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(54) **METHODS RELATED TO A STRUCTURE OF HIGH-AFFINITY HUMAN PD-1/PD-L2 COMPLEX**

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CPC ... ***G01N 33/68*** (2013.01); *G01N 2333/70521* (2013.01); ***G16C 20/64*** (2019.02); ***G16C 20/30*** (2019.02)

(57) **ABSTRACT**

Variants of human PD-1 comprising one or more of amino acid substitutions in residues corresponding to N74, T76 and A132 of SEQ ID NO:1 are described. Also described are structures, obtained using X-ray crystallography, of the human PD-1/PD-L2 complex and mutant PD-1 variants. The structures of human PD-1 described in the present disclosure are useful in drug discovery, including small-molecule drug discovery. Accordingly, methods of using the structures in drug discovery are also described.

Specification includes a Sequence Listing.

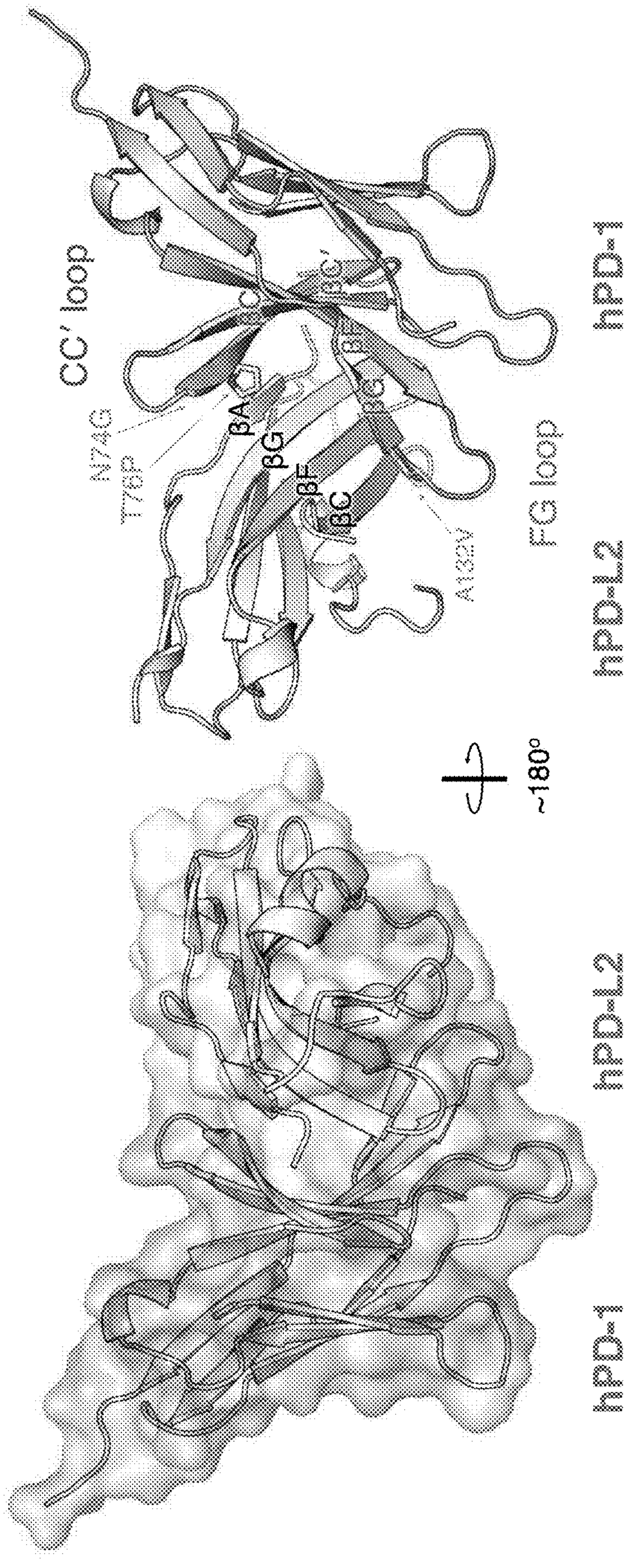

FIGURE 1A

FIGURE 1B

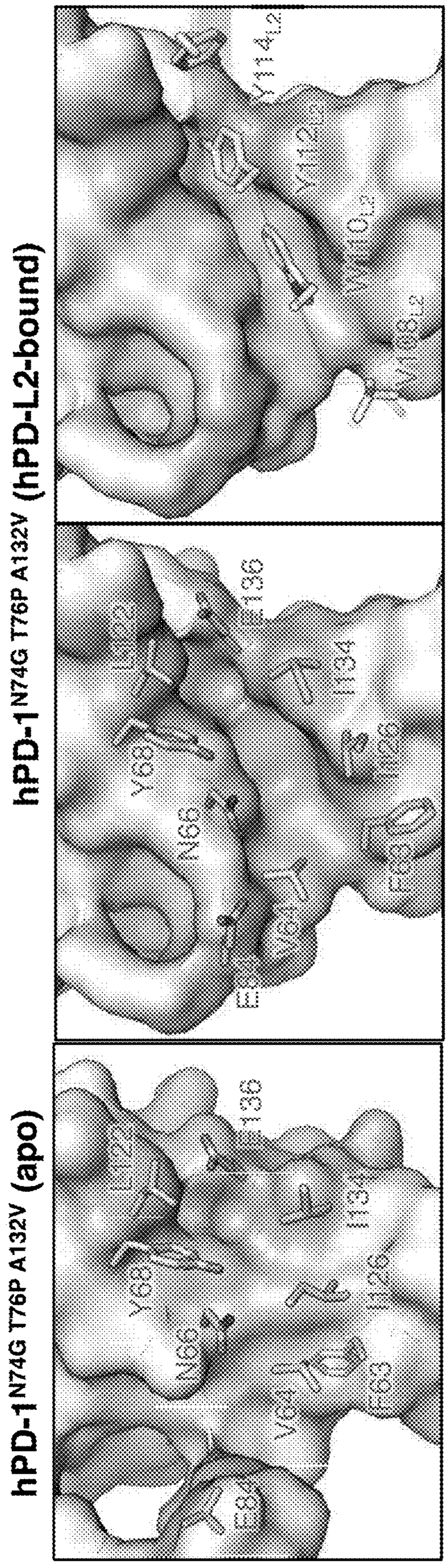

FIGURE 2C

FIGURE 2B

FIGURE 2A

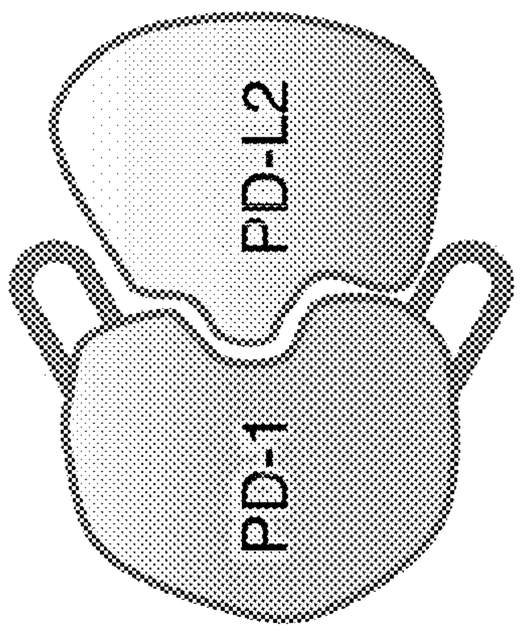

FIGURE 3A

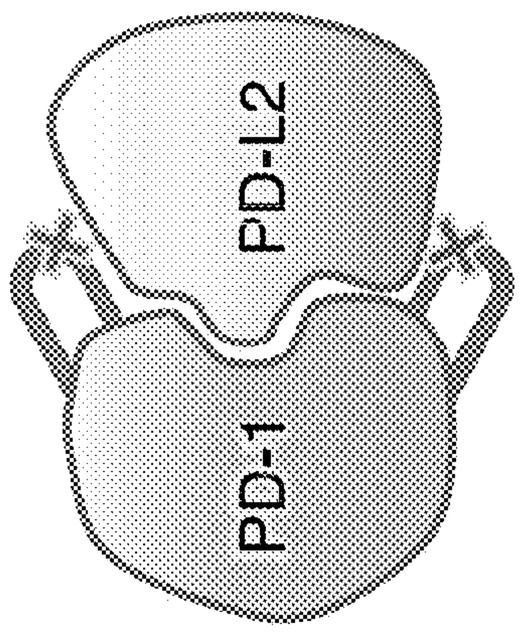

FIGURE 3B

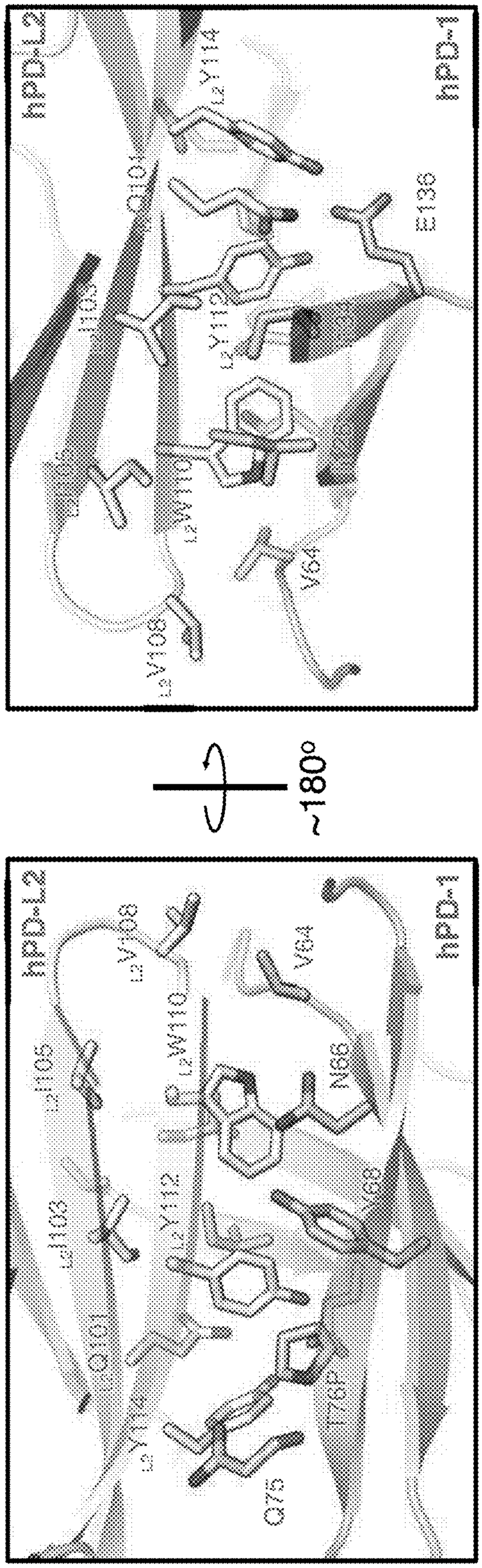

FIGURE 4B

FIGURE 4A

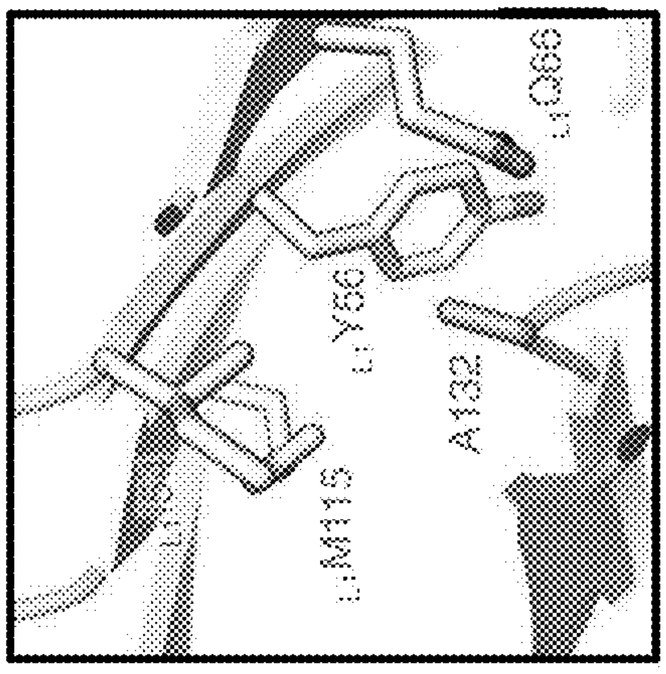

FIGURE 5A

FIGURE 5B

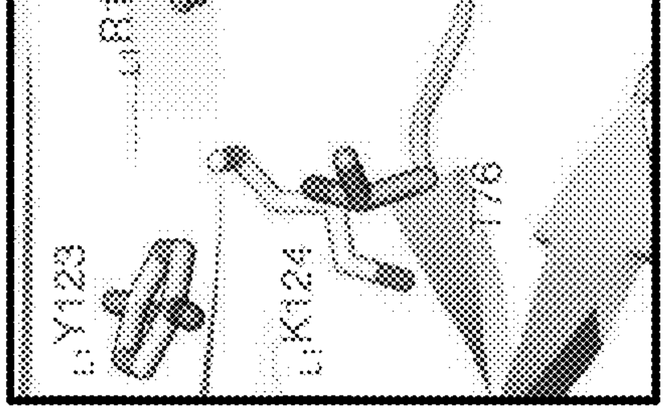

FIGURE 5C

FIGURE 5D

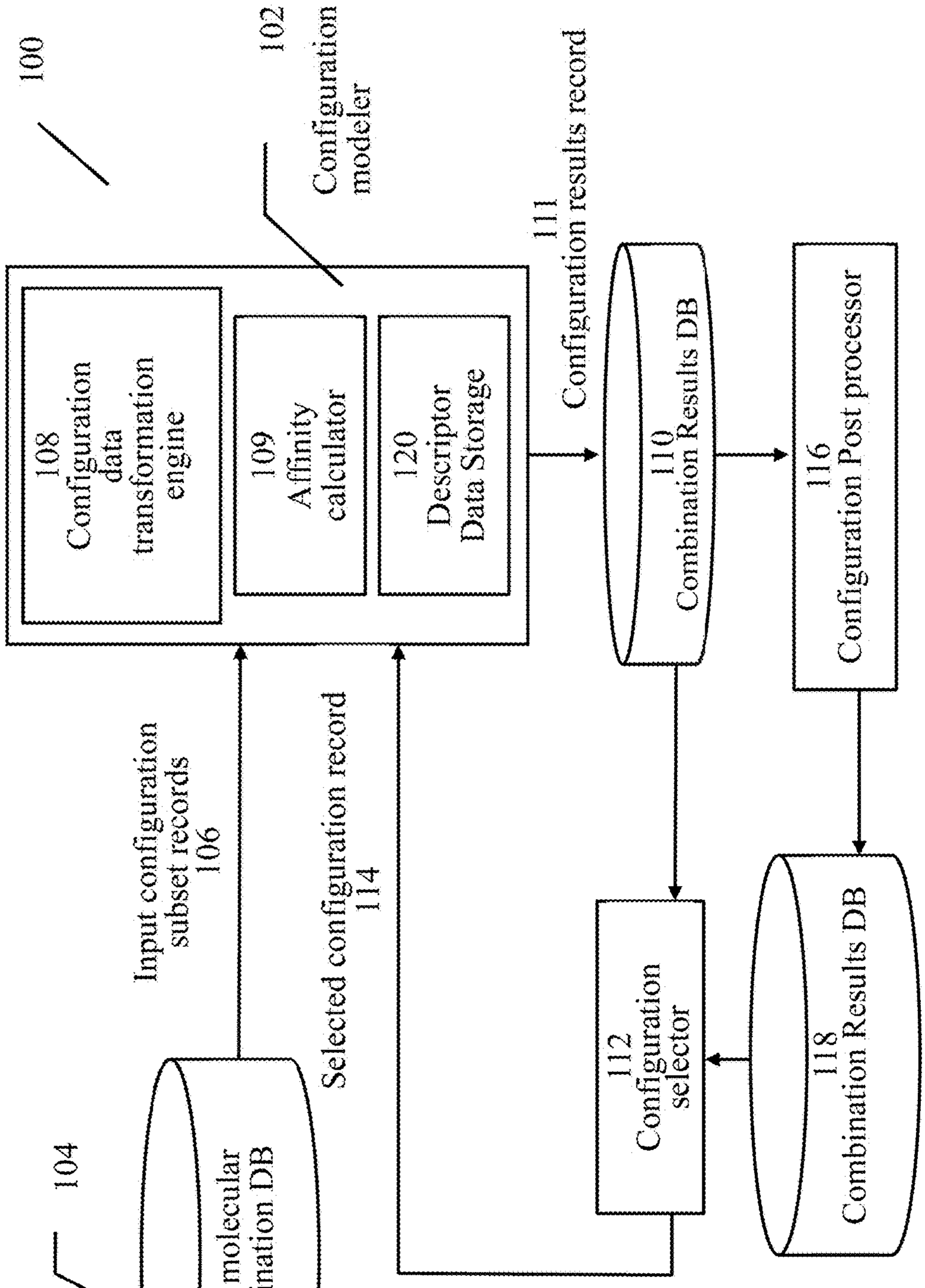
100
102
Configuration modeler
108 Configuration data transformation engine
109 Affinity calculator
120 Descriptor Data Storage
111 Configuration results record
Input configuration subset records 106
Selected configuration record 114
104
Input molecular combination DB
110 Combination Results DB
116 Configuration Post processor
112 Configuration selector
118 Combination Results DB

FIGURE 6

METHODS RELATED TO A STRUCTURE OF HIGH-AFFINITY HUMAN PD-1/PD-L2 COMPLEX

CROSS REFERENCE TO RELATED APPLICATIONS

[0001] This application is a continuation of U.S. patent application Ser. No. 16/786,409, filed Feb. 10, 2020, which claims the benefit of U.S. Provisional Application No. 62/904,515, filed Sep. 23, 2019, and U.S. Provisional Application No. 62/907,335, filed Sep. 27, 2019. All of the foregoing applications are incorporated by reference in their entirety herein.

STATEMENT AS TO RIGHTS TO INVENTIONS MADE UNDER FEDERALLY SPONSORED RESEARCH AND DEVELOPMENT

[0002] This invention was made with Government support under Contracts DA043893 and GM103393 awarded by the National Institutes of Health and DE-AC02-76F00515 awarded by the U.S. Department of Energy. The government has certain rights in the invention.

BACKGROUND

[0003] Immune checkpoint blockade of programmed death 1 (PD-1) and its ligand 1 (PD-L1) has dramatically increased progression-free survival for many cancers (1-3). For example, a monoclonal antibody (mAb) drug, pembrolizumab (Keytruda®), received regulatory approval for use in patients with microsatellite instability-high (MSI-H) or mismatch repair deficient (dMMR) solid tumors (4, 5). While mAb drugs inhibiting immune checkpoints are highly useful in oncology, there is a desire for other types of inhibitors of immune checkpoints, such as small-molecules. Small-molecule drugs targeting PD-1 may lead to increases in efficacy and safety of cancer treatment, as well to improved access to cancer treatments.

SUMMARY

[0004] Other than mAbs, compounds targeting human PD-1 so far have been out of reach. Development of human PD-1-binding drugs is hindered by the fact that the ligand-binding surface of human PD-1 is generally flat, lacking identifiable binding pockets that can serve as drug targets during computational screening of small molecule libraries and computational drug modelling efforts. Only a small cavity forms when human PD-1 binds one of its in-vivo ligands, PD-L1. The small volume of the PD-L1 binding cavity in human PD-1 prevents its use for computational modelling of PD-1 interactions with its ligands. While it is known that, in murine PD-1, the PD-L1-binding cavity extends upon binding of a different in-vivo ligand, PD-L2, the cavity of murine PD-1 cannot provide a structural model due to low sequence similarity between human and murine PD-1 proteins. As described in more detail further in the present disclosure, the inventors were able to design a substituted variant of human PD-1 that binds PD-L2 with an affinity that is two orders of magnitude higher than that of the wild-type protein, and to crystallize and, using X-ray crystallography, determine to high resolution the structures of the human PD-1 variant and the complex of the human PD-1 variant with PD-L2. As a result, a prominent pocket on the ligand-binding surface of human PD-1 was identified. The structure of the PD-L2 binding pocket of human PD-1 is described in the present disclosure. The structure of the PD-L2 binding pocket of human PD-1 is useful, for example, in the drug discovery, design and optimization methods, such as, but not limited to, the methods that involve computational (in silico) screening of small molecule libraries for candidate small molecules capable of binding to of the PD-L2 binding pocket of human PD-1, the methods that involve computational identification of ligands capable of interacting with the PD-L2 binding pocket of human PD-1, and any methods that involve computational docking of ligands to the PD-L2 binding pocket of human PD-1. Such methods are included among the embodiments of the present invention and are described in the present disclosure.

[0005] The terms "invention," "the invention," "this invention" and "the present invention," as used in this document, are intended to refer broadly to all of the subject matter of this patent application and the claims below. Statements containing these terms should be understood not to limit the subject matter described herein or to limit the meaning or scope of the patent claims below. Covered embodiments of the invention are defined by the claims, not this summary. This summary is a high-level overview of various aspects of the invention and introduces some of the concepts that are described and illustrated in the present document and the accompanying figures. This summary is not intended to identify key or essential features of the claimed subject matter, nor is it intended to be used in isolation to determine the scope of the claimed subject matter. The subject matter should be understood by reference to appropriate portions of the entire specification, any or all figures and each claim. Some of the exemplary embodiments of the present invention are discussed below.

[0006] Included among the embodiments of the present invention are proteins comprising a ligand binding pocket with a three-dimensional structure corresponding to a structure of PD-L2 binding pocket of a variant of human PD-1 with one or more of amino acid substitutions in residues corresponding to N74, T76 or A132 of SEQ ID NO:1. A variant of human PD-1 can further comprises amino acid substitutions removing one or more N-linked glycosylation sites. In a protein according to the embodiments of the present invention, the one or more of the amino acid substitutions are two or three amino acid substitutions. The amino acid substitutions can be N74G, T76P or A132V. The amino acid substitutions can be N74G, T76P, A132V or A132L. A protein according to the embodiments of the present invention can comprise amino acid substitutions N74G, T76P and A132L. A protein according to the embodiments of the present invention amino acid substitutions N74G and A132V. A protein according to the embodiments of the present invention can be a variant of human PD-1. In a protein according to the embodiments of the present invention, the PD-L2 binding pocket of the variant of human PD-1 can include bound PD-L2. In a protein according to the embodiments of the present invention, a ligand binding pocket can form upon binding of a non-PD-L2 ligand to the protein. The non-PD-L2 ligand can be a small-molecule ligand. In a protein according to the embodiments of the present invention, a binding pocket can exist in the absence of a bound ligand. Embodiments of the present invention encompass crystal forms of the proteins described in the present disclosure.

[0007] Also included among the embodiments of the present invention are variants of human PD-1, wherein the variant of human PD-1 comprising one or more of amino acid substitutions in residues corresponding to N74, T76 and A132 of SEQ ID NO:1. A variant of human PD-1 can be in crystal form. A variant of human PD-1 according to the embodiments of the present invention can include two or three amino acid substitutions. The amino acid substitutions can be N74G, T76P or A132V. In an exemplary embodiment, a variant of human PD-1 includes amino acid substitutions N74G, T76P and A132L. In another exemplary embodiment, a variant of human PD-1 includes amino acid substitutions N74G and A132V. A variant of human PD-1 can further include amino acid substitutions removing one or more N-linked glycosylation sites. A variant of human PD-1 can be capable of binding PD-L2 or be bound to PD-L2.

[0008] Also included among the embodiments of the present invention are methods for identifying a small molecule capable of binding to PD-L2 binding pocket of human PD-1. A method according to the embodiments of the present invention can comprise the steps of: I) screening small molecule libraries using in silico docking for candidate small molecules that are identified based on a docking score being above a threshold for binding to a binding pocket with a three-dimensional structure corresponding to a structure of the PD-L2 binding pocket of human PD-1; and II) evaluating the candidate small molecules identified in step (I) through one or more in vitro or in vivo assays for their ability to bind to surface residues of the PD-L2 binding pocket of human PD-1 to thereby identify the small molecule capable of binding to the PD-L2 binding pocket of human PD-1. In a method, the candidate small molecules can be identified as binding with the PD-L2 binding pocket of human PD-1 via the docking score that includes one or more interactions of (a) to (k): a) the candidate small molecules interact via hydrogen bonds with one or more amino acid residues in the PD-L2 binding pocket of human PD-1; b) the candidate small molecules interact via hydrogen bonds with the PD-L2 binding pocket of human PD-1; c) the candidate small molecules interact via ionic interactions with one or more amino acid residues in the PD-L2 binding pocket of human PD-1; d) the candidate small molecules interact via ionic interactions with the PD-L2 binding pocket of human PD-1; e) the candidate small molecules interact via one or more water molecules with one or more amino acid residues in the PD-L2 binding pocket of human PD-1; f) the candidate small molecules interact via one or more water molecules with the PD-L2 binding pocket of human PD-1; g) the candidate small molecules interact via π-π interactions with one or more amino acid residues in the in the PD-L2 binding pocket of human PD-1; h) the candidate small molecules interact via van der Waals interactions to one or more amino acid residues in the in the PD-L2 binding pocket of human PD-1; i) the candidate small molecules interact via van der Waals interactions with the PD-L2 binding pocket of human PD-1; j) the candidate small molecules interact via steric interactions to one or more amino acid residues in the in the PD-L2 binding pocket of human PD-1; k) the candidate small molecules interact via steric interactions with the PD-L2 binding pocket of human PD-1. In some embodiments, the candidate small molecules are not endogenous ligands of human PD-1. In some embodiments, the candidate small molecules have 1, 2, 3, 4, 5, 6, 7, 8, 9, 10 or 11 of the interactions (a)-(k). In some embodiments, the candidate small molecules bind via 1-20 hydrogen bonds to one or more amino acid residues in the PD-L2 binding pocket of human PD-1. In some embodiments, the candidate small molecules bind via 1-20 hydrogen bonds to the PD-L2 binding pocket of human PD-1. In some embodiments, the candidate small molecules bind via 1-20 water molecules in the PD-L2 binding pocket of human PD-1. In some embodiments, the candidate small molecules bind via 1-20 water molecules to one or more amino acid residues in the PD-L2 binding pocket of human PD-1. In some embodiments, a model of the structure of the PD-L2 binding pocket of human PD-1 is computationally derived from crystallographic data. In some embodiments, model of the PD-L2 binding pocket of human PD-1 is computationally derived from crystallographic data obtained using crystals of a variant of human PD-1 according to the embodiments of the present invention and described elsewhere in the present disclosure. In some embodiments of the methods, in silico docking comprises computational docking three-dimensional structures of small molecules from the small molecule libraries onto surface exposed amino acid residues of the model of the PD-L2 binding pocket of human PD-1. In some embodiments, the surface exposed amino acid residues comprise one or more amino acids corresponding to F63, V64, N66, Y68, E84, L122, I126, I134 or E136 of SEQ ID NO:1. In some embodiments, the computational docking comprises sampling, scoring, and binning of docking scores of a plurality of docked orientations of the small molecules relative to the model of the PD-L2 binding pocket of human PD-1. In some embodiments, the computation docking further comprising assigning a distance cutoff to match atoms of the small molecules to exposed atoms of the PD-L2 binding pocket of human PD-1. The exposed atoms can include one or more of CB of F63, CE1 of F63, CD1 of F63, CE1 of F63, CG2 of V64, CG2 of V64, O of V64, ND2 of N66, ND2 of N66, CE1 of Y68, OH of Y68, OE1 of E84, OE2 of E84, OE2 of E84, OE1 of E84, OE2 of E84, OE1 of E84, CD1 of L122, CG2 of I126, CD1 of I126, CD1 of I126, CG2 of I126, CD1 of I126, CB of I134, CG1 of I134, CG1 of I134, CD1 of I134, CD1 of I134, OE2 of E136, OE2 of E136 or OE2 of E136, wherein numbering of amino acids containing the exposed atoms is based on SEQ ID NO:1. In some embodiments, the scoring comprises determining, for complexes of the small molecules and the PD-L2 binding pocket of human PD-1, one or more of binding forces, configurational entropy, local minimal in Gibbs free energy landscape, or energy barriers between the local minima of the Gibbs free energy landscape, or combinations of two or more thereof.

[0009] Also described herein and included among the embodiments of the present invention are in silico method of identifying a compound that binds to PD-L2 binding pocket of human PD-1. The methods can comprise the steps of: (a) receiving, by a computer system, information on a three-dimensional structure of PD-L2 binding pocket of human PD-1 comprising a plurality of amino acids; (b) receiving, by the computer system, information on a three-dimensional structure of a candidate compound; (c) using the computer system and the information received into the computer system in steps (a) and (b), performing one or more of molecular dynamic simulations, kinetic Monte Carlo (KMC) simulations, direct simulations Monte Carlo (DSMC), or density functional theory (DFT) simulations to determine if the candidate compound binds to the PD-L2 binding pocket

of human PD-1, thereby identifying the compound that binds to PD-L2 binding pocket of human PD-1. In the above methods, the three-dimensional structure of the PD-L2 binding pocket of human PD-1 can be computationally derived from crystallographic data. The crystallographic data can be obtained using crystals of a variant of human PD-1 according to the embodiments of the present invention and described elsewhere in the present disclosure. In a method according to the embodiments of the present invention, step (c) can include computational docking of small molecules from small molecule libraries onto surface exposed amino acid residues of the three-dimensional structure of the PD-L2 binding pocket of human PD-1. The surface exposed amino acid residues can include one or more amino acids corresponding to F63, V64, N66, Y68, E84, L122, I126, I134 or E136 of SEQ ID NO:1. In a method according to the embodiments of the present invention, step (c) can include determining, using the computer system, a docking score of the candidate compound to the PD-L2 binding pocket of human PD-1. The determining of the docking score can include sampling, scoring and binning of docking scores of a plurality of docked orientations of the small molecules relative to the model of the PD-L2 binding pocket of human PD-1, and assigning a distance cutoff to match atoms of the small molecules to exposed atoms of the PD-L2 binding pocket of human PD-1. The exposed atoms can include one or more of CB of F63, CE1 of F63, CD1 of F63, CE1 of F63, CG2 of V64, CG2 of V64, O of V64, ND2 of N66, ND2 of N66, CE1 of Y68, OH of Y68, OE1 of E84, OE2 of E84, OE2 of E84, OE1 of E84, OE2 of E84, OE1 of E84, CD1 of L122, CG2 of I126, CD1 of I126, CD1 of I126, CG2 of I126, CD1 of I126, CB of I134, CG1 of I134, CG1 of I134, CD1 of I134, CD1 of I134, OE2 of E136, OE2 of E136 or OE2 of E136, wherein numbering of amino acids containing the exposed atoms is based on SEQ ID NO:1. In a method according to the embodiments of the present invention, step (c) can include determining, for the complexes of the compound and the PD-L2 binding pocket of human PD-1, one or more of binding forces, configurational entropy, local minimal in Gibbs free energy landscape or energy barriers between the local minima of the Gibbs free energy landscape, or combinations of two or more thereof.

[0010] Also included among the embodiments of the present invention are methods for identifying interactions between a ligand and a PD-L2 binding pocket of human PD-1. A method according to the embodiments of the present invention cam comprise the steps of: (a) receiving, by a computer system, test ligand molecular data corresponding to a test ligand that is a candidate drug; (b) receiving, by the computer system, protein molecular data corresponding to a three-dimensional structure of PD-L2 binding pocket of human PD-1; (c) calculating an interaction score between the PD-L2 binding pocket of human PD-1 and the candidate drug. In A method according to the embodiments of the present invention can further comprise a step of comparing the interaction score to a threshold score to determine whether or not an interaction exists between the PD-L2 binding pocket of human PD-1 and the candidate drug. An interaction score can be determined for each of a plurality of test ligands, including the test ligand, and the method can further comprise the steps of: determining a ranking the plurality of the interactions scores; and comparing the ranking of the test ligand to a threshold to determine whether or not an interaction exists between the PD-L2 binding pocket of human PD-1 and the candidate drug. In a method according to the embodiments of the present invention, step (c) can include performing one or more of molecular dynamic simulations, kinetic Monte Carlo (KMC) simulations, direct simulations Monte Carlo (DSMC), or density functional theory (DFT) simulations, or combinations of two or more thereof. In a method according to the embodiments of the present invention, step (c) can include determining, for the complexes of the test ligand and the PD-L2 binding pocket of human PD-1, one or more of binding forces, configurational entropy, local minimal in Gibbs free energy landscape, or energy barriers between the local minima of the Gibbs free energy landscape. In a method according to the embodiments of the present invention, the three-dimensional structure of the PD-L2 binding pocket of human PD-1 is computationally derived from crystallographic data. The crystallographic data can be obtained using crystals of a variant of human PD-1 according to the embodiments of the present invention and described elsewhere in the present disclosure. In a method according to the embodiments of the present invention, step (c) can include computational docking of small molecules from the small molecule libraries onto surface exposed amino acid residues of the model of the PD-L2 binding pocket of human PD-1. The surface exposed amino acid residues can comprise one or more amino acids corresponding to F63, V64, N66, Y68, E84, L122, I126, I134 or E136 of SEQ ID NO:1. In a method according to the embodiments of the present invention, step (c) can include determining, using the computer system, a docking score of the candidate compound to the PD-L2 binding pocket of human PD-1. The determining of the docking score can include sampling, scoring and binning of docking scores of a plurality of docked orientations of the small molecules relative to the model of the PD-L2 binding pocket of human PD-1, and assigning a distance cutoff to match atoms of the small molecules to exposed atoms of the PD-L2 binding pocket of human PD-1. The exposed atoms can include one or more of CB of F63, CE1 of F63, CD1 of F63, CE1 of F63, CG2 of V64, CG2 of V64, O of V64, ND2 of N66, ND2 of N66, CE1 of Y68, OH of Y68, OE1 of E84, OE2 of E84, OE2 of E84, OE1 of E84, OE2 of E84, OE1 of E84, CD1 of L122, CG2 of I126, CD1 of I126, CD1 of I126, CG2 of I126, CD1 of I126, CB of I134, CG1 of I134, CG1 of I134, CD1 of I134, CD1 of I134, OE2 of E136, OE2 of E136 or OE2 of E136, wherein numbering of amino acids containing the exposed atoms is based on SEQ ID NO:1.

[0011] In some embodiments of the methods described in the present disclosure, a candidate compound, such as a candidate small molecule, can be a candidate anti-cancer drug. The methods can therefore include testing the candidate anti-cancer drug in an in vitro or in vivo assay to determine its anti-cancer efficacy. The methods can also include determining toxicity of the candidate anti-cancer drug. The methods can also include determining if the candidate anti-cancer drug has an off-target effect. The toxicity or the off-target effect can be determined by an in vitro assay, by an in vivo assay, in silico, or by a combination of two or more thereof. The methods can also include optimizing the candidate anti-cancer drug. For example, the candidate anti-cancer drug can be optimized to one or more of: reduce an off-target effect, reduce toxicity, increase or decrease binding affinity for the PD-L2 binding pocket of human PD-1, decrease binding affinity for the PD-L2 binding pocket of human PD-1. Also included among the

embodiments of the present invention are computer products comprising a non-transitory computer readable medium storing a plurality of instructions that when executed control a computer system to identity protein-drug interactions by performing the methods according to the embodiments of the present invention.

BRIEF DESCRIPTION OF THE FIGURES

[0012] FIGS. **1**A and **1**B schematically illustrates the X-ray crystal structure of the human PD-1/PD-L2 complex. FIG. **1**A shows a space-filling and ribbon diagram overlay of the human PD-$1^{N74G\ T76P\ A132V}$ (dark grey)/PD-$L2^{IgV}$ (light grey)), showing the overall architecture of the human PD-1/PD-L2 complex. FIG. **1**B shows a ribbon diagram of a ~180° rotation view of the ribbon diagram shown in FIG. **1**A. Substitutions of N74G, T76P, and A132V are labeled and their sidechains are indicated with sticks. The β-sheets on the interacting faces of each protein are labeled.

[0013] FIGS. **2**A, **2**B and **2**C schematically illustrate the formation of a prominent pocket in human PD-1 upon binding PD-L2. FIGS. **2**A and **2**B show the close-up views of space-filling models of apo-human PD-$1^{N74G\ T76P\ A132V}$ (FIG. **2**A), and human PD-L2-bound human PD-$1^{N74G\ T76P\ A132V}$ overlaid with pocket-residues in sticks (FIG. **2**B). The pocket shown in FIG. **2**B adopts a funnel-shaped architecture (left: entrance, and right: end) with a volume measured as 130 $Å^3$. FIG. **2**C shows a space-filling models of pockets of human PD-L2-bound human PD-$1^{N74G\ T76P\ A132V}$ with a ribbon diagram of the PG of PD-L2. The PD-L2 interacting-residues are overlaid in sticks and labeled with an L2 subscript. A 130 $Å^3$ funnel-shaped pocket (left, entrance; right, exit) when human PD-1 binds PD-L2

[0014] FIGS. **3**A and **3**B schematically illustrate a model for conformational coupling for PD-L2 binding to PD-1. Schematic cartoon model shown in FIG. **3**A is that of human PD-1 with a flat interface (left) in equilibrium with the PD-L2-bound conformation in the absence of PD-L2 (middle). Schematic cartoon model shown in FIG. **3**B is that of the PD-1 loop variant with increased population of the PD-L2-bound conformations in the absence of PD-L2. For clarity, only two of the states in the conformational ensembles are depicted in the schematic cartoon models. Crosses indicate the loop substitutions. Binding of PD-L2 stabilizes the bound conformation of PD-1 (right).

[0015] FIGS. **4**A and **4**B show ribbon diagrams schematically illustrating human PD-1/PD-L2 binding interface. FIGS. **4**A and **4**B show ribbon diagrams of human PD-1/PD-L2 interface overlaid with interacting residues in sticks. ~180° rotation between views shown in FIGS. **4**A and **4**B.

[0016] FIGS. **5**A, **5**B, **5**C and **5**D show ribbon diagrams schematically illustrating human PD-1/PD-L2 binding interface. FIGS. **5**A and **5**B show close-up ribbon diagrams of the localizations of the loop substitutions overlaid in sticks of the mutated G74, P76 (FIG. **5**A), and V132 (FIG. **5**B) in the human PD-1/PD-L2 structure. The PD-L2 residues are overlaid in sticks and labeled with an L2 subscript. P76 of the CC' loop of PD-1 localizes in between sidechains of Y112L2 and Y114L2. V132 of the FG loop localizes to a groove of $T56_{L2}$ $S58_{L2}$ $I103_{L2}$ and $I105_{L2}$. FIGS. **5**C and **5**D show close-up ribbon diagrams of the localizations of the loop substitutions overlaid in sticks of N74, T76 (FIG. **5**C), and A132 (FIG. **5**D) in the human PD-1/PD-L1 structure (PDB: 4ZQK). The PD-L1 residues are overlaid in sticks and labeled with an L1 subscript. Compared to PD-L2, the corresponding Y114L2 is substituted by $R125_{L1}$. A132 of the FG loop localizes to a groove of $I54_{L1}$, $Y56_{L1}$, $Q66_{L1}$, and $M115_{L1}$ in PD-L1.

[0017] FIG. **6** is a schematic illustration of a system for performing exemplary methods according to the embodiments of the present invention.

DETAILED DESCRIPTION

[0018] PD-1 is a receptor expressed by T cells, B cells, and monocytes, and is a potent regulator of immune responses (16). PD-1 is an attractive target for anti-cancer pharmaceuticals. PD-1 has two known protein ligands in vivo, PD-L1 and PD-L2, which bind to the same region on the surface of PD-1. It would be desirable to identify other ligands, including, but not limited to small molecule compounds, that would bind to this region of human PD-1 and interfere with its binding to PD-L1 and/or PD-L2. Such ligands, once identified, may be used as lead compounds for drug development and tested for potential biological activity, such as anti-cancer activity, by suitable in vitro and/or in vivo assays. However, it is currently impossible to identify in silico the ligands that would specifically and efficiently bind to PD-1 ligand-binding site, because the PD-1 ligand-binding site lacks a defined binding pocket in the absence of its in vivo ligands. Although the structure of human PD-1/PD-L1 complex has been determined, and a model of PD-L1 binding cavity of human PD-1 exists, the volume of PD-1 binding cavity in the above model is too small for the model to be used effectively in computational studies of PD-1/ligand interactions. As a consequence, until the discoveries described in the present disclosure, effective computational of PD-1/ligand interactions were intractable, making it impossible, for example, to pre-select a reasonable number of lead ligands, such as small-molecule compounds for further testing with in vitro and/or in vivo assays for PD-1 signaling in order to identify biologically active ligands that can be used as drug candidates in pre-clinical and/or clinical testing. The absence of a model of binding PD-1/PD-L1 binding cavity also prevented in silico rational drug design and optimization studies.

[0019] The available structures of murine PD-1/PD-L1 and PD-1/PD-L2 complexes showed that a modest binding cavity was formed upon PD-L1 binding, and the cavity extended to a volume suitable for small-molecule ligands only upon PD-L2 binding to murine PD-1. However, the model of the structure of murine PD-1/PD-L2 complex is unsuitable for human drug development due to low sequence similarity between the human and murine PD-1 proteins. Since human PD-1 protein has a very mobile structure, all the multiple previous attempts to crystalize human PD-1/PD-L2 complex and determine the structure of PD-1 ligand binding pocket failed. As described in the present disclosure, the inventors were able to stabilize the structure of PD-1/PD-L2 complex by mutating several residues in two mobile loops (CC' and FG) of PD-1, which increased the affinity of PD-1 for PD-L2. The inventors were then able to crystallize the PD-1/PD-L2 complex and determine the structure of the PD-L2 binding pocket. The model of the structure of human PD-1/PD-L2 binding pocket can now be used for drug discovery and development. One non-limiting example of the drug discovery and development process in which the structure of human PD-1/PD-L2 binding pocket can be used, is a process that involves computational screening of compounds to identify PD-1 ligands ("leads"). In the above

process, screened compounds can be small molecules. For example, libraries of small compounds (small-molecule libraries) can be computationally screed according to various procedures, some of which are described in the present disclosure, to identify candidate small molecules capable of binding to a PD-L2 binding pocket of human PD-1. Based on the results of the computational screening, potential leads can be tested by appropriate in vitro and/or in vivo testing to identify the compounds that affect PD-1 signaling. Another non-limiting example in which the structure of human PD-1/PD-L2 binding pocket can be used is a process that involves computational design and testing of candidate ligands ("leads"), which can subsequently be tested by appropriate in vitro and/or in vivo testing to identify the compounds that affect PD-1 signaling. Prior to the determination of the structure, described in the present disclosure, of human PD-1/PD-L2 binding pocket, it was impossible to identify computationally (in silico) the leads for subsequent in vitro and/or in vivo testing identify the compounds that affect PD-1 signaling. Although in vitro and/or in vivo testing without prior in silico lead identification was theoretically possible, it was, in practice, unworkable due to the high costs (including monetary, time, labor and animal lives required for the testing) that would be required to test large numbers of essentially randomly selected compounds with low probability of success. The discoveries described in the present disclosure permit carrying out the processes related to drug discovery, such as, but not limited to, screening of small molecules and rational drug design, in which in vitro and/or in vivo testing of lead compounds can be implement practically and effectively due to the now available capability to perform the initial steps of lead screening and/or design computationally, thereby drastically reducing the number of the leads that need to be tested in vitro and/or in vivo to identify biologically active PD-1 ligands that can serve as drug candidates in subsequent pre-clinical and clinical testing.

An exemplary amino acid sequence of human PD-1 (SEQ ID NO: 1), UniProt database entry Q15116

```
        10         20         30         40
MQIPQAPWPV VWAVLQLGWR PGWFLDSPDR PWNPPTFSPA

        50         60         70         80
LLVVTEGDNA TFTCSFSNTS ESFVLNWYRM SPSNQTDKLA

        90        100        110        120
AFPEDRSQPG QDCRFRVTQL PNGRDFHMSV VRARRNDSGT

       130        140        150        160
YLCGAISLAP KAQIKESLRA ELRVTERRAE VPTAHPSPSP

       170        180        190        200
RPAGOFQTLV VGVVGGLLGS LVLLVWVLAV ICSRAARGTI

       210        220        230        240
GARRTGQPLK EDPSAVPVFS VDYGELDFQW REKTPEPPVP

       250        260        270        280
CVPEQTEYAT IVFPSGMGTS SPARRGSADG PRSAQPLRPE DGHCSWPL
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[0020] An exemplary amino acid sequence of human PD-1 protein is shown as SEQ ID NO:1. The present disclosure describes, among other things, structures of the human triple-mutant PD-1/PD-L2 complex and the apo triple-mutant PD-1 variant obtained using X-ray crystallography at 2.0 Å and 1.2 Å resolution, respectively. The structures described in the present disclosure revealed that binding of PD-L2 to human PD-1 was accompanied by formation of a prominent pocket in human PD-1, as well as substantial conformational changes of the CC' and FG loops. The structure of human apo triple-mutant PD-1 revealed that the CC' loop adopted the ligand-bound conformation, providing support for allostery between the loop and pocket. The structures of human PD-1/PD-L2 described in the present disclosure are useful for design and discovery of small-molecule PD-1 inhibitors. While mAb drugs inhibiting immune checkpoints, such as pembrolizumab, are highly useful in oncology, small-molecule inhibitors of immune checkpoints are highly desirable. Small molecule inhibitors are expected to penetrate more effectively than mAbs in the tumor microenvironment, which can enhance their efficacy (6). In addition, if penetration into the brain is desired, small molecule inhibitors can be effective (7, 8). Also, there are rare but severe immune-related side effects of checkpoint inhibition that call for immediate drug discontinuation (9, 10). Since mAbs have long half-lives in the body (typically, weeks) (11), the treatment of such severe immune-related side effects is primarily supportive. Small-molecule checkpoint inhibitors can offer the potential for convenient dosing (e.g., once a day), while allowing for prompt drug removal, if desired (12). Small-molecule immune checkpoint inhibitors can facilitate treatment of cancers in low- and middle-income countries by reducing production costs and eliminating the need for refrigeration during transportation and storage, as compared to mAbs (13). Despite substantial efforts, currently there are no well-characterized small-molecule ligands for PD-1 (14, 15).

[0021] In vivo, PD-1 binds two distinct ligands, PD-L1 (also known as B7-H1 or CD274) and PD-L2 (also known as B7-DC) (16). The ligand-binding surface of human PD-1 is generally flat, lacking pockets considered suitable for binding small molecules (16). However, upon binding to PD-L1, a modest cavity forms on the ligand binding surface of PD-1 (17). A similar cavity is formed in murine PD-1 upon binding PD-L1 (18). When murine PD-1 binds PD-L2 (19), this cavity extends to a volume comparable to that occupied by established small-molecule inhibitors (20, 21). Unfortunately, currently available structure of murine PD-1/PD-L2 complex is insufficient to provide a structural model for the analogous pocket in the human PD-1/PD-L2 complex, as the human and murine PD-1 proteins share sequence identities of only about 63% (22). Although the structure of murine PD-1/PD-L2 complex was determined over a decade ago, the structure of the human complex has not yet been obtained due to various difficulties. Previous attempts to obtain diffraction-quality crystals of human PD-1/PD-L2 complex were unsuccessful.

[0022] The inventors realized that formation of cavities on the ligand-binding surface of PD-1 is accompanied by changes in the structures of the CC' and FG loops. The inventors further realized that substitutions in these loops can have an allosteric effect on the conformations of PD-1 in the pocket region and alter its affinity for PD-L2. Using deep-mutational scanning (24) and yeast-surface display (25), the CC' and FG loop variants of human PD-1 with enhanced PD-L2 binding were selected. A triple-mutant PD-1 was identified that binds PD-L2 with nanomolar affinity and is amenable to crystallization, both alone and as a complex. The formation of a prominent pocket in human PD-1 upon binding PD-L2 revealed by the X-ray crystal

structures described in the present disclosure supports the notion of allostery between the pocket and the CC' and FG loops. The pocket identified in human PD-1 can serve as a template for virtual drug discovery (26) and opens up additional avenues for the discovery of small-molecule PD-1 inhibitors.

[0023] The prominent pocket formed in human PD-1 upon binding PD-L2 has a volume of 130 $Å^3$, comparable to those pockets that bind small-molecule drugs (20, 21, 35). The structure of the pocket in human PD-1 described in the present disclosure is quite distinct from the corresponding pocket in murine PD-1 when bound to PD-L2 (19). The pocket in human PD-1 described in the present disclosure represents an attractive drug target. It is envisioned that a small molecule binding to PD-1 contacting all or many of the residues that form the pocket, particularly F63, V64, N66, Y68, E84, L122, G124, I126, I134, and E136 in a conformation similar to that formed in the complex with PD-L2, as illustrated in FIG. **2**B. The structure of human PD-1/PD-L2 complex is useful for virtual drug screening to identify potential lead compounds (see e.g., (26)). In addition, the structures of the indole and phenyl rings and neighboring sidechains of PD-L2 when bound to the pocket, as illustrated in FIG. **2**C, are useful for the design of fragment-based screening scaffolds (36, 37).

[0024] Conformational changes in the CC' and FG loops can be coupled to formation of pockets in the ligand-binding interface of PD-1 (FIG. **3**). In this model, PD-1 exists in an ensemble of conformations in the absence of ligands, populating predominantly structures containing a flat ligand-binding face ($K_1<1$). PD-1 molecules with a pre-formed pocket have a higher affinity for PD-L2 (i.e., $K_3>K_2$). Thermodynamics dictates that $K_1K_3=K_2K_4$, so $K_4>K_1$. In this model, the PD-1 loop variants studied here increase K_1, and lead to a higher proportion of apo-PD-1 in the PD-L2-bound conformation. The increased association constants (k_{on}) for binding ligands by the mutant PD-1s, as compared to wild-type PD-1 support this model. Such kinetic properties are consistent with an increase fraction of unliganded mutant PD-1 molecules that are in a ligand-bound conformation as compared to wild-type PD-1 (38, 39). In addition, the CC' loop shifts toward the PD-L2-bound conformation in the apo-PD-1 triple and double mutants. While there are only minimal changes in the pocket of human PD-1, as illustrated in FIG. **2**A, the pocket residues and a neighboring FG loop have substantial crystal contacts in the lattice that likely interfere with conformational changes. Such coupling can stabilize the pocket in the absence of a ligand, for example, if the two loops were held in their PD-L2-bound conformations with antibodies or aptamers. Thus, the structures of human PD-1 described in the present disclosure are useful in drug development, such as, but not limited, to small-molecule drug discovery, such as by high-throughput screening (40, 41), and rational drug design. The structures described in the present disclosure can be used to discover, design and/or optimize PD-1 ligands, including small-molecule ligands, and can also be used in the discovery of allosteric regulators of PD-1 activity.

Terms and Concepts

[0025] A number of terms and concepts are discussed below. They are intended to facilitate the understanding of various embodiments of the invention in conjunction with the rest of the present document and the accompanying figures. These terms and concepts may be further clarified and understood based on the accepted conventions in the fields of the present invention. the description provided throughout the present document and/or the accompanying figures. Some other terms can be explicitly or implicitly defined in other sections of this document and in the accompanying figures, and may be used and understood based on the accepted conventions in the fields of the present invention, the description provided throughout the present document and/or the accompanying figures. The terms not explicitly defined can also be defined and understood based on the accepted conventions in the fields of the present invention and interpreted in the context of the present document and/or the accompanying figures.

[0026] Further, unless otherwise required by context, singular terms shall include pluralities and plural terms shall include the singular. Generally, nomenclatures used in connection with, and techniques of, cell and tissue culture, molecular biology, immunology, microbiology, genetics and protein and nucleic acid chemistry are those well-known and commonly used. Known methods and techniques are generally performed according to conventional methods well known and as described in various general and more specific references that are discussed throughout the present disclosure, unless otherwise indicated. For example, enzymatic reactions and purification techniques are performed according to manufacturer's specifications, as commonly accomplished. The nomenclatures used in connection with the laboratory procedures and techniques described in the present disclosure are those well-known and commonly used.

[0027] As used herein, the terms "a", "an", and "the" can refer to one or more unless specifically noted otherwise.

[0028] The use of the term "or" is used to mean "and/or" unless explicitly indicated to refer to alternatives only or the alternatives are mutually exclusive, although the disclosure supports a definition that refers to only alternatives and "and/or." As used herein "another" can mean at least a second or more.

[0029] As used herein, the amino acid residues are abbreviated as follows: alanine (Ala; A), asparagine (Asn; N), aspartic acid (Asp; D), arginine (Arg; R), cysteine (Cys; C), glutamic acid (Glu; E), glutamine (Gln; Q), glycine (Gly; G), histidine (His; H), isoleucine (Ile), leucine (Leu), lysine (Lys; K), methionine (Met; M), phenylalanine (Phe; F), proline (Pro; P), serine (Ser; S), threonine (Thr; T), tryptophan (Trp; W), tyrosine (Tyr; Y), and valine (Val; V). In the broadest sense, the naturally occurring amino acids can be divided into groups based upon the chemical characteristic of the side chain of the respective amino acids. By "hydrophobic" amino acid is meant either His, Leu, Met, Phe, Trp, Tyr, Val, Ala, Cys or Pro. By "hydrophilic" amino acid is meant either Gly, Asn, Gln, Ser, Thr, Asp, Glu, Lys, Arg or His. This grouping of amino acids can be further sub-classed as follows: by "uncharged hydrophilic" amino acid is meant either Ser, Thr, Asn or Gln. By "acidic" amino acid is meant either Glu or Asp. By "basic" amino acid is meant either Lys, Arg or His.

[0030] The term "variant," when used in the present disclosure in reference to a protein or a polypeptide, encompasses homologues, variants, isoforms, fragments, mutants, modified forms and other variations of the protein, polypeptide or amino acid sequences described in this document. The term "homologous," "homologues" and other related terms used in this document in reference to various amino

acid, are intended to describe a degree of sequence similarity among amino acid sequences, calculated according to an accepted procedure. Homologous sequences may be at least 60%, 65%, 70%, 75%, 80%, 85%, 90%, 91%, 92%, 93%, 94%, 95%, 96%, 97%, 98% 99% or 100% homologous. As used herein, "percent homology" of two amino acid sequences is determined using the algorithm of Karlin and Altschul, which is incorporated into the NBLAST and XBLAST programs, available for public use through the website of the National Institutes of Health (U.S.A.). To obtain gapped alignments for comparison purposes, Gapped BLAST is utilized. When utilizing BLAST and Gapped BLAST programs, the default parameters of the respective programs (e.g.,)(BLAST and NBLAST) are used. "Percent homology" may be used in this document to describe fragments, variants or isoforms of amino acids sequences, but other ways of describing fragments, variants or isoforms may be employed alternatively to or in conjunction with homology.

[0031] The term "ligand" and the related terms used in the present disclosure refer to a compound or compounds that form a complex with PD-1 protein. The term "ligand" encompassess all compounds, regardless of their size or origin. For example, inorganic molecules, organic molecules, small molecules, biological molecules, non-biological molecules are all encompassed by the term "ligand."

[0032] The term "interaction" and the related terms refer to a type of physical or chemical interaction of one or more molecular subsets with itself (intramolecular) or other molecular subsets (intermolecular) or with components of an environment (environmental). Interaction types may be either enthalpic or entropic in nature and may reflect either nonbonded or bonded interactions. Examples of nonbonded interaction types include, but are not limited to, electrostatic interactions, van der Waals (or dispersion) interactions between time-varying dipole moments (often related to steric complementarity), short range repulsion between overlapping atomic orbitals, hydrogen bonding, interactions involved with metal ion coordination, or interactions with one or more ordered or structural waters. Other examples of nonbonded interaction types may also include one or more solvation effects such as electrostatic desolvation (including self-reaction field polarization effects, solvent screening in a dielectric medium or interactions with a solvent-based ionic atmosphere), the hydrophobic effect, cavitation energy, and surface tension. Examples of bonded interactions include, but are not limited to, the intramolecular strain associated with distortions of equilibrium bond lengths, angles, torsions, etc., or the energy gap between cis-trans modes or the energy differential associated with changes in chirality of one or more chiral center. Examples of entropic-based interactions include the loss of conformational entropy of molecular subsets (including loss of rotameric entropy for protein side chains) upon binding or the favorable entropy gain obtained by the release of one or more ordered waters. Other more exotic interaction types may include π-π stacking, charge transfer, or other quantum mechanical phenomena.

[0033] The term "hydrogen-bonding," "hydrogen bonds," and related terms relate to a partially electrostatic attraction between a hydrogen (H) which is bound to a more electronegative atom such as nitrogen (N) or oxygen (O) and another adjacent atom bearing a lone pair of electrons. For example, when it is stated that the nitrogen acts as a "hydrogen bond donor" it means that a hydrogen (H) bound to a nitrogen (N) is donated by the nitrogen as it electrostatically attracted to or accepted by an adjacent atom bearing a lone pair of electrons such as an oxygen. Similarly, when it is stated that an oxygen acts as a "hydrogen bond acceptor," it means that a hydrogen (H) bound to a more electronegative atom such as nitrogen (N) is electrostatically attracted to or "accepted by" an adjacent atom such as oxygen bearing a lone pair of electrons. Sometimes the hydrogen bonded atoms are called out without explicitly stating the origin and presence of an intermediate hydrogen atom. The term "hydrogen bonding" is used wherever LigPlot Plus software predicts a hydrogen bonding interaction using its algorithm and applied parameters of 3.35 Å for maximum distance between hydrogen bond donor and acceptor. Not all hydrogen bonds may actually be in place simultaneously; this is evident for atoms that are shown to form 4 putative hydrogen bonds, where however, at any given time only 3 hydrogen bonds are chemically possible. In general, although crystal structures such as the co-crystal structural information herein does not directly show or detect hydrogen bonding, the software used to describe the co-crystal does predict such H-bonding exists. Therefore, throughout the disclosure when a H-bond is present and described, it may be said to be "predicted" by software to be present.

[0034] The term "ionic bonding" and related terms include a type of chemical bond that involves the electrostatic attraction between oppositely charged ions, and is the primary interaction occurring in ionic compounds.

[0035] The term "van der Waals interaction" and related terms include weak, short-range electrostatic attractive forces between uncharged molecules, arising from the interaction of permanent or transient electric dipole moments.

[0036] The term "π-π interaction or π-π stacking" and related terms include attractive, noncovalent interactions between aromatic rings that are oriented either roughly parallel or roughly perpendicular (such as in "edge-face" interactions) to each other, since they contain 7C bonds.

[0037] The term "steric interactions," "steric effects" and the related terms describe molecular and/or atomic interactions that may arise in a number of ways. Steric effects are described, for example, in (48). For example, steric effects may result from repulsions between valence electrons or nonbonded atoms, leading to in an increase in the energy of the system. In the formation of a ligand-receptor complex, any group of atoms that is in van der Waals contact with the receptor or the biomolecule can be or is involved in the binding event. If a ligand binding pocket can adjust to any ligand, then no steric effect will be observed. If, however, the binding pocket has limited conformational flexibility, and this flexibility is not equivalent in all directions, then a steric effect will be observed. The steric effect will be dependent on conformational states, and the minimal steric interaction principle will probably be observed. This principle states that a substituent whose steric effect is conformationally variable will prefer a conformation that minimizes steric repulsions and will give rise to the smallest steric strain.

[0038] The term "binding site" and related terms refer to an area on the protein wherein a small molecule can interact with such as a region, which can be located on the surface or interior of the protein molecule. The term "pocket," "binding pocket" or related terms can refer to a cavity on the surface or in the interior of a protein molecule that possesses

suitable properties for binding a ligand. Amino acid and other residues (such as co-factors) around a pocket determine its physicochemical characteristics. Residues outside the binding site can also have a long-range effect on the properties of the binding pocket. Binding pocket can have a concave surface presenting amino acid residues in a suitable configuration for binding low molecular weight compounds (which can be referred to as "small molecules"). The mobility of a protein molecule can permit opening, closing, and adaptation of binding pockets to regulate binding processes. The influence of protein flexibility on binding pockets can vary from small changes to an already existent pocket to the formation of a completely new pocket. Pockets and binding sites are described, for example, in (47).

[0039] Typically, a set of appropriate molecular descriptors describing each distinct configuration will be used to distinguish one configuration from another. Molecular descriptors may include, but are not limited to, a) chemical descriptors (e.g., element, atom type, chemical group, residue, bond type, hybridization state, ionization state, tautomeric state, chirality, stereochemistry, protonation, hydrogen bond donor or acceptor capacity, aromaticity, etc.); b) physical descriptors (e.g., charge, both formal and partial, mass, polarizability, ionization energy, characteristic size parameters, such as van der Waals [vdW] radii, vdW well depths, hydrophobicity, hydrogen bonding potential parameters, solubility, equilibrium bond parameters relating bond energies to bond geometries, etc.); c) geometrical descriptors (e.g., atomic coordinates, bond vectors, bond lengths, bond angles, bond torsions, suitable structural descriptors for rings, descriptors for molecular surfaces and volumes, such as solvent accessible surfaces and solvent-excluded volumes, etc.); and d) environmental descriptors (e.g., temperature, pH, ionic strength, pressure, etc.). Chemical descriptors may be assigned based on application of one or more rules or concepts of organic (or inorganic, if appropriate) chemistry to represent chemical structures that must at least stipulate basic structural information such as element type and bond connectivity (i.e., minimally which nonhydrogen atoms are connected to one another) but may also contain some form of coordinate information. Such chemical structures may be stored and received in a number of different data representations. One common example of data representation, though many others are also possible, is that of a PDB file. Examples of currently available software programs that can be used to assign chemical descriptors include SYBYL™ from Tripos, Chimera™ from UCSF, and WhatIf' (for proteins), etc. Correct assignment of chemical descriptors may also include additional input regarding chiral centers and stereochemistry or even environmental factors, such as expected pH as related to assignment of ionization states.

[0040] The term "affinity formulation" and the related term refer to the energy model used to calculate approximate quantitative values for a given interaction type for a configuration associated with a molecular combination. Typically, there may be many different affinity formulations for a given interaction type from which to choose. The choice of affinity formulation may affect the amount of error associated with the quantitative approximation of a given interaction type. The choice of affinity formulation may also involve very different levels of modeling sophistication and hence computational complexity. A given affinity formulation may require one or more molecular descriptors for evaluation. Two different affinity formulations for a given interaction type may require a very different set of molecular descriptors, while others may share multiple molecular descriptors in common. For example, electrostatic interactions may be modeled according to an affinity formulation involving the use of a modified form of Coulomb's law with distance-dependent dielectric function as applied to a set of partial charges assigned to atomic centers in each molecular subset via use of a suitable force field. In another example, both electrostatic and electrostatic desolvation interactions may be modeled according to an affinity formulation involving a solution of the Poisson-Boltzmann equation (linear or nonlinear) along with an assumption of point charges embedded in solute spherical cavities with size defined by van der Waal radius of each atom and the solute spheres placed in a homogeneous dielectric medium representing water with and possibly containing an ionic atmosphere. Alternatively, electrostatic interactions may be modeled based on quantum-mechanical solution of electronic ground states for each molecular subset. In most scenarios the modified Coulomb with distance-dependent dielectric formulation will be cheaper to compute but less accurate than a Poisson-Boltzmann-based formulation let alone a full quantum-mechanical solution. As further examples, van der Waals interactions may be modeled according to an affinity formulation based on use of a generalized Lennard-Jones potential or alternatively based on a steric complementarity. Hydrogen-bonding interactions may be modeled according to an affinity formulation based on use of a 12-10 Lennard-Jones potential with an angular weighting function or by rescaling of partial charges and van der Waals radii of hydrogen bond donor and acceptor atoms such as that found in the Amber force field. The hydrophobic effect may be modeled according to an affinity formulation based on the fragmental volume approach or the solvent accessible surface area-based formalism. Intramolecular strain associated with dihedral changes may be modeled according to an affinity formulation based on use of Pitzer potentials or by inverse Gaussian torsional constraints. As yet another example, instead of using a Poisson Boltzmann-based formulation, electrostatic desolvation for a configuration may be modeled via an affinity formulation based on use of a variant of the Generalized Born approximation.

[0041] The term "computation strategy" herein refers to the computational technique used to quantitatively evaluate a given affinity formulation for one or more interaction types. The choice of computation strategy may be influenced by the available computational systems, apparatus, means and/or methods, the available memory capacity, and/or computing time constraints. As an example of different computational strategies for the same affinity formulation, consider the electrostatic interaction for target-ligand combination, for which a modified Coulombic affinity formulation with distance-dependent dielectric may be computed according to a computation strategy involving direct summation of pair-wise calculation between all possible pairs of partial charges across the protein and ligand. For a ligand with 100 atoms and a protein with 3000 atoms, this would entail the calculation of 300 K intermolecular distances let alone the number of distinct intramolecular pairs. An alternative computation strategy is to instead utilize a probe grid map approximation, whereby an electrostatic potential function associated with source charges on the protein is evaluated and stored on 3-D grid for coordinate locations enclos-

ing the protein. Then for each ligand charge a corresponding electrostatic potential value is accessed from memory (or other storage) and the direct product of the charge and the potential is then accumulated over all charges in the ligand. This may significantly reduce computational effort especially in the context of screening a molecule library where many molecular combinations may feature the same target protein but different ligands. Of course, the probe grid map approximation may require significant storage in order to reduce numerical errors related to variation of the potential function. Moreover, such an approximation is only suitable when the source charges of the protein do not change positions between different configurations. An alternative for a target protein featuring a flexible binding pocket, may be to use a hybrid computation strategy involving the use of the pair-wise strategy for the portion of the protein containing mobile source charges and the probe grid map strategy for the remainder of the protein. In general, various different computation strategies may be applied to other affinity formulations for other interaction types. On the other hand, the choice of computation strategy may be limited by the nature of the affinity formulation or interaction type in question. For example, it is unlikely that one would a strategy appropriate for evaluation of intermolecular electrostatics interactions to instead compute intramolecular strain components involving bonded interactions. Other types of computational strategies exist than those based on pair-wise (e.g., interactions between pairs of atoms) or map or potential field (e.g., interactions of an atom with a potential field) calculations. For example, the evaluation of a Generalized Born solvation model based on the calculation of either volume integrals over the solvent excluded volume or on the calculation of surface integrals on the solvent accessible surface area. As yet another example, various formulations of bonded interactions may be evaluated according to a computation strategy featuring traversal of an appropriate data structure containing relevant coordinate and bond descriptors.

[0042] An "affinity function" is a composition of affinity components each of which corresponds to a combination of an interaction type, an affinity formulation, and a computation strategy. An affinity component may represent interactions for the whole or parts of one or more molecular subsets. An affinity function may contain multiple affinity components relating to the same interaction type. For example, two affinity components may represent the same interaction type but differ in either their affinity formulation and/or their computation strategy. Each distinct molecular configuration for a given molecular combination may produce different quantitative results for an affinity component and hence for the corresponding affinity function. In one embodiment, the analysis of a molecular combination may be based on determination of the configuration with the best value for the affinity function. In other embodiments, multiple favorable values for the affinity function corresponding to molecular configurations associated with one or more potential binding modes may be considered. In yet another embodiment, multiple affinity functions may be computed on one or more configurations of a molecular combination and some decision or action based on their joint consideration, such as for example the scenario of consensus scoring of a small finite number of configurations for each molecular combination explored in the course of screening a molecule library against a target molecule.

[0043] The terms "about" and "approximately" as used herein shall generally mean an acceptable degree of error for the quantity measured given the nature or precision of the measurements. Typical, exemplary degrees of error are within 20 percent (%); preferably, within 10%; and more preferably, within 5% of a given value or range of values. Any reference to "about X" specifically indicates at least the values X, 0.95X, 0.96X, 0.97X, 0.98X, 0.99X, 1.01X, 1.02X, 1.03X, 1.04X, and 1.05X. Thus, "about X" is intended to teach and provide written support for a claim limitation of, e.g., "0.98X." Alternatively, in biological systems, the terms "about" and "approximately" may mean values that are within an order of magnitude, preferably within 5-fold, and more preferably within 2-fold of a given value. Numerical quantities given herein are approximate unless stated otherwise, meaning that the term "about" or "approximately" can be inferred when not expressly stated. When "about" is applied to the beginning of a numerical range, it applies to both ends of the range.

[0044] As used herein, the terms "small molecule," "small organic molecule" and "small inorganic molecule" includes molecules (either organic, organometallic, or inorganic), organic molecules, and inorganic molecules, respectively, which have a molecular weight of more than about 50 Da and less than about 2500 Da. Small organic (for example) molecules may be less than about 2000 Da, between about 100 Da to about 1000 Da, or between about 100 Da to about 600 Da, or between about 200 Da to about 500 Da.

Drug Design and Discovery

[0045] Drug design and discovery processes (which can also be referred to as "drug development") can be divided into the following subprocesses: (1) target validation; (2) lead generation/optimization; (3) preclinical testing; and (4) clinical trials and approval. Target validation includes determination of one or more targets that have disease relevance. Results of the target validation phase might include a determination that the presence or action of the target molecule in an organism causes or influences some effect that initiates, exacerbates, or contributes to a disease for which a cure or treatment is sought. In some cases a natural binder or substrate for the target may also be determined via experimental methods. In the context of the present disclosure, a target is human PD-1 protein, with the examples of disease relevance being cancer start and/or progression, with or without treatment, some exemplary types of cancers being solid tumors and blood cancers, including metastatic cancer and cancers with high microsatellite instability and mismatch-repair deficient cancers. The types of cancers that may be relevant in the context of the present disclosure include, but are not limited to, colorectal cancer, gastrointestinal cancer, including stomach and esophageal cancer, endometrial cancer, breast cancer, prostate cancer, prostate cancer, bladder cancer, thyroid cancer, melanoma, lung cancer, head and neck cancer, including head and neck squamous cell carcinoma, or lymphoma, including Hodgkin lymphoma. Another examples of disease relevance are inherited disorders that lead to increased cancer predisposition, such as the syndromes that include mismatch repair deficiency and/or microsatellite instability, for example, Lynch syndrome.

[0046] Lead generation typically involves the identification of lead compounds, i.e., ligands, that can bind to the target molecule and that may alter the effects of the target

through either activation, deactivation, catalysis, or inhibition of the function of the target, in which case the lead would be a viewed as a suitable candidate ligand to be used in the drug application process. In the context of the present disclosure, initial leads can be compounds that are identified in silico as being able to bind to a PD-L2 binding pocket of human PD-1 and determined to exert biological activity by in vitro and/or in vivo testing. Lead optimization involves the chemical and structural refinement of lead candidates into drug precursors in order to improve binding affinity to the desired target (human PD-1 in the context of the present disclosure), increase selectivity, and also to address basic issues of toxicity, solubility, and metabolism. Together lead generation and lead optimization can result in one or more chemically distinct leads for further consideration. In preclinical testing, biochemical assays and animal models are used to test the selected leads for various pharmacokinetic factors related to drug absorption, distribution, metabolism, excretion, toxicity, side effects, and required dosages. After the preclinical testing period, clinical trials and approval take place, during which the drug candidates are tested on human subjects for safety and efficacy.

[0047] A number of laboratory methods exist for measuring or estimating affinity between a target molecule and a ligand. Often the target might be first isolated and then mixed with the ligand in vitro and the molecular interaction assessed experimentally such as in the myriad biochemical and functional assays associated with high throughput screening. However, such methods are most useful where the target is simple to isolate, the ligand is simple to manufacture and the molecular interaction easily measured, but is more problematic when the target cannot be easily isolated, isolation interferes with the biological process or disease pathway, the ligand is difficult to synthesize in sufficient quantity, or where the particular target or ligand is not well characterized ahead of time. In the latter case, many thousands or millions of experiments might be needed for all possible combinations of the target and ligands, making the use of laboratory methods unfeasible.

[0048] While a number of attempts have been made to resolve this bottleneck by first using specialized knowledge of various chemical and biological properties of the target (or even related targets such as protein family members) and/or one or more already known natural binders or substrates to the target, to reduce the number of combinations required for lab processing, this is still impractical and too expensive in most cases. Instead of actually combining molecules in a laboratory setting and measuring experimental results, another approach is to use computers to simulate or characterize molecular interactions between two or more molecules (i.e., molecular combinations modeled in silico). The use of computational methods to assess molecular combinations and interactions is usually associated with one or more stages of rational drug design, whether structure-based, ligand-based, or both.

Computational Methods

[0049] Rational drug design can use structural information about drug targets (structure-based) and/or their natural ligands (ligand-based) as a basis for the design of effective lead candidate generation and optimization. In the context of the present disclosure, PD-L2 binding pocket of human PD-1 can serve as a drug target in the drug design process. In some cases, natural ligands PD-L1 and/or PD-L2 can serve as a basis for generating lead candidates. Structure-based rational drug design can utilize a three-dimensional model of the structure for the target. For target proteins or nucleic acids, such structures may be the result of X-ray crystallography/NMR or other measurement procedures or may result from homology modeling, analysis of protein motifs and conserved domains, and/or computational modeling of protein folding or the nucleic acid equivalent.

[0050] In the context of the present disclosure, the structure of the target can be a three-dimensional model of the PD-L2 binding pocket of human PD-1 that is computationally derived (generated) from the structures of the PD-L2 binding pocket of human PD-1 described in the present disclosure. For example, the three-dimensional model of the PD-L2 binding pocket of human PD-1 can be computationally derived from atomic coordinates, provided elsewhere in the present disclosure, corresponding to crystals of a variant of human PD-1 comprising amino acid substitutions, such as substitutions in one or more of the residues (for example, each of the residues) corresponding to N74, T76 or A132 of SEQ ID NO:1. In some examples, in addition of a three-dimensional model of the PD-L2 binding pocket of human PD-1 that is computationally derived (generated) from the structures of the PD-L2 binding pocket of human PD-1 described in the present disclosure, structure-based in silico design, testing and/or optimization of human PD-1 ligands can also employ a three-dimensional model of human apo-PD-1 (meaning PD-1 without a ligand) that lacks a PD-2 binding pocket in a process that models formation of the PD-2 binding pocket and ligand-binding. The structure of a ligand may be computationally generated based on natural in vivo ligands, such as PD-1 and/or PD-2, or previously identified ligands. The ligand structure may instead be constructed ab initio from a known 2-D chemical representation using fundamental physics and chemistry principles, for example, when the ligand is not a biopolymer.

[0051] Rational drug design may incorporate the use of any of a number of computational components ranging from computational modeling of target-ligand molecular interactions and combinations to lead optimization to computational prediction of desired drug-like biological properties. The use of computational modeling in the context of rational drug design has been largely motivated by a desire both to reduce the required time and to improve the focus and efficiency of drug research and development, by avoiding often time consuming and costly efforts in biological "wet" lab testing and the like.

[0052] Computational modeling of target-ligand molecular combinations in the context of lead generation may involve the large-scale in silico screening of compound libraries, such as small-molecule libraries (i.e., library screening), whether the libraries are virtually generated and stored as one or more compound structural databases or constructed via combinatorial chemistry and organic synthesis, using computational methods to rank a selected subset of ligands based on computational prediction of bioactivity (or an equivalent measure) with respect to the intended target molecule.

[0053] In the context of the present disclosure, the target molecule is PD-1, and the structure of the target employed in the library screening can be a three-dimensional model of the PD-L2 binding pocket of human PD-1 that is computationally derived (generated) from the structures of the PD-L2 binding pocket of human PD-1 described in the

present disclosure. For example, the three-dimensional model of the PD-L2 binding pocket of human PD-1 can be computationally derived from atomic coordinates, provided elsewhere in the present disclosure, corresponding to crystals of a variant of human PD-1 comprising amino acid substitutions, such as substitutions in one or more of the residues (for example, each of the residues) corresponding to N74, T76 or A132 of SEQ ID NO:1. In some examples, in addition of a three-dimensional model of the PD-L2 binding pocket of human PD-1 that is computationally derived (generated) from the structures of the PD-L2 binding pocket of human PD-1 described in the present disclosure, computational library screending of human PD-1 ligands can also employ a three-dimensional model of human apo-PD-1 (meaning PD-1 without a ligand) that lacks a PD-2 binding pocket in a process that models formation of the PD-2 binding pocket and ligand-binding.

[0054] Fragment-based drug discovery (FBDD), discussed, for example, in (114) and (115), is another tool for discovering leads for drug development. FBDD first identifies starting points: low-molecular-weight ligands (~150 Da) (fragments) that bind to a target, for example, human PD-1. The fragments may bind to the target with the very low affinity. The identified fragments may be them grown or combined to produce leads with higher affinity. The three-dimensional binding mode of the fragments may be determined in silico and/or experimentally, using X-ray crystallography or NMR spectroscopy, and is used to facilitate their optimization into leads with higher activity. FBLD can be combined with screening.

[0055] Various terms and concepts are employed in computational modeling. For example, "binding mode" refers to the 3-D molecular structure of a potential molecular complex in a bound state at or near a minimum of the binding energy (i.e., maximum of the binding affinity), where the term "binding energy" (sometimes interchanged with "binding free energy" or with its conceptually antipodal counterpart "binding affinity") refers to the change in free energy of a molecular system upon formation of a potential molecular complex, i.e., the transition from an unbound to a (potential) bound state for the ligand and target. The term "system pose" is also sometimes used to refer to the binding mode. Here the term free energy generally refers to both enthalpic and entropic effects as the result of physical interactions between the constituent atoms and bonds of the molecules between themselves (i.e., both intermolecular and intramolecular interactions) and with their surrounding environment. Examples of the free energy are the Gibbs free energy encountered in the canonical or grand canonical ensembles of equilibrium statistical mechanics.

[0056] In general, the optimal binding free energy of a given target-ligand pair directly correlates to the likelihood of combination or formation of a potential molecular complex between the two molecules in chemical equilibrium, though, in truth, the binding free energy describes an ensemble of (putative) complexed structures and not one single binding mode. However, in computational modeling, it is usually assumed that the change in free energy is dominated by a single structure corresponding to a minimal energy. This is certainly true for tight binders (pK ~0.1 to 10 nanomolar) but questionable for weak ones (pK ~10 to 100 micromolar). The dominating structure is usually taken to be the binding mode. In some cases, it may be necessary to consider more than one alternative binding mode when the associated system states are nearly degenerate in terms of energy.

[0057] Binding affinity is of direct interest to drug discovery and rational drug design because the interaction of two molecules, such as a protein that is part of a biological process or pathway and a drug candidate sought for targeting a modification of the biological process or pathway, often helps indicate how well the drug candidate will serve its purpose. Furthermore, where the binding mode is determinable, the action of the drug on the target can be better understood. Such understanding may be useful when, for example, it is desirable to further modify one or more characteristics of the ligand so as to improve its potency (with respect to the target), binding specificity (with respect to other target biopolymers), or other chemical and metabolic properties.

[0058] When computationally modeling the nature and/or likelihood of a potential molecular combination for a given target-ligand pair, the actual computational prediction of binding mode and affinity is customarily accomplished in two parts: (a) "docking", in which the computational system attempts to predict the optimal binding mode for the ligand and the target and (b) "scoring", in which the computational system attempts to refine the estimate of the binding affinity associated with the computed binding mode. During library screening, scoring may also be used to predict a relative binding affinity for one ligand vs. another ligand with respect to the target molecule and thereby rank prioritize the ligands or assign a probability for binding.

[0059] Docking may involve a search or function optimization algorithm, whether deterministic or stochastic in nature, with the intent to find one or more system poses that have favorable affinity. Scoring may involve a more refined estimation of an affinity function, where the affinity is represented in terms of a combination of one or more empirical, molecular-mechanics-based, quantum mechanics-based, or knowledge-based expressions, i.e., a scoring function. Individuals scoring functions may themselves be combined to form a more robust consensus-scoring scheme using a variety of formulations. In practice, there are many different docking strategies and scoring schemes employed in the context of today's computational drug design.

[0060] Whatever the choice of computational method there are inherent trade-offs between the computational complexity of both the underlying molecular models and the intrinsic numerical algorithms, and the amount of computing resources (time, number of CPUs, number of simulations) that must be allocated to process each molecular combination. For example, while highly sophisticated molecular dynamics simulations (MD) of the two molecules surrounded by explicit water molecules and evolved over trillions of time steps may lead to higher accuracy in modeling the potential molecular combination, the resultant computational cost (i.e., time and computing power) is so enormous that such simulations are intractable for use with more than just a few molecular combinations. On the other hand, the use of more primitive models for representing molecular interactions, in conjunction with multiple, and often error-prone, modeling shortcuts and approximations, may result in more acceptable computational cost, but will decrease modeling accuracy and predictive power.

[0061] Methods and concepts related to computational aspects of drug discovery and drug design are described in

the publications summarized below. The process of high throughput docking and scoring and its applications are discussed in (46) and (49). A general approach to the design, docking, and virtual screening of multiple combinatorial libraries against a family of proteins is described in (50). The use of multiple computers to accelerate virtual screening of a large ligand library against a specific target by assigning groups of ligands to specific computers is described in (51). A number of examples of software tools are used to perform docking simulations. These methods involve a wide range of computational techniques, including use of a) rigid-body pattern-matching algorithms, either based on surface correlations, use of geometric hashing, pose clustering, or graph pattern-matching; b) fragmental-based methods, including incremental construction or 'place and join' operators; c) stochastic optimization methods including use of Monte Carlo, simulated annealing, or genetic (or memetic) algorithms; d) molecular dynamics simulations or e) hybrids strategies derived thereof.

[0062] The earliest docking software tool was a graph-based rigid-body pattern-matching algorithm called DOCK, developed at UCSF back in 1982 (v1.0), with more recent versions including extensions to include incremental construction. Other examples of graph-based pattern-matching algorithms are described in include CLIX (which in turn uses GRID), FLOG and LIGIN. The above and other software tools are described in (52-56). Other rigid-body pattern-matching docking software tools are described in (57-60) and include the shape-based correlation methods of FTDOCK and HEX, the geometric hashing and the pose clustering. In general, rigid-body pattern-matching algorithms assume that both the target and ligand are rigid (i.e., not flexible) and hence may be appropriate for docking small, rigid molecules (or molecular fragments) to a simple protein with a well-defined, nearly rigid active site. Thus, this class of docking tools may be suitable for de novo ligand design, combinatorial library design, or straightforward rigid-body screening of a molecule library containing multiple conformers per ligand. Incremental construction based docking software tools include FlexX (61, 62) from Tripos (licensed from EMBL), Hammerhead (63), DOCK v4.0 (as an option), and the nongreedy, backtracking algorithm of (64). Programs using incremental construction in the context of de novo ligand design include LUDI (65) (from Accelrys) and GrowMol (66_. Docking software tools also include the tools based on 'place and join' strategies (67).

[0063] Incremental construction algorithms may be used to model docking of flexible ligands to a rigid target molecule with a well-characterized active site. They may be used when screening a library of flexible ligands against one or more targets. They are often comparatively less compute intensive, yet consequently less accurate, than many of their stochastic optimization based competitors. Incremental construction algorithms often employ one or more scoring functions to evaluate and rank different system poses encountered during computations. For example, FlexX was extended to FlexE (68) to attempt to account for partial flexibility of the target molecule's active site via use of user-defined ensembles of certain active site rotamers. Computational docking software tools based on stochastic optimization (69) are described in (70-72) and include ICM (from MolSoft), GLIDE (from Schrodinger), and LigandFit (from Accelrys), all based on modified Monte Carlo techniques, as well as AutoDock v.2.5 (from Scripps Institute) based on simulated annealing. Other software tools based on genetic or memetic algorithms are described in (73-76) and include GOLD, DARWIN, and AutoDock v.3.0 (also from Scripps).

[0064] Stochastic optimization-based methods may be used to model docking of flexible ligands to a target molecule. They generally use a molecular-mechanics-based formulation of the affinity function and employ various strategies to search for one or more favorable system energy minima. They are often more computer intensive, yet also more robust, than their incremental construction competitors. As they are stochastic in nature, different runs or simulations may often result in different predictions. Traditionally most docking software tools using stochastic optimization assume the target to be nearly rigid (i.e., hydrogen bond donor and acceptor groups in the active site may rotate), since otherwise the combinatorial complexity increases rapidly making the problem difficult to robustly solve in reasonable time.

[0065] Molecular dynamics simulations have also been used in the context of computational modeling of target-ligand combinations. This includes the implementations presented in (77) and (71) (along with Monte Carlo). In principle, molecular dynamics simulations may be able to model protein flexibility to an arbitrary degree. On the other hand, they may also require evaluation of many fine-grained, time steps and are thus often very time-consuming (one order of hours or even days per target-ligand combination). They also often require user interaction for selection of valid trajectories. Use of molecular dynamics simulations in lead discovery can be more suited to local minimization of predicted complexes featuring a small number of promising lead candidates. Hybrid methods may involve use of rigid-body pattern-matching techniques for fast screening of selected low-energy ligand conformations, followed by Monte Carlo torsional optimization of surviving poses, and finally even molecular dynamics refinement of a few choice ligand structures in combination with a (potentially) flexible protein active site. An example of this type of docking software strategy is (78).

[0066] There are a number of examples of scoring functions implemented in software and used to estimate target-ligand affinity, rank prioritize different ligands as per a library screen, or rank intermediate docking poses in order to predict binding modes. Scoring functions traditionally fall into three distinct categories: a) empirical scoring functions, b) molecular-mechanics-based expressions, or I knowledge-based scoring functions or hybrid schemes derived thereof. Empirically derived scoring functions (as applied to target-ligand combinations) were first inspired by the linear free-energy relationships often utilized in QSAR studies. An early example is that of Böhm et al. (65, 79) (used in LUDI). Other empirical scoring functions are described in (80-84) and include SCORE (used in FlexX), ChemScore, PLP, Fresno, and GlideScore v.2.0+(modified form of ChemScore, used by GLIDE).

[0067] In general, empirical scoring functions comprise the bulk of scoring functions used today, especially in the context of large compound library screening. The basic premise is to calibrate a linear combination of empirical energy models, each multiplied by an associated numerical weight and each representing one of a set of interaction components represented in a (so-called) 'master scoring equation', where said equation attempts to well approximate

the binding free energy of a molecular combination. The numerical weight factors may be obtained by fitting to experimental binding free energy data composed for a training set of target-ligand complexes. Molecular-mechanics-based scoring functions were first developed for use in molecular modeling in the context of molecular mechanics force fields like AMBER, OPLS, MMFF, and CHARMM (described in (85-89)). Examples of molecular-mechanics-based scoring functions include both the chemical and energy-based scoring functions of DOCK v.4.0 (based on AMBER), the objective functions used in GOLD, AutoDock v.3.0 (with empirical weights), and FLOG. In general, molecular-mechanics-based scoring functions may closely resemble the objective functions utilized by many stochastic optimization-based docking programs. Such functions typically require atomic (or chemical group) level parameterization of various attributes (e.g., charge, mass, van der Waals radii, bond equilibrium constants, etc.) based on one or more molecular mechanics force fields (e.g., AMBER, MMFF, OPLS, etc.). In some cases, the relevant parameters for the ligand may also be assigned based on usage of other molecular modeling software packages, e.g., ligand partial charges assigned via use of MOPAC (90), AMPAC (91) or AMSOL (92). They may also include intramolecular interactions (i.e., self-energy of molecules), as well as long range interactions such as electrostatics. In some cases, the combination of energy terms may again be accomplished via numerical weights optimized for reproduction of test ligand-target complexes.

[0068] Knowledge-based scoring functions were first inspired by the potential of mean force statistical mechanics methods for modeling liquids. Examples include DrugScore, PMF and BLEEP (93-95). In general, knowledge-based scoring functions do not require partitioning of the affinity function. However, they do require usage of a large database of 3-D structures of relevant molecular complexes. There is also usually no need for regression against a data set of molecular complexes with known experimental binding affinities. These methods are based on the underlying assumption that the more favorable an interaction is between two atoms, at a given distance, the more frequent its occurrence relative to expectations in a bulk, disordered medium. These schemes are sometimes referred to as 'inverse Boltzmann' schemes, but in fact the presence of local, optimized structures in macromolecules and protein folds means that distance-dependent pair-wise preference distributions need not be strictly Boltzmann. It is also possible to introduce the concept of singlet preferences based on other molecular descriptors, e.g., solvent accessible surface area for approximation of solvation effects. Hybrid scoring functions may be a mixture of one or more scoring functions of distinct type. One example is VALIDATE (96), which is a molecular-mechanics/empirical hybrid function. Other combinations of scoring functions may include the concept of consensus scoring in which multiple functions may be evaluated for each molecular combination and some form of 'consensus' decision is made based on a set of rules or statistical criteria, e.g., states that occur in the top 10% rank list of each scoring function (intersection-based), states that have a high mean rank (average-based), etc. A useful review discussion of consensus scoring can be found in (97). Various file formats exist for the digital representation of structural and chemical information for both target proteins and compounds as related to structural databases. Examples include the pdb, mol2 (from Tripos), and the SMILES formats.

[0069] A discussion on the calculation of total electrostatic energies involved in the formation of a potential molecular complex can be found in (98). Computational solutions of electrostatic potentials in the classical regime range from simpler formulations, like those involving distance-dependent dielectric functions, to more complex formulations, like those involving solution of the Poisson-Boltzmann equation (99, 100), a second order, generally nonlinear, elliptic partial differential equation. Other classical formalisms that attempt to model electrostatic desolvation include those based on the Generalized Born solvation model (101, 102), methods that involve representation of reaction field effects via additional solvent accessible or fragmental volume terms (103-105), or explicit representation of solvent in the context of molecular dynamics simulations (106-108). A lengthy review of full quantum mechanical treatment of electrostatics interactions can be found in (109).

[0070] FIG. **6** illustrates a modeling system **100** for the analysis of molecular combinations according to embodiments of the present disclosure. As shown, a configuration modeler **102** receives one or more input configuration records **106**, including both the identities of and molecular descriptors for input structures for one or more molecular subsets from an input molecular combination database **104**. The configuration modeler **102** comprises a configuration data transformation engine **108**, an affinity calculator **109**, and descriptor data storage **120**. Results from the configuration modeler **102** are output as configuration results records **111** to a results database (DB) **110**. Modeling system **100** may be used to determine or characterize one or more molecular combinations. In some embodiments, this may include, but is not limited to, prediction of likelihood of formation of a potential molecular complex, or a proxy thereof, the estimation of the binding affinity or binding energy between molecular subsets in an environment, the prediction of the binding mode (or even additional alternative modes) for the molecular combination, or the rank prioritization of a collection of molecular subsets (e.g., ligands) based on predicted bioactivity with a target molecular subset, and would therefore also include usage associated with computational target-ligand docking and scoring.

[0071] In a typical operation, many molecular combinations, each featuring many different molecular configurations, may be modeled. Since the total possible number of configurations may be enormous, the modeling system may sample a subset of configurations during the modeling procedure, though the sampling subset may still be very large (e.g., millions or billions of configurations per combination) and the selection strategy for configuration sampling is specified by one or more search and/or optimization techniques (e.g., steepest descent, conjugate gradient, modified Newton's methods, Monte Carlo, simulated annealing, genetic or memetic algorithms, brute force sampling, pattern matching, incremental construction, fragment place-and-join, etc.). An affinity function is evaluated for each visited configuration and the results for one or more configurations recorded in a storage medium.

[0072] The molecular combination may then be assessed by examination of the set of configuration results including the corresponding computed affinity function values. Once the cycle of computation is complete for one molecular combination, modeling of the next molecular combination

may ensue. Alternatively, in some embodiments of the modeling system **100**, multiple molecular combinations may be modeled in parallel as opposed to in sequence. Likewise, in some embodiments, during modeling of a molecular combination, more than one configuration may be processed in parallel as opposed to in sequence.

[0073] In one embodiment, modeling system **100** may be implemented on a dedicated microprocessor, ASIC, or FPGA. In another embodiment, modeling system **100** may be implemented on an electronic or system board featuring multiple microprocessors, ASICs, or FPGAs. In yet another embodiment, modeling system **100** may be implemented on or across multiple boards housed in one or more electronic devices. In yet another embodiment, modeling system **100** may be implemented across multiple devices containing one or more microprocessors, ASICs, or FPGAs on one or more electronic boards and the devices connected across a network.

[0074] In some embodiments, modeling system **100** may also include one or more storage media devices for the storage of various, required data elements used in or produced by the analysis. Alternatively, in some other embodiments, some or all of the storage media devices may be externally located but networked or otherwise connected to the modeling system **100**. Examples of external storage media devices may include one or more database servers or file systems. In some embodiments involving implementations featuring one or more boards, the modeling system **100** may also include one or more software processing components in order to assist the computational process. Alternatively, in some other embodiments, some or all of the software processing components may be externally located but networked or otherwise connected to the modeling system **100**.

[0075] In some embodiments, results records from database **110** may be further subjected to a configuration selector **112** during which one or more molecular configurations may be selected based on various selection criteria and then resubmitted to the configuration modeler **102** (possibly under different operational conditions) for further scrutiny (i.e., a feedback cycle). In such embodiments, the molecular configurations are transmitted as inputs to the configuration modeler **102** in the form of selected configuration records **114**. In another embodiment, the configuration selector **112** may also send instructions to the configuration data transformation engine on how to construct one or more new configurations to be subsequently modeled by configuration modeler **102**. For example, if the configuration modeler modeled ten target-ligand configurations for a given target-ligand pair (the target, in the context of the present disclosure, can be a PD-L2 binding pocket of human PD-1, and the ligand is a test ligand capable of interacting with the PD-L2 binding pocket of human PD-1), and two of the configurations had substantially higher estimated affinity than the other eight, then the configuration selector **112** may generate instructions for the configuration data transformation engine on how to construct further additional configurations (i.e., both target and ligand poses) that are structurally similar to the top two high-scoring configurations, which are then subsequently processed by the remainder of the configuration modeler **102**. In some embodiments, the transmitted instructions may relate to construction from the resubmitted configurations whereas in other cases they relate to construction from the original input reference configuration(s).

[0076] In some embodiments, once analysis of a molecular combination is completed (i.e., all desired configurations assessed) a combination postprocessor **116** may be used to select one or more configuration results records from database **110** in order to generate one or more qualitative or quantitative measures for the combination, such as a combination score, a combination summary, a combination grade, etc., and the resultant combination measures are then stored in a combination results database **118**. In one embodiment, the combination measure may reflect the configuration record stored in database **110** with the best observed affinity. In another embodiment, multiple high affinity configurations are submitted to the combination postprocessor **116** and a set of combination measures written to the combination results database **118**. In another embodiment, the selection of multiple configurations for use by the combination postprocessor **116** may involve one or more thresholds or other decision-based criteria.

[0077] In a further embodiment, the selected configurations are also chosen based on criteria involving structural diversity or, alternatively, structural similarity (e.g., consideration of mutual rmsd of configurations, use of structure-based clustering or niching strategies, etc.). In yet another embodiment, the combination measures output to the combination results database **118** are based on various statistical analysis of a sampling of possibly a large number of configuration results records stored in database **110**. In other embodiment the selection sampling itself may be based on statistical methods (e.g., principal component analysis, multidimensional clustering, multivariate regression, etc.) or on pattern-matching methods (e.g., neural networks, support vector machines, etc.)

[0078] In yet another embodiment, the combination results records stored in database **118** may not only include the relevant combination measures, but may also include some or all of the various configuration records selected by the combination postprocessor **116** in order to construct a given combination measure. For example, combination results records stored in database **118** may include representations of the predicted binding mode or of other alternative, high affinity (possibly structurally diverse) modes for the molecular combination. In another embodiment, the combination postprocessor **116** may be applied dynamically (i.e., on-the-fly) to the configuration results database **110** in conjunction with the analysis of the molecular combination as configuration results records become available. In yet another embodiment, the combination postprocessor **116** may be used to rank different configurations in order to store a sorted list of either all or a subset of the configurations stored in database **110** that are associated with the combination in question. In yet other embodiments, once the final combination results records, reflecting the complete analysis of the molecular combination by the configuration modeler **102**, have been stored in database **118**, some or all of the configuration records in database **110** may be removed or deleted in order to conserve storage in the context of a library screen involving possibly many different molecular combinations. Alternatively, some form of garbage collection or equivalent may be used in other embodiments to dynamically remove poor affinity configuration records from database **110**.

[0079] In one embodiment, the molecular combination record database **104** may comprise one or more molecule records databases (e.g., flat file, relational, object oriented,

etc.) or file systems and the configuration modeler **102** receives an input molecule record corresponding to an input structure for each molecular subset of the combination, and possibly a set of environmental descriptors for an associated environment. In another embodiment, when modeling target protein-ligand molecular combinations, the molecular combination record database **104** is replaced by an input target record database and an input ligand (or drug candidate) record database. In a further embodiment, the input target molecular records may be based on that are experimentally derived (e.g., X-ray crystallography, NMR, etc.), energy minimized, and/or model-built structures. In another embodiment, the input ligand molecular records may reflect energy minimized or randomized 3-D structures or other 3-D structures converted from a 2-D chemical representation, or even a sampling of low energy conformers of the ligand in isolation. In yet another embodiment, the input ligand molecular records may correspond to naturally existing compounds or even to virtually generated compounds, which may or may not be synthesizable.

[0080] In one embodiment the configuration data transformation engine **108** may transform one or more input molecular configurations into one or more other new configurations by application of various geometrical operators characterized by sets of geometrical descriptors. Transformation of molecular configurations into newer variants may be accomplished by one or more unary operations (i.e., acting on one input configuration, such as the mutation operator in a genetic algorithm), binary operations (i.e., acting on two input configurations, such as a binary crossover in a genetic algorithm), other n-ary operations (i.e., acting on a plurality of input configurations, such as a transform operator based on a population of configurations), or a combination thereof. In another embodiment, the transformation of molecular configurations into newer variants may result in multiple new configurations from one configuration, such as, for example, the construction of a suitable (often randomized) initial population for use in a genetic algorithm. In some embodiments, the configuration data transformation engine **108** may be able to construct ab initio one or more entirely new configurations without the requirement of input geometrical descriptors from an input molecular combination database **104**, though other types of molecular descriptors may still be needed.

[0081] As already discussed, in some embodiments, the set of configurations generated via transformation during the course of an analysis of a molecular combination may be determined according to a schedule or sampling scheme specified by one or more search and/or optimization techniques used to drive the modeling processes of the configuration modeler **102**. In some embodiments, the search strategy or optimization technique may be an iterative process whereby one or more configurations are generated from one or more input configurations, then affinities are calculated for each configuration, decisions are made based on affinity and/or structure, and all or part of the new set of configurations are used as input seeds for the next iteration; the process continuing until a specified number of iterations are completed configuration modeler **102** or some other convergence criteria satisfied. In such embodiments, the input configuration records **106** obtained or derived from data in the input molecular combination database **104**, may serve only to initiate (or also possibly reset) the iterative process (i.e., prime the pump). For example, in the context of the present disclosure, the input target molecular records may be based on atomic coordinates of PD-L2 binding pocket of human PD-1 included in the present disclosure, which are determined from co-crystals of a variant of human PD-1 with PD-L2 ligand. In one example, the variant of human PD-1 is a variant comprising amino acid substitutions in one or more of (such as in each) of residues corresponding to N74, T76 or A132 of SEQ ID NO:1,

[0082] In some embodiments, the search strategy or optimization technique may be stochastic in nature meaning that the set of configurations visited during analysis of a molecular combination may involve some random component and thus be possibly different between different runs of the configuration modeler **102** as applied to the same molecular combination. Here the term run refers to two different initiations of (possibly iterative) cycles of computation for analysis of the same molecular combination. In some embodiments, the combination postprocessor **116** may then base its results or decisions on configuration results records stored in database **110** but obtained from different runs. In some embodiments, the configuration data transformation engine **108** may produce new configurations sequentially, such as a new possible state associated with a given iteration of a Monte Carlo-based technique, and feed them to the affinity calculator **109** in a sequential manner. In other embodiments, the configuration data transformation engine **108** may produce multiple new configurations in parallel, such as a population associated with a given iteration of a genetic algorithm, and submit them in parallel to the affinity calculator **109**. In other embodiments, the configuration data transformation engine **108** may not generate additional configurations and instead the configuration modeler **102** may operate solely on one or more input configuration records from the input molecular combination database **104**, such as for example in some usages of modeling system **100** related to scoring of a set of known molecular configurations. In such embodiments, the configuration data modeler **102** may not include a search or optimization strategy and instead be used to perform affinity calculations on an enumerated set of input configuration records.

[0083] In some embodiments, various descriptor data related to the configurations of a given molecular combination may be stored or cached in one or more components of a descriptor data storage **120** via one or more storage (or memory) allocation means, structure or apparatus for efficient access and storage during the cycle of computations performed by the configuration modeler **102**. In one embodiment, the descriptor data storage **120** may contain chemical or physical descriptors assigned to atoms, bonds, groups, residues, etc. in each of the molecular subsets or may even also contain environmental descriptors. In another embodiment, the descriptor data common to all configurations for a given molecular combination is compactly represented via a storage allocation means in one or more lookup tables. For example, often many physical and chemical descriptors may be identical for different configurations of a combination whereas one or more geometric descriptors are not. In yet another embodiment, the descriptor data storage **120** may also contain relevant geometric descriptors for the configurations arranged in one or more storage formats via a prescribed storage allocation means. As examples, such formats may involve, but are not limited to, records analogous to pdb or mol2 file formats. Additional examples include various data structures such as those associated with

the molecular representation partitioning shown in Ahuja I. As a further example, perhaps stored descriptors for atoms and bonds may represent individual nodes in one or more lists or arrays, or may alternatively be attached, respectively, to nodes and edges of a tree or directed graph.

[0084] The whole or parts of the input configuration records **106**, and, if applicable, selected configuration records **114** chosen by configuration selector **112**, may be converted to data representations used in the storage allocation means of the descriptor data storage **120**. Data constructs contained in the descriptor data storage **120** may be either read (i.e., accessed) for use by the configuration data transformation engine **108** or the affinity calculator **109** and may be written either at the inception of or during the execution of a cycle of computation by the configuration modeler **102**. The layout and access patterns for the associated descriptor data storage **120** will likely depend on the needs of the affinity calculator **109** as well as the configuration data transformation engine **108**.

[0085] The affinity calculator **109** may comprise one or more processing (i.e., affinity) engines, where each affinity engine may be dedicated to performing calculations related to one or more affinity components as defined previously in regard to interaction types, affinity formulations, and computation strategies. In some embodiments, different affinity engines are assigned to each unique affinity component. In other embodiments, one or more affinity engines may compute multiple affinity components according to similarity of processing requirements. In yet other embodiments, different affinity engines may be grouped or otherwise arranged together to take advantage of common subsets of required input data in order to improve any caching scheme and/or to reduce the number of, the bandwidth requirements for, or the routing requirements for various associated data paths.

[0086] For example, in one embodiment, affinity components for both the electrostatic and van der Waals interactions involving field-based computation strategies utilizing stored pregenerated probe grid maps, may be computed on the same affinity engine, where said engine requires access to both types of probe grid maps in storage and to various numerical parameters used in evaluating the affinity formulation for the two different interactions. As another example, affinity components for both the hydrogen bonding and van der Waals interactions using affinity formulations featuring generalized Lennard-Jones potentials computed according to a pair-based computation strategy may be computed on the same affinity engine. In an alternative embodiment, the same two affinity components may be computed using two different affinity engines but grouped together in order to share common input data such as that relating to spatial coordinates and a subset of relevant chemical or physical descriptors.

In Vitro and In Vivo Methods

[0087] The methods related to drug design and discovery described in the present disclosure can include determining biological activity (including presence, absence or amount of biological activity, which can be also referred of "efficacy," of a candidate compound or molecule (which can be, but is not limited to, a small molecule) identified and/or designed by computational (in silico) methods in an in vitro biological assay or in vivo in a subject (such as a model animal, for example, a wild-type animal, a laboratory-bred animal, or a transgenic animal model). The methods disclosed in the present disclosure can also include validating or confirming in silico predicted activities of a ligand, for example, in silico binding of the ligand to PD-1 conformation of the target protein, with the results of an in vitro biological assay, and/or with the results of an in vivo study in an animal model.

[0088] One assay in vitro platform suitable for evaluation of the ability of candidate compounds to block PD-1 interaction with its in vivo ligands is described in (116). The platform uses fluorescence-base transcriptional reporters based on the human Jurkat T cell line in conjunction with engineered T cell stimulator cell lines for investigating immune checkpoint signaling pathways, including PD-1 activity. A PD-1:PD-L2 cell-based inhibitor screening assay kit for conducting is a bioluminescent cell-based assay that can be used to screen and profile inhibitors of the PD-1:PD-L2 interaction is available from BPS Bioscience (San Diego, Calif.). In the above assay, as described in the assay data sheet, PD-1/NFAT Reporter/Jurkat T cells are used as effector cells; HEK293 cells over-expressing PD-L2 and an engineered T cell receptor (TCR) activator by transient transfection are used as target cells. When the cells are co-cultivated, TCR complexes on effector cells are activated by TCR activator on target cells, resulting in expression of the NFAT luciferase reporter. However, PD-1 and PD-L2 binding prevents TCR activation and suppresses the NFAT-responsive luciferase activity. In both scenarios, this inhibition can be specifically reversed by anti-PD-1 antibodies. This interaction also can be blocked by anti-PD-L2 antibodies. These neutralizing antibodies block PD-1 signaling and promote T cell activation, resulting in reactivation of the NFAT-responsive luciferase reporter. Another example of an in vitro assay suitable for evaluation of the ability of candidade compounds to block PD-1 interaction with its ligand in vitro is competition ELISA described in (117). As described in (117), the assay measures the amount of biotin tagged PD-1 that is able to bind to the wells coated with PD-L1. Similarly, PD-L2 can be used as an in vivo ligand. An example of an in vitro assay for testing biological activity of candidate compounds, also described in (117), is an assay testing the ability of candidate compounds to promote T cell function. As described in (117), the production of IL-2 by peripheral blood mononuclear cells (PBMCs) pre-treated with PD-1/PD-L1 antagonists (or inhibitors): neutralizing mAbs or candidate compounds before stimulation with Staphylococcal enterotoxin B (SEB) for 72 hours. PBMCs include the cells that express/up-regulate both PD-1 (T cells) and PD-L1 (T cells, APCs) upon stimulation. In this assay, cytokine levels from cell culture supernatants would indicate that stimulated T cells treated with a-PD-1/PD-L1 antagonist produced significantly higher concentrations of IL-2 compared to untreated and stimulated cells, with the cells pre-treated by neutralizing mAbs serving as a positive control. Some other in vitro assays suitable for evaluating biologica activity of candidate compounds are described in (118). In one assay, PBMC from normal healthy donors are seeded at 1×10^5 cells/well and stimulated with SEB in the presence of candidate compounds. IL-2 secretion by PMBC is measured by ELISA on day 3 after the stimulation. In another assay, mixed lymphocyte response is assessed by co-culturing 1×10^5 cells $CD4^+$ T cells with allogeneic monocyte-derived dendritic cells (DC) at a ratio of 10:1 (T:DC) in flat-bottom 96-well microtiter plates. $CD4^+$ T cells and DC are incubated for 6 days in the presence or absence of a

candidate compound. Culture supernatants are harvested on day 5 for ELISA analysis of IFN-γ secretion. One more assay measures nonspecific T cell activation. In this assay, candidate compounds are mixed with samples of heparinized fresh human whole blood to measure cytokine release. After a 4-hour incubation at 37° C., the cells are pelleted, and the plasma fraction collected for measurement of IFN-γ, TNF-α, IL-2, IL-4, IL-6, and IL-10 using a cytokine cytometric bead array assay. Studies of potential anti-cancer effects of candidate compounds can also be performed in vitro in tumor-derived cell ilnes, such as D4m melanoma lines.

[0089] In vivo assays can be performed using animals, such as mice, with chemically induced or implanted tumors. Examples of in vivo assays using mouse models are described in (118). MC38 tumor cells are cultured in DMEM and implanted subcutaneously into female C57/B16 mice or B6.129S7-Ifngtm1Ts/J C57BL/6 mice. CT26 tumor cells are cultured in DMEM and implanted subcutaneously in female BALB/c mice. Tumor measurements are made 2-3 times weekly using an electronic caliper. Candidate compounds are administered to mice intraperitoneally on days 7, 10, and 13. For T-cell depletion studies, 500 μg of depleting antibodies for CD4 (GK1.5) or CD8 (53.6.72; BioXCell, W. Lebanon, N.H.) are administered on day 7. following subcutaneous implantation of MC38 tumor cells in the hind flank. The efficiency of $CD4^+$ or $CD8^+$ T cell depletion (>90%) is confirmed by FACS analysis of blood samples collected four days after administration of the depleting antibodies. Mice are sacrificed at the study termination or pre-determined endpoints. For immune response monitoring, tumors are harvested and processed using cell disruptors. The cell suspensions are clarified, pelleted, resuspended buffer or media, and counted. Cells are incubated with anti-CD16/32 mAb 24G.2 (BioXCell) to reduce background FcγR binding and then stained with antibodies specific for CD8, CD4, and CD45. Cells are also stained with the a fixable viability. For intracellular staining (ICS), cell samples are fixed, permeabilized, and stained with antibodies specific for FoxP3, Ki67, CTLA-4, IFN-γ, and TNF-α CT26 tumor antigen-specific $CD8^+$ T cells are identified using AH-1 MHC class I tetramers. Ex vivo AH-1 peptide stimulation is performed by culturing tumor or splenic cells with 2 μM AH-1 peptide (MBL) in the presence of brefeldin-A for 4 hours at 37° C. Ex vivo cytokine staining is performed by fixing and staining cells as described above, directly after tissue harvest. Samples are analyzed on FACS flow cytometers. Cytokine assays of harvested tumor cells can also be performed using bead-bays cytokine arrays. Immunohistochemical studies of tumor sections can also be performed according to established procedures.

[0090] Any of the methods described in the present disclosure can further comprise determining the toxicity of the ligand in an in vitro, in vivo or in silico assay. As used in the present disclosure, toxicity refers to a harmful effect on a cell or organism. For example, and not to be limiting, the cardiotoxicity or neurotoxicity of a compound can be determined. In vitro methods for assessing cardiotoxicity are known in the art. For example, electrophysiology measurements can be performed in cells, including, for example single cardiac cells. The effect of one or more compounds can be assessed in cell lines that express the human ether-a-go-go related gene (hERG1) or in cells transfected with hERG1. The hERG safety assay from Cyprotex (Watertown, Mass.) can also be used. Cardiotoxicity can also be measured in vivo by conducting an electrocardiogram (ECG) in a subject (e.g., a wild type animal or transgenic animal) expressing hERG1 after administering the compound to the animal. In vitro cytotoxicity panels can also be used to measure toxicity in individual cells. For example, assays that measure nuclear size, mitochondrial membrane potential, intracellular calcium, membrane permeability and/or cell number can be used. See, for example, the ADME-Tox panel available from EuroFins PanLabs, Inc. (Redmond, Wash.). In this assay, all five parameters are measured. Intracellular calcium and membrane permeability will increase in the presence of a cytotoxic compound. Conversely, nuclear size, cell number and mitochondrial membrane potential will decrease in the presence of a cytotoxic compound.

[0091] Genotoxicity studies can also be performed to identify mutagenic compounds. Gene mutations can be detected in bacteria, where they cause a change in growth requirements. The Ames test, which is conducted using *Salmonella typhimurium* is a widely used bacterial assay for the identification of compounds that can produce gene mutations, and it shows high predictive value with rodent carcinogenicity tests. Micronucleus assays can also be used to identify mutagenic compounds. Micronucleus formation is a hallmark of genotoxicity. Micronuclei are chromatin-containing bodies that represent fragments or even whole chromosomes that were not incorporated into a daughter cell nucleus at mitosis. The purpose of the assay is to detect those agents that induce chromosome damage leading to the induction of micronuclei in interphase cells. Assays that measure Cytochrome p450 (CYP) inhibition, CYP induction or drug transporter inhibition can also be performed.

[0092] Any of the methods provided in the present disclosure can further comprise determining if a candidate compound or molecule has an adverse drug reaction (ADR) or off-target effect in an in vitro, in vivo or in silico assay. It should be noted that off-target effects may be desirable or undesirable effects. In silico methods for determining off-target effects are known in the art. See, for example (110-112). In vitro assays for assessing off-target effects are also known in the art. See (113) for a review of in vitro assays that can identify undesirable off-target activity. Any of the methods provided herein can further comprise optimizing the ligand. A candidate compound or molecule can be modified or optimized for certain properties. For example, a candidate compound or molecule can be modified to reduce its toxicity, to reduce an undesirable off-target effect, to increase the binding affinity to a target protein, to decrease the binding affinity to a target protein, to increase a desirable off-target activity or to decrease an off-target activity.

Computer Systems

[0093] Any of the computer systems mentioned in the present disclosure may utilize any suitable number of subsystems. In some embodiments, a computer system includes a single computer apparatus, where the subsystems can be the components of the computer apparatus. In other embodiments, a computer system can include multiple computer apparatuses, each being a subsystem, with internal components. The subsystems can be interconnected via a system bus. Additional subsystems such as a printer, keyboard, storage device(s), monitor, which is coupled to display adapter, and others are shown. Peripherals and input/output

(I/O) devices, which couple to I/O controller, can be connected to the computer system by any number of means known in the art, such as serial port. For example, serial port or external interface (e.g. Ethernet, Wi-Fi, etc.) can be used to connect computer system to a wide area network such as the Internet, a mouse input device, or a scanner. The interconnection via system bus allows the central processor to communicate with each subsystem and to control the execution of instructions from system memory or the storage device(s) (e.g., a fixed disk, such as a hard drive or optical disk), as well as the exchange of information between subsystems. The system memory and/or the storage device (s) may embody a computer readable medium. Any of the data mentioned herein can be output from one component to another component and can be output to the user.

[0094] A computer system can include a plurality of the same components or subsystems, e.g., connected together by external interface or by an internal interface. In some embodiments, computer systems, subsystem, or apparatuses can communicate over a network. In such instances, one computer can be considered a client and another computer a server, where each can be part of a same computer system. A client and a server can each include multiple systems, subsystems, or components.

[0095] It should be understood that any of the embodiments of the present invention can be implemented in the form of control logic using hardware (e.g. an application specific integrated circuit or field programmable gate array) and/or using computer software with a generally programmable processor in a modular or integrated manner. As user herein, a processor includes a multi-core processor on a same integrated chip, or multiple processing units on a single circuit board or networked. Based on the disclosure and teachings provided herein, a person of ordinary skill in the art will know and appreciate other ways and/or methods to implement embodiments of the present invention using hardware and a combination of hardware and software.

[0096] Any of the software components or functions described in this application may be implemented as software code to be executed by a processor using any suitable computer language such as, for example, Java, C++ or Perl using, for example, conventional or object-oriented techniques. The software code may be stored as a series of instructions or commands on a computer readable medium for storage and/or transmission, suitable media include random access memory (RAM), a read only memory (ROM), a magnetic medium such as a hard-drive or a floppy disk, or an optical medium such as a compact disk (CD) or DVD (digital versatile disk), flash memory, and the like. The computer readable medium may be any combination of such storage or transmission devices.

[0097] Such programs may also be encoded and transmitted using carrier signals adapted for transmission via wired, optical, and/or wireless networks conforming to a variety of protocols, including the Internet. As such, a computer readable medium according to an embodiment of the present invention may be created using a data signal encoded with such programs. Computer readable media encoded with the program code may be packaged with a compatible device or provided separately from other devices (e.g., via Internet download). Any such computer readable medium may reside on or within a single computer product (e.g. a hard drive, a CD, or an entire computer system), and may be present on or within different computer products within a system or network. A computer system may include a monitor, printer, or other suitable display for providing any of the results mentioned herein to a user.

[0098] The methods described herein may be totally or partially performed with a computer system including one or more processors, which can be configured to perform the steps. Thus, embodiments can be directed to computer systems configured to perform the steps of any of the methods described herein, potentially with different components performing a respective steps or a respective group of steps. Although presented as numbered steps, steps of methods herein can be performed at a same time or in a different order. Additionally, portions of these steps may be used with portions of other steps from other methods. Also, all or portions of a step may be optional. Additionally, any of the steps of any of the methods can be performed with modules, circuits, or other means for performing these steps.

EXAMPLES

[0099] The following examples are offered to illustrate, but not to limit the claimed invention.

Example 1: Materials and Methods

[0100] A. Yeast-Surface Display

[0101] Deep mutational scanning of the CC' and FG loops of human PD-1 was performed using a previously described PCR-based method (24). The PD-1 loop variant libraries were constructed using the *Saccharomyces cerevisiae* EBY100 strain. MACS and FACS experiments were performed using recombinant human PD-L2-Fc or PD-L1-Fc proteins. The yeast strains and plasmids used in the study are summarized in Table 1.

TABLE 1

Plasmids and yeast strain.

Yeast Strain (45)	Genotype
EBY100	MATa AGA1::P_{GAL1}-AGA1::URA3 ura3-52 trp1 leu2Δ200 his3Δ200 pep4Δ::HIS3 prb1Δ1.6R can1 GAL

Plasmid	Description
pST892	pRS414 P_{GAL1}-AGA2-PD-1(P21-E150)
pST992	pRS414 P_{GAL1}-AGA2-PD-1(P21-E150) N74G
pST993	pRS414 P_{GAL1}-AGA2-PD-1(P21-E150) T76P
pST995	pRS414 P_{GAL1}-AGA2-PD-1(P21-E150) A132V
pST1013	pRS414 P_{GAL1}-AGA2-PD-1(P21-E150) N74G T76P A132V
pST1132	pET23d PD-1(N33-E150)-StrepII C93S N74G T76P A132V
pST1167	pET23d PD-1(N33-E150)-StrepII C93S T76P A132V
pST971	pADD2 PD-L1-Fc
pST972	pADD2 PD-L2-Fc
pST980	pADD2 Fc
pST981	pADD2 PD-1-Fc
pST982	pADD2 PD-1-Fc N74G
pST983	pADD2 PD-1-Fc T76P
pST985	pADD2 PD-1-Fc A132V
pST1008	pADD2 PD-1-Fc N74G A132V
pST1009	pADD2 PD-1-Fc T76P A132V
pST1010	pADD2 PD-1-Fc N74G T76P A132V
pST739	pADD2 PD-L1-His_6
pST700	pADD2 PD-L2-His_6
pST963	pADD2 PD-1-Fc C93S
pST964	pADD2 PD-1-Fc C93S CC' loop-mutant (S71G P72G S73G N74G Q75G T76G D77G)
pST965	pADD2 PD-1-Fc C93S FG loop-mutant (L128G A129G P130G K131G A132G Q133G)

TABLE 1-continued

Plasmids and yeast strain.

pST966	pADD2 PD-1-Fc C93S Pocket-mutant (Y68A I126A I134A E136A)
pST1195	pADD2 PD-1(N33-E150)-Ctag C93S N74G T76P A132V N49S N58S N116D
pST1228	pADD2 PD-1(N33-E150)-Ctag N49D N58D N74D N116D
pST1207	pADD2 PD-L2(M1-Y123) N37D N64D
pST1249	pADD2 PD-1-Fc V64E
pST1250	pADD2 PD-1-Fc N66A
pST1251	pADD2 PD-1-Fc Y68A
pST1252	pADD2 PD-1-Fc Q75A
pST1253	pADD2 PD-1-Fc I126D
pST1254	pADD2 PD-1-Fc I134D
pST1255	pADD2 PD-1-Fc E136A
pST1262	pADD2 PD-L2-His_6 I103D
pST1263	pADD2 PD-L2-His_6 I105D
pST1266	pADD2 PD-L2-His_6 Y112A
pST1267	pADD2 PD-L2-His_6 Y114A

[0102] B. Bio-Layer Interferometry

[0103] BLI was performed on an Octet RED96® system at 30° C. in a buffer of 150 mM NaCl, 20 mM HEPES:NaOH pH 7.4, 0.1% BSA and 0.05% Tween 20. The human PD-1-Fc proteins were loaded onto anti-human IgG Fc capture (AHC) biosensors, associated in defined concentrations of human PD-L2-His6 or PD-L1-His6 proteins, and then dissociated in buffer.

[0104] C. Protein Crystallization and X-Ray Crystallography

[0105] The human apo-PD-1N74G T76P A132V and human apo-PD-1T76P A132V proteins were over-expressed in and refolded from the inclusion bodies of *Escherichia coli* BL21(DE3) cells. The human apo-PD-1N74G T76P A132V protein was crystallized in 100 mM NaCl, 100 mM Tris:HCl pH 8.0, 27% (w/v) PEG-MME 5,000. The human apo-PD-1T76P A132V protein was crystallized in 100 mM NaCl, 100 mM Tris:HCl pH 8.0, 36% (w/v) PEG 3,350. The human PD-1N74G T76P A132V and human PD-L2IgV protein complex was produced using the human Expi293F cell line. The complex was crystallized in 200 mM magnesium acetate, 10% (w/v) PEG 8000. All X-ray diffraction data were collected at the SSRL beam lines 12-2 or 14-1, and processed using HKL-3000 (42). Molecular replacement, refinement and density modification were performed in Phenix (43) and model building in Coot (44). The crystallographic data collection and refinement statistics are summarized in Table 2.

Example 2: Engineering Human PD-1 Loop Variants with Enhanced PD-L2 Affinity

[0106] Substantial earlier efforts (23) to crystalize the human PD-1/PD-L2 complex were unsuccessful. Previous

TABLE 2

Crystallographic data collection and refinement statistics.

	$PD1^{N74G\ T76P\ A132V}$/ $PD\text{-}L2^{Igv}$	$Apo\text{-}PD1^{N74G\ T76P\ A132V}$	$Apo\text{-}PD1^{T76P\ A132V}$
Wavelength (Å)	0.978	0.978	0.978
Resolution range (Å)	37.5-1.99 (2.06-1.99)	36.5-1.18 (1.23-1.18)	36.5-1.42 (1.48-1.42)
Space group	P 2_1 2_1 2_1	P 3_2 2 1	P 3_2 2 1
Unit cell	41.3 67.8 89.7 90 90 90	46.2 46.2 89.3 90 90 120	46.2 46.2 89.4 90 90 120
Total reflections	185797 (11081)	400313 (24984)	171335 (11683)
Unique reflections	17750 (1645)	36661 (3544)	21301 (2090)
Multiplicity	10.4 (6.7)	10.9 (7.0)	8.0 (5.6)
Completeness (%)	98.6 (90.6)	99.7 (98.8)	99.7 (98.2)
Mean I/sigma(I)	16.1 (2.28)	28.5 (2.79)	23.3 (2.40)
Wilson B-factor	35.8	16.7	21.9
R_{merge}	0.139 (0.723)	0.0521 (0.539)	0.0903 (1.03)
$CC_{1/2}$	0.992 (0.780)	0.999 (0.856)	0.998 (0.769)
CC*	0.998 (0.936)	1.00 (0.960)	0.999 (0.932)
R_{work}	0.196 (0.292)	0.154 (0.192)	0.158 (0.193)
R_{free}	0.226 (0.339)	0.164 (0.233)	0.189 (0.263)
Number of non-hydrogen atoms	1782	1156	1143
macromolecules	1654	1001	1056
water	127	144	82
Protein residues	210	112	116
RMS(bonds) (Å)	0.013	0.009	0.016
RMS(angles) (°)	1.48	1.35	1.60
Ramachandran favored (%)	99	100	99
Ramachandran outliers (%)	0	0	0
Clashscore	8.32	0.99	5.66
Average B-factor	50.8	23.4	30.3
macromolecules	50.6	21.1	30.9
solvent	53.8	38.2	39.1

Statistics for the highest-resolution shell are shown in parentheses.

studies (16, 17, 19) indicated that the PD-1 ligand-binding interface comprises a hydrophobic core, the CC' loop and the FG loop, and that formation of a complex with ligands results in loop movement and pocket formation in the hydrophobic core. In the present study, it was conceived that mutations in these two loops of PD-1 were coupled to pocket formation and may alter the affinity for PD-L2. It was then experimentally confirmed that poly-glycine mutants of these loops in human PD-1 significantly decreased its affinities for PD-L2 (data not shown). The binding of sensor-loaded PD-1, the glycine-loop-mutants and the pocket mutant to 1.9 μM PD-L2 (left) and 17 μM PD-L1 (right) was measured using biolayer interferometry. Corresponding PD-1-Fc proteins were loaded onto anti-human IgG Fc capture (AHC) biosensors. Association was monitored for 2 min and dissociation for 2 min. Since the present study was particularly interested in the structure of the PD-1 pocket when bound to PD-L2, the residues in the hydrophobic core were maintained, and directed evolution was performed exclusively in the CC' loop (residues 70-78) and the FG loop (residues 127-133) of human PD-1. Deep mutational scanning (24, 27) was used to construct loop-variant libraries with trinucleotides encoding each of 20 residues at each position. Next, yeast-surface display (25) was used with a recombinant human PD-L2-human Fc fusion protein as the selection agent. After two rounds of selection using magnetic- and fluorescent-activated cell sorting (MACS and FACS), human PD-1 loop-variant clones with single-residue substitutions were isolated (data not shown). Substitutions at two residues were identified in the CC' loop (N74G and T76P), and at one residue in the FG loop (A132V, A132L). In contrast, when the same yeast library was used for section with PD-L1-Fc, only the A132 substitutions were isolated as high-affinity variants (data not shown). This result suggested that the N74G and T76P variants were PD-L2-binding specific. PD-1^{T76P} was chosen as a template to generate a second PD-1 loop variant library and selected for further enhancement of PD-L2 binding. As a result, a PD-1 triple mutant was obtained, which contained all three substitutions identified from the first library, N74G, T76P and A132V.

Example 3: PD-1 Loop Variants Showed Increased Binding Affinity and Association Kinetics for PD-L2 and PD-L1

[0107] To validate the enhanced affinity of PD-1 loop variants, human PD-1 and the loop variants, as well as human PD-L2 and PD-L1 ectodomain proteins, were recombinantly expressed and purified. Using bio-layer interferometry (BLI), the binding of PD-L2 to wild-type PD-1 and the variants was compared (data not shown). The binding of sensor-loaded PD-1 and the loop variants to 190 nM PD-L2 and 1.1 μM PD-L1 was measured using biolayer interferometry. Corresponding PD-1-Fc proteins were loaded on anti-human IgG Fc capture (AHC) biosensors. Association was monitored for 2 min and dissociation for 2 min. Fitting of binding curves was performed in Graphpad Prism 8 software using built-in equations of "Receptor binding—kinetics" models. Means and standard deviations were calculated from 3-4 independent experiments. Wild-type PD-1 bound PD-L2 with a K_D of 500 nM. The variants all exhibited increased PD-L2 affinity, with K_D of 170 nM for N74G, 12 nM for T76P, and 69 nM for A132V. Remarkably, the PD-1 triple mutant had a K_D of 2.6 nM, exhibiting a ~200-fold increase in PD-L2 binding affinity. Table 3 summarizes the binding affinity (K_D) and kinetic parameters (association constant k_{on}, dissociation constant k_{off}) for the PD-1 loop variants binding to PD-L2 or PD-L1. Fitting of binding curves was performed in Graphpad Prism 8 using built-in equations of "Receptor binding—kinetics" models. Means and standard deviations were calculated from 3-4 independent experiments. The triple-mutant also showed substantially increased affinity for PD-L1. The A132V mutant showed increased affinity for PD-L1, consistent with previous reports (19, 23, 28, 29), but the N74G and T76P single mutants had minor effects. Thus, a human PD-1 triple-mutant exhibited potent binding affinity enhancement for both PD-L1 and PD-L2. Kinetic measurements of binding of the ligands by PD-1 with BLI also permitted the determination of association constants (k_{on}). Compared to wild-type PD-1, all loop variants showed increased k_{on} for binding PD-L2. The PD-1 triple mutant showed a 3-fold increase of k_{on} for PD-L2, and 14-fold for PD-L1. These results suggested that these amino acid substitutions in the loops stabilized the ligand-bound state among the conformational ensembles of apo-PD-1 (17, 19).

TABLE 3

Binding affinity (K_D) and kinetic parameters (association constant k_{on}, dissociation constant k_{off}) for the PD-1 loop variants binding to PD-L2 or PD-L1.

	Binding hPD-L2			Binding hPD-L1		
hPD-1	K_D (nM)	k_{on} (10^5/M · s)	k_{off} (10^{-2}/s)	K_D (nM)	k_{on} (10^5/M · s)	k_{off} (10^{-2}/s)
Wild-Type	500 ± 82	1.8 ± 0.44	8.4 ± 0.50	4,100 ± 110	0.36 ± 0.025	15 ± 1.4
N74G	170 ± 24	2.9 ± 0.39	4.7 ± 0.07	20,000 ± 430	0.097 ± 0.026	17 ± 3.0
T76P	12 ± 5.4	5.0 ± 0.96	0.56 ± 0.11	2,700 ± 290	0.42 ± 0.024	11 ± 1.3
A132V	69 ± 9.6	4.8 ± 0.76	3.3 ± 0.47	90 ± 23	5.3 ± 0.52	4.7 ± 0.73
N74G T76P A132V	2.6 ± 0.62	5.8 ± 0.74	0.14 ± 0.01	72 ± 20	5.2 ± 0.80	3.6 ± 0.41
N74G T76P	92 ± 1.3	3.5 ± 0.25	0.32 ± 0.03	2,700 ± 130	0.33 ± 0.020	89 ± 0.080
N74G A132V	22 ± 4.9	4.5 ± 0.41	0.96 ± 0.12	94 ± 23	5.2 ± 0.85	4.7 ± 0.35
T76P A132V	2.6 ± 0.29	5.5 ± 0.18	0.14 ± 0.010	82 ± 18	4.8 ± 0.69	3.9 ± 0.28

Example 4: X-Ray Crystal Structure of the Human PD-1/PD-L2 Complex

[0108] The human PD-1/PD-L2 complex was crystallized using the PD-1 triple mutant. Site-directed mutagenesis was used to remove all N-linked glycosylation sites in each protein in an effort to aid crystallization, as illustrated by the protein sequences summarized in Table 4. Co-expression of the PD-1 triple mutant and the PD-L2 IgV domain yielded a stable and 1:1 stoichiometric complex, which was purified. The crystals of the human PD-$1^{N74G\ T76P\ A132V}$/PD-$L2^{IgV}$ complex were successfully obtained, and a 2.0 Å resolution structure of the complex by X-ray crystallography was determined. The structure is illustrated, for example, in FIG. **1**A. The crystal contained one PD-1/PD-L2 complex per asymmetric unit, with space group P 2_1 2_1 2_1. The crystallographic data collection and refinement statistics are summarized in Table 2. The human PD-1/PD-L2 complex adopted an architecture similar to the previously determined murine PD-1/PD-L2 complex (19) with a Ca root-mean-square deviation (R.M.S.D.) of 3.8 Å.

TABLE 4

Amino acid sequences.

Amino acid sequence	Plasmid (Parent)
>PD-1_N74G_T76P_A132V MNPPTFSPALLVVTEGDNATFTCSFSNTSESFVLNWYRMSPSGQPDKLA AFPEDRSQPGQDSRFRVTQLPNGRDFHMSVVRARRNDSGTYLCGAISLA PKVQIKESLRAELRVTERRAE*GS*WSHPQFEK (SEQ ID NO: 2)	pST1132 (pET23d)
>PD-1_T76P_A132V MNPPTFSPALLVVTEGDNATFTCSFSNTSESFVLNWYRMSPSNQPDKLA AFPEDRSQPGQDSRFRVTQLPNGRDFHMSVVRARRNDSGTYLCGAISLA PKVQIKESLRAELRVTERRAE*GS*WSHPQFEK (SEQ ID NO: 3) *Linker*, Strep-tag®II	pST1167 (pET23d)
>PD-1_N74G_T76P_A132V *MGWSCIILFLVATATGVHS*NPPTFSPALLVVTEGDSATFTCSFSSTSESFVL NWYRMSPSGQPDKLAAFPEDRSQPGQDSRFRVTQLPNGRDFHMSVVRA RRDDSGTYLCGAISLAPKVQIKESLRAELRVTERRAEPEA (SEQ ID NO: 4)	pST1195 (pADD2)
>PD-L2_IgV *MIFLLLMLSLELQLHQIA*ALFTVTVPKELYIIEHGSDVTLECNFDTGSHVNL GAITASLQKVEDDTSPHRERATLLEEQLPLGKASFHIPQVQVRDEGQYQ CIIIYGVAWDYKYLTLKVKASY (SEQ ID NO: 5) *Signal sequence*, C-tag	pST1207 (pADD2)

[0109] The structure of human PD-1/PD-L2 complex revealed that human PD-1/PD-L2 interface was formed by the front β-sheets of both IgV domains, as illustrated in FIG. **1**B, burying 1,840 $Å^2$ (14% of the total) of solvent-accessible surface area. In the interface, notable interacting residues included the three highly conserved aromatics $W110_{L2}$, $Y112_{L2}$ and $Y114_{L2}$ from PG of the PD-L2 IgV domain. The sidechains of these residues pointed into the center of the PD-1 ligand-binding surface, as illustrated in FIGS. **4**A and **4**B. To validate the interactions observed at the PD-1/PD-L2 interface, site-directed mutagenesis on several PD-1 and PD-L2 interfacial residues was performed. Using BLI, reduced binding of PD-1 interface mutants to PD-L2, and PD-L2 interface mutants to PD-1 was observed. The observed reduced binding was consistent with the structure of human PD-1/PD-L2 complex. The high-affinity loop substitutions of PD-1 localized to the interface, as illustrated in FIG. **1**B. Among them, T76P and A132V made additional contacts to PD-L2, likely contributing to the increase in affinity, as illustrated in FIG. **5**.

Example 5: X-Ray Crystal Structures of Human Apo-PD-1 Loop Variants

[0110] To assist analyses of the conformational change of PD-1 associated with PD-L2 binding, two human apo-PD-1 loop variants (see Table 4 for the amino acid sequences) were crystallized and their X-ray crystal structures were determined at 1.2 Å and 1.4 Å resolution, for PD-$1^{N74G\ T76P\ A132V}$ and PD-$1^{T76P\ A132V}$ respectively. Crystals of both variants contain a single PD-1 molecule per asymmetric unit, with space group P 3_2 2 1 (see Table 2 for crystallographic data collection and refinement statistics). Both PD-1 variants were well-defined by the electron density maps with a notable exception of the CC' loop discussed further below. Superimposing the apo and PD-L2-bound PD-$1^{N74G\ T76P\ A132V}$ structures resulted in a C_α R.M.S.D. of 1.6 Å. The C'D loop of PD-1 (residues 83-92) was previously known to be a major part of the pembrolizumab epitope (30-32). This loop was not previously resolved in structures of human PD-1 without pembrolizumab (17, 23, 33), but it was clearly in both apo-PD-1 structures described in the present disclosure. The results of the structure determination indicated that the conformation of the loop changed significantly upon antibody binding.

Example 6: Formation of a Prominent Pocket in Human PD-1 Upon Binding PD-L2, with Human PD-1 Pocket Having Architecture Distinct from that of Murine PD-1 Pocket

[0111] The structures of the human PD-1/PD-L2 complex and apo-PD-1 variants described in the present disclosure

permitted the examination of formation of human PD-1 pocket in the PD-1/PD-L2 interface. Although human apo-PD-1 has a flat ligand-binding interface, as illustrated in FIG. **2**A, the structures described in the present disclosure revealed that there were rearrangements in this interface upon binding of PD-L2. These rearrangements involved residues in βC (F63, V64, N66, Y68), βF (L122, G124, I126), βG (I134, E136) and the C'D loop (E84) forming a deep and extended pocket (illustrated in FIG. **2**B), accommodating PD-L2 sidechains including the aromatic residues $W110_{L2}$ and $Y112_{L2}$, as illustrated in FIG. **2**C. Each of these residues in PD-1 is within 4.4 Å of a PD-L2 residue (Table 5).

TABLE 5

A list of atoms from PD-L2 residues within 6.0 Å distance of the PD-1 pocket residues shown in FIG. 2B. Distance measurements were generated by COCOMAPS.

PD-1				PD-L2			Distance
Residue		Number	Atom	Residue	Number	Atom	(Å)
βC	Phe	63	CB	Trp	110	NE1	4.7
	Phe	63	CE1	Ile	105	CG2	4.2
	Phe	63	CD1	Val	108	O	4.0
	Phe	63	CE1	Gly	107	O	4.2
	Val	64	CG2	Ala	109	N	4.1
	Val	64	CG2	Val	108	O	3.0
	Val	64	O	Trp	110	NE1	3.0
	Asn	66	ND2	Asp	111	CA	4.4
	Asn	66	ND2	Trp	110	O	2.9
	Tyr	68	CE1	Lys	113	NZ	5.3
	Tyr	68	OH	Trp	110	CZ3	3.5
C'D loop	Glu	84	OE1	Ala	109	CB	3.4
	Glu	84	OE2	Phe	21	N	3.0
	Glu	84	OE2	Thr	22	N	6.0
	Glu	84	OE1	Trp	110	N	4.6
	Glu	84	OE2	Leu	20	CD2	3.2
	Glu	84	OE1	Val	108	O	5.5
βF	Leu	122	CD1	Tyr	112	OH	4.3
	Ile	126	CG2	Val	108	O	5.7
	Ile	126	CD1	Ile	104	O	5.8
	Ile	126	CD1	Ile	103	CG2	3.8
	Ile	126	CG2	Trp	110	NE1	3.5
	Ile	126	CD1	Ile	105	CD1	3.5
βG	Ile	134	CB	Gln	101	NE2	4.0
	Ile	134	CG1	Tyr	112	CG	3.9
	Ile	134	CG1	Ile	103	CD1	3.7
	Ile	134	CD1	Trp	110	CZ3	3.4
	Ile	134	CD1	Asp	111	O	5.6
	Glu	136	OE2	Tyr	114	OH	2.6
	Glu	136	OE2	Gln	101	NE2	4.4
	Glu	136	OE2	Tyr	112	OH	2.6

[0112] Comparison of the PD-1 pockets in the human and murine PD-1/PD-L2 complexes demonstrated striking differences in pocket geometries. Human PD-1 pocket adopted an open, funnel-shaped architecture. Compared to murine PD-1 pocket, human PD-1 pocket has a wider entrance and a narrower exit (illustrated in FIG. **2**B). The structured described in the present disclosure revealed that distinct pocket geometries arise from at least two considerations. First, human PD-1 was revealed to employ a different subset of interfacial residues to form the pocket, as compared to murine PD-1. Human PD-1 lacks an ordered PC" strand, and thus the open pocket in human PD-1 is formed by rearranging residues F63, V64 and E84. In contrast, murine PD-1 pocket is closed with sidechains of A81 and S83 forming a boundary. Second, several sequence variations exist among the residues that form the pocket. For example, V64 and Y68 in human PD-1 are substituted with M64 and N68 in murine PD-1, respectively. To quantitatively evaluate the pocket dimensions, pocket volumes were measured using POCASA 1.1 (34). Human and murine PD-1 pockets were measured to have volumes of 130 $Å^3$ and 154 $Å^3$, respectively. Notably, these pockets were comparable in size to other protein cavities with established small-molecule inhibitors (20, 21, 35).

[0113] The structure of human PD-1/PD-L2 described in the present disclosure was compared with the previously determined human PD-1/PD-L1 structure (17). Superimposing the two structures resulted in a Ca R.M.S.D. of 1.5 Å for PD-1 residues. Binding PD-L1 triggered formation a much smaller cavity in human PD-1, as compared to binding of PD-L2, with the cavity having a measured volume of 40 $Å^3$. PD-L1 lacks a large aromatic sidechain corresponding to $W110_{L2}$, so the PD-1 rearrangement was revealed to involve only a small subset of the interfacial residues to accommodate the sidechain of $Y123_{L1}$, corresponding to PD-L2 residue Y112L2. These results showed that the core of the human PD-1 interface had remarkable structural plasticity and the ability to form pockets with varied dimensions, permitting the interactions with different PD-1 ligands.

Example 7: The CC' Loop in the Triple-Mutant PD-1 Adopts a Ligand-Bound Conformation in the Absence of Ligand

[0114] Conformational changes in the CC' and FG loops upon binding of PD-L2 to human PD-1 were observed (data not shown). Earlier studies showed that the CC' loop underwent a substantial conformational change when human PD-1 binds PD-L1 (17, 33). This CC' loop conformational change was even larger in the human PD-1/PD-L2 structure described in the present disclosure. Strikingly, in the absence of ligands, the CC' loop conformations of the PD-1 triple and double mutants resembled that of the ligand-bound conformations. For example, a 4.8 Å shift was observed between the Ca of T76 and P76 in the PD-1 triple mutant of apo-PD-1. When the triple-mutant PD-1 bound PD-L2, the sidechain of P76 maintained the same conformation. An increased population of the ligand-bound conformations in the mutant apo-PD-1 proteins was consistent with increased association constants (k_{on}) of the PD-1 variants.

[0115] In contrast, the conformations of the FG loop were the same in all three apo-PD-1 structures (one with an A132L substitution in the FG loop (23) and the triple and double mutants described in the present disclosure. Upon binding PD-L1 (17), there were no significant conformational changes in the FG loop. There was, however, a substantial shift in the FG loop conformation upon binding PD-L2.

Example 8: Structural plasticity of the human PD-1 ligand-binding interface

[0116] To further investigate how the loop changes were associated with pocket formation, the apo and PD-L2-bound structures of the human triple-mutant PD-1 were superimposed (data not shown). Upon binding PD-L2, a large conformational change I in the PD-1 ligand-binding interface. A three-residue shortening of βC was observed, and βC and βF moved apart to create a deep cleft. The rearrangements that I in the pocket propagated to the edge of the FG loop, resulting in a remarkable 8.2 Å lateral shift. The

overall change was less dramatic in murine PD-1. The closed architecture of the murine pocket did not require flipping of residues E84 and F63, as seen in human PD-1, and there was no secondary structure change of βC in murine PD-1. Taken together, the results described in the present disclosure provide a structural basis for systematic rearrangements at the human PD-1 ligand-binding interface coupling pocket formation and changes in the loops of PD-1 when it binds PD-L2.

Example 9: Coordinates and Structure Factors

[0117] The atomic coordinates and structure factors for human PD-$1^{N74G\ T76P\ A132V}$/PD-$L2^{IgV}$ complex, human apo-PD-$1^{N74G\ T76P\ A132V}$ and apo-PD-$1^{T76P\ A132V}$ is included as Tables 6-8, respectively, which are found in an Appendix.

REFERENCE TO A SEQUENCE LISTING SUBMITTED AS A TEXT FILE VIA EFS-WEB

[0118] The official copy of the sequence listing is submitted electronically via EFS-Web as an ASCII formatted sequence listing with a file named 103182-1163588-003620US_Seq_Listing.txt, created on Apr. 23, 2020, and having a size of 7 kilobytes, which is filed concurrently with the specification. The sequence listing contained in this ASCII formatted document is part of the specification and is herein incorporated by reference in its entirety.

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[0238] In the foregoing description, numerous specific details are set forth to provide a more thorough understanding of the present invention. However, it will be apparent to one of skill in the art that the invention described in this disclosure may be practiced without one or more of these specific details. In other instances, well-known features and procedures well known to those skilled in the art have not been described in order to avoid obscuring the invention. Embodiments of the disclosure have been described for illustrative and not restrictive purposes. Although the present invention is described primarily with reference to specific embodiments, it is also envisioned that other embodiments will become apparent to those skilled in the art upon reading the present disclosure, and it is intended that such embodiments be contained within the present inventive methods. Accordingly, the present disclosure is not limited to the embodiments described above or depicted in the drawings, and various embodiments and modifications can be made without departing from the scope of the claims below. All publications, patents, and patent applications cited herein are hereby incorporated by reference in their entirety for all purposes.

APPENDIX

[0239]

TABLE 6

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

CRYST1	41.291	67.798	89.701	90.00	90.00	90.00	P 21 21 21				
SCALE1		0.024218	0.000000	0.000000		0.00000					
SCALE2		0.000000	0.014750	0.000000		0.00000					
SCALE3		0.000000	0.000000	0.011148		0.00000					
ATOM	1	O	ASN A	33	−21.189	−9.931	21.441	1.00101.06			O
ANISOU	1	O	ASN A	33	12153	12425	13822	−1086	−350	−3162	O
ATOM	2	N	ASN A	33	−24.027	−9.539	19.170	1.00111.31			N
ANISOU	2	N	ASN A	33	12657	14221	15414	−1189	−1298	−4138	N
ATOM	3	CA	ASN A	33	−23.199	−10.217	20.160	1.00108.35			C
ANISOU	3	CA	ASN A	33	12515	13486	15165	−1354	−857	−3959	C
ATOM	4	C	ASN A	33	−21.841	−9.544	20.469	1.00	99.06		C
ANISOU	4	C	ASN A	33	11702	12421	13515	−1050	−713	−3465	C
ATOM	5	CB	ASN A	33	−22.990	−11.673	19.738	1.00117.04			C
ANISOU	5	CB	ASN A	33	13811	14236	16424	−1494	−767	−4198	C
ATOM	6	CG	ASN A	33	−24.293	−12.464	19.739	1.00126.13			C
ANISOU	6	CG	ASN A	33	14633	15208	18082	−1793	−735	−4454	C
ATOM	7	OD1	ASN A	33	−25.348	−11.936	20.099	1.00128.87			O
ANISOU	7	OD1	ASN A	33	14584	15691	18689	−1896	−755	−4480	O
ATOM	8	ND2	ASN A	33	−24.230	−13.727	19.323	1.00130.65			M
ANISOU	8	ND2	ASN A	33	15361	15477	18804	−1918	−674	−4657	N

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	9	N	PRO A	34	−21.406	−8.542	19.665	1.00	83.38		N
ANISOU	9	N	PRO A	34	9812	10792	11076	−746	−988	−3389	N
ATOM	10	C	PRO A	34	−21.072	−6.991	21.522	1.00	57.91		C
ANISOU	10	C	PRO A	34	6522	7668	7811	−674	−635	−2704	C
ATOM	11	O	PRO A	34	−22.283	−6.799	21.518	1.00	57.97		O
ANISOU	11	O	PRO A	34	6198	7745	8083	−806	−767	−2918	O
ATOM	12	CA	PRO A	34	−20.437	−7.630	20.294	1.00	70.58		C
ANISOU	12	CA	PRO A	34	8364	9278	9176	−553	−802	−2919	C
ATOM	13	CB	PRO A	34	−20.177	−6.572	19.220	1.00	71.52		C
ANISOU	13	CB	PRO A	34	8581	9745	8847	−265	−1094	−2905	C
ATOM	14	CG	PRO A	34	−20.529	−7.209	17.951	1.00	75.86		C
ANISOU	14	CG	PRO A	34	9187	10337	9300	−230	−1392	−3325	C
ATOM	15	CD	PRO A	34	−21.520	−8.309	18.213	1.00	81.93		C
ANISOU	15	CD	PRO A	34	9694	10865	10569	−546	−1405	−3685	C
ATOM	16	N	PRO A	35	−20.283	−6.644	22.545	1.00	49.94		N
ANISOU	16	N	PRO A	35	5665	6595	6714	−610	−366	−2322	N
ATOM	17	CA	PRO A	35	−20.963	−6.060	23.705	1.00	46.59		C
ANISOU	17	CA	PRO A	35	5050	6163	6489	−715	−199	−2154	C
ATOM	18	C	PRO A	35	−21.633	−4.748	23.352	1.00	47.39		C
ANISOU	18	C	PRO A	35	4920	6581	6503	−599	−450	−2180	C
ATOM	19	O	PRO A	35	−21.251	−4.083	22.386	1.00	41.97		O
ANISOU	19	O	PRO A	35	4329	6117	5500	−383	−706	−2188	O
ATOM	20	CB	PRO A	35	−19.832	−5.808	24.717	1.00	41.10		C
ANISOU	20	CB	PRO A	35	4615	5394	5608	−589	39	−1769	C
ATOM	21	CG	PRO A	35	−18.623	−6.495	24.148	1.00	40.77		C
ANISOU	21	CG	PRO A	35	4843	5271	5375	−457	29	−1764	C
ATOM	22	CD	PRO A	35	−18.821	−6.534	22.664	1.00	43.69		C
ANISOU	22	CD	PRO A	35	5171	5801	5628	−408	−251	−2054	C
ATOM	23	N	THR A	36	−22.653	−4.389	24.121	1.00	49.01		N
ANISOU	23	N	THR A	36	4845	6786	6990	−727	−350	−2192	N
ATOM	24	CA	THR A	36	−23.241	−3.073	23.972	1.00	48.00		C
ANISOU	24	CA	THR A	36	4516	6929	6791	−572	−557	−2174	C
ATOM	25	C	THR A	36	−22.754	−2.242	25.152	1.00	42.95		C
ANISOU	25	C	THR A	36	4003	6277	6041	−501	−306	−1810	C
ATOM	26	O	THR A	36	−22.334	−2.781	26.167	1.00	39.95		O
ANISOU	26	O	THR A	36	3776	5686	5717	−606	13	−1640	O
ATOM	27	CB	THR A	36	−24.757	−3.132	23.911	1.00	51.22		C
ANISOU	27	CB	THR A	36	4462	7389	7610	−717	−665	−2501	C
ATOM	28	OG1	THR A	36	−25.245	−3.728	25.112	1.00	56.97		O
ANISOU	28	OG1	THR A	36	5059	7872	8715	−994	−241	−2467	O
ATOM	29	CG2	THR A	36	−25.219	−3.968	22.694	1.00	54.62		C
ANISOU	29	CG2	THR A	36	4758	7844	8152	−780	−988	−2933	C
ATOM	30	N	PHE A	37	−22.799	−0.928	25.006	1.00	42.88		N
ANISOU	30	N	PHE A	37	3965	6475	5852	−298	−465	−1702	N
ATOM	31	CA	PHE A	37	−22.126	−0.050	25.939	1.00	42.42		C
ANISOU	31	CA	PHE A	37	4075	6413	5630	−202	−289	−1391	C
ATOM	32	C	PHE A	37	−22.893	1.261	25.947	1.00	43.95		C
ANISOU	32	C	PHE A	37	4087	6775	5837	−57	−425	−1388	C
ATOM	33	O	PHE A	37	−23.025	1.900	24.898	1.00	43.18		O
ANISOU	33	O	PHE A	37	3989	6838	5580	128	−724	−1452	O
ATOM	34	CB	PHE A	37	−20.673	0.141	25.507	1.00	42.11		C
ANISOU	34	CB	PHE A	37	4355	6392	5252	−63	−327	−1214	C
ATOM	35	CG	PHE A	37	−19.811	0.814	26.536	1.00	41.18		C
ANISOU	35	CG	PHE A	37	4397	6235	5015	−4	−154	−952	C
ATOM	36	CD1	PHE A	37	−19.221	2.030	26.261	1.00	42.27		C
ANISOU	36	CD1	PHE A	37	4629	6481	4950	150	−239	−820	C
ATOM	37	CD2	PHE A	37	−19.587	0.220	27.768	1.00	39.98		C
ANISOU	37	CD2	PHE A	37	4326	5917	4945	−94	90	−852	C
ATOM	38	CE1	PHE A	37	−18.391	2.647	27.184	1.00	39.97		C
ANISOU	38	CE1	PHE A	37	4453	6149	4585	185	−114	−641	C
ATOM	39	CE2	PHE A	37	−18.790	0.825	28.704	1.00	39.54		C
ANISOU	39	CE2	PHE A	37	4422	5847	4755	−9	179	−662	C
ATOM	40	CZ	PHE A	37	−18.181	2.046	28.408	1.00	39.80		C
ANISOU	40	CZ	PHE A	37	4487	6004	4630	118	61	−581	C
ATOM	41	O	SER A	38	−23.717	3.063	29.391	1.00	42.91		O
ANISOU	41	O	SER A	38	3867	6531	5906	−53	229	−1042	O
ATOM	42	N	SER A	38	−23.442	1.646	27.100	1.00	40.45		N
ANISOU	42	N	SER A	38	3518	6284	5567	−112	−201	−1320	N
ATOM	43	C	SER A	38	−24.207	3.590	28.388	1.00	44.20		C
ANISOU	43	C	SER A	38	3858	6843	6092	71	−62	−1170	C
ATOM	44	CA	SER A	38	−24.375	2.769	27.105	1.00	42.20		C
ANISOU	44	CA	SER A	38	3507	6648	5881	31	−322	−1378	C
ATOM	45	CB	SER A	38	−25.818	2.250	26.963	1.00	50.60		C
ANISOU	45	CB	SER A	38	4116	7750	7359	−93	−360	−1699	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	46	OG	SER A	38	−26.193	1.570	28.143	1.00	51.89		O
ANISOU	46	OG	SER A	38	4187	7736	7794	−340	64	−1692	O
ATOM	47	N	PRO A	39	−24.609	4.877	28.364	1.00	42.13		N
ANISOU	47	N	PRO A	39	3528	6683	5798	273	−180	−1144	N
ATOM	48	CA	PRO A	39	−25.211	5.580	27.221	1.00	42.61		C
ANISOU	48	CA	PRO A	39	3445	6902	5841	496	−547	−1267	C
ATOM	49	C	PRO A	39	−24.159	6.005	26.227	1.00	41.21		C
ANISOU	49	C	PRO A	39	3616	6748	5293	648	−752	−1117	C
ATOM	50	O	PRO A	39	−22.966	6.034	26.577	1.00	36.56		O
ANISOU	50	O	PRO A	39	3314	6062	4514	586	−589	−919	O
ATOM	51	CB	PRO A	39	−25.884	6.792	27.873	1.00	46.77		C
ANISOU	51	CB	PRO A	39	3852	7454	6464	665	−493	−1239	C
ATOM	52	CG	PRO A	39	−25.040	7.075	29.062	1.00	42.57		C
ANISOU	52	CG	PRO A	39	3592	6784	5798	588	−179	−1020	C
ATOM	53	CD	PRO A	39	−24.573	5.719	29.574	1.00	42.15		C
ANISOU	53	CD	PRO A	39	3613	6626	5775	324	53	−1004	C
ATOM	54	N	ALA A	40	−24.571	6.315	25.007	1.00	42.34		N
ANISOU	54	N	ALA A	40	3740	7017	5330	854	−1096	−1221	N
ATOM	55	CA	ALA A	40	−23.631	6.754	23.977	1.00	40.44		C
ANISOU	55	CA	ALA A	40	3882	6782	4703	1015	−1234	−1063	C
ATOM	56	C	ALA A	40	−22.950	8.050	24.389	1.00	43.29		C
ANISOU	56	C	ALA A	40	4504	7037	4906	1125	−1089	−793	C
ATOM	57	O	ALA A	40	−21.808	8.304	23.985	1.00	40.86		O
ANISOU	57	O	ALA A	40	4518	6657	4352	1126	−1001	−615	O
ATOM	58	CB	ALA A	40	−24.360	6.931	22.585	1.00	41.32		C
ANISOU	58	CB	ALA A	40	3983	7050	4666	1292	−1663	−1228	C
ATOM	59	N	LEU A	41	−23.659	8.869	25.171	1.00	43.52		N
ANISOU	59	N	LEU A	41	4381	7045	5109	1209	−1043	−791	N
ATOM	60	CA	LEU A	41	−23.142	10.151	25.660	1.00	39.16		C
ANISOU	60	CA	LEU A	41	4059	6358	4462	1305	−908	−583	C
ATOM	61	C	LEU A	41	−23.457	10.291	27.152	1.00	38.91		C
ANISOU	61	C	LEU A	41	3854	6267	4662	1189	−666	−613	C
ATOM	62	O	LEU A	41	−24.600	10.380	27.538	1.00	39.67		O
ANISOU	62	O	LEU A	41	3664	6426	4984	1260	−685	−758	O
ATOM	63	CB	LEU A	41	−23.756	11.330	24.892	1.00	38.46		C
ANISOU	63	CB	LEU A	41	4078	6270	4264	1656	−1144	−540	C
ATOM	64	CG	LEU A	41	−23.569	12.725	25.539	1.00	39.47		C
ANISOU	64	CG	LEU A	41	4385	6217	4396	1769	−999	−380	C
ATOM	65	CD1	LEU A	41	−22.083	13.004	25.798	1.00	37.63		C
ANISOU	65	CD1	LEU A	41	4466	5809	4024	1575	−744	−188	C
ATOM	66	CD2	LEU A	41	−24.107	13.816	24.629	1.00	42.71		C
ANISOU	66	CD2	LEU A	41	4987	6584	4658	2157	−1239	−304	C
ATOM	67	N	LEU A	42	−22.431	10.308	27.976	1.00	36.39		N
ANISOU	67	N	LEU A	42	3711	5835	4280	1029	−440	−495	N
ATOM	68	C	LEU A	42	−21.992	11.678	29.943	1.00	36.30		C
ANISOU	68	C	LEU A	42	3859	5627	4308	1020	−140	−412	C
ATOM	69	O	LEU A	42	−20.832	11.976	29.667	1.00	36.38		O
ANISOU	69	O	LEU A	42	4090	5552	4180	965	−138	−305	O
ATOM	70	CD1	LEU A	42	−23.306	9.093	32.109	1.00	39.82		C
ANISOU	70	CD1	LEU A	42	3913	6159	5059	669	340	−626	C
ATOM	71	CD2	LEU A	42	−21.099	7.841	32.101	1.00	38.26		C
ANISOU	71	CD2	LEU A	42	4087	5884	4564	480	317	−463	C
ATOM	72	CA	LEU A	42	−22.585	10.372	29.435	1.00	38.27		C
ANISOU	72	CA	LEU A	42	3882	6014	4643	937	−206	−517	C
ATOM	73	CB	LEU A	42	−21.878	9.183	30.087	1.00	35.67		C
ANISOU	73	CB	LEU A	42	3598	5665	4290	711	−42	−506	C
ATOM	74	CG	LEU A	42	−21.882	9.100	31.625	1.00	38.22		C
ANISOU	74	CG	LEU A	42	3964	5918	4638	640	207	−504	C
ATOM	75	N	VAL A	43	−22.774	12.474	30.652	1.00	36.07		N
ANISOU	75	N	VAL A	43	3759	5559	4388	1144	−70	−467	N
ATOM	76	CA	VAL A	43	−22.306	13.784	31.082	1.00	34.96		C
ANISOU	76	CA	VAL A	43	3841	5251	4191	1233	−22	−404	C
ATOM	77	C	VAL A	43	−22.431	13.835	32.595	1.00	38.56		C
ANISOU	77	C	VAL A	43	4295	5671	4684	1178	191	−488	C
ATOM	78	O	VAL A	43	−23.509	13.615	33.130	1.00	41.78		O
ANISOU	78	O	VAL A	43	4501	6149	5225	1233	305	−591	O
ATOM	79	CB	VAL A	43	−23.109	14.943	30.444	1.00	40.48		C
ANISOU	79	CB	VAL A	43	4551	5888	4941	1519	−154	−392	C
ATOM	80	CG1	VAL A	43	−22.628	16.281	30.961	1.00	42.09		C
ANISOU	80	CG1	VAL A	43	5013	5859	5122	1586	−64	−342	C
ATOM	81	CG2	VAL A	43	−23.057	14.897	28.893	1.00	49.38		C
ANISOU	81	CG2	VAL A	43	5760	7054	5947	1638	−385	−297	C
ATOM	82	N	AVAL A	44	−21.318	14.134	33.267	0.42	35.68		N
ANISOU	82	N	AVAL A	44	4155	5200	4203	1079	247	−464	N

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	83	CA	AVAL A	44	−21.217	14.103	34.730	0.42	36.28		C
ANISOU	83	CA	AVAL A	44	4322	5249	4215	1047	409	−550	C
ATOM	84	C	AVAL A	44	−20.440	15.329	35.240	0.42	36.32		C
ANISOU	84	C	AVAL A	44	4553	5078	4168	1075	384	−598	C
ATOM	85	O	AVAL A	44	−19.559	15.832	34.545	0.42	35.50		O
ANISOU	85	O	AVAL A	44	4537	4873	4079	1014	279	−544	O
ATOM	86	CB	AVAL A	44	−20.505	12.809	35.201	0.42	34.79		C
ANISOU	86	CB	AVAL A	44	4180	5136	3901	888	448	−527	C
ATOM	87	CG1	AVAL A	44	−20.607	12.646	36.701	0.42	33.76		C
ANISOU	87	CG1	AVAL A	44	4201	4991	3638	913	623	−596	C
ATOM	88	CG2	AVAL A	44	−21.054	11.565	34.460	0.42	31.56		C
ANISOU	88	CG2	AVAL A	44	3570	4844	3576	811	455	−487	C
ATOM	89	N	BVAL A	44	−21.316	14.072	33.280	0.58	35.37		N
ANISOU	89	N	BVAL A	44	4111	5167	4162	1073	250	−465	N
ATOM	90	CA	BVAL A	44	−21.332	14.226	34.738	0.58	36.42		C
ANISOU	90	CA	BVAL A	44	4334	5259	4245	1068	414	−556	C
ATOM	91	C	BVAL A	44	−20.605	15.488	35.171	0.58	36.63		C
ANISOU	91	C	BVAL A	44	4583	5106	4229	1104	386	−599	C
ATOM	92	O	BVAL A	44	−19.922	16.151	34.390	0.58	36.08		O
ANISOU	92	O	BVAL A	44	4601	4918	4188	1079	284	−538	O
ATOM	93	CB	BVAL A	44	−20.682	13.028	35.471	0.58	34.57		C
ANISOU	93	CB	BVAL A	44	4169	5093	3874	919	484	−551	C
ATOM	94	CG1	BVAL A	44	−21.524	11.767	35.297	0.58	35.02		C
ANISOU	94	CG1	BVAL A	44	4033	5264	4010	857	594	−536	C
ATOM	95	CG2	BVAL A	44	−19.221	12.801	34.983	0.58	27.21		C
ANISOU	95	CG2	BVAL A	44	3335	4141	2864	801	324	−498	C
ATOM	96	N	THR A	45	−20.768	15.811	36.435	1.00	34.64		N
ANISOU	96	N	THR A	45	4440	4813	3909	1156	506	−717	N
ATOM	97	CA	THR A	45	−20.067	16.938	37.036	1.00	36.77		C
ANISOU	97	CA	THR A	45	4925	4904	4143	1172	468	−826	C
ATOM	98	C	THR A	45	−18.768	16.431	37.670	1.00	36.41		C
ANISOU	98	C	THR A	45	4999	4887	3946	1028	370	−891	C
ATOM	99	O	THR A	45	−18.772	15.336	38.250	1.00	33.44		O
ANISOU	99	O	THR A	45	4636	4652	3418	1012	414	−875	O
ATOM	100	CB	THR A	45	−20.967	17.609	38.085	1.00	41.43		C
ANISOU	100	CB	THR A	45	5593	5436	4711	1347	632	−965	C
ATOM	101	OG1	THR A	45	−22.164	18.071	37.437	1.00	45.85		O
ANISOU	101	OG1	THR A	45	5982	5982	5455	1518	688	−927	O
ATOM	102	CG2	THR A	45	−20.263	18.784	38.730	1.00	44.32		C
ANISOU	102	CG2	THR A	45	6199	5594	5046	1361	576	−1128	C
ATOM	103	O	GLU A	46	−17.203	17.173	40.282	1.00	35.69		O
ANISOU	103	O	GLU A	46	5349	4697	3515	1064	187	−1336	O
ATOM	104	N	GLU A	46	−17.671	17.189	37.556	1.00	36.77		N
ANISOU	104	N	GLU A	46	5126	4790	4055	932	243	−974	N
ATOM	105	CA	GLU A	46	−16.377	16.733	38.083	1.00	37.14		C
ANISOU	105	CA	GLU A	46	5209	4887	4016	816	89	−1085	C
ATOM	106	C	GLU A	46	−16.540	16.439	39.577	1.00	33.91		C
ANISOU	106	C	GLU A	46	4985	4553	3347	942	88	−1229	C
ATOM	107	CB	GLU A	46	−15.248	17.762	37.839	1.00	39.17		C
ANISOU	107	CB	GLU A	46	5470	4949	4462	671	−17	−1225	C
ATOM	108	CG	GLU A	46	−15.494	19.109	38.450	1.00	38.50		C
ANISOU	108	CG	GLU A	46	5546	4642	4441	728	13	−1404	C
ATOM	109	CD	GLU A	46	−14.355	20.145	38.300	1.00	40.05		C
ANISOU	109	CD	GLU A	46	5742	4592	4884	535	−60	−1590	C
ATOM	110	OE1	GLU A	46	−13.161	19.822	37.993	1.00	38.37		O
ANISOU	110	OE1	GLU A	46	5370	4411	4797	344	−165	−1654	O
ATOM	111	OE2	GLU A	46	−14.689	21.330	38.582	1.00	42.07		O
ANISOU	111	OE2	GLU A	46	6151	4599	5236	577	5	−1707	O
ATOM	112	O	GLY A	47	−17.059	13.117	42.652	1.00	45.08		O
ANISOU	112	O	GLY A	47	7024	6323	3782	1302	306	−1114	O
ATOM	113	N	GLY A	47	−15.983	15.325	40.039	1.00	33.51		N
ANISOU	113	N	GLY A	47	4973	4649	3110	947	−4	−1218	N
ATOM	114	CA	GLY A	47	−16.123	14.964	41.449	1.00	37.77		C
ANISOU	114	CA	GLY A	47	5781	5249	3320	1110	8	−1316	C
ATOM	115	C	GLY A	47	−17.164	13.870	41.684	1.00	40.08		C
ANISOU	115	C	GLY A	47	6137	5634	3458	1185	277	−1123	C
ATOM	116	N	ASP A	48	−18.159	13.780	40.804	1.00	34.49		N
ANISOU	116	N	ASP A	48	5210	4928	2969	1124	473	−980	N
ATOM	117	C	ASP A	48	−18.742	11.428	40.192	1.00	38.54		C
ANISOU	117	C	ASP A	48	5587	5571	3484	1015	689	−686	C
ATOM	118	O	ASP A	48	−17.794	11.428	39.395	1.00	35.78		O
ANISOU	118	O	ASP A	48	5124	5237	3232	934	449	−682	O
ATOM	119	CA	ASP A	48	−19.192	12.736	40.854	1.00	35.42		C
ANISOU	119	CA	ASP A	48	5286	5111	3062	1128	753	−833	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	120	CB	ASP A	48	−20.477	13.224	40.160	1.00	37.20		C
ANISOU	120	CB	ASP A	48	5246	5325	3563	1127	930	−811	C
ATOM	121	CG	ASP A	48	−21.252	14.265	40.987	1.00	46.36		C
ANISOU	121	CG	ASP A	48	6505	6417	4694	1282	1109	−947	C
ATOM	122	OD1	ASP A	48	−21.051	14.335	42.208	1.00	48.98		O
ANISOU	122	OD1	ASP A	48	7142	6725	4742	1381	1193	−1035	O
ATOM	123	OD2	ASP A	48	−22.073	15.008	40.414	1.00	52.93		O
ANISOU	123	OD2	ASP A	48	7129	7215	5766	1341	1158	−975	O
ATOM	124	N	SER A	49	−19.431	10.318	40.466	1.00	32.69		N
ANISOU	124	N	SER A	49	4887	4844	2689	998	941	−574	N
ATOM	125	C	SER A	49	−19.742	9.092	38.380	1.00	32.87		C
ANISOU	125	C	SER A	49	4455	4928	3105	760	888	−433	C
ATOM	126	O	SER A	49	−20.806	9.666	38.207	1.00	34.32		O
ANISOU	126	O	SER A	49	4463	5122	3456	772	1017	−482	O
ATOM	127	CA	SER A	49	−19.084	9.069	39.765	1.00	31.28		C
ANISOU	127	CA	SER A	49	4624	4688	2574	888	896	−451	C
ATOM	128	CB	SER A	49	−19.533	7.822	40.557	1.00	33.21		C
ANISOU	128	CB	SER A	49	5094	4870	2656	899	1194	−335	C
ATOM	129	OG	SER A	49	−19.073	7.830	41.924	1.00	35.52		O
ANISOU	129	OG	SER A	49	5816	5123	2557	1084	1217	−339	O
ATOM	130	N	ALA A	50	−19.101	8.457	37.415	1.00	35.34		N
ANISOU	130	N	ALA A	50	4665	5271	3493	672	720	−383	N
ATOM	131	CA	ALA A	50	−19.630	8.328	36.067	1.00	36.09		C
ANISOU	131	CA	ALA A	50	4474	5413	3823	582	668	−378	C
ATOM	132	C	ALA A	50	−19.755	6.854	35.794	1.00	36.46		C
ANISOU	132	C	ALA A	50	4496	5444	3914	475	758	−326	C
ATOM	133	O	ALA A	50	−18.745	6.164	35.806	1.00	38.85		O
ANISOU	133	O	ALA A	50	4939	5722	4099	474	664	−276	O
ATOM	134	CB	ALA A	50	−18.676	8.986	35.051	1.00	34.05		C
ANISOU	134	CB	ALA A	50	4166	5179	3591	577	413	−380	C
ATOM	135	N	THR A	51	−20.957	6.374	35.498	1.00	33.68		N
ANISOU	135	N	THR A	51	3937	5093	3766	388	925	−365	N
ATOM	136	C	THR A	51	−21.693	4.597	33.930	1.00	38.22		C
ANISOU	136	C	THR A	51	4188	5665	4668	152	914	−450	C
ATOM	137	O	THR A	51	−22.772	5.027	33.536	1.00	37.82		O
ANISOU	137	O	THR A	51	3852	5687	4831	145	914	−567	O
ATOM	138	CA	THR A	51	−21.147	4.951	35.318	1.00	34.30		C
ANISOU	138	CA	THR A	51	4003	5100	3928	252	1054	−343	C
ATOM	139	CB	THR A	51	−22.070	4.393	36.412	1.00	40.09		C
ANISOU	139	CB	THR A	51	4808	5718	4707	187	1460	−324	C
ATOM	140	OG1	THR A	51	−21.456	4.623	37.686	1.00	38.41		O
ANISOU	140	OG1	THR A	51	4979	5445	4172	326	1554	−223	O
ATOM	141	CG2	THR A	51	−22.268	2.904	36.231	1.00	44.07		C
ANISOU	141	CG2	THR A	51	5327	6080	5337	16	1639	−300	C
ATOM	142	N	PHE A	52	−20.900	3.841	33.168	1.00	37.06		N
ANISOU	142	N	PHE A	52	4101	5505	4475	111	763	−431	N
ATOM	143	CA	PHE A	52	−21.390	3.213	31.950	1.00	39.21		C
ANISOU	143	CA	PHE A	52	4149	5816	4932	13	647	−558	C
ATOM	144	C	PHE A	52	−21.939	1.820	32.235	1.00	41.84		C
ANISOU	144	C	PHE A	52	4460	5992	5447	−171	888	−609	C
ATOM	145	O	PHE A	52	−21.616	1.231	33.245	1.00	45.01		O
ANISOU	145	O	PHE A	52	5114	6236	5753	−192	1125	−485	O
ATOM	146	CB	PHE A	52	−20.281	3.086	30.937	1.00	35.29		C
ANISOU	146	CB	PHE A	52	3750	5368	4290	65	408	−535	C
ATOM	147	CG	PHE A	52	−19.824	4.378	30.340	1.00	38.05		C
ANISOU	147	CG	PHE A	52	4108	5833	4516	201	209	−500	C
ATOM	148	CD1	PHE A	52	−18.606	4.943	30.725	1.00	36.80		C
ANISOU	148	CD1	PHE A	52	4132	5658	4191	270	185	−394	C
ATOM	149	CD2	PHE A	52	−20.556	4.982	29.322	1.00	36.63		C
ANISOU	149	CD2	PHE A	52	3765	5760	4394	267	37	−585	C
ATOM	150	CE1	PHE A	52	−18.144	6.108	30.127	1.00	36.62		C
ANISOU	150	CE1	PHE A	52	4133	5685	4097	351	65	−360	C
ATOM	151	CE2	PHE A	52	−20.112	6.148	28.716	1.00	37.10		C
ANISOU	151	CE2	PHE A	52	3912	5868	4314	403	−102	−514	C
ATOM	152	CZ	PHE A	52	−18.896	6.713	29.108	1.00	36.59		C
AMISOU	152	CZ	PHE A	52	4036	5748	4118	419	−53	−394	C
ATOM	153	N	THR A	53	−22.748	1.276	31.333	1.00	39.44		N
ANISOU	153	N	THR A	53	3879	5708	5397	−297	821	−800	N
ATOM	154	C	THR A	53	−22.712	−0.899	30.219	1.00	38.09		C
ANISOU	154	C	THR A	53	3685	5337	5451	−553	804	−1002	C
ATOM	155	O	THR A	53	−23.034	−0.500	29.090	1.00	41.35		O
ANISOU	155	O	THR A	53	3880	5930	5903	−502	498	−1175	O
ATOM	156	CA	THR A	53	−23.129	−0.114	31.453	1.00	35.98		C
ANISOU	156	CA	THR A	53	3431	5072	5169	−511	1045	−874	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	157	CB	THR A	53	−24.658	−0.264	31.662	1.00	41.97		C
ANISOU	157	CB	THR A	53	3813	5802	6333	−697	1266	−1071	C
ATOM	158	OG1	THR A	53	−25.048	0.459	32.838	1.00	42.98		O
ANISOU	158	OG1	THR A	53	3977	5926	6428	−642	1545	−957	O
ATOM	159	CG2	THR A	53	−25.014	−1.723	31.818	1.00	43.33		C
ANISOU	159	CG2	THR A	53	3994	5703	6767	−968	1562	−1150	C
ATOM	160	N	CYS A	54	−21.967	−1.986	30.437	1.00	39.25		N
ANISOU	160	N	CYS A	54	4109	5276	5530	−603	932	−916	N
ATOM	161	C	CYS A	54	−22.428	−4.162	29.455	1.00	47.40		C
ANISOU	161	C	CYS A	54	5072	5992	6945	−921	1009	−1224	C
ATOM	162	O	CYS A	54	−22.680	−4.677	30.538	1.00	49.13		O
ANISOU	162	O	CYS A	54	5437	5968	7261	−1034	1389	−1098	O
ATOM	163	CA	ACYS A	54	−21.571	−2.912	29.378	0.99	42.45		C
ANISOU	163	CA	ACYS A	54	4541	5624	5963	−649	771	−1055	C
ATOM	164	CB	ACYS A	54	−20.083	−3.283	29.482	0.99	43.81		C
ANISOU	164	CB	ACYS A	54	5068	5723	5853	−488	737	−875	C
ATOM	165	SG	ACYS A	54	−19.492	−4.434	28.153	0.99	51.80		S
ANISOU	165	SG	ACYS A	54	6149	6654	6877	−504	573	−1060	S
ATOM	166	CA	BCYS A	54	−21.592	−2.892	29.365	0.01	42.20		C
ANISOU	166	CA	BCYS A	54	4502	5598	5935	−649	767	−1059	C
ATOM	167	CB	BCYS A	54	−20.100	−3.223	29.426	0.01	41.78		C
ANISOU	167	CB	BCYS A	54	4797	5483	5596	−485	720	−882	C
ATOM	168	SG	BCYS A	54	−19.491	−4.198	28.028	0.01	51.66		S
ANISOU	168	SG	BCYS A	54	6099	6696	6832	−482	525	−1066	S
ATOM	169	N	ASER A	55	−22.887	−4.644	28.302	0.55	46.27		N
ANISOU	169	N	ASER A	55	4706	5883	6990	−1029	800	−1524	N
ATOM	170	C	ASER A	55	−23.086	−6.877	27.331	0.55	46.64		C
ANISOU	170	C	ASER A	55	4787	5528	7407	−1346	853	−1905	C
ATOM	171	O	ASER A	55	−22.757	−6.576	26.176	0.55	43.82		O
ANISOU	171	O	ASER A	55	4385	5398	6868	−1198	471	−2053	O
ATOM	172	CA	ASER A	55	−23.718	−5.838	28.244	0.55	47.01		C
ANISOU	172	CA	ASER A	55	4658	5712	7491	−1331	1000	−1760	C
ATOM	173	CB	ASER A	55	−25.117	−5.493	27.743	0.55	49.65		C
ANISOU	173	CB	ASER A	55	4460	6207	8197	−1481	862	−2106	C
ATOM	174	OG	ASER A	55	−25.628	−4.354	28.408	0.55	49.97		O
ANISOU	174	OG	ASER A	55	4323	6429	8233	−1391	931	−1992	O
ATOM	175	N	BSER A	55	−22.862	−4.658	28.301	0.45	46.12		N
ANISOU	175	N	BSER A	55	4696	5861	6967	−1027	800	−1521	N
ATOM	176	C	BSER A	55	−23.106	−6.885	27.321	0.45	46.61		C
ANISOU	176	C	BSER A	55	4777	5523	7410	−1350	852	−1911	C
ATOM	177	O	BSER A	55	−22.812	−6.600	26.155	0.45	44.13		O
ANISOU	177	O	BSER A	55	4408	5434	6924	−1209	469	−2070	O
ATOM	178	CA	BSER A	55	−23.709	−5.836	28.244	0.45	47.03		C
ANISOU	178	CA	BSER A	55	4663	5714	7491	−1329	999	−1758	C
ATOM	179	CB	BSER A	55	−25.109	−5.458	27.768	0.45	49.61		C
ANISOU	179	CB	BSER A	55	4458	6207	8185	−1475	865	−2096	C
ATOM	180	OG	BSER A	55	−25.938	−6.599	27.686	0.45	54.16		O
ANISOU	180	OG	BSER A	55	4827	6518	9233	−1814	1062	−2384	O
ATOM	181	N	PHE A	56	−22.928	−8.095	27.842	1.00	47.19		N
ANISOU	181	N	PHE A	56	5097	5204	7630	−1505	1179	−1858	N
ATOM	182	CA	PHE A	56	−22.288	−9.167	27.092	1.00	48.37		C
ANISOU	182	CA	PHE A	56	5459	5160	7759	−1504	1091	−1990	C
ATOM	183	C	PHE A	56	−22.551	−10.508	27.737	1.00	54.27		C
ANISOU	183	C	PHE A	56	6407	5399	8815	−1754	1519	−1985	C
ATOM	184	O	PHE A	56	−22.617	−10.614	28.958	1.00	57.38		O
ANISOU	184	O	PHE A	56	7007	5574	9220	−1791	1912	−1702	O
ATOM	185	CB	PHE A	56	−20.765	−8.963	27.002	1.00	47.95		C
ANISOU	185	CB	PHE A	56	5764	5200	7254	−1162	953	−1737	C
ATOM	186	CG	PHE A	56	−20.063	−10.061	26.251	1.00	52.72		C
ANISOU	186	CG	PHE A	56	6591	5604	7836	−1121	892	−1877	C
ATOM	187	CD1	PHE A	56	−20.131	−10.121	24.858	1.00	53.31		C
ANISOU	187	CD1	PHE A	56	6526	5850	7881	−1108	568	−2208	C
ATOM	188	CD2	PHE A	56	−19.369	−11.049	26.923	1.00	55.03		C
ANISOU	188	CD2	PHE A	56	7266	5524	8118	−1064	1153	−1692	C
ATOM	189	CE1	PHE A	56	−19.516	−11.143	24.153	1.00	53.35		C
ANISOU	189	CE1	PHE A	56	6747	5661	7860	−1063	533	−2371	C
ATOM	190	CE2	PHE A	56	−18.747	−12.081	26.223	1.00	54.15		C
ANISOU	190	CE2	PHE A	56	7360	5202	8013	−1004	1108	−1843	C
ATOM	191	CZ	PHE A	56	−18.820	−12.128	24.834	1.00	53.49		C
ANISOU	191	CZ	PHE A	56	7113	5295	7915	−1016	811	−2194	C
ATOM	192	O	SER A	57	−22.499	−13.749	25.210	1.00	72.55		O
ANISOU	192	O	SER A	57	8875	7001	11689	−2134	1303	−2927	O
ATOM	193	N	SER A	57	−22.674	−11.540	26.917	1.00	54.77		N
ANISOU	193	N	SER A	57	6463	5247	9102	−1911	1458	−2295	N

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	194	CA	SER A	57	−22.829	−12.886	27.431	1.00	63.73		C
ANISOU	194	CA	SER A	57	7850	5826	10539	−2148	1879	−2293	C
ATOM	195	C	SER A	57	−22.294	−13.895	26.421	1.00	71.20		C
ANISOU	195	C	SER A	57	8967	6581	11506	−2129	1702	−2552	C
ATOM	196	CB	SER A	57	−24.298	−13.167	27.764	1.00	68.64		C
ANISOU	196	CB	SER A	57	8099	6250	11730	−2592	2191	−2530	C
ATOM	197	OG	SER A	57	−24.534	−14.557	27.873	1.00	78.92		O
ANISOU	197	OG	SER A	57	9591	7002	13395	−2873	2543	−2647	O
ATOM	198	O	SER A	58	−21.133	−17.551	27.921	1.00	86.40		O
ANISOU	198	O	SER A	58	12282	6804	13742	−2219	2780	−2141	O
ATOM	199	N	SER A	58	−21.588	−14.902	26.927	1.00	73.98		N
ANISOU	199	N	SER A	58	9798	6487	11823	−2063	1989	−2348	N
ATOM	200	CA	SER A	58	−21.089	−15.994	26.099	1.00	79.23		C
ANISOU	200	CA	SER A	58	10678	6876	12549	−2044	1902	−2588	C
ATOM	201	C	SER A	58	−21.439	−17.315	26.751	1.00	87.23		C
ANISOU	201	C	SER A	58	11995	7205	13944	−2313	2401	−2561	C
ATOM	202	CB	SER A	58	−19.575	−15.903	25.883	1.00	76.07		C
ANISOU	202	CB	SER A	58	10618	6615	11669	−1576	1701	−2367	C
ATOM	203	OG	SER A	58	−19.115	−17.077	25.231	1.00	79.00		O
ANISOU	203	OG	SER A	58	11243	6641	12130	−1549	1704	−2583	O
ATOM	204	O	THR A	59	−21.514	−21.565	27.024	1.00113.78			O
ANISOU	204	O	THR A	59	16241	9103	17886	−2570	3157	−2540	O
ATOM	205	N	THR A	59	−22.082	−18.183	25.987	1.00	93.91		N
ANISOU	205	N	THR A	59	12655	7925	15103	−2548	2333	−2921	N
ATOM	206	CA	THR A	59	−22.535	−19.440	26.546	1.00104.73			C
ANISOU	206	CA	THR A	59	14226	8803	16762	−2751	2750	−2828	C
ATOM	207	C	THR A	59	−21.433	−20.491	26.426	1.00108.86			C
ANISOU	207	C	THR A	59	15299	8944	17121	−2500	2791	−2713	C
ATOM	208	CB	THR A	59	−23.845	−19.923	25.856	1.00111.67			C
ANISOU	208	CB	THR A	59	14615	9721	18095	−3124	2675	−3272	C
ATOM	209	OG1	THR A	59	−23.725	−19.805	24.431	1.00110.73			O
ANISOU	209	OG1	THR A	59	14272	9905	17893	−3047	2126	−3697	O
ATOM	210	CG2	THR A	59	−25.025	−19.076	26.309	1.00111.67			C
ANISOU	210	CG2	THR A	59	14111	10000	18317	−3340	2773	−3308	C
ATOM	211	O	SER A	60	−17.034	−21.457	25.544	1.00105.57			O
ANISOU	211	O	SER A	60	16118	8287	15707	−1109	2327	−2423	O
ATOM	212	N	SER A	60	−20.368	−20.119	25.742	1.00105.90			N
ANISOU	212	N	SER A	60	15046	8775	16417	−2167	2444	−2780	N
ATOM	213	CA	SER A	60	−19.374	−21.076	25.319	1.00108.06			C
ANISOU	213	CA	SER A	60	15719	8778	16561	−1902	2388	−2794	C
ATOM	214	C	SER A	60	−17.946	−20.659	25.648	1.00103.18			C
ANISOU	214	C	SER A	60	15460	8223	15519	−1403	2326	−2495	C
ATOM	215	CB	SER A	60	−19.519	−21.353	23.828	1.00110.78			C
ANISOU	215	CB	SER A	60	15824	9308	16959	−1964	1999	−3305	C
ATOM	216	OG	SER A	60	−19.036	−20.278	23.081	1.00105.77			O
ANISOU	216	OG	SER A	60	15004	9180	16003	−1749	1626	−3450	O
ATOM	217	O	GLU A	61	−17.288	−17.552	28.110	1.00105.37			O
ANISOU	217	O	GLU A	61	15623	9428	14984	−894	2287	−1470	O
ATOM	218	N	GLU A	61	−17.732	−19.423	26.087	1.00101.10			N
ANISOU	218	N	GLU A	61	15056	8364	14993	−1256	2228	−2276	N
ATOM	219	CA	GLU A	61	−16.380	−18.983	26.441	1.00	99.80		C
ANISOU	219	CA	GLU A	61	15101	8438	14381	−737	2074	−1939	C
ATOM	220	C	GLU A	61	−16.329	−18.195	27.763	1.00110.21			C
ANISOU	220	C	GLU A	61	16494	9894	15488	−613	2196	−1484	C
ATOM	221	CB	GLU A	61	−15.745	−18.199	25.285	1.00	88.19		C
ANISOU	221	CB	GLU A	61	13328	7535	12644	−533	1648	−2152	C
ATOM	222	CG	GLU A	61	−15.563	−18.990	23.998	1.00	88.07		C
ANISOU	222	CG	GLU A	61	13343	7401	12718	−543	1520	−2582	C
ATOM	223	CD	GLU A	61	−15.206	−18.134	22.787	1.00	81.57		C
ANISOU	223	CD	GLU A	61	12233	7146	11616	−409	1157	−2812	C
ATOM	224	OE1	GLU A	61	−15.937	−17.199	22.472	1.00	78.07		O
ANISOU	224	OE1	GLU A	61	11450	7080	11134	−587	980	−2905	O
ATOM	225	OE2	GLU A	61	−14.193	−18.404	22.143	1.00	79.38		O
ANISOU	225	OE2	GLU A	61	12090	6921	11150	−107	1073	−2897	O
ATOM	226	O	SER A	62	−15.732	−15.486	30.530	1.00127.79			O
ANISOU	226	O	SER A	62	18744	12881	16928	−112	2130	−561	O
ATOM	227	N	SER A	62	−15.219	−18.284	28.492	1.00125.02			N
ANISOU	227	N	SER A	62	18722	11712	17068	−171	2184	−1149	N
ATOM	228	CA	SER A	62	−15.046	−17.641	29.791	1.00129.26			C
ANISOU	228	CA	SER A	62	19419	12347	17347	16	2262	−739	C
ATOM	229	C	SER A	62	−15.107	−16.138	29.693	1.00124.89			C
ANISOU	229	C	SER A	62	18419	12425	16608	8	1993	−742	C
ATOM	230	CB	SER A	62	−13.707	−18.050	30.419	1.00135.84			C
ANISOU	230	CB	SER A	62	20679	13045	17889	566	2173	−466	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	231	OG	SER A	62	−12.551	−17.631	29.699	1.00136.69			O
ANISOU	231	OG	SER A	62	20556	13552	17829	896	1791	−596	O
ATOM	232	O	PHE A	63	−14.740	−13.234	29.854	1.00	61.43		O
ANISOU	232	O	PHE A	63	9730	5483	8128	171	1496	−622	O
ATOM	233	N	PHE A	63	−14.458	−15.574	28.685	1.00102.45			N
ANISOU	233	N	PHE A	63	15274	9998	13655	142	1648	−941	N
ATOM	234	CA	PHE A	63	−13.242	−14.818	28.870	1.00	79.01		C
ANISOU	234	CA	PHE A	63	12253	7389	10377	537	1386	−795	C
ATOM	235	C	PHE A	63	−13.602	−13.572	29.706	1.00	64.66		C
ANISOU	235	C	PHE A	63	10280	5883	8405	492	1354	−596	C
ATOM	236	CB	PHE A	63	−12.700	−14.368	27.512	1.00	71.68		C
ANISOU	236	CB	PHE A	63	10997	6833	9406	586	1124	−1072	C
ATOM	237	CG	PHE A	63	−11.889	−15.407	26.766	1.00	72.15		C
ANISOU	237	CG	PHE A	63	11220	6682	9514	791	1107	−1248	C
ATOM	238	CD1	PHE A	63	−10.580	−15.687	27.120	1.00	70.21		C
ANISOU	238	CD1	PHE A	63	11126	6406	9142	1226	1031	−1124	C
ATOM	239	CD2	PHE A	63	−12.410	−16.057	25.675	1.00	69.52		C
ANISOU	239	CD2	PHE A	63	10855	6206	9352	574	1137	−1578	C
ATOM	240	CE1	PHE A	63	−9.830	−16.614	26.421	1.00	68.61		C
ANISOU	240	CE1	PHE A	63	11049	6018	9001	1444	1031	−1304	C
ATOM	241	CE2	PHE A	63	−11.666	−16.984	24.981	1.00	68.87		C
ANISOU	241	CE2	PHE A	63	10939	5928	9300	777	1135	−1762	C
ATOM	242	CZ	PHE A	63	−10.376	−17.259	25.352	1.00	68.06		C
ANISOU	242	CZ	PHE A	63	10989	5785	9085	1215	1102	−1616	C
ATOM	243	N	VAL A	64	−12.598	−12.935	30.267	1.00	56.73		N
ANISOU	243	N	VAL A	64	9293	5116	7147	829	1163	−427	N
ATOM	244	CA	VAL A	64	−12.707	−11.657	30.951	1.00	48.70		C
ANISOU	244	CA	VAL A	64	8115	4430	5958	837	1068	−289	C
ATOM	245	C	VAL A	64	−13.228	−10.536	30.047	1.00	44.29		C
ANISOU	245	C	VAL A	64	7102	4266	5459	590	941	−474	C
ATOM	246	O	VAL A	64	−13.023	−10.556	28.861	1.00	42.88		O
ANISOU	246	O	VAL A	64	6730	4219	5344	547	826	−690	O
ATOM	247	CB	VAL A	64	−11.309	−11.250	31.437	1.00	48.17		C
ANISOU	247	CB	VAL A	64	8077	4563	5664	1259	807	−187	C
ATOM	248	CG1	VAL A	64	−11.286	−9.875	32.026	1.00	40.43		C
ANISOU	248	CG1	VAL A	64	6905	3933	4525	1269	667	−110	C
ATOM	249	CG2	VAL A	64	−10.763	−12.254	32.413	1.00	52.29		C
ANISOU	249	CG2	VAL A	64	9080	4725	6063	1597	860	14	C
ATOM	250	N	LEU A	65	−13.931	−9.578	30.638	1.00	38.97		N
ANISOU	250	N	LEU A	65	6309	3757	4739	458	976	−382	N
ATOM	251	C	LEU A	65	−13.665	−7.212	30.233	1.00	35.26		C
ANISOU	251	C	LEU A	65	5342	3954	4103	467	653	−426	C
ATOM	252	O	LEU A	65	−13.419	−6.944	31.392	1.00	35.04		O
ANISOU	252	O	LEU A	65	5476	3902	3936	608	670	−251	O
ATOM	253	CA	LEU A	65	−14.485	−8.458	29.913	1.00	36.70		C
ANISOU	253	CA	LEU A	65	5644	3811	4490	274	852	−520	C
ATOM	254	CB	LEU A	65	−15.953	−8.259	30.306	1.00	42.15		C
ANISOU	254	CB	LEU A	65	6242	4432	5341	−19	1053	−526	C
ATOM	255	CG	LEU A	65	−16.781	−7.263	29.499	1.00	46.09		C
ANISOU	255	CG	LEU A	65	6352	5231	5929	−199	917	−701	C
ATOM	256	CD1	LEU A	65	−17.018	−7.821	28.091	1.00	50.52		C
ANISOU	256	CD1	LEU A	65	6769	5795	6630	−316	793	−988	C
ATOM	257	CD2	LEU A	65	−18.118	−6.981	30.199	1.00	49.54		C
ANISOU	257	CD2	LEU A	65	6673	5611	6537	−422	1135	−684	C
ATOM	258	N	ASN A	66	−13.269	−6.442	29.222	1.00	34.31		N
ANISOU	258	N	ASN A	66	4965	4115	3957	469	480	−552	N
ATOM	259	CA	ASN A	66	−12.354	−5.314	29.436	1.00	34.32		C
ANISOU	259	CA	ASN A	66	4839	4375	3828	622	326	−495	C
ATOM	260	C	ASN A	66	−12.989	−3.969	29.200	1.00	34.62		C
ANISOU	260	C	ASN A	66	4666	4641	3846	481	279	−504	C
ATOM	261	O	ASN A	66	−13.823	−3.813	28.315	1.00	34.81		O
ANISOU	261	O	ASN A	66	4572	4723	3932	323	279	−611	O
ATOM	262	CB	ASN A	66	−11.123	−5.394	28.516	1.00	36.02		C
ANISOU	262	CB	ASN A	66	4949	4704	4034	768	230	−607	C
ATOM	263	CG	ASN A	66	−10.152	−6.502	28.893	1.00	37.61		C
ANISOU	263	CG	ASN A	66	5319	4723	4247	1016	219	−596	C
ATOM	264	OD1	ASN A	66	−10.355	−7.237	29.860	1.00	38.67		O
ANISOU	264	OD1	ASN A	66	5714	4621	4357	1103	272	−476	O
ATOM	265	ND2	ASN A	66	−9.086	−6.631	28.104	1.00	36.89		N
ANISOU	265	ND2	ASN A	66	5099	4727	4188	1153	175	−719	N
ATOM	266	N	TRP A	67	−12.559	−2.981	29.971	1.00	31.20		N
ANISOU	266	N	TRP A	67	4196	4333	3325	567	207	−415	N
ATOM	267	CA	TRP A	67	−13.016	−1.624	29.765	1.00	29.46		C
ANISOU	267	CA	TRP A	67	3806	4298	3090	470	164	−417	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	268	C	TRP A	67	−11.857	−0.754	29.256	1.00	31.37		C
ANISOU	268	C	TRP A	67	3907	4708	3306	545	66	−455	C
ATOM	269	O	TRP A	67	−10.777	−0.796	29.848	1.00	30.79		O
ANISOU	269	O	TRP A	67	3831	4642	3224	689	−6	−454	O
ATOM	270	CB	TRP A	67	−13.580	−1.100	31.086	1.00	31.97		C
ANISOU	270	CB	TRP A	67	4207	4587	3354	473	210	−312	C
ATOM	271	CG	TRP A	67	−14.127	0.260	31.040	1.00	30.78		C
ANISOU	271	CG	TRP A	67	3913	4579	3202	400	181	−315	C
ATOM	272	CD1	TRP A	67	−14.596	0.919	29.956	1.00	30.81		C
ANISOU	272	CD1	TRP A	67	3757	4693	3255	314	141	−377	C
ATOM	273	CD2	TRP A	67	−14.258	1.152	32.150	1.00	31.04		C
ANISOU	273	CD2	TRP A	67	3996	4641	3158	447	181	−257	C
ATOM	274	NE1	TRP A	67	−14.995	2.177	30.312	1.00	32.30		N
ANISOU	274	NE1	TRP A	67	3886	4959	3427	309	123	−346	N
ATOM	275	CE2	TRP A	67	−14.794	2.341	31.661	1.00	30.40		C
ANISOU	275	CE2	TRP A	67	3760	4670	3122	375	154	−287	C
ATOM	276	CE3	TRP A	67	−13.981	1.047	33.511	1.00	37.56		C
ANISOU	276	CE3	TRP A	67	5025	5400	3848	573	191	−188	C
ATOM	277	CZ2	TRP A	67	−15.068	3.424	32.484	1.00	36.15		C
ANISOU	277	CZ2	TRP A	67	4503	5428	3805	404	157	−266	C
ATOM	278	CZ3	TRP A	67	−14.259	2.134	34.335	1.00	39.10		C
ANISOU	278	CZ3	TRP A	67	5243	5650	3962	600	184	−181	C
ATOM	279	CH2	TRP A	67	−14.789	3.304	33.816	1.00	35.93		C
ANISOU	279	CH2	TRP A	67	4657	5345	3650	504	175	−228	C
ATOM	280	N	TYR A	68	−12.092	0.033	28.195	1.00	32.47		N
ANISOU	280	N	TYR A	68	3934	4965	3439	458	68	−494	N
ATOM	281	CA	TYR A	68	−11.053	0.818	27.488	1.00	31.88		C
ANISOU	281	CA	TYR A	68	3751	5001	3359	483	77	−522	C
ATOM	282	C	TYR A	68	−11.368	2.284	27.359	1.00	31.80		C
ANISOU	282	C	TYR A	68	3691	5066	3327	412	82	−469	C
ATOM	283	O	TYR A	68	−12.529	2.676	27.178	1.00	34.10		O
ANISOU	283	O	TYR A	68	4016	5366	3575	362	59	−437	O
ATOM	284	CB	TYR A	68	−10.824	0.310	26.034	1.00	31.12		C
ANISOU	284	CB	TYR A	68	3677	4932	3215	485	147	−604	C
ATOM	285	CG	TYR A	68	−10.124	−0.996	26.010	1.00	31.07		C
ANISOU	285	CG	TYR A	68	3703	4844	3256	585	169	−682	C
ATOM	286	CD1	TYR A	68	−8.733	−1.067	26.222	1.00	28.94		C
ANISOU	286	CD1	TYR A	68	3318	4601	3075	704	191	−725	C
ATOM	287	CD2	TYR A	68	−10.824	−2.170	25.840	1.00	31.06		C
ANISOU	287	CD2	TYR A	68	3827	4717	3256	570	163	−739	C
ATOM	288	CE1	TYR A	68	−8.089	−2.276	26.238	1.00	28.27		C
ANISOU	288	CE1	TYR A	68	3267	4430	3046	851	193	−801	C
ATOM	289	CE2	TYR A	68	−10.171	−3.401	25.833	1.00	30.90		C
ANISOU	289	CE2	TYR A	68	3881	4572	3289	687	193	−808	C
ATOM	290	CZ	TYR A	68	−8.803	−3.439	26.046	1.00	36.07		C
ANISOU	290	CZ	TYR A	68	4440	5264	4000	851	201	−828	C
ATOM	291	OH	TYR A	68	−8.150	−4.656	26.061	1.00	38.03		O
ANISOU	291	OH	TYR A	68	4762	5378	4309	1020	215	−900	O
ATOM	292	N	ARG A	69	−10.317	3.088	27.402	1.00	30.18		N
ANISOU	292	N	ARG A	69	3387	4897	3184	413	117	−480	N
ATOM	293	CA	ARG A	69	−10.379	4.472	26.952	1.00	29.68		C
ANISOU	293	CA	ARG A	69	3313	4849	3115	338	188	−429	C
ATOM	294	C	ARG A	69	−9.518	4.606	25.689	1.00	34.40		C
ANISOU	294	C	ARG A	69	3900	5467	3704	316	367	−445	C
ATOM	295	O	ARG A	69	−8.414	4.044	25.619	1.00	34.43		O
ANISOU	295	O	ARG A	69	3780	5489	3813	343	433	−535	O
ATOM	296	CB	ARG A	69	−9.907	5.431	28.044	1.00	31.56		C
ANISOU	296	CB	ARG A	69	3459	5064	3468	309	140	−449	C
ATOM	297	CG	ARG A	69	−9.783	6.861	27.573	1.00	32.21		C
ANISOU	297	CG	ARG A	69	3547	5097	3596	214	258	−406	C
ATOM	298	CD	ARG A	69	−9.533	7.841	28.706	1.00	33.39		C
ANISOU	298	CD	ARG A	69	3626	5193	3867	171	185	−466	C
ATOM	299	NE	ARG A	69	−9.475	9.212	28.219	1.00	36.21		N
ANISOU	299	NE	ARG A	69	4027	5439	4292	67	333	−418	N
ATOM	300	CZ	ARG A	69	−9.163	10.246	28.984	1.00	37.74		C
ANISOU	300	CZ	ARG A	69	4167	5541	4630	−6	311	−498	C
ATOM	301	NH1	ARG A	69	−8.866	10.038	30.260	1.00	38.48		N
ANISOU	301	NH1	ARG A	69	4163	5683	4776	37	112	−644	N
ATOM	302	NH2	ARG A	69	−9.107	11.469	28.476	1.00	42.52		N
ANISOU	302	NH2	ARG A	69	4853	5987	5316	−110	487	−441	N
ATOM	303	O	MET A	70	−8.955	7.844	23.711	1.00	47.21		O
ANISOU	303	O	MET A	70	5776	6908	5253	138	894	−202	O
ATOM	304	N	MET A	70	−10.048	5.287	24.671	1.00	32.95		N
ANISOU	304	N	MET A	70	3867	5275	3376	299	454	−360	N

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	305	C	MET A	70	−8.472	6.749	23.422	1.00	42.54		C
ANISOU	305	C	MET A	70	5109	6400	4656	178	911	−292	C
ATOM	306	CA	MET A	70	−9.328	5.482	23.416	1.00	35.38		C
ANISOU	306	CA	MET A	70	4257	5580	3604	293	688	−341	C
ATOM	307	CB	MET A	70	−10.323	5.537	22.245	1.00	40.35		C
ANISOU	307	CB	MET A	70	5159	6234	3938	381	659	−270	C
ATOM	308	CG	MET A	70	−11.330	4.408	22.281	1.00	41.35		C
ANISOU	308	CG	MET A	70	5295	6424	3992	447	420	−365	C
ATOM	309	SD	MET A	70	−10.548	2.775	22.405	1.00	54.68		S
ANISOU	309	SD	MET A	70	6876	8119	5782	460	446	−523	S
ATOM	310	CE	MET A	70	−9.805	2.752	20.772	1.00	43.48		C
ANISOU	310	CE	MET A	70	5649	6733	4138	527	692	−543	C
ATOM	311	O	SER A	71	−7.451	8.318	20.978	1.00	59.66		O
ANISOU	311	O	SER A	71	7686	8372	6610	90	1653	−64	O
ATOM	312	N	SER A	71	−7.195	6.587	23.106	1.00	43.34		N
ANISOU	312	N	SER A	71	5057	6500	4911	120	1141	−375	N
ATOM	313	CA	SER A	71	−6.247	7.690	22.992	1.00	53.52		C
ANISOU	313	CA	SER A	71	6243	7679	6414	−40	1431	−371	C
ATOM	314	C	SER A	71	−6.567	8.617	21.806	1.00	66.57		C
ANISOU	314	C	SER A	71	8248	9206	7841	−61	1719	−173	C
ATOM	315	CB	SER A	71	−4.834	7.130	22.839	1.00	52.34		C
ANISOU	315	CB	SER A	71	5792	7577	6517	−83	1633	−544	C
ATOM	316	OG	SER A	71	−4.674	6.627	21.526	1.00	59.64		O
ANISOU	316	OG	SER A	71	6909	8523	7229	−19	1904	−497	O
ATOM	317	O	PRO A	72	−6.525	9.773	18.325	1.00	95.84		O
ANISOU	317	O	PRO A	72	12964	12663	10790	60	2601	276	O
ATOM	318	N	PRO A	72	−5.854	9.755	21.722	1.00	85.13		N
ANISOU	318	N	PRO A	72	10565	11384	10397	−239	2035	−136	N
ATOM	319	CA	PRO A	72	−5.928	10.573	20.502	1.00	91.13		C
ANISOU	319	CA	PRO A	72	11721	11975	10928	−247	2412	81	C
ATOM	320	C	PRO A	72	−5.691	9.766	19.231	1.00	90.80		C
ANISOU	320	C	PRO A	72	11890	12020	10591	−128	2638	115	C
ATOM	321	CB	PRO A	72	−4.796	11.586	20.698	1.00	98.04		C
ANISOU	321	CB	PRO A	72	12398	12640	12211	−525	2807	33	C
ATOM	322	CG	PRO A	72	−4.708	11.739	22.182	1.00	95.56		C
ANISOU	322	CG	PRO A	72	11699	12362	12246	−615	2464	−167	C
ATOM	323	CD	PRO A	72	−4.993	10.379	22.747	1.00	88.12		C
ANISOU	323	CD	PRO A	72	10576	11685	11220	−438	2055	−300	C
ATOM	324	O	SER A	73	−4.904	6.347	16.821	1.00	76.70		O
ANISOU	324	O	SER A	73	10310	10631	8200	269	2882	−164	O
ATOM	325	N	SER A	73	−4.565	9.059	19.193	1.00	83.79		N
ANISOU	325	N	SER A	73	10685	11210	9939	−205	2838	−65	N
ATOM	326	CA	SER A	73	−4.163	8.283	18.024	1.00	78.73		C
ANISOU	326	CA	SER A	73	10215	10641	9058	−99	3119	−75	C
ATOM	327	C	SER A	73	−5.060	7.068	17.802	1.00	72.65		C
ANISOU	327	C	SER A	73	9599	10053	7950	143	2724	−129	C
ATOM	328	CB	SER A	73	−2.701	7.842	18.154	1.00	80.04		C
ANISOU	328	CB	SER A	73	9920	10844	9646	−228	3418	−297	C
ATOM	329	OG	SER A	73	−2.503	6.917	19.209	1.00	79.23		O
ANISOU	329	OG	SER A	73	9394	10900	9808	−172	3026	−525	O
ATOM	330	O	GLY A	74	−7.182	3.421	18.845	1.00	53.62		O
ANISOU	330	O	GLY A	74	7049	7995	5330	523	1520	−514	O
ATOM	331	N	GLY A	74	−5.998	6.840	18.712	1.00	63.68		N
ANISOU	331	N	GLY A	74	8376	8982	6836	195	2241	−156	N
ATOM	332	CA	GLY A	74	−6.962	5.771	18.545	1.00	58.59		C
ANISOU	332	CA	GLY A	74	7860	8467	5936	373	1884	−221	C
ATOM	333	C	GLY A	74	−6.554	4.437	19.146	1.00	55.08		C
ANISOU	333	C	GLY A	74	7116	8116	5697	402	1725	−430	C
ATOM	334	O	GLN A	75	−6.241	3.875	22.804	1.00	32.68		O
ANISOU	334	O	GLN A	75	3522	5304	3593	322	1088	−630	O
ATOM	335	N	GLN A	75	−5.515	4.431	19.989	1.00	50.13		N
ANISOU	335	N	GLN A	75	6112	7481	5455	306	1800	−532	N
ATOM	336	CA	GLN A	75	−5.137	3.235	20.725	1.00	40.00		C
ANISOU	336	CA	GLN A	75	4572	6260	4365	387	1600	−706	C
ATOM	337	C	GLN A	75	−5.999	2.984	21.970	1.00	36.89		C
ANISOU	337	C	GLN A	75	4130	5867	4020	409	1194	−694	C
ATOM	338	CB	GLN A	75	−3.654	3.295	21.149	1.00	37.80		C
ANISOU	338	CB	GLN A	75	3888	5994	4479	336	1785	−855	C
ATOM	339	CG	GLN A	75	−2.682	3.317	19.972	1.00	44.26		C
ANISOU	339	CG	GLN A	75	4693	6811	5314	316	2263	−908	C
ATOM	340	CD	GLN A	75	−2.576	1.971	19.248	1.00	43.08		C
ANISOU	340	CD	GLN A	75	4658	6715	4995	508	2302	−1021	C
ATOM	341	OE1	GLN A	75	−3.222	0.976	19.626	1.00	41.84		O
ANISOU	341	OE1	GLN A	75	4587	6571	4739	641	1965	−1065	O

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	342	NE2	GLN A	75	−1.768	1.940	18.211	1.00	46.53		N
ANISOU	342	NE2	GLN A	75	5116	7155	5408	515	2751	−1076	N
ATOM	343	O	PRO A	76	−5.406	0.521	24.557	1.00	37.77		O
ANISOU	343	O	PRO A	76	3591	5966	4793	196	728	−1132	O
ATOM	344	N	PRO A	76	−6.422	1.736	22.147	1.00	30.84		N
ANISOU	344	N	PRO A	76	3281	5135	3301	54	1119	−1031	N
ATOM	345	C	PRO A	76	−6.357	1.294	24.577	1.00	35.24		C
ANISOU	345	C	PRO A	76	3458	5690	4240	151	679	−982	C
ATOM	346	CA	PRO A	76	−7.232	1.459	23.333	1.00	30.42		C
ANISOU	346	CA	PRO A	76	3141	5108	3309	121	781	−933	C
ATOM	347	CB	PRO A	76	−7.946	0.154	22.962	1.00	31.30		C
ANISOU	347	CB	PRO A	76	3327	5215	3350	194	650	−986	C
ATOM	348	CG	PRO A	76	−6.932	−0.540	22.084	1.00	33.08		C
ANISOU	348	CG	PRO A	76	3512	5402	3656	197	886	−1172	C
ATOM	349	CD	PRO A	76	−6.275	0.554	21.276	1.00	32.29		C
ANISOU	349	CD	PRO A	76	3521	5302	3444	98	1207	−1181	C
ATOM	350	O	ASP A	77	−7.847	1.613	28.260	1.00	29.72		O
ANISOU	350	O	ASP A	77	2760	4992	3541	246	36	−690	O
ATOM	351	N	ASP A	77	−6.668	2.024	25.650	1.00	34.03		N
ANISOU	351	N	ASP A	77	3276	5553	4100	142	519	−874	N
ATOM	352	CA	ASP A	77	−5.895	1.902	26.904	1.00	39.25		C
ANISOU	352	CA	ASP A	77	3721	6186	5006	193	347	−924	C
ATOM	353	C	ASP A	77	−6.736	1.173	27.933	1.00	32.62		C
ANISOU	353	C	ASP A	77	2972	5332	4090	278	84	−818	C
ATOM	354	CB	ASP A	77	−5.489	3.270	27.443	1.00	44.76		C
ANISOU	354	CB	ASP A	77	4346	6890	5771	112	372	−918	C
ATOM	355	CG	ASP A	77	−4.729	3.177	28.779	1.00	56.00		C
ANISOU	355	CG	ASP A	77	5576	8287	7414	182	118	−996	C
ATOM	356	OD1	ASP A	77	−3.911	2.250	28.952	1.00	58.46		O
ANISOU	356	OD1	ASP A	77	5712	8554	7946	282	11	−1119	O
ATOM	357	OD2	ASP A	77	−4.958	4.027	29.673	1.00	59.65		O
ANISOU	357	OD2	ASP A	77	6079	8761	7824	155	−3	−945	O
ATOM	358	N	LYS A	78	−6.225	0.054	28.436	1.00	32.49		N
ANISOU	358	N	LYS A	78	2871	5247	4228	389	−65	−874	N
ATOM	359	C	LYS A	78	−7.209	−0.178	30.657	1.00	32.62		C
ANISOU	359	C	LYS A	78	3126	5201	4065	467	−413	−660	C
ATOM	360	O	LYS A	78	−6.217	0.020	31.342	1.00	30.01		O
ANISOU	360	O	LYS A	78	2687	4851	3864	534	−572	−730	O
ATOM	361	CA	LYS A	78	−7.050	−0.806	29.285	1.00	33.85		C
ANISOU	361	CA	LYS A	78	3199	5358	4305	457	−246	−756	C
ATOM	362	CB	LYS A	78	−6.411	−2.184	29.403	1.00	33.16		C
ANISOU	362	CB	LYS A	78	3048	5153	4398	589	−358	−828	C
ATOM	363	CG	LYS A	78	−7.229	−3.242	30.122	1.00	31.84		C
ANISOU	363	CG	LYS A	78	3086	4866	4145	647	−481	−699	C
ATOM	364	CD	LYS A	78	−6.474	−4.570	30.085	1.00	32.88		C
ANISOU	364	CD	LYS A	78	3156	4848	4491	794	−584	−780	C
ATOM	365	CE	LYS A	78	−7.005	−5.641	31.017	1.00	33.31		C
ANISOU	365	CE	LYS A	78	3450	4718	4488	875	−726	−633	C
ATOM	366	NZ	LYS A	78	−6.195	−6.917	30.919	1.00	33.02		N
ANISOU	366	NZ	LYS A	78	3352	4499	4694	1045	−844	−716	N
ATOM	367	O	LEU A	79	−8.418	−0.148	34.601	1.00	31.04		O
ANISOU	367	O	LEU A	79	3565	4844	3383	566	−818	−339	O
ATOM	368	N	LEU A	79	−8.437	0.118	31.059	1.00	32.65		N
ANISOU	368	N	LEU A	79	3312	5218	3874	407	−384	−532	N
ATOM	369	CA	LEU A	79	−8.678	0.740	32.377	1.00	33.94		C
ANISOU	369	CA	LEU A	79	3605	5375	3916	406	−492	−454	C
ATOM	370	C	LEU A	79	−8.924	−0.274	33.483	1.00	31.65		C
ANISOU	370	C	LEU A	79	3529	4962	3534	490	−628	−357	C
ATOM	371	CB	LEU A	79	−9.898	1.660	32.324	1.00	30.79		C
ANISOU	371	CB	LEU A	79	3291	5029	3380	298	−348	−384	C
ATOM	372	CG	LEU A	79	−9.903	2.724	31.243	1.00	30.97		C
ANISOU	372	CG	LEU A	79	3204	5133	3430	224	−214	−429	C
ATOM	373	CD1	LEU A	79	−11.303	3.320	31.137	1.00	32.39		C
ANISOU	373	CD1	LEU A	79	3471	5326	3510	166	−127	−360	C
ATOM	374	CD2	LEU A	79	−8.840	3.789	31.495	1.00	34.87		C
ANISOU	374	CD2	LEU A	79	3590	5654	4006	201	−237	−504	C
ATOM	375	N	ALA A	80	−9.795	−1.232	33.195	1.00	34.83		N
ANISOU	375	N	ALA A	80	4027	5287	3919	469	−523	−293	N
ATOM	376	CA	ALA A	80	−10.134	−2.232	34.190	1.00	40.96		C
ANISOU	376	CA	ALA A	80	5062	5899	4602	523	−578	−175	C
ATOM	377	C	ALA A	80	−10.776	−3.367	33.470	1.00	39.77		C
ANISOU	377	C	ALA A	80	4905	5650	4555	491	−453	−173	C
ATOM	378	O	ALA A	80	−10.981	−3.297	32.252	1.00	37.25		O
ANISOU	378	O	ALA A	80	4395	5414	4343	436	−359	−275	O

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	379	CB	ALA A	80	−11.075	−1.667	35.252	1.00	42.76		C
ANISOU	379	CB	ALA A	80	5526	6106	4614	444	−478	−70	C
ATOM	380	N	ALA A	81	−11.136	−4.390	34.231	1.00	39.22		N
ANISOU	380	N	ALA A	81	5080	5386	4436	518	−444	−60	N
ATOM	381	CA	ALA A	81	−11.687	−5.618	33.665	1.00	41.75		C
ANISOU	381	CA	ALA A	81	5408	5558	4897	485	−330	−70	C
ATOM	382	C	ALA A	81	−12.448	−6.422	34.713	1.00	44.08		C
ANISOU	382	C	ALA A	81	6036	5614	5098	443	−207	90	C
ATOM	383	O	ALA A	81	−12.228	−6.265	35.907	1.00	42.96		O
ANISOU	383	O	ALA A	81	6181	5398	4743	500	−273	225	O
ATOM	384	CB	ALA A	81	−10.589	−6.460	33.080	1.00	37.41		C
ANISOU	384	CB	ALA A	81	4746	4947	4521	628	−485	−155	C
ATOM	385	O	PHE A	82	−14.190	−9.841	33.411	1.00	51.73		O
ANISOU	385	O	PHE A	82	7018	6009	6628	243	194	−10	O
ATOM	386	N	PHE A	82	−13.322	−7.304	34.255	1.00	44.49		N
ANISOU	386	N	PHE A	82	6073	5526	5305	339	−21	64	N
ATOM	387	CA	PHE A	82	−13.965	−8.242	35.162	1.00	48.69		C
ANISOU	387	CA	PHE A	82	6931	5770	5798	281	155	213	C
ATOM	388	C	PHE A	82	−13.919	−9.645	34.599	1.00	49.92		C
ANISOU	388	C	PHE A	82	7081	5704	6180	301	171	175	C
ATOM	389	CB	PHE A	82	−15.417	−7.847	35.426	1.00	49.60		C
ANISOU	389	CB	PHE A	82	7043	5868	5933	64	482	205	C
ATOM	390	CG	PHE A	82	−16.100	−8.707	36.469	1.00	55.78		C
ANISOU	390	CG	PHE A	82	8203	6329	6663	−34	763	364	C
ATOM	391	CD1	PHE A	82	−16.133	−8.310	37.798	1.00	58.59		C
ANISOU	391	CD1	PHE A	82	8950	6613	6700	−31	863	537	C
ATOM	392	CD2	PHE A	82	−16.690	−9.915	36.124	1.00	57.19		C
ANISOU	392	CD2	PHE A	82	8379	6255	7096	−137	948	333	C
ATOM	393	CE1	PHE A	82	−16.756	−9.094	38.761	1.00	63.12		C
ANISOU	393	CE1	PHE A	82	9945	6861	7176	−133	1182	701	C
ATOM	394	CE2	PHE A	82	−17.307	−10.707	37.092	1.00	60.47		C
ANISOU	394	CE2	PHE A	82	9175	6329	7470	−251	1269	493	C
ATOM	395	CZ	PHE A	82	−17.342	−10.292	38.400	1.00	64.04		C
ANISOU	395	CZ	PHE A	82	10052	6708	7573	−251	1404	687	C
ATOM	396	O	PRO A	83	−10.824	−11.071	35.880	1.00	70.44		O
ANISOU	396	O	PRO A	83	10150	7959	8655	908	−555	407	O
ATOM	397	N	PRO A	83	−13.547	−10.620	35.434	1.00	50.73		N
ANISOU	397	N	PRO A	83	7539	5519	6217	399	137	346	N
ATOM	398	CA	PRO A	83	−12.933	−10.360	36.747	1.00	59.77		C
ANISOU	398	CA	PRO A	83	9070	6597	7045	538	−15	549	C
ATOM	399	C	PRO A	83	−11.414	−10.265	36.604	1.00	71.30		C
ANISOU	399	C	PRO A	83	10422	8151	8519	801	−437	500	C
ATOM	400	CB	PRO A	83	−13.336	−11.579	37.573	1.00	55.89		C
ANISOU	400	CB	PRO A	83	9045	5698	6492	523	154	756	C
ATOM	401	CG	PRO A	83	−13.416	−12.704	36.555	1.00	54.35		C
ANISOU	401	CG	PRO A	83	8641	5346	6662	501	203	634	C
ATOM	402	CD	PRO A	83	−13.806	−12.056	35.213	1.00	50.88		C
ANISOU	402	CD	PRO A	83	7664	5219	6449	375	250	358	C
ATOM	403	O	GLU A	84	−9.846	−7.331	38.624	1.00	93.91		O
ANISOU	403	O	GLU A	84	13474	11462	10745	1028	−1025	536	O
ATOM	404	N	GLU A	84	−10.796	−9.240	37.163	1.00	79.85		N
ANISOU	404	N	GLU A	84	11520	9415	9402	890	−647	509	N
ATOM	405	CA	GLU A	84	−9.342	−9.165	37.219	1.00	88.54		C
ANISOU	405	CA	GLU A	84	12514	10566	10563	1141	−1061	443	C
ATOM	406	C	GLU A	84	−9.012	−8.145	38.305	1.00	96.12		C
ANISOU	406	C	GLU A	84	13673	11632	11214	1200	−1253	504	C
ATOM	407	CB	GLU A	84	−8.794	−8.768	35.834	1.00	84.53		C
ANISOU	407	CB	GLU A	84	11464	10289	10363	1127	−1077	189	C
ATOM	408	CG	GLU A	84	−7.375	−9.199	35.485	1.00	83.91		C
ANISOU	408	CG	GLU A	84	11162	10177	10544	1360	−1385	53	C
ATOM	409	CD	GLU A	84	−6.919	−8.727	34.103	1.00	78.72		C
ANISOU	409	CD	GLU A	84	10019	9740	10152	1300	−1284	−201	C
ATOM	410	OE1	GLU A	84	−7.648	−8.910	33.136	1.00	73.30		O
ANISOU	410	OE1	GLU A	84	9226	9100	9526	1146	−1017	−267	O
ATOM	411	OE2	GLU A	84	−5.822	−8.178	33.992	1.00	77.18		O
ANISOU	411	OE2	GLU A	84	9566	9657	10103	1405	−1468	−345	O
ATOM	412	O	ASP A	85	−5.447	−6.546	38.532	1.00105.79			O
ANISOU	412	O	ASP A	85	14234	13193	12770	1683	−2317	70	O
ATOM	413	N	ASP A	85	−7.812	−8.194	38.876	1.00101.42			N
ANISOU	413	N	ASP A	85	14415	12260	11861	1452	−1686	493	N
ATOM	414	CA	ASP A	85	−7.353	−7.205	39.837	1.00104.52			C
ANISOU	414	CA	ASP A	85	14956	12764	11993	1527	−1946	489	C
ATOM	415	C	ASP A	85	−6.391	−6.187	39.242	1.00103.99			C
ANISOU	415	C	ASP A	85	14369	12960	12182	1557	−2142	230	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	416	O	ARG A	86	−5.966	−1.524	38.587	1.00	81.91		O
ANISOU	416	O	ARG A	86	10691	10927	9503	1148	−1973	−272	O
ATOM	417	N	ARG A	86	−6.632	−4.911	39.534	1.00	99.94		N
ANISOU	417	N	ARG A	86	13820	12644	11510	1431	−2076	174	N
ATOM	418	CA	ARG A	86	−5.743	−3.851	39.096	1.00	91.73		C
ANISOU	418	CA	ARG A	86	12336	11817	10703	1431	−2229	−64	C
ATOM	419	C	ARG A	86	−6.503	−2.634	38.613	1.00	84.28		C
ANISOU	419	C	ARG A	86	11220	11080	9721	1183	−1884	−116	C
ATOM	420	N	SER A	93	−8.138	2.009	43.366	1.00	62.39		N
ANISOU	420	N	SER A	93	9731	8513	5459	921	−1892	−158	N
ATOM	421	CA	SER A	93	−8.283	2.182	41.930	1.00	59.24		C
ANISOU	421	CA	SER A	93	8804	8223	5482	800	−1655	−210	C
ATOM	422	C	SER A	93	−9.359	3.245	41.598	1.00	53.78		C
ANISOU	422	C	SER A	93	8004	7623	4809	593	−1249	−236	C
ATOM	423	O	SER A	93	−10.355	3.408	42.297	1.00	56.09		O
ANISOU	423	O	SER A	93	8612	7862	4840	515	−1000	−162	O
ATOM	424	CB	SER A	93	−8.603	0.834	41.254	1.00	63.80		C
ANISOU	424	CB	SER A	93	9362	8701	6180	824	−1522	−61	C
ATOM	425	OG	SER A	93	−8.517	0.910	39.826	1.00	63.73		O
ANISOU	425	OG	SER A	93	8872	8793	6549	747	−1377	−140	O
ATOM	426	N	ARG A	94	−9.109	3.992	40.535	1.00	47.65		N
ANISOU	426	N	ARG A	94	6787	6963	4355	515	−1183	−353	N
ATOM	427	CA	ARG A	94	−9.997	5.038	40.074	1.00	42.51		C
ANISOU	427	CA	ARG A	94	5999	6379	3775	360	−870	−382	C
ATOM	428	C	ARG A	94	−11.170	4.474	39.284	1.00	38.15		C
ANISOU	428	C	ARG A	94	5386	5806	3303	279	−550	−264	C
ATOM	429	O	ARG A	94	−12.161	5.167	39.059	1.00	36.17		O
ANISOU	429	O	ARG A	94	5078	5574	3089	177	−299	−272	O
ATOM	430	CB	ARG A	94	−9.238	6.017	39.169	1.00	46.10		C
ANISOU	430	CB	ARG A	94	6060	6925	4530	313	−918	−528	C
ATOM	431	CG	ARG A	94	−8.134	6.831	39.814	1.00	49.99		C
ANISOU	431	CG	ARG A	94	6502	7435	5059	348	−1200	−710	C
ATOM	432	CD	ARG A	94	−7.832	8.045	38.925	1.00	49.21		C
ANISOU	432	CD	ARG A	94	6068	7382	5249	229	−1067	−829	C
ATOM	433	NE	ARG A	94	−9.059	8.832	38.797	1.00	48.07		N
ANISOU	433	NE	ARG A	94	6008	7234	5023	126	−767	−763	N
ATOM	434	CZ	ARG A	94	−9.591	9.248	37.649	1.00	45.03		C
ANISOU	434	CZ	ARG A	94	5453	6860	4796	51	−528	−705	C
ATOM	435	NH1	ARG A	94	−8.978	8.974	36.508	1.00	43.52		N
ANISOU	435	NH1	ARG A	94	5035	6692	4809	43	−507	−702	N
ATOM	436	NH2	ARG A	94	−10.754	9.925	37.653	1.00	38.80		N
ANISOU	436	NH2	ARG A	94	4743	6046	3955	−3	−314	−661	N
ATOM	437	N	PHE A	95	−10.991	3.245	38.797	1.00	34.87		N
ANISOU	437	N	PHE A	95	4941	5344	2965	336	−596	−188	N
ATOM	438	C	PHE A	95	−12.497	1.332	38.539	1.00	45.78		C
ANISOU	438	C	PHE A	95	6511	6544	4341	280	−267	8	C
ATOM	439	O	PHE A	95	−11.806	0.608	39.261	1.00	52.15		O
ANISOU	439	O	PHE A	95	7561	7254	4998	394	−465	73	O
ATOM	440	CA	PHE A	95	−11.919	2.562	37.902	1.00	36.87		C
ANISOU	440	CA	PHE A	95	5087	5572	3350	270	−363	−120	C
ATOM	441	CB	PHE A	95	−11.207	2.223	36.594	1.00	38.04		C
ANISOU	441	CB	PHE A	95	4930	5782	3743	305	−453	−175	C
ATOM	442	CG	PHE A	95	−10.579	3.417	35.987	1.00	37.70		C
ANISOU	442	CG	PHE A	95	4647	5850	3827	276	−489	−287	C
ATOM	443	CD1	PHE A	95	−11.371	4.420	35.468	1.00	35.57		C
ANISOU	443	CD1	PHE A	95	4291	5631	3592	182	−309	−299	C
ATOM	444	CD2	PHE A	95	−9.220	3.606	36.044	1.00	40.96		C
ANISOU	444	CD2	PHE A	95	4933	6288	4343	342	−702	−389	C
ATOM	445	CE1	PHE A	95	−10.807	5.564	34.972	1.00	36.43		C
ANISOU	445	CE1	PHE A	95	4242	5799	3803	146	−312	−378	C
ATOM	446	CE2	PHE A	95	−8.657	4.743	35.525	1.00	43.70		C
ANISOU	446	CE2	PHE A	95	5068	6702	4836	281	−673	−499	C
ATOM	447	CZ	PHE A	95	−9.456	5.726	35.000	1.00	37.86		C
ANISOU	447	CZ	PHE A	95	4300	5995	4090	178	−465	−476	C
ATOM	448	N	ARG A	96	−13.797	1.131	38.335	1.00	45.58		N
ANISOU	448	N	ARG A	96	6476	6465	4376	162	39	38	N
ATOM	449	C	ARG A	96	−15.410	−0.696	38.041	1.00	41.36		C
ANISOU	449	C	ARG A	96	6013	5688	4013	28	430	132	C
ATOM	450	O	ARG A	96	−16.194	−0.061	37.315	1.00	38.73		O
ANISOU	450	O	ARG A	96	5398	5442	3875	−52	548	30	O
ATOM	451	CG	ARG A	96	−15.844	−0.632	40.971	1.00	54.23		C
ANISOU	451	CG	ARG A	96	8553	7059	4995	−12	726	320	C
ATOM	452	CD	ARG A	96	−16.399	−0.130	42.282	1.00	57.72		C
ANISOU	452	CD	ARG A	96	9392	7414	5123	−82	988	347	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	453	NE	ARG A	96	−15.412	0.657	43.024	1.00	57.44		N
ANISOU	453	NE	ARG A	96	9576	7472	4775	46	675	325	N
ATOM	454	CZ	ARG A	96	−15.718	1.404	44.086	1.00	59.25		C
ANISOU	454	CZ	ARG A	96	10125	7681	4707	6	831	291	C
ATOM	455	NH1	ARG A	96	−16.974	1.466	44.508	1.00	59.90		N
ANISOU	455	NH1	ARG A	96	10323	7651	4787	−161	1337	278	N
ATOM	456	NH2	ARG A	96	−14.783	2.095	44.722	1.00	57.32		N
ANISOU	456	NH2	ARG A	96	10065	7518	4196	126	494	236	N
ATOM	457	CA	ARG A	96	−14.455	0.018	38.978	1.00	45.36		C
ANISOU	457	CA	ARG A	96	6737	6249	4248	126	222	154	C
ATOM	458	CB	ARG A	96	−15.188	0.486	40.220	1.00	47.55		C
ANISOU	458	CB	ARG A	96	7338	6448	4282	49	463	186	C
ATOM	459	N	VAL A	97	−15.324	−2.019	38.054	1.00	41.24		N
ANISOU	459	N	VAL A	97	6136	5511	4022	50	437	215	N
ATOM	460	CA	VAL A	97	−16.192	−2.869	37.233	1.00	42.09		C
ANISOU	460	CA	VAL A	97	6059	5530	4405	−49	616	170	C
ATOM	461	C	VAL A	97	−16.885	−3.879	38.095	1.00	42.31		C
ANISOU	461	C	VAL A	97	6407	5288	4380	−141	901	283	C
ATOM	462	O	VAL A	97	−16.224	−4.614	38.825	1.00	42.00		O
ANISOU	462	O	VAL A	97	6731	5095	4133	−49	812	432	O
ATOM	463	CB	VAL A	97	−15.419	−3.653	36.135	1.00	44.71		C
ANISOU	463	CB	VAL A	97	6204	5884	4900	45	390	126	C
ATOM	464	CGI	VAL A	97	−16.412	−4.406	35.254	1.00	42.83		C
ANISOU	464	CGI	VAL A	97	5764	5565	4945	−69	554	31	C
ATOM	465	CG2	VAL A	97	−14.603	−2.718	35.298	1.00	43.88		C
ANISOU	465	CG2	VAL A	97	5838	6010	4824	125	166	27	C
ATOM	466	N	THR A	98	−18.208	−3.924	38.008	1.00	42.14		N
ANISOU	466	N	THR A	98	6256	5186	4570	−318	1242	204	N
ATOM	467	CA	THR A	98	−18.983	−4.827	38.844	1.00	49.46		C
ANISOU	467	CA	THR A	98	7480	5821	5490	−456	1623	295	C
ATOM	468	C	THR A	98	−20.077	−5.496	38.016	1.00	52.20		C
ANISOU	468	C	THR A	98	7489	6060	6284	−618	1840	143	C
ATOM	469	O	THR A	98	−20.599	−4.901	37.074	1.00	54.32		O
ANISOU	469	O	THR A	98	7319	6495	6824	−644	1762	−49	O
ATOM	470	CB	THR A	98	−19.631	−4.080	40.028	1.00	58.99		C
ANISOU	470	CB	THR A	98	8940	6979	6494	−557	1958	323	C
ATOM	471	OG1	THR A	98	−20.489	−3.058	39.511	1.00	62.76		O
ANISOU	471	OG1	THR A	98	8990	7613	7242	−639	2062	121	O
ATOM	472	CG2	THR A	98	−18.575	−3.426	40.916	1.00	59.23		C
ANISOU	472	CG2	THR A	98	9339	7102	6063	−398	1712	442	C
ATOM	473	N	GLN A	99	−20.420	−6.728	38.362	1.00	53.29		N
ANISOU	473	N	GLN A	99	7844	5900	6505	−719	2090	222	N
ATOM	474	CA	GLN A	99	−21.403	−7.497	37.602	1.00	53.42		C
ANISOU	474	CA	GLN A	99	7534	5774	6989	−885	2282	48	C
ATOM	475	C	GLN A	99	−22.780	−7.377	38.229	1.00	55.44		C
ANISOU	475	C	GLN A	99	7738	5854	7471	−1128	2810	−44	C
ATOM	476	O	GLN A	99	−22.952	−7.666	39.397	1.00	57.95		O
ANISOU	476	O	GLN A	99	8497	5942	7578	−1220	3183	118	O
ATOM	477	CB	GLN A	99	−20.981	−8.964	37.522	1.00	56.06		C
ANISOU	477	CB	GLN A	99	8092	5843	7366	−873	2271	154	C
ATOM	478	CG	GLN A	99	−21.942	−9.864	36.745	1.00	59.38		C
ANISOU	478	CG	GLN A	99	8186	6081	8293	−1056	2456	−52	C
ATOM	479	CD	GLN A	99	−21.483	−11.304	36.736	1.00	64.04		C
ANISOU	479	CD	GLN A	99	9038	6371	8923	−1041	2463	61	C
ATOM	480	OE1	GLN A	99	−21.051	−11.827	37.765	1.00	68.35		O
ANISOU	480	OE1	GLN A	99	10112	6676	9180	−1007	2604	326	O
ATOM	481	NE2	GLN A	99	−21.558	−11.952	35.573	1.00	62.25		N
ANISOU	481	NE2	GLN A	99	8480	6141	9033	−1049	2290	−142	N
ATOM	482	N	LEU A	100	−23.765	−6.946	37.457	1.00	55.90		N
ANISOU	482	N	LEU A	100	7269	6004	7965	−1224	2846	−317	N
ATOM	483	CA	LEU A	100	−25.113	−6.745	38.005	1.00	58.90		C
ANISOU	483	CA	LEU A	100	7493	6221	8666	−1453	3357	−468	C
ATOM	484	C	LEU A	100	−25.831	−8.087	38.182	1.00	62.43		C
ANISOU	484	C	LEU A	100	7979	6289	9454	−1686	3777	−508	C
ATOM	485	O	LEU A	100	−25.315	−9.123	37.762	1.00	63.47		O
ANISOU	485	O	LEU A	100	8222	6304	9589	−1652	3615	−436	O
ATOM	486	CB	LEU A	100	−25.916	−5.798	37.109	1.00	61.88		C
ANISOU	486	CB	LEU A	100	7258	6808	9444	−1440	3187	−771	C
ATOM	487	CG	LEU A	100	−25.262	−4.440	36.827	1.00	63.14		C
ANISOU	487	CG	LEU A	100	7370	7305	9315	−1222	2791	−736	C
ATOM	488	CD1	LEU A	100	−26.349	−3.487	36.371	1.00	65.89		C
ANISOU	488	CD1	LEU A	100	7214	7745	10077	−1244	2793	−1012	C
ATOM	489	CD2	LEU A	100	−24.507	−3.876	38.044	1.00	63.96		C
ANISOU	489	CD2	LEU A	100	7978	7438	8887	−1160	2904	−495	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	490	O	PRO A	101	−27.903	−11.467	38.073	1.00	77.58		O
ANISOU	490	O	PRO A	101	9745	7331	12400	−2107	4498	−829	O
ATOM	491	N	PRO A	101	−26.998	−8.089	38.852	1.00	66.52		N
ANISOU	491	N	PRO A	101	8452	6627	10197	−1814	4163	−645	N
ATOM	492	C	PRO A	101	−28.000	−10.246	37.963	1.00	74.24		C
ANISOU	492	C	PRO A	101	9103	7180	11926	−2027	4335	−909	C
ATOM	493	CA	PRO A	101	−27.619	−9.381	39.164	1.00	71.13		C
ANISOU	493	CA	PRO A	101	9160	6854	11011	−1959	4495	−678	C
ATOM	494	CB	PRO A	101	−28.874	−8.972	39.943	1.00	72.61		C
ANISOU	494	CB	PRO A	101	9271	6918	11397	−2046	4872	−864	C
ATOM	495	CG	PRO A	101	−28.472	−7.708	40.646	1.00	69.54		C
ANISOU	495	CG	PRO A	101	9105	6730	10587	−1939	4821	−743	C
ATOM	496	CD	PRO A	101	−27.603	−6.992	39.639	1.00	66.07		C
ANISOU	496	CD	PRO A	101	8408	6638	10058	−1794	4325	−716	C
ATOM	497	O	ASN A	102	−28.008	−12.069	34.150	1.00	76.70		O
ANISOU	497	O	ASN A	102	8301	7562	13278	−2029	3360	−1550	O
ATOM	498	N	ASN A	102	−28.412	−9.654	36.845	1.00	72.16		N
ANISOU	498	N	ASN A	102	8259	7146	12013	−1974	3988	−1194	N
ATOM	499	CA	ASN A	102	−28.873	−10.474	35.718	1.00	74.38		C
ANISOU	499	CA	ASN A	102	8131	7361	12767	−2016	3786	−1463	C
ATOM	500	C	ASN A	102	−27.755	−11.252	35.028	1.00	72.75		C
ANISOU	500	C	ASN A	102	8053	7146	12444	−1997	3527	−1340	C
ATOM	501	CB	ASN A	102	−29.622	−9.613	34.692	1.00	73.03		C
ANISOU	501	CB	ASN A	102	7381	7429	12936	−1911	3398	−1800	C
ATOM	502	CG	ASN A	102	−28.748	−8.569	34.030	1.00	67.03		C
ANISOU	502	CG	ASN A	102	6538	7032	11899	−1741	2943	−1730	C
ATOM	503	OD1	ASN A	102	−27.529	−8.716	33.929	1.00	65.91		O
ANISOU	503	OD1	ASN A	102	6652	6982	11409	−1693	2809	−1509	O
ATOM	504	ND2	ASN A	102	−29.376	−7.496	33.567	1.00	65.25		N
ANISOU	504	ND2	ASN A	102	5980	6996	11814	−1616	2682	−1920	N
ATOM	505	O	GLY A	103	−23.588	−11.472	33.355	1.00	65.17		O
ANISOU	505	O	GLY A	103	7716	6751	10295	−1280	2165	−859	O
ATOM	506	N	GLY A	103	−26.517	−10.982	35.423	1.00	68.04		N
ANISOU	506	N	GLY A	103	7885	6653	11314	−1866	3410	−1016	N
ATOM	507	CA	GLY A	103	−25.378	−11.725	34.914	1.00	66.51		C
ANISOU	507	CA	GLY A	103	7927	6472	10871	−1695	3055	−877	C
ATOM	508	C	GLY A	103	−24.757	−11.190	33.634	1.00	63.73		C
ANISOU	508	C	GLY A	103	7303	6488	10424	−1467	2454	−1007	C
ATOM	509	O	ARG A	104	−23.992	−8.098	30.518	1.00	45.47		O
ANISOU	509	O	ARG A	104	4270	5255	7753	−916	1100	−1362	O
ATOM	510	N	ARG A	104	−25.507	−10.424	32.845	1.00	61.46		N
ANISOU	510	N	ARG A	104	6543	6405	10403	−1469	2266	−1287	N
ATOM	511	CA	ARG A	104	−24.982	−10.018	31.532	1.00	57.81		C
ANISOU	511	CA	ARG A	104	5889	6246	9831	−1266	1723	−1414	C
ATOM	512	C	ARG A	104	−24.679	−8.532	31.439	1.00	49.81		C
ANISOU	512	C	ARG A	104	4838	5564	8523	−1097	1491	−1347	C
ATOM	513	CB	ARG A	104	−25.945	−10.422	30.421	1.00	61.80		C
ANISOU	513	CB	ARG A	104	5941	6714	10826	−1348	1548	−1803	C
ATOM	514	CG	ARG A	104	−27.335	−9.902	30.613	1.00	63.43		C
ANISOU	514	CG	ARG A	104	5740	6868	11494	−1496	1721	−2044	C
ATOM	515	CD	ARG A	104	−28.260	−10.382	29.518	1.00	68.74		C
ANISOU	515	CD	ARG A	104	6012	7497	12610	−1509	1457	−2432	C
ATOM	516	NE	ARG A	104	−29.649	−10.078	29.856	1.00	72.02		N
ANISOU	516	NE	ARG A	104	6188	7812	13364	−1529	1629	−2601	N
ATOM	517	CZ	ARG A	104	−30.163	−8.862	29.752	1.00	73.38		C
ANISOU	517	CZ	ARG A	104	6194	8158	13530	−1395	1449	−2663	C
ATOM	518	NH1	ARG A	104	−29.395	−7.868	29.311	1.00	71.31		N
ANISOU	518	NH1	ARG A	104	5996	8189	12911	−1228	1106	−2547	N
ATOM	519	NH2	ARG A	104	−31.430	−8.637	30.089	1.00	75.78		N
ANISOU	519	NH2	ARG A	104	6273	8321	14198	−1422	1623	−2850	N
ATOM	520	N	ASP A	105	−25.148	−7.763	32.418	1.00	49.77		N
ANISOU	520	N	ASP A	105	4861	5547	8503	−1163	1771	−1269	N
ATOM	521	CA	ASP A	105	−24.821	−6.340	32.496	1.00	50.67		C
ANISOU	521	CA	ASP A	105	4984	5932	8337	−1012	1598	−1187	C
ATOM	522	C	ASP A	105	−23.700	−6.076	33.526	1.00	49.16		C
ANISOU	522	C	ASP A	105	5259	5773	7648	−932	1688	−863	C
ATOM	523	O	ASP A	105	−23.596	−6.782	34.541	1.00	50.64		O
ANISOU	523	O	ASP A	105	5765	5733	7742	−1028	2007	−704	O
ATOM	524	CB	ASP A	105	−26.081	−5.509	32.845	1.00	54.34		C
ANISOU	524	CB	ASP A	105	5135	6377	9135	−1108	1803	−1363	C
ATOM	525	CG	ASP A	105	−27.136	−5.539	31.735	1.00	61.72		C
ANISOU	525	CG	ASP A	105	5557	7321	10571	−1124	1569	−1719	C
ATOM	526	OD1	ASP A	105	−26.763	−5.703	30.557	1.00	61.59		O
ANISOU	526	OD1	ASP A	105	5475	7438	10487	−994	1138	−1801	O

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	527	OD2	ASP A	105	−28.346	−5.412	32.035	1.00	68.95		O
ANISOU	527	OD2	ASP A	105	6194	8097	11906	−1233	1783	−1918	O
ATOM	528	N	PHE A	106	−22.867	−5.072	33.238	1.00	46.08		N
ANISOU	528	N	PHE A	106	4920	5643	6947	−754	1393	−779	N
ATOM	529	CA	PHE A	106	−21.722	−4.683	34.075	1.00	40.91		C
ANISOU	529	CA	PHE A	106	4637	5054	5855	−651	1371	−531	C
ATOM	530	C	PHE A	106	−21.691	−3.186	34.224	1.00	43.39		C
ANISOU	530	C	PHE A	106	4886	5568	6031	−578	1290	−530	C
ATOM	531	O	PHE A	106	−21.726	−2.466	33.217	1.00	45.14		O
ANISOU	531	O	PHE A	106	4866	5967	6317	−491	1031	−638	O
ATOM	532	CB	PHE A	106	−20.381	−5.153	33.475	1.00	32.17		C
ANISOU	532	CB	PHE A	106	3655	4030	4539	−497	1061	−444	C
ATOM	533	CG	PHE A	106	−20.295	−6.618	33.342	1.00	38.54		C
ANISOU	533	CG	PHE A	106	4551	4619	5475	−542	1121	−441	C
ATOM	534	CD1	PHE A	106	−20.886	−7.256	32.262	1.00	38.88		C
ANISOU	534	CD1	PHE A	106	4321	4622	5830	−599	1051	−654	C
ATOM	535	CD2	PHE A	106	−19.694	−7.379	34.326	1.00	38.77		C
ANISOU	535	CD2	PHE A	106	4958	4451	5322	−525	1238	−236	C
ATOM	536	CE1	PHE A	106	−20.834	−8.640	32.144	1.00	42.56		C
ANISOU	536	CE1	PHE A	106	4868	4853	6451	−653	1125	−672	C
ATOM	537	CE2	PHE A	106	−19.654	−8.780	34.229	1.00	43.16		C
ANISOU	537	CE2	PHE A	106	5622	4751	6026	−564	1311	−223	C
ATOM	538	CZ	PHE A	106	−20.229	−9.405	33.136	1.00	44.62		C
ANISOU	538	CZ	PHE A	106	5506	4895	6553	−639	1274	−447	C
ATOM	539	N	HIS A	107	−21.624	−2.700	35.458	1.00	41.04		N
ANISOU	539	N	HIS A	107	4842	5228	5525	−607	1508	−410	N
ATOM	540	CA	HIS A	107	−21.315	−1.283	35.652	1.00	39.78		C
ANISOU	540	CA	HIS A	107	4676	5251	5186	−519	1398	−396	C
ATOM	541	C	HIS A	107	−19.800	−1.019	35.544	1.00	38.66		C
ANISOU	541	C	HIS A	107	4718	5256	4716	−365	1087	−264	C
ATOM	542	O	HIS A	107	−19.000	−1.639	36.229	1.00	36.62		O
ANISOU	542	O	HIS A	107	4762	4920	4231	−328	1071	−124	O
ATOM	543	CB	HIS A	107	−21.857	−0.791	37.005	1.00	45.04		C
ANISOU	543	CB	HIS A	107	5542	5817	5756	−613	1758	−366	C
ATOM	544	CG	HIS A	107	−23.304	−0.412	36.967	1.00	52.22		C
ANISOU	544	CG	HIS A	107	6133	6652	7055	−732	2030	−565	C
ATOM	545	ND1	HIS A	107	−24.039	−0.144	38.101	1.00	57.47		N
ANISOU	545	ND1	HIS A	107	6925	7179	7734	−858	2468	−595	N
ATOM	546	CD2	HIS A	107	−24.157	−0.270	35.923	1.00	53.31		C
ANISOU	546	CD2	HIS A	107	5824	6825	7608	−733	1914	−770	C
ATOM	547	CE1	HIS A	107	−25.278	0.164	37.756	1.00	59.47		C
ANISOU	547	CE1	HIS A	107	6762	7382	8452	−935	2631	−826	C
ATOM	548	NE2	HIS A	107	−25.382	0.071	36.445	1.00	58.49		N
ANISOU	548	NE2	HIS A	107	6283	7358	8582	−853	2266	−935	N
ATOM	549	O	MET A	108	−18.599	2.672	34.310	1.00	33.12		O
ANISOU	549	O	MET A	108	3728	5027	3831	−130	580	−335	O
ATOM	550	N	MET A	108	−19.427	−0.102	34.659	1.00	33.60		N
ANISOU	550	N	MET A	108	3887	4802	4079	−272	841	−320	N
ATOM	551	C	MET A	108	−18.015	1.814	34.977	1.00	34.87		C
ANISOU	551	C	MET A	108	4154	5185	3912	−137	608	−251	C
ATOM	552	CA	AMET A	108	−18.042	0.349	34.555	0.73	34.55		C
ANISOU	552	CA	AMET A	108	4112	5051	3964	−155	605	−240	C
ATOM	553	CB	AMET A	108	−17.519	0.142	33.130	0.73	33.13		C
ANISOU	553	CB	AMET A	108	3759	4971	3856	−84	382	−296	C
ATOM	554	CG	AMET A	108	−17.668	−1.320	32.722	0.73	35.17		C
ANISOU	554	CG	AMET A	108	4009	5115	4238	−109	396	−322	C
ATOM	555	SD	AMET A	108	−17.063	−1.780	31.097	0.73	41.12		S
ANISOU	555	SD	AMET A	108	4624	5959	5042	−33	182	−419	S
ATOM	556	CE	AMET A	108	−16.695	−3.545	31.344	0.73	39.78		C
ANISOU	556	CE	AMET A	108	4560	5588	4966	−54	243	−404	C
ATOM	557	CA	BMET A	108	−18.045	0.370	34.532	0.27	34.11		C
ANISOU	557	CA	BMET A	108	4051	4998	3911	−154	602	−242	C
ATOM	558	CB	BMET A	108	−17.529	0.269	33.093	0.27	32.64		C
ANISOU	558	CB	BMET A	108	3686	4922	3793	−82	376	−300	C
ATOM	559	CG	BMET A	108	−16.988	−1.085	32.705	0.27	33.74		C
ANISOU	559	CG	BMET A	108	3870	4991	3960	−57	312	−289	C
ATOM	560	SD	BMET A	108	−18.292	−2.298	32.503	0.27	36.80		S
ANISOU	560	SD	BMET A	108	4168	5202	4612	−172	475	−377	S
ATOM	561	CE	BMET A	108	−17.355	−3.671	31.842	0.27	39.03		C
ANISOU	561	CE	BMET A	108	4504	5420	4907	−106	344	−380	C
ATOM	562	O	SER A	109	−15.198	3.453	37.319	1.00	31.33		O
ANISOU	562	O	SER A	109	4228	4847	2831	9	300	−140	O
ATOM	563	N	SER A	109	−17.376	2.088	36.105	1.00	31.74		N
ANISOU	563	N	SER A	109	4006	4772	3280	−121	623	−177	N

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	564	CA	SER A	109	−17.480	3.418	36.689	1.00	32.08		C
ANISOU	564	CA	SER A	109	4079	4865	3245	−126	672	−215	C
ATOM	565	C	SER A	109	−16.148	4.084	36.863	1.00	33.21		C
ANISOU	565	C	SER A	109	4297	5103	3219	−47	444	−198	C
ATOM	566	CB	SER A	109	−18.167	3.348	38.071	1.00	34.28		C
ANISOU	566	CB	SER A	109	4614	5017	3394	−206	959	−201	C
ATOM	567	OG	SER A	109	−19.447	2.783	37.973	1.00	37.08		O
ANISOU	567	OG	SER A	109	4855	5256	3979	−309	1234	−253	O
ATOM	568	N	VAL A	110	−16.090	5.356	36.493	1.00	33.21		N
ANISOU	568	N	VAL A	110	4159	5179	3281	−40	403	−262	N
ATOM	569	CA	VAL A	110	−15.059	6.250	36.993	1.00	32.83		C
ANISOU	569	CA	VAL A	110	4187	5180	3109	−9	267	−291	C
ATOM	570	C	VAL A	110	−15.515	6.692	38.402	1.00	31.69		C
ANISOU	570	C	VAL A	110	4285	4970	2785	−45	411	−322	C
ATOM	571	O	VAL A	110	−16.566	7.332	38.524	1.00	31.03		O
ANISOU	571	O	VAL A	110	4148	4849	2795	−95	621	−378	O
ATOM	572	CB	VAL A	110	−14.891	7.481	36.132	1.00	31.93		C
ANISOU	572	CB	VAL A	110	3878	5121	3131	−7	224	−343	C
ATOM	573	CG1	VAL A	110	−13.708	8.297	36.685	1.00	30.11		C
ANISOU	573	CG1	VAL A	110	3700	4916	2825	0	88	−404	C
ATOM	574	CG2	VAL A	110	−14.666	7.099	34.658	1.00	32.57		C
ANISOU	574	CG2	VAL A	110	3786	5250	3340	19	149	−314	C
ATOM	575	O	VAL A	111	−16.511	8.389	41.679	1.00	32.39		O
ANISOU	575	O	VAL A	111	5032	4905	2370	−142	835	−507	O
ATOM	576	N	VAL A	111	−14.781	6.326	39.444	1.00	32.38		N
ANISOU	576	N	VAL A	111	4652	5031	2621	−9	298	−298	N
ATOM	577	C	VAL A	111	−15.453	7.977	41.167	1.00	35.58		C
ANISOU	577	C	VAL A	111	5362	5376	2779	−76	532	−451	C
ATOM	578	CA	VAL A	111	−15.310	6.506	40.807	1.00	33.76		C
ANISOU	578	CA	VAL A	111	5162	5121	2544	−46	476	−315	C
ATOM	579	CB	VAL A	111	−14.469	5.762	41.825	1.00	37.11		C
ANISOU	579	CB	VAL A	111	5969	5494	2637	32	282	−249	C
ATOM	580	CG1	VAL A	111	−14.921	6.093	43.267	1.00	40.92		C
ANISOU	580	CG1	VAL A	111	6892	5888	2768	−1	461	−276	C
ATOM	581	CG2	VAL A	111	−14.570	4.247	41.545	1.00	35.93		C
ANISOU	581	CG2	VAL A	111	5890	5260	2502	55	302	−102	C
ATOM	582	N	ARG A	112	−14.443	8.777	40.844	1.00	32.56		N
ANISOU	582	N	ARG A	112	4839	5070	2464	−38	281	−525	N
ATOM	583	CA	ARG A	112	−14.539	10.227	41.027	1.00	34.44		C
ANISOU	583	CA	ARG A	112	5013	5304	2769	−73	331	−662	C
ATOM	584	C	ARG A	112	−14.057	10.952	39.757	1.00	34.54		C
ANISOU	584	C	ARG A	112	4686	5362	3075	−74	227	−678	C
ATOM	585	O	ARG A	112	−12.860	11.079	39.525	1.00	35.15		O
ANISOU	585	O	ARG A	112	4680	5480	3194	−56	2	−715	O
ATOM	586	CB	ARG A	112	−13.717	10.687	42.248	1.00	37.82		C
ANISOU	586	CB	ARG A	112	5716	5724	2930	−51	151	−779	C
ATOM	587	CG	ARG A	112	−14.139	10.079	43.565	1.00	46.73		C
ANISOU	587	CG	ARG A	112	7297	6785	3674	−43	262	−755	C
ATOM	588	CD	ARG A	112	−13.240	10.515	44.766	1.00	45.63		C
ANISOU	588	CD	ARG A	112	7488	6640	3209	10	−9	−890	C
ATOM	589	NE	ARG A	112	−13.762	9.942	46.011	1.00	55.86		N
ANISOU	589	NE	ARG A	112	9318	7846	4060	17	150	−844	N
ATOM	590	CZ	ARG A	112	−14.514	10.599	46.896	1.00	60.76		C
ANISOU	590	CZ	ARG A	112	10157	8401	4527	−45	436	−941	C
ATOM	591	NH1	ARG A	112	−14.833	11.875	46.696	1.00	60.00		N
ANISOU	591	NH1	ARG A	112	9880	8312	4606	−109	574	−1126	N
ATOM	592	NH2	ARG A	112	−14.941	9.983	47.992	1.00	67.02		N
ANISOU	592	NH2	ARG A	112	11291	9100	5072	−41	584	−843	N
ATOM	593	N	ALA A	113	−14.986	11.437	38.942	1.00	30.42		N
ANISOU	593	N	ALA A	113	3981	4812	2766	−90	393	−658	N
ATOM	594	CA	ALA A	113	−14.627	11.937	37.609	1.00	26.49		C
ANISOU	594	CA	ALA A	113	3251	4331	2482	−80	317	−622	C
ATOM	595	C	ALA A	113	−13.811	13.207	37.688	1.00	29.11		C
ANISOU	595	C	ALA A	113	3553	4625	2884	−112	252	−720	C
ATOM	596	O	ALA A	113	−14.085	14.072	38.505	1.00	33.62		O
ANISOU	596	O	ALA A	113	4215	5132	3428	−135	322	−829	O
ATOM	597	CB	ALA A	113	−15.876	12.171	36.792	1.00	30.39		C
ANISOU	597	CB	ALA A	113	3611	4780	3156	−54	448	−583	C
ATOM	598	CD	ARG A	114	−8.699	12.801	38.038	1.00	45.78		C
ANISOU	598	CD	ARG A	114	5351	6839	5205	−155	−473	−1057	C
ATOM	599	NE	ARG A	114	−8.314	12.206	39.314	1.00	53.81		N
ANISOU	599	NE	ARG A	114	6543	7886	6017	−71	−746	−1141	N
ATOM	600	CZ	ARG A	114	−7.175	11.557	39.538	1.00	58.39		C
ANISOU	600	CZ	ARG A	114	7026	8491	6667	−2	−1035	−1235	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	601	NH1	ARG A	114	−6.287	11.407	38.555	1.00	55.66		N
ANISOU	601	NH1	ARG A	114	6362	8150	6635	−30	−1029	−1279	N
ATOM	602	NH2	ARG A	114	−6.925	11.071	40.752	1.00	59.80		N
ANISOU	602	NH2	ARG A	114	7445	8674	6602	105	−1327	−1294	N
ATOM	603	N	ARG A	114	−12.758	13.277	36.876	1.00	30.88		N
ANISOU	603	N	ARG A	114	3651	4871	3209	−129	144	−703	N
ATOM	604	CA	ARG A	114	−11.941	14.474	36.732	1.00	32.62		C
ANISOU	604	CA	ARG A	114	3799	5021	3572	−192	129	−797	C
ATOM	605	C	ARG A	114	−12.187	15.053	35.347	1.00	30.47		C
ANISOU	605	C	ARG A	114	3444	4678	3455	−198	246	−688	C
ATOM	606	O	ARG A	114	−12.519	14.310	34.425	1.00	32.29		O
ANISOU	606	O	ARG A	114	3649	4958	3663	−152	256	−566	O
ATOM	607	CB	ARG A	114	−10.439	14.159	36.875	1.00	34.69		C
ANISOU	607	CB	ARG A	114	3969	5328	3885	−225	−45	−894	C
ATOM	608	CG	ARG A	114	−10.057	13.492	38.183	1.00	39.36		C
ANISOU	608	CG	ARG A	114	4690	5977	4288	−177	−254	−988	C
ATOM	609	N	ARG A	115	−12.018	16.363	35.192	1.00	32.26		N
ANISOU	609	N	ARG A	115	3667	4770	3819	−249	325	−734	N
ATOM	610	C	ARG A	115	−11.336	16.174	32.824	1.00	36.23		C
ANISOU	610	C	ARG A	115	4126	5234	4406	−273	442	−525	C
ATOM	611	O	ARG A	115	−11.831	15.953	31.714	1.00	33.03		O
ANISOU	611	O	ARG A	115	3793	4818	3939	−214	480	−380	O
ATOM	612	CA	ARG A	115	−12.139	16.972	33.872	1.00	33.33		C
ANISOU	612	CA	ARG A	115	3809	4797	4056	−247	432	−605	C
ATOM	613	CB	ARG A	115	−11.680	18.437	33.886	1.00	34.75		C
ANISOU	613	CB	ARG A	115	4010	4786	4408	−333	536	−672	C
ATOM	614	CG	ARG A	115	−12.572	19.384	34.677	1.00	37.98		C
ANISOU	614	CG	ARG A	115	4485	5081	4866	−293	564	−749	C
ATOM	615	CD	ARG A	115	−14.011	19.486	34.099	1.00	35.98		C
ANISOU	615	CD	ARG A	115	4289	4770	4613	−147	581	−615	C
ATOM	616	NE	ARG A	115	−14.013	19.699	32.657	1.00	33.90		N
ANISOU	616	NE	ARG A	115	4106	4414	4363	−104	601	−427	N
ATOM	617	CZ	ARG A	115	−13.806	20.873	32.063	1.00	34.28		C
ANISOU	617	CZ	ARG A	115	4271	4234	4519	−123	695	−359	C
ATOM	618	NH1	ARG A	115	−13.591	21.975	32.769	1.00	34.88		N
ANISOU	618	NH1	ARG A	115	4351	4147	4755	−190	777	−483	N
ATOM	619	NH2	ARG A	115	−13.829	20.949	30.751	1.00	38.97		N
ANISOU	619	NH2	ARG A	115	5021	4741	5044	−72	713	−165	N
ATOM	620	N	ASP A	116	−10.117	15.720	33.153	1.00	26.58		N
ANISOU	620	N	ASP A	116	2781	4076	3242	−345	394	−638	N
ATOM	621	CA	ASP A	116	−9.325	15.073	32.133	1.00	31.95		C
ANISOU	621	CA	ASP A	116	3391	4792	3957	−376	461	−597	C
ATOM	622	C	ASP A	116	−9.781	13.654	31.856	1.00	33.78		C
ANISOU	622	C	ASP A	116	3635	5166	4035	−277	367	−518	C
ATOM	623	O	ASP A	116	−9.182	12.990	31.032	1.00	35.83		O
ANISOU	623	O	ASP A	116	3844	5461	4309	−288	423	−502	O
ATOM	624	CB	ASP A	116	−7.823	15.076	32.491	1.00	40.25		C
ANISOU	624	CB	ASP A	116	4236	5838	5220	−479	444	−785	C
ATOM	625	CG	ASP A	116	−7.576	14.572	33.906	1.00	52.12		C
ANISOU	625	CG	ASP A	116	5673	7435	6693	−429	176	−934	C
ATOM	626	OD1	ASP A	116	−7.538	15.407	34.824	1.00	60.35		O
ANISOU	626	OD1	ASP A	116	6735	8420	7777	−465	107	−1058	O
ATOM	627	OD2	ASP A	116	−7.470	13.350	34.106	1.00	56.75		O
ANISOU	627	OD2	ASP A	116	6236	8135	7189	−343	29	−923	O
ATOM	628	N	ASP A	117	−10.848	13.181	32.497	1.00	31.31		N
ANISOU	628	N	ASP A	117	3388	4911	3596	−192	265	−483	N
ATOM	629	CA	ASP A	117	−11.400	11.886	32.101	1.00	29.12		C
ANISOU	629	CA	ASP A	117	3125	4727	3212	−116	210	−408	C
ATOM	630	C	ASP A	117	−12.318	11.994	30.876	1.00	33.46		C
ANISOU	630	C	ASP A	117	3755	5245	3713	−63	260	−291	C
ATOM	631	O	ASP A	117	−12.712	10.976	30.321	1.00	32.02		O
ANISOU	631	O	ASP A	117	3575	5126	3465	−11	212	−254	O
ATOM	632	CB	ASP A	117	−12.208	11.248	33.214	1.00	26.65		C
ANISOU	632	CB	ASP A	117	2858	4458	2810	−69	133	−423	C
ATOM	633	CG	ASP A	117	−11.366	10.735	34.351	1.00	31.91		C
ANISOU	633	CG	ASP A	117	3529	5162	3433	−74	12	−511	C
ATOM	634	OD1	ASP A	117	−10.331	10.057	34.115	1.00	30.96		O
ANISOU	634	OD1	ASP A	117	3322	5080	3363	−66	−73	−545	O
ATOM	635	OD2	ASP A	117	−11.774	11.000	35.513	1.00	32.13		O
ANISOU	635	OD2	ASP A	117	3668	5171	3369	−72	−7	−557	O
ATOM	636	N	SER A	118	−12.708	13.210	30.495	1.00	31.63		N
ANISOU	636	N	SER A	118	3606	4899	3513	−59	321	−242	N
ATOM	637	CA	SER A	118	−13.559	13.367	29.316	1.00	29.70		C
ANISOU	637	CA	SER A	118	3482	4605	3200	30	294	−130	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	638	C	SER A	118	−12.893	12.718	28.096	1.00	30.75		C
ANISOU	638	C	SER A	118	3693	4774	3216	17	343	−80	C
ATOM	639	O	SER A	118	−11.706	12.912	27.844	1.00	34.08		O
ANISOU	639	O	SER A	118	4114	5169	3665	−83	497	−102	O
ATOM	640	CB	SER A	118	−13.838	14.831	29.007	1.00	27.79		C
ANISOU	640	CB	SER A	118	3367	4188	3003	50	346	−65	C
ATOM	641	OG	SER A	118	−14.514	15.469	30.040	1.00	34.25		O
ANISOU	641	OG	SER A	118	4118	4955	3942	73	323	−133	O
ATOM	642	N	GLY A	119	−13.659	11.936	27.362	1.00	29.88		N
ANISOU	642	N	GLY A	119	3635	4716	3000	109	226	−46	N
ATOM	643	CA	GLY A	119	−13.121	11.261	26.199	1.00	32.11		C
ANISOU	643	CA	GLY A	119	4030	5034	3137	105	276	−24	C
ATOM	644	C	GLY A	119	−13.982	10.127	25.708	1.00	33.96		C
ANISOU	644	C	GLY A	119	4259	5350	3295	198	101	−52	C
ATOM	645	O	GLY A	119	−15.163	10.001	26.056	1.00	32.98		O
ANISOU	645	O	GLY A	119	4053	5230	3247	275	−65	−76	O
ATOM	646	N	THR A	120	−13.345	9.252	24.949	1.00	34.08		N
ANISOU	646	N	THR A	120	4327	5419	3203	177	162	−85	N
ATOM	647	CA	THR A	120	−14.018	8.170	24.270	1.00	34.03		C
ANISOU	647	CA	THR A	120	4350	5470	3109	252	7	−136	C
ATOM	648	C	THR A	120	−13.763	6.833	24.941	1.00	33.41		C
ANISOU	648	C	THR A	120	4063	5471	3160	214	5	−239	C
ATOM	649	O	THR A	120	−12.618	6.521	25.251	1.00	31.96		O
ANISOU	649	O	THR A	120	3802	5306	3034	147	148	−274	O
ATOM	650	CB	THR A	120	−13.526	8.140	22.829	1.00	36.48		C
ANISOU	650	CB	THR A	120	4941	5757	3162	266	93	−111	C
ATOM	651	OG1	THR A	120	−13.789	9.425	22.269	1.00	40.75		O
ANISOU	651	OG1	THR A	120	5743	6183	3558	312	91	20	O
ATOM	652	CG2	THR A	120	−14.193	7.034	22.024	1.00	37.74		C
ANISOU	652	CG2	THR A	120	5166	5972	3203	348	−95	−199	C
ATOM	653	N	TYR A	121	−14.811	6.041	25.156	1.00	30.08		N
ANISOU	653	N	TYR A	121	3544	5069	2816	260	−156	−297	N
ATOM	654	CA	TYR A	121	−14.681	4.788	25.921	1.00	31.48		C
ANISOU	654	CA	TYR A	121	3565	5273	3125	222	−143	−366	C
ATOM	655	C	TYR A	121	−15.399	3.651	25.236	1.00	34.73		C
ANISOU	655	C	TYR A	121	3963	5686	3546	257	−263	−463	C
ATOM	656	O	TYR A	121	−16.335	3.882	24.477	1.00	35.79		O
ANISOU	656	O	TYR A	121	4151	5811	3638	321	−422	−498	O
ATOM	657	CB	TYR A	121	−15.259	4.917	27.338	1.00	27.88		C
ANISOU	657	CB	TYR A	121	2984	4790	2820	193	−137	−350	C
ATOM	658	CG	TYR A	121	−14.530	5.881	28.248	1.00	31.05		C
ANISOU	658	CG	TYR A	121	3388	5185	3225	152	−45	−296	C
ATOM	659	CD1	TYR A	121	−14.680	7.250	28.116	1.00	30.61		C
ANISOU	659	CD1	TYR A	121	3388	5096	3146	160	−27	−248	C
ATOM	660	CD2	TYR A	121	−13.652	5.403	29.227	1.00	30.66		C
ANISOU	660	CD2	TYR A	121	3300	5142	3207	119	−7	−306	C
ATOM	661	CE1	TYR A	121	−13.969	8.141	28.981	1.00	31.39		C
ANISOU	661	CE1	TYR A	121	3478	5174	3275	108	55	−235	C
ATOM	662	CE2	TYR A	121	−12.963	6.259	30.074	1.00	31.36		C
ANISOU	662	CE2	TYR A	121	3385	5224	3306	87	25	−298	C
ATOM	663	CZ	TYR A	121	−13.115	7.627	29.946	1.00	33.17		C
ANISOU	663	CZ	TYR A	121	3645	5426	3532	69	69	−274	C
ATOM	664	OH	TYR A	121	−12.391	8.481	30.783	1.00	30.39		O
ANISOU	664	OH	TYR A	121	3278	5052	3214	24	95	−302	O
ATOM	665	N	LEU A	122	−15.008	2.416	25.547	1.00	33.30		N
ANISOU	665	N	LEU A	122	3708	5497	3447	227	−221	−522	N
ATOM	666	CA	LEU A	122	−15.722	1.266	24.992	1.00	33.83		C
ANISOU	666	CA	LEU A	122	3743	5537	3572	241	−324	−642	C
ATOM	667	C	LEU A	122	−15.420	0.064	25.855	1.00	34.53		C
ANISOU	667	C	LEU A	122	3743	5563	3814	197	−249	−660	C
ATOM	668	O	LEU A	122	−14.543	0.116	26.716	1.00	34.68		O
ANISOU	668	O	LEU A	122	3756	5574	3846	186	−160	−584	O
ATOM	669	CB	LEU A	122	−15.329	0.991	23.507	1.00	31.64		C
ANISOU	669	CB	LEU A	122	3627	5294	3100	286	−363	−725	C
ATOM	670	CG	LEU A	122	−13.854	0.666	23.152	1.00	35.53		C
ANISOU	670	CG	LEU A	122	4187	5803	3509	270	−175	−739	C
ATOM	671	CD1	LEU A	122	−13.530	−0.773	23.469	1.00	39.44		C
ANISOU	671	CD1	LEU A	122	4571	6245	4168	260	−149	−835	C
ATOM	672	CD2	LEU A	122	−13.542	0.895	21.632	1.00	38.46		C
ANISOU	672	CD2	LEU A	122	4809	6201	3602	303	−138	−795	C
ATOM	673	N	CYS A	123	−16.177	−1.000	25.631	1.00	36.76		N
ANISOU	673	N	CYS A	123	3967	5779	4221	180	−308	−769	N
ATOM	674	C	CYS A	123	−15.651	−3.318	25.200	1.00	38.24		C
ANISOU	674	C	CYS A	123	4149	5830	4549	170	−277	−932	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	675	O	CYS A	123	−16.195	−3.249	24.091	1.00	39.11		O
ANISOU	675	O	CYS A	123	4285	5985	4590	190	−397	−1057	O
ATOM	676	CA	ACYS A	123	−16.015	−2.293	26.278	0.37	37.02		C
ANISOU	676	CA	ACYS A	123	3963	5699	4404	142	−236	−787	C
ATOM	677	CB	ACYS A	123	−17.318	−2.658	27.004	0.37	36.61		C
ANISOU	677	CB	ACYS A	123	3809	5537	4563	63	−203	−812	C
ATOM	678	SG	ACYS A	123	−17.513	−4.322	27.676	0.37	53.19		S
ANISOU	678	SG	ACYS A	123	5910	7424	6875	−13	−82	−838	S
ATOM	679	CA	BCYS A	123	−15.830	−2.261	26.262	0.63	37.27		C
ANISOU	679	CA	BCYS A	123	4006	5739	4416	149	−230	−779	C
ATOM	680	CB	BCYS A	123	−16.860	−2.692	27.308	0.63	37.76		C
ANISOU	680	CB	BCYS A	123	3996	5681	4672	71	−165	−760	C
ATOM	681	SG	BCYS A	123	−18.515	−3.004	26.705	0.63	35.46		S
ANISOU	681	SG	BCYS A	123	3540	5331	4604	16	−255	−945	S
ATOM	682	N	GLY A	124	−14.776	−4.266	25.514	1.00	37.42		N
ANISOU	682	N	GLY A	124	4060	5645	4513	187	−203	−930	N
ATOM	683	CA	GLY A	124	−14.397	−5.246	24.534	1.00	36.38		C
ANISOU	683	CA	GLY A	124	3954	5473	4396	217	−212	−1090	C
ATOM	684	C	GLY A	124	−14.460	−6.623	25.131	1.00	37.42		C
ANISOU	684	C	GLY A	124	4059	5412	4748	199	−176	−1114	C
ATOM	685	O	GLY A	124	−14.205	−6.808	26.332	1.00	35.35		O
ANISOU	685	O	GLV A	124	3817	5055	4561	202	−124	−966	O
ATOM	686	N	ALA A	125	−14.842	−7.564	24.281	1.00	38.76		N
ANISOU	686	N	ALA A	125	4222	5506	5000	183	−214	−1303	N
ATOM	687	CA	ALA A	125	−14.786	−8.987	24.558	1.00	41.58		C
ANISOU	687	CA	ALA A	125	4575	5643	5579	172	−167	−1364	C
ATOM	688	C	ALA A	125	−13.855	−9.645	23.550	1.00	42.84		C
ANISOU	688	C	ALA A	125	4770	5794	5714	251	−151	−1537	C
ATOM	689	O	ALA A	125	−13.607	−9.107	22.475	1.00	44.02		O
ANISOU	689	O	ALA A	125	4968	6099	5661	278	−169	−1650	O
ATOM	690	CB	ALA A	125	−16.163	−9.611	24.469	1.00	38.43		C
ANISOU	690	CB	ALA A	125	4104	5116	5381	56	−198	−1490	C
ATOM	691	N	ILE A	126	−13.410	−10.846	23.867	1.00	42.53		N
ANISOU	691	N	ILE A	126	4736	5545	5878	287	−102	−1569	N
ATOM	692	CA	ILE A	126	−12.572	−11.585	22.954	1.00	43.11		C
ANISOU	692	CA	ILE A	126	4820	5572	5986	365	−59	−1769	C
ATOM	693	C	ILE A	126	−13.172	−12.966	22.678	1.00	49.76		C
ANISOU	693	C	ILE A	126	5671	6179	7058	318	−67	−1946	C
ATOM	694	O	ILE A	126	−13.793	−13.568	23.550	1.00	51.93		O
ANISOU	694	O	ILE A	126	5947	6249	7534	254	−54	−1847	O
ATOM	695	CB	ILE A	126	−11.154	−11.691	23.537	1.00	40.17		C
ANISOU	695	CB	ILE A	126	4410	5150	5702	499	−3	−1677	C
ATOM	696	CG1	ILE A	126	−10.201	−12.425	22.605	1.00	39.61		C
ANISOU	696	CG1	ILE A	126	4307	5019	5723	589	88	−1914	C
ATOM	697	CG2	ILE A	126	−11.171	−12.364	24.888	1.00	40.17		C
ANISOU	697	CG2	ILE A	126	4449	4920	5893	536	−48	−1486	C
ATOM	698	CD1	ILE A	126	−8.743	−12.233	23.089	1.00	40.14		C
ANISOU	698	CD1	ILE A	126	4255	5080	5916	731	126	−1863	C
ATOM	699	O	SER A	127	−11.610	−14.784	19.717	1.00	48.68		O
ANISOU	699	O	SER A	127	5634	5942	6922	469	100	−2684	O
ATOM	700	N	SER A	127	−13.017	−13.466	21.456	1.00	48.94		N
ANISOU	700	N	SER A	127	5596	6082	6918	335	−63	−2221	N
ATOM	701	CA	SER A	127	−13.480	−14.813	21.156	1.00	48.02		C
ANISOU	701	CA	SER A	127	5480	5719	7048	292	−70	−2429	C
ATOM	702	C	SER A	127	−12.411	−15.475	20.345	1.00	46.45		C
ANISOU	702	C	SER A	127	5317	5464	6866	402	25	−2641	C
ATOM	703	CB	SER A	127	−14.814	−14.817	20.392	1.00	52.12		C
ANISOU	703	CB	SER A	127	5987	6280	7537	167	−213	−2643	C
ATOM	704	OG	SER A	127	−15.130	−16.132	19.910	1.00	55.10		O
ANISOU	704	OG	SER A	127	6359	6419	8158	122	−220	−2915	O
ATOM	705	O	LEU A	128	−11.302	−18.686	17.482	1.00	56.68		O
ANISOU	705	O	LEU A	128	6761	6307	8470	526	255	−3664	O
ATOM	706	N	LEU A	128	−12.389	−16.807	20.365	1.00	45.63		N
ANISOU	706	N	LEU A	128	5210	5071	7057	413	59	−2781	N
ATOM	707	CA	LEU A	128	−11.432	−17.574	19.587	1.00	50.69		C
ANISOU	707	CA	LEU A	128	5868	5615	7777	522	168	−3030	C
ATOM	708	C	LEU A	128	−12.022	−18.091	18.290	1.00	54.19		C
ANISOU	708	C	LEU A	128	6397	6055	8137	450	135	−3403	C
ATOM	709	CB	LEU A	128	−10.913	−18.771	20.383	1.00	55.08		C
ANISOU	709	CB	LEU A	128	6391	5812	8727	618	211	−2972	C
ATOM	710	CG	LEU A	128	−10.604	−18.636	21.865	1.00	57.74		C
ANISOU	710	CG	LEU A	128	6718	6035	9187	691	167	−2603	C
ATOM	711	CD1	LEU A	128	−9.963	−19.929	22.338	1.00	59.13		C
ANISOU	711	CD1	LEU A	128	6919	5825	9723	835	181	−2606	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	712	CD2	LEU A	128	−9.691	−17.450	22.101	1.00	59.48		C
ANISOU	712	CD2	LEU A	128	6863	6526	9212	787	163	−2454	C
ATOM	713	O	ALA A	129	−15.233	−16.529	16.493	1.00	56.84		O
ANISOU	713	O	ALA A	129	6879	6854	7862	176	−454	−3736	O
ATOM	714	N	ALA A	129	−13.328	−17.916	18.091	1.00	52.57		N
ANISOU	714	N	ALA A	129	6204	5899	7872	310	−34	−3465	N
ATOM	715	CA	ALA A	129	−13.937	−18.518	16.910	1.00	55.45		C
ANISOU	715	CA	ALA A	129	6650	6228	8191	251	−137	−3858	C
ATOM	716	C	ALA A	129	−14.595	−17.469	16.007	1.00	55.57		C
ANISOU	716	C	ALA A	129	6784	6547	7783	220	−332	−3951	C
ATOM	717	CB	ALA A	129	−14.932	−19.588	17.318	1.00	55.07		C
ANISOU	717	CB	ALA A	129	6492	5871	8559	121	−210	−3968	C
ATOM	718	O	PRO A	130	−11.448	−19.471	13.748	1.00	62.27		O
ANISOU	718	O	PRO A	130	7964	7184	8513	475	311	−4479	O
ATOM	719	N	PRO A	130	−14.426	−17.619	14.683	1.00	56.85		N
ANISOU	719	N	PRO A	130	7155	6795	7652	256	−360	−4231	N
ATOM	720	CA	PRO A	130	−13.710	−18.721	14.014	1.00	60.20		C
ANISOU	720	CA	PRO A	130	7668	7059	8147	298	−191	−4422	C
ATOM	721	C	PRO A	130	−12.193	−18.547	14.088	1.00	58.25		C
ANISOU	721	C	PRO A	130	7443	6837	7850	421	133	−4347	C
ATOM	722	CB	PRO A	130	−14.202	−18.630	12.563	1.00	62.12		C
ANISOU	722	CB	PRO A	130	8186	7438	7979	280	−352	−4607	C
ATOM	723	CG	PRO A	130	−14.444	−17.171	12.361	1.00	60.39		C
ANISOU	723	CG	PRO A	130	8108	7501	7338	301	−469	−4433	C
ATOM	724	CD	PRO A	130	−14.910	−16.613	13.719	1.00	59.38		C
ANISOU	724	CD	PRO A	130	7693	7383	7484	264	−550	−4223	C
ATOM	725	O	LYS A	131	−11.300	−15.554	16.330	1.00	59.86		O
ANISOU	725	O	LYS A	131	7402	7459	7883	486	240	−3482	O
ATOM	726	N	LYS A	131	−11.759	−17.368	14.537	1.00	57.89		N
ANISOU	726	N	LYS A	131	7376	6989	7632	462	205	−4141	N
ATOM	727	CA	LYS A	131	−10.335	−17.076	14.762	1.00	59.58		C
ANISOU	727	CA	LYS A	131	7524	7230	7883	567	506	−4047	C
ATOM	728	C	LYS A	131	−10.259	−16.071	15.913	1.00	57.87		C
ANISOU	728	C	LYS A	131	7154	7128	7704	567	460	−3648	C
ATOM	729	CB	LYS A	131	−9.665	−16.538	13.480	1.00	62.67		C
ANISOU	729	CB	LYS A	131	8177	7795	7840	575	718	−4113	C
ATOM	730	CG	LYS A	131	−10.155	−15.149	13.018	1.00	61.10		C
ANISOU	730	CG	LYS A	131	8212	7865	7140	528	629	−3979	C
ATOM	731	CD	LYS A	131	−9.798	−14.887	11.540	1.00	63.14		C
ANISOU	731	CD	LYS A	131	8875	8197	6919	527	799	−4074	C
ATOM	732	O	VAL A	132	−8.961	−12.998	16.012	1.00	52.94		O
ANISOU	732	O	VAL A	132	6589	7007	6520	574	743	−3200	O
ATOM	733	N	VAL A	132	−9.069	−15.798	16.456	1.00	51.31		N
ANISOU	733	N	VAL A	132	6178	6296	7022	656	649	−3513	N
ATOM	734	CA	VAL A	132	−8.993	−14.830	17.559	1.00	51.06		C
ANISOU	734	CA	VAL A	132	6020	6371	7009	655	576	−3157	C
ATOM	735	C	VAL A	132	−9.424	−13.453	17.057	1.00	50.05		C
ANISOU	735	C	VAL A	132	6051	6520	6445	577	556	−3058	C
ATOM	736	CB	VAL A	132	−7.577	−14.722	18.174	1.00	50.08		C
ANISOU	736	CB	VAL A	132	5689	6201	7139	777	736	−3080	C
ATOM	737	CG1	VAL A	132	−7.606	−13.755	19.261	1.00	44.23		C
ANISOU	737	CG1	VAL A	132	4857	5567	6383	767	618	−2756	C
ATOM	738	CG2	VAL A	132	−7.112	−16.054	18.714	1.00	52.93		C
ANISOU	738	CG2	VAL A	132	5912	6257	7942	899	707	−3155	C
ATOM	739	O	GLN A	133	−11.827	−11.260	19.557	1.00	42.56		O
ANISOU	739	O	GLN A	133	4962	5790	5419	412	48	−2311	O
ATOM	740	N	GLN A	133	−10.306	−12.793	17.797	1.00	50.48		N
ANISOU	740	N	GLN A	133	6077	6651	6454	518	353	−2816	N
ATOM	741	CA	GLN A	133	−10.848	−11.494	17.401	1.00	51.28		C
ANISOU	741	CA	GLN A	133	6326	6977	6182	465	281	−2707	C
ATOM	742	C	GLN A	133	−11.280	−10.702	18.625	1.00	45.41		C
ANISOU	742	C	GLN A	133	5448	6283	5522	435	159	−2398	C
ATOM	743	CB	GLN A	133	−12.049	−11.658	16.444	1.00	56.21		C
ANISOU	743	CB	GLN A	133	7142	7636	6579	419	64	−2896	C
ATOM	744	CG	GLN A	133	−13.107	−12.636	16.960	1.00	60.12		C
ANISOU	744	CG	GLN A	133	7489	7958	7396	364	−146	−2967	C
ATOM	745	CD	GLN A	133	−14.469	−12.447	16.306	1.00	64.69		C
ANISOU	74b	CD	GLN A	133	81bb	8b99	782b	314	−446	−3111	C
ATOM	746	OE1	GLN A	133	−14.932	−11.313	16.133	1.00	66.19		O
ANISOU	746	OE1	GLN A	133	8431	8960	7759	323	−582	−2992	O
ATOM	747	NE2	GLN A	133	−15.126	−13.562	15.948	1.00	63.73		N
ANISOU	747	NE2	GLN A	133	7997	8317	7901	269	−577	−3387	N
ATOM	748	O	ILE a	134	−13.112	−7.866	17.928	1.00	50.86		O
ANISOU	748	O	ILE A	134	6434	7355	5534	367	−170	−2151	O

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	749	N	ILE A	134	−10.992	−9.410	18.645	1.00	45.08		N
ANISOU	749	N	ILE A	134	5455	6410	5265	428	217	−2237	N
ATOM	750	CA	ILE A	134	−11.589	−8.546	19.648	1.00	44.28		C
ANISOU	750	CA	ILE A	134	5271	6370	5185	393	87	−1984	C
ATOM	751	C	ILE A	134	−12.957	−8.130	19.126	1.00	46.76		C
ANISOU	751	C	ILE A	134	5698	6757	5313	350	−133	−2017	C
ATOM	752	CB	ILE A	134	−10.754	−7.328	19.923	1.00	40.89		C
ANISOU	752	CB	ILE A	134	4828	6059	4649	400	224	−1820	C
ATOM	753	CG1	ILE A	134	−9.348	−7.767	20.348	1.00	43.21		C
ANISOU	753	CG1	ILE A	134	4956	6274	5189	459	402	−1854	C
ATOM	754	CG2	ILE A	134	−11.402	−6.433	21.016	1.00	36.69		C
ANISOU	754	CG2	ILE A	134	4220	5578	4141	366	91	−1580	C
ATOM	755	CD1	ILE A	134	−9.316	−8.758	21.521	1.00	40.56		C
ANISOU	755	CD1	ILE A	134	4460	5766	5184	514	282	−1793	C
ATOM	756	N	LYS A	135	−13.956	−8.112	19.997	1.00	44.24		N
ANISOU	756	N	LYS A	135	5244	6392	5174	302	−283	−1916	N
ATOM	757	CA	LYS A	135	−15.235	−7.512	19.616	1.00	43.24		C
ANISOU	757	CA	LYS A	135	5150	6337	4943	280	−513	−1948	C
ATOM	758	C	LYS A	135	−15.394	−6.245	20.420	1.00	39.05		C
ANISOU	758	C	LYS A	135	4567	5897	4375	274	−510	−1704	C
ATOM	759	O	LYS A	135	−15.603	−6.312	21.639	1.00	39.58		O
ANISOU	759	O	LYS A	135	4476	5893	4668	228	−460	−1570	O
ATOM	760	CB	LYS A	135	−16.413	−8.467	19.857	1.00	47.69		C
ANISOU	760	CB	LYS A	135	5555	6755	5809	211	−663	−2097	C
ATOM	761	CG	LYS A	135	−16.470	−9.670	18.898	1.00	52.49		C
ANISOU	761	CG	LYS A	135	6226	7265	6453	210	−723	−2397	C
ATOM	762	CD	LYS A	135	−17.638	−10.592	19.225	1.00	56.02		C
ANISOU	762	CD	LYS A	135	6474	7533	7277	110	−842	−2557	C
ATOM	763	N	GLU A	136	−15.268	−5.097	19.758	1.00	35.71		N
ANISOU	763	N	GLU A	136	4315	5604	3648	321	−542	−1643	N
ATOM	764	C	GLU A	136	−16.836	−3.422	20.476	1.00	35.76		C
ANISOU	764	C	GLU A	136	4211	5679	3699	328	−791	−1458	C
ATOM	765	O	GLU A	136	−17.523	−3.626	19.487	1.00	36.05		O
ANISOU	765	O	GLU A	136	4339	5722	3638	375	−1018	−1629	O
ATOM	766	CG	GLU A	136	−13.022	−2.978	19.626	1.00	47.50		C
ANISOU	766	CG	GLU A	136	6035	7254	4759	340	−111	−1346	C
ATOM	767	CD	GLU A	136	−12.323	−1.796	18.915	1.00	50.24		C
ANISOU	767	CD	GLU A	136	6617	7659	4811	339	69	−1261	C
ATOM	768	OE1	GLU A	136	−13.023	−1.028	18.212	1.00	51.42		O
ANISOU	768	OE1	GLU A	136	7008	7840	4688	379	−73	−1216	O
ATOM	769	OE2	GLU A	136	−11.084	−1.617	19.056	1.00	46.12		O
ANISOU	769	OE2	GLU A	136	6042	7130	4352	302	350	−1244	O
ATOM	770	CA	GLU A	136	−15.370	−3.823	20.467	1.00	32.90		C
ANISOU	770	CA	GLU A	136	3922	5315	3262	319	−530	−1425	C
ATOM	771	CB	GLU A	136	−14.548	−2.728	19.798	1.00	36.80		C
ANISOU	771	CB	GLU A	136	4642	5903	3439	355	−411	−1331	C
ATOM	772	N	SER A	137	−17.314	−2.834	21.561	1.00	34.32		N
ANISOU	772	N	SER A	137	3863	5483	3694	294	−772	−1323	N
ATOM	773	CA	SER A	137	−18.638	−2.222	21.521	1.00	38.59		C
ANISOU	773	CA	SER A	137	4305	6025	4334	321	−999	−1366	C
ATOM	774	C	SER A	137	−18.560	−0.969	20.651	1.00	40.09		C
ANISOU	774	C	SER A	137	4731	6301	4199	432	−1135	−1291	C
ATOM	775	O	SER A	137	−17.484	−0.502	20.322	1.00	38.35		O
ANISOU	775	O	SER A	137	4726	6132	3715	445	−971	−1176	O
ATOM	776	CB	SER A	137	−19.102	−1.851	22.919	1.00	36.52		C
ANISOU	776	CB	SER A	137	3832	5714	4331	253	−877	−1250	C
ATOM	777	OG	SER A	137	−18.306	−0.795	23.461	1.00	32.93		O
ANISOU	777	OG	SER A	137	3470	5322	3720	268	−732	−1043	O
ATOM	778	N	LEU A	138	−19.698	−0.397	20.310	1.00	37.05		N
ANISOU	778	N	LEU A	138	4306	5910	3863	513	−1424	−1356	N
ATOM	779	CA	LEU A	138	−19.717	0.977	19.829	1.00	40.16		C
ANISOU	779	CA	LEU A	138	4919	6338	4000	628	−1541	−1220	C
ATOM	780	C	LEU A	138	−19.149	1.894	20.899	1.00	40.98		C
ANISOU	780	C	LEU A	138	4966	6448	4158	572	−1274	−999	C
ATOM	781	O	LEU A	138	−19.180	1.586	22.119	1.00	41.48		O
ANISOU	781	O	LEU A	138	4779	6486	4496	471	−1096	−975	O
ATOM	782	CB	LEU A	138	−21.136	1.413	19.436	1.00	45.42		C
ANISOU	782	CB	LEU A	138	5489	6966	4802	756	−1952	−1345	C
ATOM	783	CG	LEU A	138	−21.800	0.509	18.404	1.00	46.57		C
ANISOU	783	CG	LEU A	138	5667	7073	4955	804	−2246	−1583	C
ATOM	784	CD1	LEU A	138	−23.325	0.761	18.372	1.00	51.66		C
ANISOU	784	CD1	LEU A	138	6055	7602	5970	875	−2531	−1696	C
ATOM	785	CD2	LEU A	138	−21.176	0.757	17.058	1.00	48.44		C
ANISOU	785	CD2	LEU A	138	6391	7320	4693	888	−2292	−1506	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	786	N	ARG A	139	−18.577	3.002	20.447	1.00	39.20		N
ANISOU	786	N	ARG A	139	5011	6236	3647	630	−1227	−841	N
ATOM	787	CA	ARG A	139	−17.828	3.873	21.349	1.00	38.07		C
ANISOU	787	CA	ARG A	139	4839	6091	3534	562	−962	−659	C
ATOM	788	C	ARG A	139	−18.773	4.900	21.947	1.00	40.93		C
ANISOU	788	C	ARG A	139	5073	6402	4075	621	−1088	−606	C
ATOM	789	O	ARG A	139	−19.701	5.352	21.287	1.00	45.61		O
ANISOU	789	O	ARG A	139	5732	6955	4645	756	−1383	−648	O
ATOM	790	CB	ARG A	139	−16.666	4.523	20.601	1.00	40.39		C
ANISOU	790	CB	ARG A	139	5463	6388	3495	558	−773	−537	C
ATOM	791	CG	ARG A	139	−15.742	3.453	20.037	1.00	42.66		C
ANISOU	791	CG	ARG A	139	5833	6715	3662	500	−607	−633	C
ATOM	792	CD	ARG A	139	−14.610	3.975	19.153	1.00	49.30		C
ANISOU	792	CD	ARG A	139	7004	7539	4190	475	−351	−558	C
ATOM	793	NE	ARG A	139	−13.801	2.853	18.672	1.00	51.57		N
ANISOU	793	NE	ARG A	139	7311	7854	4429	425	−175	−698	N
ATOM	794	CZ	ARG A	139	−12.568	2.973	18.197	1.00	53.58		C
ANISOU	794	CZ	ARG A	139	7712	8092	4555	355	170	−694	C
ATOM	795	NH1	ARG A	139	−12.024	4.186	18.126	1.00	54.33		N
ANISOU	795	NH1	ARG A	139	7963	8133	4549	310	379	−544	N
ATOM	796	NH2	ARG A	139	−11.890	1.888	17.787	1.00	50.34		N
ANISOU	796	NH2	ARG A	139	7280	7694	4154	324	329	−857	N
ATOM	797	O	ALA A	140	−17.363	7.181	24.502	1.00	38.21		O
ANISOU	797	O	ALA A	140	4612	6008	3900	452	−545	−297	O
ATOM	798	N	ALA A	140	−18.559	5.233	23.210	1.00	38.22		N
ANISOU	798	N	ALA A	140	4551	6051	3921	535	−887	−538	N
ATOM	799	CA	ALA A	140	−19.432	6.168	23.915	1.00	41.12		C
ANISOU	799	CA	ALA A	140	4771	6358	4493	576	−944	−518	C
ATOM	800	C	ALA A	140	−18.578	7.326	24.374	1.00	39.26		C
ANISOU	800	C	ALA A	140	4659	6101	4155	542	−750	−358	C
ATOM	801	CB	ALA A	140	−20.095	5.506	25.096	1.00	41.31		C
ANISOU	801	CB	ALA A	140	4490	6366	4841	488	−848	−618	C
ATOM	802	N	AGLU A	141	−19.200	8.466	24.639	0.50	36.77		N
ANISOU	802	N	AGLU A	141	4324	5707	3940	614	−817	−317	N
ATOM	803	CA	AGLU A	141	−18.442	9.641	25.026	0.50	36.21		C
ANISOU	803	CA	AGLU A	141	4375	5584	3799	578	−642	−186	C
ATOM	804	C	AGLU A	141	−18.774	10.053	26.448	0.50	33.98		C
ANISOU	804	C	AGLU A	141	3878	5275	3757	520	−514	−225	C
ATOM	805	O	AGLU A	141	−19.945	10.089	26.836	0.50	35.04		O
ANISOU	805	O	AGLU A	141	3823	5368	4124	577	−605	−321	O
ATOM	806	CB	AGLU A	141	−18.706	10.783	24.041	0.50	41.97		C
ANISOU	806	CB	AGLU A	141	5367	6198	4383	718	−797	−80	C
ATOM	807	CG	AGLU A	141	−18.197	10.453	22.638	0.50	45.67		C
ANISOU	807	CG	AGLU A	141	6163	6679	4511	759	−858	−22	C
ATOM	808	CD	AGLU A	141	−18.398	11.563	21.623	0.50	57.19		C
ANISOU	808	CD	AGLU A	141	7998	7990	5742	907	−1004	121	C
ATOM	809	OE1	AGLU A	141	−18.821	12.678	22.013	0.50	60.61		O
ANISOU	809	OE1	AGLU A	141	8423	8295	6312	977	−1047	189	O
ATOM	810	OE2	AGLU A	141	−18.127	11.316	20.424	0.50	61.11		O
ANISOU	810	OE2	AGLU A	141	8838	8479	5904	959	−1068	167	O
ATOM	811	N	BGLU A	141	−19.168	8.494	24.587	0.50	36.84		N
ANISOU	811	N	BGLU A	141	4347	5715	3935	617	−819	−312	N
ATOM	812	CA	BGLU A	141	−18.335	9.591	25.040	0.50	35.54		C
ANISOU	812	CA	BGLU A	141	4295	5507	3703	566	−623	−183	C
ATOM	813	C	BGLU A	141	−18.746	10.015	26.432	0.50	33.89		C
ANISOU	813	C	BGLU A	141	3869	5267	3740	518	−513	−225	C
ATOM	814	O	BGLU A	141	−19.930	10.007	26.787	0.50	34.96		O
ANISOU	814	O	BGLU A	141	3814	5363	4105	575	−610	−323	O
ATOM	815	CB	BGLU A	141	−18.364	10.772	24.056	0.50	41.41		C
ANISOU	815	CB	BGLU A	141	5328	6137	4269	683	−729	−60	C
ATOM	816	CG	BGLU A	141	−19.536	11.698	24.125	0.50	47.62		C
ANISOU	816	CG	BGLU A	141	6062	6803	5229	836	−941	−67	C
ATOM	817	CD	BGLU A	141	−19.258	13.048	23.449	0.50	56.78		C
ANISOU	817	CD	BGLU A	141	7561	7802	6211	926	−962	107	C
ATOM	818	OE1	BGLU A	141	−18.106	13.256	23.009	0.50	58.96		O
ANISOU	818	OE1	BGLU A	141	8096	8063	6242	829	−744	226	O
ATOM	819	OE2	BGLU A	141	−20.179	13.897	23.354	0.50	58.94		O
ANISOU	819	OE2	BGLU A	141	7841	7939	6615	1093	−1178	118	O
ATOM	820	N	LEU A	142	−17.737	10.328	27.232	1.00	29.18		N
ANISOU	820	N	LEU A	142	3293	4686	3107	405	−299	−179	N
ATOM	821	CA	LEU A	142	−17.913	10.860	28.578	1.00	28.20		C
ANISOU	821	CA	LEU A	142	3052	4529	3134	352	−174	−218	C
ATOM	822	C	LEU A	142	−17.525	12.349	28.559	1.00	28.54		C
ANISOU	822	C	LEU A	142	3219	4465	3162	365	−120	−147	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	823	O	LEU A	142	−16.449	12.707	28.054	1.00	29.52		O
ANISOU	823	O	LEU A	142	3492	4573	3150	314	−43	−69	O
ATOM	824	CB	LEU A	142	−17.031	10.075	29.583	1.00	30.01		C
ANISOU	824	CB	LEU A	142	3243	4839	3321	230	−31	−245	C
ATOM	825	CG	LEU A	142	−16.923	10.660	31.001	1.00	31.30		C
ANISOU	825	CG	LEU A	142	3384	4972	3537	169	95	−286	C
ATOM	826	CD1	LEU A	142	−18.279	10.680	31.645	1.00	31.83		C
ANISOU	826	CD1	LEU A	142	3340	4987	3768	194	140	−366	C
ATOM	827	CD2	LEU A	142	−15.922	9.878	31.925	1.00	26.31		C
ANISOU	827	CD2	LEU A	142	2782	4408	2809	88	150	−302	C
ATOM	828	N	ARG A	143	−18.380	13.214	29.091	1.00	27.94		N
ANISOU	828	N	ARG A	143	3072	4290	3255	423	−129	−189	N
ATOM	829	C	ARG A	143	−18.148	14.943	30.693	1.00	31.81		C
ANISOU	829	C	ARG A	143	3555	4636	3896	352	89	−254	C
ATOM	830	O	ARG A	143	−19.211	14.743	31.289	1.00	30.81		O
ANISOU	830	O	ARG A	143	3277	4500	3929	392	102	−359	O
ATOM	831	CA	ARG A	143	−18.016	14.621	29.220	1.00	29.12		C
ANISOU	831	CA	ARG A	143	3334	4306	3426	425	−58	−137	C
ATOM	832	CB	ARG A	143	−18.900	15.598	28.399	1.00	32.20		C
ANISOU	832	CB	ARG A	143	3811	4527	3894	599	−225	−78	C
ATOM	833	CG	ARG A	143	−18.742	15.605	26.851	1.00	72.08		C
ANISOU	833	CG	ARG A	143	9122	9534	8730	699	−389	67	C
ATOM	834	CD	ARG A	143	−17.356	16.075	26.328	1.00	68.54		C
ANISOU	834	CD	ARG A	143	8941	9034	8068	584	−195	203	C
ATOM	835	NE	ARG A	143	−16.472	14.925	26.184	1.00	65.66		N
ANISOU	835	NE	ARG A	143	8544	8841	7564	460	−92	175	N
ATOM	836	CZ	ARG A	143	−16.127	14.364	25.035	1.00	65.27		C
ANISOU	836	CZ	ARG A	143	8688	8827	7286	478	−117	241	C
ATOM	837	NH1	ARG A	143	−16.527	14.865	23.871	1.00	68.09		N
ANISOU	837	NH1	ARG A	143	9353	9060	7458	612	−251	364	N
ATOM	838	NH2	ARG A	143	−15.356	13.300	25.059	1.00	64.84		N
ANISOU	838	NH2	ARG A	143	8549	8916	7173	372	−12	179	N
ATOM	839	N	VAL A	144	−17.054	15.426	31.274	1.00	31.58		N
ANISOU	839	N	VAL A	144	3595	4599	3804	239	213	−261	N
ATOM	840	CA	VAL A	144	−17.060	15.813	32.671	1.00	33.73		C
ANISOU	840	CA	VAL A	144	3825	4856	4136	173	329	−387	C
ATOM	841	C	VAL A	144	−17.126	17.330	32.681	1.00	35.73		C
ANISOU	841	C	VAL A	144	4139	4924	4514	200	374	−398	C
ATOM	842	O	VAL A	144	−16.283	17.992	32.061	1.00	34.95		O
ANISOU	842	O	VAL A	144	4149	4740	4391	160	390	−319	O
ATOM	843	CB	VAL A	144	−15.810	15.300	33.407	1.00	30.37		C
ANISOU	843	CB	VAL A	144	3428	4536	3576	49	366	−432	C
ATOM	844	CG1	VAL A	144	−15.869	15.688	34.866	1.00	25.47		C
ANISOU	844	CG1	VAL A	144	2836	3895	2948	−1	447	−573	C
ATOM	845	CG2	VAL A	144	−15.731	13.767	33.277	1.00	28.73		C
ANISOU	845	CG2	VAL A	144	3184	4472	3260	46	309	−400	C
ATOM	846	N	THR A	145	−18.123	17.885	33.363	1.00	34.70		N
ANISOU	846	N	THR A	145	3940	4703	4543	260	428	−504	N
ATOM	847	CA	THR A	145	−18.271	19.329	33.386	1.00	38.67		C
ANISOU	847	CA	THR A	145	4497	4997	5201	305	467	−528	C
ATOM	848	C	THR A	145	−17.688	19.973	34.650	1.00	39.11		C
ANISOU	848	C	THR A	145	4590	5015	5255	185	613	−685	C
ATOM	849	O	THR A	145	−17.593	19.345	35.698	1.00	40.05		O
ANISOU	849	O	THR A	145	4697	5258	5261	110	680	−801	O
ATOM	850	CB	THR A	145	−19.746	19.728	33.225	1.00	43.79		C
ANISOU	850	CB	THR A	145	5026	5519	6092	479	414	−577	C
ATOM	851	OG1	THR A	145	−20.542	19.124	34.250	1.00	47.54		O
ANISOU	851	OG1	THR A	145	5341	6073	6648	456	543	−746	O
ATOM	852	CG2	THR A	145	−20.265	19.255	31.844	1.00	47.11		C
ANISOU	852	CG2	THR A	145	5442	5947	6510	624	181	−436	C
ATOM	853	O	GLU A	146	−19.018	22.626	36.400	1.00	48.08		O
ANISOU	853	O	GLU A	146	5715	5721	6833	266	891	−1062	O
ATOM	854	N	GLU A	146	−17.281	21.223	34.522	1.00	34.62		N
ANISOU	854	N	GLU A	146	4105	4254	4794	168	651	−689	N
ATOM	855	CA	GLU A	146	−16.800	22.005	35.653	1.00	37.67		C
ANISOU	855	CA	GLU A	146	4528	4567	5218	64	762	−877	C
ATOM	856	C	GLU A	146	−17.894	22.193	36.709	1.00	44.41		C
ANISOU	856	C	GLU A	146	5330	5388	6154	123	875	−1060	C
ATOM	857	CB	GLU A	146	−16.275	23.353	35.133	1.00	39.38		C
ANISOU	857	CB	GLU A	146	4838	4529	5596	37	801	−838	C
ATOM	858	CG	GLU A	146	−15.174	24.083	35.976	1.00	46.35		C
ANISOU	858	CG	GLU A	146	5752	5338	6518	−137	877	−1024	C
ATOM	859	CD	GLU A	146	−14.011	23.192	36.426	1.00	44.09		C
ANISOU	859	CD	GLU A	146	5419	5271	6062	−276	806	−1099	C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ATOM	860	OE1	GLU A	146	−13.718	22.203	35.738	1.00	38.29		O
ANISOU	860	OE1	GLU A	146	4648	4689	5212	−270	741	−954	O
ATOM	861	OE2	GLU A	146	−13.404	23.480	37.506	1.00	35.48		O
ANISOU	861	OE2	GLU A	146	4331	4190	4959	−377	788	−1326	O
ATOM	862	O	ARG A	147	−17.523	24.215	39.276	1.00	46.46		O
ANISOU	862	O	ARG A	147	5768	5400	6486	−29	1145	−1593	O
ATOM	863	N	ARG A	147	−17.589	21.856	37.962	1.00	43.22		N
ANISOU	863	N	ARG A	147	5237	5346	5838	23	953	−1230	N
ATOM	864	CA	ARG A	147	−18.543	22.093	39.030	1.00	40.73		C
ANISOU	864	CA	ARG A	147	4929	4980	5565	51	1138	−1426	C
ATOM	865	C	ARG A	147	−18.561	23.575	39.319	1.00	45.72		C
ANISOU	865	C	ARG A	147	5598	5376	6399	61	1215	−1572	C
ATOM	866	CB	ARG A	147	−18.188	21.304	40.289	1.00	39.75		C
ANISOU	866	CB	ARG A	147	4961	5017	5124	−51	1203	−1547	C
ATOM	867	CG	ARG A	147	−19.242	21.450	41.419	1.00	53.91		C
ANISOU	867	CG	ARG A	147	6821	6751	6912	−41	1484	−1753	C
ATOM	868	CD	ARG A	147	−18.911	20.580	42.645	1.00	55.20		C
ANISOU	868	CD	ARG A	147	7249	7055	6670	−133	1556	−1833	C
ATOM	869	NE	ARG A	147	−18.748	19.158	42.308	1.00	55.18		N
ANISOU	869	NE	ARG A	147	7248	7220	6499	−143	1464	−1643	N
ATOM	870	CZ	ARG A	147	−19.726	18.247	42.335	1.00	53.32		C
ANISOU	870	CZ	ARG A	147	6961	7013	6285	−132	1657	−1595	C
ATOM	871	NH1	ARG A	147	−20.956	18.606	42.660	1.00	58.92		N
ANISOU	871	NH1	ARG A	147	7576	7604	7208	−110	1962	−1734	N
ATOM	872	NH2	ARG A	147	−19.483	16.976	42.010	1.00	45.09		N
ANISOU	872	NH2	ARG A	147	5932	6097	5102	−148	1559	−1428	N
ATOM	873	O	ARG A	148	−18.922	25.010	42.085	1.00	64.66		O
ANISOU	873	O	ARG A	148	8258	7587	8722	−40	1601	−2179	O
ATOM	874	N	ARG A	148	−19.729	24.139	39.611	1.00	49.33		N
ANISOU	874	N	ARG A	148	5976	5683	7083	164	1374	−1698	N
ATOM	875	CA	ARG A	148	−19.797	25.572	39.908	1.00	59.43		C
ANISOU	875	CA	ARG A	148	7292	6703	8586	188	1458	−1856	C
ATOM	876	C	ARG A	148	−19.120	25.893	41.249	1.00	66.19		C
ANISOU	876	C	ARG A	148	8334	7582	9233	40	1562	−2110	C
ATOM	877	CB	ARG A	148	−21.254	26.062	39.925	1.00	61.22		C
ANISOU	877	CB	ARG A	148	7352	6751	9156	359	1602	−1966	C
ATOM	878	O	ALA A	149	−19.341	27.591	44.936	1.00	90.72		O
ANISOU	878	O	ALA A	149	11937	10471	12064	−125	2082	−3022	O
ATOM	879	N	ALA A	149	−18.741	27.151	41.441	1.00	73.74		N
ANISOU	879	N	ALA A	149	9350	8315	10355	10	1584	−2250	N
ATOM	880	CA	ALA A	149	−18.303	27.606	42.757	1.00	81.09		C
ANISOU	880	CA	ALA A	149	10459	9228	11124	−104	1675	−2557	C
ATOM	881	C	ALA A	149	−19.497	27.637	43.712	1.00	86.57		C
ANISOU	881	C	ALA A	149	11190	9887	11817	−40	1966	−2779	C
ATOM	882	CB	ALA A	149	−17.646	28.978	42.661	1.00	84.53		C
ANISOU	882	CB	ALA A	149	10924	9396	11799	−162	1641	−2676	C
TER											
ATOM	883	O	LEU B	20	−1.649	−5.434	33.856	1.00	58.08		O
ANISOU	883	O	LEU B	20	7988	9726	4354	1942	402	750	O
ATOM	884	N	LEU B	20	−3.012	−5.202	36.329	1.00	62.51		N
ANISOU	884	N	LEU B	20	9807	9782	4160	2346	1138	760	N
ATOM	885	CA	LEU B	20	−3.676	−5.607	35.106	1.00	58.15		C
ANISOU	885	CA	LEU B	20	8804	8611	4682	2971	1236	992	C
ATOM	886	C	LEU B	20	−2.682	−6.066	34.062	1.00	56.80		C
ANISOU	886	C	LEU B	20	7765	9094	4723	2746	714	1049	C
ATOM	887	CB	LEU B	20	−4.487	−4.469	34.521	1.00	62.55		C
ANISOU	887	CB	LEU B	20	10141	8069	5557	2835	1708	751	C
ATOM	888	CG	LEU B	20	−5.846	−4.191	35.138	1.00	71.78		C
ANISOU	888	CG	LEU B	20	12027	8200	7048	3362	2409	907	C
ATOM	889	CD1	LEU B	20	−6.577	−3.220	34.232	1.00	73.47		C
ANISOU	889	CD1	LEU B	20	12506	7590	7818	3013	2649	929	C
ATOM	890	CD2	LEU B	20	−6.627	−5.482	35.330	1.00	70.22		C
ANISOU	890	CD2	LEU B	20	10977	8255	7449	3520	2121	1346	C
ATOM	891	N	PHE B	21	−3.008	−7.160	33.393	1.00	52.83		N
ANISOU	891	N	PHE B	21	6487	8553	5033	3417	684	1415	N
ATOM	892	CA	PHE B	21	−2.252	−7.576	32.236	1.00	49.20		C
ANISOU	892	CA	PHE B	21	5469	8298	4926	2899	406	1312	C
ATOM	893	C	PHE B	21	−2.431	−6.524	31.140	1.00	45.14		C
ANISOU	893	C	PHE B	21	5281	7328	4542	2877	401	1134	C
ATOM	894	O	PHE B	21	−3.572	−6.224	30.766	1.00	41.12		O
ANISOU	894	O	PHE B	21	5200	5942	4480	2791	684	1034	O
ATOM	895	CB	PHE B	21	−2.720	−8.955	31.778	1.00	45.59		C
ANISOU	895	CB	PHE B	21	4890	7268	5164	2397	452	1215	C
ATOM	896	CG	PHE B	21	−2.020	−9.444	30.541	1.00	44.10		C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	896	CG	PHE B	21	4442	7169	5145	2128	355	1205	C
ATOM	897	CD1	PHE B	21	−0.744	−9.943	30.619	1.00	47.89		C
ANISOU	897	CD1	PHE B	21	4549	8169	5478	1984	244	1336	C
ATOM	898	CD2	PHE B	21	−2.637	−9.366	29.306	1.00	47.32		C
ANISOU	898	CD2	PHE B	21	4991	7151	5836	2001	390	1102	C
ATOM	899	CE1	PHE B	21	−0.084	−10.378	29.501	1.00	50.70		C
ANISOU	899	CE1	PHE B	21	4757	8513	5995	1768	221	1360	C
ATOM	900	CE2	PHE B	21	−1.982	−9.802	28.164	1.00	45.35		C
ANISOU	900	CE2	PHE B	21	4563	6948	5722	1794	315	1081	C
ATOM	901	CZ	PHE B	21	−0.700	−10.310	28.263	1.00	46.66		C
ANISOU	901	CZ	PHE B	21	4431	7530	5766	1695	253	1205	C
ATOM	902	N	THR B	22	−1.327	−5.933	30.650	1.00	45.73		N
ANISOU	902	N	THR B	22	5337	7801	4237	2149	103	874	N
ATOM	903	CA	THR B	22	−1.426	−4.916	29.583	1.00	42.62		C
ANISOU	903	CA	THR B	22	5349	6854	3992	1799	187	587	C
ATOM	904	C	THR B	22	−0.482	−5.153	28.398	1.00	41.92		C
ANISOU	904	C	THR B	22	4707	7116	4103	1531	−132	581	C
ATOM	905	O	THR B	22	0.589	−5.754	28.538	1.00	39.02		O
ANISOU	905	O	THR B	22	3771	7487	3567	1326	−435	709	O
ATOM	906	CB	THR B	22	−1.122	−3.507	30.104	1.00	47.30		C
ANISOU	906	CB	THR B	22	6763	7288	3921	1074	338	142	C
ATOM	907	OG1	THR B	22	0.190	−3.506	30.667	1.00	50.41		O
ANISOU	907	OG1	THR B	22	6942	8564	3648	444	−62	0	O
ATOM	908	CG2	THR B	22	−2.154	−3.066	31.181	1.00	49.21		C
ANISOU	908	CG2	THR B	22	7764	6949	3984	1273	836	100	C
ATOM	909	N	VAL B	23	−0.885	−4.639	27.248	1.00	35.34		N
ANISOU	909	N	VAL B	23	4057	5738	3634	1526	−19	490	N
ATOM	910	CA	VAL B	23	−0.111	−4.746	26.005	1.00	33.17		C
ANISOU	910	CA	VAL B	23	3403	5644	3557	1286	−233	458	C
ATOM	911	C	VAL B	23	0.206	−3.352	25.560	1.00	35.04		C
ANISOU	911	C	VAL B	23	4186	5587	3543	737	−146	120	C
ATOM	912	O	VAL B	23	−0.678	−2.487	25.619	1.00	35.02		O
ANISOU	912	O	VAL B	23	4758	4964	3583	793	202	41	O
ATOM	913	CB	VAL B	23	−0.906	−5.507	24.908	1.00	42.34		C
ANISOU	913	CB	VAL B	23	4319	6393	5376	1655	−158	633	C
ATOM	914	CG1	VAL B	23	−0.344	−5.249	23.495	1.00	38.71		C
ANISOU	914	CG1	VAL B	23	3720	5942	5047	1427	−273	557	C
ATOM	915	CG2	VAL B	23	−0.913	−7.010	25.247	1.00	38.47		C
ANISOU	915	CG2	VAL B	23	3718	5765	5135	1412	−155	591	C
ATOM	916	N	THR B	24	1.462	−3.101	25.174	1.00	35.92		N
ANISOU	916	N	THR B	24	4108	6094	3445	219	−382	−36	N
ATOM	917	CA	THR B	24	1.863	−1.787	24.655	1.00	38.14		C
ANISOU	917	CA	THR B	24	4840	6085	3568	−291	−254	−370	C
ATOM	918	C	THR B	24	2.542	−1.884	23.277	1.00	40.73		C
ANISOU	918	C	THR B	24	4833	6443	4201	−378	−389	−329	C
ATOM	919	O	THR B	24	3.043	−2.944	22.917	1.00	43.51		O
ANISOU	919	O	THR B	24	4608	7161	4762	−229	−607	−95	O
ATOM	920	CB	THR B	24	2.827	−1.091	25.595	1.00	46.28		C
ANISOU	920	CB	THR B	24	6103	7498	3985	−979	−360	−693	C
ATOM	921	OG1	THR B	24	3.982	−1.911	25.769	1.00	46.89		O
ANISOU	921	OG1	THR B	24	5526	8343	3949	−1168	−801	−505	O
ATOM	922	CG2	THR B	24	2.174	−0.857	26.957	1.00	47.29		C
ANISOU	922	CG2	THR B	24	6720	7552	3697	−995	−155	−807	C
ATOM	923	N	VAL B	25	2.549	−0.793	22.514	1.00	38.94		N
ANISOU	923	N	VAL B	25	4973	5795	4028	−599	−173	−525	N
ATOM	924	CA	VAL B	25	3.189	−0.797	21.197	1.00	40.66		C
ANISOU	924	CA	VAL B	25	4953	5998	4498	−675	−254	−492	C
ATOM	925	C	VAL B	25	4.116	0.374	21.098	1.00	49.10		C
ANISOU	925	C	VAL B	25	6279	7003	5372	−1232	−160	−817	C
ATOM	926	O	VAL B	25	3.672	1.509	20.933	1.00	53.14		O
ANISOU	926	O	VAL B	25	7264	7039	5889	−1327	220	−994	O
ATOM	927	CB	VAL B	25	2.183	−0.710	20.021	1.00	54.36		C
ANISOU	927	CB	VAL B	25	6786	7270	6597	−287	−66	−305	C
ATOM	928	CG1	VAL B	25	2.906	−0.596	18.712	1.00	59.16		C
ANISOU	928	CG1	VAL B	25	7254	7870	7356	−425	−110	−312	C
ATOM	929	CG2	VAL B	25	1.237	−1.924	20.019	1.00	51.02		C
ANISOU	929	CG2	VAL B	25	6067	6894	6423	228	−170	−4	C
ATOM	930	N	PRO B	26	5.421	0.113	21.192	1.00	53.75		N
ANISOU	930	N	PRO B	26	6517	8048	5857	−1601	−448	−851	N
ATOM	931	CA	PRO B	26	6.367	1.232	21.186	1.00	57.08		C
ANISOU	931	CA	PRO B	26	7149	8423	6116	−2184	−379	−1185	C
ATOM	932	C	PRO B	26	6.514	1.805	19.778	1.00	52.07		C
ANISOU	932	C	PRO B	26	6595	7343	5848	−2093	−141	−1199	C
ATOM	933	O	PRO B	26	6.907	2.947	19.616	1.00	54.90		O

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	933	O	PRO B	26	7244	7429	6186	−2431	115	−1491	O
ATOM	934	CB	PRO B	26	7.667	0.604	21.707	1.00	62.67		C
ANISOU	934	CB	PRO B	26	7328	9804	6678	−2553	−816	−1057	C
ATOM	935	CG	PRO B	26	7.572	−0.819	21.361	1.00	61.18		C
ANISOU	935	CG	PRO B	26	6596	9851	6797	−2078	−975	−596	C
ATOM	936	CD	PRO B	26	6.089	−1.191	21.326	1.00	56.87		C
ANISOU	936	CD	PRO B	26	6271	8989	6349	−1508	−781	−528	C
ATOM	937	N	LYS B	27	6.116	1.044	18.770	1.00	48.04		N
ANISOU	937	N	LYS B	27	5864	6737	5653	−1640	−169	−897	N
ATOM	938	CA	LYS B	27	6.121	1.574	17.418	1.00	47.65		C
ANISOU	938	CA	LYS B	27	5936	6300	5870	−1525	61	−871	C
ATOM	939	C	LYS B	27	4.809	1.202	16.758	1.00	43.30		C
ANISOU	939	C	LYS B	27	5455	5533	5462	−1033	155	−615	C
ATOM	940	O	LYS B	27	4.538	0.025	16.564	1.00	43.91		O
ANISOU	940	O	LYS B	27	5241	5816	5625	−784	−54	−405	O
ATOM	941	CB	LYS B	27	7.325	1.029	16.652	1.00	50.64		C
ANISOU	941	CB	LYS B	27	5951	6835	6454	−1637	−97	−757	C
ATOM	942	CG	LYS B	27	7.419	1.471	15.203	1.00	53.14		C
ANISOU	942	CG	LYS B	27	6406	6777	7009	−1504	141	−711	C
ATOM	943	CD	LYS B	27	8.634	0.840	14.533	1.00	55.35		C
ANISOU	943	CD	LYS B	27	6369	7136	7526	−1609	60	−568	C
ATOM	944	CE	LYS B	27	8.934	1.499	13.201	1.00	58.42		C
ANISOU	944	CE	LYS B	27	6965	7121	8110	−1542	342	−576	C
ATOM	945	NZ	LYS B	27	9.728	0.608	12.336	1.00	59.37		N
ANISOU	945	NZ	LYS B	27	6870	7211	8476	−1508	360	−358	N
ATOM	946	N	GLU B	28	3.974	2.184	16.430	1.00	40.82		N
ANISOU	946	N	GLU B	28	5487	4813	5209	−909	504	−590	N
ATOM	947	CA	GLU B	28	2.655	1.841	15.917	1.00	44.01		C
ANISOU	947	CA	GLU B	28	5894	5079	5749	−480	535	−249	C
ATOM	948	C	GLU B	28	2.562	1.849	14.390	1.00	44.43		C
ANISOU	948	C	GLU B	28	5880	5066	5936	−338	548	−30	C
ATOM	949	O	GLU B	28	1.615	1.293	13.833	1.00	45.11		O
ANISOU	949	O	GLU B	28	5867	5193	6081	−68	428	267	O
ATOM	950	CB	GLU B	28	1.585	2.760	16.502	1.00	51.11		C
ANISOU	950	CB	GLU B	28	7137	5585	6696	−364	941	−155	C
ATOM	951	CG	GLU B	28	1.802	4.241	16.332	1.00	60.68		C
ANISOU	951	CG	GLU B	28	8673	6401	7982	−569	1478	−281	C
ATOM	952	CD	GLU B	28	0.794	5.079	17.152	1.00	65.46		C
ANISOU	952	CD	GLU B	28	9655	6542	8676	−503	2034	−191	C
ATOM	953	OE1	GLU B	28	−0.050	4.488	17.874	1.00	56.50		O
ANISOU	953	OE1	GLU B	28	8540	5398	7530	−281	1942	−26	O
ATOM	954	OE2	GLU B	28	0.852	6.332	17.068	1.00	74.70		O
ANISOU	954	OE2	GLU B	28	11104	7297	9982	−661	2649	−268	O
ATOM	955	N	LEU B	29	3.545	2.447	13.721	1.00	40.79		N
ANISOU	955	N	LEU B	29	5469	4524	5507	−541	680	−170	N
ATOM	956	CA	LEU B	29	3.527	2.546	12.267	1.00	39.31		C
ANISOU	956	CA	LEU B	29	5277	4273	5386	−420	738	34	C
ATOM	957	C	LEU B	29	4.800	1.981	11.631	1.00	38.09		C
ANISOU	957	C	LEU B	29	4989	4230	5254	−597	609	−105	C
ATOM	958	O	LEU B	29	5.900	2.392	11.950	1.00	37.80		O
ANISOU	958	O	LEU B	29	4942	4128	5293	−841	690	−327	O
ATOM	959	CB	LEU B	29	3.346	3.999	11.835	1.00	44.93		C
ANISOU	959	CB	LEU B	29	6213	4638	6222	−380	1213	125	C
ATOM	960	CG	LEU B	29	3.402	4.281	10.336	1.00	47.96		C
ANISOU	960	CG	LEU B	29	6598	4986	6640	−245	1322	377	C
ATOM	961	CD1	LEU B	29	2.344	3.481	9.572	1.00	46.93		C
ANISOU	961	CD1	LEU B	29	6352	5112	6365	−38	1026	764	C
ATOM	962	CD2	LEU B	29	3.175	5.756	10.142	1.00	53.43		C
ANISOU	962	CD2	LEU B	29	7440	5327	7536	−155	1903	524	C
ATOM	963	N	TYR B	30	4.617	1.027	10.726	1.00	33.10		N
ANISOU	963	N	TYR B	30	4264	3738	4576	−502	446	46	N
ATOM	964	CA	TYR B	30	5.703	0.406	10.010	1.00	35.59		C
ANISOU	964	CA	TYR B	30	4508	4057	4957	−645	452	−17	C
ATOM	965	C	TYR B	30	5.574	0.797	8.541	1.00	39.60		C
ANISOU	965	C	TYR B	30	5235	4430	5381	−573	612	125	C
ATOM	966	O	TYR B	30	4.509	0.663	7.931	1.00	38.67		O
ANISOU	966	O	TYR B	30	5181	4438	5073	−445	519	331	O
ATOM	967	CB	TYR B	30	5.648	−1.106	10.169	1.00	32.27		C
ANISOU	967	CB	TYR B	30	3850	3864	4547	−653	272	10	C
ATOM	968	CG	TYR B	30	5.931	−1.620	11.574	1.00	34.35		C
ANISOU	968	CG	TYR B	30	3821	4331	4899	−698	133	−47	C
ATOM	969	CD1	TYR B	30	7.171	−2.148	11.892	1.00	35.46		C
ANISOU	969	CD1	TYR B	30	3693	4550	5229	−883	164	−35	C
ATOM	970	CD2	TYR B	30	4.953	−1.572	12.573	1.00	37.16		C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	970	CD2	TYR B	30	4152	4806	5163	−546	−4	−35	C
ATOM	971	CE1	TYR B	30	7.450	−2.613	13.160	1.00	40.40		C
ANISOU	971	CE1	TYR B	30	3990	5466	5892	−936	13	6	C
ATOM	972	CE2	TYR B	30	5.208	−2.046	13.861	1.00	35.61		C
ANISOU	972	CE2	TYR B	30	3706	4844	4981	−580	−129	−64	C
ATOM	973	CZ	TYR B	30	6.450	−2.574	14.151	1.00	38.84		C
ANISOU	973	CZ	TYR B	30	3807	5431	5519	−781	−147	−33	C
ATOM	974	OH	TYR B	30	6.709	−3.064	15.417	1.00	37.39		O
ANISOU	974	OH	TYR B	30	3310	5586	5310	−820	−296	32	O
ATOM	975	N	ILE B	31	6.653	1.290	7.973	1.00	38.79		N
ANISOU	975	N	ILE B	31	5228	4095	5417	−660	843	54	N
ATOM	976	CA	ILE B	31	6.641	1.686	6.582	1.00	38.51		C
ANISOU	976	CA	ILE B	31	5420	3930	5283	−572	1037	201	C
ATOM	977	C	ILE B	31	7.670	0.824	5.868	1.00	43.88		C
ANISOU	977	C	ILE B	31	6155	4480	6037	−718	1141	139	C
ATOM	978	O	ILE B	31	8.849	0.939	6.117	1.00	46.53		O
ANISOU	978	O	ILE B	31	6412	4584	6683	−819	1298	50	O
ATOM	979	CB	ILE B	31	6.948	3.171	6.442	1.00	43.79		C
ANISOU	979	CB	ILE B	31	6191	4319	6127	−471	1377	219	C
ATOM	980	CG1	ILE B	31	5.761	3.992	6.965	1.00	47.95		C
ANISOU	980	CG1	ILE B	31	6704	4902	6612	−311	1439	382	C
ATOM	981	CG2	ILE B	31	7.230	3.528	5.005	1.00	44.84		C
ANISOU	981	CG2	ILE B	31	6529	4303	6205	−354	1627	386	C
ATOM	982	CD1	ILE B	31	6.084	5.446	7.279	1.00	51.11		C
ANISOU	982	CD1	ILE B	31	7166	4964	7288	−275	1906	310	C
ATOM	983	N	ILE B	32	7.220	−0.089	5.020	1.00	42.96		N
ANISOU	983	N	ILE B	32	6170	4495	5659	−773	1086	201	N
ATOM	984	CA	ILE B	32	8.123	−1.097	4.462	1.00	43.12		C
ANISOU	984	CA	ILE B	32	6274	4325	5785	−954	1307	135	C
ATOM	985	C	ILE B	32	8.120	−1.054	2.932	1.00	45.07		C
ANISOU	985	C	ILE B	32	6939	4453	5734	−1000	1523	193	C
ATOM	986	O	ILE B	32	7.065	−0.878	2.312	1.00	46.79		O
ANISOU	986	O	ILE B	32	7302	4963	5514	−980	1335	297	O
ATOM	987	CB	ILE B	32	7.717	−2.501	4.951	1.00	41.14		C
ANISOU	987	CB	ILE B	32	5827	4288	5515	−1080	1183	72	C
ATOM	988	CG1	ILE B	32	7.667	−2.509	6.493	1.00	43.57		C
ANISOU	988	CG1	ILE B	32	5728	4772	6053	−1001	956	58	C
ATOM	989	CG2	ILE B	32	8.670	−3.556	4.425	1.00	42.51		C
ANISOU	989	CG2	ILE B	32	6073	4181	5900	−1278	1587	50	C
ATOM	990	CD1	ILE B	32	8.978	−2.111	7.138	1.00	47.81		C
ANISOU	990	CD1	ILE B	32	6066	5123	6975	−1063	1081	74	C
ATOM	991	O	GLU B	33	8.893	−3.626	0.909	1.00	51.23		O
ANISOU	991	O	GLU B	33	8407	4825	6234	−1618	2264	−19	O
ATOM	992	N	GLU B	33	9.292	−1.206	2.329	1.00	47.25		N
ANISOU	992	N	GLU B	33	7398	4311	6243	−1071	1922	181	N
ATOM	993	CA	GLU B	33	9.390	−1.266	0.878	1.00	51.43		C
ANISOU	993	CA	GLU B	33	8403	4680	6459	−1144	2198	214	C
ATOM	994	C	GLU B	33	8.730	−2.523	0.355	1.00	48.95		C
ANISOU	994	C	GLU B	33	8293	4581	5724	−1451	2169	92	C
ATOM	995	CB	GLU B	33	10.842	−1.217	0.416	1.00	59.64		C
ANISOU	995	CB	GLU B	33	9507	5260	7894	−1047	2594	200	C
ATOM	996	CG	GLU B	33	11.622	−0.080	0.998	1.00	64.78		C
ANISOU	996	CG	GLU B	33	9851	5788	8976	−786	2570	246	C
ATOM	997	CD	GLU B	33	12.555	0.549	0.001	1.00	77.49		C
ANISOU	997	CD	GLU B	33	11587	7179	10676	−562	2848	268	C
ATOM	998	OE1	GLU B	33	12.894	−0.122	−1.006	1.00	81.94		O
ANISOU	998	OE1	GLU B	33	12412	7654	11067	−592	3069	227	O
ATOM	999	OE2	GLU B	33	12.942	1.724	0.223	1.00	82.24		O
ANISOU	999	OE2	GLU B	33	12025	7703	11520	−371	2889	301	O
ATOM	1000	O	HIS B	34	9.374	−4.436	−2.071	1.00	42.45		O
ANISOU	1000	O	HIS B	34	4652	7423	4053	−463	507	−501	O
ATOM	1001	N	HIS B	34	7.929	−2.334	−0.676	1.00	44.67		N
ANISOU	1001	N	HIS B	34	4623	8075	4274	780	−88	192	N
ATOM	1002	CA	HIS B	34	7.298	−3.433	−1.384	1.00	48.78		C
ANISOU	1002	CA	HIS B	34	4864	9335	4335	137	25	−163	C
ATOM	1003	C	HIS B	34	8.246	−4.623	−1.634	1.00	46.34		C
ANISOU	1003	C	HIS B	34	4848	8489	4270	−488	387	−595	C
ATOM	1004	CB	HIS B	34	6.763	−2.935	−2.722	1.00	56.08		C
ANISOU	1004	CB	HIS B	34	5459	11213	4636	123	−114	92	C
ATOM	1005	CG	HIS B	34	5.878	−3.927	−3.392	1.00	62.90		C
ANISOU	1005	CG	HIS B	34	5962	13061	4875	−595	−58	−263	C
ATOM	1006	ND1	HIS B	34	6.324	−4.763	−4.393	1.00	71.37		N
ANISOU	1006	ND1	HIS B	34	7164	14274	5678	−1324	195	−654	N
ATOM	1007	CD2	HIS B	34	4.589	−4.264	−3.159	1.00	65.10		C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1007	CD2	HIS B	34	5777	14207	4749	−770	−177	−330	C
ATOM	1008	CE1	HIS B	34	5.331	−5.549	−4.777	1.00	78.01		C
ANISOU	1008	CE1	HIS B	34	7651	16034	5954	−1968	221	−976	C
ATOM	1009	NE2	HIS B	34	4.271	−5.272	−4.038	1.00	75.05		N
ANISOU	1009	NE2	HIS B	34	6884	16089	5542	−1636	−19	−762	N
ATOM	1010	N	GLY B	35	7.778	−5.843	−1.370	1.00	46.16		N
ANISOU	1010	N	GLY B	35	4738	8627	4175	−1038	626	−1040	N
ATOM	1011	CA	GLY B	35	8.616	−7.019	−1.521	1.00	47.19		C
ANISOU	1011	CA	GLY B	35	5155	8160	4617	−1588	1113	−1416	C
ATOM	1012	C	GLY B	35	9.688	−7.266	−0.438	1.00	41.02		C
ANISOU	1012	C	GLY B	35	4676	6302	4608	−1363	1285	−1304	C
ATOM	1013	O	GLY B	35	10.420	−8.245	−0.528	1.00	44.43		O
ANISOU	1013	O	GLY B	35	5308	6190	5382	−1739	1764	−1503	O
ATOM	1014	N	ASER B	36	9.775	−6.418	0.582	0.24	37.94		N
ANISOU	1014	N	ASER B	36	4308	5630	4477	−791	948	−970	N
ATOM	1015	CA	ASER B	36	10.718	−6.697	1.668	0.24	36.07		C
ANISOU	1015	CA	ASER B	36	4282	4558	4867	−669	1060	−836	C
ATOM	1016	C	ASER B	36	10.004	−7.122	2.951	0.24	35.38		C
ANISOU	1016	C	ASER B	36	4068	4524	4852	−627	1018	−928	C
ATOM	1017	O	ASER B	36	8.863	−6.733	3.201	0.24	34.94		O
ANISOU	1017	O	ASER B	36	3804	5040	4432	−465	778	−975	O
ATOM	1018	CB	ASER B	36	11.613	−5.488	1.941	0.24	36.35		C
ANISOU	1018	CB	ASER B	36	4513	4132	5166	−189	767	−419	C
ATOM	1019	OG	ASER B	36	10.858	−4.361	2.329	0.24	37.10		O
ANISOU	1019	OG	ASER B	36	4540	4548	5009	255	394	−261	O
ATOM	1020	N	BSER B	36	9.786	−6.394	0.564	0.76	37.11		N
ANISOU	1020	N	BSER B	36	4205	5526	4370	−784	943	−963	N
ATOM	1021	CA	BSER B	36	10.704	−6.653	1.676	0.76	36.59		C
ANISOU	1021	CA	BSER B	36	4346	4632	4925	−652	1044	−827	C
ATOM	1022	C	BSER B	36	9.953	−7.316	2.830	0.76	36.23		C
ANISOU	1022	C	BSER B	36	4160	4670	4935	−717	1084	−989	C
ATOM	1023	O	BSER B	36	8.724	−7.301	2.850	0.76	35.46		O
ANISOU	1023	O	BSER B	36	3817	5235	4422	−745	954	−1152	O
ATOM	1024	CB	BSER B	36	11.383	−5.364	2.150	0.76	36.69		C
ANISOU	1024	CB	BSER B	36	4526	4252	5163	−119	695	−414	C
ATOM	1025	OG	BSER B	36	12.329	−4.899	1.186	0.76	39.16		O
ANISOU	1025	OG	BSER B	36	5002	4309	5570	−86	739	−235	O
ATOM	1026	N	ASP B	37	10.698	−7.923	3.754	1.00	36.58		N
ANISOU	1026	N	ASP B	37	4318	4092	5487	−747	1282	−890	N
ATOM	1027	CA	ASP B	37	10.130	−8.523	4.984	1.00	37.16		C
ANISOU	1027	CA	ASP B	37	4280	4172	5669	−761	1328	−962	C
ATOM	1028	C	ASP B	37	9.856	−7.496	6.085	1.00	35.60		C
ANISOU	1028	C	ASP B	37	4103	4009	5414	−299	877	−735	C
ATOM	1029	O	ASP B	37	10.470	−6.457	6.119	1.00	36.66		O
ANISOU	1029	O	ASP B	37	4403	3919	5608	−4	611	−480	O
ATOM	1030	CB	ASP B	37	11.083	−9.583	5.575	1.00	38.44		C
ANISOU	1030	CB	ASP B	37	4514	3691	6402	−937	1751	−826	C
ATOM	1031	CG	ASP B	37	11.277	−10.783	4.673	1.00	43.73		C
ANISOU	1031	CG	ASP B	37	5311	4367	6939	−1103	2102	−1054	C
ATOM	1032	OD1	ASP B	37	10.839	−10.752	3.517	1.00	44.18		O
ANISOU	1032	OD1	ASP B	37	5386	4702	6697	−1423	2215	−1364	O
ATOM	1033	OD2	ASP B	37	11.841	−11.788	5.126	1.00	44.73		O
ANISOU	1033	OD2	ASP B	37	5497	4257	7241	−937	2273	−951	O
ATOM	1034	N	VAL B	38	8.970	−7.814	7.024	1.00	35.97		N
ANISOU	1034	N	VAL B	38	4016	4286	5364	−273	854	−848	N
ATOM	1035	CA	VAL B	38	8.783	−6.937	8.176	1.00	33.62		C
ANISOU	1035	CA	VAL B	38	3808	3936	5033	106	532	−670	C
ATOM	1036	C	VAL B	38	8.447	−7.770	9.404	1.00	34.40		C
ANISOU	1036	C	VAL B	38	3822	3988	5259	4	666	−717	C
ATOM	1037	O	VAL B	38	7.878	−8.855	9.295	1.00	34.50		O
ANISOU	1037	O	VAL B	38	3648	4186	5275	−284	971	−943	O
ATOM	1038	CB	VAL B	38	7.692	−5.892	7.944	1.00	33.86		C
ANISOU	1038	CB	VAL B	38	3754	4465	4644	444	285	−697	C
ATOM	1039	CG1	VAL B	38	6.288	−6.541	7.830	1.00	36.65		C
ANISOU	1039	CG1	VAL B	38	3763	5477	4684	297	391	−950	C
ATOM	1040	CG2	VAL B	38	7.674	−4.885	9.085	1.00	37.72		C
ANISOU	1040	CG2	VAL B	38	4457	4732	5143	817	73	−536	C
ATOM	1041	N	THR B	39	8.856	−7.279	10.564	1.00	37.67		N
ANISOU	1041	N	THR B	39	4392	4152	5770	189	471	−504	N
ATOM	1042	CA	THR B	39	8.531	−7.921	11.831	1.00	36.24		C
ANISOU	1042	CA	THR B	39	4139	3981	5649	135	553	−488	C
ATOM	1043	C	THR B	39	7.718	−6.941	12.674	1.00	34.97		C
ANISOU	1043	C	THR B	39	4090	4029	5168	437	300	−542	C
ATOM	1044	O	THR B	39	8.221	−5.906	13.110	1.00	38.33		O

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1044	O	THR B	39	4781	4243	5538	597	71	−409	O
ATOM	1045	CB	THR B	39	9.795	−8.354	12.590	1.00	43.86		C
ANISOU	1045	CB	THR B	39	5159	4530	6978	9	595	−129	C
ATOM	1046	OG1	THR B	39	10.460	−9.401	11.863	1.00	42.54		O
ANISOU	1046	OG1	THR B	39	4869	4111	7184	−230	984	−42	O
ATOM	1047	CG2	THR B	39	9.413	−8.872	13.954	1.00	47.38		C
ANISOU	1047	CG2	THR B	39	5524	5071	7406	−11	636	−55	C
ATOM	1048	N	LEU B	40	6.435	−7.223	12.841	1.00	30.76		N
ANISOU	1048	N	LEU B	40	3364	3903	4419	494	392	−753	N
ATOM	1049	CA	LEU B	40	5.551	−6.330	13.601	1.00	32.50		C
ANISOU	1049	CA	LEU B	40	3676	4308	4365	823	262	−790	C
ATOM	1050	C	LEU B	40	5.532	−6.811	15.075	1.00	37.02		C
ANISOU	1050	C	LEU B	40	4311	4781	4973	743	313	−755	C
ATOM	1051	O	LEU B	40	5.585	−8.017	15.341	1.00	37.31		O
ANISOU	1051	O	LEU B	40	4157	4829	5192	491	514	−751	O
ATOM	1052	CB	LEU B	40	4.139	−6.329	13.019	1.00	36.32		C
ANISOU	1052	CB	LEU B	40	3850	5363	4588	960	332	−947	C
ATOM	1053	CG	LEU B	40	4.041	−6.109	11.490	1.00	45.78		C
ANISOU	1053	CG	LEU B	40	4870	6857	5668	941	294	−955	C
ATOM	1054	CD1	LEU B	40	2.646	−6.421	10.967	1.00	48.96		C
ANISOU	1054	CD1	LEU B	40	4836	7996	5770	915	358	−1076	C
ATOM	1055	CD2	LEU B	40	4.397	−4.681	11.142	1.00	47.82		C
ANISOU	1055	CD2	LEU B	40	5366	6934	5870	1330	119	−745	C
ATOM	1056	N	GLU B	41	5.446	−5.880	16.017	1.00	34.50		N
ANISOU	1056	N	GLU B	41	4277	4359	4474	938	190	−728	N
ATOM	1057	CA	GLU B	41	5.673	−6.243	17.410	1.00	36.14		C
ANISOU	1057	CA	GLU B	41	4590	4488	4653	793	193	−654	C
ATOM	1058	C	GLU B	41	4.801	−5.494	18.382	1.00	35.37		C
ANISOU	1058	C	GLU B	41	4708	4481	4250	1017	225	−788	C
ATOM	1059	O	GLU B	41	4.434	−4.331	18.165	1.00	35.79		O
ANISOU	1059	O	GLU B	41	4988	4460	4152	1301	225	−869	O
ATOM	1060	CB	GLU B	41	7.139	−6.005	17.773	1.00	41.04		C
ANISOU	1060	CB	GLU B	41	5426	4789	5379	563	0	−408	C
ATOM	1061	CG	GLU B	41	8.104	−6.958	17.074	1.00	49.77		C
ANISOU	1061	CG	GLU B	41	6292	5756	6863	340	67	−177	C
ATOM	1062	CD	GLU B	41	9.578	−6.630	17.356	1.00	57.67		C
ANISOU	1062	CD	GLU B	41	7427	6508	7977	137	−147	157	C
ATOM	1063	OE1	GLU B	41	9.882	−5.449	17.648	1.00	58.68		O
ANISOU	1063	OE1	GLU B	41	7885	6534	7876	145	−375	107	O
ATOM	1064	OE2	GLU B	41	10.424	−7.551	17.289	1.00	61.84		O
ANISOU	1064	OE2	GLU B	41	7721	6940	8834	−43	−41	490	O
ATOM	1065	N	CYS B	42	4.458	−6.166	19.469	1.00	31.20		N
ANISOU	1065	N	CYS B	42	4119	4085	3653	909	321	−784	N
ATOM	1066	CA	CYS B	42	3.902	−5.459	20.588	1.00	33.63		C
ANISOU	1066	CA	CYS B	42	4725	4400	3653	1037	373	−897	C
ATOM	1067	C	CYS B	42	4.404	−6.176	21.834	1.00	34.18		C
ANISOU	1067	C	CYS B	42	4815	4520	3653	725	339	−747	C
ATOM	1068	O	CYS B	42	4.823	−7.349	21.766	1.00	35.93		O
ANISOU	1068	O	CYS B	42	4713	4812	4127	531	371	−536	O
ATOM	1069	CB	CYS B	42	2.349	−5.381	20.534	1.00	47.34		C
ANISOU	1069	CB	CYS B	42	6285	6418	5283	1388	612	−1061	C
ATOM	1070	SG	CYS B	42	1.472	−6.981	20.617	1.00	54.11		S
ANISOU	1070	SG	CYS B	42	6605	7676	6276	1269	806	−1080	S
ATOM	1071	N	ASN B	43	4.430	−5.438	22.940	1.00	36.79		N
ANISOU	1071	N	ASN B	43	5539	4802	3638	656	315	−828	N
ATOM	1072	CA	ASN B	43	5.008	−5.917	24.168	1.00	38.29		C
ANISOU	1072	CA	ASN B	43	5777	5131	3642	310	222	−640	C
ATOM	1073	C	ASN B	43	3.931	−6.211	25.187	1.00	44.90		C
ANISOU	1073	C	ASN B	43	6626	6187	4245	411	453	−764	C
ATOM	1074	O	ASN B	43	2.837	−5.661	25.112	1.00	41.32		O
ANISOU	1074	O	ASN B	43	6294	5706	3700	736	677	−1032	O
ATOM	1075	CB	ASN B	43	5.969	−4.877	24.742	1.00	48.08		C
ANISOU	1075	CB	ASN B	43	7481	6232	4553	−12	3	−660	C
ATOM	1076	CG	ASN B	43	7.024	−4.462	23.739	1.00	50.32		C
ANISOU	1076	CG	ASN B	43	7775	6275	5068	−102	−212	−541	C
ATOM	1077	OD1	ASN B	43	7.325	−3.290	23.587	1.00	57.91		O
ANISOU	1077	OD1	ASN B	43	9149	6978	5877	−149	−254	−733	O
ATOM	1078	ND2	ASN B	43	7.574	−5.423	23.044	1.00	44.09		N
ANISOU	1078	ND2	ASN B	43	6554	5525	4673	−124	−277	−232	N
ATOM	1079	O	PHE B	44	5.112	−7.564	28.721	1.00	52.80		O
ANISOU	1079	O	PHE B	44	7615	7986	4459	−503	239	−56	O
ATOM	1080	N	PHE B	44	4.234	−7.060	26.162	1.00	43.33		N
ANISOU	1080	N	PHE B	44	6281	6226	3957	159	428	−510	N
ATOM	1081	CA	PHE B	44	3.262	−7.240	27.227	1.00	45.35		C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1081	CA	PHE B	44	6609	6685	3936	233	653	−629	C
ATOM	1082	C	PHE B	44	3.932	−7.209	28.581	1.00	53.45		C
ANISOU	1082	C	PHE B	44	7849	7939	4521	−174	505	−446	C
ATOM	1083	CB	PHE B	44	2.460	−8.525	27.017	1.00	44.67		C
ANISOU	1083	CB	PHE B	44	6024	6763	4187	413	903	−530	C
ATOM	1084	CG	PHE B	44	3.297	−9.747	26.877	1.00	48.05		C
ANISOU	1084	CG	PHE B	44	6052	7242	4965	211	877	−101	C
ATOM	1085	CD1	PHE B	44	3.613	−10.508	27.985	1.00	53.57		C
ANISOU	1085	CD1	PHE B	44	6616	8174	5564	25	918	270	C
ATOM	1086	CD2	PHE B	44	3.765	−10.146	25.622	1.00	52.78		C
ANISOU	1086	CD2	PHE B	44	6404	7647	6004	224	877	−29	C
ATOM	1087	CE1	PHE B	44	4.386	−11.648	27.858	1.00	56.93		C
ANISOU	1087	CE1	PHE B	44	6641	8603	6387	−90	1000	768	C
ATOM	1088	CE2	PHE B	44	4.537	−11.288	25.478	1.00	52.65		C
ANISOU	1088	CE2	PHE B	44	6042	7584	6377	72	989	391	C
ATOM	1089	CZ	PHE B	44	4.850	−12.041	26.609	1.00	55.11		C
ANISOU	1089	CZ	PHE B	44	6196	8093	6649	−57	1072	822	C
ATOM	1090	O	ASP B	45	1.640	−7.122	32.030	1.00	76.11		O
ANISOU	1090	O	ASP B	45	11338	11369	6213	−211	1171	−855	O
ATOM	1091	N	ASP B	45	3.155	−6.759	29.566	1.00	60.34		N
ANISOU	1091	N	ASP B	45	9058	8898	4972	−159	700	−704	N
ATOM	1092	CA	ASP B	45	3.655	−6.433	30.889	1.00	69.25		C
ANISOU	1092	CA	ASP B	45	10529	10277	5505	−614	586	−666	C
ATOM	1093	C	ASP B	45	2.883	−7.200	31.942	1.00	78.36		C
ANISOU	1093	C	ASP B	45	11552	11755	6468	−573	812	−569	C
ATOM	1094	CB	ASP B	45	3.554	−4.929	31.156	1.00	71.36		C
ANISOU	1094	CB	ASP B	45	11510	10264	5339	−742	692	−1162	C
ATOM	1095	O	THR B	46	5.354	−8.573	34.718	1.00128.01			O
ANISOU	1095	O	THR B	46	19514	15362	13762	−1288	753	−976	O
ATOM	1096	N	THR B	46	3.654	−7.942	32.725	1.00117.53			N
ANISOU	1096	N	THR B	46	18518	13246	12891	−716	857	−1346	N
ATOM	1097	CA	THR B	46	3.159	−8.792	33.785	1.00122.03			C
ANISOU	1097	CA	THR B	46	18844	14174	13349	−633	1011	−1350	C
ATOM	1098	C	THR B	46	4.152	−8.726	34.941	1.00125.08			C
ANISOU	1098	C	THR B	46	19190	14916	13418	−1019	900	−1209	C
ATOM	1099	CB	THR B	46	2.995	−10.241	33.306	1.00124.30			C
ANISOU	1099	CB	THR B	46	18746	14629	13853	−407	1185	−1043	C
ATOM	1100	OG1	THR B	46	4.257	−10.735	32.850	1.00124.51			O
ANISOU	1100	OG1	THR B	46	18550	14813	13946	−597	1092	−637	O
ATOM	1101	CG2	THR B	46	1.990	−10.313	32.155	1.00123.96			C
ANISOU	1101	CG2	THR B	46	18739	14229	14130	−13	1291	−1192	C
ATOM	1102	O	GLY B	47	5.089	−10.155	39.186	1.00120.05			O
ANISOU	1102	O	GLY B	47	18382	15439	11790	−1710	814	−934	O
ATOM	1103	N	GLY B	47	3.658	−8.837	36.170	1.00125.72			N
ANISOU	1103	N	GLY B	47	19292	15218	13255	−1067	970	−1377	N
ATOM	1104	CA	GLY B	47	4.515	−8.742	37.342	1.00122.62			C
ANISOU	1104	CA	GLY B	47	18916	15139	12537	−1426	842	−1269	C
ATOM	1105	C	GLY B	47	4.897	−10.072	37.975	1.00116.92			C
ANISOU	1105	C	GLY B	47	17915	14796	11712	−1485	867	−929	C
ATOM	1106	O	SER B	48	5.763	−12.937	35.410	1.00	98.98		O
ANISOU	1106	O	SER B	48	14774	12605	10229	−991	934	−28	O
ATOM	1107	N	SER B	48	4.995	−11.095	37.155	1.00112.19			N
ANISOU	1107	N	SER B	48	17038	14218	11371	−1287	925	−643	N
ATOM	1108	CA	SER B	48	5.372	−12.390	37.667	1.00107.95			C
ANISOU	1108	CA	SER B	48	16268	13993	10755	−1315	894	−313	C
ATOM	1109	C	SER B	48	6.014	−13.170	36.570	1.00104.79			C
ANISOU	1109	C	SER B	48	15547	13588	10680	−1173	842	14	C
ATOM	1110	CB	SER B	48	4.136	−13.109	38.185	1.00103.44			C
ANISOU	1110	CB	SER B	48	15726	13493	10082	−1158	1140	−433	C
ATOM	1111	O	HIS B	49	5.643	−15.491	35.257	1.00110.33			O
ANISOU	1111	O	HIS B	49	15713	14352	11854	−677	1012	489	O
ATOM	1112	N	HIS B	49	6.807	−14.142	36.949	1.00106.08			N
ANISOU	1112	N	HIS B	49	15492	14016	10799	−1247	678	326	N
ATOM	1113	CA	HIS B	49	7.725	−14.723	36.032	1.00109.44			C
ANISOU	1113	CA	HIS B	49	15581	14485	11516	−1189	558	591	C
ATOM	1114	C	HIS B	49	6.799	−15.237	34.976	1.00109.74			C
ANISOU	1114	C	HIS B	49	15515	14332	11849	−845	808	610	C
ATOM	1115	CB	HIS B	49	8.432	−15.892	36.690	1.00111.32			C
ANISOU	1115	CB	HIS B	49	15610	15015	11670	−1226	328	883	C
ATOM	1116	O	VAL B	50	6.870	−17.628	32.146	1.00100.44			O
ANISOU	1116	O	VAL B	50	13531	13068	11562	−202	992	1166	O
ATOM	1117	N	VAL B	50	7.253	−15.286	33.737	1.00108.29			N
ANISOU	1117	N	VAL B	50	15126	14033	11987	−761	815	711	N
ATOM	1118	CA	VAL B	50	6.320	−15.373	32.640	1.00103.91			C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1118	CA	VAL B	50	14573	13208	11701	−462	1049	650	C
ATOM	1119	C	VAL B	50	6.006	−16.830	32.475	1.00100.58			C
ANISOU	1119	C	VAL B	50	13867	12923	11427	−203	1127	904	C
ATOM	1120	CB	VAL B	50	6.881	−14.791	31.330	1.00102.46			C
ANISOU	1120	CB	VAL B	50	14355	12807	11769	−517	1040	645	C
ATOM	1121	O	ASN B	51	3.504	−20.481	32.483	1.00	88.57		O
ANISOU	1121	O	ASN B	51	12002	11577	10076	573	1613	1295	O
ATOM	1122	N	ASN B	51	4.760	−17.172	32.721	1.00	99.47		N
ANISOU	1122	N	ASN B	51	13835	12720	11240	11	1339	792	N
ATOM	1123	CA	ASN B	51	4.456	−18.463	33.287	1.00	96.35		C
ANISOU	1123	CA	ASN B	51	13313	12537	10760	111	1373	993	C
ATOM	1124	C	ASN B	51	4.031	−19.417	32.210	1.00	91.66		C
ANISOU	1124	C	ASN B	51	12464	11860	10504	439	1523	1164	C
ATOM	1125	CB	ASN B	51	3.376	−18.330	34.345	1.00	96.71		C
ANISOU	1125	CB	ASN B	51	13633	12621	10492	66	1543	740	C
ATOM	1126	O	LEU B	52	4.971	−19.273	28.248	1.00	85.97		O
ANISOU	1126	O	LEU B	52	11233	10645	10785	772	1611	1388	O
ATOM	1127	N	LEU B	52	4.222	−18.995	30.969	1.00	90.63		N
ANISOU	1127	N	LEU B	52	12236	11516	10683	545	1559	1148	N
ATOM	1128	CA	LEU B	52	3.307	−19.377	29.924	1.00	88.19		C
ANISOU	1128	CA	LEU B	52	11845	10996	10666	882	1789	1126	C
ATOM	1129	C	LEU B	52	4.058	−19.906	28.728	1.00	86.56		C
ANISOU	1129	C	LEU B	52	11328	10766	10794	968	1736	1386	C
ATOM	1130	CB	LEU B	52	2.465	−18.176	29.546	1.00	87.40		C
ANISOU	1130	CB	LEU B	52	12047	10564	10597	956	1908	749	C
ATOM	1131	O	GLY B	53	0.462	−22.179	27.767	1.00	86.95		O
ANISOU	1131	O	GLY B	53	11206	10585	11247	1953	2471	1307	O
ATOM	1132	N	GLY B	53	3.656	−21.059	28.230	1.00	84.58		N
ANISOU	1132	N	GLY B	53	10839	10549	10747	1240	1849	1579	N
ATOM	1133	CA	GLY B	53	2.529	−21.119	27.340	1.00	84.37		C
ANISOU	1133	CA	GLY B	53	10850	10259	10948	1555	2095	1462	C
ATOM	1134	C	GLY B	53	1.215	−21.273	28.051	1.00	85.94		C
ANISOU	1134	C	GLY B	53	11213	10451	10989	1700	2294	1243	C
ATOM	1135	O	ALA B	54	−1.678	−17.977	28.102	1.00	71.58		O
ANISOU	1135	O	ALA B	54	10269	7822	9106	1969	2529	−144	O
ATOM	1136	N	ALA B	54	0.926	−20.332	28.932	1.00	83.82		N
ANISOU	1136	N	ALA B	54	11232	10166	10448	1525	2279	944	N
ATOM	1137	CA	ALA B	54	−0.398	−19.766	29.090	1.00	77.01		C
ANISOU	1137	CA	ALA B	54	10581	9123	9555	1680	2477	521	C
ATOM	1138	C	ALA B	54	−0.627	−18.587	28.134	1.00	71.62		C
ANISOU	1138	C	ALA B	54	10094	8043	9075	1795	2434	260	C
ATOM	1139	CB	ALA B	54	−0.604	−19.342	30.530	1.00	76.88		C
ANISOU	1139	CB	ALA B	54	10777	9291	9144	1426	2475	290	C
ATOM	1140	N	ILE B	55	0.376	−18.272	27.353	1.00	67.24		N
ANISOU	1140	N	ILE B	55	9520	7385	8645	1680	2273	468	N
ATOM	1141	CA	ILE B	55	0.261	−17.136	26.461	1.00	66.95		C
ANISOU	1141	CA	ILE B	55	9762	6940	8736	1717	2194	252	C
ATOM	1142	C	ILE B	55	−0.165	−17.553	25.067	1.00	67.05		C
ANISOU	1142	C	ILE B	55	9688	6686	9103	2023	2285	333	C
ATOM	1143	O	ILE B	55	0.413	−18.453	24.466	1.00	66.51		O
ANISOU	1143	O	ILE B	55	9325	6746	9200	2041	2320	679	O
ATOM	1144	CB	ILE B	55	1.564	−16.359	26.360	1.00	67.80		C
ANISOU	1144	CB	ILE B	55	9989	7041	8732	1340	1982	365	C
ATOM	1145	CG1	ILE B	55	1.631	−15.346	27.493	1.00	72.90		C
ANISOU	1145	CG1	ILE B	55	10914	7730	9053	1096	1865	103	C
ATOM	1146	CG2	ILE B	55	1.631	−15.601	25.034	1.00	65.66		C
ANISOU	1146	CG2	ILE B	55	9961	6339	8646	1360	1918	298	C
ATOM	1147	CD1	ILE B	55	2.955	−14.685	27.623	1.00	76.41		C
ANISOU	1147	CD1	ILE B	55	11438	8252	9345	687	1670	213	C
ATOM	1148	N	THR B	56	−1.217	−16.911	24.585	1.00	47.66		N
ANISOU	1148	N	THR B	56	8634	4154	5321	642	2450	802	N
ATOM	1149	CA	THR B	56	−1.536	−16.897	23.172	1.00	51.32		C
ANISOU	1149	CA	THR B	56	8646	4778	6076	310	2315	562	C
ATOM	1150	C	THR B	56	−1.153	−15.501	22.668	1.00	49.38		C
ANISOU	1150	C	THR B	56	7913	5043	5808	283	1829	539	C
ATOM	1151	O	THR B	56	−1.229	−14.530	23.418	1.00	51.68		O
ANISOU	1151	O	THR B	56	8163	5456	6019	328	1732	629	O
ATOM	1152	CB	THR B	56	−3.043	−17.190	22.918	1.00	71.03		C
ANISOU	1152	CB	THR B	56	11004	7017	8969	−160	2661	363	C
ATOM	1153	OG1	THR B	56	−3.392	−18.445	23.501	1.00	74.68		O
ANISOU	1153	OG1	THR B	56	11963	6931	9481	−162	3206	391	O
ATOM	1154	CG2	THR B	56	−3.354	−17.244	21.424	1.00	70.90		C
ANISOU	1154	CG2	THR B	56	10553	7209	9177	−477	2444	84	C
ATOM	1155	N	ALA B	57	−0.700	−15.387	21.427	1.00	41.89		N

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1155	N	ALA B	57	6653	4356	4905	224	1567	422	N
ATOM	1156	CA	ALA B	57	−0.611	−14.082	20.809	1.00	33.93		C
ANISOU	1156	CA	ALA B	57	5202	3751	3940	128	1222	392	C
ATOM	1157	C	ALA B	57	−1.081	−14.236	19.399	1.00	35.37		C
ANISOU	1157	C	ALA B	57	5115	4048	4278	−121	1144	196	C
ATOM	1158	O	ALA B	57	−0.800	−15.244	18.771	1.00	38.28		O
ANISOU	1158	O	ALA B	57	5632	4294	4616	−113	1231	91	O
ATOM	1159	CB	ALA B	57	0.857	−13.530	20.835	1.00	36.33		C
ANISOU	1159	CB	ALA B	57	5430	4344	4029	426	919	505	C
ATOM	1160	N	SER B	58	−1.749	−13.224	18.873	1.00	35.97		N
ANISOU	1160	N	SER B	58	4823	4361	4482	−305	969	149	N
ATOM	1161	CA	SER B	58	−2.133	−13.252	17.472	1.00	38.71		C
ANISOU	1161	CA	SER B	58	4923	4898	4886	−483	804	−26	C
ATOM	1162	C	SER B	58	−2.071	−11.861	16.920	1.00	37.40		C
ANISOU	1162	C	SER B	58	4439	5079	4693	−447	534	63	C
ATOM	1163	O	SER B	58	−2.246	−10.867	17.651	1.00	35.31		O
ANISOU	1163	O	SER B	58	4080	4849	4486	−405	533	201	O
ATOM	1164	CB	SER B	58	−3.550	−13.819	17.295	1.00	53.43		C
ANISOU	1164	CB	SER B	58	6670	6615	7014	−815	939	−237	C
ATOM	1165	OG	SER B	58	−3.592	−15.182	17.691	1.00	64.20		O
ANISOU	1165	OG	SER B	58	8381	7587	8426	−884	1266	−339	O
ATOM	1166	N	LEU B	59	−1.827	−11.788	15.617	1.00	32.74		N
ANISOU	1166	N	LEU B	59	3739	4711	3990	−452	346	−16	N
ATOM	1167	CA	LEU B	59	−1.876	−10.533	14.926	1.00	33.05		C
ANISOU	1167	CA	LEU B	59	3528	5044	3984	−404	137	82	C
ATOM	1168	C	LEU B	59	−3.023	−10.604	13.914	1.00	43.26		C
ANISOU	1168	C	LEU B	59	4615	6503	5320	−573	−36	−80	C
ATOM	1169	O	LEU B	59	−2.955	−11.349	12.937	1.00	47.27		O
ANISOU	1169	O	LEU B	59	5211	7069	5679	−635	−123	−265	O
ATOM	1170	CB	LEU B	59	−0.544	−10.237	14.247	1.00	35.74		C
ANISOU	1170	CB	LEU B	59	3937	5528	4113	−214	79	168	C
ATOM	1171	CG	LEU B	59	−0.479	−8.825	13.679	1.00	36.52		C
ANISOU	1171	CG	LEU B	59	3849	5853	4173	−142	−37	322	C
ATOM	1172	CD1	LEU B	59	−0.232	−7.796	14.759	1.00	35.91		C
ANISOU	1172	CD1	LEU B	59	3705	5716	4223	−100	31	481	C
ATOM	1173	CD2	LEU B	59	0.580	−8.796	12.670	1.00	39.62		C
ANISOU	1173	CD2	LEU B	59	4320	6366	4367	−13	−33	350	C
ATOM	1174	N	GLN B	60	−4.081	−9.846	14.153	1.00	39.57		N
ANISOU	1174	N	GLN B	60	3869	6119	5047	−635	−96	−28	N
ATOM	1175	CA	GLN B	60	−5.260	−9.955	13.305	1.00	44.90		C
ANISOU	1175	CA	GLN B	60	4262	6996	5803	−782	−315	−200	C
ATOM	1176	C	GLN B	60	−5.456	−8.737	12.424	1.00	42.61		C
ANISOU	1176	C	GLN B	60	3772	7041	5378	−591	−578	−38	C
ATOM	1177	O	GLN B	60	−5.641	−7.623	12.914	1.00	38.62		O
ANISOU	1177	O	GLN B	60	3138	6547	4989	−453	−519	192	O
ATOM	1178	CB	GLN B	60	−6.487	−10.178	14.165	1.00	46.57		C
ANISOU	1178	CB	GLN B	60	4236	7057	6401	−985	−165	−284	C
ATOM	1179	CG	GLN B	60	−6.467	−11.510	14.903	1.00	54.37		C
ANISOU	1179	CG	GLN B	60	5469	7672	7519	−1191	144	−457	C
ATOM	1180	CD	GLN B	60	−6.650	−12.710	13.974	1.00	64.33		C
ANISOU	1180	CD	GLN B	60	6785	8929	8728	−1425	48	−798	C
ATOM	1181	OE1	GLN B	60	−7.229	−12.588	12.885	1.00	71.72		O
ANISOU	1181	OE1	GLN B	60	7460	10177	9613	−1514	−290	−971	O
ATOM	1182	NE2	GLN B	60	−6.177	−13.874	14.408	1.00	63.52		N
ANISOU	1182	NE2	GLN B	60	7052	8463	8617	−1509	346	−901	N
ATOM	1183	N	LYS B	61	−5.452	−8.952	11.110	1.00	42.99		N
ANISOU	1183	N	LYS B	61	3842	7340	5154	−565	−847	−157	N
ATOM	1184	CA	LYS B	61	−5.655	−7.833	10.207	1.00	38.43		C
ANISOU	1184	CA	LYS B	61	3146	7075	4380	−323	−1088	32	C
ATOM	1185	C	LYS B	61	−7.097	−7.330	10.336	1.00	41.13		C
ANISOU	1185	C	LYS B	61	3039	7593	4995	−332	−1270	42	C
ATOM	1186	O	LYS B	61	−8.078	−8.102	10.326	1.00	44.45		O
ANISOU	1186	O	LYS B	61	3189	8076	5623	−575	−1409	−238	O
ATOM	1187	CB	LYS B	61	−5.309	−8.216	8.759	1.00	49.92		C
ANISOU	1187	CB	LYS B	61	4809	8762	5395	−256	−1328	−97	C
ATOM	1188	CG	LYS B	61	−5.010	−7.020	7.886	1.00	50.07		C
ANISOU	1188	CG	LYS B	61	4916	9005	5104	83	−1430	198	C
ATOM	1189	CD	LYS B	61	−4.664	−7.435	6.472	1.00	54.24		C
ANISOU	1189	CD	LYS B	61	5734	9743	5130	171	−1626	72	C
ATOM	1190	CE	LYS B	61	−4.271	−6.245	5.603	1.00	51.21		C
ANISOU	1190	CE	LYS B	61	5538	9521	4396	545	−1630	414	C
ATOM	1191	NZ	LYS B	61	−5.303	−5.218	5.441	1.00	50.86		N
ANISOU	1191	NZ	LYS B	61	5226	9714	4385	773	−1875	630	N
ATOM	1192	N	VAL B	62	−7.245	−6.020	10.449	1.00	43.87		N

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1192	N	VAL B	62	3278	8008	5381	−66	−1244	358	N
ATOM	1193	CA	VAL B	62	−8.584	−5.457	10.571	1.00	44.83		C
ANISOU	1193	CA	VAL B	62	2946	8300	5787	7	−1387	416	C
ATOM	1194	C	VAL B	62	−9.384	−5.557	9.276	1.00	52.62		C
ANISOU	1194	C	VAL B	62	3716	9701	6577	102	−1875	291	C
ATOM	1195	O	VAL B	62	−10.520	−6.015	9.299	1.00	56.68		O
ANISOU	1195	O	VAL B	62	3886	10258	7390	−61	−2037	64	O
ATOM	1196	CB	VAL B	62	−8.555	−3.977	11.004	1.00	43.44		C
ANISOU	1196	CB	VAL B	62	2763	8040	5703	315	−1187	803	C
ATOM	1197	CG1	VAL B	62	−9.985	−3.405	10.995	1.00	50.36		C
ANISOU	1197	CG1	VAL B	62	3205	9057	6874	462	−1319	858	C
ATOM	1198	CG2	VAL B	62	−7.969	−3.849	12.397	1.00	41.17		C
ANISOU	1198	CG2	VAL B	62	2669	7343	5631	192	−748	861	C
ATOM	1199	O	GLU B	63	−11.560	−5.909	5.991	1.00	92.29		O
ANISOU	1199	O	GLU B	63	8497	15454	11114	309	−3144	−98	O
ATOM	1200	N	GLU B	63	−8.803	−5.127	8.156	1.00	55.98		N
ANISOU	1200	N	GLU B	63	4451	10290	6529	363	−2045	425	N
ATOM	1201	CA	GLU B	63	−9.603	−4.907	6.931	1.00	70.47		C
ANISOU	1201	CA	GLU B	63	6241	12377	8157	552	−2458	383	C
ATOM	1202	C	GLU B	63	−10.460	−6.093	6.519	1.00	84.42		C
ANISOU	1202	C	GLU B	63	7778	14280	10017	235	−2803	−52	C
ATOM	1203	CB	GLU B	63	−8.716	−4.535	5.741	1.00	70.62		C
ANISOU	1203	CB	GLU B	63	6742	12504	7587	822	−2525	542	C
ATOM	1204	O	ASP B	64	−12.942	−8.390	5.647	1.00112.02			O
ANISOU	1204	O	ASP B	64	10559	18045	13960	−535	−3581	−975	O
ATOM	1205	N	ASP B	64	−9.955	−7.301	6.751	1.00	85.46		N
ANISOU	1205	N	ASP B	64	8028	14318	10126	−125	−2707	−370	N
ATOM	1206	CA	ASP B	64	−10.612	−8.517	6.258	1.00	97.58		C
ANISOU	1206	CA	ASP B	64	9451	15923	11702	−478	−2979	−827	C
ATOM	1207	C	ASP B	64	−12.114	−8.618	6.540	1.00104.54			C
ANISOU	1207	C	ASP B	64	9782	16839	13100	−645	−3152	−952	C
ATOM	1208	CB	ASP B	64	−9.906	−9.717	6.848	1.00	97.62		C
ANISOU	1208	CB	ASP B	64	9637	15696	11759	−859	−2687	−1128	C
ATOM	1209	CG	ASP B	64	−8.446	−9.708	6.546	1.00	95.55		C
ANISOU	1209	CG	ASP B	64	9892	15387	11024	−701	−2511	−1008	C
ATOM	1210	OD1	ASP B	64	−8.067	−9.230	5.456	1.00	98.14		O
ANISOU	1210	OD1	ASP B	64	10490	15933	10866	−411	−2716	−880	O
ATOM	1211	OD2	ASP B	64	−7.672	−10.145	7.407	1.00	91.84		O
ANISOU	1211	OD2	ASP B	64	9661	14510	10724	−811	−2073	−967	O
ATOM	1212	O	PRO B	68	−7.396	−14.242	5.894	1.00100.74			O
ANISOU	1212	O	PRO B	68	11578	15240	11460	−1752	−2074	−2335	O
ATOM	1213	N	PRO B	68	−10.494	−14.729	5.787	1.00116.51			N
ANISOU	1213	N	PRO B	68	12523	17506	14238	−2372	−2688	−2893	N
ATOM	1214	CA	PRO B	68	−9.523	−14.470	4.739	1.00115.35			C
ANISOU	1214	CA	PRO B	68	12851	17560	13416	−2073	−2862	−2825	C
ATOM	1215	C	PRO B	68	−8.097	−14.880	5.116	1.00108.70			C
ANISOU	1215	C	PRO B	68	12519	16424	12358	−2030	−2399	−2785	C
ATOM	1216	CB	PRO B	68	−9.677	−12.976	4.532	1.00114.27			C
ANISOU	1216	CB	PRO B	68	12501	17767	13148	−1604	−3110	−2344	C
ATOM	1217	CG	PRO B	68	−11.141	−12.739	4.750	1.00118.30			C
ANISOU	1217	CG	PRO B	68	12431	18385	14134	−1717	−3353	−2358	C
ATOM	1218	CD	PRO B	68	−11.641	−13.810	5.677	1.00119.42			C
ANISOU	1218	CD	PRO B	68	12368	18178	14830	−2207	−3038	−2678	C
ATOM	1219	O	HIS B	69	−6.646	−18.953	4.114	1.00120.78			O
ANISOU	1219	O	HIS B	69	15599	16807	13485	−2796	−1566	−3991	O
ATOM	1220	N	HIS B	69	−7.700	−16.015	4.583	1.00111.88			N
ANISOU	1220	N	HIS B	69	13358	16609	12542	−2250	−2284	−3167	N
ATOM	1221	CA	HIS B	69	−7.040	−16.999	5.387	1.00110.83			C
ANISOU	1221	CA	HIS B	69	13567	15888	12656	−2396	−1698	−3209	C
ATOM	1222	C	HIS B	69	−6.190	−17.916	4.549	1.00115.95			C
ANISOU	1222	C	HIS B	69	14844	16336	12877	−2402	−1536	−3468	C
ATOM	1223	CB	HIS B	69	−8.037	−17.782	6.242	1.00112.06			C
ANISOU	1223	CB	HIS B	69	13413	15751	13414	−2880	−1520	−3510	C
ATOM	1224	CG	HIS B	69	−9.089	−18.535	5.473	1.00118.11			C
ANISOU	1224	CG	HIS B	69	14038	16580	14259	−3248	−1819	−3981	C
ATOM	1225	ND1	HIS B	69	−10.171	−17.934	4.866	1.00121.55			N
ANISOU	1225	ND1	HIS B	69	14012	17446	14725	−3209	−2368	−3968	N
ATOM	1226	CD2	HIS B	69	−9.249	−19.866	5.280	1.00122.49			C
ANISOU	1226	CD2	HIS B	69	14879	16737	14925	−3601	−1596	−4383	C
ATOM	1227	CE1	HIS B	69	−10.923	−18.855	4.298	1.00128.90			C
ANISOU	1227	CE1	HIS B	69	14932	18293	15752	−3555	−2524	−4379	C
ATOM	1228	NE2	HIS B	69	−10.395	−20.036	4.551	1.00129.64			N
ANISOU	1228	NE2	HIS B	69	15468	17881	15909	−3808	−2049	−4641	N
ATOM	1229	O	ARG B	70	−2.018	−17.873	6.287	1.00105.31			O

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1229	O	ARG B	70	14427	14088	11496	−1298	−121	−2287	O
ATOM	1230	N	ARG B	70	−4.961	−17.523	4.284	1.00114.04			N
ANISOU	1230	N	ARG B	70	14970	16073	12286	−1979	−1341	−3127	N
ATOM	1231	CA	ARG B	70	−3.823	−18.258	4.776	1.00112.98			C
ANISOU	1231	CA	ARG B	70	15269	15450	12207	−1852	−776	−3017	C
ATOM	1232	C	ARG B	70	−3.127	−17.515	5.909	1.00105.58			C
ANISOU	1232	C	ARG B	70	14169	14414	11531	−1529	−516	−2474	C
ATOM	1233	CB	ARG B	70	−2.849	−18.564	3.641	1.00116.54			C
ANISOU	1233	CB	ARG B	70	16265	15900	12115	−1636	−671	−3100	C
ATOM	1234	O	GLU B	71	−1.608	−16.244	8.152	1.00	77.81		O
ANISOU	1234	O	GLU B	71	10423	10689	8452	−950	−46	−1552	O
ATOM	1235	N	GLU B	71	−3.768	−16.540	6.535	1.00100.31			N
ANISOU	1235	N	GLU B	71	13034	13965	11113	−1512	−718	−2239	N
ATOM	1236	CA	GLU B	71	−3.183	−15.221	6.679	1.00	89.47		C
ANISOU	1236	CA	GLU B	71	11517	12824	9652	−1140	−770	−1774	C
ATOM	1237	C	GLU B	71	−1.882	−15.275	7.487	1.00	76.87		C
ANISOU	1237	C	GLU B	71	10116	10939	8152	−881	−351	−1470	C
ATOM	1238	CB	GLU B	71	−4.171	−14.252	7.336	1.00	87.85		C
ANISOU	1238	CB	GLU B	71	10806	12820	9753	−1183	−988	−1602	C
ATOM	1239	CG	GLU B	71	−4.728	−13.148	6.430	1.00	86.37		C
ANISOU	1239	CG	GLU B	71	10390	13114	9313	−1029	−1427	−1504	C
ATOM	1240	CD	GLU B	71	−6.011	−12.568	6.958	1.00	82.99		C
ANISOU	1240	CD	GLU B	71	9429	12859	9243	−1144	−1655	−1477	C
ATOM	1241	OE1	GLU B	71	−6.432	−11.492	6.577	1.00	80.10		O
ANISOU	1241	OE1	GLU B	71	8830	12828	8777	−928	−1933	−1270	O
ATOM	1242	OE2	GLU B	71	−6.615	−13.201	7.802	1.00	85.14		O
ANISOU	1242	OE2	GLU B	71	9521	12900	9928	−1433	−1502	−1647	O
ATOM	1243	O	ARG B	72	2.482	−14.256	7.485	1.00	46.67		O
ANISOU	1243	O	ARG B	72	6633	7026	4076	123	399	−640	O
ATOM	1244	N	ARG B	72	−1.063	−14.245	7.308	1.00	65.86		N
ANISOU	1244	N	ARG B	72	8690	9726	6609	−570	−346	−1135	N
ATOM	1245	CA	ARG B	72	0.265	−14.288	6.735	1.00	54.71		C
ANISOU	1245	CA	ARG B	72	7564	8277	4947	−301	−115	−1017	C
ATOM	1246	C	ARG B	72	1.361	−13.956	7.725	1.00	46.15		C
ANISOU	1246	C	ARG B	72	6391	7051	4092	−79	151	−704	C
ATOM	1247	CB	ARG B	72	0.379	−13.231	5.652	1.00	51.55		C
ANISOU	1247	CB	ARG B	72	7171	8213	4203	−125	−288	−871	C
ATOM	1248	CG	ARG B	72	0.167	−13.674	4.224	1.00	53.12		C
ANISOU	1248	CG	ARG B	72	7705	8556	3923	−145	−427	−1139	C
ATOM	1249	CD	ARG B	72	0.600	−12.558	3.286	1.00	51.88		C
ANISOU	1249	CD	ARG B	72	7649	8661	3403	142	−455	−874	C
ATOM	1250	NE	ARG B	72	1.905	−12.824	2.745	1.00	55.84		N
ANISOU	1250	NE	ARG B	72	8491	9016	3709	352	−47	−805	N
ATOM	1251	CZ	ARG B	72	2.778	−11.923	2.381	1.00	55.87		C
ANISOU	1251	CZ	ARG B	72	8540	9076	3614	611	193	−489	C
ATOM	1252	NH1	ARG B	72	3.904	−12.320	1.907	1.00	61.32		N
ANISOU	1252	NH1	ARG B	72	9502	9614	4184	774	601	−473	N
ATOM	1253	NH2	ARG B	72	2.540	−10.650	2.465	1.00	58.36		N
ANISOU	1253	NH2	ARG B	72	8641	9563	3969	707	81	−196	N
ATOM	1254	N	ALA B	73	1.033	−13.313	8.822	1.00	41.84		N
ANISOU	1254	N	ALA B	73	5561	6508	3830	−110	88	−527	N
ATOM	1255	CA	ALA B	73	2.039	−12.903	9.774	1.00	39.81		C
ANISOU	1255	CA	ALA B	73	5200	6174	3751	82	255	−270	C
ATOM	1256	C	ALA B	73	2.232	−13.993	10.778	1.00	45.23		C
ANISOU	1256	C	ALA B	73	6027	6555	4605	91	438	−325	C
ATOM	1257	O	ALA B	73	1.299	−14.386	11.438	1.00	45.12		O
ANISOU	1257	O	ALA B	73	6010	6393	4740	−96	421	−421	O
ATOM	1258	CB	ALA B	73	1.632	−11.633	10.453	1.00	39.35		C
ANISOU	1258	CB	ALA B	73	4845	6248	3858	58	115	−70	C
ATOM	1259	N	THR B	74	3.442	−14.487	10.903	1.00	34.99		N
ANISOU	1259	N	THR B	74	4850	5150	3293	337	646	−247	N
ATOM	1260	CA	THR B	74	3.656	−15.619	11.770	1.00	37.57		C
ANISOU	1260	CA	THR B	74	5387	5165	3725	427	843	−269	C
ATOM	1261	C	THR B	74	4.344	−15.226	13.081	1.00	37.02		C
ANISOU	1261	C	THR B	74	5163	5105	3797	644	826	−23	C
ATOM	1262	O	THR B	74	5.317	−14.477	13.082	1.00	37.96		O
ANISOU	1262	O	THR B	74	5052	5433	3937	818	769	128	O
ATOM	1263	CB	THR B	74	4.468	−16.687	11.072	1.00	43.56		C
ANISOU	1263	CB	THR B	74	6441	5748	4361	612	1106	−364	C
ATOM	1264	OG1	THR B	74	3.836	−16.981	9.830	1.00	49.20		O
ANISOU	1264	OG1	THR B	74	7337	6480	4878	394	1083	−634	O
ATOM	1265	CG2	THR B	74	4.494	−17.946	11.920	1.00	45.70		C
ANISOU	1265	CG2	THR B	74	7009	5626	4728	713	1352	−385	C
ATOM	1266	N	LEU B	75	3.835	−15.758	14.182	1.00	34.30		N

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1266	N	LEU B	75	4964	4527	3541	620	889	−5	N
ATOM	1267	CA	LEU B	75	4.362	−15.463	15.521	1.00	33.45		C
ANISOU	1267	CA	LEU B	75	4797	4426	3485	835	836	204	C
ATOM	1268	C	LEU B	75	5.764	−16.055	15.671	1.00	35.36		C
ANISOU	1268	C	LEU B	75	5091	4659	3685	1245	925	324	C
ATOM	1269	O	LEU B	75	5.977	−17.199	15.310	1.00	38.87		O
ANISOU	1269	O	LEU B	75	5820	4860	4089	1381	1166	268	O
ATOM	1270	CB	LEU B	75	3.444	−16.027	16.606	1.00	34.03		C
ANISOU	1270	CB	LEU B	75	5124	4199	3608	748	964	207	C
ATOM	1271	CG	LEU B	75	3.881	−15.838	18.067	1.00	36.37		C
ANISOU	1271	CG	LEU B	75	5490	4473	3855	998	914	414	C
ATOM	1272	CD1	LEU B	75	3.922	−14.351	18.444	1.00	31.54		C
ANISOU	1272	CD1	LEU B	75	4543	4172	3269	910	638	477	C
ATOM	1273	CD2	LEU B	75	2.986	−16.634	19.025	1.00	38.85		C
ANISOU	1273	CD2	LEU B	75	6187	4396	4179	949	1176	431	C
ATOM	1274	N	LEU B	76	6.695	−15.274	16.214	1.00	34.81		N
ANISOU	1274	N	LEU B	76	4730	4847	3649	1435	735	470	N
ATOM	1275	CA	LEU B	76	8.029	−15.802	16.587	1.00	37.41		C
ANISOU	1275	CA	LEU B	76	5010	5224	3980	1872	753	601	C
ATOM	1276	C	LEU B	76	8.068	−16.133	18.089	1.00	41.31		C
ANISOU	1276	C	LEU B	76	5685	5625	4385	2111	654	743	C
ATOM	1277	O	LEU B	76	8.232	−15.251	18.927	1.00	40.95		O
ANISOU	1277	O	LEU B	76	5441	5795	4324	2097	383	794	O
ATOM	1278	CB	LEU B	76	9.110	−14.785	16.219	1.00	37.28		C
ANISOU	1278	CB	LEU B	76	4503	5576	4087	1923	594	635	C
ATOM	1279	CG	LEU B	76	9.029	−14.252	14.777	1.00	42.18		C
ANISOU	1279	CG	LEU B	76	4998	6287	4741	1694	718	536	C
ATOM	1280	CD1	LEU B	76	10.035	−13.122	14.567	1.00	39.49		C
ANISOU	1280	CD1	LEU B	76	4180	6255	4570	1694	631	584	C
ATOM	1281	CD2	LEU B	76	9.197	−15.374	13.688	1.00	38.51		C
ANISOU	1281	CD2	LEU B	76	4814	5625	4195	1822	1036	458	C
ATOM	1282	N	GLU B	77	7.837	−17.393	18.425	1.00	39.69		N
ANISOU	1282	N	GLU B	77	4778	5378	4924	1296	363	625	N
ATOM	1283	CA	GLU B	77	7.582	−17.774	19.811	1.00	44.60		C
ANISOU	1283	CA	GLU B	77	5477	6106	5362	1498	410	791	C
ATOM	1284	C	GLU B	77	8.796	−17.544	20.715	1.00	45.19		C
ANISOU	1284	C	GLU B	77	5476	6439	5256	1685	181	920	C
ATOM	1285	O	GLU B	77	8.660	−17.279	21.907	1.00	50.57		O
ANISOU	1285	O	GLU B	77	6241	7303	5670	1821	74	971	O
ATOM	1286	CB	GLU B	77	7.165	−19.248	19.893	1.00	53.70		C
ANISOU	1286	CB	GLU B	77	6705	7051	6646	1605	766	988	C
ATOM	1287	CG	GLU B	77	5.752	−19.535	19.448	1.00	60.50		C
ANISOU	1287	CG	GLU B	77	7642	7685	7661	1442	969	884	C
ATOM	1288	CD	GLU B	77	5.413	−21.020	19.487	1.00	69.41		C
ANISOU	1288	CD	GLU B	77	8826	8562	8985	1522	1338	1059	C
ATOM	1289	OE1	GLU B	77	6.328	−21.864	19.283	1.00	71.22		O
ANISOU	1289	OE1	GLU B	77	9036	8718	9305	1636	1471	1204	O
ATOM	1290	OE2	GLU B	77	4.226	−21.339	19.734	1.00	71.86		O
ANISOU	1290	OE2	GLU B	77	9184	8725	9396	1475	1521	1065	O
ATOM	1291	N	GLU B	78	9.979	−17.635	20.132	1.00	43.81		N
ANISOU	1291	N	GLU B	78	5142	6279	5226	1691	102	975	N
ATOM	1292	CA	GLU B	78	11.199	−17.584	20.904	1.00	49.48		C
ANISOU	1292	CA	GLU B	78	5724	7232	5845	1865	−125	1140	C
ATOM	1293	C	GLU B	78	11.365	−16.221	21.569	1.00	52.51		C
ANISOU	1293	C	GLU B	78	6084	7858	6011	1793	−512	944	C
ATOM	1294	O	GLU B	78	12.129	−16.083	22.505	1.00	56.31		O
ANISOU	1294	O	GLU B	78	6500	8583	6313	1928	−767	1039	O
ATOM	1295	CB	GLU B	78	12.406	−17.900	20.023	1.00	49.92		C
ANISOU	1295	CB	GLU B	78	5573	7213	6183	1872	−96	1247	C
ATOM	1296	CG	GLU B	78	12.947	−16.717	19.222	1.00	50.53		C
ANISOU	1296	CG	GLU B	78	5498	7306	6396	1674	−312	1035	C
ATOM	1297	CD	GLU B	78	12.175	−16.483	17.911	1.00	50.44		C
ANISOU	1297	CD	GLU B	78	5589	7055	6520	1461	−123	828	C
ATOM	1298	OE1	GLU B	78	11.111	−17.143	17.702	1.00	49.57		O
ANISOU	1298	OE1	GLU B	78	5663	6787	6385	1430	115	802	O
ATOM	1299	OE2	GLU B	78	12.624	−15.622	17.113	1.00	46.37		O
ANISOU	1299	OE2	GLU B	78	4963	6517	6139	1328	−223	699	O
ATOM	1300	N	GLN B	79	10.655	−15.206	21.103	1.00	49.31		N
ANISOU	1300	N	GLN B	79	5732	7386	5619	1580	−564	668	N
ATOM	1301	CA	GLN B	79	10.848	−13.899	21.717	1.00	54.81		C
ANISOU	1301	CA	GLN B	79	6416	8265	6144	1502	−894	461	C
ATOM	1302	C	GLN B	79	9.832	−13.573	22.824	1.00	51.84		C
ANISOU	1302	C	GLN B	79	6290	7972	5437	1563	−887	380	C
ATOM	1303	O	GLN B	79	9.952	−12.548	23.510	1.00	50.98		O

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1303	O	GLN B	79	6233	8009	5127	1520	−1140	193	O
ATOM	1304	CB	GLN B	79	10.857	−12.834	20.623	1.00	64.12		C
ANISOU	1304	CB	GLN B	79	7485	9325	7551	1261	−952	231	C
ATOM	1305	CG	GLN B	79	12.236	−12.808	19.927	1.00	71.51		C
ANISOU	1305	CG	GLN B	79	8155	10262	8754	1237	−1060	304	C
ATOM	1306	CD	GLN B	79	12.219	−12.131	18.588	1.00	75.16		C
ANISOU	1306	CD	GLN B	79	8532	10547	9479	1051	−979	170	C
ATOM	1307	OE1	GLN B	79	11.348	−11.304	18.305	1.00	75.81		O
ANISOU	1307	OE1	GLN B	79	8707	10563	9535	913	−961	−20	O
ATOM	1308	NE2	GLN B	79	13.186	−12.481	17.740	1.00	77.35		N
ANISOU	1308	NE2	GLN B	79	8634	10739	10016	1067	−901	296	N
ATOM	1309	N	LEU B	80	8.870	−14.465	23.035	1.00	49.02		N
ANISOU	1309	N	LEU B	80	6090	7501	5034	1671	−577	525	N
ATOM	1310	CA	LEU B	80	7.907	−14.277	24.108	1.00	51.73		C
ANISOU	1310	CA	LEU B	80	6675	7895	5085	1773	−492	506	C
ATOM	1311	C	LEU B	80	8.547	−14.120	25.503	1.00	55.40		C
ANISOU	1311	C	LEU B	80	7257	8653	5139	1971	−739	557	C
ATOM	1312	O	LEU B	80	8.093	−13.287	26.285	1.00	56.56		O
ANISOU	1312	O	LEU B	80	7598	8886	5005	1972	−825	386	O
ATOM	1313	CB	LEU B	80	6.910	−15.428	24.115	1.00	50.36		C
ANISOU	1313	CB	LEU B	80	6604	7532	5000	1878	−91	711	C
ATOM	1314	CG	LEU B	80	5.920	−15.352	22.953	1.00	48.15		C
ANISOU	1314	CG	LEU B	80	6266	6987	5041	1656	104	593	C
ATOM	1315	CD1	LEU B	80	5.095	−16.625	22.877	1.00	51.51		C
ANISOU	1315	CD1	LEU B	80	6739	7201	5631	1727	475	791	C
ATOM	1316	CD2	LEU B	80	5.013	−14.117	23.041	1.00	44.05		C
ANISOU	1316	CD2	LEU B	80	5818	6449	4469	1525	62	373	C
ATOM	1317	N	PRO B	81	9.599	−14.902	25.824	1.00	58.66		N
ANISOU	1317	N	PRO B	81	7562	9223	5503	2144	−855	794	N
ATOM	1318	CA	PRO B	81	10.204	−14.675	27.148	1.00	62.15		C
ANISOU	1318	CA	PRO B	81	8116	9988	5509	2323	−1161	831	C
ATOM	1319	C	PRO B	81	10.839	−13.287	27.307	1.00	63.28		C
ANISOU	1319	C	PRO B	81	8200	10292	5553	2132	−1607	496	C
ATOM	1320	O	PRO B	81	11.115	−12.879	28.430	1.00	65.62		O
ANISOU	1320	O	PRO B	81	8658	10843	5434	2227	−1883	422	O
ATOM	1321	CB	PRO B	81	11.286	−15.758	27.241	1.00	65.57		C
ANISOU	1321	CB	PRO B	81	8359	10546	6008	2527	−1216	1180	C
ATOM	1322	CG	PRO B	81	10.900	−16.781	26.236	1.00	63.57		C
ANISOU	1322	CG	PRO B	81	8019	9984	6149	2519	−790	1356	C
ATOM	1323	CD	PRO B	81	10.182	−16.078	25.148	1.00	60.09		C
ANISOU	1323	CD	PRO B	81	7558	9299	5974	2223	−686	1063	C
ATOM	1324	N	LEU B	82	11.072	−12.585	26.201	1.00	62.19		N
ANISOU	1324	N	LEU B	82	7846	9999	5783	1870	−1667	298	N
ATOM	1325	CA	LEU B	82	11.525	−11.189	26.246	1.00	65.18		C
ANISOU	1325	CA	LEU B	82	8163	10447	6155	1656	−2014	−43	C
ATOM	1326	C	LEU B	82	10.360	−10.223	26.447	1.00	61.76		C
ANISOU	1326	C	LEU B	82	7990	9888	5589	1545	−1879	−321	C
ATOM	1327	O	LEU B	82	10.544	−9.011	26.413	1.00	62.06		O
ANISOU	1327	O	LEU B	82	8007	9912	5662	1354	−2080	−625	O
ATOM	1328	CB	LEU B	82	12.276	−10.803	24.961	1.00	66.50		C
ANISOU	1328	CB	LEU B	82	7986	10475	6805	1446	−2081	−103	C
ATOM	1329	CG	LEU B	82	13.649	−11.418	24.722	1.00	71.74		C
ANISOU	1329	CG	LEU B	82	8331	11249	7678	1515	−2261	126	C
ATOM	1330	CD1	LEU B	82	14.531	−10.423	23.985	1.00	74.30		C
ANISOU	1330	CD1	LEU B	82	8354	11514	8360	1282	−2484	−56	C
ATOM	1331	CD2	LEU B	82	14.270	−11.826	26.055	1.00	76.78		C
ANISOU	1331	CD2	LEU B	82	9014	12217	7941	1724	−2566	269	C
ATOM	1332	N	GLY B	83	9.162	−10.765	26.628	1.00	57.80		N
ANISOU	1332	N	GLY B	83	7708	9265	4987	1666	−1507	−202	N
ATOM	1333	CA	GLY B	83	7.969	−9.942	26.760	1.00	52.94		C
ANISOU	1333	CA	GLY B	83	7308	8497	4309	1588	−1308	−403	C
ATOM	1334	C	GLY B	83	7.471	−9.300	25.469	1.00	49.05		C
ANISOU	1334	C	GLY B	83	6645	7753	4239	1351	−1170	−532	C
ATOM	1335	O	GLY B	83	6.804	−8.269	25.501	1.00	43.27		O
ANISOU	1335	O	GLY B	83	6015	6912	3512	1244	−1106	−744	O
ATOM	1336	N	LYS B	84	7.776	−9.906	24.331	1.00	41.11		N
ANISOU	1336	N	LYS B	84	5397	6648	3573	1284	−1104	−393	N
ATOM	1337	C	LYS B	84	6.620	−10.405	22.248	1.00	40.66		C
ANISOU	1337	C	LYS B	84	5158	6226	4065	1101	−700	−291	C
ATOM	1338	O	LYS B	84	6.992	−11.577	22.219	1.00	39.22		O
ANISOU	1338	O	LYS B	84	4943	6063	3896	1215	−630	−87	O
ATOM	1339	CA	LYS B	84	7.350	−9.358	23.055	1.00	45.90		C
ANISOU	1339	CA	LYS B	84	5858	7048	4532	1083	−992	−487	C
ATOM	1340	CB	LYS B	84	8.524	−8.860	22.197	1.00	53.74		C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1340	CB	LYS B	84	6590	8049	5780	937	−1214	−567	C
ATOM	1341	CG	LYS B	84	9.560	−8.016	22.877	1.00	65.52		C
ANISOU	1341	CG	LYS B	84	8027	9698	7171	889	−1563	−745	C
ATOM	1342	CD	LYS B	84	10.240	−7.076	21.866	1.00	69.89		C
ANISOU	1342	CD	LYS B	84	8328	10143	8083	687	−1668	−879	C
ATOM	1343	CE	LYS B	84	11.012	−7.826	20.787	1.00	69.93		C
ANISOU	1343	CE	LYS B	84	8093	10097	8379	694	−1612	−673	C
ATOM	1344	NZ	LYS B	84	12.040	−8.704	21.395	1.00	73.12		N
ANISOU	1344	NZ	LYS B	84	8402	10686	8695	838	−1789	−497	N
ATOM	1345	N	ALA B	85	5.593	−9.945	21.572	1.00	33.88		N
ANISOU	1345	N	ALA B	85	4293	5201	3377	979	−539	−357	N
ATOM	1346	CA	ALA B	85	4.914	−10.732	20.581	1.00	33.81		C
ANISOU	1346	CA	ALA B	85	4215	5034	3596	924	−334	−238	C
ATOM	1347	C	ALA B	85	5.343	−10.155	19.238	1.00	33.43		C
ANISOU	1347	C	ALA B	85	3995	4924	3782	750	−429	−331	C
ATOM	1348	O	ALA B	85	5.006	−8.999	18.917	1.00	34.59		O
ANISOU	1348	O	ALA B	85	4106	5032	4005	640	−471	−465	O
ATOM	1349	CB	ALA B	85	3.397	−10.645	20.783	1.00	31.76		C
ANISOU	1349	CB	ALA B	85	4043	4651	3372	919	−106	−215	C
ATOM	1350	N	SER B	86	6.131	−10.940	18.503	1.00	34.85		N
ANISOU	1350	N	SER B	86	4084	5085	4070	749	−433	−242	N
ATOM	1351	CA	SER B	86	6.682	−10.528	17.217	1.00	33.15		C
ANISOU	1351	CA	SER B	86	3738	4810	4049	625	−483	−294	C
ATOM	1352	C	SER B	86	6.126	−11.391	16.148	1.00	31.01		C
ANISOU	1352	C	SER B	86	3489	4402	3892	567	−315	−230	C
ATOM	1353	O	SER B	86	6.130	−12.622	16.269	1.00	32.28		O
ANISOU	1353	O	SER B	86	3707	4513	4046	641	−186	−116	O
ATOM	1354	CB	SER B	86	8.216	−10.643	17.180	1.00	35.86		C
ANISOU	1354	CB	SER B	86	3957	5228	4442	677	−612	−249	C
ATOM	1355	OG	SER B	86	8.796	−9.895	18.223	1.00	40.58		O
ANISOU	1355	OG	SER B	86	4523	5970	4927	710	−828	−332	O
ATOM	1356	N	PHE B	87	5.726	−10.742	15.070	1.00	31.21		N
ANISOU	1356	N	PHE B	87	3473	4363	4024	436	−321	−303	N
ATOM	1357	CA	PHE B	87	5.101	−11.404	13.940	1.00	27.28		C
ANISOU	1357	CA	PHE B	87	3015	3752	3596	346	−217	−288	C
ATOM	1358	C	PHE B	87	5.822	−11.039	12.654	1.00	32.24		C
ANISOU	1358	C	PHE B	87	3606	4351	4291	290	−238	−315	C
ATOM	1359	O	PHE B	87	5.979	−9.865	12.330	1.00	34.68		O
ANISOU	1359	O	PHE B	87	3837	4693	4645	252	−317	−360	O
ATOM	1360	CB	PHE B	87	3.625	−10.991	13.834	1.00	25.29		C
ANISOU	1360	CB	PHE B	87	2761	3469	3378	253	−206	−318	C
ATOM	1361	CG	PHE B	87	2.820	−11.332	15.064	1.00	28.39		C
ANISOU	1361	CG	PHE B	87	3197	3857	3733	325	−120	−267	C
ATOM	1362	CD1	PHE B	87	2.136	−12.538	15.156	1.00	29.94		C
ANISOU	1362	CD1	PHE B	87	3439	3952	3984	321	20	−195	C
ATOM	1363	CD2	PHE B	87	2.747	−10.437	16.121	1.00	30.93		C
ANISOU	1363	CD2	PHE B	87	3529	4251	3971	398	−152	−295	C
ATOM	1364	CE1	PHE B	87	1.368	−12.851	16.304	1.00	31.78		C
ANISOU	1364	CE1	PHE B	87	3711	4159	4206	412	154	−110	C
ATOM	1365	CE2	PHE B	87	2.011	−10.745	17.276	1.00	32.26		C
ANISOU	1365	CE2	PHE B	87	3779	4408	4070	496	−28	−231	C
ATOM	1366	CZ	PHE B	87	1.315	−11.956	17.348	1.00	32.61		C
ANISOU	1366	CZ	PHE B	87	3850	4352	4188	513	138	−119	C
ATOM	1367	N	HIS B	88	6.279	−12.026	11.918	1.00	28.66		N
ANISOU	1367	N	HIS B	88	3223	3813	3852	298	−129	−279	N
ATOM	1368	CA	HIS B	88	7.042	−11.797	10.715	1.00	30.79		C
ANISOU	1368	CA	HIS B	88	3501	4038	4160	282	−90	−282	C
ATOM	1369	C	HIS B	88	6.187	−11.988	9.487	1.00	34.45		C
ANISOU	1369	C	HIS B	88	4088	4439	4562	165	−63	−345	C
ATOM	1370	O	HIS B	88	5.472	−12.936	9.382	1.00	31.09		O
ANISOU	1370	O	HIS B	88	3765	3945	4104	105	−14	−381	O
ATOM	1371	CB	HIS B	88	8.250	−12.701	10.701	1.00	31.36		C
ANISOU	1371	CB	HIS B	88	3585	4046	4286	393	42	−191	C
ATOM	1372	CG	HIS B	88	9.123	−12.589	9.498	1.00	37.07		C
ANISOU	1372	CG	HIS B	88	4334	4688	5064	411	156	−164	C
ATOM	1373	ND1	HIS B	88	8.888	−13.313	8.359	1.00	39.72		N
ANISOU	1373	ND1	HIS B	88	4870	4900	5324	368	309	−206	N
ATOM	1374	CD2	HIS B	88	10.272	−11.918	9.282	1.00	35.70		C
ANISOU	1374	CD2	HIS B	88	4022	4519	5023	477	168	−94	C
ATOM	1375	CE1	HIS B	88	9.832	−13.072	7.483	1.00	42.00		C
ANISOU	1375	CE1	HIS B	88	5172	5124	5660	430	436	−152	C
ATOM	1376	NE2	HIS B	88	10.691	−12.234	8.020	1.00	39.53		N
ANISOU	1376	NE2	HIS B	88	4634	4879	5506	498	365	−67	N
ATOM	1377	N	ILE B	89	6.258	−11.028	8.585	1.00	31.70		N

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1377	N	ILE B	89	3721	4121	4204	133	−106	−356	N
ATOM	1378	CA	ILE B	89	5.730	−11.176	7.254	1.00	30.60		C
ANISOU	1378	CA	ILE B	89	3723	3952	3950	52	−99	−400	C
ATOM	1379	C	ILE B	89	6.807	−11.086	6.194	1.00	31.44		C
ANISOU	1379	C	ILE B	89	3921	4002	4024	124	37	−361	C
ATOM	1380	O	ILE B	89	7.513	−10.135	6.075	1.00	31.62		O
ANISOU	1380	O	ILE B	89	3834	4044	4135	192	60	−290	O
ATOM	1381	CB	ILE B	89	4.631	−10.161	6.916	1.00	34.20		C
ANISOU	1381	CB	ILE B	89	4109	4503	4382	−27	−250	−401	C
ATOM	1382	CG1	ILE B	89	3.588	−10.098	8.013	1.00	35.29		C
ANISOU	1382	CG1	ILE B	89	4134	4676	4598	−72	−334	−408	C
ATOM	1383	CG2	ILE B	89	3.975	−10.522	5.603	1.00	35.86		C
ANISOU	1383	CG2	ILE B	89	4479	4720	4427	−119	−301	−449	C
ATOM	1384	CD1	ILE B	89	2.793	−8.834	8.010	1.00	36.18		C
ANISOU	1384	CD1	ILE B	89	4112	4865	4768	−94	−430	−361	C
ATOM	1385	O	PRO B	90	6.262	−11.581	2.730	1.00	37.74		O
ANISOU	1385	O	PRO B	90	5291	4752	4295	38	122	−478	O
ATOM	1386	N	PRO B	90	6.858	−12.201	5.391	1.00	33.41		N
ANISOU	1386	N	PRO B	90	4399	4147	4150	100	159	−420	N
ATOM	1387	CA	PRO B	90	7.860	−12.159	4.332	1.00	36.58		C
ANISOU	1387	CA	PRO B	90	4932	4469	4496	192	346	−374	C
ATOM	1388	C	PRO B	90	7.382	−11.436	3.079	1.00	38.46		C
ANISOU	1388	C	PRO B	90	5296	4775	4540	161	289	−386	C
ATOM	1389	CB	PRO B	90	8.115	−13.622	4.069	1.00	38.28		C
ANISOU	1389	CB	PRO B	90	5368	4524	4653	194	534	−441	C
ATOM	1390	CG	PRO B	90	6.803	−14.214	4.176	1.00	39.61		C
ANISOU	1390	CG	PRO B	90	5614	4707	4728	28	380	−584	C
ATOM	1391	CD	PRO B	90	6.176	−13.565	5.324	1.00	32.57		C
ANISOU	1391	CD	PRO B	90	4465	3944	3968	1	190	−535	C
ATOM	1392	O	GLN B	91	5.747	−10.014	0.390	1.00	37.38		O
ANISOU	1392	O	GLN B	91	5459	4900	3845	91	24	−371	O
ATOM	1393	N	GLN B	91	8.237	−10.663	2.439	1.00	37.21		N
ANISOU	1393	N	GLN B	91	5130	4599	4409	280	427	−270	N
ATOM	1394	CA	GLN B	91	7.973	−10.168	1.108	1.00	37.62		C
ANISOU	1394	CA	GLN B	91	5371	4697	4225	302	445	−245	C
ATOM	1395	C	GLN B	91	6.620	−9.500	1.003	1.00	37.27		C
ANISOU	1395	C	GLN B	91	5263	4826	4071	194	163	−266	C
ATOM	1396	CB	GLN B	91	8.170	−11.243	0.051	1.00	41.56		C
ANISOU	1396	CB	GLN B	91	6247	5092	4452	312	611	−342	C
ATOM	1397	CG	GLN B	91	9.581	−11.768	0.003	1.00	50.35		C
ANISOU	1397	CG	GLN B	91	7413	6010	5706	463	961	−262	C
ATOM	1398	CD	GLN B	91	9.836	−12.792	−1.076	1.00	63.63		C
ANISOU	1398	CD	GLN B	91	9513	7546	7117	496	1198	−361	C
ATOM	1399	OE1	GLN B	91	8.967	−13.177	−1.807	1.00	69.50		O
ANISOU	1399	OE1	GLN B	91	10533	8340	7533	383	1069	−528	O
ATOM	1400	NE2	GLN B	91	11.053	−13.224	−1.167	1.00	68.09		N
ANISOU	1400	NE2	GLN B	91	10119	7920	7832	650	1549	−258	N
ATOM	1401	N	VAL B	92	6.439	−8.404	1.708	1.00	35.54		N
ANISOU	1401	N	VAL B	92	4766	4674	4064	206	74	−174	N
ATOM	1402	CA	VAL B	92	5.139	−7.812	1.852	1.00	34.02		C
ANISOU	1402	CA	VAL B	92	4458	4618	3849	117	−161	−166	C
ATOM	1403	C	VAL B	92	4.561	−7.375	0.522	1.00	35.12		C
ANISOU	1403	C	VAL B	92	4743	4873	3729	136	−239	−93	C
ATOM	1404	O	VAL B	92	5.243	−6.929	−0.328	1.00	33.80		O
ANISOU	1404	O	VAL B	92	4686	4686	3471	263	−78	12	O
ATOM	1405	CB	VAL B	92	5.149	−6.613	2.800	1.00	34.52		C
ANISOU	1405	CB	VAL B	92	4230	4693	4194	150	−177	−79	C
ATOM	1406	CG1	VAL B	92	5.715	−6.978	4.144	1.00	35.55		C
ANISOU	1406	CG1	VAL B	92	4236	4749	4523	140	−145	−152	C
ATOM	1407	CG2	VAL B	92	5.943	−5.496	2.215	1.00	38.30		C
ANISOU	1407	CG2	VAL B	92	4653	5132	4767	279	−14	70	C
ATOM	1408	N	GLN B	93	3.267	−7.530	0.392	1.00	36.05		N
ANISOU	1408	N	GLN B	93	4844	5115	3736	13	−492	−135	N
ATOM	1409	CA	GLN B	93	2.515	−7.217	−0.816	1.00	36.76		C
ANISOU	1409	CA	GLN B	93	5055	5367	3545	10	−659	−67	C
ATOM	1410	C	GLN B	93	1.576	−6.059	−0.492	1.00	38.51		C
ANISOU	1410	C	GLN B	93	4982	5707	3942	21	−803	109	C
ATOM	1411	O	GLN B	93	1.367	−5.724	0.689	1.00	37.05		O
ANISOU	1411	O	GLN B	93	4551	5463	4063	−6	−784	117	O
ATOM	1412	CB	GLN B	93	1.721	−8.447	−1.287	1.00	39.53		C
ANISOU	1412	CB	GLN B	93	5606	5766	3650	−171	−880	−268	C
ATOM	1413	CG	GLN B	93	2.574	−9.701	−1.673	1.00	48.34		C
ANISOU	1413	CG	GLN B	93	7058	6723	4584	−188	−700	−464	C
ATOM	1414	CD	GLN B	93	1.739	−10.982	−1.845	1.00	47.61		C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1414	CD	GLN B	93	7120	6614	4357	−412	−902	−712	C
ATOM	1415	OE1	GLN B	93	0.552	−10.924	−2.161	1.00	44.52		O
ANISOU	1415	OE1	GLN B	93	6657	6375	3883	−552	−1225	−739	O
ATOM	1416	NE2	GLN B	93	2.356	−12.143	−1.601	1.00	46.87		N
ANISOU	1416	NE2	GLN B	93	7204	6315	4288	−450	−706	−883	N
ATOM	1417	N	VAL B	94	1.024	−5.438	−1.530	1.00	37.85		N
ANISOU	1417	N	VAL B	94	4938	5788	3656	79	−927	263	N
ATOM	1418	CA	VAL B	94	−0.031	−4.450	−1.384	1.00	42.05		C
ANISOU	1418	CA	VAL B	94	5193	6444	4339	94	−1078	461	C
ATOM	1419	C	VAL B	94	−1.129	−4.946	−0.416	1.00	42.32		C
ANISOU	1419	C	VAL B	94	5012	6482	4585	−84	−1275	368	C
ATOM	1420	O	VAL B	94	−1.591	−4.191	0.425	1.00	39.68		O
ANISOU	1420	O	VAL B	94	4407	6114	4555	−58	−1231	482	O
ATOM	1421	CB	VAL B	94	−0.653	−4.094	−2.768	1.00	45.84		C
ANISOU	1421	CB	VAL B	94	5783	7152	4481	157	−1276	629	C
ATOM	1422	CG1	VAL B	94	−1.864	−3.240	−2.599	1.00	44.44		C
ANISOU	1422	CG1	VAL B	94	5285	7109	4489	164	−1458	853	C
ATOM	1423	CG2	VAL B	94	0.372	−3.384	−3.650	1.00	43.42		C
ANISOU	1423	CG2	VAL B	94	5660	6826	4013	384	−1010	796	C
ATOM	1424	N	ARG B	95	−1.523	−6.215	−0.516	1.00	38.35		N
ANISOU	1424	N	ARG B	95	4638	5989	3946	−259	−1450	160	N
ATOM	1425	CA	ARG B	95	−2.574	−6.735	0.361	1.00	42.00		C
ANISOU	1425	CA	ARG B	95	4885	6428	4647	−422	−1601	95	C
ATOM	1426	C	ARG B	95	−2.225	−6.737	1.860	1.00	40.15		C
ANISOU	1426	C	ARG B	95	4510	6014	4732	−399	−1374	53	C
ATOM	1427	O	ARG B	95	−3.117	−6.889	2.702	1.00	43.99		O
ANISOU	1427	O	ARG B	95	4790	6469	5456	−479	−1427	67	O
ATOM	1428	CB	ARG B	95	−2.953	−8.163	−0.031	1.00	40.54		C
ANISOU	1428	CB	ARG B	95	4875	6235	4294	−628	−1791	−145	C
ATOM	1429	CG	ARG B	95	−1.852	−9.233	0.131	1.00	38.83		C
ANISOU	1429	CG	ARG B	95	4942	5834	3979	−644	−1575	−372	C
ATOM	1430	CD	ARG B	95	−2.483	−10.588	−0.172	1.00	46.45		C
ANISOU	1430	CD	ARG B	95	6034	6757	4858	−875	−1763	−609	C
ATOM	1431	NE	ARG B	95	−1.572	−11.724	−0.327	1.00	50.98		N
ANISOU	1431	NE	ARG B	95	6929	7151	5292	−904	−1570	−832	N
ATOM	1432	CZ	ARG B	95	−1.718	−12.889	0.308	1.00	53.62		C
ANISOU	1432	CZ	ARG B	95	7276	7302	5793	−1040	−1504	−1002	C
ATOM	1433	NH1	ARG B	95	−0.882	−13.893	0.075	1.00	50.51		N
ANISOU	1433	NH1	ARG B	95	7183	6731	5277	−1046	−1299	−1182	N
ATOM	1434	NH2	ARG B	95	−2.719	−13.054	1.167	1.00	57.43		N
ANISOU	1434	NH2	ARG B	95	7470	7760	6591	−1155	−1608	−970	N
ATOM	1435	N	ASP B	96	−0.944	−6.609	2.195	1.00	35.98		N
ANISOU	1435	N	ASP B	96	4093	5370	4207	−289	−1129	8	N
ATOM	1436	CA	ASP B	96	−0.544	−6.602	3.624	1.00	36.54		C
ANISOU	1436	CA	ASP B	96	4055	5305	4525	−261	−957	−40	C
ATOM	1437	C	ASP B	96	−0.744	−5.239	4.281	1.00	40.24		C
ANISOU	1437	C	ASP B	96	4303	5763	5223	−164	−869	108	C
ATOM	1438	O	ASP B	96	−0.668	−5.109	5.517	1.00	36.55		O
ANISOU	1438	O	ASP B	96	3748	5205	4935	−149	−763	66	O
ATOM	1439	CB	ASP B	96	0.928	−7.027	3.778	1.00	32.01		C
ANISOU	1439	CB	ASP B	96	3647	4620	3894	−191	−765	−139	C
ATOM	1440	CG	ASP B	96	1.187	−8.461	3.290	1.00	37.69		C
ANISOU	1440	CG	ASP B	96	4602	5290	4427	−274	−775	−296	C
ATOM	1441	OD1	ASP B	96	0.476	−9.407	3.724	1.00	35.26		O
ANISOU	1441	OD1	ASP B	96	4287	4946	4165	−398	−853	−394	O
ATOM	1442	OD2	ASP B	96	2.091	−8.643	2.443	1.00	38.06		O
ANISOU	1442	OD2	ASP B	96	4850	5309	4301	−209	−670	−316	O
ATOM	1443	N	GLU B	97	−0.944	−4.219	3.455	1.00	43.03		N
ANISOU	1443	N	GLU B	97	4596	6198	5554	−86	−890	281	N
ATOM	1444	CA	GLU B	97	−1.061	−2.847	3.944	1.00	41.46		C
ANISOU	1444	CA	GLU B	97	4207	5950	5595	17	−755	426	C
ATOM	1445	C	GLU B	97	−2.360	−2.700	4.709	1.00	36.02		C
ANISOU	1445	C	GLU B	97	3315	5263	5109	−30	−810	494	C
ATOM	1446	O	GLU B	97	−3.407	−3.174	4.270	1.00	38.79		O
ANISOU	1446	O	GLU B	97	3593	5720	5424	−111	−1006	558	O
ATOM	1447	CB	GLU B	97	−1.015	−1.802	2.794	1.00	43.33		C
ANISOU	1447	CB	GLU B	97	4422	6263	5779	139	−728	646	C
ATOM	1448	CG	GLU B	97	−0.911	−0.348	3.330	1.00	57.97		C
ANISOU	1448	CG	GLU B	97	6096	7996	7933	251	−511	777	C
ATOM	1449	CD	GLU B	97	−0.720	0.742	2.260	1.00	59.34		C
ANISOU	1449	CD	GLU B	97	6241	8199	8106	403	−405	1026	C
ATOM	1450	OE1	GLU B	97	0.391	0.848	1.670	1.00	55.03		O
ANISOU	1450	OE1	GLU B	97	5828	7606	7474	475	−275	1022	O
ATOM	1451	OE2	GLU B	97	−1.679	1.523	2.039	1.00	62.85		O

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1451	OE2	GLU B	97	6514	8698	8669	471	−418	1257	O
ATOM	1452	N	GLY B	98	−2.291	−2.059	5.869	1.00	42.74		N
ANISOU	1452	N	GLY B	98	5399	7196	3643	28	−802	992	N
ATOM	1453	CA	GLY B	98	−3.497	−1.734	6.603	1.00	40.83		C
ANISOU	1453	CA	GLY B	98	4890	7044	3580	220	−1011	1094	C
ATOM	1454	C	GLY B	98	−3.244	−1.824	8.103	1.00	39.89		C
ANISOU	1454	C	GLY B	98	4757	6465	3934	312	−878	888	C
ATOM	1455	O	GLY B	98	−2.102	−1.907	8.561	1.00	38.24		O
ANISOU	1455	O	GLY B	98	4711	5897	3920	280	−674	756	O
ATOM	1456	N	GLN B	99	−4.341	−1.837	8.848	1.00	39.23		N
ANISOU	1456	N	GLN B	99	4445	6464	3996	412	−1000	865	N
ATOM	1457	C	GLN B	99	−4.461	−3.303	10.792	1.00	34.54		C
ANISOU	1457	C	GLN B	99	3822	5575	3727	257	−826	343	C
ATOM	1458	O	GLN B	99	−5.124	−4.128	10.161	1.00	37.11		O
ANISOU	1458	O	GLN B	99	4057	6225	3818	38	−902	212	O
ATOM	1459	CA	GLN B	99	−4.321	−1.868	10.293	1.00	40.04		C
ANISOU	1459	CA	GLN B	99	4522	6229	4462	500	−889	696	C
ATOM	1460	CB	GLN B	99	−5.458	−0.990	10.841	1.00	46.09		C
ANISOU	1460	CB	GLN B	99	5052	7017	5444	770	−973	888	C
ATOM	1461	CG	GLN B	99	−5.293	−0.610	12.270	1.00	53.11		C
ANISOU	1461	CG	GLN B	99	5973	7526	6680	884	−807	749	C
ATOM	1462	CD	GLN B	99	−6.473	0.184	12.768	1.00	62.24		C
ANISOU	1462	CD	GLN B	99	6894	8682	8072	1143	−812	895	C
ATOM	1463	OE1	GLN B	99	−7.618	−0.141	12.465	1.00	63.39		O
ANISOU	1463	OE1	GLN B	99	6767	9183	8136	1165	−964	966	O
ATOM	1464	NE2	GLN B	99	−6.202	1.235	13.536	1.00	66.04		N
ANISOU	1464	NE2	GLN B	99	7455	8769	8868	1322	−615	912	N
ATOM	1465	N	TYR B	100	−3.827	−3.578	11.926	1.00	31.25		N
ANISOU	1465	N	TYR B	100	3498	4841	3535	283	−671	201	N
ATOM	1466	CA	TYR B	100	−3.766	−4.904	12.533	1.00	31.65		C
ANISOU	1466	CA	TYR B	100	3590	4824	3611	121	−534	−41	C
ATOM	1467	C	TYR B	100	−4.054	−4.734	14.015	1.00	34.48		C
ANISOU	1467	C	TYR B	100	3892	5032	4177	259	−489	−62	C
ATOM	1468	O	TYR B	100	−3.684	−3.709	14.576	1.00	32.70		O
ANISOU	1468	O	TYR B	100	3680	4666	4077	426	−502	23	O
ATOM	1469	CB	TYR B	100	−2.371	−5.534	12.374	1.00	29.13		C
ANISOU	1469	CB	TYR B	100	3465	4298	3306	47	−352	−115	C
ATOM	1470	CG	TYR B	100	−1.989	−5.952	10.938	1.00	29.04		C
ANISOU	1470	CG	TYR B	100	3561	4408	3065	−148	−291	−178	C
ATOM	1471	CD1	TYR B	100	−2.038	−7.280	10.549	1.00	26.45		C
ANISOU	1472	CD1	TYR B	100	3309	4079	2662	−391	−100	−424	C
ATOM	1472	CD2	TYR B	100	−1.535	−5.013	10.023	1.00	29.08		C
ANISOU	1472	CD2	TYR B	100	3618	4490	2939	−101	−361	−4	C
ATOM	1473	CE1	TYR B	100	−1.684	−7.671	9.238	1.00	31.66		C
ANISOU	1473	CE1	TYR B	100	4093	4863	3074	−618	8	−558	C
ATOM	1474	CE2	TYR B	100	−1.164	−5.390	8.733	1.00	31.74		C
ANISOU	1474	CE2	TYR B	100	4079	4978	3002	−298	−275	−71	C
ATOM	1475	CZ	TYR B	100	−1.245	−6.719	8.357	1.00	33.45		C
ANISOU	1475	CZ	TYR B	100	4369	5234	3108	−567	−96	−376	C
ATOM	1476	OH	TYR B	100	−0.902	−7.081	7.081	1.00	36.51		O
ANISOU	1476	OH	TYR B	100	4900	5788	3186	−805	31	−509	O
ATOM	1477	N	GLN B	101	−4.684	−5.715	14.649	1.00	36.18		N
ANISOU	1477	N	GLN B	101	4063	5265	4420	159	−392	−196	N
ATOM	1478	C	GLN B	101	−3.656	−6.753	16.637	1.00	31.33		C
ANISOU	1478	C	GLN B	101	3622	4343	3938	242	−128	−216	C
ATOM	1479	O	GLN B	101	−3.618	−7.931	16.239	1.00	33.85		O
ANISOU	1479	O	GLN B	101	4007	4596	4258	100	33	−283	O
ATOM	1480	CA	GLN B	101	−4.710	−5.780	16.126	1.00	32.90		C
ANISOU	1480	CA	GLN B	101	3661	4713	4126	263	−290	−212	C
ATOM	1481	CB	GLN B	101	−6.098	−6.212	16.648	1.00	29.75		C
ANISOU	1481	CB	GLN B	101	3103	4429	3771	198	−231	−294	C
ATOM	1482	CG	GLN B	101	−7.218	−5.282	16.242	1.00	35.27		C
ANISOU	1482	CG	GLN B	101	3556	5336	4511	280	−385	−238	C
ATOM	1483	CD	GLN B	101	−8.606	−5.895	16.366	1.00	43.66		C
ANISOU	1483	CD	GLN B	101	4374	6601	5613	142	−342	−345	C
ATOM	1484	OE1	GLN B	101	−8.820	−7.073	16.071	1.00	47.85		O
ANISOU	1484	OE1	GLN B	101	4912	7182	6085	−126	−243	−502	O
ATOM	1485	NE2	GLN B	101	−9.554	−5.085	16.807	1.00	41.56		N
ANISOU	1485	NE2	GLN B	101	3875	6427	5489	311	−366	−282	N
ATOM	1486	N	CYS B	102	−2.806	−6.273	17.537	1.00	28.72		N
ANISOU	1486	N	CYS B	102	3336	3950	3627	381	−147	−145	N
ATOM	1487	CA	CYS B	102	−1.849	−7.136	18.208	1.00	30.40		C
ANISOU	1487	CA	CYS B	102	3625	4084	3840	434	−31	−59	C
ATOM	1488	C	CYS B	102	−2.483	−7.620	19.485	1.00	35.08		C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1488	C	CYS B	102	4225	4714	4390	473	69	−20	C
ATOM	1489	O	CYS B	102	−2.691	−6.804	20.371	1.00	35.21		O
ANISOU	1489	O	CYS B	102	4207	4840	4330	530	−10	−52	O
ATOM	1490	CB	CYS B	102	−0.567	−6.361	18.511	1.00	31.66		C
ANISOU	1490	CB	CYS B	102	3762	4278	3989	526	−147	−4	C
ATOM	1491	SG	CYS B	102	0.908	−7.387	18.669	1.00	52.31		S
ANISOU	1491	SG	CYS B	102	6371	6851	6655	627	−45	174	S
ATOM	1492	N	ILE B	103	−2.786	−8.919	19.595	1.00	33.75		N
ANISOU	1492	N	ILE B	103	4122	4429	4274	426	297	33	N
ATOM	1493	CA	ILE B	103	−3.660	−9.415	20.674	1.00	34.24		C
ANISOU	1493	CA	ILE B	103	4202	4506	4302	423	456	77	C
ATOM	1494	C	ILE B	103	−2.896	−10.420	21.490	1.00	38.10		C
ANISOU	1494	C	ILE B	103	4799	4905	4774	566	638	347	C
ATOM	1495	O	ILE B	103	−2.285	−11.339	20.955	1.00	38.66		O
ANISOU	1495	O	ILE B	103	4936	4761	4994	590	814	446	O
ATOM	1496	CB	ILE B	103	−4.962	−10.076	20.135	1.00	37.37		C
ANISOU	1496	CB	ILE B	103	4555	4831	4813	202	631	−87	C
ATOM	1497	CG1	ILE B	103	−5.729	−9.100	19.243	1.00	38.13		C
ANISOU	1497	CG1	ILE B	103	4476	5105	4906	109	407	−271	C
ATOM	1498	CG2	ILE B	103	−5.864	−10.591	21.266	1.00	39.83		C
ANISOU	1498	CG2	ILE B	103	4878	5132	5121	177	859	−39	C
ATOM	1499	CD1	ILE B	103	−6.847	−9.744	18.430	1.00	40.86		C
ANISOU	1499	CD1	ILE B	103	4699	5507	5320	−160	495	−461	C
ATOM	1500	N	ILE B	104	−2.876	−10.223	22.795	1.00	34.98		N
ANISOU	1500	N	ILE B	104	4418	4687	4185	682	613	491	N
ATOM	1501	CA	ILE B	104	−2.132	−11.140	23.620	1.00	36.61		C
ANISOU	1501	CA	ILE B	104	4699	4890	4323	874	750	852	C
ATOM	1502	C	ILE B	104	−3.049	−11.596	24.749	1.00	38.22		C
ANISOU	1502	C	ILE B	104	4995	5137	4390	867	969	972	C
ATOM	1503	O	ILE B	104	−3.690	−10.777	25.418	1.00	38.53		O
ANISOU	1503	O	ILE B	104	5008	5401	4229	799	877	813	O
ATOM	1504	CB	ILE B	104	−0.826	−10.487	24.135	1.00	38.06		C
ANISOU	1504	CB	ILE B	104	4778	5385	4297	1038	456	990	C
ATOM	1505	CGI	ILE B	104	−0.063	−9.851	22.953	1.00	38.30		C
ANISOU	1505	CGI	ILE B	104	4708	5354	4489	988	278	811	C
ATOM	1506	CG2	ILE B	104	0.029	−11.508	24.881	1.00	37.06		C
ANISOU	1506	CG2	ILE B	104	4657	5319	4106	1303	563	1465	C
ATOM	1507	CD1	ILE B	104	1.276	−9.246	23.299	1.00	44.53		C
ANISOU	1507	CD1	ILE B	104	5339	6433	5148	1090	18	898	C
ATOM	1508	N	ILE B	105	−3.131	−12.915	24.894	1.00	39.09		N
ANISOU	1508	N	ILE B	105	5228	4974	4652	927	1328	1240	N
ATOM	1509	CA	ILE B	105	−3.963	−13.578	25.867	1.00	43.63		C
ANISOU	1509	CA	ILE B	105	5924	5501	5153	915	1645	1419	C
ATOM	1510	C	ILE B	105	−3.053	−14.276	26.871	1.00	47.53		C
ANISOU	1510	C	ILE B	105	6506	6090	5464	1236	1733	1983	C
ATOM	1511	O	ILE B	105	−2.060	−14.924	26.481	1.00	46.72		O
ANISOU	1511	O	ILE B	105	6395	5808	5549	1444	1794	2260	O
ATOM	1512	CB	ILE B	105	−4.883	−14.630	25.228	1.00	48.68		C
ANISOU	1512	CB	ILE B	105	6643	5691	6160	693	2084	1298	C
ATOM	1513	CG1	ILE B	105	−5.767	−14.013	24.149	1.00	51.06		C
ANISOU	1513	CG1	ILE B	105	6790	6007	6603	382	1946	786	C
ATOM	1514	CG2	ILE B	105	−5.727	−15.315	26.301	1.00	51.55		C
ANISOU	1514	CG2	ILE B	105	7139	5978	6471	667	2474	1511	C
ATOM	1515	CD1	ILE B	105	−6.645	−15.048	23.441	1.00	56.20		C
ANISOU	1515	CD1	ILE B	105	7466	6306	7580	70	2343	578	C
ATOM	1516	O	TYR B	106	−4.196	−14.555	31.052	1.00	60.34		O
ANISOU	1516	O	TYR B	106	8479	8599	5850	1435	2087	2804	O
ATOM	1517	N	TYR B	106	−3.396	−14.143	28.146	1.00	48.76		N
ANISOU	1517	N	TYR B	106	6730	6551	5247	1290	1755	2172	N
ATOM	1518	CA	TYR B	106	−2.626	−14.729	29.242	1.00	56.60		C
ANISOU	1518	CA	TYR B	106	7788	7781	5938	1608	1792	2776	C
ATOM	1519	C	TYR B	106	−3.608	−15.297	30.250	1.00	59.64		C
ANISOU	1519	C	TYR B	106	8370	8137	6152	1570	2181	2993	C
ATOM	1520	CB	TYR B	106	−1.716	−13.671	29.879	1.00	59.27		C
ANISOU	1520	CB	TYR B	106	7966	8773	5783	1693	1275	2768	C
ATOM	1521	CG	TYR B	106	−0.729	−14.164	30.926	1.00	65.71		C
ANISOU	1521	CG	TYR B	106	8700	9952	6313	1961	1129	3252	C
ATOM	1522	CD1	TYR B	106	0.158	−15.195	30.643	1.00	68.62		C
ANISOU	1522	CD1	TYR B	106	8969	10069	7035	2227	1233	3613	C
ATOM	1523	CD2	TYR B	106	−0.635	−13.547	32.169	1.00	69.13		C
ANISOU	1523	CD2	TYR B	106	9104	10975	6186	1889	870	3215	C
ATOM	1524	CE1	TYR B	106	1.080	−15.631	31.579	1.00	75.75		C
ANISOU	1524	CE1	TYR B	106	9719	11324	7737	2455	1084	3997	C
ATOM	1525	CE2	TYR B	106	0.299	−13.986	33.124	1.00	76.21		C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1525	CE2	TYR B	106	9873	12235	6849	2075	691	3585	C
ATOM	1526	CZ	TYR B	106	1.151	−15.030	32.810	1.00	79.07		C
ANISOU	1526	CZ	TYR B	106	10106	12363	7573	2379	793	4004	C
ATOM	1527	OH	TYR B	106	2.091	−15.488	33.707	1.00	86.71		O
ANISOU	1527	OH	TYR B	106	10904	13718	8325	2600	639	4414	O
ATOM	1528	O	GLY B	107	−6.517	−17.060	29.267	1.00	65.57		O
ANISOU	1528	O	GLY B	107	9341	7677	7894	922	3346	2502	O
ATOM	1529	N	GLY B	107	−3.818	−16.608	30.194	1.00	62.02		N
ANISOU	1529	N	GLY B	107	8782	7944	6838	1627	2591	3225	N
ATOM	1530	CA	GLY B	107	−4.861	−17.221	31.004	1.00	64.59		C
ANISOU	1530	CA	GLY B	107	9263	8129	7149	1511	2959	3290	C
ATOM	1531	C	GLY B	107	−6.211	−16.799	30.443	1.00	65.16		C
ANISOU	1531	C	GLY B	107	9335	8024	7397	1117	3180	2789	C
ATOM	1532	O	VAL B	108	−9.096	−13.411	30.140	1.00	59.94		O
ANISOU	1532	O	VAL B	108	8195	8022	6559	389	2796	1233	O
ATOM	1533	N	VAL B	108	−7.020	−16.134	31.262	1.00	63.74		N
ANISOU	1533	N	VAL B	108	9165	8177	6877	976	3181	2633	N
ATOM	1534	CA	VAL B	108	−8.264	−15.567	30.764	1.00	60.51		C
ANISOU	1534	CA	VAL B	108	8638	7701	6652	641	3327	2116	C
ATOM	1535	C	VAL B	108	−8.163	−14.048	30.627	1.00	57.38		C
ANISOU	1535	C	VAL B	108	8051	7719	6031	605	2819	1686	C
ATOM	1536	CB	VAL B	108	−9.485	−15.931	31.653	1.00	66.32		C
ANISOU	1536	CB	VAL B	108	9432	8396	7370	456	3685	2073	C
ATOM	1537	CGI	VAL B	108	−9.923	−17.362	31.384	1.00	70.30		C
ANISOU	1537	CGI	VAL B	108	10020	8342	8347	347	4087	2182	C
ATOM	1538	CG2	VAL B	108	−9.194	−15.701	33.143	1.00	68.15		C
ANISOU	1538	CG2	VAL B	108	9811	9069	7015	619	3596	2371	C
ATOM	1539	N	ALA B	109	−7.027	−13.488	31.028	1.00	51.92		N
ANISOU	1539	N	ALA B	109	7375	7394	4959	815	2435	1841	N
ATOM	1540	CA	ALA B	109	−6.759	−12.069	30.868	1.00	47.80		C
ANISOU	1540	CA	ALA B	109	6703	7187	4273	764	2005	1433	C
ATOM	1541	C	ALA B	109	−6.228	−11.758	29.465	1.00	47.65		C
ANISOU	1541	C	ALA B	109	6523	6958	4623	754	1718	1220	C
ATOM	1542	O	ALA B	109	−5.648	−12.625	28.797	1.00	50.58		O
ANISOU	1542	O	ALA B	109	6918	7061	5241	844	1771	1447	O
ATOM	1543	CB	ALA B	109	−5.781	−11.604	31.904	1.00	50.21		C
ANISOU	1543	CB	ALA B	109	7068	8014	3997	904	1738	1621	C
ATOM	1544	N	TRP B	110	−6.409	−10.520	29.014	1.00	40.75		N
ANISOU	1544	N	TRP B	110	5503	6183	3796	653	1463	801	N
ATOM	1545	CA	TRP B	110	−5.962	−10.158	27.670	1.00	35.45		C
ANISOU	1545	CA	TRP B	110	4699	5341	3430	637	1214	627	C
ATOM	1546	C	TRP B	110	−5.938	−8.649	27.468	1.00	33.56		C
ANISOU	1546	C	TRP B	110	4343	5251	3159	591	948	271	C
ATOM	1547	O	TRP B	110	−6.520	−7.889	28.251	1.00	34.91		O
ANISOU	1547	O	TRP B	110	4517	5579	3168	539	1019	74	O
ATOM	1548	CB	TRP B	110	−6.876	−10.806	26.630	1.00	37.60		C
ANISOU	1548	CB	TRP B	110	4896	5279	4111	484	1415	507	C
ATOM	1549	CG	TRP B	110	−8.307	−10.389	26.811	1.00	36.45		C
ANISOU	1549	CG	TRP B	110	4623	5165	4061	331	1575	248	C
ATOM	1550	CD1	TRP B	110	−9.220	−10.921	27.674	1.00	41.65		C
ANISOU	1550	CD1	TRP B	110	5329	5816	4681	252	1936	305	C
ATOM	1551	CD2	TRP B	110	−8.972	−9.323	26.131	1.00	35.59		C
ANISOU	1551	CD2	TRP B	110	4289	5110	4125	273	1406	−65	C
ATOM	1552	NE1	TRP B	110	−10.427	−10.269	27.556	1.00	41.88		N
ANISOU	1552	NE1	TRP B	110	5138	5901	4875	134	2002	8	N
ATOM	1553	CE2	TRP B	110	−10.306	−9.291	26.605	1.00	39.69		C
ANISOU	1553	CE2	TRP B	110	4679	5663	4737	171	1671	−196	C
ATOM	1554	CE3	TRP B	110	−8.583	−8.427	25.122	1.00	33.97		C
ANISOU	1554	CE3	TRP B	110	3964	4914	4027	316	1088	−202	C
ATOM	1555	CZ2	TRP B	110	−11.249	−8.363	26.138	1.00	38.06		C
ANISOU	1555	CZ2	TRP B	110	4188	5524	4747	156	1604	−437	C
ATOM	1556	CZ3	TRP B	110	−9.513	−7.513	24.665	1.00	35.12		C
ANISOU	1556	CZ3	TRP B	110	3875	5109	4359	305	1028	−403	C
ATOM	1557	CH2	TRP B	110	−10.833	−7.486	25.168	1.00	34.32		C
ANISOU	1557	CH2	TRP B	110	3608	5061	4371	245	1273	−509	C
ATOM	1558	N	ASP B	111	−5.268	−8.223	26.403	1.00	34.63		N
ANISOU	1558	N	ASP B	111	4391	5293	3473	606	704	190	N
ATOM	1559	CA	ASP B	111	−5.205	−6.818	26.016	1.00	33.87		C
ANISOU	1559	CA	ASP B	111	4200	5229	3440	573	509	−99	C
ATOM	1560	C	ASP B	111	−4.785	−6.784	24.538	1.00	33.04		C
ANISOU	1560	C	ASP B	111	4014	4936	3602	574	351	−101	C
ATOM	1561	O	ASP B	111	−4.424	−7.808	23.980	1.00	34.78		O
ANISOU	1561	O	ASP B	111	4267	5039	3908	584	395	69	O
ATOM	1562	CB	ASP B	111	−4.225	−6.034	26.905	1.00	34.02		C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1562	CB	ASP B	111	4265	5522	3138	575	348	−173	C
ATOM	1563	CG	ASP B	111	−4.444	−4.517	26.845	1.00	36.61		C
ANISOU	1563	CG	ASP B	111	4546	5809	3555	498	313	−538	C
ATOM	1564	OD1	ASP B	111	−3.551	−3.755	27.285	1.00	36.03		O
ANISOU	1564	OD1	ASP B	111	4489	5904	3297	422	181	−695	O
ATOM	1565	OD2	ASP B	111	−5.501	−4.071	26.361	1.00	35.08		O
ANISOU	1565	OD2	ASP B	111	4278	5412	3639	509	440	−666	O
ATOM	1566	N	TYR B	112	−4.871	−5.625	23.909	1.00	35.61		N
ANISOU	1566	N	TYR B	112	4255	5211	4064	564	224	−286	N
ATOM	1567	CA	TYR B	112	−4.484	−5.480	22.509	1.00	32.86		C
ANISOU	1567	CA	TYR B	112	3851	4734	3900	560	84	−266	C
ATOM	1568	C	TYR B	112	−4.129	−4.035	22.174	1.00	32.50		C
ANISOU	1568	C	TYR B	112	3770	4640	3938	585	−36	−395	C
ATOM	1569	O	TYR B	112	−4.454	−3.114	22.942	1.00	30.73		O
ANISOU	1569	O	TYR B	112	3549	4426	3702	592	35	−557	O
ATOM	1570	CB	TYR B	112	−5.615	−5.973	21.578	1.00	33.54		C
ANISOU	1570	CB	TYR B	112	3829	4756	4157	494	146	−277	C
ATOM	1571	CG	TYR B	112	−6.837	−5.066	21.496	1.00	34.88		C
ANISOU	1571	CG	TYR B	112	3828	4961	4465	529	160	−386	C
ATOM	1572	CD1	TYR B	112	−7.158	−4.385	20.311	1.00	32.29		C
ANISOU	1572	CD1	TYR B	112	3357	4636	4275	570	15	−363	C
ATOM	1573	CD2	TYR B	112	−7.649	−4.849	22.616	1.00	35.84		C
ANISOU	1573	CD2	TYR B	112	3915	5126	4576	552	341	−473	C
ATOM	1574	CE1	TYR B	112	−8.287	−3.538	20.242	1.00	34.35		C
ANISOU	1574	CE1	TYR B	112	3405	4938	4710	680	38	−377	C
ATOM	1575	CE2	TYR B	112	−8.743	−4.013	22.562	1.00	36.31		C
ANISOU	1575	CE2	TYR B	112	3778	5191	4828	632	404	−553	C
ATOM	1576	CZ	TYR B	112	−9.078	−3.365	21.361	1.00	36.45		C
ANISOU	1576	CZ	TYR B	112	3611	5206	5034	719	245	−481	C
ATOM	1577	OH	TYR B	112	−10.201	−2.530	21.315	1.00	35.18		O
ANISOU	1577	OH	TYR B	112	3195	5059	5112	872	322	−480	O
ATOM	1578	N	LYS B	113	−3.441	−3.849	21.039	1.00	28.94		N
ANISOU	1578	N	LYS B	113	3311	4103	3583	583	−155	−334	N
ATOM	1579	CA	LYS B	113	−3.166	−2.526	20.496	1.00	26.59		C
ANISOU	1579	CA	LYS B	113	2995	3686	3421	607	−209	−396	C
ATOM	1580	C	LYS B	113	−3.337	−2.586	18.969	1.00	31.07		C
ANISOU	1580	C	LYS B	113	3521	4198	4086	624	−283	−259	C
ATOM	1581	O	LYS B	113	−3.412	−3.676	18.397	1.00	29.01		O
ANISOU	1581	O	LYS B	113	3261	4003	3757	562	−296	−195	O
ATOM	1582	CB	LYS B	113	−1.756	−2.070	20.860	1.00	28.04		C
ANISOU	1582	CB	LYS B	113	3227	3886	3541	539	−268	−467	C
ATOM	1583	CG	LYS B	113	−1.579	−1.710	22.400	1.00	32.02		C
ANISOU	1583	CG	LYS B	113	3757	4547	3862	467	−227	−666	C
ATOM	1584	CD	LYS B	113	−2.429	−0.535	22.774	1.00	34.30		C
ANISOU	1584	CD	LYS B	113	4066	4678	4288	467	−62	−880	C
ATOM	1585	CE	LYS B	113	−2.374	−0.238	24.298	1.00	35.99		C
ANISOU	1585	CE	LYS B	113	4339	5083	4255	340	29	−1150	C
ATOM	1586	NZ	LYS B	113	−3.056	−1.333	25.025	1.00	36.79		N
ANISOU	1586	NZ	LYS B	113	4455	5395	4128	392	66	−1031	N
ATOM	1587	N	TYR B	114	−3.385	−1.431	18.321	1.00	31.27		N
ANISOU	1587	N	TYR B	114	3528	4101	4254	693	−296	−215	N
ATOM	1588	CA	TYR B	114	−3.408	−1.389	16.859	1.00	30.07		C
ANISOU	1588	CA	TYR B	114	3354	3967	4102	708	−382	−39	C
ATOM	1589	C	TYR B	114	−1.996	−1.114	16.351	1.00	33.63		C
ANISOU	1589	C	TYR B	114	3918	4310	4549	641	−380	−14	C
ATOM	1590	O	TYR B	114	−1.247	−0.378	17.002	1.00	29.21		O
ANISOU	1590	O	TYR B	114	3399	3616	4082	614	−316	−120	O
ATOM	1591	CB	TYR B	114	−4.371	−0.313	16.372	1.00	33.29		C
ANISOU	1591	CB	TYR B	114	3652	4326	4668	881	−378	112	C
ATOM	1592	CG	TYR B	114	−5.850	−0.705	16.509	1.00	37.98		C
ANISOU	1592	CG	TYR B	114	4036	5118	5276	946	−410	133	C
ATOM	1593	CD1	TYR B	114	−6.430	−1.596	15.617	1.00	40.03		C
ANISOU	1593	CD1	TYR B	114	4174	5667	5369	848	−553	197	C
ATOM	1594	CD2	TYR B	114	−6.656	−0.159	17.501	1.00	37.64		C
ANISOU	1594	CD2	TYR B	114	3898	4988	5418	1069	−266	51	C
ATOM	1595	CE1	TYR B	114	−7.775	−1.958	15.710	1.00	42.70		C
ANISOU	1595	CE1	TYR B	114	4255	6236	5734	855	−587	188	C
ATOM	1596	CE2	TYR B	114	−8.007	−0.528	17.628	1.00	40.31		C
ANISOU	1596	CE2	TYR B	114	3988	5524	5805	1121	−268	69	C
ATOM	1597	CZ	TYR B	114	−8.558	−1.443	16.734	1.00	43.63		C
ANISOU	1597	CZ	TYR B	114	4245	6263	6069	1005	−445	141	C
ATOM	1598	OH	TYR B	114	−9.903	−1.819	16.804	1.00	47.57		O
ANISOU	1598	OH	TYR B	114	4431	7015	6630	1003	−457	132	O
ATOM	1599	N	LEU B	115	−1.647	−1.747	15.224	1.00	31.19		N

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1599	N	LEU B	115	3646	4083	4124	572	−422	80	N
ATOM	1600	CA	LEU B	115	−0.421	−1.507	14.463	1.00	33.70		C
ANISOU	1600	CA	LEU B	115	4049	4313	4441	510	−378	135	C
ATOM	1601	C	LEU B	115	−0.811	−1.213	13.026	1.00	35.12		C
ANISOU	1601	C	LEU B	115	4259	4574	4510	523	−413	329	C
ATOM	1602	O	LEU B	115	−1.764	−1.810	12.523	1.00	32.02		O
ANISOU	1602	O	LEU B	115	3807	4405	3955	499	−506	356	O
ATOM	1603	CB	LEU B	115	0.497	−2.735	14.480	1.00	36.04		C
ANISOU	1603	CB	LEU B	115	4372	4655	4667	413	−327	60	C
ATOM	1604	CG	LEU B	115	1.133	−3.203	15.772	1.00	40.21		C
ANISOU	1604	CG	LEU B	115	4845	5193	5238	428	−315	−28	C
ATOM	1605	CD1	LEU B	115	1.877	−4.523	15.615	1.00	35.56		C
ANISOU	1605	CD1	LEU B	115	4259	4618	4634	416	−218	2	C
ATOM	1606	CD2	LEU B	115	2.050	−2.102	16.264	1.00	44.19		C
ANISOU	1606	CD2	LEU B	115	5303	5637	5850	399	−325	−90	C
ATOM	1607	N	THR B	116	−0.082	−0.333	12.349	1.00	36.33		N
ANISOU	1607	N	THR B	116	4495	4590	4719	533	−335	464	N
ATOM	1608	CA	THR B	116	−0.366	−0.074	10.942	1.00	37.35		C
ANISOU	1608	CA	THR B	116	4677	4856	4658	551	−365	711	C
ATOM	1609	C	THR B	116	0.857	−0.407	10.095	1.00	38.10		C
ANISOU	1609	C	THR B	116	4902	4932	4641	396	−232	696	C
ATOM	1610	O	THR B	116	1.973	−0.056	10.449	1.00	34.51		O
ANISOU	1610	O	THR B	116	4474	4255	4383	349	−89	623	O
ATOM	1611	CB	THR B	116	−0.786	1.391	10.692	1.00	44.84		C
ANISOU	1611	CB	THR B	116	5628	5641	5768	756	−321	1009	C
ATOM	1612	OG1	THR B	116	−2.013	1.658	11.383	1.00	50.90		O
ANISOU	1612	OG1	THR B	116	6240	6436	6662	931	−404	1033	O
ATOM	1613	CG2	THR B	116	−1.028	1.639	9.181	1.00	40.61		C
ANISOU	1613	CG2	THR B	116	5148	5331	4953	803	−373	1364	C
ATOM	1614	N	LEU B	117	0.625	−1.103	8.978	1.00	36.95		N
ANISOU	1614	N	LEU B	117	4814	5057	4168	286	−264	728	N
ATOM	1615	CA	LEU B	117	1.677	−1.385	8.033	1.00	35.28		C
ANISOU	1615	CA	LEU B	117	4743	4843	3817	137	−81	713	C
ATOM	1616	C	LEU B	117	1.396	−0.640	6.758	1.00	33.83		C
ANISOU	1616	C	LEU B	117	4661	4842	3350	162	−98	1032	C
ATOM	1617	O	LEU B	117	0.330	−0.776	6.187	1.00	38.44		O
ANISOU	1617	O	LEU B	117	5195	5783	3625	171	−295	1147	O
ATOM	1618	CB	LEU B	117	1.787	−2.875	7.759	1.00	35.26		C
ANISOU	1618	CB	LEU B	117	4775	4980	3642	−55	−6	435	C
ATOM	1619	CG	LEU B	117	2.755	−3.382	6.693	1.00	37.15		C
ANISOU	1619	CG	LEU B	117	5167	5236	3711	−233	250	349	C
ATOM	1620	CD1	LEU B	117	4.210	−2.932	6.918	1.00	37.68		C
ANISOU	1620	CD1	LEU B	117	5230	5007	4081	−192	476	382	C
ATOM	1621	CD2	LEU B	117	2.638	−4.874	6.787	1.00	39.90		C
ANISOU	1621	CD2	LEU B	117	5528	5608	4023	−386	368	29	C
ATOM	1622	N	ALYS B	118	2.356	0.171	6.333	0.51	35.23		N
ANISOU	1622	N	ALYS B	118	4956	4803	3627	168	111	1199	N
ATOM	1623	CA	ALYS B	118	2.270	0.879	5.061	0.51	41.08		C
ANISOU	1623	CA	ALYS B	118	5839	5699	4071	198	162	1573	C
ATOM	1624	C	ALYS B	118	3.351	0.347	4.119	0.51	44.17		C
ANISOU	1624	C	ALYS B	118	6399	6147	4238	−35	422	1462	C
ATOM	1625	O	ALYS B	118	4.494	0.128	4.517	0.51	43.43		O
ANISOU	1625	O	ALYS B	118	6294	5774	4434	−128	653	1243	O
ATOM	1626	CB	ALYS B	118	2.416	2.392	5.262	0.51	43.62		C
ANISOU	1626	CB	ALYS B	118	6195	5654	4725	403	292	1920	C
ATOM	1627	CG	ALYS B	118	1.184	3.054	5.870	0.51	44.10		C
ANISOU	1627	CG	ALYS B	118	6114	5684	4959	680	101	2122	C
ATOM	1628	N	BLYS B	118	2.377	0.154	6.339	0.49	35.20		N
ANISOU	1628	N	BLYS B	118	4953	4797	3626	165	114	1192	N
ATOM	1629	CA	BLYS B	118	2.341	0.913	5.091	0.49	41.26		C
ANISOU	1629	CA	BLYS B	118	5865	5695	4119	198	178	1570	C
ATOM	1630	C	BLYS B	118	3.371	0.329	4.119	0.49	44.12		C
ANISOU	1630	C	BLYS B	118	6393	6139	4232	−39	427	1455	C
ATOM	1631	O	BLYS B	118	4.509	0.060	4.501	0.49	43.29		O
ANISOU	1631	O	BLYS B	118	6277	5765	4405	−138	656	1227	O
ATOM	1632	CB	BLYS B	118	2.632	2.398	5.356	0.49	43.61		C
ANISOU	1632	CB	BLYS B	118	6199	5589	4781	380	335	1876	C
ATOM	1633	CG	BLYS B	118	2.546	3.294	4.131	0.49	47.86		C
ANISOU	1633	CG	BLYS B	118	6903	6203	5081	483	444	2389	C
ATOM	1634	N	VAL B	119	2.968	0.118	2.873	1.00	45.61		N
ANISOU	1634	N	VAL B	119	6707	6742	3879	−135	386	1603	N
ATOM	1635	CA	VAL B	119	3.862	−0.469	1.880	1.00	51.10		C
ANISOU	1635	CA	VAL B	119	7590	7546	4278	−387	673	1452	C
ATOM	1636	C	VAL B	119	4.182	0.580	0.832	1.00	54.41		C

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

ANISOU	1636	C	VAL B	119	8200	8020	4451	−343	836	1914	C
ATOM	1637	O	VAL B	119	3.282	0.984	0.111	1.00	59.47		O
ANISOU	1637	O	VAL B	119	8880	9065	4651	−255	621	2278	O
ATOM	1638	CB	VAL B	119	3.201	−1.712	1.242	1.00	52.68		C
ANISOU	1638	CB	VAL B	119	7824	8227	3964	−636	564	1144	C
ATOM	1639	CG1	VAL B	119	4.074	−2.326	0.208	1.00	57.21		C
ANISOU	1639	CG1	VAL B	119	8619	8899	4221	−916	925	931	C
ATOM	1640	CG2	VAL B	119	2.873	−2.739	2.334	1.00	48.97		C
ANISOU	1640	CG2	VAL B	119	7186	7613	3806	−666	474	734	C
ATOM	1641	N	LYS B	120	5.404	1.102	0.809	1.00	57.03		N
ANISOU	1641	N	LYS B	120	8615	7960	5094	−377	1205	1956	N
ATOM	1642	C	LYS B	120	6.414	1.226	−1.478	1.00	66.76		C
ANISOU	1642	C	LYS B	120	10283	9533	5550	−672	1734	2224	C
ATOM	1643	O	LYS B	120	6.823	0.105	−1.364	1.00	66.57		O
ANISOU	1643	O	LYS B	120	10220	9531	5543	−866	1845	1734	O
ATOM	1644	CA	LYS B	120	5.932	1.965	−0.264	1.00	64.53		C
ANISOU	1644	CA	LYS B	120	9793	8905	5822	−396	1494	2364	C
ATOM	1645	CB	LYS B	120	7.161	2.723	0.183	1.00	69.57		C
ANISOU	1645	CB	LYS B	120	10412	8975	7048	−413	1872	2372	C
ATOM	1646	CG	LYS B	120	7.195	3.214	1.594	1.00	67.42		C
ANISOU	1646	CG	LYS B	120	9915	8276	7426	−286	1772	2241	C
ATOM	1647	CD	LYS B	120	8.585	3.689	1.930	1.00	69.90		C
ANISOU	1647	CD	LYS B	120	10160	8159	8240	−439	2159	2098	C
ATOM	1648	CE	LYS B	120	9.624	2.639	1.621	1.00	71.34		C
ANISOU	1648	CE	LYS B	120	10279	8451	8374	−655	2382	1744	C
ATOM	1649	NZ	LYS B	120	10.830	2.828	2.455	1.00	72.38		N
ANISOU	1649	NZ	LYS B	120	10146	8260	9096	−770	2583	1482	N
ATOM	1650	O	ALA B	121	8.913	2.828	−3.416	1.00	77.21		O
ANISOU	1650	O	ALA B	121	11983	10459	6895	−908	2779	2744	O
ATOM	1651	N	ALA B	121	6.461	1.886	−2.630	1.00	69.76		N
ANISOU	1651	N	ALA B	121	10901	10137	5469	−684	1889	2666	N
ATOM	1652	CA	ALA B	121	7.093	1.309	−3.806	1.00	75.66		C
ANISOU	1652	CA	ALA B	121	11823	11181	5741	−951	2189	2499	C
ATOM	1653	C	ALA B	121	8.553	1.752	−3.897	1.00	76.62		C
ANISOU	1653	C	ALA B	121	11952	10834	6325	−1041	2680	2465	C
ATOM	1654	CB	ALA B	121	6.347	1.704	−5.038	1.00	84.92		C
ANISOU	1654	CB	ALA B	121	13224	12772	6271	−818	2038	2848	C
TER											
HETATM	1655	MG	MG C	1	−12.423	21.789	37.851	1.00	10.21		Mg
TER											
HETATM	1656	O	HOH S	1	−11.900	7.714	39.918	1.00	36.82		O
HETATM	1657	O	HOH S	2	5.380	−1.733	18.078	1.00	42.03		O
HETATM	1658	O	HOH S	3	−3.752	−1.172	27.706	1.00	30.61		O
HETATM	1659	O	HOH S	4	−10.403	9.535	25.067	1.00	36.60		O
HETATM	1660	O	HOH S	5	−10.109	8.110	32.307	1.00	33.09		O
HETATM	1661	O	HOH S	6	−8.230	−8.835	30.592	1.00	36.54		O
HETATM	1662	O	HOH S	7	−6.450	−3.897	7.581	1.00	43.31		O
HETATM	1663	O	HOH S	8	−11.226	17.652	37.643	1.00	41.73		O
HETATM	1664	O	HOH S	9	11.006	−5.310	10.589	1.00	41.18		O
HETATM	1665	O	HOH S	10	6.936	−13.148	20.077	1.00	42.17		O
HETATM	1666	O	HOH S	11	−7.618	7.364	31.834	1.00	35.02		O
HETATM	1667	O	HOH S	12	−23.200	−0.301	40.120	1.00	39.37		O
HETATM	1668	O	HOH S	13	−10.349	11.123	41.000	1.00	42.33		O
HETATM	1669	O	HOH S	14	−8.911	−19.801	17.605	1.00	54.02		O
HETATM	1670	O	HOH S	15	−12.611	15.391	40.612	1.00	39.82		O
HETATM	1671	O	HOH 5	16	−18.344	3.513	17.529	1.00	40.36		O
HETATM	1672	O	HOH S	17	−14.904	13.729	44.439	1.00	43.93		O
HETATM	1673	O	HOH S	18	−7.828	10.805	33.107	1.00	47.89		O
HETATM	1674	O	HOH S	19	−23.034	14.524	38.000	1.00	40.79		O
HETATM	1675	O	HOH S	20	−23.090	8.084	36.258	1.00	44.88		O
HETATM	1676	O	HOH S	21	−22.806	9.951	40.206	1.00	54.76		O
HETATM	1677	O	HOH S	22	0.813	1.581	23.702	1.00	57.37		O
HETATM	1678	O	HOH S	23	11.708	−14.287	3.627	1.00	52.01		O
HETATM	1679	O	HOH S	24	−14.338	−11.481	26.493	1.00	44.42		O
HETATM	1680	O	HOH S	25	9.131	−3.175	16.236	1.00	42.13		O
HETATM	1681	O	HOH S	26	−1.105	2.064	14.167	1.00	60.92		O
HETATM	1682	O	HOH S	27	11.909	−5.197	−1.529	1.00	51.43		O
HETATM	1683	O	HOH S	28	13.293	−15.900	14.555	1.00	39.68		O
HETATM	1684	O	HOH S	29	7.650	−19.522	16.191	1.00	43.67		O
HETATM	1685	O	HOH S	30	1.348	−17.126	14.225	1.00	42.61		O
HETATM	1686	O	HOH S	31	−14.905	23.868	39.927	1.00	45.13		O
HETATM	1687	O	HOH S	32	−10.080	14.900	28.889	1.00	37.23		O
HETATM	1688	O	HOH S	33	−8.426	−10.736	11.463	1.00	55.62		O
HETATM	1689	O	HOH S	34	−18.847	0.126	38.624	1.00	43.58		O

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

HETATM	1690	O	HOH S	35	−15.672	0.253	18.397	1.00	44.41	O
HETATM	1691	O	HOH S	36	13.643	−7.930	3.769	1.00	42.90	O
HETATM	1692	O	HOH S	37	−10.654	−8.957	15.970	1.00	47.50	O
HETATM	1693	O	HOH S	38	−21.135	−14.442	22.657	1.00	54.40	O
HETATM	1694	O	HOH S	39	−21.281	20.925	35.993	1.00	50.08	O
HETATM	1695	O	HOH S	40	−13.418	17.631	41.547	1.00	50.58	O
HETATM	1696	O	HOH S	41	−27.329	5.575	24.313	1.00	59.43	O
HETATM	1697	O	HOH S	42	−14.776	−4.993	16.979	1.00	49.61	O
HETATM	1698	O	HOH S	43	−0.676	−9.652	6.203	1.00	43.69	O
HETATM	1699	O	HOH S	44	−25.252	−1.782	28.133	1.00	54.09	O
HETATM	1700	O	HOH S	45	−22.083	−2.141	20.937	1.00	41.28	O
HETATM	1701	O	HOH S	46	6.716	−24.401	18.382	1.00	56.79	O
HETATM	1702	O	HOH S	47	−19.242	−7.960	40.741	1.00	55.27	O
HETATM	1703	O	HOH S	48	−24.885	3.029	32.595	1.00	47.29	O
HETATM	1704	O	HOH S	49	−6.222	1.301	35.492	1.00	47.37	O
HETATM	1705	O	HOH S	50	−6.853	−1.015	7.397	1.00	54.42	O
HETATM	1706	O	HOH S	51	−9.238	3.184	16.875	1.00	56.84	O
HETATM	1707	O	HOH S	52	5.516	−14.125	0.045	1.00	59.28	O
HETATM	1708	O	HOH S	53	−9.526	11.881	25.225	1.00	51.94	O
HETATM	1709	O	HOH S	54	−3.550	2.482	14.129	1.00	55.95	O
HETATM	1710	O	HOH S	55	−17.418	22.428	31.944	1.00	40.14	O
HETATM	1711	O	HOH S	56	−4.486	−3.749	1.719	1.00	45.17	O
HETATM	1712	O	HOH S	57	5.103	4.636	14.892	1.00	66.66	O
HETATM	1713	O	HOH S	58	−23.492	−0.094	22.392	1.00	47.19	O
HETATM	1714	O	HOH S	59	−26.738	3.100	30.515	1.00	57.55	O
HETATM	1715	O	HOH S	60	−24.686	10.560	35.917	1.00	46.11	O
HETATM	1716	O	HOH S	61	13.398	−18.359	23.686	1.00	51.45	O
HETATM	1717	O	HOH S	62	−21.258	−0.014	40.488	1.00	59.28	O
HETATM	1718	O	HOH S	63	−21.450	9.546	21.544	1.00	44.60	O
HETATM	1719	O	HOH S	64	−15.980	19.531	42.414	1.00	54.58	O
HETATM	1720	O	HOH S	65	−26.583	9.077	25.046	1.00	67.01	O
HETATM	1721	O	HOH S	66	−25.031	6.323	34.427	1.00	49.13	O
HETATM	1722	O	HOH S	67	4.323	−19.716	14.727	1.00	60.95	O
HETATM	1723	O	HOH S	68	9.220	2.118	9.552	1.00	49.01	O
HETATM	1724	O	HOH S	69	−26.836	7.978	32.921	1.00	49.25	O
HETATM	1725	O	HOH S	70	−23.972	−5.676	19.453	1.00	56.39	O
HETATM	1726	O	HOH S	71	14.673	−7.560	1.360	1.00	55.30	O
HETATM	1727	O	HOH S	72	−6.648	−17.237	15.642	1.00	53.29	O
HETATM	1728	O	HOH S	73	0.200	−17.959	20.530	1.00	49.36	O
HETATM	1729	O	HOH S	74	12.672	−11.935	1.844	1.00	53.58	O
HETATM	1730	O	HOH S	75	−5.701	13.730	36.592	1.00	58.09	O
HETATM	1731	O	HOH S	76	−5.766	−19.056	27.135	1.00	51.70	O
HETATM	1732	O	HOH S	77	−25.610	11.969	30.497	1.00	45.95	O
HETATM	1733	O	HOH S	78	10.560	−2.550	−4.237	1.00	57.19	O
HETATM	1734	O	HOH S	79	−25.261	12.245	34.406	1.00	52.54	O
HETATM	1735	O	HOH S	80	6.500	−27.035	18.000	1.00	50.83	O
HETATM	1736	O	HOH S	81	−12.866	−16.068	33.587	1.00	63.38	O
HETATM	1737	O	HOH S	82	−6.248	8.367	35.809	1.00	44.88	O
HETATM	1738	O	HOH S	83	13.594	−2.415	−2.493	1.00	62.89	O
HETATM	1739	O	HOH S	85	1.990	−6.171	−4.313	1.00	46.07	O
HETATM	1740	O	HOH S	86	−6.321	6.088	29.395	1.00	43.19	O
HETATM	1741	O	HOH S	87	−5.277	−11.712	9.904	1.00	41.48	O
HETATM	1742	O	HOH S	88	−0.692	−21.465	15.484	1.00	65.91	O
HETATM	1743	O	HOH S	89	−10.486	8.212	42.653	1.00	58.03	O
HETATM	1744	O	HOH S	90	−9.955	−4.337	37.118	1.00	56.18	O
HETATM	1745	O	HOH S	91	3.767	−23.040	34.067	1.00	59.96	O
HETATM	1746	O	HOH S	92	0.653	−0.503	30.031	1.00	51.73	O
HETATM	1747	O	HOH S	93	−18.336	−14.096	21.741	1.00	59.29	O
HETATM	1748	O	HOH S	94	3.479	−25.209	38.916	1.00	63.56	O
HETATM	1749	O	HOH S	95	−26.605	10.470	22.549	1.00	52.94	O
HETATM	1750	O	HOH S	96	−12.820	14.810	43.469	1.00	60.93	O
HETATM	1751	O	HOH S	97	−11.877	−22.060	17.397	1.00	57.27	O
HETATM	1752	O	HOH S	98	−11.511	−6.158	13.611	1.00	61.64	O
HETATM	1753	O	HOH S	99	−6.402	3.744	38.398	1.00	58.98	O
HETATM	1754	O	HOH S	100	−12.627	−6.523	39.220	1.00	65.30	O
HETATM	1755	O	HOH S	101	−24.129	−11.311	39.009	1.00	73.80	O
HETATM	1756	O	HOH S	102	−3.142	−18.704	9.848	1.00	65.08	O
HETATM	1757	O	HOH S	103	7.671	−5.745	27.881	1.00	60.74	O
HETATM	1758	O	HOH S	104	−0.042	2.480	25.710	1.00	60.35	O
HETATM	1759	O	HOH S	105	−4.587	−10.265	34.955	1.00	61.56	O
HETATM	1760	O	HOH S	106	−24.323	5.290	19.367	1.00	61.98	O
HETATM	1761	O	HOH S	107	−25.459	7.824	19.064	1.00	67.53	O
HETATM	1762	O	HOH S	108	−24.758	1.839	41.011	1.00	71.29	O
HETATM	1763	O	HOH S	109	5.609	−12.232	−2.646	1.00	69.92	O

TABLE 6-continued

Atomic coordinates and structure factors for the human PD $1^{N74G\ T76P\ A132V}$/PD-L2IgV complex (based on a PDB file).

HETATM	1764	O	HOH S	110	−22.882	16.125	43.554	1.00	63.16	O
HETATM	1765	O	HOH S	112	−16.657	12.218	48.606	1.00	69.31	O
HETATM	1766	O	HOH S	113	−24.809	15.560	34.889	1.00	69.17	O
HETATM	1767	O	HOH S	114	−17.404	6.366	16.634	1.00	62.38	O
HETATM	1768	O	HOH S	115	14.658	−12.079	2.681	1.00	67.54	O
HETATM	1769	O	HOH S	116	13.040	−9.195	13.096	1.00	55.34	O
HETATM	1770	O	HOH S	118	−16.739	11.026	49.721	1.00	69.52	O
HETATM	1771	O	HOH S	119	−12.669	6.257	18.282	1.00	61.46	O
HETATM	1772	O	HOH S	120	12.775	−6.171	14.964	1.00	65.93	O
HETATM	1773	O	HOH S	122	11.291	−2.217	13.161	1.00	63.39	O
HETATM	1774	O	HOH S	123	−11.161	−2.151	14.499	1.00	68.03	O
HETATM	1775	O	HOH S	124	−8.793	2.192	14.011	1.00	73.70	O
HETATM	1776	O	HOH S	125	−11.481	−15.730	36.023	1.00	71.36	O
HETATM	1777	O	HOH S	126	−5.104	1.400	43.064	1.00	68.56	O
HETATM	1778	O	HOH S	127	3.229	−28.600	36.834	1.00	78.22	O
HETATM	1779	O	HOH S	128	5.055	−12.031	−1.300	1.00	69.82	O
HETATM	1780	O	HOH S	130	−16.498	18.765	29.401	1.00	57.18	O
HETATM	1781	O	HOH S	131	−27.516	8.450	17.962	1.00	79.87	O
HETATM	1782	O	HOH S	132	1.844	8.012	23.188	1.00	76.81	O
TER										
END										

TABLE 7

Atomic coordinates and structure factors for human apo-PD-$1^{N74G\ T76P\ A132V}$ (based on a PDB file).

CRYST1	46.172	46.172	89.270	90.00	90.00	120.00	P 32 2 1			
SCALE1		0.021658	0.012504	0.000000		0.00000				
SCALE2		0.000000	0.025009	0.000000		0.00000				
SCALE3		0.000000	0.000000	0.011202		0.00000				
ATOM	1	O	MET A	32	79.830	72.727	114.713	1.00	33.51	O
ANISOU	1	O	MET A	32	4442	4896	3394	−702	−1149	301 O
ATOM	2	N	MET A	32	78.909	75.195	115.710	1.00	37.88	N
ANISOU	2	N	MET A	32	5485	5060	3848	−66	−935	−491 N
ATOM	3	C	MET A	32	78.636	72.854	114.996	1.00	31.86	C
ANISOU	3	C	MET A	32	4346	4552	3207	−68	−941	−549 C
ATOM	4	CA	AMET A	32	77.995	74.240	115.087	0.49	30.75	C
ANISOU	4	CA	AMET A	32	4520	4029	3135	44	−1085	−722 C
ATOM	5	CB	AMET A	32	77.560	74.735	113.696	0.49	32.29	C
ANISOU	5	CB	AMET A	32	4539	4040	3688	−153	−1019	−383 C
ATOM	6	CG	AMET A	32	76.475	73.892	113.023	0.49	29.96	C
ANISOU	6	CG	AMET A	32	4316	3395	3674	−172	−944	−240 C
ATOM	7	SD	AMET A	32	75.859	74.568	111.459	0.49	25.76	S
ANISOU	7	SD	AMET A	32	3894	2513	3382	−170	−830	42 S
ATOM	8	CE	AMET A	32	77.360	74.632	110.485	0.49	24.73	C
ANISOU	8	CE	AMET A	32	3990	2249	3158	−46	−746	−0 C
ATOM	9	CA	BMET A	32	77.988	74.230	115.126	0.51	31.28	C
ANISOU	9	CA	BMET A	32	4697	4033	3155	190	−922	−701 C
ATOM	10	CB	BMET A	32	77.504	74.711	113.760	0.51	34.88	C
ANISOU	10	CB	BMET A	32	5128	4374	3750	550	−604	−347 C
ATOM	11	CG	BMET A	32	78.611	74.790	112.734	0.51	29.06	C
ANISOU	11	CG	BMET A	32	4499	3462	3079	949	−286	−26 C
ATOM	12	SD	BMET A	32	78.032	75.208	111.094	0.51	22.29	S
ANISOU	12	SD	BMET A	32	3320	2568	2581	−86	−682	98 S
ATOM	13	CE	BMET A	32	76.765	73.972	110.841	0.51	21.47	C
ANISOU	13	CE	BMET A	32	3037	2508	2612	−312	−458	−483 C
ATOM	14	N	ASN A	33	77.838	71.825	115.236	1.00	27.27	N
ANISOU	14	N	ASN A	33	3793	3937	2629	415	−354	−960 N
ATOM	15	CA	ASN A	33	78.278	70.448	115.106	1.00	25.75	C
ANISOU	15	CA	ASN A	33	3582	3665	2536	−312	−207	−1117 C
ATOM	16	C	ASN A	33	77.907	69.965	113.725	1.00	22.88	C
ANISOU	16	C	ASN A	33	2433	3822	2438	444	−531	−1185 C
ATOM	17	O	ASN A	33	76.936	70.447	113.146	1.00	27.75	O
ANISOU	17	O	ASN A	33	2891	4625	3026	1444	−982	−1681 O
ATOM	18	CB	ASN A	33	77.529	69.583	116.118	1.00	30.67	C
ANISOU	18	CB	ASN A	33	4226	4744	2683	−940	184	−1015 C
ATOM	19	CG	ASN A	33	77.341	70.278	117.443	1.00	34.68	C
ANISOU	19	CG	ASN A	33	4200	5911	3064	−76	292	−796 C
ATOM	20	OD1	ASN A	33	76.219	70.417	117.946	1.00	37.76	O
ANISOU	20	OD1	ASN A	33	4804	6206	3335	−264	280	−880 O

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	21	ND2	ASN A	33	78.440	70.734	118.016	1.00	29.13		N
ANISOU	21	ND2	ASN A	33	3681	5301	2088	595	−673	−893	N
ATOM	22	N	PRO A	34	78.655	68.998	113.179	1.00	18.36		N
ANISOU	22	N	PRO A	34	1952	2987	2038	257	−510	−597	N
ATOM	23	C	PRO A	34	76.953	67.611	112.049	1.00	15.80		C
ANISOU	23	C	PRO A	34	1875	2665	1462	379	−368	−360	C
ATOM	24	O	PRO A	34	76.706	67.033	113.102	1.00	18.22		O
ANISOU	24	O	PRO A	34	2174	3378	1372	68	−220	30	O
ATOM	25	CA	APRO A	34	78.235	68.417	111.903	0.47	16.78		C
ANISOU	25	CA	APRO A	34	1807	2637	1930	289	−434	−220	C
ATOM	26	CB	APRO A	34	79.384	67.461	111.555	0.47	19.28		C
ANISOU	26	CB	APRO A	34	2070	2646	2609	16	−131	−137	C
ATOM	27	CG	APRO A	34	80.526	67.879	112.418	0.47	16.73		C
ANISOU	27	CG	APRO A	34	1848	2450	2059	82	−671	−184	C
ATOM	28	CD	APRO A	34	79.925	68.430	113.662	0.47	17.94		C
ANISOU	28	CD	APRO A	34	1726	3066	2023	172	−701	−345	C
ATOM	29	CA	BPRO A	34	78.196	68.473	111.896	0.53	16.26		C
ANISOU	29	CA	BPRO A	34	1714	2648	1817	420	−357	−563	C
ATOM	30	CB	BPRO A	34	79.373	67.613	111.430	0.53	19.36		C
ANISOU	30	CB	BPRO A	34	2073	2908	2374	459	−177	−544	C
ATOM	31	CG	BPRO A	34	80.037	67.196	112.684	0.53	21.73		C
ANISOU	31	CG	BPRO A	34	2467	3366	2422	687	−363	−378	C
ATOM	32	CD	BPRO A	34	79.900	68.354	113.632	0.53	21.39		C
ANISOU	32	CD	BPRO A	34	2149	3605	2373	528	−424	−408	C
ATOM	33	N	PRO A	35	76.153	67.545	110.992	1.00	14.87		N
ANISOU	33	N	PRO A	35	1860	2567	1222	320	−286	−531	N
ATOM	34	CA	PRO A	35	75.029	66.611	110.996	1.00	15.01		C
ANISOU	34	CA	PRO A	35	1992	2294	1417	421	−354	−385	C
ATOM	35	C	PRO A	35	75.547	65.175	110.811	1.00	14.70		C
ANISOU	35	C	PRO A	35	1862	2629	1094	194	−229	−323	C
ATOM	36	O	PRO A	35	76.677	64.987	110.362	1.00	15.42		O
ANISOU	36	O	PRO A	35	1899	2377	1584	386	−97	−146	O
ATOM	37	CB	PRO A	35	74.232	67.048	109.767	1.00	16.89		C
ANISOU	37	CB	PRO A	35	2063	2934	1420	365	−287	−270	C
ATOM	38	CG	PRO A	35	75.269	67.639	108.845	1.00	17.84		C
ANISOU	38	CG	PRO A	35	2804	2536	1438	746	−662	−274	C
ATOM	39	CD	PRO A	35	76.296	68.267	109.713	1.00	16.05		C
ANISOU	39	CD	PRO A	35	2802	2289	1009	546	−449	−215	C
ATOM	40	N	THR A	36	74.718	64.185	111.117	1.00	15.08		N
ANISOU	40	N	THR A	36	2017	2363	1351	225	−228	−344	N
ATOM	41	CA	THR A	36	75.023	62.793	110.803	1.00	16.35		C
ANISOU	41	CA	THR A	36	2124	2588	1502	246	−309	−222	C
ATOM	42	C	THR A	36	74.028	62.296	109.759	1.00	15.16		C
ANISOU	42	C	THR A	36	1801	2402	1557	206	−204	−398	C
ATOM	43	O	THR A	36	72.916	62.814	109.646	1.00	18.63		O
ANISOU	43	O	THR A	36	2032	3001	2046	688	−368	−1001	O
ATOM	44	CB	THR A	36	74.965	61.892	112.042	1.00	20.81		C
ANISOU	44	CB	THR A	36	2401	3485	2019	275	−138	105	C
ATOM	45	OG1	THR A	36	73.631	61.886	112.555	1.00	24.03		O
ANISOU	45	OG1	THR A	36	3055	3856	2219	497	207	636	O
ATOM	46	CG2	THR A	36	75.933	62.383	113.114	1.00	20.93		C
ANISOU	46	CG2	THR A	36	2980	3430	1543	429	−566	−172	C
ATOM	47	N	PHE A	37	74.431	61.308	108.976	1.00	14.36		N
ANISOU	47	N	PHE A	37	2089	2035	1331	309	−60	−217	N
ATOM	48	CA	PHE A	37	73.640	60.887	107.830	1.00	13.70		C
ANISOU	48	CA	PHE A	37	2134	1944	1126	100	−174	−165	C
ATOM	49	C	PHE A	37	73.624	59.369	107.792	1.00	14.15		C
ANISOU	49	C	PHE A	37	2000	2138	1240	407	−90	−88	C
ATOM	50	O	PHE A	37	74.684	58.740	107.782	1.00	17.72		O
ANISOU	50	O	PHE A	37	2211	2296	2225	259	84	−36	O
ATOM	51	CB	PHE A	37	74.274	61.468	106.576	1.00	14.18		C
ANISOU	51	CB	PHE A	37	2209	2159	1019	39	−98	−76	C
ATOM	52	CG	PHE A	37	73.369	61.532	105.387	1.00	14.61		C
ANISOU	52	CG	PHE A	37	2445	1869	1238	−149	50	−21	C
ATOM	53	CD1	PHE A	37	73.812	61.078	104.163	1.00	19.33		C
ANISOU	53	CD1	PHE A	37	3032	3221	1090	−913	193	−167	C
ATOM	54	CD2	PHE A	37	72.111	62.105	105.465	1.00	17.12		C
ANISOU	54	CD2	PHE A	37	2497	2187	1820	−100	−524	−2	C
ATOM	55	CE1	PHE A	37	73.010	61.163	103.046	1.00	23.99		C
ANISOU	55	CE1	PHE A	37	3414	4289	1414	−1415	108	90	C
ATOM	56	CE2	PHE A	37	71.308	62.201	104.347	1.00	19.30		C
ANISOU	56	CE2	PHE A	37	2914	2529	1892	−612	−721	455	C
ATOM	57	CZ	PHE A	37	71.765	61.734	103.141	1.00	21.04		C
ANISOU	57	CZ	PHE A	37	2905	3608	1483	−1397	−469	732	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	58	O	SER A	38	70.289	57.574	106.613	1.00	15.97		O
ANISOU	58	O	SER A	38	2359	2030	1679	215	−282	−3	O
ATOM	59	N	SER A	38	72.431	58.785	107.767	1.00	14.16		N
ANISOU	59	N	SER A	38	2349	1917	1113	58	−180	−60	N
ATOM	60	C	SER A	38	71.160	56.826	107.016	1.00	14.91		C
ANISOU	60	C	SER A	38	2287	2034	1342	−75	−143	61	C
ATOM	61	CA	ASER A	38	72.288	57.343	107.907	0.56	15.15		C
ANISOU	61	CA	ASER A	38	2420	2246	1091	304	−249	23	C
ATOM	62	CB	ASER A	38	72.023	56.979	109.374	0.56	20.63		C
ANISOU	62	CB	ASER A	38	3585	2419	1836	181	3	16	C
ATOM	63	OG	ASER A	38	70.756	57.451	109.795	0.56	21.87		O
ANISOU	63	OG	ASER A	38	4075	2401	1835	−72	389	78	O
ATOM	64	CA	BSER A	38	72.260	57.348	107.941	0.16	15.76		C
ANISOU	64	CA	BSER A	38	2456	2292	1239	113	−273	11	C
ATOM	65	CB	BSER A	38	71.909	57.057	109.408	0.16	17.69		C
ANISOU	65	CB	BSER A	38	2714	2621	1285	139	−331	−33	C
ATOM	66	OG	BSER A	38	71.329	55.775	109.576	0.16	16.34		O
ANISOU	66	OG	BSER A	38	2597	2720	890	117	−526	0	O
ATOM	67	CA	CSER A	38	72.263	57.344	107.930	0.28	15.41		C
ANISOU	67	CA	CSER A	38	2481	2242	1132	167	−273	15	C
ATOM	68	CB	CSER A	38	71.896	57.020	109.381	0.28	17.88		C
ANISOU	68	CB	CSER A	38	3115	2347	1332	−64	−223	−42	C
ATOM	69	OG	CSER A	38	72.827	57.580	110.283	0.28	17.98		O
ANISOU	69	OG	CSER A	38	3241	2377	1212	−387	−254	133	O
ATOM	70	N	PRO A	39	71.197	55.524	106.669	1.00	16.19		N
ANISOU	70	N	PRO A	39	2436	1977	1737	65	−316	85	N
ATOM	71	CA	PRO A	39	72.243	54.535	106.948	1.00	16.60		C
ANISOU	71	CA	PRO A	39	2454	1838	2014	41	−99	41	C
ATOM	72	C	PRO A	39	73.419	54.778	106.016	1.00	15.97		C
ANISOU	72	C	PRO A	39	2658	1744	1666	131	−207	245	C
ATOM	73	O	PRO A	39	73.264	55.425	104.971	1.00	16.75		O
ANISOU	73	O	PRO A	39	2523	2165	1675	191	−88	230	O
ATOM	74	CB	PRO A	39	71.571	53.210	106.600	1.00	19.16		C
ANISOU	74	CB	PRO A	39	3181	1904	2195	26	−121	227	C
ATOM	75	CG	PRO A	39	70.626	53.561	105.537	1.00	19.50		C
ANISOU	75	CG	PRO A	39	3343	1919	2148	−173	−550	30	C
ATOM	76	CD	PRO A	39	70.094	54.929	105.892	1.00	18.31		C
ANISOU	76	CD	PRO A	39	2901	2007	2050	−155	−387	170	C
ATOM	77	N	ALA A	40	74.581	54.258	106.377	1.00	16.67		N
ANISOU	77	N	ALA A	40	2629	2178	1525	335	−190	183	N
ATOM	78	CA	ALA A	40	75.768	54.444	105.561	1.00	16.37		C
ANISOU	78	CA	ALA A	40	2306	2449	1465	144	−236	−117	C
ATOM	79	C	ALA A	40	75.627	53.797	104.190	1.00	15.01		C
ANISOU	79	C	ALA A	40	2233	2025	1446	215	−251	236	C
ATOM	80	O	ALA A	40	76.222	54.262	103.222	1.00	15.34		O
ANISOU	80	O	ALA A	40	2262	2060	1505	−20	−202	134	O
ATOM	81	CB	ALA A	40	76.990	53.897	106.276	1.00	20.28		C
ANISOU	81	CB	ALA A	40	2826	3357	1522	643	−539	−171	C
ATOM	82	N	LEU A	41	74.855	52.717	104.120	1.00	15.59		N
ANISOU	82	N	LEU A	41	2571	2135	1218	360	−160	−76	N
ATOM	83	CA	LEU A	41	74.588	52.042	102.856	1.00	15.63		C
ANISOU	83	CA	LEU A	41	2477	2052	1411	62	−23	116	C
ATOM	84	C	LEU A	41	73.105	51.734	102.800	1.00	14.98		C
ANISOU	84	C	LEU A	41	2489	1902	1299	64	−72	11	C
ATOM	85	O	LEU A	41	72.569	51.088	103.699	1.00	18.14		O
ANISOU	85	O	LEU A	41	2947	2224	1719	36	−31	345	O
ATOM	86	CB	LEU A	41	75.385	50.742	102.740	1.00	16.61		C
ANISOU	86	CB	LEU A	41	2618	2152	1540	286	−109	−298	C
ATOM	87	CG	LEU A	41	75.066	49.870	101.518	1.00	18.17		C
ANISOU	87	CG	LEU A	41	2906	2231	1768	387	−18	−173	C
ATOM	88	CD1	LEU A	41	75.352	50.581	100.207	1.00	18.57		C
ANISOU	88	CD1	LEU A	41	2888	2659	1508	−9	232	−249	C
ATOM	89	CD2	LEU A	41	75.842	48.564	101.591	1.00	20.17		C
ANISOU	89	CD2	LEU A	41	3236	2167	2259	336	121	−279	C
ATOM	90	N	LEU A	42	72.452	52.211	101.750	1.00	14.97		N
ANISOU	90	N	LEU A	42	2285	2045	1357	139	8	−66	N
ATOM	91	C	LEU A	42	70.899	51.271	100.172	1.00	14.15		C
ANISOU	91	C	LEU A	42	1938	2233	1205	97	48	87	C
ATOM	92	O	LEU A	42	71.321	51.808	99.151	1.00	15.43		O
ANISOU	92	O	LEU A	42	2382	2214	1268	−9	151	−67	O
ATOM	93	CD1	LEU A	42	68.105	52.322	102.336	1.00	24.90		C
ANISOU	93	CD1	LEU A	42	2747	4393	2320	341	253	409	C
ATOM	94	CD2	LEU A	42	68.209	54.656	101.428	1.00	23.22		C
ANISOU	94	CD2	LEU A	42	2935	3807	2082	1510	−20	−37	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	95	CA	LEU A	42	71.040	51.961	101.525	1.00	15.55		C
ANISOU	95	CA	LEU A	42	2344	2269	1296	392	147	156	C
ATOM	96	CB	LEU A	42	70.285	53.287	101.519	1.00	17.74		C
ANISOU	96	CB	LEU A	42	2446	2867	1427	690	−24	−381	C
ATOM	97	CG	LEU A	42	68.772	53.247	101.324	1.00	19.78		C
ANISOU	97	CG	LEU A	42	2418	3446	1654	505	−170	185	C
ATOM	98	N	VAL A	43	70.315	50.078	100.172	1.00	15.80		N
ANISOU	98	N	VAL A	43	2433	2143	1428	71	101	162	N
ATOM	99	CA	VAL A	43	70.124	49.313	98.949	1.00	16.71		C
ANISOU	99	CA	VAL A	43	2287	1993	2069	−25	33	5	C
ATOM	100	C	VAL A	43	68.630	49.186	98.706	1.00	16.06		C
ANISOU	100	C	VAL A	43	2498	1838	1768	−45	78	291	C
ATOM	101	O	VAL A	43	67.887	48.701	99.568	1.00	19.81		O
ANISOU	101	O	VAL A	43	2835	2613	2078	−283	−37	558	O
ATOM	102	CB	VAL A	43	70.750	47.902	99.057	1.00	19.48		C
ANISOU	102	CB	VAL A	43	2787	2163	2452	227	−314	−188	C
ATOM	103	CG1	VAL A	43	70.563	47.128	97.749	1.00	22.59		C
ANISOU	103	CG1	VAL A	43	3225	2444	2913	70	−423	−342	C
ATOM	104	CG2	VAL A	43	72.217	48.010	99.427	1.00	20.81		C
ANISOU	104	CG2	VAL A	43	2974	2305	2628	409	−228	156	C
ATOM	105	N	VAL A	44	68.188	49.625	97.535	1.00	15.96		N
ANISOU	105	N	VAL A	44	2101	2113	1849	−158	−56	66	N
ATOM	106	CA	VAL A	44	66.786	49.525	97.156	1.00	16.74		C
ANISOU	106	CA	VAL A	44	2428	1970	1962	−130	69	−14	C
ATOM	107	C	VAL A	44	66.691	49.006	95.727	1.00	16.45		C
ANISOU	107	C	VAL A	44	2440	1820	1990	−201	−140	−306	C
ATOM	108	O	VAL A	44	67.665	49.018	94.985	1.00	19.18		O
ANISOU	108	O	VAL A	44	2609	2599	2079	−243	181	−421	O
ATOM	109	CB	VAL A	44	66.044	50.886	97.255	1.00	17.02		C
ANISOU	109	CB	VAL A	44	2823	2239	1406	229	12	−137	C
ATOM	110	CG1	VAL A	44	66.197	51.487	98.646	1.00	17.74		C
ANISOU	110	CG1	VAL A	44	2799	2493	1450	−41	108	−102	C
ATOM	111	CG2	VAL A	44	66.530	51.855	96.190	1.00	17.52		C
ANISOU	111	CG2	VAL A	44	3101	1940	1617	−142	2	35	C
ATOM	112	N	ATHR A	45	65.497	48.571	95.351	0.71	16.45		N
ANISOU	112	N	ATHR A	45	2256	1846	2150	−433	−9	−362	N
ATOM	113	CA	ATHR A	45	65.228	48.128	93.991	0.71	18.16		C
ANISOU	113	CA	ATHR A	45	2516	2138	2248	−655	−58	−612	C
ATOM	114	C	ATHR A	45	64.713	49.293	93.160	0.71	17.67		C
ANISOU	114	C	ATHR A	45	2553	2219	1944	−325	−54	−749	C
ATOM	115	O	ATHR A	45	63.957	50.122	93.664	0.71	15.17		O
ANISOU	115	O	ATHR A	45	2130	1995	1638	−252	−15	−517	O
ATOM	116	CB	ATHR A	45	64.179	47.003	93.993	0.71	23.21		C
ANISOU	116	CB	ATHR A	45	3391	2475	2951	−714	−299	−438	C
ATOM	117	OG1	ATHR A	45	64.605	45.975	94.892	0.71	24.08		O
ANISOU	117	OG1	ATHR A	45	3734	2170	3248	−460	−132	−208	O
ATOM	118	CG2	ATHR A	45	64.002	46.410	92.594	0.71	22.72		C
ANISOU	118	CG2	ATHR A	45	3321	2345	2966	−575	−443	−535	C
ATOM	119	N	BTHR A	45	65.522	48.507	95.349	0.29	19.88		N
ANISOU	119	N	BTHR A	45	2704	2333	2518	−233	−162	−303	N
ATOM	120	CA	BTHR A	45	65.315	48.117	93.963	0.29	21.66		C
ANISOU	120	CA	BTHR A	45	2882	2599	2751	−272	−188	−417	C
ATOM	121	C	BTHR A	45	64.831	49.328	93.188	0.29	19.03		C
ANISOU	121	C	BTHR A	45	2370	2457	2404	−478	−15	−488	C
ATOM	122	O	BTHR A	45	64.225	50.234	93.760	0.29	25.66		O
ANISOU	122	O	BTHR A	45	3197	3384	3168	−379	219	−258	O
ATOM	123	CB	BTHR A	45	64.294	46.973	93.820	0.29	25.92		C
ANISOU	123	CB	BTHR A	45	3398	3210	3241	−149	−347	−434	C
ATOM	124	OG1	BTHR A	45	63.092	47.308	94.522	0.29	27.14		O
ANISOU	124	OG1	BTHR A	45	3544	3390	3377	−241	−219	−550	O
ATOM	125	CG2	BTHR A	45	64.858	45.679	94.381	0.29	25.55		C
ANISOU	125	CG2	BTHR A	45	3258	3145	3303	−81	−414	−354	C
ATOM	126	N	AGLU A	46	65.114	49.353	91.891	0.71	17.63		N
ANISOU	126	N	AGLU A	46	2589	2242	1868	−98	−13	−582	N
ATOM	127	C	AGLU A	46	63.082	50.480	91.088	0.71	16.75		C
ANISOU	127	C	AGLU A	46	2581	2539	1245	−614	−77	−562	C
ATOM	128	O	AGLU A	46	62.386	49.461	91.045	0.71	18.68		O
ANISOU	128	O	AGLU A	46	2753	2659	1685	−631	−213	−575	O
ATOM	129	CD	AGLU A	46	65.212	48.836	87.533	0.71	33.06		C
ANISOU	129	CD	AGLU A	46	5116	4718	2725	−733	−70	−1224	C
ATOM	130	OE1	AGLU A	46	65.296	49.890	86.867	0.71	36.61		O
ANISOU	130	OE1	AGLU A	46	5669	5242	2997	−929	−172	−1456	O
ATOM	131	OE2	AGLU A	46	65.450	47.707	87.057	0.71	33.49		O
ANISOU	131	OE2	AGLU A	46	5216	5046	2462	−129	64	−1320	O

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	132	CG	AGLU A	46	64.794	48.925	88.984	0.71	26.90		C
ANISOU	132	CG	AGLU A	46	4032	3916	2271	−762	−109	−1017	C
ATOM	133	CA	AGLU A	46	64.605	50.416	91.037	0.71	18.78		C
ANISOU	133	CA	AGLU A	46	2648	2748	1739	−235	95	−535	C
ATOM	134	CB	AGLU A	46	65.105	50.263	89.599	0.71	23.48		C
ANISOU	134	CB	AGLU A	46	3012	3787	2124	−371	−57	−714	C
ATOM	135	N	BGLU A	46	65.079	49.332	91.912	0.29	19.95		N
ANISOU	135	N	BGLU A	46	2619	2589	2373	−318	102	−529	N
ATOM	136	C	BGLU A	46	63.075	50.471	91.126	0.29	18.27		C
ANISOU	136	C	BGLU A	46	2602	2552	1786	−566	57	−502	C
ATOM	137	O	BGLU A	46	62.393	49.480	91.117	0.29	21.67		O
ANISOU	137	O	BGLU A	46	3051	2850	2334	−445	85	−432	O
ATOM	138	CD	BGLU A	46	65.685	50.905	87.353	0.29	29.27		C
ANISOU	138	CD	BGLU A	46	4288	4449	2384	17	217	−1220	C
ATOM	139	OE1	BGLU A	46	65.554	49.697	86.977	0.29	28.44		O
ANISOU	139	OE1	BGLU A	46	4611	4037	2157	−159	2	−1571	O
ATOM	140	OE2	BGLU A	46	66.221	51.892	86.715	0.29	26.39		O
ANISOU	140	OE2	BGLU A	46	3311	4592	2124	−1012	230	−1032	O
ATOM	141	CG	BGLU A	46	65.103	51.196	88.740	0.29	28.25		C
ANISOU	141	CG	BGLU A	46	4004	4129	2599	3	459	−877	C
ATOM	142	CA	BGLU A	46	64.579	50.340	91.043	0.29	19.89		C
ANISOU	142	CA	BGLU A	46	2644	2768	2147	−376	277	−573	C
ATOM	143	CB	BGLU A	46	65.003	50.000	89.611	0.29	22.64		C
ANISOU	143	CB	BGLU A	46	2924	3355	2324	−393	506	−676	C
ATOM	144	N	GLY A	47	62.578	51.700	91.211	1.00	16.83		N
ANISOU	144	N	GLY A	47	2563	2385	1445	−516	−94	−315	N
ATOM	145	CA	GLY A	47	61.157	51.931	91.349	1.00	17.00		C
ANISOU	145	CA	GLY A	47	2295	2743	1422	−102	−326	−304	C
ATOM	146	C	GLY A	47	60.739	52.183	92.791	1.00	16.71		C
ANISOU	146	C	GLY A	47	2189	2753	1406	−346	−282	−90	C
ATOM	147	O	GLY A	47	59.705	52.807	93.037	1.00	17.82		O
ANISOU	147	O	GLY A	47	2076	2916	1780	−261	−343	−48	O
ATOM	148	N	ASP A	48	61.524	51.706	93.758	1.00	16.20		N
ANISOU	148	N	ASP A	48	2414	2424	1317	−142	−195	−254	N
ATOM	149	C	ASP A	48	61.540	53.383	95.542	1.00	14.98		C
ANISOU	149	C	ASP A	48	2004	2400	1289	−423	−86	−322	C
ATOM	150	O	ASP A	48	62.274	54.085	94.853	1.00	17.23		O
ANISOU	150	O	ASP A	48	2320	2516	1711	−587	296	−202	O
ATOM	151	OD1	ASP A	48	60.858	49.221	95.553	1.00	25.99		O
ANISOU	151	OD1	ASP A	48	4034	2673	3167	−827	839	−366	O
ATOM	152	OD2	ASP A	48	62.827	48.965	96.533	1.00	27.11		O
ANISOU	152	OD2	ASP A	48	3064	3221	4017	−880	939	−583	O
ATOM	153	CG	ASP A	48	61.916	49.675	96.039	1.00	28.36		C
ANISOU	153	CG	ASP A	48	3675	3712	3391	25	908	−239	C
ATOM	154	CA	ASP A	48	61.227	51.956	95.169	1.00	14.96		C
ANISOU	154	CA	ASP A	48	2268	2050	1366	−318	−298	−133	C
ATOM	155	CB	ASP A	48	62.146	51.150	96.088	1.00	21.71		C
ANISOU	155	CB	ASP A	48	3615	2510	2123	360	15	−122	C
ATOM	156	N	ASN A	49	61.035	53.812	96.688	1.00	14.25		N
ANISOU	156	N	ASN A	49	1950	2081	1382	−420	−76	−203	N
ATOM	157	C	ASN A	49	62.763	54.746	98.109	1.00	14.83		C
ANISOU	157	C	ASN A	49	2202	1989	1443	−229	−206	31	C
ATOM	158	O	ASN A	49	63.021	53.609	98.464	1.00	16.68		O
ANISOU	158	O	ASN A	49	2375	2165	1796	−386	−391	32	O
ATOM	159	CA	AASN A	49	61.504	55.031	97.329	0.79	14.54		C
ANISOU	159	CA	AASN A	49	2109	2039	1375	−330	−232	−311	C
ATOM	160	OD1	AASN A	49	59.174	56.327	96.449	0.79	18.64		O
ANISOU	160	OD1	AASN A	49	2021	2630	2431	−267	−296	86	O
ATOM	161	ND2	AASN A	49	58.033	55.612	98.245	0.79	17.53		N
ANISOU	161	ND2	AASN A	49	2076	2453	2134	461	−141	−505	N
ATOM	162	CB	AASN A	49	60.441	55.544	98.287	0.79	18.02		C
ANISOU	162	CB	AASN A	49	2691	2333	1825	−31	−47	−586	C
ATOM	163	CG	AASN A	49	59.158	55.870	97.589	0.79	17.41		C
ANISOU	163	CG	AASN A	49	2051	2395	2170	−29	−278	−365	C
ATOM	164	CA	BASN A	49	61.547	55.049	97.237	0.21	15.93		C
ANISOU	164	CA	BASN A	49	2103	2270	1679	−379	−37	−79	C
ATOM	165	OD1	BASN A	49	60.303	54.472	99.874	0.21	12.57		O
ANISOU	165	OD1	BASN A	49	1619	2027	1132	−354	262	256	O
ATOM	166	ND2	BASN A	49	58.372	55.043	98.869	0.21	11.68		N
ANISOU	166	ND2	BASN A	49	1088	2516	833	144	−71	206	N
ATOM	167	CB	BASN A	49	60.459	55.868	97.951	0.21	15.89		C
ANISOU	167	CB	BASN A	49	1964	2391	1683	−2	243	150	C
ATOM	168	CG	BASN A	49	59.702	55.068	98.984	0.21	13.93		C
ANISOU	168	CG	BASN A	49	1668	2210	1414	−76	247	166	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	169	N	ALA A	50	63.545	55.770	98.395	1.00	14.97		N
ANISOU	169	N	ALA A	50	2221	1884	1584	−223	−509	−146	N
ATOM	170	CA	ALA A	50	64.733	55.609	99.215	1.00	15.39		C
ANISOU	170	CA	ALA A	50	2057	2050	1739	75	−572	−316	C
ATOM	171	C	ALA A	50	64.804	56.796	100.149	1.00	13.56		C
ANISOU	171	C	ALA A	50	1987	1839	1326	−116	−460	−25	C
ATOM	172	O	ALA A	50	64.684	57.940	99.717	1.00	16.01		O
ANISOU	172	O	ALA A	50	2995	1848	1241	20	−628	−15	O
ATOM	173	CB	ALA A	50	65.971	55.565	98.362	1.00	17.18		C
ANISOU	173	CB	ALA A	50	2215	2124	2188	142	−393	−543	C
ATOM	174	N	THR A	51	65.032	56.531	101.430	1.00	12.96		N
ANISOU	174	N	THR A	51	1948	1665	1312	−147	−223	−37	N
ATOM	175	C	THR A	51	66.290	57.466	103.330	1.00	12.69		C
ANISOU	175	C	THR A	51	1967	1768	1086	66	−112	57	C
ATOM	176	O	THR A	51	66.484	56.453	103.997	1.00	14.73		O
ANISOU	176	O	THR A	51	2193	1930	1475	−249	−319	98	O
ATOM	177	CA	THR A	51	65.076	57.587	102.423	1.00	13.04		C
ANISOU	177	CA	THR A	51	1772	1928	1254	−72	−84	−74	C
ATOM	178	CB	THR A	51	63.795	57.569	103.296	1.00	16.11		C
ANISOU	178	CB	THR A	51	1860	2543	1719	−171	−49	−138	C
ATOM	179	OG1	THR A	51	62.661	57.803	102.460	1.00	17.62		O
ANISOU	179	OG1	THR A	51	1895	2845	1956	−9	50	49	O
ATOM	180	CG2	THR A	51	63.856	58.646	104.369	1.00	17.63		C
ANISOU	180	CG2	THR A	51	2141	2903	1654	−42	311	−439	C
ATOM	181	N	PHE A	52	67.099	58.517	103.341	1.00	12.45		N
ANISOU	181	N	PHE A	52	1755	1780	1196	−46	−94	−77	N
ATOM	182	CA	PHE A	52	68.149	58.690	104.333	1.00	12.35		C
ANISOU	182	CA	PHE A	52	1693	1780	1220	−87	−117	−170	C
ATOM	183	C	PHE A	52	67.637	59.574	105.461	1.00	11.78		C
ANISOU	183	C	PHE A	52	1775	1819	883	−47	88	−103	C
ATOM	184	O	PHE A	52	66.713	60.363	105.272	1.00	13.68		O
ANISOU	184	O	PHE A	52	1862	1996	1339	171	49	−54	O
ATOM	185	CB	PHE A	52	69.362	59.373	103.707	1.00	13.20		C
ANISOU	185	CB	PHE A	52	1674	2082	1259	−74	36	−193	C
ATOM	186	CG	PHE A	52	70.060	58.558	102.656	1.00	13.65		C
ANISOU	186	CG	PHE A	52	1859	2063	1265	101	−80	−294	C
ATOM	187	CD1	PHE A	52	69.867	58.808	101.304	1.00	15.96		C
ANISOU	187	CD1	PHE A	52	2344	2424	1297	450	−110	−262	C
ATOM	188	CD2	PHE A	52	70.960	57.571	103.022	1.00	13.80		C
ANISOU	188	CD2	PHE A	52	2050	1952	1242	55	36	−380	C
ATOM	189	CE1	PHE A	52	70.550	58.070	100.353	1.00	19.56		C
ANISOU	189	CE1	PHE A	52	2890	3357	1187	1033	−244	−404	C
ATOM	190	CE2	PHE A	52	71.627	56.830	102.065	1.00	15.86		C
ANISOU	190	CE2	PHE A	52	2309	2450	1266	185	−126	−442	C
ATOM	191	CZ	PHE A	52	71.424	57.083	100.741	1.00	19.49		C
ANISOU	191	CZ	PHE A	52	2993	3185	1230	972	−96	−537	C
ATOM	192	N	THR A	53	68.267	59.457	106.624	1.00	13.11		N
ANISOU	192	N	THR A	53	2050	2005	927	−107	−0	−249	N
ATOM	193	C	THR A	53	69.175	61.189	108.078	1.00	13.81		C
ANISOU	193	C	THR A	53	2110	2108	1027	154	153	−327	C
ATOM	194	O	THR A	53	70.271	60.665	108.336	1.00	14.96		O
ANISOU	194	O	THR A	53	2204	2189	1291	268	−121	−186	O
ATOM	195	CA	THR A	53	67.961	60.342	107.741	1.00	14.27		C
ANISOU	195	CA	THR A	53	2236	2258	928	−320	144	−150	C
ATOM	196	CB	THR A	53	67.523	59.561	108.986	1.00	17.46		C
ANISOU	196	CB	THR A	53	2645	2908	1081	−531	119	−197	C
ATOM	197	OG1	THR A	53	66.366	58.783	108.662	1.00	19.30		O
ANISOU	197	OG1	THR A	53	2767	2883	1685	−568	468	−5	O
ATOM	198	CG2	THR A	53	67.179	60.511	110.122	1.00	19.57		C
ANISOU	198	CG2	THR A	53	3268	2842	1325	−217	518	−202	C
ATOM	199	N	CYS A	54	68.980	62.502	108.044	1.00	14.25		N
ANISOU	199	N	CYS A	54	1903	2111	1400	24	72	−436	N
ATOM	200	C	CYS A	54	69.602	63.910	109.883	1.00	15.35		C
ANISOU	200	C	CYS A	54	1932	2469	1432	93	−224	−449	C
ATOM	201	O	CYS A	54	68.469	64.334	110.093	1.00	18.07		O
ANISOU	201	O	CYS A	54	1863	3055	1949	414	−68	−659	O
ATOM	202	CA	ACYS A	54	69.994	63.454	108.488	0.71	15.23		C
ANISOU	202	CA	ACYS A	54	1763	2153	1872	−72	−154	−232	C
ATOM	203	CB	ACYS A	54	70.071	64.655	107.530	0.71	16.71		C
ANISOU	203	CB	ACYS A	54	1744	2158	2448	−209	−168	−78	C
ATOM	204	SG	ACYS A	54	71.243	65.962	107.970	0.71	20.97		S
ANISOU	204	SG	ACYS A	54	2659	2312	2996	50	−627	−398	S
ATOM	205	CA	BCYS A	54	69.994	63.439	108.493	0.29	15.64		C
ANISOU	205	CA	BCYS A	54	1955	2443	1545	60	−10	−399	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	206	CB	BCYS A	54	70.075	64.624	107.534	0.29	14.54		C
ANISOU	206	CB	BCYS A	54	1615	2621	1290	266	242	−351	C
ATOM	207	SG	BCYS A	54	71.443	65.750	107.821	0.29	13.09		S
ANISOU	207	SG	BCYS A	54	1527	2428	1017	−145	345	−322	S
ATOM	208	N	SER A	55	70.526	63.806	110.831	1.00	15.37		N
ANISOU	208	N	SER A	55	1956	2468	1416	46	5	−417	N
ATOM	209	C	SER A	55	71.142	65.460	112.496	1.00	16.48		C
ANISOU	209	C	SER A	55	1830	3049	1382	24	125	−573	C
ATOM	210	O	SER A	55	72.350	65.437	112.281	1.00	17.81		O
ANISOU	210	O	SER A	55	1932	2900	1934	159	−87	−946	O
ATOM	211	CA	ASER A	55	70.266	64.254	112.192	0.78	15.56		C
ANISOU	211	CA	ASER A	55	2144	2606	1164	7	−121	−405	C
ATOM	212	CB	ASER A	55	70.518	63.126	113.188	0.78	19.67		C
ANISOU	212	CB	ASER A	55	2608	3009	1855	−145	229	−201	C
ATOM	213	OG	ASER A	55	69.698	62.006	112.896	0.78	21.82		O
ANISOU	213	OG	ASER A	55	3024	3035	2229	57	171	−66	O
ATOM	214	CA	BSER A	55	70.282	64.241	112.201	0.22	20.24		C
ANISOU	214	CA	BSER A	55	2673	3100	1917	113	135	−321	C
ATOM	215	CB	BSER A	55	70.607	63.112	113.178	0.22	25.20		C
ANISOU	215	CB	BSER A	55	3703	3356	2516	254	323	24	C
ATOM	216	OG	BSER A	55	70.412	63.518	114.520	0.22	23.63		O
ANISOU	216	OG	BSER A	55	3875	2988	2116	1127	401	391	O
ATOM	217	N	PHE A	56	70.531	66.530	112.985	1.00	15.78		N
ANISOU	217	N	PHE A	56	2052	2746	1197	228	47	−380	N
ATOM	218	CA	PHE A	56	71.276	67.759	113.197	1.00	14.92		C
ANISOU	218	CA	PHE A	56	2201	2450	1019	72	91	−351	C
ATOM	219	C	PHE A	56	70.784	68.461	114.429	1.00	17.96		C
ANISOU	219	C	PHE A	56	2383	2975	1468	236	46	−328	C
ATOM	220	O	PHE A	56	69.590	68.729	114.551	1.00	19.12		O
ANISOU	220	O	PHE A	56	2334	2899	2034	347	318	−520	O
ATOM	221	CB	PHE A	56	71.130	68.693	111.994	1.00	17.02		C
ANISOU	221	CB	PHE A	56	2329	2970	1168	306	−88	−170	C
ATOM	222	CG	PHE A	56	71.801	70.029	112.177	1.00	15.82		C
ANISOU	222	CG	PHE A	56	2302	2580	1128	340	−120	−92	C
ATOM	223	CD1	PHE A	56	73.177	70.112	112.330	1.00	16.84		C
ANISOU	223	CD1	PHE A	56	2452	2880	1068	404	−23	−167	C
ATOM	224	CD2	PHE A	56	71.055	71.201	112.196	1.00	18.24		C
ANISOU	224	CD2	PHE A	56	2931	2790	1208	698	−216	−242	C
ATOM	225	CE1	PHE A	56	73.799	71.336	112.489	1.00	18.09		C
ANISOU	225	CE1	PHE A	56	2671	2660	1543	254	−135	33	C
ATOM	226	CE2	PHE A	56	71.672	72.424	112.350	1.00	18.75		C
ANISOU	226	CE2	PHE A	56	3314	2594	1215	992	−146	47	C
ATOM	227	CZ	PHE A	56	73.044	72.498	112.499	1.00	19.20		C
ANISOU	227	CZ	PHE A	56	2868	2945	1483	769	−282	209	C
ATOM	228	O	SER A	57	72.963	71.288	116.247	1.00	28.67		O
ANISOU	228	O	SER A	57	4434	4296	2164	−383	−224	−589	O
ATOM	229	N	SER A	57	71.717	68.753	115.329	1.00	18.02		N
ANISOU	229	N	SER A	57	2800	2847	1201	188	−7	−553	N
ATOM	230	C	SER A	57	71.786	70.943	116.340	1.00	23.95		C
ANISOU	230	C	SER A	57	3948	3464	1686	−163	413	−550	C
ATOM	231	CA	ASER A	57	71.423	69.491	116.554	0.77	22.72		C
ANISOU	231	CA	ASER A	57	4043	2959	1631	−461	30	−474	C
ATOM	232	CB	ASER A	57	72.223	68.928	117.732	0.77	30.41		C
ANISOU	232	CB	ASER A	57	5609	3756	2191	474	327	−332	C
ATOM	233	OG	ASER A	57	71.849	67.590	118.015	0.77	34.14		O
ANISOU	233	OG	ASER A	57	6172	4402	2398	991	1022	349	O
ATOM	234	CA	BSER A	57	71.420	69.486	116.550	0.23	23.72		C
ANISOU	234	CA	BSER A	57	3848	3512	1653	84	94	−637	C
ATOM	235	CB	BSER A	57	72.202	68.908	117.731	0.23	23.65		C
ANISOU	235	CB	BSER A	57	4045	3455	1488	84	−21	−1017	C
ATOM	236	OG	BSER A	57	73.594	68.900	117.466	0.23	28.42		O
ANISOU	236	OG	BSER A	57	4828	4290	1681	482	−25	−918	O
ATOM	237	O	ASN A	58	71.189	73.518	118.344	1.00	27.11		O
ANISOU	237	O	ASN A	58	5348	3155	1798	104	864	119	O
ATOM	238	N	ASN A	58	70.768	71.791	116.263	1.00	24.93		N
ANISOU	238	N	ASN A	58	3932	3386	2153	284	553	−276	N
ATOM	239	C	ASN A	58	71.354	73.991	117.220	1.00	23.37		C
ANISOU	239	C	ASN A	58	3886	3066	1928	−258	482	−469	C
ATOM	240	CG	ASN A	58	68.497	73.622	116.272	1.00	31.16		C
ANISOU	240	CG	ASN A	58	5146	3958	2735	1225	93	−339	C
ATOM	241	ND2	ASN A	58	67.605	74.596	116.245	1.00	31.49		N
ANISOU	241	ND2	ASN A	58	5592	3808	2565	763	50	−124	N
ATOM	242	CA	ASN A	58	70.970	73.202	115.979	1.00	24.89		C
ANISOU	242	CA	ASN A	58	4103	3002	2353	77	363	−317	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	243	CB	ASN A	58	69.700	73.793	115.373	1.00	27.45		C
ANISOU	243	CB	ASN A	58	4410	3654	2366	886	364	−69	C
ATOM	244	O	THR A	59	69.822	76.582	117.228	1.00	26.47		O
ANISOU	244	O	THR A	59	3897	4075	2086	−1292	108	100	O
ATOM	245	N	THR A	59	71.881	75.192	117.011	1.00	22.79		N
ANISOU	245	N	THR A	59	4037	2360	2261	114	694	−58	N
ATOM	246	CA	THR A	59	72.007	76.168	118.077	1.00	24.12		C
ANISOU	246	CA	THR A	59	4022	2483	2661	152	127	127	C
ATOM	247	C	THR A	59	70.733	76.974	117.958	1.00	19.72		C
ANISOU	247	C	THR A	59	3618	2271	1605	−534	396	56	C
ATOM	248	CB	THR A	59	73.225	77.093	117.891	1.00	26.52		C
ANISOU	248	CB	THR A	59	3290	3353	3436	71	−94	377	C
ATOM	249	OG1	THR A	59	73.068	77.870	116.696	1.00	24.62		O
ANISOU	249	OG1	THR A	59	3011	2918	3424	131	388	426	O
ATOM	250	N	SER A	60	70.659	78.091	118.656	1.00	23.62		N
ANISOU	250	N	SER A	60	4120	3135	1719	228	275	266	N
ATOM	251	C	SER A	60	69.462	79.724	117.267	1.00	24.75		C
ANISOU	251	C	SER A	60	3898	3733	1775	879	−15	362	C
ATOM	252	O	SER A	60	68.482	80.399	116.961	1.00	28.56		O
ANISOU	252	O	SER A	60	3860	4779	2210	1292	−166	218	O
ATOM	253	CA	ASER A	60	69.477	78.931	118.566	0.91	29.40		C
ANISOU	253	CA	ASER A	60	4487	4650	2035	1254	49	231	C
ATOM	254	CB	ASER A	60	69.417	79.880	119.760	0.91	34.07		C
ANISOU	254	CB	ASER A	60	5625	5190	2128	1589	57	−218	C
ATOM	255	OG	ASER A	60	70.576	80.690	119.801	0.91	37.81		O
ANISOU	255	OG	ASER A	60	6811	5070	2486	1709	−350	−846	O
ATOM	256	CA	BSER A	60	69.495	78.964	118.584	0.09	26.73		C
ANISOU	256	CA	BSER A	60	4577	3723	1857	980	101	224	C
ATOM	257	CB	BSER A	60	69.509	79.968	119.738	0.09	29.68		C
ANISOU	257	CB	BSER A	60	5463	3900	1913	1377	73	6	C
ATOM	258	OG	BSER A	60	69.485	79.315	120.993	0.09	31.59		O
ANISOU	258	OG	BSER A	60	5970	4055	1977	1408	12	−150	O
ATOM	259	O	GLU A	61	69.922	78.569	113.979	1.00	17.86		O
ANISOU	259	O	GLU A	61	3074	2315	1398	262	−62	−145	O
ATOM	260	N	GLU A	61	70.541	79.620	116.497	1.00	20.99		N
ANISOU	260	N	GLU A	61	3855	2731	1388	240	−25	71	N
ATOM	261	CA	GLU A	61	70.682	80.431	115.297	1.00	22.03		C
ANISOU	261	CA	GLU A	61	4064	3020	1286	325	−243	−275	C
ATOM	262	C	GLU A	61	70.069	79.789	114.059	1.00	17.74		C
ANISOU	262	C	GLU A	61	3292	2150	1298	203	−150	−12	C
ATOM	263	CB	GLU A	61	72.154	80.747	115.040	1.00	24.81		C
ANISOU	263	CB	GLU A	61	4484	3178	1763	−889	−577	−100	C
ATOM	264	CG	GLU A	61	72.879	81.390	116.212	1.00	33.93		C
ANISOU	264	CG	GLU A	61	6075	3794	3025	−353	−757	77	C
ATOM	265	CD	GLU A	61	72.273	82.716	116.634	1.00	37.67		C
ANISOU	265	CD	GLU A	61	6657	4334	3321	234	−1045	278	C
ATOM	266	OE1	GLU A	61	71.806	83.471	115.757	1.00	38.90		O
ANISOU	266	OE1	GLU A	61	7305	3901	3575	48	−1107	129	O
ATOM	267	N	SER A	62	69.721	80.633	113.095	1.00	18.16		N
ANISOU	267	N	SER A	62	3209	2204	1488	428	−98	−51	N
ATOM	268	C	SER A	62	70.110	79.264	111.090	1.00	14.71		C
ANISOU	268	C	SER A	62	2356	2015	1219	150	5	−155	C
ATOM	269	O	SER A	62	71.315	79.448	111.147	1.00	15.97		O
ANISOU	269	O	SER A	62	2723	2245	1101	106	89	−133	O
ATOM	270	CA	ASER A	62	69.160	80.196	111.815	0.84	17.43		C
ANISOU	270	CA	ASER A	62	3105	2302	1217	519	−145	−350	C
ATOM	271	CB	ASER A	62	68.895	81.411	110.920	0.84	20.15		C
ANISOU	271	CB	ASER A	62	3728	2145	1786	558	84	166	C
ATOM	272	OG	ASER A	62	68.170	82.409	111.607	0.84	22.31		O
ANISOU	272	OG	ASER A	62	3725	2681	2070	549	133	184	O
ATOM	273	CA	BSER A	62	69.143	80.170	111.842	0.16	17.49		C
ANISOU	273	CA	BSER A	62	2955	2302	1390	589	−90	−341	C
ATOM	274	CB	BSER A	62	68.752	81.362	110.966	0.16	18.11		C
ANISOU	274	CB	BSER A	62	3065	2452	1364	1104	−73	−581	C
ATOM	275	OG	BSER A	62	69.863	82.206	110.724	0.16	20.38		O
ANISOU	275	OG	BSER A	62	3356	2821	1568	1249	51	−638	O
ATOM	276	N	PHE A	63	69.559	78.286	110.382	1.00	14.78		N
ANISOU	276	N	PHE A	63	2556	1904	1155	149	−15	−152	N
ATOM	277	CA	PHE A	63	70.374	77.366	109.612	1.00	13.93		C
ANISOU	277	CA	PHE A	63	2492	1811	989	305	−72	−44	C
ATOM	278	C	PHE A	63	69.632	76.896	108.376	1.00	13.38		C
ANISOU	278	C	PHE A	63	2341	1838	903	306	7	78	C
ATOM	279	O	PHE A	63	68.421	77.053	108.270	1.00	14.28		O
ANISOU	279	O	PHE A	63	2286	2024	1115	481	−106	37	O

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	280	CB	PHE A	63	70.785	76.151	110.449	1.00	15.23		C
ANISOU	280	CB	PHE A	63	2609	1969	1207	−50	−307	57	C
ATOM	281	CG	PHE A	63	69.633	75.271	110.865	1.00	14.79		C
ANISOU	281	CG	PHE A	63	2488	2036	1097	138	−282	−4	C
ATOM	282	CD1	PHE A	63	69.309	74.123	110.149	1.00	15.78		C
ANISOU	282	CD1	PHE A	63	2928	1697	1370	180	−222	237	C
ATOM	283	CD2	PHE A	63	68.898	75.570	112.005	1.00	16.83		C
ANISOU	283	CD2	PHE A	63	2847	2287	1261	11	−267	148	C
ATOM	284	CE1	PHE A	63	68.257	73.305	110.549	1.00	16.54		C
ANISOU	284	CE1	PHE A	63	3050	1963	1271	−3	33	−29	C
ATOM	285	CE2	PHE A	63	67.846	74.762	112.403	1.00	18.09		C
ANISOU	285	CE2	PHE A	63	2936	2408	1528	−214	127	21	C
ATOM	286	CZ	PHE A	63	67.529	73.623	111.672	1.00	18.05		C
ANISOU	286	CZ	PHE A	63	3212	2134	1513	−102	172	111	C
ATOM	287	N	VAL A	64	70.387	76.321	107.449	1.00	13.89		N
ANISOU	287	N	VAL A	64	2374	1895	1010	58	47	−203	N
ATOM	288	CA	VAL A	64	69.842	75.618	106.293	1.00	13.59		C
ANISOU	288	CA	VAL A	64	2410	1726	1029	122	23	−66	C
ATOM	289	C	VAL A	64	70.497	74.244	106.268	1.00	12.85		C
ANISOU	289	C	VAL A	64	1989	1701	1191	50	−17	−70	C
ATOM	290	O	VAL A	64	71.683	74.104	106.576	1.00	14.71		O
ANISOU	290	O	VAL A	64	1853	1840	1898	25	−186	−210	O
ATOM	291	CB	VAL A	64	70.160	76.379	104.979	1.00	15.12		C
ANISOU	291	CB	VAL A	64	2695	2026	1022	254	−124	−25	C
ATOM	292	CG1	VAL A	64	69.871	75.536	103.725	1.00	17.25		C
ANISOU	292	CG1	VAL A	64	3344	2244	966	69	66	−56	C
ATOM	293	CG2	VAL A	64	69.387	77.690	104.961	1.00	16.93		C
ANISOU	293	CG2	VAL A	64	3099	1948	1385	291	17	−32	C
ATOM	294	N	LEU A	65	69.709	73.230	105.941	1.00	13.31		N
ANISOU	294	N	LEU A	65	1854	1781	1422	68	−105	−12	N
ATOM	295	C	LEU A	65	70.026	71.455	104.347	1.00	14.47		C
ANISOU	295	C	LEU A	65	1918	1888	1692	375	−298	−235	C
ATOM	296	O	LEU A	65	68.898	71.352	103.873	1.00	17.15		O
ANISOU	296	O	LEU A	65	2053	2382	2080	402	−545	−622	O
ATOM	297	CA	ALEU A	65	70.221	71.884	105.802	0.73	13.54		C
ANISOU	297	CA	ALEU A	65	1945	1514	1686	26	−65	33	C
ATOM	298	CB	ALEU A	65	69.452	70.978	106.760	0.73	16.36		C
ANISOU	298	CB	ALEU A	65	2096	1694	2425	114	−107	411	C
ATOM	299	CG	ALEU A	65	70.018	69.616	107.123	0.73	17.07		C
ANISOU	299	CG	ALEU A	65	1843	2185	2458	15	290	105	C
ATOM	300	CD1	ALEU A	65	71.343	69.787	107.861	0.73	17.78		C
ANISOU	300	CD1	ALEU A	65	1801	2494	2460	14	−263	515	C
ATOM	301	CD2	ALEU A	65	69.029	68.890	107.989	0.73	18.56		C
ANISOU	301	CD2	ALEU A	65	2107	2515	2431	−227	372	212	C
ATOM	302	CA	BLEU A	65	70.206	71.869	105.784	0.27	16.45		C
ANISOU	302	CA	BLEU A	65	2203	2063	1984	84	−176	−18	C
ATOM	303	CB	BLEU A	65	69.407	70.899	106.641	0.27	19.74		C
ANISOU	303	CB	BLEU A	65	2579	2463	2458	144	−233	152	C
ATOM	304	CG	BLEU A	65	69.630	70.897	108.141	0.27	17.01		C
ANISOU	304	CG	BLEU A	65	2026	2263	2174	−162	−201	59	C
ATOM	305	CD1	BLEU A	65	69.071	69.622	108.692	0.27	14.06		C
ANISOU	305	CD1	BLEU A	65	1786	1776	1779	−382	−127	354	C
ATOM	306	CD2	BLEU A	65	71.087	70.997	108.451	0.27	13.64		C
ANISOU	306	CD2	BLEU A	65	1756	1684	1743	−256	45	97	C
ATOM	307	N	ASN A	66	71.133	71.229	103.651	1.00	14.31		N
ANISOU	307	N	ASN A	66	1991	1772	1674	206	−314	−424	N
ATOM	308	CA	ASN A	66	71.105	70.858	102.249	1.00	15.36		C
ANISOU	308	CA	ASN A	66	2298	1848	1689	290	−272	−387	C
ATOM	309	C	ASN A	66	71.382	69.361	102.106	1.00	14.40		C
ANISOU	309	C	ASN A	66	1958	1893	1620	429	−324	−227	C
ATOM	310	O	ASN A	66	72.203	68.783	102.842	1.00	16.44		O
ANISOU	310	O	ASN A	66	2291	2094	1862	406	−601	−403	O
ATOM	311	CB	ASN A	66	72.175	71.616	101.467	1.00	17.15		C
ANISOU	311	CB	ASN A	66	2706	1917	1891	287	−81	−163	C
ATOM	312	CG	ASN A	66	71.791	73.042	101.133	1.00	18.64		C
ANISOU	312	CG	ASN A	66	3139	1723	2220	102	−338	−95	C
ATOM	313	OD1	ASN A	66	70.624	73.420	101.153	1.00	20.60		O
ANISOU	313	OD1	ASN A	66	3423	2061	2342	712	−486	−88	O
ATOM	314	ND2	ASN A	66	72.793	73.835	100.790	1.00	21.57		N
ANISOU	314	ND2	ASN A	66	3650	1939	2606	5	−455	−177	N
ATOM	315	N	TRP A	67	70.722	68.738	101.138	1.00	12.75		N
ANISOU	315	N	TRP A	67	1839	1829	1177	182	−127	−220	N
ATOM	316	CA	TRP A	67	71.006	67.362	100.746	1.00	12.34		C
ANISOU	316	CA	TRP A	67	1935	1769	983	336	85	4	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	317	C	TRP A	67	71.748	67.412	99.428	1.00	12.12		C
ANISOU	317	C	TRP A	67	1745	1726	1132	38	−118	−121	C
ATOM	318	O	TRP A	67	71.255	68.022	98.487	1.00	12.76		O
ANISOU	318	O	TRP A	67	1765	1909	1173	40	−90	97	O
ATOM	319	CB	TRP A	67	69.687	66.619	100.566	1.00	12.68		C
ANISOU	319	CB	TRP A	67	1649	1773	1396	−95	44	−48	C
ATOM	320	CG	TRP A	67	69.816	65.171	100.211	1.00	11.92		C
ANISOU	320	CG	TRP A	67	1671	2022	836	43	34	5	C
ATOM	321	CD1	TRP A	67	70.914	64.362	100.346	1.00	13.13		C
ANISOU	321	CD1	TRP A	67	1850	1870	1269	−3	−103	−134	C
ATOM	322	CD2	TRP A	67	68.780	64.353	99.670	1.00	11.88		C
ANISOU	322	CD2	TRP A	67	1715	1951	848	3	217	75	C
ATOM	323	NE1	TRP A	67	70.614	63.082	99.912	1.00	12.66		N
ANISOU	323	NE1	TRP A	67	1567	2116	1129	−51	157	−68	N
ATOM	324	CE2	TRP A	67	69.313	63.058	99.494	1.00	11.56		C
ANISOU	324	CE2	TRP A	67	1601	2028	763	−78	283	−48	C
ATOM	325	CE3	TRP A	67	67.443	64.590	99.334	1.00	13.96		C
ANISOU	325	CE3	TRP A	67	1526	2406	1370	−12	75	149	C
ATOM	326	CZ2	TRP A	67	68.545	62.004	99.001	1.00	13.02		C
ANISOU	326	CZ2	TRP A	67	1706	2270	971	−215	253	−82	C
ATOM	327	CZ3	TRP A	67	66.687	63.547	98.857	1.00	14.78		C
ANISOU	327	CZ3	TRP A	67	1737	2393	1484	−350	−53	101	C
ATOM	328	CH2	TRP A	67	67.240	62.277	98.680	1.00	14.74		C
ANISOU	328	CH2	TRP A	67	1988	2096	1519	−57	−105	−40	C
ATOM	329	N	TYR A	68	72.924	66.784	99.370	1.00	12.48		N
ANISOU	329	N	TYR A	68	1803	1913	1027	133	118	−62	N
ATOM	330	CA	TYR A	68	73.749	66.782	98.173	1.00	13.15		C
ANISOU	330	CA	TYR A	68	2092	1608	1295	−25	24	−8	C
ATOM	331	C	TYR A	68	73.969	65.385	97.631	1.00	12.46		C
ANISOU	331	C	TYR A	68	1801	1927	1008	105	167	−18	C
ATOM	332	O	TYR A	68	74.116	64.411	98.386	1.00	13.68		O
ANISOU	332	O	TYR A	68	2142	2007	1049	282	−33	39	O
ATOM	333	CB	TYR A	68	75.143	67.323	98.478	1.00	15.77		C
ANISOU	333	CB	TYR A	68	2074	2117	1802	−148	286	−228	C
ATOM	334	CG	TYR A	68	75.178	68.725	99.014	1.00	15.67		C
ANISOU	334	CG	TYR A	68	2062	2014	1878	−115	−125	−226	C
ATOM	335	CD1	TYR A	68	75.113	69.821	98.166	1.00	17.48		C
ANISOU	335	CD1	TYR A	68	2477	2023	2140	−49	−324	232	C
ATOM	336	CD2	TYR A	68	75.288	68.955	100.372	1.00	18.50		C
ANISOU	336	CD2	TYR A	68	2933	2221	1875	183	−251	−541	C
ATOM	337	CE1	TYR A	68	75.175	71.111	98.659	1.00	19.19		C
ANISOU	337	CE1	TYR A	68	2777	1944	2571	−58	−346	−164	C
ATOM	338	CE2	TYR A	68	75.348	70.238	100.873	1.00	21.38		C
ANISOU	338	CE2	TYR A	68	3262	2316	2547	−13	−230	−261	C
ATOM	339	CZ	TYR A	68	75.294	71.308	100.011	1.00	19.89		C
ANISOU	339	CZ	TYR A	68	2755	1961	2842	−64	−353	−521	C
ATOM	340	OH	TYR A	68	75.357	72.575	100.515	1.00	25.60		O
ANISOU	340	OH	TYR A	68	3976	2269	3481	419	−449	−816	O
ATOM	341	N	ARG A	69	74.047	65.292	96.309	1.00	13.12		N
ANISOU	341	N	ARG A	69	1946	1920	1120	27	134	−12	N
ATOM	342	CA	ARG A	69	74.641	64.137	95.662	1.00	13.65		C
ANISOU	342	CA	ARG A	69	2058	2055	1073	−134	188	−182	C
ATOM	343	C	ARG A	69	76.071	64.515	95.332	1.00	15.57		C
ANISOU	343	C	ARG A	69	2385	1745	1788	−99	292	85	C
ATOM	344	O	ARG A	69	76.319	65.587	94.782	1.00	17.91		O
ANISOU	344	O	ARG A	69	2389	2222	2193	−37	486	148	O
ATOM	345	CB	ARG A	69	73.878	63.763	94.406	1.00	15.79		C
ANISOU	345	CB	ARG A	69	2497	2444	1061	−107	199	−400	C
ATOM	346	CG	ARG A	69	74.444	62.548	93.739	1.00	18.45		C
ANISOU	346	CG	ARG A	69	2955	2486	1571	134	−4	−437	C
ATOM	347	CD	ARG A	69	73.515	62.067	92.657	1.00	20.16		C
ANISOU	347	CD	ARG A	69	3537	2681	1443	−116	−15	−668	C
ATOM	348	NE	ARG A	69	74.000	60.832	92.066	1.00	22.13		N
ANISOU	348	NE	ARG A	69	3985	3058	1364	207	37	−248	N
ATOM	349	CZ	ARG A	69	73.401	60.204	91.056	1.00	20.16		C
ANISOU	349	CZ	ARG A	69	4133	2458	1069	−241	106	−1	C
ATOM	350	NH1	ARG A	69	72.297	60.705	90.521	1.00	24.37		N
ANISOU	350	NH1	ARG A	69	4156	3285	1817	−776	398	−325	N
ATOM	351	NH2	ARG A	69	73.922	59.100	90.559	1.00	25.49		N
ANISOU	351	NH2	ARG A	69	5407	2586	1692	156	20	145	N
ATOM	352	O	MET A	70	78.519	62.145	93.955	1.00	26.67		O
ANISOU	352	O	MET A	70	3096	3335	3703	−118	826	−479	O
ATOM	353	N	MET A	70	77.005	63.634	95.676	1.00	16.93		N
ANISOU	353	N	MET A	70	2006	1914	2513	15	292	−133	N

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	354	C	MET A	70	79.055	63.153	94.403	1.00	24.24		C
ANISOU	354	C	MET A	70	2963	2574	3672	42	501	42	C
ATOM	355	CA	AMET A	70	78.443	63.891	95.587	0.74	19.88		C
ANISOU	355	CA	AMET A	70	2329	2256	2967	244	−102	64	C
ATOM	356	CB	AMET A	70	79.155	63.453	96.880	0.74	18.43		C
ANISOU	356	CB	AMET A	70	2519	1941	2543	176	−335	133	C
ATOM	357	CG	AMET A	70	78.608	64.127	98.134	0.74	19.82		C
ANISOU	357	CG	AMET A	70	2393	2745	2395	−235	−82	−231	C
ATOM	358	SD	AMET A	70	78.836	65.908	98.115	0.74	19.75		S
ANISOU	358	SD	AMET A	70	2392	2996	2117	19	95	−115	S
ATOM	359	CE	AMET A	70	80.624	65.982	98.207	0.74	23.24		C
ANISOU	359	CE	AMET A	70	2813	3622	2394	−88	133	−425	C
ATOM	360	CA	BMET A	70	78.408	63.972	95.506	0.26	25.11		C
ANISOU	360	CA	BMET A	70	2866	2847	3829	41	410	−103	C
ATOM	361	CB	BMET A	70	79.172	63.793	96.817	0.26	32.43		C
ANISOU	361	CB	BMET A	70	3612	3793	4915	33	576	−150	C
ATOM	362	CG	BMET A	70	80.538	64.448	96.821	0.26	38.99		C
ANISOU	362	CG	BMET A	70	4371	4666	5779	124	765	−201	C
ATOM	363	SD	BMET A	70	80.492	66.247	96.836	0.26	41.31		S
ANISOU	363	SD	BMET A	70	4516	5319	5860	755	920	−426	S
ATOM	364	CE	BMET A	70	79.803	66.560	98.459	0.26	39.32		C
ANISOU	364	CE	BMET A	70	4138	4795	6006	163	1008	−422	C
ATOM	365	O	GLN A	75	79.533	67.314	93.156	1.00	59.81		O
ANISOU	365	O	GLN A	75	5496	6775	10454	−367	3926	570	O
ATOM	366	N	GLN A	75	82.467	67.453	93.351	1.00	65.58		N
ANISOU	366	N	GLN A	75	6279	7002	11637	−69	3815	−22	N
ATOM	367	CA	GLN A	75	81.558	68.591	93.278	1.00	64.14		C
ANISOU	367	CA	GLN A	75	6119	6868	11382	−99	3743	161	C
ATOM	368	C	GLN A	75	80.156	68.203	93.734	1.00	61.67		C
ANISOU	368	C	GLN A	75	5856	6752	10823	−38	3546	338	C
ATOM	369	CB	GLN A	75	81.512	69.152	91.856	1.00	69.11		C
ANISOU	369	CB	GLN A	75	6803	7535	11921	435	3706	68	C
ATOM	370	O	PRO A	76	77.317	70.261	93.947	1.00	37.41		O
ANISOU	370	O	PRO A	76	4445	2739	7031	−487	1773	1170	O
ATOM	371	N	PRO A	76	79.659	68.865	94.784	1.00	47.65		N
ANISOU	371	N	PRO A	76	4178	4699	9229	−429	2977	379	N
ATOM	372	C	PRO A	76	77.209	69.141	94.450	1.00	34.74		C
ANISOU	372	C	PRO A	76	3765	2706	6728	−488	2096	632	C
ATOM	373	CA	PRO A	76	78.326	68.582	95.323	1.00	41.79		C
ANISOU	373	CA	PRO A	76	3727	3934	8216	−348	2638	391	C
ATOM	374	CB	PRO A	76	78.341	69.304	96.672	1.00	48.42		C
ANISOU	374	CB	PRO A	76	4224	5386	8785	205	2965	611	C
ATOM	375	CG	PRO A	76	79.296	70.429	96.478	1.00	51.38		C
ANISOU	375	CG	PRO A	76	4505	5874	9144	453	3196	784	C
ATOM	376	CD	PRO A	76	80.361	69.905	95.557	1.00	51.62		C
ANISOU	376	CD	PRO A	76	4374	5909	9329	579	3152	626	C
ATOM	377	O	ASP A	77	73.450	67.872	95.183	1.00	17.09		O
ANISOU	377	O	ASP A	77	2573	1931	1989	−78	179	418	O
ATOM	378	N	ASP A	77	76.148	68.364	94.274	1.00	27.61		N
ANISOU	378	N	ASP A	77	3182	2248	5058	−51	2019	303	N
ATOM	379	CA	ASP A	77	74.960	68.844	93.585	1.00	25.29		C
ANISOU	379	CA	ASP A	77	3260	2429	3921	108	1406	651	C
ATOM	380	C	ASP A	77	73.819	68.890	94.596	1.00	19.12		C
ANISOU	380	C	ASP A	77	2645	1864	2756	−154	388	395	C
ATOM	381	CB	ASP A	77	74.587	67.934	92.417	1.00	33.66		C
ANISOU	381	CB	ASP A	77	4555	3599	4635	53	1470	606	C
ATOM	382	CG	ASP A	77	73.296	68.361	91.738	1.00	39.65		C
ANISOU	382	CG	ASP A	77	5496	4491	5077	−212	1645	670	C
ATOM	383	OD2	ASP A	77	72.636	67.506	91.111	1.00	43.65		O
ANISOU	383	OD2	ASP A	77	5964	5343	5278	−604	1573	886	O
ATOM	384	N	LYS A	78	73.265	70.077	94.812	1.00	18.13		N
ANISOU	384	N	LYS A	78	2656	2021	2211	−292	128	738	N
ATOM	385	C	LYS A	78	70.900	69.679	95.252	1.00	17.91		C
ANISOU	385	C	LYS A	78	2582	2405	1820	110	−120	778	C
ATOM	386	O	LYS A	78	70.459	70.061	94.175	1.00	23.29		O
ANISOU	386	O	LYS A	78	3262	3409	2177	−475	−462	1288	O
ATOM	387	CD	LYS A	78	70.844	73.246	97.792	1.00	31.36		C
ANISOU	387	CD	LYS A	78	5027	3368	3521	167	147	139	C
ATOM	388	CE	LYS A	78	70.602	74.229	96.682	1.00	36.57		C
ANISOU	388	CE	LYS A	78	5609	4344	3941	9	135	−87	C
ATOM	389	CA	LYS A	78	72.205	70.235	95.798	1.00	18.66		C
ANISOU	389	CA	LYS A	78	2733	1988	2368	−187	219	468	C
ATOM	390	CB	LYS A	78	72.024	71.697	96.202	1.00	20.26		C
ANISOU	390	CB	LYS A	78	2983	2140	2575	−67	194	403	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	391	CG	LYS A	78	70.942	71.840	97.253	1.00	23.00		C
ANISOU	391	CG	LYS A	78	3743	2305	2690	17	188	328	C
ATOM	392	N	LEU A	79	70.300	68.761	95.995	1.00	14.93		N
ANISOU	392	N	LEU A	79	2193	2021	1459	60	11	346	N
ATOM	393	CA	LEU A	79	69.061	68.106	95.585	1.00	14.87		C
ANISOU	393	CA	LEU A	79	2146	2203	1299	80	−138	17	C
ATOM	394	C	LEU A	79	67.813	68.749	96.155	1.00	15.07		C
ANISOU	394	C	LEU A	79	2034	2226	1466	197	−275	−45	C
ATOM	395	O	LEU A	79	66.782	68.816	95.495	1.00	17.12		O
ANISOU	395	O	LEU A	79	2255	2712	1537	228	−311	11	O
ATOM	396	CB	LEU A	79	69.085	66.648	96.040	1.00	15.38		C
ANISOU	396	CB	LEU A	79	2206	2080	1556	238	145	−62	C
ATOM	397	CG	LEU A	79	70.270	65.839	95.514	1.00	15.34		C
ANISOU	397	CG	LEU A	79	2239	2083	1505	70	32	8	C
ATOM	398	CD1	LEU A	79	70.353	64.513	96.244	1.00	16.98		C
ANISOU	398	CD1	LEU A	79	2645	1939	1867	38	426	−10	C
ATOM	399	CD2	LEU A	79	70.165	65.634	94.019	1.00	18.66		C
ANISOU	399	CD2	LEU A	79	2815	3182	1095	460	48	−201	C
ATOM	400	N	ALA A	80	67.907	69.182	97.401	1.00	15.22		N
ANISOU	400	N	ALA A	80	2270	2164	1350	219	−209	−35	N
ATOM	401	CA	ALA A	80	66.769	69.690	98.152	1.00	14.17		C
ANISOU	401	CA	ALA A	80	1958	2196	1229	123	−92	−176	C
ATOM	402	C	ALA A	80	67.304	70.274	99.444	1.00	13.34		C
ANISOU	402	C	ALA A	80	1931	1846	1290	167	−139	151	C
ATOM	403	O	ALA A	80	68.460	70.050	99.797	1.00	14.84		O
ANISOU	403	O	ALA A	80	2009	2141	1489	297	−266	−77	O
ATOM	404	CB	ALA A	80	65.763	68.572	98.437	1.00	17.46		C
ANISOU	404	CB	ALA A	80	2376	2541	1717	−366	2	−212	C
ATOM	405	N	ALA A	81	66.476	71.050	100.129	1.00	14.26		N
ANISOU	405	N	ALA A	81	1911	1978	1529	347	−270	−112	N
ATOM	406	CA	ALA A	81	66.912	71.740	101.333	1.00	15.46		C
ANISOU	406	CA	ALA A	81	2038	2197	1641	−10	−151	−273	C
ATOM	407	C	ALA A	81	65.792	71.876	102.346	1.00	13.84		C
ANISOU	407	C	ALA A	81	1708	1729	1820	230	−67	11	C
ATOM	408	O	ALA A	81	64.607	71.836	101.996	1.00	14.92		O
ANISOU	408	O	ALA A	81	1770	2029	1870	55	−148	−141	O
ATOM	409	CB	ALA A	81	67.444	73.129	100.979	1.00	19.24		C
ANISOU	409	CB	ALA A	81	2786	2332	2194	−609	230	−380	C
ATOM	410	O	PHE A	82	67.093	73.937	105.446	1.00	17.78		O
ANISOU	410	O	PHE A	82	1865	2618	2271	447	−361	−609	O
ATOM	411	N	PHE A	82	66.194	72.068	103.599	1.00	14.65		N
ANISOU	411	N	PHE A	82	2045	2056	1468	294	−98	−213	N
ATOM	412	CA	PHE A	82	65.325	72.541	104.665	1.00	15.78		C
ANISOU	412	CA	PHE A	82	2180	1991	1827	128	−46	−218	C
ATOM	413	C	PHE A	82	65.901	73.845	105.213	1.00	15.26		C
ANISOU	413	C	PHE A	82	2013	2063	1722	386	−47	−247	C
ATOM	414	CB	PHE A	82	65.234	71.552	105.828	1.00	17.84		C
ANISOU	414	CB	PHE A	82	2955	2220	1603	557	−3	151	C
ATOM	415	CG	PHE A	82	64.555	72.136	107.043	1.00	17.96		C
ANISOU	415	CG	PHE A	82	3276	2085	1465	469	−43	138	C
ATOM	416	CD1	PHE A	82	63.187	72.065	107.164	1.00	20.00		C
ANISOU	416	CD1	PHE A	82	2822	2710	2069	−17	230	445	C
ATOM	417	CD2	PHE A	82	65.277	72.803	108.032	1.00	20.15		C
ANISOU	417	CD2	PHE A	82	4186	2211	1258	819	−276	−34	C
ATOM	418	CE1	PHE A	82	62.546	72.627	108.257	1.00	20.60		C
ANISOU	418	CE1	PHE A	82	3319	2722	1785	298	551	94	C
ATOM	419	CE2	PHE A	82	64.641	73.377	109.121	1.00	21.22		C
ANISOU	419	CE2	PHE A	82	4330	1975	1759	257	8	264	C
ATOM	420	CZ	PHE A	82	63.275	73.276	109.236	1.00	21.54		C
ANISOU	420	CZ	PHE A	82	3444	2628	2110	138	374	212	C
ATOM	421	O	APRO A	83	64.534	75.084	102.806	0.78	17.31		O
ANISOU	421	O	APRO A	83	2881	2017	1681	−373	95	−57	O
ATOM	422	N	APRO A	83	65.057	74.863	105.424	0.78	13.97		N
ANISOU	422	N	APRO A	83	1879	1971	1456	265	26	18	N
ATOM	423	CA	APRO A	83	63.649	74.965	105.036	0.78	14.86		C
ANISOU	423	CA	APRO A	83	2040	2040	1566	477	6	−17	C
ATOM	424	C	APRO A	83	63.534	74.923	103.518	0.78	15.20		C
ANISOU	424	C	APRO A	83	2282	1663	1830	−51	0	91	C
ATOM	425	CB	APRO A	83	63.245	76.357	105.547	0.78	17.53		C
ANISOU	425	CB	APRO A	83	2598	2308	1753	749	−85	−356	C
ATOM	426	CG	APRO A	83	64.219	76.672	106.610	0.78	19.00		C
ANISOU	426	CG	APRO A	83	2894	2303	2023	780	−236	−334	C
ATOM	427	CD	APRO A	83	65.509	76.055	106.161	0.78	16.76		C
ANISOU	427	CD	APRO A	83	2557	2022	1790	498	−384	−407	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	428	O	BPRO A	83	64.504	75.290	102.883	0.22	16.75		O
ANISOU	428	O	BPRO A	83	2733	2012	1618	429	−43	747	O
ATOM	429	N	BPRO A	83	65.052	74.862	105.416	0.22	19.74		N
ANISOU	429	N	BPRO A	83	2486	2470	2545	100	85	13	N
ATOM	430	CA	BPRO A	83	63.634	74.855	105.058	0.22	20.73		C
ANISOU	430	CA	BPRO A	83	2647	2668	2563	256	1	190	C
ATOM	431	C	BPRO A	83	63.513	74.970	103.550	0.22	20.60		C
ANISOU	431	C	BPRO A	83	2844	2629	2354	123	−151	511	C
ATOM	432	CB	BPRO A	83	63.107	76.121	105.731	0.22	21.65		C
ANISOU	432	CB	BPRO A	83	2699	2693	2834	91	139	153	C
ATOM	433	CG	BPRO A	83	64.268	77.037	105.735	0.22	19.42		C
ANISOU	433	CG	BPRO A	83	2355	2419	2605	124	166	236	C
ATOM	434	CD	BPRO A	83	65.477	76.166	105.954	0.22	17.84		C
ANISOU	434	CD	BPRO A	83	2283	2088	2407	−41	259	152	C
ATOM	435	O	GLU A	84	62.190	77.212	101.837	1.00	23.62		O
ANISOU	435	O	GLU A	84	3166	3247	2561	−336	−386	1188	O
ATOM	436	N	GLU A	84	62.333	74.688	103.015	1.00	19.02		N
ANISOU	436	N	GLU A	84	2551	2553	2124	−411	−461	633	N
ATOM	437	C	GLU A	84	62.522	76.236	101.167	1.00	23.36		C
ANISOU	437	C	GLU A	84	3268	3027	2579	−822	−552	684	C
ATOM	438	CA	AGLU A	84	62.118	74.820	101.583	0.78	22.42		C
ANISOU	438	CA	AGLU A	84	3205	3051	2263	−774	−859	684	C
ATOM	439	CB	AGLU A	84	60.665	74.546	101.218	0.78	26.82		C
ANISOU	439	CB	AGLU A	84	3306	4177	2706	−1277	−1119	711	C
ATOM	440	CG	AGLU A	84	60.416	74.454	99.721	0.78	31.73		C
ANISOU	440	CG	AGLU A	84	3984	4919	3152	−1016	−1297	512	C
ATOM	441	CA	BGLU A	84	62.129	74.823	101.582	0.22	23.88		C
ANISOU	441	CA	BGLU A	84	3269	3142	2660	−325	−468	620	C
ATOM	442	CB	BGLU A	84	60.685	74.506	101.189	0.22	28.06		C
ANISOU	442	CB	BGLU A	84	3669	3804	3189	206	−366	532	C
ATOM	443	CG	BGLU A	84	59.638	75.324	101.920	0.22	24.44		C
ANISOU	443	CG	BGLU A	84	3119	3391	2774	862	−219	455	C
ATOM	444	O	ASP A	85	61.949	78.209	98.274	1.00	25.20		O
ANISOU	444	O	ASP A	85	3930	3398	2248	−53	−857	48	O
ATOM	445	N	ASP A	85	63.268	76.331	100.081	1.00	21.43		N
ANISOU	445	N	ASP A	85	3677	2558	1909	−557	−542	607	N
ATOM	446	C	ASP A	85	62.725	78.547	99.165	1.00	21.13		C
ANISOU	446	C	ASP A	85	3274	2668	2086	−480	−587	278	C
ATOM	447	CG	ASP A	85	65.361	78.608	97.908	1.00	22.45		C
ANISOU	447	CG	ASP A	85	3991	2525	2014	−834	−400	−112	C
ATOM	448	OD1	ASP A	85	65.532	79.599	98.641	1.00	20.09		O
ANISOU	448	OD1	ASP A	85	2992	2515	2125	−310	−400	42	O
ATOM	449	OD2	ASP A	85	65.626	78.606	96.696	1.00	28.08		O
ANISOU	449	OD2	ASP A	85	5417	3188	2066	−1047	29	−280	O
ATOM	450	CA	AASP A	85	63.823	77.599	99.639	0.50	21.48		C
ANISOU	450	CA	AASP A	85	3594	2559	2009	−607	−498	404	C
ATOM	451	CB	AASP A	85	64.821	77.340	98.512	0.50	22.67		C
ANISOU	451	CB	AASP A	85	3962	2620	2032	−713	−443	111	C
ATOM	452	CA	BASP A	85	63.823	77.599	99.639	0.50	21.47		C
ANISOU	452	CA	BASP A	85	3593	2557	2008	−606	−497	405	C
ATOM	453	CB	BASP A	85	64.821	77.340	98.512	0.50	22.69		C
ANISOU	453	CB	BASP A	85	3964	2622	2034	−714	−442	113	C
ATOM	454	O	ARG A	86	61.763	82.988	98.452	1.00	22.95		O
ANISOU	454	O	ARG A	86	2562	2977	3179	−9	−100	682	O
ATOM	455	N	ARG A	86	62.665	79.733	99.766	1.00	20.17		N
ANISOU	455	N	ARG A	86	2853	2802	2009	−407	−366	458	N
ATOM	456	CA	ARG A	86	61.711	80.764	99.362	1.00	20.70		C
ANISOU	456	CA	ARG A	86	2371	3069	2423	−796	70	134	C
ATOM	457	C	ARG A	86	62.392	81.958	98.685	1.00	20.61		C
ANISOU	457	C	ARG A	86	2465	2787	2577	−296	−394	292	C
ATOM	458	CB	ARG A	86	60.891	81.237	100.561	1.00	26.57		C
ANISOU	458	CB	ARG A	86	3126	3810	3159	−519	363	443	C
ATOM	459	CG	ARG A	86	59.936	80.187	101.095	1.00	28.39		C
ANISOU	459	CG	ARG A	86	3490	3724	3573	−743	369	492	C
ATOM	460	CD	ARG A	86	58.831	79.901	100.093	1.00	31.18		C
ANISOU	460	CD	ARG A	86	3877	4040	3929	−1020	436	425	C
ATOM	461	O	SER A	87	64.635	83.665	95.428	1.00	20.78		O
ANISOU	461	O	SER A	87	3764	2006	2125	−347	−216	27	O
ATOM	462	N	SER A	87	63.678	81.824	98.373	1.00	17.97		N
ANISOU	462	N	SER A	87	2511	2503	1812	−510	−166	−102	N
ATOM	463	CA	SER A	87	64.399	82.880	97.670	1.00	17.63		C
ANISOU	463	CA	SER A	87	2430	2367	1901	−463	4	−332	C
ATOM	464	C	SER A	87	64.296	82.740	96.160	1.00	17.95		C
ANISOU	464	C	SER A	87	2911	1944	1967	−267	−225	−86	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	465	CB	SER A	87	65.876	82.882	98.068	1.00	17.44		C
ANISOU	465	CB	SER A	87	2583	2262	1780	−372	125	−606	C
ATOM	466	OG	SER A	87	66.572	81.799	97.475	1.00	17.39		O
ANISOU	466	OG	SER A	87	2815	2448	1346	−305	−12	−237	O
ATOM	467	O	GLN A	88	61.787	80.040	95.023	1.00	20.77		O
ANISOU	467	O	GLN A	88	3440	2502	1950	−582	−513	267	O
ATOM	468	N	GLN A	88	63.852	81.572	95.705	1.00	18.09		N
ANISOU	468	N	GLN A	88	2977	2093	1805	−272	−409	42	N
ATOM	469	CA	GLN A	88	63.696	81.272	94.289	1.00	19.08		C
ANISOU	469	CA	GLN A	88	3031	2430	1788	−132	−535	−12	C
ATOM	470	C	GLN A	88	62.354	80.595	94.076	1.00	19.03		C
ANISOU	470	C	GLN A	88	3191	2241	1801	−454	−468	355	C
ATOM	471	CB	GLN A	88	64.812	80.326	93.837	1.00	20.35		C
ANISOU	471	CB	GLN A	88	2830	3218	1684	−3	−456	−330	C
ATOM	472	CG	GLN A	88	66.212	80.903	93.946	1.00	22.21		C
ANISOU	472	CG	GLN A	88	3071	3837	1530	−58	−336	−146	C
ATOM	473	CD	GLN A	88	66.479	81.994	92.928	1.00	23.77		C
ANISOU	473	CD	GLN A	88	3083	4614	1336	55	−482	−412	C
ATOM	474	OE1	GLN A	88	65.631	82.310	92.087	1.00	28.49		O
ANISOU	474	OE1	GLN A	88	3633	5636	1555	−355	−399	475	O
ATOM	475	NE2	GLN A	88	67.671	82.572	92.993	1.00	24.25		N
ANISOU	475	NE2	GLN A	88	2930	4646	1637	−287	−219	−420	N
ATOM	476	O	PRO A	89	61.745	77.831	92.863	1.00	25.02		O
ANISOU	476	O	PRO A	89	4635	2982	1888	−1212	−947	440	O
ATOM	477	N	PRO A	89	61.852	80.600	92.827	1.00	21.31		N
ANISOU	477	N	PRO A	89	3510	2583	2004	−597	−717	541	N
ATOM	478	CA	PRO A	89	60.590	79.906	92.557	1.00	23.52		C
ANISOU	478	CA	PRO A	89	3804	3239	1893	−1177	−974	676	C
ATOM	479	C	PRO A	89	60.665	78.422	92.888	1.00	26.08		C
ANISOU	479	C	PRO A	89	4289	3537	2084	−1006	−978	478	C
ATOM	480	CB	PRO A	89	60.410	80.072	91.047	1.00	25.55		C
ANISOU	480	CB	PRO A	89	4076	3659	1971	−856	−1060	627	C
ATOM	481	CG	PRO A	89	61.262	81.200	90.662	1.00	25.71		C
ANISOU	481	CG	PRO A	89	4079	3550	2141	−1092	−950	630	C
ATOM	482	CD	PRO A	89	62.413	81.216	91.614	1.00	21.71		C
ANISOU	482	CD	PRO A	89	3670	2839	1738	−419	−612	884	C
ATOM	483	O	GLY A	90	59.812	76.050	91.128	1.00	30.52		O
ANISOU	483	O	GLY A	90	5742	3916	1938	−1347	−515	151	O
ATOM	484	N	GLY A	90	59.515	77.833	93.186	1.00	26.56		N
ANISOU	484	N	GLY A	90	4633	3065	2395	−1226	−554	414	N
ATOM	485	CA	GLY A	90	59.443	76.416	93.473	1.00	28.69		C
ANISOU	485	CA	GLY A	90	5254	3596	2052	−1124	−258	209	C
ATOM	486	C	GLY A	90	59.880	75.596	92.278	1.00	27.73		C
ANISOU	486	C	GLY A	90	5532	3423	1582	−1150	−191	296	C
ATOM	487	O	GLN A	91	60.118	71.649	92.899	1.00	36.65		O
ANISOU	487	O	GLN A	91	7341	4045	2540	−647	−838	−23	O
ATOM	488	N	GLN A	91	60.346	74.387	92.555	1.00	30.58		N
ANISOU	488	N	GLN A	91	6500	3296	1822	−339	−451	−108	N
ATOM	489	CA	GLN A	91	60.777	73.483	91.507	1.00	32.88		C
ANISOU	489	CA	GLN A	91	6550	3649	2294	−431	−957	−253	C
ATOM	490	C	GLN A	91	60.198	72.101	91.759	1.00	35.00		C
ANISOU	490	C	GLN A	91	6948	3585	2767	−337	−981	83	C
ATOM	491	CB	GLN A	91	62.305	73.415	91.450	1.00	37.68		C
ANISOU	491	CB	GLN A	91	6800	4675	2842	−139	−1191	58	C
ATOM	492	O	ASP A	92	61.544	69.405	90.352	1.00	38.12		O
ANISOU	492	O	ASP A	92	6240	3836	4407	521	−84	2149	O
ATOM	493	N	ASP A	92	59.775	71.443	90.688	1.00	32.54		N
ANISOU	493	N	ASP A	92	6408	2878	3078	−125	−1248	−106	N
ATOM	494	CA	ASP A	92	59.289	70.075	90.779	1.00	33.32		C
ANISOU	494	CA	ASP A	92	6009	2884	3766	291	−1087	238	C
ATOM	495	C	ASP A	92	60.488	69.159	90.930	1.00	33.55		C
ANISOU	495	C	ASP A	92	5699	3030	4018	−227	−662	1287	C
ATOM	496	CB	ASP A	92	58.495	69.702	89.530	1.00	35.93		C
ANISOU	496	CB	ASP A	92	6034	3526	4091	988	−1266	−315	C
ATOM	497	CG	ASP A	92	57.367	70.670	89.253	1.00	39.20		C
ANISOU	497	CG	ASP A	92	6283	4264	4349	1570	−1146	−250	C
ATOM	498	OD1	ASP A	92	57.594	71.644	88.503	1.00	40.93		O
ANISOU	498	OD1	ASP A	92	6607	4537	4406	1865	−994	−332	O
ATOM	499	N	SER A	93	60.331	68.095	91.704	1.00	31.37		N
ANISOU	499	N	SER A	93	5045	3069	3807	−406	−1308	977	N
ATOM	500	CA	SER A	93	61.484	67.293	92.067	1.00	29.30		C
ANISOU	500	CA	SER A	93	4388	3190	3555	−688	−1461	996	C
ATOM	501	C	SER A	93	61.095	65.911	92.569	1.00	26.29		C
ANISOU	501	C	SER A	93	3690	3021	3277	−553	−841	720	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	502	O	SER A	93	60.028	65.746	93.153	1.00	28.27		O
ANISOU	502	O	SER A	93	3223	3405	4113	319	−267	910	O
ATOM	503	CB	SER A	93	62.265	68.024	93.157	1.00	33.85		C
ANISOU	503	CB	SER A	93	5574	3390	3898	−1246	−1329	860	C
ATOM	504	OG	SER A	93	63.428	67.315	93.509	1.00	32.62		O
ANISOU	504	OG	SER A	93	5489	3552	3354	−1242	−1481	1245	O
ATOM	505	N	ARG A	94	61.963	64.926	92.342	1.00	20.30		N
ANISOU	505	N	ARG A	94	3048	2960	1704	−444	−480	450	N
ATOM	506	CA	ARG A	94	61.815	63.616	92.977	1.00	17.72		C
ANISOU	506	CA	ARG A	94	2618	2603	1514	−456	−264	284	C
ATOM	507	C	ARG A	94	62.415	63.607	94.374	1.00	15.29		C
ANISOU	507	C	ARG A	94	2054	2523	1233	−370	−64	327	C
ATOM	508	O	ARG A	94	62.303	62.615	95.078	1.00	17.63		O
ANISOU	508	O	ARG A	94	2799	2200	1700	−251	−196	418	O
ATOM	509	CB	ARG A	94	62.489	62.507	92.154	1.00	19.40		C
ANISOU	509	CB	ARG A	94	2916	2914	1541	177	−230	−45	C
ATOM	510	CG	ARG A	94	61.767	62.182	90.868	1.00	20.14		C
ANISOU	510	CG	ARG A	94	2701	3291	1660	−101	−596	396	C
ATOM	511	CD	ARG A	94	62.369	60.974	90.166	1.00	21.38		C
ANISOU	511	CD	ARG A	94	2991	3172	1961	131	−257	257	C
ATOM	512	NE	ARG A	94	63.783	61.189	89.899	1.00	19.16		N
ANISOU	512	NE	ARG A	94	2513	3131	1636	282	98	213	N
ATOM	513	CZ	ARG A	94	64.774	60.418	90.323	1.00	16.67		C
ANISOU	513	CZ	ARG A	94	2308	2686	1339	97	−15	55	C
ATOM	514	NH1	ARG A	94	64.532	59.314	91.014	1.00	18.26		N
ANISOU	514	NH1	ARG A	94	2371	3039	1528	−139	−16	269	N
ATOM	515	NH2	ARG A	94	66.019	60.752	90.022	1.00	17.67		N
ANISOU	515	NH2	ARG A	94	2506	2575	1632	−145	79	81	N
ATOM	516	N	PHE A	95	63.042	64.712	94.767	1.00	15.48		N
ANISOU	516	N	PHE A	95	2362	2305	1217	−366	−227	307	N
ATOM	517	C	PHE A	95	63.115	65.661	97.029	1.00	16.60		C
ANISOU	517	C	PHE A	95	2787	2168	1352	−19	56	166	C
ATOM	518	O	PHE A	95	62.652	66.756	96.706	1.00	21.26		O
ANISOU	518	O	PHE A	95	4079	2218	1783	440	−147	155	O
ATOM	519	CA	APHE A	95	63.802	64.764	96.008	0.60	15.40		C
ANISOU	519	CA	APHE A	95	2374	2299	1177	−447	−5	95	C
ATOM	520	CB	APHE A	95	65.241	65.225	95.738	0.60	17.70		C
ANISOU	520	CB	APHE A	95	2505	3070	1152	−728	−107	100	C
ATOM	521	CG	APHE A	95	66.005	64.304	94.818	0.60	17.06		C
ANISOU	521	CG	APHE A	95	2251	3242	987	−813	130	53	C
ATOM	522	CD1	APHE A	95	66.807	63.294	95.328	0.60	17.27		C
ANISOU	522	CD1	APHE A	95	2597	2718	1246	−1015	141	−247	C
ATOM	523	CD2	APHE A	95	65.905	64.434	93.440	0.60	20.26		C
ANISOU	523	CD2	APHE A	95	2394	4067	1236	−571	330	140	C
ATOM	524	CE1	APHE A	95	67.501	62.438	94.481	0.60	17.41		C
ANISOU	524	CE1	APHE A	95	2279	3093	1244	−940	−186	−347	C
ATOM	525	CE2	APHE A	95	66.596	63.582	92.593	0.60	21.17		C
ANISOU	525	CE2	APHE A	95	2329	4064	1650	−693	184	74	C
ATOM	526	CZ	APHE A	95	67.390	62.582	93.113	0.60	20.82		C
ANISOU	526	CZ	APHE A	95	2461	3930	1519	−763	98	−117	C
ATOM	527	CA	BPHE A	95	63.803	64.784	96.013	0.40	16.16		C
ANISOU	527	CA	BPHE A	95	2520	2210	1411	−371	67	144	C
ATOM	528	CB	BPHE A	95	65.197	65.343	95.753	0.40	17.84		C
ANISOU	528	CB	BPHE A	95	2637	2532	1608	−594	232	4	C
ATOM	529	CG	BPHE A	95	65.877	64.703	94.598	0.40	16.16		C
ANISOU	529	CG	BPHE A	95	2311	2590	1238	−798	417	−95	C
ATOM	530	CD1	BPHE A	95	66.381	63.420	94.708	0.40	18.96		C
ANISOU	530	CD1	BPHE A	95	2670	3203	1332	−218	432	−455	C
ATOM	531	CD2	BPHE A	95	65.990	65.366	93.389	0.40	19.75		C
ANISOU	531	CD2	BPHE A	95	2728	2891	1885	−726	169	−115	C
ATOM	532	CE1	BPHE A	95	66.998	62.811	93.634	0.40	17.68		C
ANISOU	532	CE1	BPHE A	95	2183	3157	1377	−1008	407	−220	C
ATOM	533	CE2	BPHE A	95	66.610	64.764	92.313	0.40	20.84		C
ANISOU	533	CE2	BPHE A	95	2649	3464	1804	−666	39	−127	C
ATOM	534	CZ	BPHE A	95	67.115	63.486	92.435	0.40	20.23		C
ANISOU	534	CZ	BPHE A	95	2400	3543	1744	−520	130	−205	C
ATOM	535	N	ARG A	96	63.058	65.186	98.264	1.00	15.57		N
ANISOU	535	N	ARG A	96	1877	2794	1246	141	43	160	N
ATOM	536	C	ARG A	96	63.220	65.897	100.582	1.00	15.94		C
ANISOU	536	C	ARG A	96	2303	2502	1250	282	324	−96	C
ATOM	537	O	ARG A	96	63.883	64.905	100.880	1.00	15.74		O
ANISOU	537	O	ARG A	96	2571	1970	1438	402	−38	−83	O
ATOM	538	CG	AARG A	96	60.052	65.904	100.483	0.74	32.33		C
ANISOU	538	CG	AARG A	96	3554	5716	3016	736	−21	140	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	539	CD	AARG A	96	58.847	65.011	100.784	0.74	36.28		C
ANISOU	539	CD	AARG A	96	3912	5949	3924	−79	−103	−10	C
ATOM	540	NE	AARG A	96	57.943	64.855	99.646	0.74	34.69		N
ANISOU	540	NE	AARG A	96	3628	5549	4004	−469	258	307	N
ATOM	541	CZ	AARG A	96	56.791	64.189	99.693	0.74	35.88		C
ANISOU	541	CZ	AARG A	96	3718	5640	4274	−391	252	499	C
ATOM	542	NH1	AARG A	96	56.400	63.611	100.823	0.74	30.40		N
ANISOU	542	NH1	AARG A	96	3104	4637	3810	−282	554	836	N
ATOM	543	NH2	AARG A	96	56.028	64.100	98.611	0.74	41.38		N
ANISOU	543	NH2	AARG A	96	4540	6283	4901	−253	164	525	N
ATOM	544	CA	AARG A	96	62.362	65.896	99.317	0.74	19.49		C
ANISOU	544	CA	AARG A	96	2563	3664	1178	1066	222	56	C
ATOM	545	CB	AARG A	96	61.021	65.190	99.577	0.74	24.85		C
ANISOU	545	CB	AARG A	96	2264	5235	1942	1177	−175	−196	C
ATOM	546	CG	BARG A	96	60.088	65.290	98.485	0.26	30.44		C
ANISOU	546	CG	BARG A	96	3116	5402	3047	504	−45	56	C
ATOM	547	CD	BARG A	96	58.797	64.585	98.906	0.26	36.84		C
ANISOU	547	CD	BARG A	96	3987	6035	3975	316	17	116	C
ATOM	548	NE	BARG A	96	57.772	64.582	97.864	0.26	37.27		N
ANISOU	548	NE	BARG A	96	4071	5829	4260	−192	−48	152	N
ATOM	549	CZ	BARG A	96	56.614	63.931	97.958	0.26	37.23		C
ANISOU	549	CZ	BARG A	96	4054	5704	4388	−379	−16	259	C
ATOM	550	NH1	BARG A	96	56.331	63.225	99.046	0.26	32.06		N
ANISOU	550	NH1	BARG A	96	3381	4903	3897	−797	119	344	N
ATOM	551	NH2	BARG A	96	55.737	63.986	96.963	0.26	39.77		N
ANISOU	551	NH2	BARG A	96	4382	6063	4667	−215	−67	258	N
ATOM	552	CA	BARG A	96	62.462	65.896	99.317	0.26	19.09		C
ANISOU	552	CA	BARG A	96	2389	3427	1436	655	153	22	C
ATOM	553	CB	BARG A	96	61.121	65.190	99.577	0.26	26.16		C
ANISOU	553	CB	BARG A	96	2800	4814	2326	776	−32	−87	C
ATOM	554	N	VAL A	97	63.208	67.013	101.311	1.00	16.57		N
ANISOU	554	N	VAL A	97	2509	2406	1379	657	448	463	N
ATOM	555	CA	VAL A	97	63.741	67.064	102.662	1.00	15.24		C
ANISOU	555	CA	VAL A	97	2030	2151	1611	315	690	232	C
ATOM	556	C	VAL A	97	62.600	67.464	103.566	1.00	15.96		C
ANISOU	556	C	VAL A	97	2173	1951	1940	99	564	−94	C
ATOM	557	O	VAL A	97	61.918	68.460	103.320	1.00	17.51		O
ANISOU	557	O	VAL A	97	2300	2147	2206	502	494	106	O
ATOM	558	CB	VAL A	97	64.897	68.070	102.850	1.00	16.53		C
ANISOU	558	CB	VAL A	97	2032	2122	2125	147	563	216	C
ATOM	559	CG1	VAL A	97	65.341	68.085	104.307	1.00	18.83		C
ANISOU	559	CG1	VAL A	97	2266	2364	2526	−305	626	−540	C
ATOM	560	CG2	VAL A	97	66.068	67.715	101.960	1.00	17.60		C
ANISOU	560	CG2	VAL A	97	1986	2366	2335	175	453	398	C
ATOM	561	N	ATHR A	98	62.352	66.673	104.602	0.48	15.93		N
ANISOU	561	N	ATHR A	98	1793	2361	1897	−631	158	−349	N
ATOM	562	CA	ATHR A	98	61.291	66.993	105.553	0.48	22.15		C
ANISOU	562	CA	ATHR A	98	2567	3200	2648	−365	144	−387	C
ATOM	563	C	ATHR A	98	61.769	66.857	106.982	0.48	17.38		C
ANISOU	563	C	ATHR A	98	1729	3166	1707	61	309	−547	C
ATOM	564	O	ATHR A	98	62.313	65.826	107.373	0.48	19.03		O
ANISOU	564	O	ATHR A	98	2103	3872	1254	348	172	−428	O
ATOM	565	CB	ATHR A	98	60.077	66.065	105.408	0.48	21.66		C
ANISOU	565	CB	ATHR A	98	2887	2550	2793	−654	72	−204	C
ATOM	566	OG1	ATHR A	98	60.494	64.707	105.595	0.48	21.51		O
ANISOU	566	OG1	ATHR A	98	2728	2805	2641	−502	627	563	O
ATOM	567	CG2	ATHR A	98	59.430	66.225	104.051	0.48	21.26		C
ANISOU	567	CG2	ATHR A	98	2704	2440	2935	−493	−414	−49	C
ATOM	568	N	BTHR A	98	62.398	66.700	104.623	0.52	13.91		N
ANISOU	568	N	BTHR A	98	1623	2373	1290	590	627	142	N
ATOM	569	CA	BTHR A	98	61.323	66.996	105.538	0.52	14.20		C
ANISOU	569	CA	BTHR A	98	1773	2260	1365	172	587	245	C
ATOM	570	C	BTHR A	98	61.861	66.907	106.954	0.52	14.38		C
ANISOU	570	C	BTHR A	98	1555	2283	1627	89	636	−66	C
ATOM	571	O	BTHR A	98	62.591	65.981	107.291	0.52	17.26		O
ANISOU	571	O	BTHR A	98	2643	2172	1741	1137	460	243	O
ATOM	572	CB	BTHR A	98	60.157	66.020	105.321	0.52	16.05		C
ANISOU	572	CB	BTHR A	98	1919	3050	1131	96	521	66	C
ATOM	573	OG1	BTHR A	98	59.816	65.993	103.927	0.52	17.77		O
ANISOU	573	OG1	BTHR A	98	2067	3177	1509	92	36	−18	O
ATOM	574	CG2	BTHR A	98	58.944	66.439	106.132	0.52	17.76		C
ANISOU	574	CG2	BTHR A	98	1974	3490	1282	−250	465	19	C
ATOM	575	N	GLN A	99	61.522	67.891	107.773	1.00	16.48		N
ANISOU	575	N	GLN A	99	1987	2588	1687	231	214	−483	N

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	576	CA	GLN A	99	61.857	67.853	109.172	1.00	15.12		C
ANISOU	576	CA	GLN A	99	1907	2066	1770	−125	375	−261	C
ATOM	577	C	GLN A	99	60.842	66.993	109.896	1.00	16.11		C
ANISOU	577	C	GLN A	99	1777	2258	2087	80	114	−346	C
ATOM	578	O	GLN A	99	59.647	67.216	109.763	1.00	18.16		O
ANISOU	578	O	GLN A	99	1838	2472	2591	−32	284	−379	O
ATOM	579	CB	GLN A	99	61.834	69.257	109.738	1.00	16.41		C
ANISOU	579	CB	GLN A	99	2386	2191	1657	−188	379	−423	C
ATOM	580	CG	GLN A	99	62.258	69.318	111.172	1.00	17.42		C
ANISOU	580	CG	GLN A	99	2535	2335	1751	−417	218	−300	C
ATOM	581	CD	GLN A	99	62.333	70.741	111.658	1.00	19.11		C
ANISOU	581	CD	GLN A	99	2949	2372	1939	136	276	−149	C
ATOM	582	OE1	GLN A	99	61.439	71.545	111.383	1.00	21.45		O
ANISOU	582	OE1	GLN A	99	3307	2763	2080	548	242	−130	O
ATOM	583	NE2	GLN A	99	63.410	71.074	112.362	1.00	20.48		N
ANISOU	583	NE2	GLN A	99	3155	2423	2201	−377	120	−401	N
ATOM	584	N	LEU A	100	61.301	66.004	110.655	1.00	15.04		N
ANISOU	584	N	LEU A	100	1871	2386	1459	−205	531	−266	N
ATOM	585	CA	LEU A	100	60.383	65.158	111.409	1.00	16.78		C
ANISOU	585	CA	LEU A	100	2203	2488	1684	−457	440	−398	C
ATOM	586	C	LEU A	100	59.901	65.913	112.646	1.00	17.14		C
ANISOU	586	C	LEU A	100	2145	2711	1657	−639	604	−720	C
ATOM	587	O	LEU A	100	60.516	66.901	113.061	1.00	18.94		O
ANISOU	587	O	LEU A	100	2393	2806	1999	−577	627	−691	O
ATOM	588	CB	LEU A	100	61.066	63.850	111.790	1.00	17.20		C
ANISOU	588	CB	LEU A	100	2408	2341	1785	−370	582	−186	C
ATOM	589	CG	LEU A	100	61.464	62.989	110.584	1.00	20.20		C
ANISOU	589	CG	LEU A	100	2679	2491	2504	−374	69	−754	C
ATOM	590	CD1	LEU A	100	62.072	61.676	111.039	1.00	24.69		C
ANISOU	590	CD1	LEU A	100	3217	2849	3315	−237	44	−306	C
ATOM	591	CD2	LEU A	100	60.296	62.745	109.648	1.00	24.32		C
ANISOU	591	CD2	LEU A	100	3287	3342	2610	337	−381	−985	C
ATOM	592	O	PRO A	101	58.879	67.123	116.438	1.00	28.28		O
ANISOU	592	O	PRO A	101	3373	4523	2848	−683	778	−1915	O
ATOM	593	N	PRO A	101	58.788	65.471	113.241	1.00	18.27		N
ANISOU	593	N	PRO A	101	2137	2770	2034	−574	700	−584	N
ATOM	594	C	PRO A	101	59.154	66.304	115.582	1.00	23.89		C
ANISOU	594	C	PRO A	101	2816	3818	2444	−1282	989	−1029	C
ATOM	595	CA	PRO A	101	58.231	66.199	114.382	1.00	21.55		C
ANISOU	595	CA	PRO A	101	2293	3662	2233	−815	984	−1149	C
ATOM	596	CB	PRO A	101	56.990	65.386	114.730	1.00	24.55		C
ANISOU	596	CB	PRO A	101	2332	4634	2363	−1116	884	−1196	C
ATOM	597	CG	PRO A	101	56.555	64.838	113.423	1.00	23.37		C
ANISOU	597	CG	PRO A	101	2468	3806	2607	−1008	918	−1023	C
ATOM	598	CD	PRO A	101	57.829	64.490	112.709	1.00	19.04		C
ANISOU	598	CD	PRO A	101	2120	3111	2003	−968	748	−801	C
ATOM	599	O	ASN A	102	62.906	67.290	117.402	1.00	21.80		O
ANISOU	599	O	ASN A	102	3401	3297	1586	−840	52	−564	O
ATOM	600	N	ASN A	102	60.227	65.534	115.661	1.00	22.60		N
ANISOU	600	N	ASN A	102	2582	4131	1874	−1060	613	−989	N
ATOM	601	CA	ASN A	102	61.164	65.749	116.763	1.00	22.20		C
ANISOU	601	CA	ASN A	102	2926	3793	1718	−970	330	−576	C
ATOM	602	C	ASN A	102	62.156	66.893	116.510	1.00	19.28		C
ANISOU	602	C	ASN A	102	2628	3282	1418	−849	292	−265	C
ATOM	603	CB	ASN A	102	61.876	64.453	117.168	1.00	22.66		C
ANISOU	603	CB	ASN A	102	3580	3404	1626	39	777	239	C
ATOM	604	CG	ASN A	102	62.942	64.015	116.171	1.00	26.42		C
ANISOU	604	CG	ASN A	102	4159	3706	2172	80	875	387	C
ATOM	605	OD1	ASN A	102	63.103	64.589	115.091	1.00	25.28		O
ANISOU	605	OD1	ASN A	102	3760	4004	1841	−237	1014	215	O
ATOM	606	ND2	ASN A	102	63.680	62.975	116.540	1.00	31.94		N
ANISOU	606	ND2	ASN A	102	4324	4873	2939	938	1039	494	N
ATOM	607	O	GLY A	103	65.039	68.934	113.819	1.00	22.76		O
ANISOU	607	O	GLY A	103	2323	3746	2580	−626	396	638	O
ATOM	608	N	GLY A	103	62.147	67.435	115.297	1.00	18.77		N
ANISOU	608	N	GLY A	103	2325	2931	1877	−439	312	−559	N
ATOM	609	CA	GLY A	103	62.990	68.571	114.963	1.00	19.17		C
ANISOU	609	CA	GLY A	103	2196	2956	2132	−591	318	−542	C
ATOM	610	C	GLY A	103	64.439	68.256	114.648	1.00	18.04		C
ANISOU	610	C	GLY A	103	2428	2448	1978	−426	101	−524	C
ATOM	611	O	ARG A	104	67.673	66.097	113.234	1.00	17.80		O
ANISOU	611	O	ARG A	104	2167	3047	1550	−143	135	−284	O
ATOM	612	N	ARG A	104	64.987	67.225	115.281	1.00	18.37		N
ANISOU	612	N	ARG A	104	2522	2933	1523	−215	349	−197	N

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	613	CA	ARG A	104	66.385	66.830	115.106	1.00	19.14		C
ANISOU	613	CA	ARG A	104	2564	3213	1496	−84	83	−183	C
ATOM	614	C	ARG A	104	66.619	66.005	113.853	1.00	17.14		C
ANISOU	614	C	ARG A	104	2167	2919	1425	−338	159	−126	C
ATOM	615	CB	ARG A	104	66.836	66.009	116.312	1.00	26.16		C
ANISOU	615	CB	ARG A	104	3444	4974	1523	883	−139	62	C
ATOM	616	CG	ARG A	104	68.186	65.337	116.143	1.00	32.58		C
ANISOU	616	CG	ARG A	104	4231	6092	2055	1415	−467	249	C
ATOM	617	CD	ARG A	104	68.456	64.357	117.264	1.00	43.56		C
ANISOU	617	CD	ARG A	104	5603	7615	3334	1456	−429	598	C
ATOM	618	NE	ARG A	104	67.465	63.285	117.299	1.00	50.09		N
ANISOU	618	NE	ARG A	104	6396	8712	3925	1615	−537	468	N
ATOM	619	CZ	ARG A	104	67.672	62.059	116.832	1.00	52.21		C
ANISOU	619	CZ	ARG A	104	6792	8990	4056	1621	−521	386	C
ATOM	620	NH1	ARG A	104	68.840	61.739	116.289	1.00	52.44		N
ANISOU	620	NH1	ARG A	104	6927	9017	3982	1539	−468	439	N
ATOM	621	NH2	ARG A	104	66.709	61.149	116.908	1.00	50.96		N
ANISOU	621	NH2	ARG A	104	6677	8757	3929	1701	−569	575	N
ATOM	622	N	ASP A	105	65.656	65.158	113.516	1.00	17.04		N
ANISOU	622	N	ASP A	105	2326	3181	967	−339	202	−316	N
ATOM	623	CA	ASP A	105	65.801	64.283	112.363	1.00	15.90		C
ANISOU	623	CA	ASP A	105	2141	2691	1210	−349	224	−29	C
ATOM	624	C	ASP A	105	65.086	64.831	111.154	1.00	14.57		C
ANISOU	624	C	ASP A	105	1894	2359	1284	−205	173	−121	C
ATOM	625	O	ASP A	105	64.027	65.455	111.280	1.00	15.84		O
ANISOU	625	O	ASP A	105	1716	2919	1383	64	311	−209	O
ATOM	626	CB	ASP A	105	65.272	62.886	112.675	1.00	17.68		C
ANISOU	626	CB	ASP A	105	2521	2919	1278	−111	150	−39	C
ATOM	627	CG	ASP A	105	66.041	62.212	113.790	1.00	23.87		C
ANISOU	627	CG	ASP A	105	2847	4344	1878	−120	171	467	C
ATOM	628	OD1	ASP A	105	67.270	62.424	113.898	1.00	25.21		O
ANISOU	628	OD1	ASP A	105	3180	4770	1626	−9	49	616	O
ATOM	629	OD2	ASP A	105	65.407	61.466	114.560	1.00	28.54		O
ANISOU	629	OD2	ASP A	105	3737	4506	2600	−286	99	1368	O
ATOM	630	N	PHE A	106	65.675	64.566	109.987	1.00	13.84		N
ANISOU	630	N	PHE A	106	1942	2274	1040	−176	299	−381	N
ATOM	631	CA	PHE A	106	65.158	65.007	108.704	1.00	14.06		C
ANISOU	631	CA	PHE A	106	1954	2333	1055	−259	212	−306	C
ATOM	632	C	PHE A	106	65.202	63.831	107.744	1.00	14.26		C
ANISOU	632	C	PHE A	106	1884	2333	1203	−243	67	−317	C
ATOM	633	O	PHE A	106	66.201	63.118	107.676	1.00	17.69		O
ANISOU	633	O	PHE A	106	1819	2691	2212	389	−136	−752	O
ATOM	634	CB	PHE A	106	66.001	66.154	108.130	1.00	14.75		C
ANISOU	634	CB	PHE A	106	1894	2273	1436	26	278	−69	C
ATOM	635	CG	PHE A	106	66.058	67.372	109.018	1.00	14.13		C
ANISOU	635	CG	PHE A	106	1766	2134	1467	−60	325	−145	C
ATOM	636	CD1	PHE A	106	66.865	67.385	110.154	1.00	14.24		C
ANISOU	636	CD1	PHE A	106	1939	1908	1562	−177	434	−147	C
ATOM	637	CD2	PHE A	106	65.325	68.513	108.716	1.00	15.05		C
ANISOU	637	CD2	PHE A	106	1755	2257	1704	75	410	41	C
ATOM	638	CE1	PHE A	106	66.915	68.485	110.984	1.00	15.99		C
ANISOU	638	CE1	PHE A	106	2097	2131	1847	−151	213	100	C
ATOM	639	CE2	PHE A	106	65.389	69.634	109.535	1.00	16.71		C
ANISOU	639	CE2	PHE A	106	2220	2274	1854	−6	355	24	C
ATOM	640	CZ	PHE A	106	66.175	69.622	110.670	1.00	16.88		C
ANISOU	640	CZ	PHE A	106	2135	2293	1985	−167	324	−67	C
ATOM	641	N	HIS A	107	64.121	63.616	107.042	1.00	13.17		N
ANISOU	641	N	HIS A	107	1842	2409	754	−134	257	−121	N
ATOM	642	CA	HIS A	107	64.111	62.630	105.973	1.00	13.61		C
ANISOU	642	CA	HIS A	107	1835	2337	999	−219	324	69	C
ATOM	643	C	HIS A	107	64.532	63.257	104.650	1.00	12.32		C
ANISOU	643	C	HIS A	107	1682	1767	1232	110	285	−75	C
ATOM	644	O	HIS A	107	63.992	64.239	104.243	1.00	14.37		O
ANISOU	644	O	HIS A	107	1939	2092	1427	184	381	47	O
ATOM	645	CB	HIS A	107	62.735	62.005	105.804	1.00	15.09		C
ANISOU	645	CB	HIS A	107	1914	2649	1172	−367	537	−41	C
ATOM	646	CG	HIS A	107	62.480	60.891	106.751	1.00	16.86		C
ANISOU	646	CG	HIS A	107	1996	2904	1507	−597	512	−303	C
ATOM	647	ND1	HIS A	107	61.253	60.282	106.871	1.00	22.25		N
ANISOU	647	ND1	HIS A	107	2596	3704	2152	−792	577	217	N
ATOM	648	CD2	HIS A	107	63.305	60.260	107.602	1.00	17.79		C
ANISOU	648	CD2	HIS A	107	2702	2552	1506	−266	543	396	C
ATOM	649	CE1	HIS A	107	61.343	59.331	107.776	1.00	22.80		C
ANISOU	649	CE1	HIS A	107	3308	2978	2376	−745	389	402	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	650	NE2	HIS A	107	62.569	59.298	108.240	1.00	20.29		N
ANISOU	650	NE2	HIS A	107	2887	2781	2041	−632	392	104	N
ATOM	651	O	MET A	108	66.111	60.745	101.834	1.00	12.41		O
ANISOU	651	O	MET A	108	1913	1779	1024	6	−185	−42	O
ATOM	652	N	MET A	108	65.500	62.599	104.024	1.00	11.99		N
ANISOU	652	N	MET A	108	1573	1911	1071	−34	168	−23	N
ATOM	653	C	MET A	108	65.531	61.837	101.785	1.00	11.86		C
ANISOU	653	C	MET A	108	1543	1703	1260	−138	−35	93	C
ATOM	654	CA	AMET A	108	65.897	62.991	102.694	0.31	9.98		C
ANISOU	654	CA	AMET A	108	1420	1693	679	−182	283	−218	C
ATOM	655	CB	AMET A	108	67.369	63.364	102.695	0.31	11.01		C
ANISOU	655	CB	AMET A	108	1856	1622	707	313	128	−219	C
ATOM	656	CG	AMET A	108	67.561	64.586	103.573	0.31	11.16		C
ANISOU	656	CG	AMET A	108	1792	1815	632	31	238	−218	C
ATOM	657	SD	AMET A	108	69.236	65.170	103.793	0.31	11.68		S
ANISOU	657	SD	AMET A	108	1560	1813	1066	−148	50	−117	S
ATOM	658	CE	AMET A	108	68.935	66.784	104.501	0.31	13.36		C
ANISOU	658	CE	AMET A	108	2340	1343	1394	−257	392	7	C
ATOM	659	CA	BMET A	108	65.980	62.961	102.697	0.69	11.74		C
ANISOU	659	CA	BMET A	108	1508	1929	1025	−99	145	−18	C
ATOM	660	CB	BMET A	108	67.510	63.017	102.703	0.69	11.36		C
ANISOU	660	CB	BMET A	108	1464	1919	932	−137	−15	−0	C
ATOM	661	CG	BMET A	108	1819	1851	1401	0.69	13.35		C
ANISOU	661	CG	BMET A	108	67.708	64.851	104.737	−14	−68	−164	C
ATOM	662	SD	BMET A	108	2055	2065	1219	0.69	14.05		S
ANISOU	662	SD	BMET A	108	68.668	66.359	104.858	−165	155	−93	S
ATOM	663	CE	BMET A	108	2166	1900	1404	0.69	14.40		C
ANISOU	663	CE	BMET A	108	63.524	62.347	98.368	−477	−52	−276	C
ATOM	664	O	ASER A	109	63.524	62.347	98.368	0.46	13.09		O
ANISOU	664	O	ASER A	109	1510	1702	1761	−64	−206	550	O
ATOM	665	N	ASER A	109	64.481	62.066	101.006	0.46	13.22		N
ANISOU	665	N	ASER A	109	1401	2243	1378	−596	−76	297	N
ATOM	666	CA	ASER A	109	63.814	60.982	100.313	0.46	14.19		C
ANISOU	666	CA	ASER A	109	1532	2199	1660	−729	−387	316	C
ATOM	667	C	ASER A	109	63.777	61.232	98.823	0.46	15.86		C
ANISOU	667	C	ASER A	109	1881	2209	1935	−293	−523	315	C
ATOM	668	CB	ASER A	109	62.384	60.835	100.825	0.46	18.88		C
ANISOU	668	CB	ASER A	109	1932	3045	2197	−918	−420	384	C
ATOM	669	OG	ASER A	109	61.627	61.981	100.489	0.46	23.42		O
ANISOU	669	OG	ASER A	109	2235	4129	2534	−848	−302	383	O
ATOM	670	O	BSER A	109	63.893	62.301	98.210	0.54	14.06		O
ANISOU	670	O	BSER A	109	1871	2436	1035	−354	−16	−34	O
ATOM	671	N	BSER A	109	64.488	62.079	100.993	0.54	12.36		N
ANISOU	671	N	BSER A	109	1967	1671	1056	320	−262	−67	N
ATOM	672	CA	BSER A	109	63.865	61.002	100.229	0.54	13.66		C
ANISOU	672	CA	BSER A	109	2146	1688	1357	−49	−261	−97	C
ATOM	673	C	BSER A	109	63.959	61.185	98.719	0.54	12.08		C
ANISOU	673	C	BSER A	109	1760	1787	1043	−554	−173	82	C
ATOM	674	CB	BSER A	109	62.395	60.845	100.629	0.54	15.41		C
ANISOU	674	CB	BSER A	109	2028	2475	1351	−126	−44	530	C
ATOM	675	OG	BSER A	109	62.275	60.525	102.005	0.54	14.24		O
ANISOU	675	OG	BSER A	109	1704	2365	1343	−572	−47	288	O
ATOM	676	N	AVAL A	110	64.025	60.178	98.063	0.46	14.13		N
ANISOU	676	N	AVAL A	110	2189	1495	1685	−252	−781	−248	N
ATOM	677	CA	AVAL A	110	63.842	60.235	96.629	0.46	13.87		C
ANISOU	677	CA	AVAL A	110	1818	1975	1475	−693	−507	−150	C
ATOM	678	C	AVAL A	110	62.783	59.221	96.233	0.46	16.24		C
ANISOU	678	C	AVAL A	110	2276	2379	1515	−186	−521	−271	C
ATOM	679	O	AVAL A	110	62.760	58.086	96.710	0.46	15.75		O
ANISOU	679	O	AVAL A	110	2184	2287	1512	−353	−623	−124	O
ATOM	680	CB	AVAL A	110	65.153	59.981	95.871	0.46	14.17		C
ANISOU	680	CB	AVAL A	110	1908	1950	1528	−628	−360	−91	C
ATOM	681	CG1	AVAL A	110	65.725	58.620	96.231	0.46	15.64		C
ANISOU	681	CG1	AVAL A	110	1827	2141	1976	33	−239	−186	C
ATOM	682	CG2	AVAL A	110	64.935	60.110	94.367	0.46	14.09		C
ANISOU	682	CG2	AVAL A	110	2312	1705	1339	−763	−445	−16	C
ATOM	683	N	BVAL A	110	64.107	60.064	98.020	0.54	16.27		N
ANISOU	683	N	BVAL A	110	2723	2252	1207	−353	−393	40	N
ATOM	684	CA	BVAL A	110	63.987	60.007	96.570	0.54	17.67		C
ANISOU	684	CA	BVAL A	110	3012	2291	1409	22	−458	211	C
ATOM	685	C	BVAL A	110	62.749	59.177	96.257	0.54	15.31		C
ANISOU	685	C	BVAL A	110	2567	2018	1230	−464	−274	200	C
ATOM	686	O	BVAL A	110	62.572	58.100	96.821	0.54	16.94		O
ANISOU	686	O	BVAL A	110	2820	2028	1589	−420	−467	90	O

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	687	CB	BVAL A	110	65.197	59.286	95.926	0.54	18.85		C
ANISOU	687	CB	BVAL A	110	3031	2399	1733	−1070	−352	−34	C
ATOM	688	CG1	BVAL A	110	65.085	59.302	94.408	0.54	20.93		C
ANISOU	688	CG1	BVAL A	110	3622	2405	1925	−873	48	306	C
ATOM	689	CG2	BVAL A	110	66.514	59.895	96.374	0.54	27.75		C
ANISOU	689	CG2	BVAL A	110	4208	3504	2832	−400	−383	−73	C
ATOM	690	O	VAL A	111	61.952	58.746	92.749	1.00	16.30		O
ANISOU	690	O	VAL A	111	2339	2657	1196	−449	−226	−114	O
ATOM	691	N	VAL A	111	61.893	59.655	95.359	1.00	14.94		N
ANISOU	691	N	VAL A	111	1920	2579	1175	−404	−188	111	N
ATOM	692	C	VAL A	111	61.218	58.161	93.547	1.00	15.49		C
ANISOU	692	C	VAL A	111	1886	2665	1332	−439	−234	293	C
ATOM	693	CA	AVAL A	111	60.815	58.816	94.868	0.20	16.52		C
ANISOU	693	CA	AVAL A	111	1946	2767	1565	−566	−386	51	C
ATOM	694	CB	AVAL A	111	59.507	59.636	94.710	0.20	17.33		C
ANISOU	694	CB	AVAL A	111	1923	2957	1705	−241	−956	−331	C
ATOM	695	CG1	AVAL A	111	59.563	60.531	93.482	0.20	17.31		C
ANISOU	695	CG1	AVAL A	111	1995	2786	1794	212	−1057	−308	C
ATOM	696	CG2	AVAL A	111	58.298	58.729	94.641	0.20	21.58		C
ANISOU	696	CG2	AVAL A	111	2345	3687	2167	−367	−934	−421	C
ATOM	697	CA	BVAL A	111	60.826	58.804	94.863	0.80	16.66		C
ANISOU	697	CA	BVAL A	111	1976	3204	1148	−368	226	118	C
ATOM	698	CB	BVAL A	111	59.496	59.550	94.714	0.80	23.34		C
ANISOU	698	CB	BVAL A	111	2542	4811	1516	36	405	−152	C
ATOM	699	CG1	BVAL A	111	58.921	59.840	96.071	0.80	24.86		C
ANISOU	699	CG1	BVAL A	111	2781	5029	1638	670	286	−652	C
ATOM	700	CG2	BVAL A	111	59.686	60.837	93.958	0.80	28.83		C
ANISOU	700	CG2	BVAL A	111	3727	5261	1965	846	414	19	C
ATOM	701	N	ARG A	112	60.737	56.940	93.346	1.00	17.54		N
ANISOU	701	N	ARG A	112	1933	2425	2304	−250	−66	57	N
ATOM	702	CA	ARG A	112	60.950	56.185	92.126	1.00	20.77		C
ANISOU	702	CA	ARG A	112	2284	3024	2584	−132	−533	−363	C
ATOM	703	C	ARG A	112	62.422	56.147	91.753	1.00	16.79		C
ANISOU	703	C	ARG A	112	1871	2671	1837	−501	−302	48	C
ATOM	704	O	ARG A	112	62.837	56.635	90.691	1.00	19.07		O
ANISOU	704	O	ARG A	112	2796	2615	1834	−85	−473	−36	O
ATOM	705	CB	ARG A	112	60.115	56.765	90.994	1.00	21.77		C
ANISOU	705	CB	ARG A	112	2242	3200	2831	−32	−822	−806	C
ATOM	706	CG	ARG A	112	59.864	55.757	89.898	1.00	29.72		C
ANISOU	706	CG	ARG A	112	3768	3934	3592	518	−937	−878	C
ATOM	707	CD	ARG A	112	58.893	56.257	88.855	1.00	27.60		C
ANISOU	707	CD	ARG A	112	3707	3393	3389	−461	−924	−563	C
ATOM	708	NE	ARG A	112	58.584	55.192	87.912	1.00	27.35		N
ANISOU	708	NE	ARG A	112	3366	3631	3394	−952	−705	236	N
ATOM	709	CZ	ARG A	112	57.782	55.334	86.867	1.00	24.16		C
ANISOU	709	CZ	ARG A	112	2973	3152	3055	−1031	−555	768	C
ATOM	710	NH1	ARG A	112	57.218	56.510	86.619	1.00	25.29		N
ANISOU	710	NH1	ARG A	112	2961	3236	3412	−420	−598	748	N
ATOM	711	NH2	ARG A	112	57.556	54.303	86.065	1.00	26.18		N
ANISOU	711	NH2	ARG A	112	3477	3147	3323	−911	−800	374	N
ATOM	712	N	ALA A	113	63.213	55.581	92.651	1.00	16.27		N
ANISOU	712	N	ALA A	113	2134	2413	1635	−181	−171	190	N
ATOM	713	CA	ALA A	113	64.651	55.489	92.474	1.00	14.95		C
ANISOU	713	CA	ALA A	113	1739	2638	1304	−351	60	−50	C
ATOM	714	C	ALA A	113	64.989	54.748	91.191	1.00	16.73		C
ANISOU	714	C	ALA A	113	2521	2389	1445	−300	−83	−84	C
ATOM	715	O	ALA A	113	64.373	53.740	90.856	1.00	17.71		O
ANISOU	715	O	ALA A	113	2456	2409	1864	−287	86	−300	O
ATOM	716	CB	ALA A	113	65.248	54.781	93.645	1.00	16.82		C
ANISOU	716	CB	ALA A	113	2237	2998	1155	−96	−120	283	C
ATOM	717	CD	AARG A	114	66.096	58.022	87.181	0.47	22.28		C
ANISOU	717	CD	AARG A	114	4380	2235	1851	586	−454	157	C
ATOM	718	NE	AARG A	114	66.807	59.283	87.375	0.47	29.21		N
ANISOU	718	NE	AARG A	114	5121	3878	2099	561	−435	−201	N
ATOM	719	CZ	AARG A	114	66.843	60.280	86.494	0.47	29.18		C
ANISOU	719	CZ	AARG A	114	4935	4185	1969	858	−468	−157	C
ATOM	720	NH1	AARG A	114	66.210	60.173	85.334	0.47	29.51		N
ANISOU	720	NH1	AARG A	114	4913	4547	1753	313	−347	−156	N
ATOM	721	NH2	AARG A	114	67.522	61.386	86.774	0.47	28.86		N
ANISOU	721	NH2	AARG A	114	4808	4083	2075	829	−48	558	N
ATOM	722	N	AARG A	114	65.946	55.280	90.442	0.47	16.78		N
ANISOU	722	N	AARG A	114	2381	2769	1224	−787	270	−73	N
ATOM	723	CA	AARG A	114	66.390	54.651	89.200	0.47	19.86		C
ANISOU	723	CA	AARG A	114	2775	3432	1339	−871	146	−279	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	724	C	AARG A	114	67.841	54.207	89.358	0.47	19.32		C
ANISOU	724	C	AARG A	114	2730	3222	1387	−997	295	−279	C
ATOM	725	O	AARG A	114	68.543	54.707	90.237	0.47	16.91		O
ANISOU	725	O	AARG A	114	2646	2777	1005	−1122	254	−149	O
ATOM	726	CB	AARG A	114	66.215	55.607	88.011	0.47	23.44		C
ANISOU	726	CB	AARG A	114	3530	3302	2075	−1037	−16	3	C
ATOM	727	CG	AARG A	114	66.342	57.080	88.367	0.47	23.11		C
ANISOU	727	CG	AARG A	114	4394	2386	2001	231	−111	141	C
ATOM	728	CD	BARG A	114	65.114	56.925	86.490	0.53	29.64		C
ANISOU	728	CD	BARG A	114	3805	3936	3521	−303	449	68	C
ATOM	729	NE	BARG A	114	66.154	57.921	86.261	0.53	32.49		N
ANISOU	729	NE	BARG A	114	4232	4250	3861	−576	603	147	N
ATOM	730	CZ	BARG A	114	66.103	59.153	86.745	0.53	32.81		C
ANISOU	730	CZ	BARG A	114	3897	4956	3612	−1041	762	−157	C
ATOM	731	NH1	BARG A	114	65.074	59.522	87.485	0.53	39.73		N
ANISOU	731	NH1	BARG A	114	4650	6253	4193	−258	742	−234	N
ATOM	732	NH2	BARG A	114	67.081	60.011	86.501	0.53	25.77		N
ANISOU	732	NH2	BARG A	114	2917	4047	2826	−1934	578	−651	N
ATOM	733	N	BARG A	114	66.001	55.255	90.500	0.53	16.92		N
ANISOU	733	N	BARG A	114	2241	2872	1315	139	77	−334	N
ATOM	734	CA	BARG A	114	66.468	54.674	89.253	0.53	17.25		C
ANISOU	734	CA	BARG A	114	2322	3159	1073	476	214	−544	C
ATOM	735	C	BARG A	114	67.857	54.110	89.449	0.53	16.74		C
ANISOU	735	C	BARG A	114	2648	2541	1171	561	63	−720	C
ATOM	736	O	BARG A	114	68.547	54.452	90.410	0.53	17.00		O
ANISOU	736	O	BARG A	114	2578	2603	1279	390	−260	−456	O
ATOM	737	CB	BARG A	114	66.513	55.740	88.170	0.53	20.12		C
ANISOU	737	CB	BARG A	114	2607	3562	1477	550	368	−166	C
ATOM	738	CG	BARG A	114	65.175	56.371	87.896	0.53	25.17		C
ANISOU	738	CG	BARG A	114	3311	3704	2547	563	254	−46	C
ATOM	739	N	ARG A	115	68.281	53.258	88.526	1.00	19.29		N
ANISOU	739	N	ARG A	115	2678	3110	1540	−304	184	−771	N
ATOM	740	C	ARG A	115	70.647	53.879	88.645	1.00	16.53		C
ANISOU	740	C	ARG A	115	2755	2243	1284	−43	−86	−389	C
ATOM	741	O	ARG A	115	71.625	53.814	89.385	1.00	16.80		O
ANISOU	741	O	ARG A	115	2692	2558	1135	112	−127	−273	O
ATOM	742	CA	ARG A	115	69.646	52.739	88.581	1.00	18.24		C
ANISOU	742	CA	ARG A	115	2510	2720	1702	5	242	−904	C
ATOM	743	CB	ARG A	115	69.929	51.864	87.361	1.00	23.65		C
ANISOU	743	CB	ARG A	115	3131	3699	2158	292	46	−1078	C
ATOM	744	N	AASN A	116	70.383	54.934	87.887	0.36	15.37		N
ANISOU	744	N	AASN A	116	2565	2465	809	−172	−236	−368	N
ATOM	745	CA	AASN A	116	71.305	56.057	87.815	0.36	16.82		C
ANISOU	745	CA	AASN A	116	2921	2698	770	59	−152	−155	C
ATOM	746	C	AASN A	116	71.206	57.040	88.995	0.36	18.02		C
ANISOU	746	C	AASN A	116	2819	2812	1218	−441	126	−54	C
ATOM	747	O	AASN A	116	71.856	58.087	88.973	0.36	24.62		O
ANISOU	747	O	AASN A	116	3748	3859	1746	−150	506	47	O
ATOM	748	CB	AASN A	116	71.164	56.762	86.468	0.36	21.29		C
ANISOU	748	CB	AASN A	116	3591	3452	1045	549	−189	14	C
ATOM	749	CG	AASN A	116	69.749	57.111	86.163	0.36	21.89		C
ANISOU	749	CG	AASN A	116	3534	3523	1262	896	−478	77	C
ATOM	750	OD1	AASN A	116	69.040	57.593	87.031	0.36	21.41		O
ANISOU	750	OD1	AASN A	116	3203	3596	1336	1271	−19	439	O
ATOM	751	ND2	AASN A	116	69.310	56.843	84.942	0.36	23.62		N
ANISOU	751	ND2	AASN A	116	3873	3279	1823	192	−720	−107	N
ATOM	752	N	BASN A	116	70.353	54.916	87.869	0.64	17.08		N
ANISOU	752	N	BASN A	116	2786	2699	1005	−88	59	−187	N
ATOM	753	CA	BASN A	116	71.208	56.094	87.775	0.64	15.60		C
ANISOU	753	CA	BASN A	116	2635	2608	687	43	70	−37	C
ATOM	754	C	BASN A	116	71.256	56.972	89.038	0.64	13.42		C
ANISOU	754	C	BASN A	116	2121	2074	903	27	412	5	C
ATOM	755	O	BASN A	116	71.996	57.902	89.081	0.64	16.21		O
ANISOU	755	O	BASN A	116	2371	2484	1303	−334	600	−90	O
ATOM	756	CB	BASN A	116	70.812	57.080	86.651	0.64	22.22		C
ANISOU	756	CB	BASN A	116	3469	3707	1266	−333	−266	87	C
ATOM	757	CG	BASN A	116	70.430	56.447	85.356	0.64	25.18		C
ANISOU	757	CG	BASN A	116	4094	3742	1733	61	−123	279	C
ATOM	758	OD1	BASN A	116	71.115	56.674	84.383	0.64	25.75		O
ANISOU	758	OD1	BASN A	116	3866	4047	1872	604	417	344	O
ATOM	759	ND2	BASN A	116	69.305	55.736	85.307	0.64	22.01		N
ANISOU	759	ND2	BASN A	116	3700	3679	984	3	−225	247	N
ATOM	760	N	ASP A	117	70.398	56.707	90.008	1.00	14.41		N
ANISOU	760	N	ASP A	117	2158	2458	859	6	−56	−46	N

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	761	CA	ASP A	117	70.468	57.377	91.314	1.00	13.50		C
ANISOU	761	CA	ASP A	117	1970	2283	875	42	−32	−109	C
ATOM	762	C	ASP A	117	71.553	56.760	92.202	1.00	14.25		C
ANISOU	762	C	ASP A	117	1941	2161	1311	−89	95	−272	C
ATOM	763	O	ASP A	117	71.884	57.308	93.253	1.00	14.60		O
ANISOU	763	O	ASP A	117	2149	2316	1084	−47	−48	−425	O
ATOM	764	CB	ASP A	117	69.129	57.312	92.034	1.00	14.55		C
ANISOU	764	CB	ASP A	117	1989	2329	1212	42	117	−107	C
ATOM	765	CG	ASP A	117	68.074	58.194	91.396	1.00	14.39		C
ANISOU	765	CG	ASP A	117	2112	2028	1329	−159	176	−115	C
ATOM	766	OD1	ASP A	117	68.389	59.322	90.957	1.00	16.30		O
ANISOU	766	OD1	ASP A	117	2380	2449	1365	−26	−72	−54	O
ATOM	767	OD2	ASP A	117	66.908	57.774	91.385	1.00	17.53		O
ANISOU	767	OD2	ASP A	117	2155	2599	1906	−237	−77	−95	O
ATOM	768	N	SER A	118	72.099	55.613	91.813	1.00	13.49		N
ANISOU	768	N	SER A	118	1842	2339	944	−93	6	−177	N
ATOM	769	CA	SER A	118	73.164	55.007	92.598	1.00	13.65		C
ANISOU	769	CA	SER A	118	1990	2268	927	−214	6	−237	C
ATOM	770	C	SER A	118	74.331	55.971	92.703	1.00	12.92		C
ANISOU	770	C	SER A	118	2080	2062	765	28	36	−149	C
ATOM	771	O	SER A	118	74.718	56.591	91.719	1.00	15.69		O
ANISOU	771	O	SER A	118	2329	2706	927	−261	170	−129	O
ATOM	772	CB	SER A	118	73.639	53.703	91.961	1.00	14.99		C
ANISOU	772	CB	SER A	118	2105	2183	1407	−208	95	−430	C
ATOM	773	OG	SER A	118	72.591	52.757	91.905	1.00	15.64		O
ANISOU	773	OG	SER A	118	2312	2256	1373	−173	160	−360	O
ATOM	774	N	GLY A	119	74.885	56.101	93.900	1.00	12.77		N
ANISOU	774	N	GLY A	119	1890	2033	929	84	21	−288	N
ATOM	775	CA	GLY A	119	75.997	57.014	94.099	1.00	13.83		C
ANISOU	775	CA	GLY A	119	1890	2380	986	−233	14	−398	C
ATOM	776	C	GLY A	119	76.126	57.368	95.558	1.00	12.67		C
ANISOU	776	C	GLY A	119	1542	2194	1077	125	199	−49	C
ATOM	777	O	GLY A	119	75.591	56.685	96.421	1.00	14.12		O
ANISOU	777	O	GLY A	119	2112	2263	989	−113	−31	−249	O
ATOM	778	N	THR A	120	76.858	58.434	95.841	1.00	13.23		N
ANISOU	778	N	THR A	120	1669	2124	1236	14	152	−166	N
ATOM	779	CA	THR A	120	77.013	58.848	97.225	1.00	13.66		C
ANISOU	779	CA	THR A	120	1751	2209	1232	352	−268	−518	C
ATOM	780	C	THR A	120	76.419	60.219	97.444	1.00	12.85		C
ANISOU	780	C	THR A	120	1865	1759	1259	12	−232	−14	C
ATOM	781	O	THR A	120	76.339	61.058	96.542	1.00	13.74		O
ANISOU	781	O	THR A	120	1899	2053	1268	162	233	−168	O
ATOM	782	CB	THR A	120	78.435	58.821	97.752	1.00	18.06		C
ANISOU	782	CB	THR A	120	2271	2318	2275	492	27	−383	C
ATOM	783	OG1	THR A	120	79.208	59.751	97.008	1.00	18.48		O
ANISOU	783	OG1	THR A	120	2013	2529	2480	132	414	118	O
ATOM	784	CG2	THR A	120	79.016	57.434	97.676	1.00	20.53		C
ANISOU	784	CG2	THR A	120	2335	2792	2672	680	−247	−548	C
ATOM	785	N	TYR A	121	75.985	60.404	98.674	1.00	12.14		N
ANISOU	785	N	TYR A	121	1649	2006	958	63	32	−140	N
ATOM	786	CA	TYR A	121	75.174	61.527	99.065	1.00	12.31		C
ANISOU	786	CA	TYR A	121	1697	2116	865	343	20	−277	C
ATOM	787	C	TYR A	121	75.660	61.997	100.427	1.00	12.33		C
ANISOU	787	C	TYR A	121	1797	1900	990	179	73	178	C
ATOM	788	O	TYR A	121	76.284	61.230	101.167	1.00	13.90		O
ANISOU	788	O	TYR A	121	2072	1916	1294	214	−362	−104	O
ATOM	789	CB	TYR A	121	73.709	61.089	99.184	1.00	13.05		C
ANISOU	789	CB	TYR A	121	1660	2354	945	100	2	−139	C
ATOM	789	CG	TYR A	121	73.073	60.674	97.880	1.00	11.72		C
ANISOU	790	CG	TYR A	121	1673	1953	827	98	89	−65	C
ATOM	791	CD1	TYR A	121	73.308	59.416	97.319	1.00	13.22		C
ANISOU	791	CD1	TYR A	121	1739	2157	1128	24	169	68	C
ATOM	792	CD2	TYR A	121	72.231	61.542	97.208	1.00	13.26		C
ANISOU	792	CD2	TYR A	121	1977	2118	944	348	−95	−79	C
ATOM	793	CE1	TYR A	121	72.739	59.051	96.108	1.00	13.76		C
ANISOU	793	CE1	TYR A	121	1746	2072	1410	−86	90	−5	C
ATOM	794	CE2	TYR A	121	71.631	61.180	96.020	1.00	14.01		C
ANISOU	794	CE2	TYR A	121	2416	2145	761	257	−268	−233	C
ATOM	795	CZ	TYR A	121	71.888	59.940	95.475	1.00	13.00		C
ANISOU	795	CZ	TYR A	121	2198	1939	802	36	42	10	C
ATOM	796	OH	TYR A	121	71.300	59.627	94.271	1.00	14.81		O
ANISOU	796	OH	TYR A	121	2323	2303	1000	145	−199	−175	O
ATOM	797	N	LEU A	122	75.333	63.226	100.794	1.00	13.07		N
ANISOU	797	N	LEU A	122	1854	2115	997	277	−6	−236	N

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	798	CA	LEU A	122	75.613	63.680	102.146	1.00	13.79		C
ANISOU	798	CA	LEU A	122	1625	2261	1355	437	−160	−259	C
ATOM	799	C	LEU A	122	74.654	64.803	102.494	1.00	12.48		C
ANISOU	799	C	LEU A	122	1496	2110	1135	199	−134	−51	C
ATOM	800	O	LEU A	122	73.943	65.314	101.631	1.00	13.74		O
ANISOU	800	O	LEU A	122	1851	2278	1093	439	−119	−42	O
ATOM	801	CB	LEU A	122	77.067	64.116	102.333	1.00	16.34		C
ANISOU	801	CB	LEU A	122	1875	2279	2056	136	−83	−216	C
ATOM	802	CG	LEU A	122	77.649	65.347	101.648	1.00	20.27		C
ANISOU	802	CG	LEU A	122	2556	2935	2209	351	769	23	C
ATOM	803	CD1	LEU A	122	77.256	66.677	102.284	1.00	23.23		C
ANISOU	803	CD1	LEU A	122	3633	2394	2800	−118	−62	−81	C
ATOM	804	CD2	LEU A	122	79.158	65.205	101.742	1.00	24.56		C
ANISOU	804	CD2	LEU A	122	2716	3908	2710	203	452	−623	C
ATOM	805	N	CYS A	123	74.639	65.163	103.769	1.00	12.47		N
ANISOU	805	N	CYS A	123	1827	1792	1119	216	−110	−148	N
ATOM	806	C	CYS A	123	74.842	67.350	104.740	1.00	13.20		C
ANISOU	806	C	CYS A	123	1597	1955	1463	95	−204	−288	C
ATOM	807	O	CYS A	123	75.865	67.021	105.363	1.00	16.98		O
ANISOU	807	O	CYS A	123	1948	2177	2327	43	−675	−251	O
ATOM	808	CA	ACYS A	123	73.860	66.264	104.293	0.35	12.80		C
ANISOU	808	CA	ACYS A	123	1553	1897	1413	−5	−276	−173	C
ATOM	809	CB	ACYS A	123	73.080	65.736	105.492	0.35	16.64		C
ANISOU	809	CB	ACYS A	123	2030	2679	1614	375	−92	−583	C
ATOM	810	SG	ACYS A	123	72.063	66.905	106.359	0.35	19.14		S
ANISOU	810	SG	ACYS A	123	1808	3384	2080	388	−212	−661	S
ATOM	811	CA	BCYS A	123	73.888	66.342	104.155	0.65	12.35		C
ANISOU	811	CA	BCYS A	123	1942	1522	1230	361	15	−270	C
ATOM	812	CB	BCYS A	123	72.694	66.057	105.078	0.65	13.85		C
ANISOU	812	CB	BCYS A	123	1967	1926	1369	342	113	−135	C
ATOM	813	SG	BCYS A	123	73.068	65.330	106.668	0.65	14.15		S
ANISOU	813	SG	BCYS A	123	2056	2123	1198	132	−170	−279	S
ATOM	814	N	GLY A	124	74.546	68.611	104.471	1.00	13.98		N
ANISOU	814	N	GLY A	124	1932	1679	1699	68	−247	−399	N
ATOM	815	CA	GLY A	124	75.409	69.685	104.912	1.00	15.36		C
ANISOU	815	CA	GLY A	124	1979	1824	2033	149	−131	−384	C
ATOM	816	C	GLY A	124	74.597	70.727	105.640	1.00	14.07		C
ANISOU	816	C	GLY A	124	1920	1640	1786	112	−70	−99	C
ATOM	817	O	GLY A	124	73.558	71.153	105.141	1.00	16.05		O
ANISOU	817	O	GLY A	124	2049	2285	1762	432	−319	−359	O
ATOM	818	N	ALA A	125	75.056	71.118	106.823	1.00	14.15		N
ANISOU	818	N	ALA A	125	1956	1798	1621	−21	−295	−273	N
ATOM	819	CA	ALA A	125	74.405	72.152	107.612	1.00	15.07		C
ANISOU	819	CA	ALA A	125	2232	1776	1717	72	−71	−359	C
ATOM	820	C	ALA A	125	75.128	73.467	107.417	1.00	14.80		C
ANISOU	820	C	ALA A	125	2075	1672	1875	−27	−158	−353	C
ATOM	821	O	ALA A	125	76.351	73.524	107.514	1.00	17.95		O
ANISOU	821	O	ALA A	125	2024	1995	2802	−176	−410	−185	O
ATOM	822	CB	ALA A	125	74.405	71.776	109.087	1.00	17.33		C
ANISOU	822	CB	ALA A	125	2696	2349	1539	−105	−220	−144	C
ATOM	823	N	ILE A	126	74.369	74.517	107.143	1.00	14.25		N
ANISOU	823	N	ILE A	126	2188	1679	1547	−111	−76	−237	N
ATOM	824	CA	ILE A	126	74.917	75.850	106.988	1.00	14.83		C
ANISOU	824	CA	ILE A	126	2188	1996	1452	−8	−211	−135	C
ATOM	825	C	ILE A	126	74.382	76.719	108.098	1.00	15.65		C
ANISOU	825	C	ILE A	126	2310	1888	1749	27	−271	−137	C
ATOM	826	O	ILE A	126	73.171	76.924	108.203	1.00	15.71		O
ANISOU	826	O	ILE A	126	2271	2056	1644	−23	1	−290	O
ATOM	827	CB	ILE A	126	74.489	76.464	105.651	1.00	16.21		C
ANISOU	827	CB	ILE A	126	2431	2163	1566	−85	−47	85	C
ATOM	828	CG1	ILE A	126	74.933	75.566	104.496	1.00	19.33		C
ANISOU	828	CG1	ILE A	126	2837	3063	1445	53	−65	−255	C
ATOM	829	CG2	ILE A	126	75.095	77.838	105.490	1.00	18.36		C
ANISOU	829	CG2	ILE A	126	2881	2294	1801	−127	−215	152	C
ATOM	830	CD1	ILE A	126	74.276	75.888	103.175	1.00	24.69		C
ANISOU	830	CD1	ILE A	126	3413	4262	1705	−205	−124	−445	C
ATOM	831	N	SER A	127	75.275	77.201	108.948	1.00	16.52		N
ANISOU	831	N	SER A	127	2502	1703	2073	77	−398	−385	N
ATOM	832	C	SER A	127	74.814	79.540	109.297	1.00	19.59		C
ANISOU	832	C	SER A	127	2975	1877	2592	−60	65	−491	C
ATOM	833	O	SER A	127	75.710	79.923	108.535	1.00	22.57		O
ANISOU	833	O	SER A	127	2996	2333	3247	−467	230	−553	O
ATOM	834	CA	ASER A	127	74.905	78.177	109.959	0.45	20.72		C
ANISOU	834	CA	ASER A	127	3014	2320	2538	79	−393	−382	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	835	CB	ASER A	127	75.953	78.222	111.068	0.45	21.55		C
ANISOU	835	CB	ASER A	127	2952	2825	2411	−478	−634	−91	C
ATOM	836	OG	ASER A	127	77.183	78.726	110.573	0.45	21.36		O
ANISOU	836	OG	ASER A	127	3177	2582	2356	−502	−724	−36	O
ATOM	837	CA	BSER A	127	74.877	78.170	109.951	0.55	17.42		C
ANISOU	837	CA	BSER A	127	2728	1958	1934	328	−604	−768	C
ATOM	838	CB	BSER A	127	75.847	78.178	111.134	0.55	23.22		C
ANISOU	838	CB	BSER A	127	3309	3423	2093	28	−862	−1064	C
ATOM	839	OG	BSER A	127	75.401	79.056	112.153	0.55	27.03		O
ANISOU	839	OG	BSER A	127	3908	4035	2329	294	−832	−1451	O
ATOM	840	O	LEU A	128	74.050	83.859	109.583	1.00	26.89		O
ANISOU	840	O	LEU A	128	4259	2209	3748	−286	−696	−18	O
ATOM	841	N	LEU A	128	73.745	80.271	109.581	1.00	19.17		N
ANISOU	841	N	LEU A	128	3119	1801	2364	45	−196	−380	N
ATOM	842	CA	LEU A	128	73.585	81.582	108.994	1.00	21.02		C
ANISOU	842	CA	LEU A	128	3686	1656	2646	−11	33	−217	C
ATOM	843	C	LEU A	128	74.001	82.694	109.962	1.00	24.21		C
ANISOU	843	C	LEU A	128	4035	1901	3263	31	−36	−130	C
ATOM	844	CB	LEU A	128	72.150	81.757	108.525	1.00	19.79		C
ANISOU	844	CB	LEU A	128	3864	1670	1983	116	−2	−101	C
ATOM	845	CG	LEU A	128	71.735	80.768	107.437	1.00	19.99		C
ANISOU	845	CG	LEU A	128	3926	2051	1617	296	187	320	C
ATOM	846	CD1	LEU A	128	70.253	80.928	107.162	1.00	22.41		C
ANISOU	846	CD1	LEU A	128	4228	2414	1875	−136	−290	−42	C
ATOM	847	CD2	LEU A	128	72.556	80.951	106.161	1.00	24.98		C
ANISOU	847	CD2	LEU A	128	4312	3193	1986	597	103	378	C
ATOM	848	N	ALA A	129	74.328	82.313	111.197	1.00	24.94		N
ANISOU	848	N	ALA A	129	3926	2291	3261	−307	−73	−713	N
ATOM	849	CA	ALA A	129	74.789	83.235	112.234	1.00	30.35		C
ANISOU	849	CA	ALA A	129	4517	3113	3902	−95	−405	−882	C
ATOM	850	C	ALA A	129	75.338	82.423	113.412	1.00	30.47		C
ANISOU	850	C	ALA A	129	4703	2926	3947	−673	−840	−737	C
ATOM	851	O	ALA A	129	74.948	81.274	113.604	1.00	34.23		O
ANISOU	851	O	ALA A	129	4945	3845	4217	−1048	−331	−432	O
ATOM	852	CB	ALA A	129	73.648	84.129	112.687	1.00	31.92		C
ANISOU	852	CB	ALA A	129	4856	3348	3925	216	−175	−959	C
ATOM	853	O	PRO A	130	78.183	85.428	112.388	1.00	47.91		O
ANISOU	853	O	PRO A	130	8160	3729	6314	−716	−868	−970	O
ATOM	854	N	PRO A	130	76.258	83.005	114.203	1.00	40.27		N
ANISOU	854	N	PRO A	130	6003	4354	4945	−1014	−1393	−1001	N
ATOM	855	CA	PRO A	130	76.865	84.334	114.057	1.00	39.87		C
ANISOU	855	CA	PRO A	130	6281	3919	4950	−991	−1368	−1609	C
ATOM	856	C	PRO A	130	77.898	84.367	112.937	1.00	48.18		C
ANISOU	856	C	PRO A	130	7481	4483	6342	−757	−1106	−1180	C
ATOM	857	CB	PRO A	130	77.542	84.555	115.411	1.00	44.09		C
ANISOU	857	CB	PRO A	130	6803	4743	5204	−614	−1648	−1698	C
ATOM	858	CG	PRO A	130	77.852	83.187	115.894	1.00	42.21		C
ANISOU	858	CG	PRO A	130	6661	4386	4989	−755	−1733	−1537	C
ATOM	859	CD	PRO A	130	76.714	82.330	115.431	1.00	40.64		C
ANISOU	859	CD	PRO A	130	6069	4508	4865	−1218	−1748	−1134	C
ATOM	860	O	LYS A	131	78.197	81.120	110.815	1.00	43.67		O
ANISOU	860	O	LYS A	131	5793	4637	6164	−1021	−1211	−610	O
ATOM	861	N	LYS A	131	78.451	83.207	112.606	1.00	43.55		N
ANISOU	861	N	LYS A	131	6157	4263	6129	−1307	−1163	−860	N
ATOM	862	CA	LYS A	131	79.371	83.097	111.485	1.00	47.77		C
ANISOU	862	CA	LYS A	131	6227	5224	6700	−898	−1163	−802	C
ATOM	863	C	LYS A	131	78.793	82.136	110.458	1.00	39.78		C
ANISOU	863	C	LYS A	131	5208	4011	5894	−779	−1179	−607	C
ATOM	864	CB	LYS A	131	80.743	82.611	111.953	1.00	49.12		C
ANISOU	864	CB	LYS A	131	6057	5704	6901	−1072	−1087	−814	C
ATOM	865	N	VAL A	132	78.955	82.465	109.184	1.00	29.62		N
ANISOU	865	N	VAL A	132	3527	2782	4945	−791	−1052	−86	N
ATOM	866	CA	VAL A	132	78.487	81.597	108.118	1.00	26.03		C
ANISOU	866	CA	VAL A	132	3039	2262	4590	−524	−1158	439	C
ATOM	867	C	VAL A	132	79.498	80.490	107.882	1.00	26.40		C
ANISOU	867	C	VAL A	132	2871	2419	4740	−606	−794	146	C
ATOM	868	O	VAL A	132	80.650	80.738	107.549	1.00	29.54		O
ANISOU	868	O	VAL A	132	3043	2876	5305	−520	−479	284	O
ATOM	869	CB	VAL A	132	78.262	82.379	106.820	1.00	29.44		C
ANISOU	869	CB	VAL A	132	3636	2818	4731	−703	−1156	929	C
ATOM	870	CG1	VAL A	132	77.820	81.442	105.711	1.00	31.93		C
ANISOU	870	CG1	VAL A	132	3690	3734	4707	−852	−1452	549	C
ATOM	871	CG2	VAL A	132	77.241	83.470	107.044	1.00	31.15		C
ANISOU	871	CG2	VAL A	132	3843	3001	4990	−573	−1332	831	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	872	N	GLN A	133	79.062	79.256	108.071	1.00	26.20		N
ANISOU	872	N	GLN A	133	3052	2153	4751	−297	−670	179	N
ATOM	873	C	GLN A	133	79.098	76.911	107.453	1.00	24.80		C
ANISOU	873	C	GLN A	133	2769	2063	4592	−230	−91	241	C
ATOM	874	O	GLN A	133	77.906	76.834	107.762	1.00	23.24		O
ANISOU	874	O	GLN A	133	2322	2217	4290	−271	−459	−90	O
ATOM	875	CA	AGLN A	133	79.931	78.106	107.886	0.69	28.66		C
ANISOU	875	CA	AGLN A	133	3201	2799	4888	−652	−726	−38	C
ATOM	876	CB	AGLN A	133	80.646	77.767	109.185	0.69	31.24		C
ANISOU	876	CB	AGLN A	133	3488	3566	4815	−655	−1347	−395	C
ATOM	877	CA	BGLN A	133	79.931	78.107	107.879	0.31	28.06		C
ANISOU	877	CA	BGLN A	133	3161	2591	4911	−449	−575	61	C
ATOM	878	CB	BGLN A	133	80.664	77.771	109.170	0.31	32.24		C
ANISOU	878	CB	BGLN A	133	3663	3346	5240	−395	−864	−130	C
ATOM	879	N	ILE A	134	79.719	75.990	106.725	1.00	25.56		N
ANISOU	879	N	ILE A	134	2608	2544	4560	−243	412	634	N
ATOM	880	C	ILE A	134	79.831	73.576	107.058	1.00	22.31		C
ANISOU	880	C	ILE A	134	1851	2611	4015	24	212	173	C
ATOM	881	O	ILE A	134	81.066	73.563	107.084	1.00	25.41		O
ANISOU	881	O	ILE A	134	2126	2823	4707	−55	80	144	O
ATOM	882	CA	AILE A	134	79.070	74.729	106.407	0.61	22.23		C
ANISOU	882	CA	AILE A	134	2349	2093	4005	483	270	516	C
ATOM	883	CB	AILE A	134	78.897	74.493	104.868	0.61	21.09		C
ATOM	884	CG1	AILE A	134	78.105	73.198	104.615	0.61	26.12		C
ATOM	885	CG2	AILE A	134	80.249	74.520	104.143	0.61	35.37		C
ATOM	886	CA	BILE A	134	79.170	74.729	106.407	0.39	26.87		C
ANISOU	886	CA	BILE A	134	2726	2858	4624	175	328	426	C
ATOM	887	CB	BILE A	134	78.997	74.493	104.868	0.39	31.21		C
ATOM	888	CG1	BILE A	134	78.152	73.232	104.616	0.39	30.26		C
ATOM	889	CG2	BILE A	134	80.354	74.458	104.152	0.39	36.57		C
ATOM	890	N	LYS A	135	79.090	72.643	107.643	1.00	18.71		N
ANISOU	890	N	LYS A	135	1937	1951	3223	−26	−60	−126	N
ATOM	891	CA	LYS A	135	79.656	71.392	108.134	1.00	18.47		C
ANISOU	891	CA	LYS A	135	1975	1983	3061	25	−475	−353	C
ATOM	892	C	LYS A	135	78.904	70.226	107.520	1.00	17.52		C
ANISOU	892	C	LYS A	135	1889	2114	2653	−83	−452	−74	C
ATOM	893	O	LYS A	135	77.673	70.175	107.528	1.00	17.94		O
ANISOU	893	O	LYS A	135	1825	2409	2581	22	−235	−450	O
ATOM	894	CB	LYS A	135	79.598	71.319	109.651	1.00	23.31		C
ANISOU	894	CB	LYS A	135	3256	2166	3434	252	−959	−545	C
ATOM	895	CG	LYS A	135	80.420	72.422	110.286	1.00	26.16		C
ANISOU	895	CG	LYS A	135	4007	2174	3757	194	−1292	−625	C
ATOM	896	CD	LYS A	135	80.870	72.094	111.685	1.00	30.44		C
ANISOU	896	CD	LYS A	135	4405	2633	4529	−286	−1440	−164	C
ATOM	897	CE	LYS A	135	81.737	73.215	112.251	1.00	32.34		C
ANISOU	897	CE	LYS A	135	4531	2907	4851	−524	−1232	−376	C
ATOM	898	NZ	LYS A	135	83.078	73.310	111.606	1.00	39.32		N
ANISOU	898	NZ	LYS A	135	5621	3854	5462	−714	−1056	−345	N
ATOM	899	N	GLU A	136	79.667	69.288	106.988	1.00	17.58		N
ANISOU	899	N	GLU A	136	1777	2026	2878	28	−374	−303	N
ATOM	900	C	GLU A	136	79.100	66.903	107.098	1.00	15.56		C
ANISOU	900	C	GLU A	136	1660	2035	2217	209	−278	−364	C
ATOM	901	O	GLU A	136	79.993	66.668	107.928	1.00	16.23		O
ANISOU	901	O	GLU A	136	1688	2211	2267	47	−253	−457	O
ATOM	902	CG	GLU A	136	79.894	69.110	104.011	1.00	28.51		C
ANISOU	902	CG	GLU A	136	3684	3470	3677	−363	198	251	C
ATOM	903	CD	GLU A	136	80.612	68.863	102.687	1.00	44.23		C
ANISOU	903	CD	GLU A	136	5616	6070	5121	48	272	387	C
ATOM	904	OE1	GLU A	136	81.467	67.953	102.618	1.00	36.65		O
ANISOU	904	OE1	GLU A	136	4507	5310	4107	−769	586	271	O
ATOM	905	OE2	GLU A	136	80.319	69.587	101.706	1.00	45.57		O
ANISOU	905	OE2	GLU A	136	5976	6342	4998	545	182	735	O
ATOM	906	CA	AGLU A	136	79.120	68.163	106.258	0.61	16.88		C
ANISOU	906	CA	AGLU A	136	2038	1873	2502	−93	−289	−334	C
ATOM	907	CB	AGLU A	136	79.941	67.923	104.978	0.61	21.37		C
ANISOU	907	CB	AGLU A	136	2741	2372	3007	−109	112	69	C
ATOM	908	CA	BGLU A	136	79.220	68.163	106.258	0.39	19.72		C
ANISOU	908	CA	BGLU A	136	2280	2374	2840	136	−355	−389	C
ATOM	909	CB	BGLU A	136	80.041	67.923	104.978	0.39	22.35		C
ANISOU	909	CB	BGLU A	136	2709	2566	3218	−73	−31	−90	C
ATOM	910	N	SER A	137	78.092	66.072	106.850	1.00	14.12		N
ANISOU	910	N	SER A	137	1608	1959	1800	56	−141	−371	N
ATOM	911	CA	SER A	137	78.086	64.714	107.351	1.00	13.81		C
ANISOU	911	CA	SER A	137	1707	1907	1633	136	−165	−296	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	912	C	SER A	137	79.127	63.892	106.609	1.00	13.49		C
ANISOU	912	C	SER A	137	1695	2031	1399	253	−116	−298	C
ATOM	913	O	SER A	137	79.708	64.344	105.623	1.00	14.99		O
ANISOU	913	O	SER A	137	1909	2105	1680	270	20	−148	O
ATOM	914	CB	SER A	137	76.711	64.083	107.133	1.00	13.13		C
ANISOU	914	CB	SER A	137	1602	2025	1361	137	−190	−270	C
ATOM	915	OG	SER A	137	76.471	63.847	105.750	1.00	13.22		O
ANISOU	915	OG	SER A	137	1692	1979	1352	26	−263	−172	O
ATOM	916	N	LEU A	138	79.340	62.664	107.059	1.00	13.53		N
ANISOU	916	N	LEU A	138	1676	2005	1460	327	−297	−425	N
ATOM	917	CA	LEU A	138	80.035	61.714	106.213	1.00	14.24		C
ANISOU	917	CA	LEU A	138	1922	1972	1516	345	−315	−321	C
ATOM	918	C	LEU A	138	79.096	61.317	105.080	1.00	13.40		C
ANISOU	918	C	LEU A	138	1652	2005	1434	235	−335	−269	C
ATOM	919	O	LEU A	138	77.875	61.524	105.145	1.00	14.30		O
ANISOU	919	O	LEU A	138	1817	2122	1494	274	−360	−319	O
ATOM	920	CB	LEU A	138	80.430	60.481	107.007	1.00	15.80		C
ANISOU	920	CB	LEU A	138	2268	2188	1548	557	−333	−332	C
ATOM	921	CG	LEU A	138	81.395	60.733	108.163	1.00	17.06		C
ANISOU	921	CG	LEU A	138	2453	2817	1212	870	−564	−528	C
ATOM	922	CD1	LEU A	138	81.776	59.401	108.778	1.00	22.22		C
ANISOU	922	CD1	LEU A	138	3158	3685	1601	1653	−461	−182	C
ATOM	923	CD2	LEU A	138	82.634	61.495	107.697	1.00	19.04		C
ANISOU	923	CD2	LEU A	138	2123	3312	1801	659	−792	−780	C
ATOM	924	N	ARG A	139	79.644	60.724	104.032	1.00	14.60		N
ANISOU	924	N	ARG A	139	2136	2119	1294	329	−230	−295	N
ATOM	925	CA	ARG A	139	78.795	60.288	102.933	1.00	14.78		C
ANISOU	925	CA	ARG A	139	2456	2108	1053	201	−586	−331	C
ATOM	926	C	ARG A	139	77.970	59.050	103.285	1.00	16.19		C
ANISOU	926	C	ARG A	139	2699	2019	1434	268	−584	200	C
ATOM	927	O	ARG A	139	78.311	58.281	104.183	1.00	16.93		O
ANISOU	927	O	ARG A	139	2311	2414	1707	−14	−378	52	O
ATOM	928	CB	ARG A	139	79.635	60.000	101.710	1.00	18.11		C
ANISOU	928	CB	ARG A	139	2650	2549	1680	−83	−374	−173	C
ATOM	929	CG	ARG A	139	80.251	61.234	101.155	1.00	17.94		C
ANISOU	929	CG	ARG A	139	2309	2926	1581	−390	−144	−183	C
ATOM	930	CD	ARG A	139	80.614	61.028	99.730	1.00	21.55		C
ANISOU	930	CD	ARG A	139	2839	3023	2326	−472	17	227	C
ATOM	931	NE	ARG A	139	81.616	61.985	99.309	1.00	22.47		N
ANISOU	931	NE	ARG A	139	2570	3298	2671	−402	−180	505	N
ATOM	932	CZ	ARG A	139	82.194	61.959	98.117	1.00	22.50		C
ANISOU	932	CZ	ARG A	139	2436	3488	2625	279	−251	866	C
ATOM	933	NH1	ARG A	139	81.837	61.044	97.228	1.00	22.91		N
ANISOU	933	NH1	ARG A	139	2377	3500	2828	−194	−313	473	N
ATOM	934	NH2	ARG A	139	83.116	62.852	97.815	1.00	24.34		N
ANISOU	934	NH2	ARG A	139	2374	3639	3234	−246	−141	1211	N
ATOM	935	O	ALA A	140	76.007	57.992	100.187	1.00	17.70		O
ANISOU	935	O	ALA A	140	3352	2154	1218	−358	−525	123	O
ATOM	936	N	ALA A	140	76.871	58.868	102.569	1.00	15.86		N
ANISOU	936	N	ALA A	140	2543	2147	1338	−129	−583	−48	N
ATOM	937	CA	ALA A	140	76.141	57.605	102.569	1.00	15.81		C
ANISOU	937	CA	ALA A	140	2719	2111	1178	−343	−537	−18	C
ATOM	938	C	ALA A	140	76.020	57.162	101.107	1.00	15.57		C
ANISOU	938	C	ALA A	140	2655	2130	1130	−309	−530	183	C
ATOM	939	CB	ALA A	140	74.763	57.759	103.228	1.00	19.34		C
ANISOU	939	CB	ALA A	140	2752	2958	1639	−312	82	16	C
ATOM	940	N	GLU A	141	75.941	55.854	100.890	1.00	15.45		N
ANISOU	940	N	GLU A	141	2633	1949	1289	−211	−309	77	N
ATOM	941	CA	GLU A	141	75.813	55.314	99.547	1.00	14.01		C
ANISOU	941	CA	GLU A	141	2012	2090	1223	−201	−299	6	C
ATOM	942	C	GLU A	141	74.410	54.795	99.307	1.00	13.38		C
ANISOU	942	C	GLU A	141	2188	1940	957	70	110	−156	C
ATOM	943	O	GLU A	141	73.837	54.097	100.154	1.00	14.64		O
ANISOU	943	O	GLU A	141	2244	2108	1210	−51	−126	50	O
ATOM	944	CB	GLU A	141	76.798	54.169	99.341	1.00	16.38		C
ANISOU	944	CB	GLU A	141	2246	2333	1645	−93	−204	−101	C
ATOM	945	CG	GLU A	141	76.706	53.581	97.942	1.00	17.79		C
ANISOU	945	CG	GLU A	141	2312	2375	2073	154	39	16	C
ATOM	946	CD	GLU A	141	77.665	52.434	97.689	1.00	21.05		C
ANISOU	946	CD	GLU A	141	2654	3015	2328	415	61	61	C
ATOM	947	OE1	GLU A	141	78.469	52.088	98.591	1.00	22.81		O
ANISOU	947	OE1	GLU A	141	2687	3419	2559	582	314	447	O
ATOM	948	OE2	GLU A	141	77.605	51.865	96.575	1.00	23.73		O
ANISOU	948	OE2	GLU A	141	3387	3338	2291	1202	63	−157	O

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	949	N	LEU A	142	73.873	55.128	98.137	1.00	13.02		N
ANISOU	949	N	LEU A	142	2153	1950	843	49	−49	−99	N
ATOM	950	CA	LEU A	142	72.638	54.531	97.646	1.00	12.97		C
ANISOU	950	CA	LEU A	142	1770	2037	1121	−35	−95	−217	C
ATOM	951	C	LEU A	142	73.008	53.568	96.527	1.00	13.06		C
ANISOU	951	C	LEU A	142	1915	2054	995	−58	−41	−220	C
ATOM	952	O	LEU A	142	73.721	53.935	95.576	1.00	13.51		O
ANISOU	952	O	LEU A	142	1906	2100	1129	20	158	−202	O
ATOM	953	CB	LEU A	142	71.707	55.606	97.081	1.00	13.82		C
ANISOU	953	CB	LEU A	142	1990	2088	1172	84	−48	−81	C
ATOM	954	CG	LEU A	142	70.372	55.113	96.536	1.00	14.05		C
ANISOU	954	CG	LEU A	142	1902	2215	1221	224	−69	−132	C
ATOM	955	CD1	LEU A	142	69.555	54.431	97.625	1.00	16.79		C
ANISOU	955	CD1	LEU A	142	1992	2857	1529	−108	−4	284	C
ATOM	956	CD2	LEU A	142	69.624	56.273	95.925	1.00	16.01		C
ANISOU	956	CD2	LEU A	142	2119	2684	1279	183	69	−42	C
ATOM	957	N	ARG A	143	72.535	52.333	96.640	1.00	13.93		N
ANISOU	957	N	ARG A	143	2025	1842	1425	−68	110	−290	N
ATOM	958	C	ARG A	143	71.301	50.970	95.115	1.00	15.63		C
ANISOU	958	C	ARG A	143	2586	1922	1429	−182	56	−480	C
ATOM	959	O	ARG A	143	70.501	50.481	95.904	1.00	18.86		O
ANISOU	959	O	ARG A	143	2882	2606	1677	−675	169	−149	O
ATOM	960	NE	AARG A	143	76.173	48.875	96.563	0.56	26.47		N
ANISOU	960	NE	AARG A	143	3900	3059	3097	1060	401	−324	N
ATOM	961	CZ	AARG A	143	76.907	48.245	97.477	0.56	26.76		C
ANISOU	961	CZ	AARG A	143	3819	3240	3108	1146	410	−587	C
ATOM	962	NH1	AARG A	143	76.641	46.982	97.785	0.56	29.91		N
ANISOU	962	NH1	AARG A	143	4282	3270	3813	131	416	−626	N
ATOM	963	NH2	AARG A	143	77.902	48.877	98.091	0.56	23.26		N
ANISOU	963	NH2	AARG A	143	2922	2838	3077	1182	419	−81	N
ATOM	964	CA	AARG A	143	72.701	51.346	95.591	0.56	16.10		C
ANISOU	964	CA	AARG A	143	2593	1914	1609	328	138	−517	C
ATOM	965	CB	AARG A	143	73.431	50.126	96.155	0.56	20.95		C
ANISOU	965	CB	AARG A	143	3481	2306	2173	904	196	−369	C
ATOM	966	CG	AARG A	143	74.183	49.296	95.137	0.56	25.33		C
ANISOU	966	CG	AARG A	143	3915	2740	2969	341	−45	−547	C
ATOM	967	CD	AARG A	143	75.064	48.263	95.831	0.56	27.18		C
ANISOU	967	CD	AARG A	143	3894	2973	3461	402	193	−424	C
ATOM	968	NE	CARG A	143	76.869	49.400	97.299	0.44	20.33		N
ANISOU	968	NE	CARG A	143	2868	2365	2490	775	479	−119	N
ATOM	969	CZ	CARG A	143	77.606	48.570	98.026	0.44	24.33		C
ANISOU	969	CZ	CARG A	143	3292	2620	3332	337	473	187	C
ATOM	970	NH1	CARG A	143	77.159	47.352	98.307	0.44	21.51		N
ANISOU	970	NH1	CARG A	143	3104	2243	2825	1002	411	78	N
ATOM	971	NH2	CARG A	143	78.787	48.965	98.476	0.44	23.17		N
ANISOU	971	NH2	CARG A	143	2551	3234	3017	674	477	235	N
ATOM	972	CA	CARG A	143	72.679	51.360	95.567	0.44	14.97		C
ANISOU	972	CA	CARG A	143	2398	1662	1628	−371	315	−12	C
ATOM	973	CB	CARG A	143	73.411	50.112	96.038	0.44	20.30		C
ANISOU	973	CB	CARG A	143	3094	2282	2337	−62	284	19	C
ATOM	974	CG	CARG A	143	74.849	50.352	96.335	0.44	16.25		C
ANISOU	974	CG	CARG A	143	2165	2118	1891	−280	2	−532	C
ATOM	975	CD	CARG A	143	75.552	49.084	96.761	0.44	19.96		C
ANISOU	975	CD	CARG A	143	2984	2306	2293	442	486	−89	C
ATOM	976	N	VAL A	144	71.016	51.207	93.839	1.00	16.24		N
ANISOU	976	N	VAL A	144	2443	2419	1308	−39	−58	−366	N
ATOM	977	CA	VAL A	144	69.711	50.890	93.283	1.00	16.83		C
ANISOU	977	CA	VAL A	144	2617	2290	1486	−102	67	−376	C
ATOM	978	C	VAL A	144	69.870	49.716	92.337	1.00	21.07		C
ANISOU	978	C	VAL A	144	3173	2891	1942	−272	455	−634	C
ATOM	979	O	VAL A	144	70.539	49.817	91.310	1.00	23.65		O
ANISOU	979	O	VAL A	144	3734	3326	1926	−242	526	−790	O
ATOM	980	CB	VAL A	144	69.090	52.086	92.538	1.00	17.74		C
ANISOU	980	CB	VAL A	144	2482	2715	1544	−276	−194	−399	C
ATOM	981	CG1	VAL A	144	67.705	51.735	92.050	1.00	19.38		C
ANISOU	981	CG1	VAL A	144	2640	3148	1575	−493	−170	−236	C
ATOM	982	CG2	VAL A	144	69.047	53.325	93.425	1.00	16.94		C
ANISOU	982	CG2	VAL A	144	2808	2199	1430	−393	3	−259	C
ATOM	983	N	THR A	145	69.248	48.600	92.692	1.00	20.56		N
ANISOU	983	N	THR A	145	3128	2306	2378	−198	374	−729	N
ATOM	984	CA	THR A	145	69.463	47.344	91.988	1.00	23.95		C
ANISOU	984	CA	THR A	145	3461	2672	2967	74	163	−1190	C
ATOM	985	C	THR A	145	68.383	47.081	90.944	1.00	24.55		C
ANISOU	985	C	THR A	145	3347	2667	3314	−173	205	−1226	C

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

ATOM	986	O	THR A	145	67.292	47.641	91.000	1.00	23.35		O
ANISOU	986	O	THR A	145	2959	2847	3065	−151	132	−1264	O
ATOM	987	CB	THR A	145	69.520	46.177	92.981	1.00	28.34		C
ANISOU	987	CB	THR A	145	4479	2827	3462	617	205	−970	C
ATOM	988	OG1	THR A	145	68.280	46.098	93.694	1.00	31.62		O
ANISOU	988	OG1	THR A	145	5383	2817	3813	387	876	−577	O
ATOM	989	CG2	THR A	145	70.646	46.394	93.983	1.00	32.13		C
ANISOU	989	CG2	THR A	145	5294	3342	3571	787	−281	−1033	C
ATOM	990	O	GLU A	146	66.589	44.315	90.220	1.00	33.08		O
ANISOU	990	O	GLU A	146	4148	3633	4789	−465	−94	−1525	O
ATOM	991	N	GLU A	146	68.693	46.214	89.990	1.00	27.38		N
ANISOU	991	N	GLU A	146	3510	3446	3447	−49	327	−1807	N
ATOM	992	CA	GLU A	146	67.774	45.933	88.888	1.00	29.06		C
ANISOU	992	CA	GLU A	146	3956	3533	3552	−317	−30	−2047	C
ATOM	993	C	GLU A	146	66.524	45.170	89.335	1.00	31.40		C
ANISOU	993	C	GLU A	146	3972	3678	4281	−948	3	−1685	C
ATOM	994	CB	GLU A	146	68.491	45.165	87.773	1.00	34.51		C
ANISOU	994	CB	GLU A	146	4684	4966	3460	218	−200	−2294	C
ATOM	995	O	ARG A	147	64.818	43.038	87.503	1.00	41.53		O
ANISOU	995	O	ARG A	147	5166	4974	5640	−391	−426	−2644	O
ATOM	996	N	ARG A	147	65.387	45.494	88.721	1.00	31.67		N
ANISOU	996	N	ARG A	147	3749	3888	4395	−951	−11	−1878	N
ATOM	997	CA	ARG A	147	64.134	44.785	88.980	1.00	38.10		C
ANISOU	997	CA	ARG A	147	4634	4509	5332	−659	−204	−1893	C
ATOM	998	C	ARG A	147	64.241	43.330	88.547	1.00	39.30		C
ANISOU	998	C	ARG A	147	4756	4756	5420	−415	−287	−2397	C
ATOM	999	CB	ARG A	147	62.968	45.453	88.242	1.00	44.93		C
ANISOU	999	CB	ARG A	147	5572	5478	6021	−342	−499	−1680	C
ATOM	1000	CG	ARG A	147	62.252	46.530	89.042	1.00	49.71		C
ANISOU	1000	CG	ARG A	147	6135	6192	6560	−208	−730	−1375	C
ATOM	1001	CD	ARG A	147	61.567	47.538	88.129	1.00	50.17		C
ANISOU	1001	CD	ARG A	147	5985	6479	6597	−346	−933	−1156	C
TER											
HETATM	1002	CL	CL B	1	77.677	61.025	109.310	1.00	24.26		Cl
TER											
HETATM	1003	CL A	CL B	2	60.106	72.005	104.718	0.43	31.83		Cl
HETATM	1004	CL B	CL B	2	60.046	74.655	105.285	0.57	28.96		Cl
TER											
HETATM	1005	O	HOH S	1	57.430	67.141	118.746	1.00	21.21		O
HETATM	1006	O	HOH S	2	82.586	60.395	103.902	1.00	20.60		O
HETATM	1007	O	HOH S	3	78.817	63.491	111.081	1.00	22.60		O
HETATM	1008	O	HOH S	4	76.145	52.923	94.493	1.00	21.32		O
HETATM	1009	O	HOH S	5	67.052	80.545	100.696	1.00	22.45		O
HETATM	1010	O	HOH S	6	66.272	79.354	102.896	1.00	19.65		O
HETATM	1011	O	HOH S	7	71.389	60.172	110.959	1.00	26.91		O
HETATM	1012	O	HOH S	8	66.515	56.646	106.896	1.00	22.37		O
HETATM	1013	O	HOH S	9	64.255	53.753	102.197	1.00	22.29		O
HETATM	1014	O	HOH S	10	62.264	71.138	103.203	1.00	22.77		O
HETATM	1015	O	HOH S	11	63.607	79.682	102.525	1.00	24.56		O
HETATM	1016	O	HOH S	12	67.408	70.442	114.015	1.00	22.97		O
HETATM	1017	O	AHOH S	13	69.436	75.663	100.041	0.74	20.55		O
HETATM	1018	O	BHOH S	13	67.843	77.110	100.058	0.26	21.75		O
HETATM	1019	O	HOH S	14	76.851	60.191	93.207	1.00	24.68		O
HETATM	1020	O	HOH S	15	70.133	61.148	92.264	1.00	27.30		O
HETATM	1021	O	HOH S	17	58.782	55.203	94.319	1.00	24.40		O
HETATM	1022	O	AHOH S	18	59.915	70.158	106.713	0.61	20.66		O
HETATM	1023	O	BHOH S	18	59.452	69.640	106.872	0.39	27.64		O
HETATM	1024	O	HOH S	19	63.847	71.353	98.727	1.00	25.28		O
HETATM	1025	O	HOH S	20	65.339	53.944	104.582	1.00	26.63		O
HETATM	1026	O	HOH S	21	69.516	48.688	102.677	1.00	30.33		O
HETATM	1027	O	HOH S	22	62.920	51.874	100.481	1.00	27.87		O
HETATM	1028	O	HOH S	23	65.379	76.411	95.129	1.00	30.76		O
HETATM	1029	O	HOH S	24	70.432	71.724	120.013	1.00	29.49		O
HETATM	1030	O	HOH S	25	61.940	55.413	101.581	1.00	26.88		O
HETATM	1031	O	HOH S	26	76.093	85.628	109.892	1.00	30.88		O
HETATM	1032	O	HOH S	27	80.576	57.162	105.547	1.00	30.06		O
HETATM	1033	O	HOH S	28	74.611	52.689	108.918	1.00	31.81		O
HETATM	1034	O	HOH S	29	61.819	69.297	100.027	1.00	31.23		O
HETATM	1035	O	HOH S	30	77.221	58.625	106.967	1.00	26.29		O
HETATM	1036	O	HOH S	31	77.910	65.513	114.947	1.00	33.77		O
HETATM	1037	O	HOH S	32	59.000	52.395	88.751	1.00	25.46		O
HETATM	1038	O	HOH S	34	74.269	72.547	93.457	1.00	31.68		O
HETATM	1039	O	HOH S	35	59.962	61.995	102.948	1.00	30.48		O
HETATM	1040	O	HOH S	36	78.949	51.959	101.310	1.00	29.60		O

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

HETATM	1041	O	HOH S	37	60.418	77.661	103.825	1.00	32.54	O
HETATM	1042	O	HOH S	38	64.337	73.857	98.445	1.00	36.83	O
HETATM	1043	O	HOH S	39	70.282	50.025	105.056	1.00	38.23	O
HETATM	1044	O	HOH S	40	67.330	45.766	96.409	1.00	36.46	O
HETATM	1045	O	HOH S	41	66.498	68.443	92.773	1.00	42.28	O
HETATM	1046	O	HOH S	42	57.480	64.464	118.550	1.00	43.50	O
HETATM	1047	O	HOH S	43	63.919	55.879	107.942	1.00	48.40	O
HETATM	1048	O	HOH S	44	82.271	65.080	106.284	1.00	51.88	O
HETATM	1049	O	HOH S	45	67.906	70.564	118.415	1.00	35.59	O
HETATM	1050	O	HOH S	46	59.675	62.503	114.914	1.00	42.35	O
HETATM	1051	O	HOH S	47	84.504	75.303	113.293	1.00	44.45	O
HETATM	1052	O	HOH S	48	69.227	60.073	88.487	1.00	25.89	O
HETATM	1053	O	HOH S	49	56.407	56.257	94.519	1.00	29.48	O
HETATM	1054	O	HOH S	50	75.972	87.073	112.546	1.00	45.01	O
HETATM	1055	O	HOH S	51	61.016	73.535	95.375	1.00	42.26	O
HETATM	1056	O	HOH S	52	73.061	77.907	112.924	1.00	33.56	O
HETATM	1057	O	HOH S	53	82.470	82.777	106.828	1.00	53.02	O
HETATM	1058	O	AHOH S	54	79.436	59.161	94.370	0.51	24.61	O
HETATM	1059	O	BHOH S	54	81.256	59.211	95.031	0.49	27.92	O
HETATM	1060	O	HOH S	56	55.642	58.691	92.932	1.00	47.56	O
HETATM	1061	O	HOH S	57	75.933	64.200	116.451	1.00	42.90	O
HETATM	1062	O	HOH S	58	61.360	64.040	102.879	1.00	21.86	O
HETATM	1063	O	HOH S	59	70.389	63.369	90.940	1.00	26.53	O
HETATM	1064	O	HOH S	60	78.757	54.411	102.685	1.00	27.01	O
HETATM	1065	O	HOH S	61	57.378	65.660	109.331	1.00	23.47	O
HETATM	1066	O	HOH S	62	79.929	56.310	100.932	1.00	26.39	O
HETATM	1067	O	HOH S	63	74.661	50.940	106.612	1.00	28.90	O
HETATM	1068	O	HOH S	64	57.806	52.236	91.089	1.00	33.66	O
HETATM	1069	O	HOH S	65	64.127	69.714	95.525	1.00	39.44	O
HETATM	1070	O	HOH S	66	57.817	49.353	90.926	1.00	43.07	O
HETATM	1071	O	HOH S	67	82.662	76.748	106.385	1.00	42.18	O
HETATM	1072	O	HOH S	68	59.754	48.914	92.942	1.00	43.66	O
HETATM	1073	O	HOH S	69	65.932	58.157	83.638	1.00	25.25	O
HETATM	1074	O	HOH S	70	83.553	67.550	106.500	1.00	36.13	O
HETATM	1075	O	HOH S	71	79.130	49.647	103.301	1.00	44.50	O
HETATM	1076	O	HOH S	72	74.424	67.532	114.823	1.00	26.09	O
HETATM	1077	O	AHOH S	73	65.707	82.659	89.714	0.59	33.77	O
HETATM	1078	O	BHOH S	73	64.853	83.970	90.636	0.41	21.68	O
HETATM	1079	O	HOH S	74	60.223	59.329	113.439	1.00	48.46	O
HETATM	1080	O	HOH S	75	78.431	45.755	100.061	1.00	52.89	O
HETATM	1081	O	HOH S	76	71.873	78.026	121.604	1.00	44.28	O
HETATM	1082	O	HOH S	77	59.163	52.192	98.563	1.00	21.31	O
HETATM	1083	O	HOH S	78	71.545	76.150	114.323	1.00	23.97	O
HETATM	1084	O	HOH S	79	77.047	54.056	91.965	1.00	28.71	O
HETATM	1085	O	HOH S	80	55.960	64.395	120.883	1.00	34.79	O
HETATM	1086	O	HOH S	81	57.096	79.709	93.763	1.00	45.83	O
HETATM	1087	O	HOH S	82	59.224	68.879	102.307	1.00	36.88	O
HETATM	1088	O	HOH S	83	75.095	78.893	115.129	1.00	45.56	O
HETATM	1089	O	HOH S	84	82.002	64.491	104.242	1.00	37.55	O
HETATM	1090	O	HOH S	86	83.627	62.767	104.076	1.00	32.57	O
HETATM	1091	O	HOH S	87	62.350	77.030	95.671	1.00	34.75	O
HETATM	1092	O	HOH S	88	72.529	65.140	91.039	1.00	38.63	O
HETATM	1093	O	HOH S	89	62.629	54.150	105.575	1.00	49.04	O
HETATM	1094	O	HOH S	90	63.207	49.381	99.368	1.00	31.86	O
HETATM	1095	O	HOH S	91	73.193	53.654	83.945	1.00	40.40	O
HETATM	1096	O	HOH S	92	76.565	43.643	93.769	1.00	51.00	O
HETATM	1097	O	HOH S	93	73.894	44.922	93.694	1.00	51.33	O
HETATM	1098	O	HOH S	94	82.395	64.135	100.901	1.00	37.20	O
HETATM	1099	O	HOH S	95	68.694	54.383	85.476	1.00	38.52	O
HETATM	1100	O	HOH S	96	75.745	50.591	92.570	1.00	38.51	O
HETATM	1101	O	HOH S	97	57.196	74.069	89.690	1.00	44.43	O
HETATM	1102	O	HOH S	98	58.823	71.444	109.216	1.00	43.89	O
HETATM	1103	O	AHOH S	99	65.419	54.387	84.501	0.54	33.13	O
HETATM	1104	O	BHOH S	99	66.459	52.602	86.126	0.46	25.24	O
HETATM	1105	O	HOH S	100	72.132	53.131	110.463	1.00	47.44	O
HETATM	1106	O	HOH S	102	60.149	84.733	99.929	1.00	41.38	O
HETATM	1107	O	HOH S	103	67.196	55.553	83.544	1.00	47.80	O
HETATM	1108	O	HOH S	104	78.913	45.418	95.016	1.00	57.07	O
HETATM	1109	O	HOH S	105	78.173	65.188	92.355	1.00	40.00	O
HETATM	1110	O	HOH S	106	71.615	52.024	84.401	1.00	52.57	O
HETATM	1111	O	HOH S	107	77.280	77.678	115.428	1.00	48.55	O
HETATM	1112	O	HOH S	108	71.512	43.089	92.230	1.00	56.65	O
HETATM	1113	O	HOH S	110	80.509	47.126	95.603	1.00	54.92	O
HETATM	1114	O	HOH S	111	80.259	71.593	99.980	1.00	63.90	O

TABLE 7-continued

Atomic coordinates and structure factors for human apo-PD-1$^{N74G\ T76P\ A132V}$ (based on a PDB file).

HETATM	1115	O	HOH S	112	68.918	57.671	112.722	1.00	53.96	O
HETATM	1116	O	HOH S	113	70.300	83.442	113.613	1.00	29.88	O
HETATM	1117	O	AHOH S	114	66.795	76.702	101.785	0.74	23.82	O
HETATM	1118	O	BHOH S	114	66.370	77.010	102.388	0.26	24.19	O
HETATM	1119	O	AHOH S	115	59.053	62.549	106.127	0.60	19.44	O
HETATM	1120	O	BHOH S	115	57.247	65.452	103.361	0.40	15.82	O
HETATM	1121	O	HOH S	116	60.861	62.614	97.618	1.00	30.80	O
HETATM	1122	O	HOH S	117	61.573	56.997	117.632	1.00	51.95	O
HETATM	1123	O	HOH S	118	81.074	84.577	108.313	1.00	46.27	O
HETATM	1124	O	HOH S	119	73.428	55.743	81.859	1.00	34.45	O
HETATM	1125	O	HOH S	120	82.654	69.742	107.083	1.00	38.65	O
HETATM	1126	O	HOH S	122	62.374	69.829	96.978	1.00	48.84	O
HETATM	1127	O	HOH S	123	58.386	70.671	111.363	1.00	56.98	O
HETATM	1128	O	HOH S	124	78.972	58.166	91.940	1.00	52.15	O
HETATM	1129	O	HOH S	125	80.430	64.535	90.804	1.00	48.85	O
HETATM	1130	O	HOH S	126	71.469	44.836	90.528	1.00	43.98	O
HETATM	1131	O	HOH S	127	75.978	56.855	109.467	1.00	44.00	O
HETATM	1132	O	HOH S	128	70.323	59.333	116.131	1.00	57.81	O
HETATM	1133	O	HOH S	129	77.256	62.535	90.718	1.00	52.58	O
HETATM	1134	O	HOH S	130	74.334	45.315	96.792	1.00	51.31	O
HETATM	1135	O	HOH S	131	83.259	66.794	103.808	1.00	50.92	O
HETATM	1136	O	HOH S	132	59.345	79.745	96.552	1.00	47.19	O
HETATM	1137	O	HOH S	133	61.610	58.979	116.361	1.00	48.36	O
HETATM	1138	O	HOH S	134	63.162	59.836	118.024	1.00	55.93	O
HETATM	1139	O	HOH S	135	76.936	43.553	96.830	1.00	61.58	O
HETATM	1140	O	HOH S	136	57.386	68.014	92.618	1.00	49.32	O
HETATM	1141	O	HOH S	137	83.138	74.599	115.308	1.00	50.48	O
HETATM	1142	O	HOH S	138	84.189	82.738	109.005	1.00	57.05	O
HETATM	1143	O	HOH S	139	68.404	50.713	106.175	1.00	50.11	O
HETATM	1144	O	HOH S	140	65.546	48.441	100.909	1.00	45.80	O
HETATM	1145	O	HOH S	141	68.393	66.857	91.161	1.00	62.36	O
HETATM	1146	O	HOH S	142	67.813	76.089	93.906	1.00	51.02	O
HETATM	1147	O	HOH S	143	82.920	66.297	100.638	1.00	61.00	O
HETATM	1148	O	AHOH S	145	58.793	64.590	96.018	0.57	51.09	O
HETATM	1149	O	BHOH S	145	52.539	62.260	96.275	0.43	51.51	O
HETATM	1150	O	HOH S	146	61.132	37.910	86.642	1.00	63.11	O
HETATM	1151	O	HOH S	147	78.019	80.100	113.163	1.00	56.94	O
HETATM	1152	O	HOH S	148	68.878	66.327	88.863	1.00	61.15	O
HETATM	1153	O	HOH S	149	71.524	48.875	88.987	1.00	53.48	O
HETATM	1154	O	HOH S	150	62.915	37.379	84.940	1.00	65.99	O
HETATM	1155	O	AHOH S	151	64.070	58.203	110.138	0.55	27.19	O
TER										
HETATM	1156	O	BHOH S	151	68.424	55.667	109.016	0.55	36.34	O
TER										
END										

TABLE 8

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

CRYST1		46.199	46.199	89.407	90.00	90.00	120.00	P	32 2	1
SCALE1				0.021645	0.012497	0.000000	0.00000			
SCALE2				0.000000	0.024994	0.000000	0.00000			
SCALE3				0.000000	0.000000	0.011185	0.00000			
ATOM	1	O	MET A	32	−33.514	7.432	25.524	1.00	47.58	O
ANISOU	1	O	MET A	32	5753	7175	5152	−154	1784	723 O
ATOM	2	N	MET A	32	−32.396	5.090	26.810	1.00	52.12	N
ANISOU	2	N	MET A	32	7042	7125	5636	902	705	156 N
ATOM	3	C	MET A	32	−32.333	7.387	25.888	1.00	46.44	C
ANISOU	3	C	MET A	32	5888	6742	5015	461	1457	1051 C
ATOM	4	CA	AMET A	32	−31.611	6.036	26.020	0.44	47.31	C
ANISOU	4	CA	AMET A	32	6303	6386	5287	645	1240	552 C
ATOM	5	CB	AMET A	32	−31.295	5.439	24.632	0.44	46.23	C
ANISOU	5	CB	AMET A	32	6247	5879	5438	798	1190	194 C
ATOM	6	CG	AMET A	32	−30.328	6.255	23.780	0.44	41.86	C
ANISOU	6	CG	AMET A	32	5742	4789	5375	307	1475	53 C
ATOM	7	SD	AMET A	32	−29.839	5.507	22.193	0.44	37.67	S
ANISOU	7	SD	AMET A	32	5243	3605	5463	−669	1423	−221 S
ATOM	8	CE	AMET A	32	−31.424	5.296	21.385	0.44	36.56	C
ANISOU	8	CE	AMET A	32	5475	3025	5390	−623	1237	−248 C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	9	CA	BMET A	32	−31.593	6.066	26.090	0.56	48.41		C
ANISOU	9	CA	BMET A	32	6455	6487	5453	676	1273	841	C
ATOM	10	CB	BMET A	32	−31.144	5.510	24.741	0.56	49.97		C
ANISOU	10	CB	BMET A	32	6754	6243	5990	1043	1250	908	C
ATOM	11	CG	BMET A	32	−32.295	5.139	23.844	0.56	48.60		C
ANISOU	11	CG	BMET A	32	6773	5415	6276	982	1591	1293	C
ATOM	12	SD	BMET A	32	−31.726	4.762	22.201	0.56	46.23		S
ANISOU	12	SD	BMET A	32	6431	4509	6625	638	2362	1816	S
ATOM	13	CE	BMET A	32	−30.808	6.252	21.804	0.56	45.84		C
ANISOU	13	CE	BMET A	32	6576	4482	6358	127	2259	2483	C
ATOM	14	N	ASN A	33	−31.627	8.474	26.165	1.00	39.88		N
ANISOU	14	N	ASN A	33	5292	5645	4214	563	1175	2037	N
ATOM	15	CA	ASN A	33	−32.157	9.804	25.947	1.00	42.03		C
ANISOU	15	CA	ASN A	33	5949	6351	3667	1269	1131	1849	C
ATOM	16	C	ASN A	33	−31.669	10.277	24.596	1.00	33.44		C
ANISOU	16	C	ASN A	33	3743	5808	3156	1482	1232	1757	C
ATOM	17	O	ASN A	33	−30.602	9.874	24.145	1.00	35.26		O
ANISOU	17	O	ASN A	33	3938	5705	3755	1651	995	1962	O
ATOM	18	CB	ASN A	33	−31.672	10.756	27.036	1.00	46.78		C
ANISOU	18	CB	ASN A	33	7351	6823	3600	1245	1354	2231	C
ATOM	19	CG	ASN A	33	−32.138	10.334	28.401	1.00	55.32		C
ANISOU	19	CG	ASN A	33	9094	7638	4285	1888	1346	2061	C
ATOM	20	OD1	ASN A	33	−33.140	10.836	28.916	1.00	58.96		O
ANISOU	20	OD1	ASN A	33	9496	8239	4667	2705	2288	2012	O
ATOM	21	ND2	ASN A	33	−31.444	9.374	28.977	1.00	57.08		N
ANISOU	21	ND2	ASN A	33	9752	7825	4112	1789	537	2233	N
ATOM	22	N	PRO A	34	−32.450	11.127	23.928	1.00	25.03		N
ANISOU	22	N	PRO A	34	2563	4178	2769	511	766	754	N
ATOM	23	C	PRO A	34	−30.767	12.498	22.759	1.00	21.81		C
ANISOU	23	C	PRO A	34	1958	4072	2255	672	314	156	C
ATOM	24	O	PRO A	34	−30.547	13.154	23.783	1.00	25.42		O
ANISOU	24	O	PRO A	34	3358	4404	1898	286	435	166	O
ATOM	25	CA	APRO A	34	−32.035	11.666	22.632	0.47	23.20		C
ANISOU	25	CA	APRO A	34	2253	3858	2704	79	394	137	C
ATOM	26	CB	APRO A	34	−33.204	12.576	22.249	0.47	23.74		C
ANISOU	26	CB	APRO A	34	2223	3997	2800	−347	−25	64	C
ATOM	27	CG	APRO A	34	−34.359	12.136	23.140	0.47	24.04		C
ANISOU	27	CG	APRO A	34	2277	4132	2727	−649	−35	−148	C
ATOM	28	CD	APRO A	34	−33.715	11.706	24.399	0.47	25.77		C
ANISOU	28	CD	APRO A	34	2344	4530	2916	−52	245	562	C
ATOM	29	CA	BPRO A	34	−31.987	11.604	22.628	0.53	22.93		C
ANISOU	29	CA	BPRO A	34	2143	3873	2696	330	575	228	C
ATOM	30	CB	BPRO A	34	−33.181	12.399	22.103	0.53	23.06		C
ANISOU	30	CB	BPRO A	34	1926	4133	2700	387	514	289	C
ATOM	31	CG	BPRO A	34	−33.935	12.807	23.325	0.53	22.86		C
ANISOU	31	CG	BPRO A	34	2147	3935	2602	661	553	349	C
ATOM	32	CD	BPRO A	34	−33.765	11.673	24.290	0.53	25.43		C
ANISOU	32	CD	BPRO A	34	2311	4493	2857	779	527	773	C
ATOM	33	N	PRO A	35	−29.938	12.498	21.729	1.00	18.67		N
ANISOU	33	N	PRO A	35	2177	3152	1765	659	538	514	N
ATOM	34	CA	PRO A	35	−28.824	13.447	21.691	1.00	17.89		C
ANISOU	34	CA	PRO A	35	2092	2784	1920	−166	392	682	C
ATOM	35	C	PRO A	35	−29.335	14.871	21.506	1.00	19.21		C
ANISOU	35	C	PRO A	35	2469	3182	1647	472	−69	509	C
ATOM	36	O	PRO A	35	−30.457	15.077	21.047	1.00	20.66		O
ANISOU	36	O	PRO A	35	2705	3371	1774	517	−35	145	O
ATOM	37	CB	PRO A	35	−28.018	12.989	20.464	1.00	20.77		C
ANISOU	37	CB	PRO A	35	1994	4010	1888	71	280	288	C
ATOM	38	CG	PRO A	35	−29.057	12.343	19.594	1.00	23.62		C
ANISOU	38	CG	PRO A	35	3977	2987	2012	495	867	158	C
ATOM	39	CD	PRO A	35	−30.036	11.693	20.498	1.00	22.34		C
ANISOU	39	CD	PRO A	35	3666	3393	1428	777	545	64	C
ATOM	40	N	THR A	36	−28.516	15.850	21.856	1.00	19.79		N
ANISOU	40	N	THR A	36	2357	3543	1620	225	228	410	N
ATOM	41	CA	THR A	36	−28.836	17.243	21.504	1.00	21.34		C
ANISOU	41	CA	THR A	36	2300	3727	2082	407	53	429	C
ATOM	42	C	THR A	36	−27.853	17.747	20.457	1.00	19.81		C
ANISOU	42	C	THR A	36	1755	3785	1985	13	128	444	C
ATOM	43	O	THR A	36	−26.730	17.247	20.388	1.00	23.78		O
ANISOU	43	O	THR A	36	2094	4251	2690	641	492	1409	O
ATOM	44	CB	THR A	36	−28.811	18.190	22.717	1.00	25.11		C
ANISOU	44	CB	THR A	36	2832	4606	2102	22	−29	−329	C
ATOM	45	OG1	THR A	36	−27.491	18.194	23.256	1.00	30.33		O
ANISOU	45	OG1	THR A	36	3601	5178	2745	627	−419	−1114	O

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	46	CG2	THR A	36	−29.768	17.710	23.787	1.00	25.12		C
ANISOU	46	CG2	THR A	36	3469	3857	2218	79	447	−9	C
ATOM	47	N	PHE A	37	−28.262	18.714	19.642	1.00	19.41		N
ANISOU	47	N	PHE A	37	3220	2748	1406	414	49	18	N
ATOM	48	CA	PHE A	37	−27.460	19.111	18.485	1.00	17.96		C
ANISOU	48	CA	PHE A	37	2894	2853	1076	380	153	127	C
ATOM	49	C	PHE A	37	−27.464	20.626	18.460	1.00	20.12		C
ANISOU	49	C	PHE A	37	2929	2759	1958	430	284	78	C
ATOM	50	O	PHE A	37	−28.532	21.236	18.445	1.00	22.81		O
ANISOU	50	O	PHE A	37	3082	3060	2526	280	63	70	O
ATOM	51	CB	PHE A	37	−28.117	18.528	17.240	1.00	18.94		C
ANISOU	51	CB	PHE A	37	2712	3275	1211	161	105	−184	C
ATOM	52	CG	PHE A	37	−27.218	18.477	16.055	1.00	18.45		C
ANISOU	52	CG	PHE A	37	2760	2794	1458	−185	−46	−236	C
ATOM	53	CD1	PHE A	37	−27.657	18.932	14.828	1.00	24.25		C
ANISOU	53	CD1	PHE A	37	3367	4312	1533	−7.41	−281	189	C
ATOM	54	CD2	PHE A	37	−25.976	17.884	16.154	1.00	20.07		C
ANISOU	54	CD2	PHE A	37	3020	2550	2055	150	591	210	C
ATOM	55	CE1	PHE A	37	−26.816	18.847	13.735	1.00	27.38		C
ANISOU	55	CE1	PHE A	37	3908	4736	1760	−1156	−240	−120	C
ATOM	56	CE2	PHE A	37	−25.151	17.761	15.061	1.00	24.03		C
ANISOU	56	CE2	PHE A	37	3724	3298	2107	−381	532	−362	C
ATOM	57	CZ	PHE A	37	−25.565	18.241	13.859	1.00	26.10		C
ANISOU	57	CZ	PHE A	37	3415	4685	1817	−1535	193	−572	C
ATOM	58	O	SER A	38	−24.150	22.452	17.292	1.00	20.42		O
ANISOU	58	O	SER A	38	2994	2559	2205	256	293	60	O
ATOM	59	N	SER A	38	−26.280	21.221	18.458	1.00	18.09		N
ANISOU	59	N	SER A	38	2679	2283	1912	−222	210	332	N
ATOM	60	C	SER A	38	−25.018	23.195	17.712	1.00	18.62		C
ANISOU	60	C	SER A	38	2903	2295	1875	−52	224	238	C
ATOM	61	CA	ASER A	38	−26.143	22.663	18.613	0.45	19.87		C
ANISOU	61	CA	ASER A	38	3356	2275	1916	−154	391	125	C
ATOM	62	CB	ASER A	38	−25.872	23.028	20.086	0.45	23.68		C
ANISOU	62	CB	ASER A	38	3879	2993	2125	−261	−58	22	C
ATOM	63	OG	ASER A	38	−24.580	22.611	20.489	0.45	24.63		O
ANISOU	63	OG	ASER A	38	4337	2956	2063	−162	−417	−203	O
ATOM	64	CA	BSER A	38	−26.112	22.655	18.650	0.26	19.74		C
ANISOU	64	CA	BSER A	38	3038	2548	1916	−150	363	360	C
ATOM	65	CB	BSER A	38	−25.745	22.911	20.119	0.26	22.39		C
ANISOU	65	CB	BSER A	38	3098	3325	2086	−431	119	447	C
ATOM	66	OG	BSER A	38	−25.301	24.234	20.343	0.26	22.99		O
ANISOU	66	OG	BSER A	38	3212	3455	2068	−700	63	275	O
ATOM	67	CA	CSER A	38	−26.119	22.663	18.631	0.28	19.53		C
ANISOU	67	CA	CSER A	38	3234	2412	1776	52	444	165	C
ATOM	68	CB	CSER A	38	−25.755	22.986	20.087	0.28	21.98		C
ANISOU	68	CB	CSER A	38	3700	2978	1674	309	311	−6	C
ATOM	69	OG	CSER A	38	−26.670	22.392	20.982	0.28	21.91		O
ANISOU	69	OG	CSER A	38	3954	3054	1317	802	561	−208	O
ATOM	70	N	PRO A	39	−25.057	24.483	17.380	1.00	19.87		N
ANISOU	70	N	PRO A	39	2776	2564	2212	−238	114	144	N
ATOM	71	CA	PRO A	39	−26.117	25.474	17.640	1.00	20.67		C
ANISOU	71	CA	PRO A	39	2909	2582	2364	435	218	−148	C
ATOM	72	C	PRO A	39	−27.289	25.226	16.687	1.00	20.46		C
ANISOU	72	C	PRO A	39	3004	3038	1733	−76	185	−423	C
ATOM	73	O	PRO A	39	−27.126	24.581	15.640	1.00	21.86		O
ANISOU	73	O	PRO A	39	3387	3020	1898	−105	103	−514	O
ATOM	74	CB	PRO A	39	−25.441	26.808	17.293	1.00	23.73		C
ANISOU	74	CB	PRO A	39	4010	2378	2631	191	16	−199	C
ATOM	75	CG	PRO A	39	−24.458	26.432	16.236	1.00	23.37		C
ANISOU	75	CG	PRO A	39	3339	2298	3242	−45	396	−90	C
ATOM	76	CD	PRO A	39	−23.982	25.040	16.550	1.00	21.23		C
ANISOU	76	CD	PRO A	39	3038	2343	2687	−326	280	49	C
ATOM	77	N	ALA A	40	−28.462	25.717	17.025	1.00	21.41		N
ANISOU	77	N	ALA A	40	3090	2992	2051	74	43	33	N
ATOM	78	CA	ALA A	40	−29.634	25.478	16.198	1.00	21.40		C
ANISOU	78	CA	ALA A	40	3191	3174	1768	−425	257	−190	C
ATOM	79	C	ALA A	40	−29.502	26.162	14.825	1.00	20.53		C
ANISOU	79	C	ALA A	40	3396	2723	1680	84	217	−581	C
ATOM	80	O	ALA A	40	−30.052	25.679	13.847	1.00	19.65		O
ANISOU	80	O	ALA A	40	3053	2723	1689	−157	342	−385	O
ATOM	81	CB	ALA A	40	−30.898	25.935	16.937	1.00	27.12		C
ANISOU	81	CB	ALA A	40	3481	4477	2347	779	453	−68	C
ATOM	82	N	LEU A	41	−28.763	27.265	14.773	1.00	22.38		N
ANISOU	82	N	LEU A	41	3710	3141	1654	471	98	151	N

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	83	CA	LEU A	41	−28.443	27.908	13.502	1.00	20.19		C
ANISOU	83	CA	LEU A	41	3380	2378	1914	293	−187	−52	C
ATOM	84	C	LEU A	41	−26.971	28.250	13.448	1.00	21.56		C
ANISOU	84	C	LEU A	41	3473	2921	1796	−102	−124	−301	C
ATOM	85	O	LEU A	41	−26.451	28.944	14.326	1.00	24.54		O
ANISOU	85	O	LEU A	41	3684	3336	2304	−143	390	−630	O
ATOM	86	CB	LEU A	41	−29.258	29.194	13.339	1.00	21.12		C
ANISOU	86	CB	LEU A	41	3244	2777	2006	303	189	393	C
ATOM	87	CG	LEU A	41	−28.938	30.068	12.099	1.00	23.28		C
ANISOU	87	CG	LEU A	41	3860	2574	2411	255	142	243	C
ATOM	88	CD1	LEU A	41	−29.214	29.331	10.782	1.00	22.84		C
ANISOU	88	CD1	LEU A	41	3378	3307	1993	46	−395	190	C
ATOM	89	CD2	LEU A	41	−29.664	31.402	12.148	1.00	26.07		C
ANISOU	89	CD2	LEU A	41	4385	2593	2927	435	−414	−23	C
ATOM	90	N	LEU A	42	−26.292	27.748	12.415	1.00	19.00		N
ANISOU	90	N	LEU A	42	2746	2694	1778	43	−86	−24	N
ATOM	91	C	LEU A	42	−24.733	28.730	10.839	1.00	19.27		C
ANISOU	91	C	LEU A	42	3071	2391	1858	−30	386	91	C
ATOM	92	O	LEU A	42	−25.161	28.204	9.803	1.00	20.72		O
ANISOU	92	O	LEU A	42	3025	3024	1824	−33	−265	−161	O
ATOM	93	CD1	LEU A	42	−21.882	27.647	12.991	1.00	32.06		C
ANISOU	93	CD1	LEU A	42	3249	5651	3281	159	−669	−369	C
ATOM	94	CD2	LEU A	42	−22.065	25.304	12.149	1.00	30.38		C
ANISOU	94	CD2	LEU A	42	4172	4881	2490	1858	−365	−173	C
ATOM	95	CA	LEU A	42	−24.879	28.019	12.178	1.00	19.23		C
ANISOU	95	CA	LEU A	42	2674	2722	1910	−63	50	−111	C
ATOM	96	CB	LEU A	42	−24.106	26.710	12.170	1.00	24.94		C
ANISOU	96	CB	LEU A	42	3435	3581	2460	1004	−1	−442	C
ATOM	97	CG	LEU A	42	−22.587	26.731	11.994	1.00	26.64		C
ANISOU	97	CG	LEU A	42	3177	4266	2680	613	−258	−318	C
ATOM	98	N	VAL A	43	−24.175	29.933	10.855	1.00	21.69		N
ANISOU	98	N	VAL A	43	3097	2560	2585	303	−126	298	N
ATOM	99	CA	VAL A	43	−23.993	30.701	9.631	1.00	21.50		C
ANISOU	99	CA	VAL A	43	3240	2071	2859	309	−528	26	C
ATOM	100	C	VAL A	43	−22.515	30.842	9.375	1.00	23.88		C
ANISOU	100	C	VAL A	43	3547	2558	2970	79	−270	−433	C
ATOM	101	O	VAL A	43	−21.786	31.299	10.246	1.00	27.58		O
ANISOU	101	O	VAL A	43	3650	3699	3130	−529	44	−732	O
ATOM	102	CB	VAL A	43	−24.603	32.105	9.755	1.00	24.41		C
ANISOU	102	CB	VAL A	43	3490	2727	3057	67	−103	393	C
ATOM	103	CG1	VAL A	43	−24.418	32.878	8.433	1.00	28.27		C
ANISOU	103	CG1	VAL A	43	4208	3064	3470	359	149	648	C
ATOM	104	CG2	VAL A	43	−26.086	32.003	10.153	1.00	26.73		C
ANISOU	104	CG2	VAL A	43	3574	3309	3273	208	−309	160	C
ATOM	105	N	VAL A	44	−22.061	30.408	8.202	1.00	22.26		N
ANISOU	105	N	VAL A	44	2961	2776	2722	−42	15	−314	N
ATOM	106	CA	VAL A	44	−20.646	30.481	7.852	1.00	22.76		C
ANISOU	106	CA	VAL A	44	3092	2816	2738	−41	156	372	C
ATOM	107	C	VAL A	44	−20.518	31.005	6.429	1.00	22.60		C
ANISOU	107	C	VAL A	44	3086	2715	2787	−371	97	749	C
ATOM	108	O	VAL A	44	−21.487	31.009	5.672	1.00	25.09		O
ANISOU	108	O	VAL A	44	2954	3568	3012	−243	−511	683	O
ATOM	109	CB	VAL A	44	−19.925	29.101	7.961	1.00	23.66		C
ANISOU	109	CB	VAL A	44	4296	2293	2401	−43	−172	129	C
ATOM	110	CG1	VAL A	44	−20.102	28.511	9.353	1.00	26.79		C
ANISOU	110	CG1	VAL A	44	4403	3453	2323	818	95	707	C
ATOM	111	CG2	VAL A	44	−20.436	28.119	6.934	1.00	25.41		C
ANISOU	111	CG2	VAL A	44	5020	2275	2361	207	−247	−241	C
ATOM	112	N	ATHR A	45	−19.312	31.451	6.082	0.58	25.11		N
ANISOU	112	N	ATHR A	45	3256	3112	3171	−605	−172	717	N
ATOM	113	CA	ATHR A	45	−19.022	31.961	4.750	0.58	25.13		C
ANISOU	113	CA	ATHR A	45	3571	2435	3544	−764	−39	944	C
ATOM	114	C	ATHR A	45	−18.455	30.817	3.929	0.58	24.21		C
ANISOU	114	C	ATHR A	45	3450	2534	3215	−477	−241	1296	C
ATOM	115	O	ATHR A	45	−17.655	30.031	4.438	0.58	24.40		O
ANISOU	115	O	ATHR A	45	3271	2757	3244	−61	−186	1292	O
ATOM	116	CB	ATHR A	45	−17.985	33.107	4.811	0.58	28.30		C
ANISOU	116	CB	ATHR A	45	3785	2904	4064	−784	119	573	C
ATOM	117	OG1	ATHR A	45	−18.391	34.091	5.777	0.58	28.86		O
ANISOU	117	OG1	ATHR A	45	3705	3125	4136	−168	−215	267	O
ATOM	118	CG2	ATHR A	45	−17.808	33.770	3.434	0.58	28.67		C
ANISOU	118	CG2	ATHR A	45	3993	2608	4291	−921	443	934	C
ATOM	119	N	BTHR A	45	−19.334	31.461	6.031	0.42	25.74		N
ANISOU	119	N	BTHR A	45	3408	3262	3109	−824	−52	714	N

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	120	CA	BTHR A	45	−19.164	31.872	4.635	0.42	27.81		C
ANISOU	120	CA	BTHR A	45	3803	3292	3471	−805	−84	727	C
ATOM	121	C	BTHR A	45	−18.582	30.727	3.818	0.42	27.25		C
ANISOU	121	C	BTHR A	45	3384	3840	3129	−927	−111	905	C
ATOM	122	O	BTHR A	45	−17.925	29.842	4.364	0.42	26.31		O
ANISOU	122	O	BTHR A	45	3026	4011	2958	−1147	190	1007	O
ATOM	123	CB	BTHR A	45	−18.283	33.130	4.482	0.42	32.37		C
ANISOU	123	CB	BTHR A	45	4524	3726	4047	4	−302	577	C
ATOM	124	OG1	BTHR A	45	−16.997	32.889	5.056	0.42	34.11		O
ANISOU	124	OG1	BTHR A	45	4492	4153	4315	−255	−560	698	O
ATOM	125	CG2	BTHR A	45	−18.910	34.313	5.179	0.42	32.09		C
ANISOU	125	CG2	BTHR A	45	4916	3070	4206	1119	−745	508	C
ATOM	126	N	AGLU A	46	−18.870	30.713	2.670	0.58	26.06		N
ANISOU	126	N	AGLU A	46	3778	3222	2902	−39	−388	1324	N
ATOM	127	C	AGLU A	46	−16.838	29.567	1.855	0.58	25.90		C
ANISOU	127	C	AGLU A	46	3479	3836	2524	−702	−163	827	C
ATOM	128	O	AGLU A	46	−16.135	30.581	1.892	0.58	24.57		O
ANISOU	128	O	AGLU A	46	3633	2839	2865	−583	43	527	O
ATOM	129	CD	AGLU A	46	−18.932	31.333	−1.730	0.58	42.11		C
ANISOU	129	CD	AGLU A	46	6661	6106	3233	315	−229	1203	C
ATOM	130	OE1	AGLU A	46	−19.035	30.320	−2.456	0.58	42.51		O
ANISOU	130	OE1	AGLU A	46	6736	5977	3440	−1097	−212	1386	O
ATOM	131	OE2	AGLU A	46	−19.252	32.478	−2.116	0.58	45.21		O
ANISOU	131	OE2	AGLU A	46	7058	7012	3107	1316	−353	1088	O
ATOM	132	CG	AGLU A	46	−18.386	31.159	−0.311	0.58	38.08		C
ANISOU	132	CG	AGLU A	46	5954	5336	3177	734	−119	1403	C
ATOM	133	CA	AGLU A	46	−18.363	29.665	1.789	0.58	27.90		C
ANISOU	133	CA	AGLU A	46	3813	4040	2749	−117	−369	1042	C
ATOM	134	CB	AGLU A	46	−18.847	29.875	0.337	0.58	33.23		C
ANISOU	134	CB	AGLU A	46	5094	4514	3017	548	−126	1301	C
ATOM	135	N	BGLU A	46	−18.830	30.742	2.512	0.42	28.35		N
ANISOU	135	N	BGLU A	46	3447	4309	3015	−878	−506	814	N
ATOM	136	C	BGLU A	46	−16.824	29.565	1.756	0.42	26.37		C
ANISOU	136	C	BGLU A	46	3221	4440	2359	−1078	−338	1036	C
ATOM	137	O	BGLU A	46	−16.109	30.569	1.737	0.42	27.79		O
ANISOU	137	O	BGLU A	46	3360	4830	2370	−668	−244	1392	O
ATOM	138	CD	BGLU A	46	−19.653	28.824	−1.999	0.42	39.10		C
ANISOU	138	CD	BGLU A	46	5062	6154	3642	−529	−737	2020	C
ATOM	139	OE1	BGLU A	46	−19.810	29.987	−2.432	0.42	43.16		O
ANISOU	139	OE1	BGLU A	46	5577	6957	3867	−574	−804	2120	O
ATOM	140	OE2	BGLU A	46	−20.039	27.807	−2.633	0.42	34.63		O
ANISOU	140	OE2	BGLU A	46	4088	5406	3663	−1665	−247	2168	O
ATOM	141	CG	BGLU A	46	−18.964	28.633	−0.642	0.42	39.17		C
ANISOU	141	CG	BGLU A	46	5385	6075	3422	−47	−875	1363	C
ATOM	142	CA	BGLU A	46	−18.343	29.683	1.634	0.42	29.14		C
ANISOU	142	CA	BGLU A	46	3532	4723	2818	−1023	−588	924	C
ATOM	143	CB	BGLU A	46	−18.778	29.926	0.169	0.42	34.14		C
ANISOU	143	CB	BGLU A	46	4742	5118	3112	−313	−740	1260	C
ATOM	144	N	GLY A	47	−16.336	28.339	1.924	1.00	25.60		N
ANISOU	144	N	GLY A	47	3084	4465	2176	−480	149	925	N
ATOM	145	CA	GLY A	47	−14.915	28.127	2.064	1.00	24.50		C
ANISOU	145	CA	GLY A	47	2722	4641	1947	59	158	734	C
ATOM	146	C	GLY A	47	−14.499	27.850	3.507	1.00	22.87		C
ANISOU	146	C	GLY A	47	2501	4179	2009	−622	−248	478	C
ATOM	147	O	GLY A	47	−13.474	27.227	3.731	1.00	26.21		O
ANISOU	147	O	GLY A	47	2651	4800	2509	−426	−145	611	O
ATOM	148	N	AASP A	48	−15.297	28.310	4.467	0.65	22.60		N
ANISOU	148	N	AASP A	48	2947	3607	2032	−245	208	1095	N
ATOM	149	C	AASP A	48	−15.371	26.667	6.310	0.65	19.68		C
ANISOU	149	C	AASP A	48	2497	2927	2053	−392	−28	254	C
ATOM	150	O	AASP A	48	−16.083	25.950	5.636	0.65	24.35		O
ANISOU	150	O	AASP A	48	2970	3949	2332	−442	−778	262	O
ATOM	151	CA	AASP A	48	−14.985	28.074	5.870	0.65	19.93		C
ANISOU	151	CA	AASP A	48	2687	2951	1937	17	−248	434	C
ATOM	152	CB	AASP A	48	−15.719	29.071	6.760	0.65	25.63		C
ANISOU	152	CB	AASP A	48	4691	2791	2258	538	−271	−200	C
ATOM	153	CG	AASP A	48	−15.232	30.504	6.568	0.65	33.29		C
ANISOU	153	CG	AASP A	48	6202	3260	3187	2073	−1021	−390	C
ATOM	154	OD1	AASP A	48	−14.173	30.702	5.938	0.65	35.52		O
ANISOU	154	OD1	AASP A	48	6471	3105	3919	430	−1652	−118	O
ATOM	155	OD2	AASP A	48	−15.912	31.432	7.051	0.65	45.53		O
ANISOU	155	OD2	AASP A	48	8640	4673	3987	2824	−1288	−403	O
ATOM	156	N	BASP A	48	−15.274	28.336	4.479	0.35	24.42		N
ANISOU	156	N	BASP A	48	3254	3720	2303	−168	17	354	N

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	157	C	BASP A	48	−15.365	26.720	6.323	0.35	21.83		C
ANISOU	157	C	BASP A	48	3011	3003	2280	−573	213	358	C
ATOM	158	O	BASP A	48	−16.116	26.047	5.635	0.35	23.09		O
ANISOU	158	O	BASP A	48	3478	2705	2590	−1134	157	732	O
ATOM	159	CA	BASP A	48	−14.962	28.126	5.901	0.35	24.28		C
ANISOU	159	CA	BASP A	48	3535	3277	2414	−138	−13	269	C
ATOM	160	CB	BASP A	48	−15.712	29.142	6.774	0.35	30.12		C
ANISOU	160	CB	BASP A	48	5048	3562	2833	816	−62	−91	C
ATOM	161	CG	BASP A	48	−15.222	29.166	8.234	0.35	35.60		C
ANISOU	161	CG	BASP A	48	6143	3960	3422	2179	−268	−357	C
ATOM	162	OD1	BASP A	48	−14.143	28.607	8.536	0.35	34.05		O
ANISOU	162	OD1	BASP A	48	6160	3242	3535	1756	−524	−86	O
ATOM	163	OD2	BASP A	48	−15.915	29.764	9.089	0.35	42.66		O
ANISOU	163	OD2	BASP A	48	7123	5095	3992	3325	−485	−999	O
ATOM	164	N	ASN A	49	−14.861	26.256	7.459	1.00	19.71		N
ANISOU	164	N	ASN A	49	2473	3228	1789	−28	216	335	N
ATOM	165	C	ASN A	49	−16.593	25.293	8.848	1.00	20.19		C
ANISOU	165	C	ASN A	49	2582	3254	1837	−123	256	108	C
ATOM	166	O	ASN A	49	−16.840	26.429	9.225	1.00	22.09		O
ANISOU	166	O	ASN A	49	3074	3224	2094	−385	501	408	O
ATOM	167	CA	AASN A	49	−15.329	25.021	8.074	0.76	17.58		C
ANISOU	167	CA	AASN A	49	2115	2662	1901	−42	172	459	C
ATOM	168	OD1	AASN A	49	−13.020	23.767	7.187	0.76	23.75		O
ANISOU	168	OD1	AASN A	49	2516	3564	2942	−206	597	−187	O
ATOM	169	ND2	AASN A	49	−11.865	24.326	9.020	0.76	23.19		N
ANISOU	169	ND2	AASN A	49	2680	3748	2386	689	−29	720	N
ATOM	170	CB	AASN A	49	−14.264	24.499	9.038	0.76	21.43		C
ANISOU	170	CB	AASN A	49	2486	3403	2253	41	131	568	C
ATOM	171	CG	AASN A	49	−12.992	24.156	8.341	0.76	21.57		C
ANISOU	171	CG	AASN A	49	2632	3126	2437	356	422	348	C
ATOM	172	CA	BASN A	49	−15.375	25.006	7.983	0.24	18.26		C
ANISOU	172	CA	BASN A	49	2329	2832	1776	−81	−12	57	C
ATOM	173	OD1	BASN A	49	−14.105	25.588	10.650	0.24	21.94		O
ANISOU	173	OD1	BASN A	49	2934	3450	1953	−231	−787	522	O
ATOM	174	ND2	BASN A	49	−12.206	25.064	9.582	0.24	17.39		N
ANISOU	174	ND2	BASN A	49	2074	2345	2188	−48	−287	89	N
ATOM	175	CB	BASN A	49	−14.298	24.194	8.722	0.24	18.84		C
ANISOU	175	CB	BASN A	49	2475	2796	1889	221	−437	−372	C
ATOM	176	CG	BASN A	49	−13.527	25.017	9.736	0.24	18.35		C
ANISOU	176	CG	BASN A	49	2388	2573	2010	−227	−387	39	C
ATOM	177	N	ALA A	50	−17.380	24.264	9.102	1.00	18.96		N
ANISOU	177	N	ALA A	50	2511	2545	2150	−300	582	292	N
ATOM	178	CA	ALA A	50	−18.563	24.443	9.937	1.00	19.41		C
ANISOU	178	CA	ALA A	50	2594	2643	2139	−84	745	412	C
ATOM	179	C	ALA A	50	−18.640	23.264	10.885	1.00	19.32		C
ANISOU	179	C	ALA A	50	3052	2436	1852	−375	368	123	C
ATOM	180	O	ALA A	50	−18.538	22.132	10.451	1.00	20.58		O
ANISOU	180	O	ALA A	50	3728	2504	1588	5	658	134	O
ATOM	181	CB	ALA A	50	−19.835	24.519	9.080	1.00	23.14		C
ANISOU	181	CB	ALA A	50	2801	3481	2508	195	465	356	C
ATOM	182	N	THR A	51	−18.863	23.529	12.175	1.00	18.79		N
ANISOU	182	N	THR A	51	2429	2755	1957	−135	371	292	N
ATOM	183	C	THR A	51	−20.128	22.564	14.065	1.00	17.40		C
ANISOU	183	C	THR A	51	2125	2905	1580	−119	356	300	C
ATOM	184	O	THR A	51	−20.348	23.586	14.698	1.00	20.69		O
ANISOU	184	O	THR A	51	2698	3083	2079	−112	364	−1	O
ATOM	185	CA	THR A	51	−18.895	22.465	13.181	1.00	17.49		C
ANISOU	185	CA	THR A	51	2041	2661	1945	−284	−64	319	C
ATOM	186	CB	THR A	51	−17.628	22.488	14.066	1.00	20.21		C
ANISOU	186	CB	THR A	51	2247	3169	2264	−264	28	320	C
ATOM	187	OG1	THR A	51	−16.486	22.283	13.220	1.00	23.51		O
ANISOU	187	OG1	THR A	51	2846	3604	2483	−156	293	−54	O
ATOM	188	CG2	THR A	51	−17.676	21.392	15.127	1.00	21.96		C
ANISOU	188	CG2	THR A	51	2415	3488	2441	−371	−175	598	C
ATOM	189	N	PHE A	52	−20.931	21.503	14.086	1.00	16.27		N
ANISOU	189	N	PHE A	52	1851	2837	1495	−235	164	342	N
ATOM	190	CA	PHE A	52	−22.002	21.329	15.059	1.00	16.43		C
ANISOU	190	CA	PHE A	52	2151	2445	1649	−23	−92	376	C
ATOM	191	C	PHE A	52	−21.490	20.450	16.172	1.00	15.77		C
ANISOU	191	C	PHE A	52	2256	2291	1446	−14	−10	157	C
ATOM	192	O	PHE A	52	−20.551	19.675	16.001	1.00	17.77		O
ANISOU	192	O	PHE A	52	2550	2478	1723	112	−47	76	O
ATOM	193	CB	PHE A	52	−23.204	20.629	14.445	1.00	16.69		C
ANISOU	193	CB	PHE A	52	2105	2370	1866	−148	−361	68	C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	194	CG	PHE A	52	−23.901	21.418	13.371	1.00	18.07		C
ANISOU	194	CG	PHE A	52	2395	2885	1587	86	37	420	C
ATOM	195	CD1	PHE A	52	−23.722	21.120	12.023	1.00	22.08		C
ANISOU	195	CD1	PHE A	52	3299	3379	1712	205	100	473	C
ATOM	196	CD2	PHE A	52	−24.789	22.434	13.710	1.00	17.47		C
ANISOU	196	CD2	PHE A	52	2173	2461	2005	133	−169	530	C
ATOM	197	CE1	PHE A	52	−24.438	21.817	11.058	1.00	24.07		C
ANISOU	197	CE1	PHE A	52	3755	3513	1878	892	438	397	C
ATOM	198	CE2	PHE A	52	−25.480	23.128	12.740	1.00	20.34		C
ANISOU	198	CE2	PHE A	52	2935	3235	1559	257	−68	375	C
ATOM	199	CZ	PHE A	52	−25.294	22.828	11.416	1.00	23.73		C
ANISOU	199	CZ	PHE A	52	3538	4003	1476	816	161	449	C
ATOM	200	N	THR A	53	−22.125	20.574	17.331	1.00	17.89		N
ANISOU	200	N	THR A	53	2557	2970	1270	13	89	198	N
ATOM	201	C	THR A	53	−23.014	18.850	18.804	1.00	18.88		C
ANISOU	201	C	THR A	53	2732	2876	1567	72	318	259	C
ATOM	202	O	THR A	53	−24.093	19.370	19.067	1.00	19.29		O
ANISOU	202	O	THR A	53	2312	3063	1954	218	162	115	O
ATOM	203	CA	THR A	53	−21.804	19.691	18.449	1.00	18.70		C
ANISOU	203	CA	THR A	53	2888	3065	1151	−231	−149	124	C
ATOM	204	CB	THR A	53	−21.351	20.487	19.689	1.00	21.27		C
ANISOU	204	CB	THR A	53	3213	3309	1559	−398	−242	222	C
ATOM	205	OG1	THR A	53	−20.186	21.244	19.354	1.00	24.52		O
ANISOU	205	OG1	THR A	53	3505	3697	2116	−735	−349	74	O
ATOM	206	CG2	THR A	53	−20.976	19.556	20.870	1.00	25.04		C
ANISOU	206	CG2	THR A	53	3909	3789	1814	−80	−436	330	C
ATOM	207	N	CYS A	54	−22.827	17.541	18.773	1.00	18.66		N
ANISOU	207	N	CYS A	54	1992	3186	1912	−41	−36	824	N
ATOM	208	C	CYS A	54	−23.446	16.119	20.618	1.00	20.94		C
ANISOU	208	C	CYS A	54	2377	3427	2154	208	309	660	C
ATOM	209	O	CYS A	54	−22.325	15.686	20.813	1.00	23.39		O
ANISOU	209	O	CYS A	54	2485	4082	2319	598	276	800	O
ATOM	210	CA	ACYS A	54	−23.832	16.589	19.223	0.75	19.79		C
ANISOU	210	CA	ACYS A	54	2285	3111	2122	−99	359	40	C
ATOM	211	CB	ACYS A	54	−23.847	15.385	18.261	0.75	21.16		C
ANISOU	211	CB	ACYS A	54	2873	2464	2703	−89	497	18	C
ATOM	212	SG	ACYS A	54	−25.000	14.041	18.736	0.75	28.05		S
ANISOU	212	SG	ACYS A	54	4084	2849	3723	424	1078	251	S
ATOM	213	CA	BCYS A	54	−23.835	16.610	19.228	0.25	18.74		C
ANISOU	213	CA	BCYS A	54	1898	3297	1923	−31	−58	700	C
ATOM	214	CB	BCYS A	54	−23.911	15.442	18.254	0.25	16.94		C
ANISOU	214	CB	BCYS A	54	1583	3121	1734	−62	−584	873	C
ATOM	215	SG	BCYS A	54	−25.284	14.348	18.558	0.25	18.10		S
ANISOU	215	SG	BCYS A	54	1810	3267	1801	−176	−839	636	S
ATOM	216	N	SER A	55	−24.380	16.202	21.571	1.00	20.54		N
ANISOU	216	N	SER A	55	2347	3805	1654	6	−15	433	N
ATOM	217	C	SER A	55	−24.972	14.568	23.249	1.00	21.69		C
ANISOU	217	C	SER A	55	2217	4285	1739	−527	−182	643	C
ATOM	218	O	SER A	55	−26.183	14.575	23.015	1.00	23.95		O
ANISOU	218	O	SER A	55	2356	4217	2526	147	−76	1094	O
ATOM	219	CA	ASER A	55	−24.117	15.779	22.947	0.63	20.27		C
ANISOU	219	CA	ASER A	55	2377	3968	1357	−156	393	15	C
ATOM	220	CB	ASER A	55	−24.425	16.882	23.963	0.63	23.07		C
ANISOU	220	CB	ASER A	55	3136	3939	1690	−281	376	322	C
ATOM	221	OG	ASER A	55	−23.611	18.004	23.698	0.63	26.53		O
ANISOU	221	OG	ASER A	55	3951	3913	2215	−100	46	94	O
ATOM	222	CA	BSER A	55	−24.131	15.798	22.946	0.37	23.08		C
ANISOU	222	CA	BSER A	55	2792	4282	1695	66	−60	120	C
ATOM	223	CB	BSER A	55	−24.510	16.927	23.900	0.37	29.58		C
ANISOU	223	CB	BSER A	55	3989	5163	2086	773	−291	−52	C
ATOM	224	OG	BSER A	55	−24.154	16.607	25.227	0.37	34.88		O
ANISOU	224	OG	BSER A	55	4949	5865	2438	1337	−645	−542	O
ATOM	225	N	PHE A	56	−24.339	13.511	23.746	1.00	21.58		N
ANISOU	225	N	PHE A	56	2556	3987	1657	−17	45	600	N
ATOM	226	CA	PHE A	56	−25.072	12.276	23.950	1.00	21.23		C
ANISOU	226	CA	PHE A	56	2336	3971	1761	333	280	301	C
ATOM	227	C	PHE A	56	−24.508	11.559	25.143	1.00	25.58		C
ANISOU	227	C	PHE A	56	2957	4462	2299	261	24	783	C
ATOM	228	O	PHE A	56	−23.326	11.259	25.199	1.00	25.38		O
ANISOU	228	O	PHE A	56	3152	3768	2725	161	−591	622	O
ATOM	229	CB	PHE A	56	−24.960	11.368	22.717	1.00	22.98		C
ANISOU	229	CB	PHE A	56	2926	3682	2124	552	481	138	C
ATOM	230	CG	PHE A	56	−25.627	10.038	22.891	1.00	22.10		C
ANISOU	230	CG	PHE A	56	3154	3462	1780	632	214	220	C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	231	CD1	PHE A	56	−27.007	9.955	23.047	1.00	23.78		C
ANISOU	231	CD1	PHE A	56	3384	3856	1796	281	284	430	C
ATOM	232	CD2	PHE A	56	−24.882	8.871	22.925	1.00	24.70		C
ANISOU	232	CD2	PHE A	56	3554	3699	2133	600	60	−299	C
ATOM	233	CE1	PHE A	56	−27.640	8.713	23.207	1.00	24.74		C
ANISOU	233	CE1	PHE A	56	3504	3764	2131	767	−109	76	C
ATOM	234	CE2	PHE A	56	−25.491	7.628	23.078	1.00	26.53		C
ANISOU	234	CE2	PHE A	56	3852	4022	2208	992	−36	−175	C
ATOM	235	CZ	PHE A	56	−26.883	7.536	23.229	1.00	25.80		C
ANISOU	235	CZ	PHE A	56	3682	4125	1995	578	193	−96	C
ATOM	236	O	SER A	57	−26.560	8.805	27.017	1.00	36.59		O
ANISOU	236	O	SER A	57	5426	4898	3580	169	−254	1075	O
ATOM	237	N	SER A	57	−25.383	11.315	26.086	1.00	28.19		N
ANISOU	237	N	SER A	57	4093	4177	2440	344	255	1314	N
ATOM	238	C	SER A	57	−25.423	8.949	27.327	1.00	36.44		C
ANISOU	238	C	SER A	57	5525	5136	3183	674	−531	202	C
ATOM	239	CA	ASER A	57	−24.962	10.572	27.3030	0.58	36.34		C
ANISOU	239	CA	ASER A	57	559	4910	3041	1279	97	635	C
ATOM	240	CB	ASER A	57	−25.645	11.205	28.517	0.58	42.64		C
ANISOU	240	CB	ASER A	57	7399	5326	3475	2220	−87	−24	C
ATOM	241	OG	ASER A	57	−25.300	12.576	28.633	0.58	42.98		O
ANISOU	241	OG	ASER A	57	7946	4967	3418	2929	−295	−828	O
ATOM	242	CA	BSER A	57	−24.949	10.568	27.290	0.42	35.14		C
ANISOU	242	CA	BSER A	57	5347	5149	2856	796	146	1299	C
ATOM	243	CB	BSER A	57	−25.602	11.204	28.507	0.42	38.96		C
ANISOU	243	CB	BSER A	57	5926	5936	2940	812	261	1992	C
ATOM	244	OG	BSER A	57	−27.006	11.149	28.390	0.42	39.13		O
ANISOU	244	OG	BSER A	57	5539	6401	2928	529	101	2149	O
ATOM	245	O	ASN A	58	−25.004	6.449	28.983	1.00	37.84		O
ANISOU	245	O	ASN A	58	7229	3929	3219	530	−1977	−322	O
ATOM	246	N	ASN A	58	−24.459	8.132	26.972	1.00	38.69		N
ANISOU	246	N	ASN A	58	5983	5713	3006	427	−1083	−553	N
ATOM	247	C	ASN A	58	−25.150	5.985	27.899	1.00	34.43		C
ANISOU	247	C	ASN A	58	5486	4363	3232	−156	−1779	167	C
ATOM	248	CA	ASN A	58	−24.736	6.753	26.676	1.00	38.79		C
ANISOU	248	CA	ASN A	58	5811	5443	3484	350	−1094	−320	C
ATOM	249	CB	ASN A	58	−23.578	6.060	26.021	1.00	39.67		C
ANISOU	249	CB	ASN A	58	5592	5720	3763	−274	−579	−39	C
ATOM	250	CG	ASN A	58	−22.264	6.397	26.642	1.00	44.41		C
ANISOU	250	CG	ASN A	58	6590	6063	4220	834	−341	464	C
ATOM	251	OD1	ASN A	58	−21.874	7.520	26.681	1.00	46.73		O
ANISOU	251	OD1	ASN A	58	6786	6306	4662	683	−157	427	O
ATOM	252	ND2	ASN A	58	−21.554	5.399	27.060	1.00	42.66		N
ANISOU	252	ND2	ASN A	58	6985	5339	3884	884	−572	1128	N
ATOM	253	O	THR A	59	−23.731	3.373	28.098	1.00	33.37		O
ATOM	254	N	THR A	59	−25.762	4.855	27.658	1.00	33.61		N
ATOM	255	CA	THR A	59	−25.970	3.807	28.608	1.00	35.90		C
ATOM	256	C	THR A	59	−24.703	3.042	28.699	1.00	27.20		C
ATOM	257	CB	THR A	59	−27.142	2.896	28.200	1.00	48.98		C
ATOM	258	OG1	THR A	59	−26.898	2.353	26.898	1.00	48.93		O
ATOM	259	CG2	THR A	59	−28.411	3.713	28.006	1.00	56.40		C
ATOM	260	N	SER A	60	−24.739	1.978	29.446	1.00	36.19		N
ANISOU	260	N	SER A	60	6165	4140	3447	1065	−1646	−687	N
ATOM	261	C	SER A	60	−23.125	0.606	27.786	1.00	41.91		C
ANISOU	261	C	SER A	60	6752	5724	3448	1045	−285	41	C
ATOM	262	O	SER A	60	−22.334	−0.279	27.866	1.00	46.82		O
ANISOU	262	O	SER A	60	7408	6950	3430	1055	−761	678	O
ATOM	263	CA	SER A	60	−23.429	1.195	29.347	1.00	40.15		C
ANISOU	263	CA	SER A	60	6058	5185	4012	1849	−1000	−139	C
ATOM	264	CB	SER A	60	−23.436	0.031	30.340	1.00	46.31		C
ATOM	265	OG	SER A	60	−23.462	0.500	31.676	1.00	87.22		O
ATOM	266	O	GLU A	61	−23.745	1.380	24.715	1.00	28.36		O
ANISOU	266	O	GLU A	61	4989	3780	2008	−311	−244	−68	O
ATOM	267	N	GLU A	61	−24.292	0.450	27.204	1.00	35.39		N
ANISOU	267	N	GLU A	61	6241	4573	2632	−468	426	164	N
ATOM	268	CA	GLU A	61	−24.403	−0.421	26.068	1.00	36.09		C
ANISOU	268	CA	GLU A	61	6984	4145	2586	−495	636	171	C
ATOM	269	C	GLU A	61	−23.851	0.206	24.811	1.00	32.43		C
ANISOU	269	C	GLU A	61	6059	3869	2392	−29	−216	−33	C
ATOM	270	CB	GLU A	61	−25.820	−0.873	25.884	1.00	40.27		C
ANISOU	270	CB	GLU A	61	7762	4520	3019	−1470	1112	216	C
ATOM	271	CG	GLU A	61	−26.306	−1.785	27.011	1.00	48.39		C
ANISOU	271	CG	GLU A	61	9067	5656	3663	−678	1691	90	C
ATOM	272	CD	GLU A	61	−25.289	−2.840	27.427	1.00	57.83		C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	272	CD	GLU A	61	10504	6967	4500	499	1573	−288	C
ATOM	273	OE1	GLU A	61	−25.136	−3.818	26.707	1.00	59.54		O
ANISOU	273	OE1	GLU A	61	10799	6776	5049	1045	1544	−545	O
ATOM	274	OE2	GLU A	61	−24.642	−2.731	28.479	1.00	63.24		O
ANISOU	274	OE2	GLU A	61	11063	8024	4941	691	1232	−304	O
ATOM	275	N	SER A	62	−23.496	0.642	23.870	1.00	30.03		N
ANISOU	275	N	SER A	62	5078	3885	2447	284	−7	115	N
ATOM	276	C	SER A	62	−23.900	0.717	21.863	1.00	22.91		C
ANISOU	276	C	SER A	62	4253	2375	2078	−125	−59	101	C
ATOM	277	O	SER A	62	−25.111	0.522	21.914	1.00	25.03		O
ANISOU	277	O	SER A	62	4593	2868	2049	−233	−12	393	O
ATOM	278	CA	ASER A	62	−22.952	−0.209	22.583	0.75	25.32		C
ANISOU	278	CA	ASER A	62	5079	2247	2295	77	−257	158	C
ATOM	279	CB	ASER A	62	−22.746	−1.426	21.685	0.75	26.51		C
ANISOU	279	CB	ASER A	62	5064	2376	2634	443	−433	−94	C
ATOM	280	OG	ASER A	62	−21.953	−2.396	22.324	0.75	29.08		O
ANISOU	280	OG	ASER A	62	5016	3192	2839	188	−50	206	O
ATOM	281	CA	BSER A	62	−22.931	−0.187	22.609	0.25	28.34		C
ANISOU	281	CA	BSER A	62	5058	3443	2268	127	−70	291	C
ATOM	282	CB	BSER A	62	−22.584	−1.386	21.735	0.25	31.99		C
ANISOU	282	CB	BSER A	62	5478	4302	2374	124	−145	506	C
ATOM	283	OG	BSER A	62	−23.730	−2.188	21.532	0.25	34.84		O
ANISOU	283	OG	BSER A	62	5926	4950	2362	44	−120	901	O
ATOM	284	N	PHE A	63	−23.349	1.690	21.144	1.00	20.93		N
ANISOU	284	N	PHE A	63	3727	2789	1438	332	−270	10	N
ATOM	285	CA	PHE A	63	−24.170	2.619	20.363	1.00	19.10		C
ANISOU	285	CA	PHE A	63	3155	2539	1564	192	58	215	C
ATOM	286	C	PHE A	63	−23.412	3.072	19.118	1.00	19.71		C
ANISOU	286	C	PHE A	63	3196	2796	1495	138	−75	−93	C
ATOM	287	O	PHE A	63	−22.211	2.936	19.019	1.00	21.47		O
ANISOU	287	O	PHE A	63	3340	3181	1638	627	−68	−94	O
ATOM	288	CB	PHE A	63	−24.592	3.847	21.194	1.00	21.69		C
ANISOU	288	CB	PHE A	63	3646	2488	2107	−141	280	−553	C
ATOM	289	CG	PHE A	63	−23.452	4.731	21.596	1.00	21.93		C
ANISOU	289	CG	PHE A	63	3665	2561	2107	251	428	−15	C
ATOM	290	CD1	PHE A	63	−23.135	5.853	20.855	1.00	20.38		C
ANISOU	290	CD1	PHE A	63	3111	2473	2159	201	−187	−281	C
ATOM	291	CD2	PHE A	63	−22.696	4.447	22.743	1.00	24.22		C
ANISOU	291	CD2	PHE A	63	3884	3142	2176	221	136	−15	C
ATOM	292	CE1	PHE A	63	−22.108	6.695	21.237	1.00	22.60		C
ANISOU	292	CE1	PHE A	63	3640	2966	1979	220	202	−195	C
ATOM	293	CE2	PHE A	63	−21.644	5.282	23.126	1.00	22.98		C
ANISOU	293	CE2	PHE A	63	3654	3102	1976	155	−161	225	C
ATOM	294	CZ	PHE A	63	−21.355	6.421	22.356	1.00	25.17		C
ANISOU	294	CZ	PHE A	63	4351	3336	1877	22	−227	48	C
ATOM	295	N	VAL A	64	−24.155	3.623	18.176	1.00	19.04		N
ANISOU	295	N	VAL A	64	2901	2997	1335	−41	−103	203	N
ATOM	296	CA	VAL A	64	−23.607	4.315	17.020	1.00	19.45		C
ANISOU	296	CA	VAL A	64	3380	2611	1397	326	−0	291	C
ATOM	297	C	VAL A	64	−24.264	5.706	16.999	1.00	17.21		C
ANISOU	297	C	VAL A	64	2355	2399	1784	−395	164	493	C
ATOM	298	O	VAL A	64	−25.468	5.838	17.267	1.00	20.34		O
ANISOU	298	O	VAL A	64	2595	2706	2427	−183	182	351	O
ATOM	299	CB	VAL A	64	−23.972	3.535	15.734	1.00	20.05		C
ANISOU	299	CB	VAL A	64	3554	2403	1662	188	475	521	C
ATOM	300	CG1	VAL A	64	−23.750	4.384	14.483	1.00	24.84		C
ANISOU	300	CG1	VAL A	64	4319	3151	1967	−111	−23	−122	C
ATOM	301	CG2	VAL A	64	−23.155	2.243	15.695	1.00	22.81		C
ANISOU	301	CG2	VAL A	64	4007	2486	2173	738	11	409	C
ATOM	302	N	LEU A	65	−23.492	6.731	16.689	1.00	17.65		N
ANISOU	302	N	LEU A	65	2470	2373	1863	114	95	105	N
ATOM	303	C	LEU A	65	−23.834	8.496	15.056	1.00	19.14		C
ANISOU	303	C	LEU A	65	2278	2980	2017	348	144	266	C
ATOM	304	O	LEU A	65	−22.710	8.616	14.599	1.00	23.52		O
ANISOU	304	O	LEU A	65	2717	3486	2734	757	626	920	O
ATOM	305	CA	ALEU A	65	−24.017	8.077	16.523	0.76	17.01		C
ANISOU	305	CA	ALEU A	65	2800	1911	1753	436	−139	−203	C
ATOM	306	CB	ALEU A	65	−23.258	9.010	17.462	0.76	23.38		C
ANISOU	306	CB	ALEU A	65	3087	2789	3008	178	−24	−483	C
ATOM	307	CG	ALEU A	65	−23.842	10.358	17.829	0.76	23.41		C
ANISOU	307	CG	ALEU A	65	2650	2853	3390	−90	39	−451	C
ATOM	308	CD1	ALEU A	65	−25.206	10.222	18.515	0.76	22.26		C
ANISOU	308	CD1	ALEU A	65	2225	3066	3169	−116	554	−278	C
ATOM	309	CD2	ALEU A	65	−22.858	11.045	18.720	0.76	23.52		C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	309	CD2	ALEU A	65	2641	3172	3125	−323	−612	−143	C
ATOM	310	CA	BLEU A	65	−24.025	8.078	16.488	0.24	17.60		C
ANISOU	310	CA	BLEU A	65	2218	2502	1966	−16	136	341	C
ATOM	311	CB	BLEU A	65	−23.296	9.093	17.346	0.24	19.59		C
ANISOU	311	CB	BLEU A	65	2146	2886	2411	50	24	192	C
ATOM	312	CG	BLEU A	65	−23.572	9.048	18.831	0.24	17.01		C
ANISOU	312	CG	BLEU A	65	1590	2505	2367	−539	−304	270	C
ATOM	313	CD1	BLEU A	65	−22.802	10.157	19.470	0.24	15.56		C
ANISOU	313	CD1	BLEU A	65	1608	2000	2302	−462	−786	−460	C
ATOM	314	CD2	BLEU A	65	−25.032	9.207	19.115	0.24	17.29		C
ANISOU	314	CD2	BLEU A	65	2374	1904	2291	−503	−207	729	C
ATOM	315	N	ASN A	66	−24.937	8.717	14.358	1.00	19.50		N
ANISOU	315	N	ASN A	66	2956	2476	1978	262	−53	496	N
ATOM	316	CA	ASN A	66	−24.916	9.075	12.942	1.00	20.34		C
ANISOU	316	CA	ASN A	66	2925	2622	2181	332	−27	324	C
ATOM	317	C	ASN A	66	−25.205	10.582	12.804	1.00	18.94		C
ANISOU	317	C	ASN A	66	2394	2820	1983	371	282	367	C
ATOM	318	O	ASN A	66	−26.039	11.159	13.526	1.00	21.81		O
ANISOU	318	O	ASN A	66	2874	3062	2353	703	577	367	O
ATOM	319	CB	ASN A	66	−26.012	8.323	12.218	1.00	21.72		C
ANISOU	319	CB	ASN A	66	3495	2328	2432	68	−46	78	C
ATOM	320	CG	ASN A	66	−25.629	6.885	11.859	1.00	24.63		C
ANISOU	320	CG	ASN A	66	3679	2649	3031	−234	9	183	C
ATOM	321	OD1	ASN A	66	−24.464	6.506	11.844	1.00	28.62		O
ANISOU	321	OD1	ASN A	66	4225	3368	3281	867	382	392	O
ATOM	322	ND2	ASN A	66	−26.628	6.094	11.512	1.00	26.30		N
ANISOU	322	ND2	ASN A	66	3996	2551	3447	−249	244	−93	N
ATOM	323	N	TRP A	67	−24.527	11.210	11.857	1.00	16.96		N
ANISOU	323	N	TRP A	67	2219	2551	1675	403	139	202	N
ATOM	324	CA	TRP A	67	−24.821	12.582	11.466	1.00	17.35		C
ANISOU	324	CA	TRP A	67	2648	2322	1622	296	−487	80	C
ATOM	325	C	TRP A	67	−25.559	12.535	10.139	1.00	16.02		C
ANISOU	325	C	TRP A	67	2057	2340	1690	−132	188	−137	C
ATOM	326	O	TRP A	67	−25.044	11.953	9.193	1.00	17.52		O
ANISOU	326	O	TRP A	67	2341	2772	1542	192	20	−102	O
ATOM	327	CB	TRP A	67	−23.506	13.345	11.289	1.00	16.70		C
ANISOU	327	CB	TRP A	67	2291	2264	1791	−158	−88	−202	C
ATOM	328	CG	TRP A	67	−23.644	14.788	10.913	1.00	15.50		C
ANISOU	328	CG	TRP A	67	1895	2429	1566	−32	−158	−93	C
ATOM	329	CD1	TRP A	67	−24.733	15.597	11.062	1.00	16.72		C
ANISOU	329	CD1	TRP A	67	2197	2528	1627	539	−206	319	C
ATOM	330	CD2	TRP A	67	−22.605	15.614	10.379	1.00	15.69		C
ANISOU	330	CD2	TRP A	67	1896	2652	1416	−242	−150	−334	C
ATOM	331	NE1	TRP A	67	−24.447	16.880	10.638	1.00	16.73		N
ANISOU	331	NE1	TRP A	67	2145	2701	1512	−36	135	245	N
ATOM	332	CE2	TRP A	67	−23.145	16.912	10.195	1.00	15.97		C
ANISOU	332	CE2	TRP A	67	2002	2561	1506	−0	34	−116	C
ATOM	333	CE3	TRP A	67	−21.264	15.382	10.059	1.00	18.33		C
ANISOU	333	CE3	TRP A	67	1627	3525	1813	−201	87	−270	C
ATOM	334	CZ2	TRP A	67	−22.385	17.979	9.710	1.00	17.25		C
ANISOU	334	CZ2	TRP A	67	2052	2871	1631	−217	−404	−7	C
ATOM	335	CZ3	TRP A	67	−20.503	16.435	9.554	1.00	18.98		C
ANISOU	335	CZ3	TRP A	67	2015	3430	1766	−354	48	66	C
ATOM	336	CH2	TRP A	67	−21.066	17.716	9.382	1.00	19.49		C
ANISOU	336	CH2	TRP A	67	2459	2964	1984	−57	−77	37	C
ATOM	337	N	TYR A	68	−26.733	13.148	10.084	1.00	17.60		N
ANISOU	337	N	TYR A	68	2239	2803	1645	360	−334	196	N
ATOM	338	CA	TYR A	68	−27.535	13.132	8.865	1.00	18.83		C
ANISOU	338	CA	TYR A	68	2361	2956	1838	151	−193	160	C
ATOM	339	C	TYR A	68	−27.775	14.520	8.312	1.00	17.36		C
ANISOU	339	C	TYR A	68	2348	2705	1542	685	−246	369	C
ATOM	340	O	TYR A	68	−27.945	15.487	9.058	1.00	19.44		O
ANISOU	340	O	TYR A	68	2880	2839	1669	786	212	34	O
ATOM	341	CB	TYR A	68	−28.939	12.583	9.158	1.00	22.37		C
ANISOU	341	CB	TYR A	68	2629	3311	2558	−208	−229	−62	C
ATOM	342	CG	TYR A	68	−28.966	11.176	9.662	1.00	21.28		C
ANISOU	342	CG	TYR A	68	2607	2830	2649	−131	−166	262	C
ATOM	343	CD1	TYR A	68	−28.924	10.112	8.809	1.00	22.93		C
ANISOU	343	CD1	TYR A	68	3237	2732	2745	−556	−122	40	C
ATOM	344	CD2	TYR A	68	−29.104	10.914	11.020	1.00	25.46		C
ANISOU	344	CD2	TYR A	68	4086	3081	2507	341	−14	572	C
ATOM	345	CE1	TYR A	68	−28.987	8.803	9.267	1.00	25.28		C
ANISOU	345	CE1	TYR A	68	3736	2842	3027	−353	−31	504	C
ATOM	346	CE2	TYR A	68	−29.160	9.597	11.489	1.00	28.99		C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	346	CE2	TYR A	68	4540	3390	3085	673	187	212	C
ATOM	347	CZ	TYR A	68	−29.114	8.555	10.593	1.00	26.96		C
ANISOU	347	CZ	TYR A	68	3934	2885	3423	−365	55	342	C
ATOM	348	OH	TYR A	68	−29.187	7.260	11.023	1.00	32.87		O
ANISOU	348	OH	TYR A	68	5410	3215	3862	−257	148	377	O
ATOM	349	N	ARG A	69	−27.843	14.606	6.988	1.00	18.39		N
ANISOU	349	N	ARG A	69	2680	2776	1532	30	−79	388	N
ATOM	350	CA	ARG A	69	−28.398	15.774	6.357	1.00	19.02		C
ANISOU	350	CA	ARG A	69	3074	2452	1703	−487	−332	534	C
ATOM	351	C	ARG A	69	−29.832	15.410	6.025	1.00	19.80		C
ANISOU	351	C	ARG A	69	3020	2443	2061	−149	−557	−543	C
ATOM	352	O	ARG A	69	−30.102	14.356	5.461	1.00	24.21		O
ANISOU	352	O	ARG A	69	3236	3098	2867	119	−495	−783	O
ATOM	353	CB	ARG A	69	−27.645	16.133	5.082	1.00	22.34		C
ANISOU	353	CB	ARG A	69	3564	3429	1495	−177	−56	808	C
ATOM	354	CG	ARG A	69	−28.133	17.419	4.475	1.00	22.49		C
ANISOU	354	CG	ARG A	69	3915	3021	1607	−379	−19	799	C
ATOM	355	CD	ARG A	69	−27.252	17.890	3.388	1.00	26.43		C
ANISOU	355	CD	ARG A	69	4548	3361	2133	−82	137	1257	C
ATOM	356	NE	ARG A	69	−27.785	19.116	2.803	1.00	24.93		N
ANISOU	356	NE	ARG A	69	4181	3495	1796	−267	218	766	N
ATOM	357	CZ	ARG A	69	−27.190	19.754	1.795	1.00	24.72		C
ANISOU	357	CZ	ARG A	69	4062	3413	1916	−360	−424	−63	C
ATOM	358	NH1	ARG A	69	−26.063	19.279	1.278	1.00	27.53		N
ANISOU	358	NH1	ARG A	69	3709	4627	2123	−390	−768	378	N
ATOM	359	NH2	ARG A	69	−27.710	20.843	1.314	1.00	28.19		N
ANISOU	359	NH2	ARG A	69	5033	3694	1984	327	−385	−535	N
ATOM	360	O	AMET A	70	−34.121	16.404	5.088	0.63	32.94		O
ANISOU	360	O	AMET A	70	3794	4565	4158	1047	173	127	O
ATOM	361	N	AMET A	70	−30.757	16.279	6.435	0.63	21.29		N
ANISOU	361	N	AMET A	70	2374	3135	2579	639	45	−106	N
ATOM	362	C	AMET A	70	−32.961	16.726	5.350	0.63	29.17		C
ANISOU	362	C	AMET A	70	3071	4239	3774	218	−765	−262	C
ATOM	363	CA	AMET A	70	−32.204	16.001	6.427	0.63	25.67		C
ANISOU	363	CA	AMET A	70	2819	3863	3072	282	2	−344	C
ATOM	364	CB	AMET A	70	−32.865	16.415	7.762	0.63	25.85		C
ANISOU	364	CB	AMET A	70	3156	4084	2580	1193	587	−592	C
ATOM	365	CG	AMET A	70	−32.334	15.641	8.925	0.63	26.62		C
ANISOU	365	CG	AMET A	70	3310	4024	2779	29	−95	202	C
ATOM	366	SD	AMET A	70	−32.681	13.886	8.816	0.63	25.57		S
ANISOU	366	SD	AMET A	70	2915	3735	3064	55	−215	−27	S
ATOM	367	CE	AMET A	70	−34.457	13.866	9.003	0.63	29.39		C
ANISOU	367	CE	AMET A	70	2985	4948	3233	−294	−572	658	C
ATOM	368	O	BMET A	70	−33.686	16.135	4.423	0.37	32.05		O
ANISOU	368	O	BMET A	70	2704	5080	4392	−853	−1724	−463	O
ATOM	369	N	BMET A	70	−30.758	16.278	6.387	0.37	23.82		N
ANISOU	369	N	BMET A	70	2725	3374	2950	−718	−775	−187	N
ATOM	370	C	BMET A	70	−32.797	16.669	5.100	0.37	30.69		C
ANISOU	370	C	BMET A	70	2651	4926	4083	−738	−1707	−367	C
ATOM	371	CA	BMET A	70	−32.161	15.941	6.264	0.37	29.71		C
ANISOU	371	CA	BMET A	70	3118	4533	3638	−766	−1059	−301	C
ATOM	372	CB	BMET A	70	−32.899	16.289	7.556	0.37	36.52		C
ANISOU	372	CB	BMET A	70	4116	5976	3784	375	−401	105	C
ATOM	373	CG	BMET A	70	−34.246	15.651	7.647	0.37	41.35		C
ANISOU	373	CG	BMET A	70	4953	6816	3944	939	158	630	C
ATOM	374	SD	BMET A	70	−34.206	13.870	7.553	0.37	46.65		S
ANISOU	374	SD	BMET A	70	5683	7766	4278	1347	404	1179	S
ATOM	375	CE	BMET A	70	−34.938	13.419	9.126	0.37	46.19		C
ANISOU	375	CE	BMET A	70	5849	7281	4419	894	302	1210	C
ATOM	376	O	SER A	71	−30.690	19.786	3.772	1.00	27.87		O
ANISOU	376	O	SER A	71	3431	3577	3579	197	−867	105	O
ATOM	377	N	SER A	71	−32.347	17.894	4.866	1.00	30.43		N
ANISOU	377	N	SER A	71	2656	4721	4183	−120	−889	675	N
ATOM	378	CA	SER A	71	−32.842	18.692	3.756	1.00	33.99		C
ANISOU	378	CA	SER A	71	3005	5737	4173	913	−732	199	C
ATOM	379	C	SER A	71	−31.687	19.460	3.105	1.00	36.17		C
ANISOU	379	C	SER A	71	4376	4900	4466	3	−579	938	C
ATOM	380	CB	SER A	71	−33.940	19.655	4.231	1.00	33.85		C
ANISOU	380	CB	SER A	71	3149	5270	4443	496	−513	−653	C
ATOM	381	OG	SER A	71	−33.405	20.647	5.095	1.00	37.20		O
ANISOU	381	OG	SER A	71	4259	5515	4360	425	−571	−1173	O
ATOM	382	O	PRO A	72	−31.622	17.247	0.700	1.00	79.55		O
ANISOU	382	O	PRO A	72	9807	8972	11447	1413	−611	524	O
ATOM	383	N	PRO A	72	−31.930	19.711	1.760	1.00	46.66		N

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	383	N	PRO A	72	5155	6766	5809	500	−1637	509	N
ATOM	384	CA	PRO A	72	−32.981	19.189	0.882	1.00	58.56		C
ANISOU	384	CA	PRO A	72	6438	7948	7865	408	−1909	548	C
ATOM	385	C	PRO A	72	−32.715	17.754	0.447	1.00	87.61		C
ANISOU	385	C	PRO A	72	10558	10867	11864	353	−1260	528	C
ATOM	386	CB	PRO A	72	−32.915	20.123	−0.328	1.00	53.01		C
ANISOU	386	CB	PRO A	72	5911	7859	6373	1210	−1816	605	C
ATOM	387	CG	PRO A	72	−31.500	20.589	−0.359	1.00	49.25		C
ANISOU	387	CG	PRO A	72	5060	8210	5441	1261	−1901	497	C
ATOM	388	CD	PRO A	72	−31.074	20.698	1.078	1.00	45.71		C
ANISOU	388	CD	PRO A	72	4769	7373	5224	1151	−2036	1113	C
ATOM	389	O	SER A	73	−35.496	14.835	−0.740	1.00	89.31		O
ATOM	390	N	SER A	73	−33.794	17.016	0.435	1.00	131.36		N
ATOM	391	CA	SER A	73	−33.763	15.579	0.767	1.00	69.01		C
ATOM	392	C	SER A	73	−34.364	14.639	−0.297	1.00	88.91		C
ATOM	393	O	ASN A	74	−35.006	10.928	1.253	1.00	97.59		O
ATOM	394	N	ASN A	74	−33.596	13.625	−0.696	1.00	67.36		N
ATOM	395	CA	ASN A	74	−33.885	12.194	−0.474	1.00	83.94		C
ATOM	396	C	ASN A	74	−34.163	11.781	0.974	1.00	112.13		C
ATOM	397	CB	ASN A	74	−32.760	11.330	−1.052	1.00	81.23		C
ATOM	398	O	GLN A	75	−34.797	11.983	4.041	1.00	94.95		O
ATOM	399	N	GLN A	75	−33.428	12.412	1.877	1.00	116.23		N
ATOM	400	CA	GLN A	75	−32.670	11.842	2.945	1.00	75.15		C
ATOM	401	C	GLN A	75	−33.646	11.547	4.049	1.00	75.49		C
ATOM	402	CB	GLN A	75	−31.602	12.823	3.431	1.00	109.74		C
ATOM	403	O	PRO A	76	−30.775	9.537	4.735	1.00	40.28		O
ANISOU	403	O	PRO A	76	5352	3506	6447	−351	−1585	−514	O
ATOM	404	N	PRO A	76	−33.150	10.791	5.002	1.00	52.61		N
ANISOU	404	N	PRO A	76	5675	6045	8269	−2909	−1848	886	N
ATOM	405	C	PRO A	76	−30.795	10.728	5.056	1.00	37.46		C
ANISOU	405	C	PRO A	76	4497	3555	6180	−813	−1791	203	C
ATOM	406	CA	PRO A	76	−32.015	11.328	5.738	1.00	43.47		C
ANISOU	406	CA	PRO A	76	4563	4769	7184	−1137	−2010	455	C
ATOM	407	CB	PRO A	76	−32.198	10.727	7.124	1.00	46.18		C
ANISOU	407	CB	PRO A	76	4663	5522	7363	−1010	−1800	415	C
ATOM	408	CG	PRO A	76	−33.667	10.501	7.230	1.00	46.93		C
ANISOU	408	CG	PRO A	76	4916	5399	7517	−1582	−1827	169	C
ATOM	409	CD	PRO A	76	−34.113	10.107	5.879	1.00	50.47		C
ANISOU	409	CD	PRO A	76	5055	6224	7896	−1723	−1718	791	C
ATOM	410	O	ASP A	77	−27.188	12.018	5.842	1.00	21.14		O
ANISOU	410	O	ASP A	77	3066	2646	2322	−21	−356	−317	O
ATOM	411	N	ASP A	77	−29.798	11.547	4.798	1.00	31.79		N
ANISOU	411	N	ASP A	77	3417	3780	4881	−876	−1752	458	N
ATOM	412	CA	ASP A	77	−28.597	11.075	4.152	1.00	30.39		C
ANISOU	412	CA	ASP A	77	4217	3630	3700	−629	−1385	−166	C
ATOM	413	C	ASP A	77	−27.530	10.999	5.228	1.00	23.84		C
ANISOU	413	C	ASP A	77	3427	2890	2741	−879	−888	−334	C
ATOM	414	CB	ASP A	77	−28.181	12.097	3.081	1.00	35.59		C
ANISOU	414	CB	ASP A	77	6033	4101	3390	74	−1396	384	C
ATOM	415	CG	ASP A	77	−26.901	11.701	2.348	1.00	48.11		C
ANISOU	415	CG	ASP A	77	8332	5760	4188	895	−446	914	C
ATOM	416	OD1	ASP A	77	−26.453	10.541	2.501	1.00	55.44		O
ANISOU	416	OD1	ASP A	77	9101	7301	4661	458	563	1016	O
ATOM	417	OD2	ASP A	77	−26.349	12.536	1.593	1.00	54.64		O
ANISOU	417	OD2	ASP A	77	9396	7230	4135	1159	−444	445	O
ATOM	418	N	LYS A	78	−26.998	9.808	5.468	1.00	25.64		N
ANISOU	418	N	LYS A	78	3532	3634	2576	126	−286	−255	N
ATOM	419	C	LYS A	78	−24.626	10.301	5.958	1.00	23.36		C
ANISOU	419	C	LYS A	78	2636	3525	2716	−313	468	−1003	C
ATOM	420	O	LYS A	78	−24.109	9.901	4.898	1.00	31.31		O
ANISOU	420	O	LYS A	78	4100	4572	3224	−682	800	−1583	O
ATOM	421	CA	LYS A	78	−25.946	9.693	6.469	1.00	23.80		C
ANISOU	421	CA	LYS A	78	3170	3080	2793	−2	−441	−378	C
ATOM	422	CB	LYS A	78	−25.731	8.250	6.874	1.00	25.49		C
ANISOU	422	CB	LYS A	78	3701	3222	2761	284	−676	−87	C
ATOM	423	CG	LYS A	78	−24.649	8.164	7.922	1.00	28.34		C
ANISOU	423	CG	LYS A	78	4370	3575	2822	728	−689	268	C
ATOM	424	CD	LYS A	78	−24.572	6.804	8.517	1.00	39.89		C
ANISOU	424	CD	LYS A	78	6575	5112	3471	1388	98	457	C
ATOM	425	CE	LYS A	78	−24.293	5.814	7.461	1.00	45.57		C
ANISOU	425	CE	LYS A	78	7602	6017	3697	1619	654	818	C
ATOM	426	NZ	LYS A	78	−24.459	4.455	7.998	1.00	51.10		N
ANISOU	426	NZ	LYS A	78	8393	6831	4191	1793	956	1085	N
ATOM	427	N	LEU A	79	−24.051	11.246	6.690	1.00	19.32		N

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	427	N	LEU A	79	2214	3018	2108	80	−181	−403	N
ATOM	428	CA	LEU A	79	−22.807	11.898	6.278	1.00	19.20		C
ANISOU	428	CA	LEU A	79	2316	3162	1817	286	149	14	C
ATOM	429	C	LEU A	79	−21.560	11.234	6.852	1.00	19.69		C
ANISOU	429	C	LEU A	79	2365	3348	1767	−30	308	30	C
ATOM	430	O	LEU A	79	−20.502	11.174	6.211	1.00	22.91		O
ANISOU	430	O	LEU A	79	3000	3571	2132	266	439	206	O
ATOM	431	CB	LEU A	79	−22.820	13.370	6.738	1.00	19.24		C
ANISOU	431	CB	LEU A	79	2652	2849	1809	176	−144	232	C
ATOM	432	CG	LEU A	79	−24.040	14.149	6.242	1.00	19.55		C
ANISOU	432	CG	LEU A	79	2696	3082	1649	397	−173	25	C
ATOM	433	CD1	LEU A	79	−24.103	15.506	6.919	1.00	21.97		C
ANISOU	433	CD1	LEU A	79	3347	2831	2170	151	−435	−207	C
ATOM	434	CD2	LEU A	79	−23.963	14.287	4.723	1.00	22.99		C
ANISOU	434	CD2	LEU A	79	3157	4106	1471	546	−249	555	C
ATOM	435	N	ALA A	80	−21.674	10.793	8.105	1.00	19.24		N
ANISOU	435	N	ALA A	80	2934	2922	1453	460	212	114	N
ATOM	436	CA	ALA A	80	−20.524	10.293	8.859	1.00	18.60		C
ANISOU	436	CA	ALA A	80	2440	2818	1808	114	130	401	C
ATOM	437	C	ALA A	80	−21.066	9.699	10.160	1.00	17.43		C
ANISOU	437	C	ALA A	80	2430	2390	1801	119	401	112	C
ATOM	438	O	ALA A	80	−22.223	9.940	10.515	1.00	19.11		O
ANISOU	438	O	ALA A	80	2218	3148	1896	203	398	199	O
ATOM	439	CB	ALA A	80	−19.538	11.430	9.164	1.00	22.26		C
ANISOU	439	CB	ALA A	80	2913	2941	2604	−517	−136	62	C
ATOM	440	N	ALA A	81	−20.252	8.903	10.835	1.00	19.05		N
ANISOU	440	N	ALA A	81	2646	2780	1811	354	22	295	N
ATOM	441	CA	ALA A	81	−20.665	8.235	12.060	1.00	18.68		C
ANISOU	441	CA	ALA A	81	2603	2499	1995	−195	−337	275	C
ATOM	442	C	ALA A	81	−19.569	8.109	13.064	1.00	18.56		C
ANISOU	442	C	ALA A	81	2328	2498	2226	464	−121	−470	C
ATOM	443	O	ALA A	81	−18.392	8.136	12.709	1.00	20.25		O
ANISOU	443	O	ALA A	81	2360	2812	2520	444	95	−61	O
ATOM	444	CB	ALA A	81	−21.214	6.815	11.744	1.00	22.23		C
ANISOU	444	CB	ALA A	81	2855	3182	2411	−451	−528	108	C
ATOM	445	O	PHE A	82	−20.846	6.014	16.222	1.00	24.81		O
ANISOU	445	O	PHE A	82	2317	3708	3401	502	170	861	O
ATOM	446	N	PHE A	82	−19.975	7.934	14.324	1.00	20.32		N
ANISOU	446	N	PHE A	82	2866	2887	1968	203	5	321	N
ATOM	447	CA	PHE A	82	−19.108	7.430	15.394	1.00	21.19		C
ANISOU	447	CA	PHE A	82	2782	3210	2058	33	−356	258	C
ATOM	448	C	PHE A	82	−19.669	6.106	15.940	1.00	20.15		C
ANISOU	448	C	PHE A	82	2405	2780	2471	143	−253	528	C
ATOM	449	CB	PHE A	82	−19.022	8.415	16.566	1.00	23.16		C
ANISOU	449	CB	PHE A	82	3374	3419	2009	345	−510	−481	C
ATOM	450	CG	PHE A	82	−18.336	7.822	17.765	1.00	26.29		C
ANISOU	450	CG	PHE A	82	4301	3361	2328	518	−828	−708	C
ATOM	451	CD1	PHE A	82	−16.977	7.856	17.858	1.00	30.38		C
ANISOU	451	CD1	PHE A	82	4339	4414	2790	440	−802	−988	C
ATOM	452	CD2	PHE A	82	−19.065	7.164	18.763	1.00	29.00		C
ANISOU	452	CD2	PHE A	82	5248	3373	2397	1517	−321	−378	C
ATOM	453	CE1	PHE A	82	−16.326	7.262	18.968	1.00	30.08		C
ANISOU	453	CE1	PHE A	82	4657	4169	2602	3	−1011	88	C
ATOM	454	CE2	PHE A	82	−18.440	6.561	19.858	1.00	28.43		C
ANISOU	454	CE2	PHE A	82	5143	3059	2599	480	−438	287	C
ATOM	455	CZ	PHE A	82	−17.061	6.612	19.966	1.00	29.77		C
ANISOU	455	CZ	PHE A	82	5102	3359	2851	282	−1108	−171	C
ATOM	456	O	APRO A	83	−18.301	4.853	13.522	0.74	22.74		O
ANISOU	456	O	APRO A	83	3313	2768	2560	−197	−53	−17	O
ATOM	457	N	APRO A	83	−18.825	5.082	16.116	0.74	20.63		N
ANISOU	457	N	APRO A	83	2773	2904	2161	501	−83	−14	N
ATOM	458	CA	APRO A	83	−17.417	4.993	15.738	0.74	20.86		C
ANISOU	458	CA	APRO A	83	2663	2991	2270	968	−83	−17	C
ATOM	459	C	APRO A	83	−17.295	5.045	14.227	0.74	21.23		C
ANISOU	459	C	APRO A	83	3178	2409	2480	81	−222	−207	C
ATOM	460	CB	APRO A	83	−17.012	3.600	16.225	0.74	24.70		C
ANISOU	460	CB	APRO A	83	2927	3578	2880	984	183	477	C
ATOM	461	CG	APRO A	83	−17.986	3.279	17.346	0.74	25.48		C
ANISOU	461	CG	APRO A	83	3095	3505	3080	936	146	430	C
ATOM	462	CD	APRO A	83	−19.279	3.899	16.873	0.74	23.74		C
ANISOU	462	CD	APRO A	83	2911	3352	2757	531	−66	−88	C
ATOM	463	O	BPRO A	83	−18.283	4.761	13.573	0.26	25.54		O
ANISOU	463	O	BPRO A	83	3539	3224	2940	315	168	−293	O
ATOM	464	N	BPRO A	83	−18.817	5.081	16.099	0.26	21.32		N

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	464	N	BPRO A	83	2579	2907	2614	399	19	407	N
ATOM	465	CA	BPRO A	83	−17.402	5.136	15.751	0.26	21.83		C
ANISOU	465	CA	BPRO A	83	2732	2779	2785	312	208	282	C
ATOM	466	C	BPRO A	83	−17.287	5.047	14.248	0.26	24.04		C
ANISOU	466	C	BPRO A	83	3306	2902	2928	86	232	−180	C
ATOM	467	CB	BPRO A	83	−16.853	3.860	16.375	0.26	21.48		C
ANISOU	467	CB	BPRO A	83	2478	2675	3007	134	419	675	C
ATOM	468	CG	BPRO A	83	−17.978	2.899	16.235	0.26	20.85		C
ANISOU	468	CG	BPRO A	83	2249	2720	2954	454	273	542	C
ATOM	469	CD	BPRO A	83	−19.222	3.723	16.508	0.26	22.96		C
ANISOU	469	CD	BPRO A	83	2468	3434	2823	672	85	553	C
ATOM	470	O	GLU A	84	−15.904	2.794	12.572	1.00	31.21		O
ANISOU	470	O	GLU A	84	5278	3198	3384	40	173	−865	O
ATOM	471	N	GLU A	84	−16.099	5.317	13.736	1.00	25.49		N
ANISOU	471	N	GLU A	84	3646	2948	3092	−310	526	−426	N
ATOM	472	C	GLU A	84	−16.263	3.779	11.906	1.00	29.82		C
ANISOU	472	C	GLU A	84	4641	3545	3145	−386	401	−385	C
ATOM	473	CA	AGLU A	84	−15.885	5.205	12.307	0.62	29.77		C
ANISOU	473	CA	AGLU A	84	4113	3950	3248	−726	570	−493	C
ATOM	474	CB	AGLU A	84	−14.443	5.525	11.930	0.62	34.81		C
ANISOU	474	CB	AGLU A	84	4402	5228	3598	−1155	667	−774	C
ATOM	475	CG	AGLU A	84	−14.202	5.621	10.418	0.62	36.28		C
ANISOU	475	CG	AGLU A	84	4818	5426	3540	−1112	892	−907	C
ATOM	476	CA	BGLU A	84	−15.858	5.187	12.313	0.38	29.16		C
ANISOU	476	CA	BGLU A	84	4058	3758	3262	−442	446	−377	C
ATOM	477	CB	BGLU A	84	−14.388	5.452	11.991	0.38	31.91		C
ANISOU	477	CB	BGLU A	84	3976	4556	3593	−654	324	−452	C
ATOM	478	CG	BGLU A	84	−13.396	4.609	12.783	0.38	32.68		C
ANISOU	478	CG	BGLU A	84	3860	4904	3652	−430	219	−573	C
ATOM	479	O	ASP A	85	−15.707	1.834	9.028	1.00	37.07		O
ANISOU	479	O	ASP A	85	5502	5657	2927	−142	1140	−325	O
ATOM	480	N	ASP A	85	−17.040	3.687	10.843	1.00	31.28		N
ANISOU	480	N	ASP A	85	5268	3841	2777	−285	697	−454	N
ATOM	481	C	ASP A	85	−16.503	1.479	9.902	1.00	30.78		C
ANISOU	481	C	ASP A	85	4808	4235	2652	−522	569	−729	C
ATOM	482	CG	ASP A	85	−19.192	1.391	8.726	1.00	34.55		C
ANISOU	482	CG	ASP A	85	5916	4574	2639	−961	362	52	C
ATOM	483	OD1	ASP A	85	−19.395	0.418	9.473	1.00	32.78		O
ANISOU	483	OD1	ASP A	85	5362	4018	3077	−631	438	421	O
ATOM	484	OD2	ASP A	85	−19.435	1.358	7.512	1.00	40.60		O
ANISOU	484	OD2	ASP A	85	7698	5108	2620	−820	135	−409	O
ATOM	485	CA	AASP A	85	−17.599	2.422	10.405	0.50	31.21		C
ANISOU	485	CA	AASP A	85	5137	4219	2502	−567	529	−338	C
ATOM	486	CB	AASP A	85	−18.641	2.672	9.311	0.50	32.81		C
ANISOU	486	CB	AASP A	85	5417	4407	2641	−1074	290	17	C
ATOM	487	CA	BASP A	85	−17.599	2.422	10.405	0.50	31.20		C
ANISOU	487	CA	BASP A	85	5136	4218	2502	−568	530	−337	C
ATOM	488	CB	BASP A	85	−18.641	2.672	9.312	0.50	32.80		C
ANISOU	488	CB	BASP A	85	5416	4405	2641	−1077	293	19	C
ATOM	489	O	ARG A	86	−15.612	−2.973	9.130	1.00	35.85		O
ANISOU	489	O	ARG A	86	4572	3850	5200	−92	1205	−1072	O
ATOM	490	N	ARG A	86	−16.469	0.268	10.450	1.00	31.26		N
ANISOU	490	N	ARG A	86	4426	4480	2973	−240	676	−542	N
ATOM	491	CA	ARG A	86	−15.518	−0.743	10.004	1.00	32.86		C
ANISOU	491	CA	ARG A	86	4019	4586	3880	−1057	656	−628	C
ATOM	492	C	ARG A	86	−16.226	−1.913	9.330	1.00	32.39		C
ANISOU	492	C	ARG A	86	4418	3495	4394	−119	958	−886	C
ATOM	493	CB	ARG A	86	−14.680	−1.233	11.193	1.00	36.58		C
ANISOU	493	CB	ARG A	86	4355	5051	4492	−631	198	−603	C
ATOM	494	CG	ARG A	86	−13.757	−0.165	11.776	1.00	36.27		C
ANISOU	494	CG	ARG A	86	4656	4401	4726	−706	79	−1212	C
ATOM	495	CD	ARG A	86	−12.555	0.089	10.855	1.00	40.36		C
ANISOU	495	CD	ARG A	86	5035	5109	5192	−394	−322	−579	C
ATOM	496	O	SER A	87	−18.498	−3.594	6.042	1.00	34.51		O
ANISOU	496	O	SER A	87	5952	4009	3153	−80	258	305	O
ATOM	497	N	SER A	87	−17.511	−1.747	8.990	1.00	29.93		N
ANISOU	497	N	SER A	87	4223	3507	3643	−1038	1047	−242	N
ATOM	498	CA	SER A	87	−18.261	−2.819	8.303	1.00	29.09		C
ANISOU	498	CA	SER A	87	4311	3704	3038	−945	1119	−49	C
ATOM	499	C	SER A	87	−18.165	−2.667	6.793	1.00	31.24		C
ANISOU	499	C	SER A	87	5281	3609	2981	−760	779	60	C
ATOM	500	CB	SER A	87	−19.738	−2.847	8.710	1.00	28.40		C
ANISOU	500	CB	SER A	87	4171	3559	3062	−542	515	225	C
ATOM	501	OG	SER A	87	−20.450	−1.741	8.163	1.00	29.67		O

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	501	OG	SER A	87	4864	3795	2613	−369	−195	280	O
ATOM	502	O	GLN A	88	−15.661	0.062	5.677	1.00	35.65		O
ANISOU	502	O	GLN A	88	6338	4381	2827	−906	966	−716	O
ATOM	503	N	GLN A	88	−17.702	−1.503	6.360	1.00	28.54		N
ANISOU	503	N	GLN A	88	4855	3292	2697	−490	284	−173	N
ATOM	504	CA	GLN A	88	−17.569	−1.182	4.955	1.00	33.90		C
ANISOU	504	CA	GLN A	88	5221	4806	2853	−735	461	−496	C
ATOM	505	C	GLN A	88	−16.255	−0.470	4.727	1.00	35.45		C
ANISOU	505	C	GLN A	88	6005	4772	2694	−847	1039	−941	C
ATOM	506	CB	GLN A	88	−18.736	−0.289	4.509	1.00	31.31		C
ANISOU	506	CB	GLN A	88	4696	4584	2618	−922	227	−129	C
ATOM	507	CG	GLN A	88	−20.088	−0.968	4.655	1.00	32.64		C
ANISOU	507	CG	GLN A	88	4902	5292	2209	−592	648	−553	C
ATOM	508	CD	GLN A	88	−20.315	−2.105	3.658	1.00	36.25		C
ANISOU	508	CD	GLN A	88	5163	6336	2274	44	1289	−836	C
ATOM	509	OE1	GLN A	88	−19.440	−2.450	2.834	1.00	40.67		O
ANISOU	509	OE1	GLN A	88	5517	7444	2491	−712	808	−1367	O
ATOM	510	NE2	GLN A	88	−21.519	−2.675	3.702	1.00	37.45		N
ANISOU	510	NE2	GLN A	88	5002	6422	2807	−432	1077	−245	N
ATOM	511	O	PRO A	89	−15.707	2.257	3.519	1.00	42.39		O
ANISOU	511	O	PRO A	89	8235	4472	3399	−2054	790	−754	O
ATOM	512	N	PRO A	89	−15.788	−0.445	3.466	1.00	38.38		N
ANISOU	512	N	PRO A	89	6933	4791	2859	−1271	1577	−970	N
ATOM	513	CA	PRO A	89	−14.520	0.240	3.197	1.00	39.05		C
ANISOU	513	CA	PRO A	89	7344	4358	3135	−2106	1680	−255	C
ATOM	514	C	PRO A	89	−14.615	1.695	3.563	1.00	42.25		C
ANISOU	514	C	PRO A	89	8056	4672	3324	−2041	1306	−204	C
ATOM	515	CB	PRO A	89	−14.369	0.107	1.690	1.00	41.99		C
ANISOU	515	CB	PRO A	89	7688	5350	2916	−1511	1804	−188	C
ATOM	516	CG	PRO A	89	−15.213	−0.987	1.288	1.00	40.12		C
ANISOU	516	CG	PRO A	89	7391	4717	3135	−2191	1758	−122	C
ATOM	517	CD	PRO A	89	−16.325	−1.098	2.253	1.00	38.08		C
ANISOU	517	CD	PRO A	89	7289	4438	2741	−1610	1452	−1034	C
ATOM	518	O	GLY A	90	−13.766	4.053	1.897	1.00	50.07		O
ANISOU	518	O	GLY A	90	10806	4730	3490	−2299	1756	−696	O
ATOM	519	N	GLY A	90	−13.485	2.286	3.931	1.00	42.62		N
ANISOU	519	N	GLY A	90	8318	4368	3507	−2948	881	−564	N
ATOM	520	CA	GLY A	90	−13.440	3.699	4.250	1.00	46.50		C
ANISOU	520	CA	GLY A	90	9190	4754	3723	−2602	1105	−750	C
ATOM	521	C	GLY A	90	−13.821	4.527	3.038	1.00	49.51		C
ANISOU	521	C	GLY A	90	10315	4774	3723	−2032	1501	−566	C
ATOM	522	O	GLN A	91	−14.348	8.633	3.531	1.00	60.25		O
ANISOU	522	O	GLN A	91	12188	6000	4707	834	2151	46	O
ATOM	523	N	GLN A	91	−14.219	5.764	3.280	1.00	53.64		N
ANISOU	523	N	GLN A	91	11363	4889	4127	−731	1334	−315	N
ATOM	524	CA	GLN A	91	−14.641	6.655	2.210	1.00	54.13		C
ANISOU	524	CA	GLN A	91	11631	4667	4269	−384	1697	72	C
ATOM	525	C	GLN A	91	−14.110	8.062	2.466	1.00	57.56		C
ANISOU	525	C	GLN A	91	11791	5314	4767	288	1902	13	C
ATOM	526	CB	GLN A	91	−16.171	6.675	2.114	1.00	54.49		C
ANISOU	526	CB	GLN A	91	11546	4962	4196	−620	1607	−216	C
ATOM	527	O	ASP A	92	−14.923	10.911	0.914	1.00	56.66		O
ANISOU	527	O	ASP A	92	10373	5142	6015	1649	1210	−1660	O
ATOM	528	N	ASP A	92	−13.383	8.609	1.493	1.00	56.97		N
ANISOU	528	N	ASP A	92	11008	5464	5176	405	1970	251	N
ATOM	529	CA	ASP A	92	−12.820	9.957	1.599	1.00	55.51		C
ANISOU	529	CA	ASP A	92	10188	5341	5561	897	1707	−75	C
ATOM	530	C	ASP A	92	−13.592	10.985	1.684	1.00	53.27		C
ANISOU	530	C	ASP A	92	9661	4871	5709	1006	1477	−905	C
ATOM	531	CB	ASP A	92	−11.903	10.241	0.402	1.00	55.64		C
ANISOU	531	CB	ASP A	92	9800	5659	5681	505	1879	291	C
ATOM	532	N	SER A	93	−13.835	11.935	2.614	1.00	42.80		N
ANISOU	532	N	SER A	93	8122	2599	5540	451	1585	−868	N
ATOM	533	CA	SER A	93	−14.985	12.746	2.983	1.00	38.50		C
ANISOU	533	CA	SER A	93	6693	3361	4575	−257	1960	−1003	C
ATOM	534	C	SER A	93	−14.678	14.152	3.484	1.00	31.06		C
ANISOU	534	C	SER A	93	5067	2890	3853	148	1312	−950	C
ATOM	535	O	SER A	93	−13.716	14.353	4.234	1.00	37.92		O
ANISOU	535	O	SER A	93	4552	5039	4817	1141	1078	−92	O
ATOM	536	CB	SER A	93	−15.759	12.030	4.074	1.00	40.18		C
ANISOU	536	CB	SER A	93	6953	3882	4430	−772	1532	−1274	C
ATOM	537	OG	SER A	93	−16.999	12.656	4.233	1.00	38.36		O
ANISOU	537	OG	SER A	93	6253	4256	4067	−1358	1677	−1700	O
ATOM	538	N	ARG A	94	−15.533	15.114	3.121	1.00	27.17		N

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	538	N	ARG A	94	4597	3294	2431	−235	1036	−346	N
ATOM	539	CA	ARG A	94	−15.488	16.429	3.758	1.00	22.75		C
ANISOU	539	CA	ARG A	94	3400	3348	1895	−369	479	−28	C
ATOM	540	C	ARG A	94	−16.160	16.421	5.124	1.00	21.09		C
ANISOU	540	C	ARG A	94	2696	3597	1722	−432	270	−341	C
ATOM	541	O	ARG A	94	−16.126	17.410	5.789	1.00	21.86		O
ANISOU	541	O	ARG A	94	3236	3180	1890	−422	260	−138	O
ATOM	542	CB	ARG A	94	−16.186	17.502	2.898	1.00	26.10		C
ANISOU	542	CB	ARG A	94	3701	4157	2061	75	305	801	C
ATOM	543	CG	ARG A	94	−15.485	17.813	1.611	1.00	26.03		C
ANISOU	543	CG	ARG A	94	3195	4624	2073	239	224	739	C
ATOM	544	CD	ARG A	94	−16.125	19.020	0.916	1.00	27.51		C
ANISOU	544	CD	ARG A	94	3149	5362	1943	867	355	1021	C
ATOM	545	NE	ARG A	94	−17.533	18.761	0.637	1.00	28.02		N
ANISOU	545	NE	ARG A	94	2666	5611	2368	699	−110	17	N
ATOM	546	CZ	ARG A	94	−18.538	19.539	1.029	1.00	22.60		C
ANISOU	546	CZ	ARG A	94	2360	4470	1758	−60	−197	−95	C
ATOM	547	NH1	ARG A	94	−18.303	20.671	1.684	1.00	24.22		N
ANISOU	547	NH1	ARG A	94	2892	4712	1599	−407	78	−113	N
ATOM	548	NH2	ARG A	94	−19.772	19.195	0.736	1.00	24.78		N
ANISOU	548	NH2	ARG A	94	3273	4014	2128	826	−108	4	N
ATOM	549	N	PHE A	95	−16.784	15.314	5.504	1.00	20.85		N
ANISOU	549	N	PHE A	95	3394	3074	1455	−671	239	−286	N
ATOM	550	C	PHE A	95	−16.870	14.368	7.755	1.00	20.58		C
ANISOU	550	C	PHE A	95	3213	2963	1642	−63	189	308	C
ATOM	551	O	PHE A	95	−16.363	13.284	7.425	1.00	27.39		O
ANISOU	551	O	PHE A	95	4832	3034	2540	613	−91	−57	O
ATOM	552	CA	APHE A	95	−17.561	15.263	6.743	0.55	21.28		C
ANISOU	552	CA	APHE A	95	3251	3465	1371	−530	−183	71	C
ATOM	553	CB	APHE A	95	−19.004	14.812	6.473	0.55	23.58		C
ANISOU	553	CB	APHE A	95	3538	3900	1522	−836	−314	327	C
ATOM	554	CG	APHE A	95	−19.756	15.729	5.534	0.55	22.19		C
ANISOU	554	CG	APHE A	95	3107	3868	1455	−1493	−413	267	C
ATOM	555	CD1	APHE A	95	−20.546	16.758	6.027	0.55	23.63		C
ANISOU	555	CD1	APHE A	95	3583	3884	1511	−1279	−394	578	C
ATOM	556	CD2	APHE A	95	−19.674	15.570	4.153	0.55	21.24		C
ANISOU	556	CD2	APHE A	95	3457	3320	1295	−603	−166	755	C
ATOM	557	CE1	APHE A	95	−21.240	17.593	5.167	0.55	23.61		C
ANISOU	557	CE1	APHE A	95	3405	4028	1538	−1275	−145	274	C
ATOM	558	CE2	APHE A	95	−20.359	16.411	3.305	0.55	23.20		C
ANISOU	558	CE2	APHE A	95	3257	4020	1537	−6	126	−279	C
ATOM	559	CZ	APHE A	95	−21.133	17.421	3.813	0.55	23.09		C
ANISOU	559	CZ	APHE A	95	3297	3912	1564	−470	344	300	C
ATOM	560	CA	BPHE A	95	−17.576	15.217	6.740	0.45	20.30		C
ANISOU	560	CA	BPHE A	95	3171	3054	1490	−552	−106	87	C
ATOM	561	CB	BPHE A	95	−18.920	14.561	6.465	0.45	20.68		C
ANISOU	561	CB	BPHE A	95	3409	2749	1699	−615	−266	317	C
ATOM	562	CG	BPHE A	95	−19.626	15.135	5.294	0.45	18.61		C
ANISOU	562	CG	BPHE A	95	3166	2357	1548	−265	123	395	C
ATOM	563	CD1	BPHE A	95	−20.183	16.403	5.364	0.45	21.97		C
ANISOU	563	CD1	BPHE A	95	3051	3751	1548	349	80	454	C
ATOM	564	CD2	BPHE A	95	−19.710	14.433	4.103	0.45	17.20		C
ANISOU	564	CD2	BPHE A	95	2668	1958	1908	214	218	−3	C
ATOM	565	CE1	BPHE A	95	−20.830	16.948	4.285	0.45	23.41		C
ANISOU	565	CE1	BPHE A	95	2539	4629	1725	176	24	7	C
ATOM	566	CE2	BPHE A	95	−20.366	14.968	3.028	0.45	21.95		C
ANISOU	566	CE2	BPHE A	95	2908	3552	1878	642	−123	−403	C
ATOM	567	CZ	BPHE A	95	−20.919	16.229	3.113	0.45	22.35		C
ANISOU	567	CZ	BPHE A	95	1954	4668	1869	695	80	−603	C
ATOM	568	N	ARG A	96	−16.837	14.841	8.989	1.00	20.91		N
ANISOU	568	N	ARG A	96	2695	3730	1522	31	−61	49	N
ATOM	569	C	ARG A	96	−16.991	14.137	11.313	1.00	20.35		C
ANISOU	569	C	ARG A	96	3091	3020	1619	557	19	−272	C
ATOM	570	O	ARG A	96	−17.652	15.132	11.602	1.00	19.34		O
ANISOU	570	O	ARG A	96	3037	2624	1688	576	26	−56	O
ATOM	571	CG	AARG A	96	−13.712	14.155	11.035	0.72	34.13		C
ANISOU	571	CG	AARG A	96	3860	6297	2809	430	−336	−523	C
ATOM	572	CD	AARG A	96	−12.525	15.090	11.345	0.72	33.69		C
ANISOU	572	CD	AARG A	96	3252	6072	3478	−719	−259	−531	C
ATOM	573	NE	AARG A	96	−11.631	15.298	10.206	0.72	39.09		N
ANISOU	573	NE	AARG A	96	3882	6644	4327	−119	−187	−749	N
ATOM	574	CZ	AARG A	96	−10.517	16.027	10.235	0.72	39.28		C
ANISOU	574	CZ	AARG A	96	4140	6177	4610	136	1	−920	C
ATOM	575	NH1	AARG A	96	−10.139	16.648	11.343	0.72	33.42		N

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	575	NH1	AARG A	96	3843	4424	4431	39	−444	−1393	N
ATOM	576	NH2	AARG A	96	−9.778	16.137	9.135	0.72	43.24		N
ANISOU	576	NH2	AARG A	96	4516	6840	5072	381	−52	−980	N
ATOM	577	CA	AARG A	96	−16.128	14.141	10.048	0.72	22.82		C
ANISOU	577	CA	AARG A	96	3065	3917	1688	450	−384	−300	C
ATOM	578	CB	AARG A	96	−14.820	14.911	10.328	0.72	29.51		C
ANISOU	578	CB	AARG A	96	3200	5515	2496	424	−371	93	C
ATOM	579	CG	BARG A	96	−13.801	14.649	9.198	0.28	32.35		C
ANISOU	579	CG	BARG A	96	3511	5486	3296	15	73	−304	C
ATOM	580	CD	BARG A	96	−12.553	15.474	9.471	0.28	36.70		C
ANISOU	580	CD	BARG A	96	4017	6152	3776	540	−44	−530	C
ATOM	581	NE	BARG A	96	−11.775	15.718	8.259	0.28	38.49		N
ANISOU	581	NE	BARG A	96	4175	6296	4153	497	223	−803	N
ATOM	582	CZ	BARG A	96	−10.693	16.488	8.217	0.28	40.96		C
ANISOU	582	CZ	BARG A	96	4857	6214	4492	632	227	−780	C
ATOM	583	NH1	BARG A	96	−10.267	17.088	9.321	0.28	41.22		N
ANISOU	583	NH1	BARG A	96	4986	5983	4694	555	−2	−1069	N
ATOM	584	NH2	BARG A	96	−10.037	16.658	7.075	0.28	41.24		N
ANISOU	584	NH2	BARG A	96	4866	6121	4683	730	413	−642	N
ATOM	585	CA	BARG A	96	−16.159	14.110	10.049	0.28	22.57		C
ANISOU	585	CA	BARG A	96	2951	3775	1849	348	−93	−144	C
ATOM	586	CB	BARG A	96	−14.787	14.729	10.345	0.28	28.08		C
ANISOU	586	CB	BARG A	96	3086	4920	2663	293	−61	38	C
ATOM	587	N	VAL A	97	−16.968	13.015	12.034	1.00	21.53		N
ANISOU	587	N	VAL A	97	3316	3008	1855	361	−527	−109	N
ATOM	588	CA	VAL A	97	−17.528	12.949	13.376	1.00	18.82		C
ANISOU	588	CA	VAL A	97	2335	2566	2248	227	−656	−4	C
ATOM	589	C	VAL A	97	−16.381	12.558	14.291	1.00	20.67		C
ANISOU	589	C	VAL A	97	2449	2946	2459	−110	−456	201	C
ATOM	590	O	VAL A	97	−15.705	11.549	14.075	1.00	23.93		O
ANISOU	590	O	VAL A	97	3100	3292	2701	727	−620	−4	O
ATOM	591	CB	VAL A	97	−18.722	11.960	13.549	1.00	21.64		C
ANISOU	591	CB	VAL A	97	2515	3010	2698	65	−360	−128	C
ATOM	592	CG1	VAL A	97	−19.173	11.964	15.005	1.00	24.40		C
ANISOU	592	CG1	VAL A	97	3154	3368	2749	109	−322	991	C
ATOM	593	CG2	VAL A	97	−19.888	12.325	12.655	1.00	23.05		C
ANISOU	593	CG2	VAL A	97	2578	3365	2813	370	−474	−497	C
ATOM	594	N	ATHR A	98	−16.102	13.405	15.274	0.54	20.12		N
ANISOU	594	N	ATHR A	98	2232	3211	2204	−431	−432	105	N
ATOM	595	CA	ATHR A	98	−15.090	13.072	16.277	0.54	23.91		C
ANISOU	595	CA	ATHR A	98	2780	3858	2446	−609	−506	197	C
ATOM	596	C	ATHR A	98	−15.677	13.128	17.668	0.54	20.84		C
ANISOU	596	C	ATHR A	98	2301	3649	1969	−728	−365	516	C
ATOM	597	O	ATHR A	98	−16.453	14.036	17.988	0.54	21.61		O
ANISOU	597	O	ATHR A	98	3168	3407	1634	8	6	604	O
ATOM	598	CB	ATHR A	98	−13.891	14.036	16.259	0.54	30.22		C
ANISOU	598	CB	ATHR A	98	3569	4953	2961	−106	−562	534	C
ATOM	599	OG1	ATHR A	98	−14.350	15.381	16.455	0.54	31.33		O
ANISOU	599	OG1	ATHR A	98	3048	5642	3213	−215	−587	412	O
ATOM	600	CG2	ATHR A	98	−13.113	13.920	14.954	0.54	35.29		C
ANISOU	600	CG2	ATHR A	98	4475	5671	3265	313	−244	479	C
ATOM	601	N	BTHR A	98	−16.176	13.363	15.321	0.46	20.09		N
ANISOU	601	N	BTHR A	98	2038	3530	2064	549	−436	247	N
ATOM	602	CA	BTHR A	98	−15.106	13.085	16.263	0.46	21.23		C
ANISOU	602	CA	BTHR A	98	2135	3849	2082	592	−449	245	C
ATOM	603	C	BTHR A	98	−15.562	13.201	17.705	0.46	20.15		C
ANISOU	603	C	BTHR A	98	1803	3948	1904	292	−759	385	C
ATOM	604	O	BTHR A	98	−16.137	14.222	18.094	0.46	22.84		O
ANISOU	604	O	BTHR A	98	2486	4261	1932	1126	−694	205	O
ATOM	605	CB	BTHR A	98	−13.952	14.043	16.045	0.46	21.40		C
ANISOU	605	CB	BTHR A	98	2109	4039	1983	579	−109	323	C
ATOM	606	OG1	BTHR A	98	−13.601	14.042	14.653	0.46	20.44		O
ANISOU	606	OG1	BTHR A	98	1921	3731	2112	−352	334	−338	O
ATOM	607	CG2	BTHR A	98	−12.775	13.615	16.893	0.46	20.00		C
ANISOU	607	CG2	BTHR A	98	1665	4186	1747	384	5	507	C
ATOM	608	N	GLN A	99	−15.287	12.166	18.500	1.00	21.57		N
ANISOU	608	N	GLN A	99	2526	3886	1782	291	−239	647	N
ATOM	609	CA	GLN A	99	−15.642	12.176	19.911	1.00	19.60		C
ANISOU	609	CA	GLN A	99	2407	2987	2054	100	−73	555	C
ATOM	610	C	GLN A	99	−14.627	13.036	20.635	1.00	21.13		C
ANISOU	610	C	GLN A	99	2168	3429	2433	−383	−373	769	C
ATOM	611	O	GLN A	99	−13.413	12.849	20.481	1.00	25.72		O
ANISOU	611	O	GLN A	99	2265	4660	2845	205	−90	871	O
ATOM	612	CB	GLN A	99	−15.627	10.763	20.468	1.00	23.32		C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	612	CB	GLN A	99	3448	3354	2060	84	−398	944	C
ATOM	613	CG	GLN A	99	−16.121	10.657	21.911	1.00	24.29		C
ANISOU	613	CG	GLN A	99	3681	3235	2315	−359	−790	792	C
ATOM	614	CD	GLN A	99	−16.120	9.241	22.387	1.00	24.87		C
ANISOU	614	CD	GLN A	99	3340	3395	2714	−104	−658	541	C
ATOM	615	OE1	GLN A	99	−15.155	8.499	22.151	1.00	27.40		O
ANISOU	615	OE1	GLN A	99	3662	3771	2979	721	−481	14	O
ATOM	616	NE2	GLN A	99	−17.202	8.830	23.046	1.00	24.83		N
ANISOU	616	NE2	GLN A	99	3350	3346	2738	−410	−466	473	N
ATOM	617	N	LEU A	100	−15.108	13.989	21.424	1.00	20.35		N
ANISOU	617	N	LEU A	100	2427	3424	1881	−315	−846	702	N
ATOM	618	CA	LEU A	100	−14.218	14.855	22.193	1.00	22.12		C
ANISOU	618	CA	LEU A	100	2509	3354	2543	−587	−923	929	C
ATOM	619	C	LEU A	100	−13.757	14.099	23.439	1.00	25.22		C
ANISOU	619	C	LEU A	100	2833	3977	2774	−1314	−1036	1650	C
ATOM	620	O	LEU A	100	−14.376	13.116	23.851	1.00	27.84		O
ANISOU	620	O	LEU A	100	3004	4776	2798	−1252	−1055	1755	O
ATOM	621	CB	LEU A	100	−14.954	16.148	22.564	1.00	22.18		C
ANISOU	621	CB	LEU A	100	3310	2550	2569	−116	−841	571	C
ATOM	622	CG	LEU A	100	−15.310	16.980	21.323	1.00	28.57		C
ANISOU	622	CG	LEU A	100	3537	3836	3484	−505	−141	1220	C
ATOM	623	CD1	LEU A	100	−15.964	18.295	21.711	1.00	32.10		C
ANISOU	623	CD1	LEU A	100	3875	4438	3882	−661	−249	677	C
ATOM	624	CD2	LEU A	100	−14.102	17.260	20.439	1.00	31.65		C
ANISOU	624	CD2	LEU A	100	4243	4262	3519	8	165	1410	C
ATOM	625	O	PRO A	101	−12.823	12.888	27.227	1.00	42.12		O
ANISOU	625	O	PRO A	101	4341	7516	4147	−2276	−1438	2756	O
ATOM	626	N	PRO A	101	−12.641	14.524	24.022	1.00	27.37		N
ANISOU	626	N	PRO A	101	3025	4492	2883	−1042	−851	1757	N
ATOM	627	C	PRO A	101	−13.061	13.728	26.355	1.00	34.13		C
ANISOU	627	C	PRO A	101	3698	6095	3173	−1859	−1291	1925	C
ATOM	628	CA	PRO A	101	−12.108	13.796	25.173	1.00	30.26		C
ANISOU	628	CA	PRO A	101	3072	4929	3498	−1719	−1295	2197	C
ATOM	629	CB	PRO A	101	−10.870	14.603	25.543	1.00	31.58		C
ANISOU	629	CB	PRO A	101	2962	5358	3680	−1735	−1316	1898	C
ATOM	630	CG	PRO A	101	−10.423	15.192	24.260	1.00	32.58		C
ANISOU	630	CG	PRO A	101	3238	5486	3656	−1126	−1249	2046	C
ATOM	631	CD	PRO A	101	−11.707	15.540	23.537	1.00	29.39		C
ANISOU	631	CD	PRO A	101	2928	4828	3412	−1714	−1259	1811	C
ATOM	632	O	ASN A	102	−16.801	12.781	28.200	1.00	35.02		O
ANISOU	632	O	ASN A	102	4270	6614	2423	−1745	−851	1252	O
ATOM	633	N	ASN A	102	−14.091	14.557	26.448	1.00	32.58		N
ANISOU	633	N	ASN A	102	4022	5777	2581	−2080	−1029	1493	N
ATOM	634	CA	ASN A	102	−15.065	14.346	27.553	1.00	32.70		C
ANISOU	634	CA	ASN A	102	4343	5858	2224	−1815	−549	1207	C
ATOM	635	C	ASN A	102	−16.057	13.180	27.305	1.00	29.34		C
ANISOU	635	C	ASN A	102	3349	5361	2439	−1440	−802	1599	C
ATOM	636	CB	ASN A	102	−15.768	15.655	27.921	1.00	35.06		C
ANISOU	636	CB	ASN A	102	4712	6095	2516	−1470	−1263	−197	C
ATOM	637	CG	ASN A	102	−16.865	16.039	26.954	1.00	35.49		C
ANISOU	637	CG	ASN A	102	5449	5336	2698	−1224	−1270	−897	C
ATOM	638	OD1	ASN A	102	−17.007	15.447	25.897	1.00	33.75		O
ANISOU	638	OD1	ASN A	102	5435	4761	2628	−1602	−1374	−353	O
ATOM	639	ND2	ASN A	102	−17.654	17.043	27.322	1.00	41.24		N
ANISOU	639	ND2	ASN A	102	6179	6153	3335	−152	−997	−218	N
ATOM	640	O	GLY A	103	−18.907	11.008	24.825	1.00	32.45		O
ANISOU	640	O	GLY A	103	3152	4883	4296	−845	−1333	240	O
ATOM	641	N	GLY A	103	−16.123	12.691	26.101	1.00	28.97		N
ANISOU	641	N	GLY A	103	3350	5204	2454	−710	−1037	1402	N
ATOM	642	CA	GLY A	103	−16.834	11.481	25.790	1.00	28.79		C
ANISOU	642	CA	GLY A	103	3333	4748	2858	−1476	−931	1338	C
ATOM	643	C	GLY A	103	−18.305	11.747	25.543	1.00	27.31		C
ANISOU	643	C	GLY A	103	3375	4064	2938	−1613	−1087	838	C
ATOM	644	O	ARG A	104	−21.504	13.994	24.086	1.00	22.07		O
ANISOU	644	O	ARG A	104	2425	3656	2303	−471	−456	432	O
ATOM	645	N	ARG A	104	−18.832	12.829	26.061	1.00	25.93		N
ANISOU	645	N	ARG A	104	3342	4210	2300	−646	−963	1045	N
ATOM	646	CA	ARG A	104	−20.201	13.227	25.880	1.00	25.73		C
ANISOU	646	CA	ARG A	104	3272	4683	1820	3	−922	241	C
ATOM	647	C	ARG A	104	−20.466	14.039	24.630	1.00	20.90		C
ANISOU	647	C	ARG A	104	2015	3732	2192	−400	−783	59	C
ATOM	648	CB	ARG A	104	−20.638	14.047	27.057	1.00	34.48		C
ANISOU	648	CB	ARG A	104	4973	6038	2089	1169	−12	106	C
ATOM	649	CG	ARG A	104	−22.086	14.384	27.026	1.00	41.42		C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	649	CG	ARG A	104	5706	7086	2946	1174	501	−347	C
ATOM	650	CD	ARG A	104	−22.418	15.373	28.120	1.00	50.96		C
ANISOU	650	CD	ARG A	104	7134	7926	4304	1794	370	−841	C
ATOM	651	NE	ARG A	104	−21.389	16.386	28.246	1.00	60.36		N
ANISOU	651	NE	ARG A	104	8381	9038	5516	2806	225	−656	N
ATOM	652	CZ	ARG A	104	−21.471	17.644	27.836	1.00	63.89		C
ANISOU	652	CZ	ARG A	104	9252	8929	6093	2909	102	−250	C
ATOM	653	NH1	ARG A	104	−22.552	18.085	27.225	1.00	63.72		N
ANISOU	653	NH1	ARG A	104	9360	8710	6140	2947	131	−275	N
ATOM	654	NH2	ARG A	104	−20.455	18.452	28.023	1.00	64.81		N
ANISOU	654	NH2	ARG A	104	9606	8608	6413	2804	38	−321	N
ATOM	655	N	ASP A	105	−19.496	14.812	24.225	1.00	22.13		N
ANISOU	655	N	ASP A	105	2712	3885	1812	−265	−418	210	N
ATOM	656	CA	ASP A	105	−19.652	15.717	23.118	1.00	20.37		C
ANISOU	656	CA	ASP A	105	2627	3149	1964	−635	−551	381	C
ATOM	657	C	ASP A	105	−18.933	15.183	21.907	1.00	21.30		C
ANISOU	657	C	ASP A	105	2468	3720	1905	129	−110	114	C
ATOM	658	O	ASP A	105	−17.963	14.536	22.015	1.00	21.58		O
ANISOU	658	O	ASP A	105	2488	3988	1722	−86	−104	72	O
ATOM	659	CB	ASP A	105	−19.119	17.092	23.438	1.00	23.74		C
ANISOU	659	CB	ASP A	105	3191	3859	1971	−172	−224	−50	C
ATOM	660	CG	ASP A	105	−19.880	17.763	24.535	1.00	33.60		C
ANISOU	660	CG	ASP A	105	4328	5776	2664	−93	−275	−1112	C
ATOM	661	OD1	ASP A	105	−21.065	17.547	24.681	1.00	34.44		O
ANISOU	661	OD1	ASP A	105	4145	6321	2618	−284	−44	−1308	O
ATOM	662	OD2	ASP A	105	−19.246	18.521	25.249	1.00	36.25		O
ANISOU	662	OD2	ASP A	105	4728	5484	3562	−707	−265	−1489	O
ATOM	663	N	PHE A	106	−19.524	15.439	20.753	1.00	18.18		N
ANISOU	663	N	PHE A	106	2548	2696	1663	−538	−167	160	N
ATOM	664	CA	PHE A	106	−18.981	15.003	19.480	1.00	16.83		C
ANISOU	664	CA	PHE A	106	2415	2448	1531	−17	−266	248	C
ATOM	665	C	PHE A	106	−19.004	16.178	18.503	1.00	17.57		C
ANISOU	665	C	PHE A	106	1991	3059	1628	317	−319	255	C
ATOM	666	O	PHE A	106	−19.997	16.918	18.426	1.00	21.23		O
ANISOU	666	O	PHE A	106	2094	3402	2570	650	177	799	O
ATOM	667	CB	PHE A	106	−19.860	13.889	18.898	1.00	18.71		C
ANISOU	667	CB	PHE A	106	2259	3046	1805	61	−264	169	C
ATOM	668	CG	PHE A	106	−19.914	12.664	19.743	1.00	17.88		C
ANISOU	668	CG	PHE A	106	2132	2838	1822	105	−385	207	C
ATOM	669	CD1	PHE A	106	−20.717	12.626	20.877	1.00	17.86		C
ANISOU	669	CD1	PHE A	106	2273	2774	1740	−120	−307	213	C
ATOM	670	CD2	PHE A	106	−19.146	11.549	19.421	1.00	19.49		C
ANISOU	670	CD2	PHE A	106	2447	3221	1738	38	−412	243	C
ATOM	671	CE1	PHE A	106	−20.742	11.505	21.683	1.00	19.36		C
ANISOU	671	CE1	PHE A	106	2906	2398	2052	252	−233	−87	C
ATOM	672	CE2	PHE A	106	−19.206	10.404	20.208	1.00	21.47		C
ANISOU	672	CE2	PHE A	106	2787	3543	1827	9	−16	302	C
ATOM	673	CZ	PHE A	106	−19.981	10.391	21.342	1.00	20.27		C
ANISOU	673	CZ	PHE A	106	2985	2821	1895	−217	−336	217	C
ATOM	674	N	HIS A	107	−17.915	16.375	17.784	1.00	18.11		N
ANISOU	674	N	HIS A	107	2115	3526	1239	−191	−153	240	N
ATOM	675	CA	HIS A	107	−17.931	17.405	16.726	1.00	17.62		C
ANISOU	675	CA	HIS A	107	2317	3059	1319	−395	−451	134	C
ATOM	676	C	HIS A	107	−18.349	16.772	15.406	1.00	15.55		C
ANISOU	676	C	HIS A	107	2321	2421	1167	−278	−594	86	C
ATOM	677	O	HIS A	107	−17.791	15.750	15.006	1.00	19.06		O
ANISOU	677	O	HIS A	107	2768	2785	1689	358	−295	−121	O
ATOM	678	CB	HIS A	107	−16.580	18.074	16.555	1.00	19.06		C
ANISOU	678	CB	HIS A	107	2110	3144	1988	−846	−495	−173	C
ATOM	679	CG	HIS A	107	−16.336	19.176	17.532	1.00	20.90		C
ANISOU	679	CG	HIS A	107	2843	3071	2025	−955	−969	328	C
ATOM	680	ND1	HIS A	107	−15.112	19.792	17.646	1.00	27.80		N
ANISOU	680	ND1	HIS A	107	2976	4887	2700	−1398	−945	−352	N
ATOM	681	CD2	HIS A	107	−17.164	19.809	18.400	1.00	22.85		C
ANISOU	681	CD2	HIS A	107	3497	3272	1913	−257	−644	−76	C
ATOM	682	CE1	HIS A	107	−15.182	20.740	18.564	1.00	27.90		C
ANISOU	682	CE1	HIS A	107	3576	4309	2715	−871	−706	−930	C
ATOM	683	NE2	HIS A	107	−16.417	20.773	19.037	1.00	25.61		N
ANISOU	683	NE2	HIS A	107	3042	3935	2753	−1004	−432	−349	N
ATOM	684	O	MET A	108	−19.925	19.263	12.576	1.00	16.89		O
ANISOU	684	O	MET A	108	2706	2461	1251	−158	26	35	O
ATOM	685	N	MET A	108	−19.309	17.413	14.767	1.00	15.87		N
ANISOU	685	N	MET A	108	2301	2680	1049	−419	−400	230	N
ATOM	686	C	MET A	108	−19.344	18.168	12.511	1.00	15.57		C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	686	C	MET A	108	2717	2119	1078	−523	4	−128	C
ATOM	687	CA	AMET A	108	−19.700	17.022	13.431	0.32	16.16		C
ANISOU	687	CA	AMET A	108	2600	2353	1187	13	−255	80	C
ATOM	688	CB	AMET A	108	−21.169	16.659	13.433	0.32	15.94		C
ANISOU	688	CB	AMET A	108	3022	1636	1398	−223	−93	−407	C
ATOM	689	CG	AMET A	108	−21.353	15.400	14.247	0.32	17.02		C
ANISOU	689	CG	AMET A	108	2499	2421	1547	−480	49	−142	C
ATOM	690	SD	AMET A	108	−23.038	14.856	14.506	0.32	16.64		S
ANISOU	690	SD	AMET A	108	2135	2566	1621	−97	11	25	S
ATOM	691	CE	AMET A	108	−22.785	13.224	15.205	0.32	15.65		C
ANISOU	691	CE	AMET A	108	2774	1318	1854	−329	−281	154	C
ATOM	692	CA	BMET A	108	−19.777	17.045	13.417	0.68	15.05		C
ANISOU	692	CA	BMET A	108	1659	2843	1218	−474	−213	226	C
ATOM	693	CB	BMET A	108	−21.303	16.993	13.391	0.68	16.38		C
ANISOU	693	CB	BMET A	108	1378	3382	1463	−501	174	454	C
ATOM	694	CG	BMET A	108	−21.875	15.650	13.763	0.68	20.01		C
ANISOU	694	CG	BMET A	108	2285	3439	1878	61	−154	863	C
ATOM	695	SD	BMET A	108	−21.507	15.184	15.465	0.68	19.52		S
ANISOU	695	SD	BMET A	108	2548	3053	1817	−242	−231	86	S
ATOM	696	CE	BMET A	108	−22.409	13.651	15.637	0.68	20.51		C
ANISOU	696	CE	BMET A	108	2629	2942	2221	−671	−220	14	C
ATOM	697	O	ASER A	109	−17.267	17.696	9.029	0.43	18.50		O
ANISOU	697	O	ASER A	109	1959	3313	1756	234	142	−1063	O
ATOM	698	N	ASER A	109	−18.333	17.924	11.681	0.43	15.96		N
ANISOU	698	N	ASER A	109	2243	2294	1526	−857	355	−225	N
ATOM	699	CA	ASER A	109	−17.667	19.024	10.994	0.43	19.35		C
ANISOU	699	CA	ASER A	109	2447	2967	1938	−715	95	−670	C
ATOM	700	C	ASER A	109	−17.594	18.792	9.493	0.43	19.29		C
ANISOU	700	C	ASER A	109	2177	3504	1650	−318	151	−805	C
ATOM	701	CB	ASER A	109	−16.239	19.196	11.523	0.43	23.72		C
ANISOU	701	CB	ASER A	109	2616	3962	2433	114	−62	−1036	C
ATOM	702	OG	ASER A	109	−15.449	18.066	11.206	0.43	24.87		O
ANISOU	702	OG	ASER A	109	2232	4522	2694	−77	142	−378	O
ATOM	703	O	BSER A	109	−17.755	17.712	8.903	0.57	16.58		O
ANISOU	703	O	BSER A	109	2228	2680	1393	−326	36	357	O
ATOM	704	N	BSER A	109	−18.310	17.930	11.700	0.57	17.42		N
ANISOU	704	N	BSER A	109	2651	3054	915	132	261	432	N
ATOM	705	CA	BSER A	109	−17.720	19.036	10.931	0.57	18.10		C
ANISOU	705	CA	BSER A	109	2316	3142	1420	−340	18	333	C
ATOM	706	C	BSER A	109	−17.807	18.844	9.413	0.57	17.35		C
ANISOU	706	C	BSER A	109	2279	2987	1328	−363	158	232	C
ATOM	707	CB	BSER A	109	−16.233	19.249	11.301	0.57	18.35		C
ANISOU	707	CB	BSER A	109	1707	3539	1728	−560	−117	−304	C
ATOM	708	OG	BSER A	109	−16.081	19.537	12.694	0.57	18.43		O
ANISOU	708	OG	BSER A	109	2119	3280	1604	−671	−282	−272	O
ATOM	709	N	AVAL A	110	−17.879	19.848	8.749	0.43	20.22		N
ANISOU	709	N	AVAL A	110	2646	3467	1570	−274	344	−416	N
ATOM	710	CA	AVAL A	110	−17.685	19.820	7.311	0.43	18.67		C
ANISOU	710	CA	AVAL A	110	2544	3062	1489	−282	353	−386	C
ATOM	711	C	AVAL A	110	−16.617	20.829	6.918	0.43	19.25		C
ANISOU	711	C	AVAL A	110	2525	3225	1565	−86	198	−393	C
ATOM	712	O	AVAL A	110	−16.610	21.971	7.371	0.43	21.11		O
ANISOU	712	O	AVAL A	110	2862	3304	1853	−113	355	−451	O
ATOM	713	CB	AVAL A	110	−18.994	20.089	6.540	0.43	18.48		C
ANISOU	713	CB	AVAL A	110	2217	3191	1614	−484	317	−311	C
ATOM	714	CG1	AVAL A	110	−19.556	21.453	6.936	0.43	17.24		C
ANISOU	714	CG1	AVAL A	110	1865	2994	1691	261	25	−350	C
ATOM	715	CG2	AVAL A	110	−18.767	19.987	5.022	0.43	18.66		C
ANISOU	715	CG2	AVAL A	110	3126	2446	1519	−907	508	−173	C
ATOM	716	N	BVAL A	110	−17.948	19.974	8.727	0.57	20.02		N
ANISOU	716	N	BVAL A	110	3350	2884	1373	−535	−10	617	N
ATOM	717	CA	BVAL A	110	−17.806	20.049	7.276	0.57	20.16		C
ANISOU	717	CA	BVAL A	110	3309	2772	1578	−634	−7	637	C
ATOM	718	C	BVAL A	110	−16.551	20.862	6.975	0.57	19.46		C
ANISOU	718	C	BVAL A	110	3030	2682	1682	−618	345	461	C
ATOM	719	O	BVAL A	110	−16.337	21.905	7.575	0.57	22.31		O
ANISOU	719	O	BVAL A	110	3588	2840	2047	−704	622	378	O
ATOM	720	CB	BVAL A	110	−19.015	20.766	6.604	0.57	24.08		C
ANISOU	720	CB	BVAL A	110	3663	3351	2136	−1178	−128	1214	C
ATOM	721	CG1	BVAL A	110	−18.845	20.824	5.080	0.57	25.54		C
ANISOU	721	CG1	BVAL A	110	3902	3935	1869	−723	−823	696	C
ATOM	722	CG2	BVAL A	110	−20.331	20.085	6.959	0.57	30.09		C
ANISOU	722	CG2	BVAL A	110	4574	4134	2725	−626	279	1349	C
ATOM	723	O	VAL A	111	−15.710	21.304	3.526	1.00	22.48		O

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	723	O	VAL A	111	3203	3547	1793	−452	306	67	O
ATOM	724	N	VAL A	111	−15.694	20.388	6.082	1.00	20.45		N
ANISOU	724	N	VAL A	111	2564	3535	1670	−208	209	89	N
ATOM	725	C	VAL A	111	−14.992	21.904	4.327	1.00	22.78		C
ANISOU	725	C	VAL A	111	2511	3946	2197	−572	238	99	C
ATOM	726	CA	VAL A	111	−14.614	21.254	5.641	1.00	21.42		C
ANISOU	726	CA	VAL A	111	2591	3604	1944	65	−166	−44	C
ATOM	727	CB	VAL A	111	−13.256	20.545	5.502	1.00	28.54		C
ANISOU	727	CB	VAL A	111	3359	5341	2143	776	−361	122	C
ATOM	728	CG1	VAL A	111	−12.765	20.131	6.855	1.00	34.74		C
ANISOU	728	CG1	VAL A	111	3942	6915	2341	1505	−240	1042	C
ATOM	729	CG2	VAL A	111	−13.344	19.356	4.616	1.00	32.15		C
ANISOU	729	CG2	VAL A	111	4741	4959	2514	1243	−217	140	C
ATOM	730	N	AARG A	112	−14.502	23.123	4.130	0.64	25.50		N
ANISOU	730	N	AARG A	112	2338	4648	2704	560	57	482	N
ATOM	731	CA	AARG A	112	−14.716	23.863	2.899	0.64	28.16		C
ANISOU	731	CA	AARG A	112	3096	4660	2946	224	75	807	C
ATOM	732	C	AARG A	112	−16.189	23.863	2.517	0.64	25.69		C
ANISOU	732	C	AARG A	112	2940	4205	2614	−321	−431	69	C
ATOM	733	O	AARG A	112	−16.599	23.293	1.497	0.64	28.17		O
ANISOU	733	O	AARG A	112	3662	4575	2464	36	172	−354	O
ATOM	734	CB	AARG A	112	−13.881	23.264	1.784	0.64	32.74		C
ANISOU	734	CB	AARG A	112	3520	5668	3251	772	812	1196	C
ATOM	735	CG	AARG A	112	−13.672	24.222	0.641	0.64	37.11		C
ANISOU	735	CG	AARG A	112	4357	6186	3556	1108	1203	1445	C
ATOM	736	CD	AARG A	112	−12.668	23.673	−0.347	0.64	37.95		C
ANISOU	736	CD	AARG A	112	4603	5884	3933	499	1346	1205	C
ATOM	737	NE	AARG A	112	−12.339	24.695	−1.313	0.64	35.79		N
ANISOU	737	NE	AARG A	112	4011	5560	4028	−410	928	336	N
ATOM	738	CZ	AARG A	112	−11.469	24.535	−2.294	0.64	35.41		C
ANISOU	738	CZ	AARG A	112	3566	5629	4259	−1251	877	138	C
ATOM	739	NH1	AARG A	112	−10.841	23.380	−2.456	0.64	34.82		N
ANISOU	739	NH1	AARG A	112	3635	5291	4303	−780	384	68	N
ATOM	740	NH2	AARG A	112	−11.251	25.535	−3.121	0.64	37.00		N
ANISOU	740	NH2	AARG A	112	3619	5713	4724	−1464	953	−112	N
ATOM	741	N	BARG A	112	−14.507	23.128	4.129	0.36	25.39		N
ANISOU	741	N	BARG A	112	2625	4291	2730	266	157	616	N
ATOM	742	CA	BARG A	112	−14.706	23.887	2.896	0.36	26.81		C
ANISOU	742	CA	BARG A	112	2991	4095	3103	−24	272	1219	C
ATOM	743	C	BARG A	112	−16.169	23.948	2.474	0.36	24.08		C
ANISOU	743	C	BARG A	112	2848	3479	2824	−25	125	1085	C
ATOM	744	O	BARG A	112	−16.539	23.526	1.376	0.36	23.44		O
ANISOU	744	O	BARG A	112	2813	3230	2863	461	906	1647	O
ATOM	745	CB	BARG A	112	−13.827	23.325	1.781	0.36	31.96		C
ANISOU	745	CB	BARG A	112	3389	5114	3642	279	443	1177	C
ATOM	746	CG	BARG A	112	−12.347	23.407	2.107	0.36	35.35		C
ANISOU	746	CG	BARG A	112	3724	5528	4178	41	550	1210	C
ATOM	747	CD	BARG A	112	−11.473	23.126	0.904	0.36	39.31		C
ANISOU	747	CD	BARG A	112	4401	5838	4698	−159	544	1152	C
ATOM	748	NE	BARG A	112	−10.076	22.971	1.297	0.36	44.00		N
ANISOU	748	NE	BARG A	112	5216	6419	5084	84	425	1034	N
ATOM	749	CZ	BARG A	112	−9.106	22.587	0.475	0.36	45.80		C
ANISOU	749	CZ	BARG A	112	5444	6610	5349	−368	486	970	C
ATOM	750	NH1	BARG A	112	−9.375	22.314	−0.794	0.36	47.53		N
ANISOU	750	NH1	BARG A	112	5679	7004	5376	−200	445	828	N
ATOM	751	NH2	BARG A	112	−7.866	22.467	0.926	0.36	45.03		N
ANISOU	751	NH2	BARG A	112	5455	6153	5501	−891	469	1060	N
ATOM	752	N	ALA A	113	−16.999	24.471	3.367	1.00	23.98		N
ANISOU	752	N	ALA A	113	3000	3452	2658	130	−457	328	N
ATOM	753	CA	ALA A	113	−18.430	24.526	3.155	1.00	20.94		C
ANISOU	753	CA	ALA A	113	2416	3494	2046	−164	−422	331	C
ATOM	754	C	ALA A	113	−18.747	25.291	1.880	1.00	22.40		C
ANISOU	754	C	ALA A	113	3228	3217	2067	−533	−46	587	C
ATOM	755	O	ALA A	113	−18.148	26.310	1.575	1.00	25.47		O
ANISOU	755	O	ALA A	113	3626	3522	2531	−263	−590	849	O
ATOM	756	CB	ALA A	113	−19.075	25.220	4.378	1.00	24.76		C
ANISOU	756	CB	ALA A	113	3029	4434	1945	109	−90	−62	C
ATOM	757	CD	AARG A	114	−19.822	22.063	−2.196	0.44	27.73		C
ANISOU	757	CD	AARG A	114	4602	4367	1567	−229	528	927	C
ATOM	758	NE	AARG A	114	−20.565	20.821	−1.977	0.44	33.50		N
ANISOU	758	NE	AARG A	114	5210	5529	1988	984	468	594	N
ATOM	759	CZ	AARG A	114	−20.512	19.732	−2.743	0.44	33.12		C
ANISOU	759	CZ	AARG A	114	4858	5683	2042	1930	559	798	C
ATOM	760	NH1	AARG A	114	−19.738	19.691	−3.834	0.44	35.33		N

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ANISOU	760	NH1	AARG A	114	5422	5657	2345	2434	940	848	N
ATOM	761	NH2	AARG A	114	−21.248	18.668	−2.416	0.44	30.86		N
ANISOU	761	NH2	AARG A	114	3689	6042	1995	1766	−568	−101	N
ATOM	762	N	AARG A	114	−19.681	24.763	1.110	0.44	23.54		N
ANISOU	762	N	AARG A	114	3330	3855	1757	−888	−497	392	N
ATOM	763	CA	AARG A	114	−20.120	25.419	−0.113	0.44	25.85		C
ANISOU	763	CA	AARG A	114	3684	4464	1673	−514	−616	420	C
ATOM	764	C	AARG A	114	−21.587	25.822	0.037	0.44	23.92		C
ANISOU	764	C	AARG A	114	3674	3849	1565	−455	−670	680	C
ATOM	765	O	AARG A	114	−22.282	25.310	0.928	0.44	23.09		O
ANISOU	765	O	AARG A	114	4106	3262	1404	−838	−675	192	O
ATOM	766	CB	AARG A	114	−19.886	24.498	−1.311	0.44	25.68		C
ANISOU	766	CB	AARG A	114	3957	4334	1468	−1066	−593	217	C
ATOM	767	CG	AARG A	114	−20.049	23.017	−0.997	0.44	28.12		C
ANISOU	767	CG	AARG A	114	4700	4662	1320	72	−71	616	C
ATOM	768	CD	BARG A	114	−18.772	23.074	−2.774	0.56	35.82		C
ANISOU	768	CD	BARG A	114	4056	5852	3704	117	−126	2051	C
ATOM	769	NE	BARG A	114	−19.944	22.277	−3.109	0.56	40.47		N
ANISOU	769	NE	BARG A	114	4804	5911	4662	55	−389	1775	N
ATOM	770	CZ	BARG A	114	−20.098	21.011	−2.753	0.56	42.83		C
ANISOU	770	CZ	BARG A	114	4566	6379	5328	−456	−1164	1126	C
ATOM	771	NH1	BARG A	114	−19.143	20.408	−2.079	0.56	41.08		N
ANISOU	771	NH1	BARG A	114	3605	6549	5453	−1102	−2126	551	N
ATOM	772	NH2	BARG A	114	−21.198	20.343	−3.085	0.56	40.75		N
ANISOU	772	NH2	BARG A	114	4003	5819	5660	−1974	−1102	1134	N
ATOM	773	N	BARG A	114	−19.723	24.767	1.160	0.56	22.89		N
ANISOU	773	N	BARG A	114	2520	4204	1973	−596	−310	454	N
ATOM	774	CA	BARG A	114	−20.196	25.345	−0.083	0.56	25.25		C
ANISOU	774	CA	BARG A	114	2633	4796	2163	340	−129	872	C
ATOM	775	C	BARG A	114	−21.603	25.887	0.108	0.56	22.44		C
ANISOU	775	C	BARG A	114	2802	3977	1749	456	−196	1011	C
ATOM	776	O	BARG A	114	−22.282	25.517	1.077	0.56	22.28		O
ANISOU	776	O	BARG A	114	2878	3893	1695	601	343	649	O
ATOM	777	CB	BARG A	114	−20.206	24.270	−1.151	0.56	29.98		C
ANISOU	777	CB	BARG A	114	3322	5573	2495	800	−78	1057	C
ATOM	778	CG	BARG A	114	−18.866	23.604	−1.360	0.56	31.95		C
ANISOU	778	CG	BARG A	114	3493	5722	2925	46	57	1221	C
ATOM	779	N	ARG A	115	−22.046	26.749	−0.807	1.00	25.34		N
ANISOU	779	N	ARG A	115	3540	4070	2019	−88	−539	1193	N
ATOM	780	C	ARG A	115	−24.377	26.091	−0.682	1.00	23.08		C
ANISOU	780	C	ARG A	115	3190	4041	1539	265	323	1049	C
ATOM	781	O	ARG A	115	−25.342	26.113	0.082	1.00	21.35		O
ANISOU	781	O	ARG A	115	2940	3726	1447	140	188	409	O
ATOM	782	CA	ARG A	115	−23.407	27.257	−0.729	1.00	27.28		C
ANISOU	782	CA	ARG A	115	4054	4056	2257	409	−360	1570	C
ATOM	783	CB	ARG A	115	−23.724	28.110	−1.967	1.00	32.91		C
ATOM	784	CG	ARG A	115	−25.218	28.462	−2.136	1.00	41.29		C
ATOM	785	CD	ARG A	115	−25.569	28.978	−3.572	1.00	61.63		C
ATOM	786	NE	ARG A	115	−25.270	27.958	−4.585	1.00	78.38		N
ATOM	787	CZ	ARG A	115	−24.270	28.027	−5.466	1.00	72.47		C
ATOM	788	NH1	ARG A	115	−23.472	29.092	−5.502	1.00	76.77		N
ATOM	789	NH2	ARG A	115	−24.071	27.031	−6.324	1.00	56.40		N
ATOM	790	N	AASN A	116	−24.118	25.053	−1.459	1.00	22.62		N
ANISOU	790	N	AASN A	116	3265	3968	1361	477	−142	510	N
ATOM	791	CA	AASN A	116	−25.047	23.934	−1.529	0.41	21.78		C
ANISOU	791	CA	AASN A	116	3351	3780	1144	774	57	−138	C
ATOM	792	C	AASN A	116	−24.921	22.945	−0.356	0.41	21.02		C
ANISOU	792	C	AASN A	116	3012	3710	1263	656	−173	−174	C
ATOM	793	O	AASN A	116	−25.539	21.881	−0.376	0.41	23.29		O
ANISOU	793	O	AASN A	116	2655	4542	1652	1467	−582	−538	O
ATOM	794	CB	AASN A	116	−24.913	23.237	−2.880	0.41	22.43		C
ANISOU	794	CB	AASN A	116	3493	3705	1323	1047	−478	−446	C
ATOM	795	CG	AASN A	116	−23.485	22.930	−3.205	0.41	25.26		C
ANISOU	795	CG	AASN A	116	3882	4220	1494	1347	−291	−558	C
ATOM	796	OD1	AASN A	116	−22.717	22.625	−2.299	0.41	26.45		O
ANISOU	796	OD1	AASN A	116	3529	4711	1810	897	−662	−673	O
ATOM	797	ND2	AASN A	116	−23.101	23.017	−4.479	0.41	28.74		N
ANISOU	797	ND2	AASN A	116	4690	4144	2084	1089	686	−736	N
ATOM	798	N	BASN A	116	−24.061	25.048	−1.446	0.59	22.74		N
ANISOU	798	N	BASN A	116	3178	3893	1569	883	−283	821	N
ATOM	799	CA	BASN A	116	−24.905	23.864	−1.578	0.59	23.94		C
ANISOU	799	CA	BASN A	116	3529	3995	1571	978	210	258	C
ATOM	800	C	BASN A	116	−25.030	23.066	−0.288	0.59	22.23		C
ANISOU	800	C	BASN A	116	3261	3740	1447	339	−21	150	C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	801	O	BASN A	116	−25.939	22.250	−0.154	0.59	23.73		O
ANISOU	801	O	BASN A	116	3117	4220	1678	77	68	221	O
ATOM	802	CB	BASN A	116	−24.371	22.942	−2.679	0.59	27.67		C
ANISOU	802	CB	BASN A	116	4242	4299	1972	1422	−53	185	C
ATOM	803	CG	BASN A	116	−24.010	23.681	−3.939	0.59	31.37		C
ANISOU	803	CG	BASN A	116	4600	5105	2215	1349	272	242	C
ATOM	804	OD1	BASN A	116	−22.977	24.379	−4.004	0.59	35.05		O
ANISOU	804	OD1	BASN A	116	5288	6005	2023	1324	736	732	O
ATOM	805	ND2	BASN A	116	−24.850	23.519	−4.975	0.59	29.76		N
ANISOU	805	ND2	BASN A	116	3851	4866	2590	1526	−90	463	N
ATOM	806	N	ASP A	117	−24.126	23.295	0.664	1.00	18.63		N
ANISOU	806	N	ASP A	117	2614	3385	1081	348	192	244	N
ATOM	807	CA	ASP A	117	−24.216	22.614	1.978	1.00	17.28		C
ANISOU	807	CA	ASP A	117	2064	3061	1440	234	−11	463	C
ATOM	808	C	ASP A	117	−25.308	23.206	2.871	1.00	17.99		C
ANISOU	808	C	ASP A	117	2199	3074	1563	−202	−177	182	C
ATOM	809	O	ASP A	117	−25.651	22.625	3.923	1.00	19.33		O
ANISOU	809	O	ASP A	117	2538	3209	1595	280	160	127	O
ATOM	810	CB	ASP A	117	−22.882	22.714	2.707	1.00	19.14		C
ANISOU	810	CB	ASP A	117	1982	3815	1475	316	−173	286	C
ATOM	811	CG	ASP A	117	−21.810	21.821	2.075	1.00	19.54		C
ANISOU	811	CG	ASP A	117	2536	2972	1916	−9	170	274	C
ATOM	812	OD1	ASP A	117	−22.099	20.687	1.618	1.00	21.93		O
ANISOU	812	OD1	ASP A	117	2784	3055	2494	193	−92	218	O
ATOM	813	OD2	ASP A	117	−20.654	22.257	2.042	1.00	24.17		O
ANISOU	813	OD2	ASP A	117	2760	4075	2348	−325	102	183	O
ATOM	814	N	SER A	118	−25.855	24.355	2.497	1.00	18.44		N
ANISOU	814	N	SER A	118	2710	2940	1356	107	91	301	N
ATOM	815	CA	SER A	118	−26.961	24.934	3.248	1.00	19.24		C
ANISOU	815	CA	SER A	118	2740	3090	1480	123	161	578	C
ATOM	816	C	SER A	118	−28.119	23.962	3.352	1.00	17.34		C
ANISOU	816	C	SER A	118	2236	2841	1513	−195	149	411	C
ATOM	817	O	SER A	118	−28.515	23.319	2.387	1.00	21.21		O
ANISOU	817	O	SER A	118	2561	3719	1780	−7	−135	61	O
ATOM	818	CB	SER A	118	−27.435	26.240	2.609	1.00	19.56		C
ANISOU	818	CB	SER A	118	2643	2969	1821	473	211	257	C
ATOM	819	OG	SER A	118	−26.407	27.208	2.561	1.00	21.23		O
ANISOU	819	OG	SER A	118	2741	3282	2043	−67	−164	262	O
ATOM	820	N	GLY A	119	−28.681	23.830	4.541	1.00	18.54		N
ANISOU	820	N	GLY A	119	2190	3450	1404	151	216	858	N
ATOM	821	CA	GLY A	119	−29.787	22.912	4.726	1.00	17.86		C
ANISOU	821	CA	GLY A	119	2272	3347	1168	−389	142	704	C
ATOM	822	C	GLY A	119	−29.940	22.538	6.187	1.00	16.48		C
ANISOU	822	C	GLY A	119	1791	3008	1462	162	−290	376	C
ATOM	823	O	GLY A	119	−29.411	23.231	7.047	1.00	17.68		O
ANISOU	823	O	GLY A	119	2467	2930	1320	−127	−151	322	O
ATOM	824	N	THR A	120	−30.652	1.455	6.460	1.00	16.96		N
ANISOU	824	N	THR A	120	2339	2589	1515	133	50	324	N
ATOM	825	CA	THR A	120	−30.846	21.038	7.844	1.00	17.39		C
ANISOU	825	CA	THR A	120	2261	2752	1596	363	11	412	C
ATOM	826	C	THR A	120	−30.229	19.704	8.108	1.00	17.16		C
ANISOU	826	C	THR A	120	2518	2569	1433	598	188	356	C
ATOM	827	O	THR A	120	−30.087	18.854	7.204	1.00	18.43		O
ANISOU	827	O	THR A	120	2501	2862	1640	293	−322	136	O
ATOM	828	CB	THR A	120	−32.295	21.080	8.322	1.00	22.74		C
ANISOU	828	CB	THR A	120	2508	3475	2658	1017	−502	139	C
ATOM	829	OG1	THR A	120	−33.067	20.130	7.605	1.00	25.67		O
ANISOU	829	OG1	THR A	120	2845	3744	3164	458	−375	−510	O
ATOM	830	CG2	THR A	120	−32.866	22.453	8.114	1.00	25.50		C
ANISOU	830	CG2	THR A	120	2512	3674	3501	577	384	939	C
ATOM	831	N	TYR A	121	−29.785	19.560	9.357	1.00	15.89		N
ANISOU	831	N	TYR A	121	2154	2671	1212	48	−246	588	N
ATOM	832	CA	TYR A	121	−28.971	18.442	9.782	1.00	16.03		C
ANISOU	832	CA	TYR A	121	2230	2669	1190	126	−244	476	C
ATOM	833	C	TYR A	121	−29.457	17.963	11.142	1.00	17.45		C
ANISOU	833	C	TYR A	121	2751	2650	1229	−26	−107	157	C
ATOM	834	O	TYR A	121	−30.094	18.715	11.871	1.00	18.74		O
ANISOU	834	O	TYR A	121	2581	3114	1427	−4	32	−32	O
ATOM	835	CB	TYR A	121	−27.505	18.867	9.909	1.00	17.02		C
ANISOU	835	CB	TYR A	121	2030	3297	1142	−152	7	84	C
ATOM	836	CG	TYR A	121	−26.862	19.284	8.595	1.00	16.99		C
ANISOU	836	CG	TYR A	121	1923	3330	1202	303	−58	−27	C
ATOM	837	CD1	TYR A	121	−27.122	20.526	8.025	1.00	16.94		C
ANISOU	837	CD1	TYR A	121	2175	2999	1261	81	−6	91	C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	838	CD2	TYR A	121	−25.990	18.431	7.953	1.00	18.72		C
ANISOU	838	CD2	TYR A	121	2084	3636	1394	597	20	3	C
ATOM	839	CE1	TYR A	121	−26.535	20.894	6.783	1.00	17.26		C
ANISOU	839	CE1	TYR A	121	2223	2814	1521	192	−68	174	C
ATOM	840	CE2	TYR A	121	−25.396	18.786	6.753	1.00	19.09		C
ANISOU	840	CE2	TYR A	121	2817	3101	1335	803	93	136	C
ATOM	841	CZ	TYR A	121	−25.658	20.002	6.196	1.00	18.53		C
ANISOU	841	CZ	TYR A	121	2973	3026	1040	892	218	291	C
ATOM	842	OH	TYR A	121	−25.073	20.311	4.976	1.00	20.02		O
ANISOU	842	OH	TYR A	121	3173	3044	1390	410	120	244	O
ATOM	843	N	LEU A	122	−29.151	16.732	11.481	1.00	17.79		N
ANISOU	843	N	LEU A	122	2426	2656	1679	300	99	258	N
ATOM	844	CA	LEU A	122	−29.436	16.259	12.829	1.00	18.38		C
ANISOU	844	CA	LEU A	122	2257	2876	1850	383	151	362	C
ATOM	845	C	LEU A	122	−28.480	15.143	13.165	1.00	17.50		C
ANISOU	845	C	LEU A	122	2241	2673	1738	488	72	83	C
ATOM	846	O	LEU A	122	−27.747	14.642	12.323	1.00	18.44		O
ANISOU	846	O	LEU A	122	2330	3142	1533	367	83	22	O
ATOM	847	CB	LEU A	122	−30.899	15.832	13.022	1.00	21.09		C
ANISOU	847	CB	LEU A	122	2899	2911	2203	−122	97	−92	C
ATOM	848	CG	LEU A	122	−31.446	14.572	12.301	1.00	24.97		C
ANISOU	848	CG	LEU A	122	2912	3526	3050	762	−893	−350	C
ATOM	849	CD1	LEU A	122	−30.992	13.195	12.875	1.00	28.68		C
ANISOU	849	CD1	LEU A	122	4278	2844	3777	−171	−455	−198	C
ATOM	850	CD2	LEU A	122	−32.977	14.605	12.377	1.00	30.20		C
ANISOU	850	CD2	LEU A	122	2868	5067	3539	−50	77	824	C
ATOM	851	N	CYS A	123	−28.460	14.772	14.435	1.00	16.93		N
ANISOU	851	N	CYS A	123	2292	2385	1757	459	93	276	N
ATOM	852	C	CYS A	123	−28.643	12.568	15.416	1.00	17.97		C
ANISOU	852	C	CYS A	123	1816	2736	2277	−65	303	37	C
ATOM	853	O	CYS A	123	−29.644	12.887	16.062	1.00	22.06		O
ANISOU	853	O	CYS A	123	2319	3083	2978	100	651	228	O
ATOM	854	CA	ACYS A	123	−27.673	13.661	14.942	0.31	19.10		C
ANISOU	854	CA	ACYS A	123	2057	3008	2190	−6	122	39	C
ATOM	855	CB	ACYS A	123	−26.847	14.215	16.103	0.31	21.57		C
ANISOU	855	CB	ACYS A	123	2243	3416	2539	306	−33	−437	C
ATOM	856	SG	ACYS A	123	−25.899	13.084	17.129	0.31	25.01		S
ANISOU	856	SG	ACYS A	123	2756	4044	2703	677	343	464	S
ATOM	857	CA	BCYS A	123	−27.706	13.581	14.809	0.69	18.12		C
ANISOU	857	CA	BCYS A	123	2473	2531	1880	208	−102	260	C
ATOM	858	CB	BCYS A	123	−26.510	13.901	15.718	0.69	20.42		C
ANISOU	858	CB	BCYS A	123	3173	3100	1485	820	−676	149	C
ATOM	859	SG	BCYS A	123	−26.883	14.651	17.349	0.69	20.60		S
ANISOU	859	SG	BCYS A	123	2693	3083	2053	279	165	300	S
ATOM	860	N	GLY A	124	−28.353	11.317	15.140	1.00	18.85		N
ANISOU	860	N	GLY A	124	2602	2364	2197	341	27	219	N
ATOM	861	CA	GLY A	124	−29.211	10.233	15.570	1.00	21.70		C
ANISOU	861	CA	GLY A	124	2982	2486	2776	54	161	780	C
ATOM	862	C	GLY A	124	−28.392	9.209	16.333	1.00	19.89		C
ANISOU	862	C	GLY A	124	2817	2321	2418	202	−132	44	C
ATOM	863	O	GLY A	124	−27.320	8.802	15.878	1.00	21.28		O
ANISOU	863	O	GLY A	124	2637	3036	2413	337	167	453	O
ATOM	864	N	ALA A	125	−28.854	8.849	17.529	1.00	19.97		N
ANISOU	864	N	ALA A	125	2743	2795	2051	174	198	573	N
ATOM	865	CA	ALA A	125	−28.199	7.823	18.311	1.00	19.04		C
ANISOU	865	CA	ALA A	125	2651	2461	2121	−104	232	384	C
ATOM	866	C	ALA A	125	−28.897	6.474	18.131	1.00	20.41		C
ANISOU	866	C	ALA A	125	2524	2715	2516	−849	237	283	C
ATOM	867	O	ALA A	125	−30.107	6.391	18.227	1.00	22.93		O
ANISOU	867	O	ALA A	125	2463	2991	3260	−482	402	210	O
ATOM	868	CB	ALA A	125	−28.199	8.206	19.825	1.00	22.31		C
ANISOU	868	CB	ALA A	125	3434	3137	1907	148	409	112	C
ATOM	869	N	ILE A	126	−28.134	5.431	17.849	1.002	1.28		N
ANISOU	869	N	ILE A	126	3331	2307	2448	333	229	−23	N
ATOM	870	CA	ILE A	126	−28.689	4.102	17.708	1.00	21.03		C
ANISOU	870	CA	ILE A	126	2812	2984	2196	232	149	104	C
ATOM	871	C	ILE A	126	−28.141	3.249	18.823	1.00	20.32		C
ANISOU	871	C	ILE A	126	2948	2533	2241	81	381	−141	C
ATOM	872	O	ILE A	126	−26.929	3.053	18.932	1.00	21.41		O
ANISOU	872	O	ILE A	126	3035	2745	2354	236	304	359	O
ATOM	873	CB	ILE A	126	−28.299	3.468	16.357	1.00	21.73		C
ANISOU	873	CB	ILE A	126	2778	2998	2480	−196	−64	−74	C
ATOM	874	CG1	ILE A	126	−28.776	4.372	15.225	1.00	28.07		C
ANISOU	874	CG1	ILE A	126	3806	4420	2439	863	−34	−111	C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	875	CG2	ILE A	126	−28.936	2.091	16.234	1.00	23.65		C
ANISOU	875	CG2	ILE A	126	3280	2829	2876	427	198	−128	C
ATOM	876	CD1	ILE A	126	−28.124	4.074	13.911	1.00	32.06		C
ANISOU	876	CD1	ILE A	126	4119	5593	2470	1068	160	48	C
ATOM	877	N	SER A	127	−29.021	2.786	19.704	1.00	24.52		N
ANISOU	877	N	SER A	127	3469	2702	3148	134	942	513	N
ATOM	878	C	SER A	127	−28.562	0.439	20.099	1.00	26.97		C
ANISOU	878	C	SER A	127	3918	2809	3522	−161	486	365	C
ATOM	879	O	SER A	127	−29.476	0.016	19.372	1.00	30.64		O
ANISOU	879	O	SER A	127	4144	3088	4412	−524	−127	480	O
ATOM	880	CA	ASER A	127	−28.644	1.821	20.727	0.54	27.12		C
ANISOU	880	CA	ASER A	127	4183	2766	3354	−53	1116	866	C
ATOM	881	CB	ASER A	127	−29.680	1.805	21.850	0.54	30.65		C
ANISOU	881	CB	ASER A	127	4362	3651	3631	−97	1372	780	C
ATOM	882	OG	ASER A	127	−30.912	1.290	21.378	0.54	33.96		O
ANISOU	882	OG	ASER A	127	5028	4137	3738	695	1611	696	O
ATOM	883	CA	BSER A	127	−28.625	1.827	20.718	0.46	27.29		C
ANISOU	883	CA	BSER A	127	4288	2833	3249	67	1037	923	C
ATOM	884	CB	BSER A	127	−29.607	1.847	21.886	0.46	31.44		C
ANISOU	884	CB	BSER A	127	4819	3848	3277	387	1211	1189	C
ATOM	885	OG	BSER A	127	−29.173	0.977	22.908	0.46	33.58		O
ANISOU	885	OG	BSER A	127	5560	4055	3145	879	1354	1535	O
ATOM	886	O	LEU A	128	−27.899	−3.841	20.248	1.00	40.42		O
ANISOU	886	O	LEU A	128	6912	3312	5132	−4	1784	999	O
ATOM	887	N	LEU A	128	−27.490	−0.275	20.368	1.00	26.79		N
ANISOU	887	N	LEU A	128	43.71	2658	3149	562	905	370	N
ATOM	888	CA	LEU A	128	−27.366	−1.581	19.753	1.00	29.51		C
ANISOU	888	CA	LEU A	128	5014	2643	3556	242	573	395	C
ATOM	889	C	LEU A	128	−27.806	−2.701	20.682	1.00	37.60		C
ANISOU	889	C	LEU A	128	6003	3639	4645	441	1078	830	C
ATOM	890	CB	LEU A	128	−25.945	−1.775	19.240	1.00	26.66		C
ANISOU	890	CB	LEU A	128	4851	2415	2863	599	348	48	C
ATOM	891	CG	LEU A	128	−25.549	−0.733	18.186	1.00	25.31		C
ANISOU	891	CG	LEU A	128	4167	2838	2613	−13	88	−245	C
ATOM	892	CD1	LEU A	128	−24.029	−0.823	17.921	1.00	29.58		C
ANISOU	892	CD1	LEU A	128	4757	3555	2926	−46	66	−64	C
ATOM	893	CD2	LEU A	128	−26.332	−0.928	16.881	1.00	30.47		C
ANISOU	893	CD2	LEU A	128	4623	4166	2786	563	−133	−25	C
ATOM	894	N	ALA A	129	−28.110	−2.354	21.936	1.00	39.39		N
ANISOU	894	N	ALA A	129	5889	4067	5009	−75	1006	1586	N
ATOM	895	CA	ALA A	129	−28.617	−3.302	22.925	1.00	45.02		C
ANISOU	895	CA	ALA A	129	6382	5149	5573	81	1339	1287	C
ATOM	896	C	ALA A	129	−29.217	−2.550	24.109	1.00	47.61		C
ANISOU	896	C	ALA A	129	7091	5023	5976	−1056	2079	1526	C
ATOM	897	O	ALA A	129	−28.877	−1.393	24.334	1.00	50.07		O
ANISOU	897	O	ALA A	129	7454	5518	6050	−1216	2171	1360	O
ATOM	898	CB	ALA A	129	−27.500	−4.215	23.394	1.00	46.58		C
ANISOU	898	CB	ALA A	129	6533	5557	5608	790	693	916	C
ATOM	899	O	PRO A	130	−31.975	−5.426	22.814	1.00	58.16		O
ANISOU	899	O	PRO A	130	9589	4988	7521	−1059	1676	−700	O
ATOM	900	N	PRO A	130	−30.127	−3.187	24.870	1.00	52.97		N
ANISOU	900	N	PRO A	130	7755	6077	6294	−1043	2279	1376	N
ATOM	901	CA	PRO A	130	−30.751	−4.501	24.659	1.00	54.02		C
ANISOU	901	CA	PRO A	130	8326	5681	6519	−793	2163	1694	C
ATOM	902	C	PRO A	130	−31.774	−4.442	23.525	1.00	58.13		C
ANISOU	902	C	PRO A	130	8882	6003	7202	−388	1678	266	C
ATOM	903	CB	PRO A	130	−31.454	−4.770	25.994	1.00	55.97		C
ANISOU	903	CB	PRO A	130	8309	6714	6242	−233	2603	2153	C
ATOM	904	CG	PRO A	130	−31.716	−3.407	26.554	1.00	55.32		C
ANISOU	904	CG	PRO A	130	7997	7025	5998	−482	3053	2247	C
ATOM	905	CD	PRO A	130	−30.534	−2.585	26.153	1.00	56.05		C
ANISOU	905	CD	PRO A	130	8015	6969	6310	−691	2524	1488	C
ATOM	906	O	LYS A	131	−32.225	−1.083	21.638	1.00	53.26		O
ANISOU	906	O	LYS A	131	7211	6036	6988	−1277	1642	719	O
ATOM	907	N	LYS A	131	−32.408	−3.286	23.360	1.00	58.14		N
ANISOU	907	N	LYS A	131	8041	6758	7291	−26	1292	353	N
ATOM	908	CA	LYS A	131	−33.371	−3.084	22.292	1.00	55.65		C
ANISOU	908	CA	LYS A	131	7022	6953	7171	−240	1321	445	C
ATOM	909	C	LYS A	131	−32.764	−2.133	21.279	1.00	51.15		C
ANISOU	909	C	LYS A	131	6744	5717	6973	−589	1260	252	C
ATOM	910	CB	LYS A	131	−34.670	−2.498	22.848	1.00	57.23		C
ANISOU	910	CB	LYS A	131	6610	7844	7290	−149	1166	209	C
ATOM	911	N	VAL A	132	−32.830	−2.501	20.006	1.00	40.79		N
ANISOU	911	N	VAL A	132	5203	3596	6701	−1585	1163	−67	N

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	912	CA	VAL A	132	−32.317	−1.621	18.981	1.00	37.12		C
ANISOU	912	CA	VAL A	132	4764	2788	6552	−1002	756	−133	C
ATOM	913	C	VAL A	132	−33.320	−0.516	18.763	1.00	38.89		C
ANISOU	913	C	VAL A	132	4436	3429	6910	−1212	628	33	C
ATOM	914	O	VAL A	132	−34.480	−0.768	18.473	1.00	41.35		O
ANISOU	914	O	VAL A	132	4698	3917	7096	−1001	409	−245	O
ATOM	915	CB	VAL A	132	−32.025	−2.372	17.695	1.00	37.20		C
ANISOU	915	CB	VAL A	132	4556	3156	6421	−1074	845	220	C
ATOM	916	CG1	VAL A	132	−31.490	−1.421	16.657	1.00	40.18		C
ANISOU	916	CG1	VAL A	132	4267	4807	6192	−1019	938	592	C
ATOM	917	CG2	VAL A	132	−31.042	−3.488	17.975	1.00	38.97		C
ANISOU	917	CG2	VAL A	132	4858	3617	6334	−244	731	−674	C
ATOM	918	N	AGLN A	133	−32.866	0.712	18.932	0.57	36.67		N
ANISOU	918	N	AGLN A	133	4276	2779	6877	−882	1224	287	N
ATOM	919	C	AGLN A	133	−32.869	3.051	18.267	0.57	35.25		C
ANISOU	919	C	AGLN A	133	3895	2804	6695	−519	842	−196	C
ATOM	920	O	AGLN A	133	−31.672	3.115	18.576	0.57	31.91		O
ANISOU	920	O	AGLN A	133	3376	2180	6569	−290	1780	−88	O
ATOM	921	CA	AGLN A	133	−33.709	1.867	18.676	0.57	39.15		C
ANISOU	921	CA	AGLN A	133	4417	3492	6967	−647	1210	218	C
ATOM	922	CB	AGLN A	133	−34.528	2.228	19.907	0.57	42.37		C
ANISOU	922	CB	AGLN A	133	5048	3932	7118	−1063	1864	671	C
ATOM	923	CG	AGLN A	133	−33.711	2.526	21.140	0.57	44.27		C
ANISOU	923	CG	AGLN A	133	5475	4046	7297	−1184	2221	777	C
ATOM	924	CD	AGLN A	133	−34.593	2.758	22.350	0.57	50.66		C
ANISOU	924	CD	AGLN A	133	6319	5437	7492	−495	2498	616	C
ATOM	925	OE1	AGLN A	133	−35.753	3.146	22.211	0.57	53.00		O
ANISOU	925	OE1	AGLN A	133	6654	5903	7579	38	2804	382	O
ATOM	926	NE2	AGLN A	133	−34.055	2.508	23.541	0.57	52.31		N
ANISOU	926	NE2	AGLN A	133	6680	5778	7418	−349	2559	744	N
ATOM	927	N	BGLN A	133	−32.871	0.721	18.930	0.43	39.44		N
ANISOU	927	N	BGLN A	133	4607	3384	6993	−681	767	68	N
ATOM	928	C	BGLN A	133	−32.931	3.130	18.406	0.43	38.26		C
ANISOU	928	C	BGLN A	133	4343	3358	6834	−461	155	−235	C
ATOM	929	O	BGLN A	133	−31.807	3.308	18.880	0.43	38.96		O
ANISOU	929	O	BGLN A	133	4650	3298	6857	71	138	−37	O
ATOM	930	CA	BGLN A	133	−33.736	1.888	18.769	0.43	42.20		C
ANISOU	930	CA	BGLN A	133	4877	4053	7102	−322	644	−21	C
ATOM	931	CB	BGLN A	133	−34.542	2.142	20.045	0.43	47.47		C
ANISOU	931	CB	BGLN A	133	5710	4986	7340	−23	1096	59	C
ATOM	932	CG	BGLN A	133	−35.879	1.407	20.097	0.43	50.82		C
ANISOU	932	CG	BGLN A	133	6207	5567	7535	53	1489	79	C
ATOM	933	CD	BGLN A	133	−36.420	1.276	21.505	0.43	53.36		C
ANISOU	933	CD	BGLN A	133	6601	6038	7635	−66	1892	261	C
ATOM	934	OE1	BGLN A	133	−35.849	1.816	22.452	0.43	54.60		O
ANISOU	934	OE1	BGLN A	133	6745	6345	7658	208	2223	567	O
ATOM	935	NE2	BGLN A	133	−37.523	0.550	21.652	0.43	55.35		N
ANISOU	935	NE2	BGLN A	133	6841	6460	7729	−86	1819	24	N
ATOM	936	N	ILE A	134	−33.504	3.978	17.552	1.00	35.40		N
ANISOU	936	N	ILE A	134	3349	3611	6491	−583	−106	−910	N
ATOM	937	C	ILE A	134	−33.613	6.410	17.820	1.00	30.98		C
ANISOU	937	C	ILE A	134	2294	3924	5551	−178	341	−304	C
ATOM	938	O	ILE A	134	−34.846	6.473	17.819	1.00	32.63		O
ANISOU	938	O	ILE A	134	2501	3638	6258	−262	79	−693	O
ATOM	939	CA	AILE A	134	−32.875	5.234	17.194	0.68	34.85		C
ANISOU	939	CA	AILE A	134	3516	3823	5902	448	151	−865	C
ATOM	940	CB	AILE A	134	−32.704	5.418	15.648	0.68	37.88		C
ANISOU	940	CB	AILE A	134	3748	4645	6000	−417	−218	−447	C
ATOM	941	CG1	AILE A	134	−31.927	6.709	15.348	0.68	39.75		C
ANISOU	941	CG1	AILE A	134	4153	5038	5913	600	−109	−476	C
ATOM	942	CG2	AILE A	134	−34.046	5.375	14.924	0.68	40.75		C
ANISOU	942	CG2	AILE A	134	3975	5387	6121	−861	−445	−310	C
ATOM	943	CA	BILE A	134	−32.879	5.233	17.187	0.32	35.26		C
ANISOU	943	CA	BILE A	134	3339	4032	6026	184	−4	−733	C
ATOM	944	CB	BILE A	134	−32.760	5.408	15.643	0.32	38.10		C
ANISOU	944	CB	BILE A	134	3678	4648	6149	−72	−404	−621	C
ATOM	945	CG1	BILE A	134	−32.110	6.754	15.301	0.32	40.22		C
ANISOU	945	CG1	BILE A	134	4090	5057	6135	734	−370	−550	C
ATOM	946	CG2	BILE A	134	−34.114	5.246	14.962	0.32	39.37		C
ANISOU	946	CG2	BILE A	134	3826	4906	6226	−498	−624	−652	C
ATOM	947	N	LYS A	135	−32.845	7.328	18.382	1.00	26.14		N
ANISOU	947	N	LYS A	135	2711	3294	3926	−126	215	−318	N
ATOM	948	CA	LYS A	135	−33.411	8.562	18.892	1.00	24.68		C
ANISOU	948	CA	LYS A	135	3001	2979	3397	84	1008	32	C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	949	C	LYS A	135	−32.685	9.739	18.266	1.00	21.47		C
ANISOU	949	C	LYS A	135	2178	3288	2691	−290	820	252	C
ATOM	950	O	LYS A	135	−31.451	9.807	18.273	1.00	22.71		O
ANISOU	950	O	LYS A	135	2266	3535	2827	131	432	381	O
ATOM	951	CB	LYS A	135	−33.316	8.607	20.405	1.00	28.39		C
ANISOU	951	CB	LYS A	135	4369	2783	3635	−212	1253	49	C
ATOM	952	CG	LYS A	135	−34.219	7.555	21.038	1.00	33.42		C
ANISOU	952	CG	LYS A	135	5709	2756	4233	−385	1258	336	C
ATOM	953	CD	LYS A	135	−34.517	7.852	22.465	1.00	38.61		C
ANISOU	953	CD	LYS A	135	6454	3325	4891	−534	1238	−352	C
ATOM	954	CE	LYS A	135	−35.348	6.754	23.117	1.00	42.65		C
ANISOU	954	CE	LYS A	135	6800	4003	5403	−1287	528	−101	C
ATOM	955	NZ	LYS A	135	−36.471	6.331	22.237	1.00	48.04		N
ANISOU	955	NZ	LYS A	135	7318	5307	5628	−1522	511	−62	N
ATOM	956	N	GLU A	136	−33.462	10.652	17.695	1.00	23.35		N
ANISOU	956	N	GLU A	136	2991	2826	3053	197	385	578	N
ATOM	957	C	GLU A	136	−32.906	13.034	17.760	1.00	19.67		C
ANISOU	957	C	GLU A	136	2080	2737	2657	137	103	279	C
ATOM	958	O	GLU A	136	−33.805	13.251	18.574	1.00	21.83		O
ANISOU	958	O	GLU A	136	2419	3222	2653	161	571	314	O
ATOM	959	CG	GLU A	136	−33.689	10.893	14.658	1.00	31.99		C
ANISOU	959	CG	GLU A	136	4476	4059	3618	−668	−265	−348	C
ATOM	960	CD	GLU A	136	−34.524	11.190	13.402	1.00	47.16		C
ANISOU	960	CD	GLU A	136	6277	6971	4669	−88	138	−1110	C
ATOM	961	OE1	GLU A	136	−35.431	12.063	13.467	1.00	50.70		O
ANISOU	961	OE1	GLU A	136	6225	8062	4976	−713	−80	−1367	O
ATOM	962	OE2	GLU A	136	−34.258	10.562	12.340	1.00	53.59		O
ANISOU	962	OE2	GLU A	136	7551	7600	5212	716	362	−1417	O
ATOM	963	CA	AGLU A	136	−32.917	11.772	16.948	0.69	21.12		C
ANISOU	963	CA	AGLU A	136	3045	2312	2666	70	18	486	C
ATOM	964	CB	AGLU A	136	−33.740	12.028	15.672	0.69	25.77		C
ANISOU	964	CB	AGLU A	136	3767	3151	2875	−18	−244	−72	C
ATOM	965	CA	BGLU A	136	−32.915	11.768	16.942	0.31	22.97		C
ANISOU	965	CA	BGLU A	136	2977	2834	2917	−0	114	290	C
ATOM	966	CB	BGLU A	136	−33.739	12.020	15.671	0.31	27.38		C
ANISOU	966	CB	BGLU A	136	3759	3459	3184	−182	−117	−98	C
ATOM	967	N	SER A	137	−31.903	13.876	17.520	1.00	18.53		N
ANISOU	967	N	SER A	137	2157	2736	2147	−146	57	275	N
ATOM	968	CA	SER A	137	−31.894	15.241	18.028	1.00	17.46		C
ANISOU	968	CA	SER A	137	1863	2622	2149	159	−2	400	C
ATOM	969	C	SER A	137	−32.933	16.055	17.267	1.00	16.92		C
ANISOU	969	C	SER A	137	1849	2709	1870	397	416	289	C
ATOM	970	O	SER A	137	−33.534	15.580	16.290	1.00	20.16		O
ANISOU	970	O	SER A	137	2638	3004	2018	131	−138	235	O
ATOM	971	CB	SER A	137	−30.514	15.894	17.838	1.00	16.92		C
ANISOU	971	CB	SER A	137	2290	2353	1784	−490	238	202	C
ATOM	972	OG	SER A	137	−30.254	16.113	16.431	1.00	17.57		O
ANISOU	972	OG	SER A	137	2494	2424	1757	−31	353	32	O
ATOM	973	N	LEU A	138	−33.172	17.271	17.739	1.00	18.35		N
ANISOU	973	N	LEU A	138	2290	2564	2116	515	272	621	N
ATOM	974	CA	LEU A	138	−33.828	18.251	16.914	1.00	18.04		C
ANISOU	974	CA	LEU A	138	2178	2637	2038	176	20	313	C
ATOM	975	C	LEU A	138	−32.914	18.642	15.747	1.00	19.17		C
ANISOU	975	C	LEU A	138	2523	2480	2280	528	579	785	C
ATOM	976	O	LEU A	138	−31.705	18.434	15.790	1.00	19.07		O
ANISOU	976	O	LEU A	138	2245	2967	2036	426	381	312	O
ATOM	977	CB	LEU A	138	−34.196	19.465	17.730	1.00	19.59		C
ANISOU	977	CB	LEU A	138	2591	3074	1780	302	355	−25	C
ATOM	978	CG	LEU A	138	−35.195	19.212	18.866	1.00	20.19		C
ANISOU	978	CG	LEU A	138	2813	2946	1912	245	387	−11	C
ATOM	979	CD1	LEU A	138	−35.592	20.544	19.485	1.00	26.06		C
ANISOU	979	CD1	LEU A	138	3684	4248	1970	1112	267	−273	C
ATOM	980	CD2	LEU A	138	−36.419	18.476	18.367	1.00	23.97		C
ANISOU	980	CD2	LEU A	138	2422	4374	2313	401	261	461	C
ATOM	981	N	ARG A	139	−33.483	19.218	14.708	1.00	19.80		N
ANISOU	981	N	ARG A	139	2752	2550	2223	277	521	523	N
ATOM	982	CA	ARG A	139	−32.644	19.650	13.588	1.00	20.06		C
ANISOU	982	CA	ARG A	139	2831	2913	1878	−152	293	367	C
ATOM	983	C	ARG A	139	−31.837	20.911	13.925	1.00	20.13		C
ANISOU	983	C	ARG A	139	3273	2290	2087	23	633	−40	C
ATOM	984	O	ARG A	139	−32.163	21.662	14.850	1.00	23.90		O
ANISOU	984	O	ARG A	139	3342	3477	2260	86	854	−51	O
ATOM	985	CB	ARG A	139	−33.507	19.924	12.370	1.00	21.52		C
ANISOU	985	CB	ARG A	139	3053	3147	1976	−344	153	−71	C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	986	CG	ARG A	139	−34.110	18.684	11.839	1.00	24.33		C
ANISOU	986	CG	ARG A	139	2966	3883	2397	−538	256	188	C
ATOM	987	CD	ARG A	139	−34.509	18.902	10.447	1.00	29.17		C
ANISOU	987	CD	ARG A	139	3901	3995	3188	−1108	453	134	C
ATOM	988	NE	ARG A	139	−35.479	17.914	10.030	1.00	28.32		N
ANISOU	988	NE	ARG A	139	2642	4736	3380	−476	559	−548	N
ATOM	989	CZ	ARG A	139	−36.055	17.941	8.832	1.00	36.30		C
ANISOU	989	CZ	ARG A	139	3771	5894	4128	650	−37	−1418	C
ATOM	990	NH1	ARG A	139	−35.687	18.866	7.943	1.00	33.63		N
ANISOU	990	NH1	ARG A	139	3087	5737	3955	498	−139	−1344	N
ATOM	991	NH2	ARG A	139	−36.967	17.037	8.516	1.00	36.48		N
ANISOU	991	NH2	ARG A	139	3088	5936	4838	−687	164	−1380	N
ATOM	992	O	ALA A	140	−29.878	21.986	10.818	1.00	21.57		O
ANISOU	992	O	ALA A	140	3842	2652	1699	−483	500	−200	O
ATOM	993	N	ALA A	140	−30.737	21.106	13.216	1.00	20.72		N
ANISOU	993	N	ALA A	140	3539	2563	1771	−190	850	463	N
ATOM	994	CA	ALA A	140	−30.049	22.393	13.202	1.00	20.38		C
ANISOU	994	CA	ALA A	140	3678	2583	1482	−461	536	373	C
ATOM	995	C	ALA A	140	−29.896	22.818	11.744	1.00	20.49		C
ANISOU	995	C	ALA A	140	3429	2891	1465	−588	534	108	C
ATOM	996	CB	ALA A	140	−28.687	22.287	13.876	1.00	24.02		C
ANISOU	996	CB	ALA A	140	3761	3710	1654	−424	−54	139	C
ATOM	997	N	GLU A	141	−29.788	24.114	11.535	1.00	19.80		N
ANISOU	997	N	GLU A	141	3092	3005	1425	−56	194	55	N
ATOM	998	CA	GLU A	141	−29.666	24.651	10.179	1.00	17.45		C
ANISOU	998	CA	GLU A	141	2487	2728	1416	−40	185	83	C
ATOM	999	C	GLU A	141	−28.270	25.175	9.950	1.00	18.20		C
ANISOU	999	C	GLU A	141	2746	2916	1252	273	−84	−213	C
ATOM	1000	O	GLU A	141	−27.708	25.887	10.793	1.00	20.22		O
ANISOU	1000	O	GLU A	141	2999	3297	1386	2	205	60	O
ATOM	1001	CB	GLU A	141	−30.640	25.818	10.000	1.00	18.96		C
ANISOU	1001	CB	GLU A	141	2515	2785	1905	−114	387	163	C
ATOM	1002	CG	GLU A	141	−30.542	26.399	8.583	1.00	20.36		C
ANISOU	1002	CG	GLU A	141	2437	3058	2242	59	124	455	C
ATOM	1003	CD	GLU A	141	−31.480	27.549	8.318	1.00	25.04		C
ANISOU	1003	CD	GLU A	141	2830	3962	2722	283	261	507	C
ATOM	1004	OE1	GLU A	141	−32.339	27.854	9.197	1.00	30.41		O
ANISOU	1004	OE1	GLU A	141	3420	4737	3396	651	470	−34	O
ATOM	1005	OE2	GLU A	141	−31.355	28.152	7.203	1.00	28.36		O
ANISOU	1005	OE2	GLU A	141	3788	3932	3057	622	339	760	O
ATOM	1006	N	LEU A	142	−27.723	24.838	8.779	1.00	17.25		N
ANISOU	1006	N	LEU A	142	2428	2903	1224	−28	8	20	N
ATOM	1007	CA	LEU A	142	−26.477	25.425	8.309	1.00	17.05		C
ANISOU	1007	CA	LEU A	142	2050	2819	1609	−3	150	187	C
ATOM	1008	C	LEU A	142	−26.850	26.402	7.199	1.00	17.92		C
ANISOU	1008	C	LEU A	142	2317	3003	1489	−45	−177	187	C
ATOM	1009	O	LEU A	142	−27.535	26.028	6.236	1.00	18.25		O
ANISOU	1009	O	LEU A	142	2423	3093	1417	−12	−204	76	O
ATOM	1010	CB	LEU A	142	−25.520	24.366	7.721	1.00	17.75		C
ANISOU	1010	CB	LEU A	142	2189	2903	1652	274	278	224	C
ATOM	1011	CG	LEU A	142	−24.203	24.876	7.162	1.00	19.28		C
ANISOU	1011	CG	LEU A	142	2133	3338	1853	341	−77	−68	C
ATOM	1012	CD1	LEU A	142	−23.364	25.550	8.276	1.00	21.27		C
ANISOU	1012	CD1	LEU A	142	2296	3665	2121	−352	−75	−323	C
ATOM	1013	CD2	LEU A	142	−23.431	23.706	6.578	1.00	21.29		C
ANISOU	1013	CD2	LEU A	142	2604	3900	1587	701	201	137	C
ATOM	1014	N	ARG A	143	−26.389	27.641	7.317	1.00	20.55		N
ANISOU	1014	N	ARG A	143	2698	3139	1972	182	−273	545	N
ATOM	1015	C	ARG A	143	−25.145	29.038	5.782	1.00	20.92		C
ANISOU	1015	C	ARG A	143	2770	3069	2111	−89	−273	655	C
ATOM	1016	O	ARG A	143	−24.344	29.518	6.553	1.00	24.40		O
ANISOU	1016	O	ARG A	143	3181	3810	2281	−673	−356	244	O
ATOM	1017	NE	AARG A	143	−29.995	31.156	7.319	0.69	30.85		N
ANISOU	1017	NE	AARG A	143	2933	4351	4438	846	−382	−3	N
ATOM	1018	CZ	AARG A	143	−30.815	31.764	8.171	0.69	31.56		C
ANISOU	1018	CZ	AARG A	143	3699	3581	4713	967	−552	−151	C
ATOM	1019	NH1	AARG A	143	−30.637	33.043	8.479	0.69	33.62		N
ANISOU	1019	NH1	AARG A	143	4960	2737	5075	1080	−393	−97	N
ATOM	1020	NH2	AARG A	143	−31.832	31.096	8.713	0.69	31.37		N
ANISOU	1020	NH2	AARG A	143	3013	4083	4824	500	−391	−477	N
ATOM	1021	CA	AARG A	143	−26.553	28.643	6.270	0.69	21.57		C
ANISOU	1021	CA	AARG A	143	2407	3379	2410	−139	−321	135	C
ATOM	1022	CB	AARG A	143	−27.307	29.837	6.872	0.69	29.36		C
ANISOU	1022	CB	AARG A	143	3895	4148	3112	897	−360	−316	C

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

ATOM	1023	CG	AARG A	143	−27.972	30.786	5.904	0.69	30.72		C
ANISOU	1023	CG	AARG A	143	3611	4398	3664	412	−422	−299	C
ATOM	1024	CD	AARG A	143	−28.854	31.796	6.660	0.69	30.46		C
ANISOU	1024	CD	AARG A	143	3105	4349	4119	86	−230	180	C
ATOM	1025	NE	CARG A	143	−30.663	30.715	7.848	0.31	20.97		N
ANISOU	1025	NE	CARG A	143	2566	3151	2251	−254	−644	172	N
ATOM	1026	CZ	CARG A	143	−31.351	31.490	8.681	0.31	27.40		C
ANISOU	1026	CZ	CARG A	143	4013	3541	2855	810	−474	−120	C
ATOM	1027	NH1	CARG A	143	−30.839	32.633	9.124	0.31	29.22		N
ANISOU	1027	NH1	CARG A	143	5046	3171	2886	1020	−304	−41	N
ATOM	1028	NH2	CARG A	143	−32.555	31.110	9.086	0.31	28.81		N
ANISOU	1028	NH2	CARG A	143	3897	3792	3258	901	−412	−397	N
ATOM	1029	CA	CARG A	143	−26.519	28.633	6.242	0.31	20.29		C
ANISOU	1029	CA	CARG A	143	2537	3077	2097	465	−114	353	C
ATOM	1030	CB	CARG A	143	−27.229	29.889	6.718	0.31	22.01		C
ANISOU	1030	CB	CARG A	143	3063	3108	2192	1484	185	−60	C
ATOM	1031	CG	CARG A	143	−28.685	29.718	6.887	0.31	19.17		C
ANISOU	1031	CG	CARG A	143	2125	3077	2080	1098	162	148	C
ATOM	1032	CD	CARG A	143	−29.329	31.003	7.345	0.31	21.56		C
ANISOU	1032	CD	CARG A	143	2765	3212	2216	962	−641	229	C
ATOM	1033	N	VAL A	144	−24.856	28.813	4.510	1.00	21.88		N
ANISOU	1033	N	VAL A	144	3090	3346	1878	34	−90	738	N
ATOM	1034	CA	VAL A	144	−23.532	29.112	3.969	1.00	23.28		C
ANISOU	1034	CA	VAL A	144	3527	3129	2190	264	105	541	C
ATOM	1035	C	VAL A	144	−23.701	30.284	3.029	1.00	26.54		C
ANISOU	1035	C	VAL A	144	3981	3196	2907	−54	−637	803	C
ATOM	1036	O	VAL A	144	−24.371	30.151	1.992	1.00	29.52		O
ANISOU	1036	O	VAL A	144	4547	3893	2776	−172	−996	849	O
ATOM	1037	CB	VAL A	144	−22.907	27.892	3.234	1.00	23.48		C
ANISOU	1037	CB	VAL A	144	3236	3542	2145	−559	−121	429	C
ATOM	1038	CG1	VAL A	144	−21.504	28.239	2.773	1.00	26.07		C
ANISOU	1038	CG1	VAL A	144	3304	4245	2355	−565	415	374	C
ATOM	1039	CG2	VAL A	144	−22.856	26.660	4.153	1.00	22.88		C
ANISOU	1039	CG2	VAL A	144	3579	3353	1760	−117	−111	317	C
ATOM	1040	N	THR A	145	−23.087	31.409	3.391	1.00	28.09		N
ANISOU	1040	N	THR A	145	3919	2960	3793	−182	−570	1683	N
ATOM	1041	CA	THR A	145	−23.256	32.681	2.691	1.00	33.03		C
ANISOU	1041	CA	THR A	145	4297	3816	4436	−421	−291	1965	C
ATOM	1042	C	THR A	145	−22.169	32.932	1.643	1.00	34.34		C
ANISOU	1042	C	THR A	145	4694	3753	4599	−398	−357	2439	C
ATOM	1043	O	THR A	145	−21.069	32.371	1.705	1.00	35.97		O
ANISOU	1043	O	THR A	145	4824	4201	4640	−28	−1138	2306	O
ATOM	1044	CB	THR A	145	−23.298	33.869	3.684	1.00	39.34		C
ANISOU	1044	CB	THR A	145	5615	4258	5072	929	557	1765	C
ATOM	1045	OG1	THR A	145	−22.067	33.952	4.418	1.00	45.47		O
ANISOU	1045	OG1	THR A	145	6704	5069	5502	2029	253	1472	O
ATOM	1046	CG2	THR A	145	−24.447	33.694	4.671	1.00	42.22		C
ANISOU	1046	CG2	THR A	145	6522	4211	5308	1062	1015	1722	C
ATOM	1047	O	GLU A	146	−20.501	35.700	1.021	1.00	44.40		O
ANISOU	1047	O	GLU A	146	5976	4884	6011	−564	264	1951	O
ATOM	1048	N	GLU A	146	−22.476	33.813	0.697	1.00	39.17		N
ANISOU	1048	N	GLU A	146	4997	4905	4980	161	−113	2870	N
ATOM	1049	CA	GLU A	146	−21.570	34.106	−0.406	1.00	44.14		C
ANISOU	1049	CA	GLU A	146	5590	6091	5091	8	475	3151	C
ATOM	1050	C	GLU A	146	−20.372	34.889	0.104	1.00	45.57		C
ANISOU	1050	C	GLU A	146	5795	5759	5761	−390	414	2913	C
ATOM	1051	CB	GLU A	146	−22.306	34.911	−1.483	1.00	47.51		C
ANISOU	1051	CB	GLU A	146	6071	7138	4841	307	517	3122	C
ATOM	1052	O	ARG A	147	−18.730	37.060	−1.694	1.00	54.70		O
ANISOU	1052	O	ARG A	147	6744	6771	7270	−518	244	2924	O
ATOM	1053	N	ARG A	147	−19.204	34.634	−0.478	1.00	47.61		N
ANISOU	1053	N	ARG A	147	5793	5843	6454	−1135	292	3100	N
ATOM	1054	CA	ARG A	147	−17.999	35.381	−0.129	1.00	52.50		C
ANISOU	1054	CA	ARG A	147	6324	6550	7072	−725	236	2577	C
ATOM	1055	C	ARG A	147	−18.043	36.799	−0.704	1.00	53.81		C
ANISOU	1055	C	ARG A	147	6575	6666	7205	−494	135	2875	C
ATOM	1056	CB	ARG A	147	−16.741	34.649	−0.615	1.00	54.71		C
ANISOU	1056	CB	ARG A	147	6524	6912	7350	−466	422	2352	C
TER											
HETATM	1057	CL	CL B	1	−31.532	18.967	19.982	0.00	22.75		Cl
HETATM	1058	CL A	CL B	2	−14.013	7.942	15.373	0.41	43.02		Cl
HETATM	1059	CL B	CL B	2	−13.877	5.390	15.959	0.59	36.08		Cl
TER											
HETATM	1060	O	HOH S	1	−11.320	12.933	29.488	1.00	24.25		O

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

HETATM	1061	O	HOH	S	2	−29.963	27.082	5.173	1.00	26.06	O
HETATM	1062	O	HOH	S	3	−36.398	19.602	14.615	1.00	26.46	O
HETATM	1063	O	HOH	S	4	−25.179	19.890	21.690	1.00	31.16	O
HETATM	1064	O	HOH	S	5	−20.377	23.391	17.674	1.00	27.55	O
HETATM	1065	O	HOH	S	6	−32.642	16.478	21.774	1.00	29.02	O
HETATM	1066	O	HOH	S	7	−20.800	−0.588	11.468	1.00	28.91	O
HETATM	1067	O	HOH	S	8	−21.210	9.475	24.802	1.00	31.01	O
HETATM	1068	O	HOH	S	9	−23.269	4.299	10.683	1.00	32.96	O
HETATM	1069	O	HOH	S	10	−15.168	16.008	13.610	1.00	30.12	O
HETATM	1070	O	HOH	S	11	−23.000	19.897	−0.770	1.00	32.33	O
HETATM	1071	O	HOH	S	12	−16.053	8.925	14.002	1.00	28.30	O
HETATM	1072	O	HOH	S	13	−31.058	21.412	17.451	1.00	34.49	O
HETATM	1073	O	HOH	S	14	−11.148	17.070	13.522	1.00	35.55	O
HETATM	1074	O	HOH	S	15	−13.606	9.894	17.437	1.00	33.67	O
HETATM	1075	O	HOH	S	16	−17.334	0.330	13.286	1.00	29.83	O
HETATM	1076	O	HOH	S	17	−23.530	18.918	3.248	1.00	32.42	O
HETATM	1077	O	HOH	S	18	−25.398	3.755	25.094	1.00	37.41	O
HETATM	1078	O	HOH	S	19	−12.444	24.646	5.144	1.00	32.56	O
HETATM	1079	O	HOH	S	20	−23.990	−3.579	24.355	1.00	38.71	O
HETATM	1080	O	HOH	S	21	−28.227	12.362	25.591	1.00	36.43	O
HETATM	1081	O	HOH	S	22	−35.754	15.422	14.773	1.00	40.39	O
HETATM	1082	O	HOH	S	23	−15.728	24.696	12.356	1.00	32.84	O
HETATM	1083	O	HOH	S	24	−24.219	16.690	1.736	1.00	32.43	O
HETATM	1084	O	HOH	S	25	−15.646	10.746	10.757	1.00	38.67	O
HETATM	1085	O	HOH	S	26	−14.652	17.508	8.417	1.00	33.75	O
HETATM	1086	O	HOH	S	27	−17.545	8.522	9.523	1.00	33.84	O
HETATM	1087	O	AHOH	S	28	−12.876	17.475	17.095	0.54	26.63	O
HETATM	1088	O	BHOH	S	28	−11.123	14.550	14.203	0.46	25.57	O
HETATM	1089	O	HOH	S	29	−11.145	14.343	20.129	1.00	30.72	O
HETATM	1090	O	HOH	S	30	−13.826	17.975	13.783	1.00	36.95	O
HETATM	1091	O	HOH	S	31	−28.657	26.959	19.793	1.00	39.40	O
HETATM	1092	O	HOH	S	32	−14.087	2.338	14.701	1.00	42.49	O
HETATM	1093	O	HOH	S	33	−16.594	28.407	10.975	1.00	41.30	O
HETATM	1094	O	HOH	S	34	−36.440	10.244	17.770	1.00	48.54	O
HETATM	1095	O	HOH	S	35	−19.238	26.131	15.375	1.00	35.22	O
HETATM	1096	O	HOH	S	36	−24.391	30.001	15.634	1.00	45.39	O
HETATM	1097	O	HOH	S	37	−10.294	23.547	5.439	1.00	33.79	O
HETATM	1098	O	HOH	S	38	−20.262	11.381	3.588	1.00	40.36	O
HETATM	1099	O	HOH	S	39	−9.566	21.361	3.724	1.00	45.76	O
HETATM	1100	O	HOH	S	40	−31.839	14.557	25.618	1.00	39.31	O
HETATM	1101	O	HOH	S	41	−28.573	29.123	17.160	1.00	34.87	O
HETATM	1102	O	HOH	S	42	−17.837	21.890	21.041	1.00	39.71	O
HETATM	1103	O	HOH	S	43	−23.508	31.272	13.390	1.00	38.35	O
HETATM	1104	O	HOH	S	44	−14.232	23.031	15.160	1.00	45.86	O
HETATM	1105	O	HOH	S	45	−32.842	28.036	11.832	1.00	37.47	O
HETATM	1106	O	HOH	S	46	−20.017	0.581	13.613	1.00	26.90	O
HETATM	1107	O	HOH	S	47	−30.924	26.051	2.727	1.00	33.41	O
HETATM	1108	O	HOH	S	48	−17.972	6.069	9.248	1.00	44.79	O
HETATM	1109	O	HOH	S	49	−31.615	24.043	1.750	1.00	39.50	O
HETATM	1110	O	HOH	S	50	−32.977	22.499	3.078	1.00	43.12	O
HETATM	1111	O	HOH	S	51	−37.283	19.091	5.781	1.00	50.59	O
HETATM	1112	O	HOH	S	52	−16.505	25.687	16.469	1.00	47.70	O
HETATM	1113	O	HOH	S	53	−17.987	10.202	6.094	1.00	44.99	O
HETATM	1114	O	HOH	S	54	−25.817	27.114	21.137	1.00	54.54	O
HETATM	1115	O	HOH	S	55	−19.634	31.262	12.044	1.00	51.44	O
HETATM	1116	O	HOH	S	56	−19.282	3.533	5.922	1.00	44.19	O
HETATM	1117	O	HOH	S	57	−18.140	26.304	12.964	1.00	28.65	O
HETATM	1118	O	HOH	S	58	−20.503	16.347	−0.676	1.00	39.93	O
HETATM	1119	O	HOH	S	59	−20.668	28.377	16.271	1.00	54.96	O
HETATM	1120	O	AHOH	S	60	−13.046	27.984	9.370	0.58	25.01	O
HETATM	1121	O	BHOH	S	60	−17.607	32.024	8.445	0.42	30.47	O
HETATM	1122	O	HOH	S	61	−12.651	27.445	−0.487	1.00	44.24	O
HETATM	1123	O	HOH	S	62	−10.636	16.383	18.094	1.00	34.27	O
HETATM	1124	O	HOH	S	63	−19.658	21.740	−5.664	1.00	34.16	O
HETATM	1125	O	HOH	S	64	−21.399	34.434	7.059	1.00	50.31	O
HETATM	1126	O	HOH	S	65	−29.754	22.788	20.357	1.00	47.87	O
HETATM	1127	O	HOH	S	66	−29.614	29.358	3.092	1.00	46.67	O
HETATM	1128	O	HOH	S	67	−9.725	11.812	27.805	1.00	45.85	O
HETATM	1129	O	HOH	S	68	−32.790	9.593	10.674	1.00	54.56	O
HETATM	1130	O	HOH	S	69	−27.077	26.307	−5.229	1.00	51.00	O
HETATM	1131	O	HOH	S	70	−20.474	3.201	12.726	1.00	34.09	O
HETATM	1132	O	HOH	S	71	−34.490	8.897	10.790	1.00	57.99	O
HETATM	1133	O	HOH	S	72	−21.449	2.801	11.173	1.00	50.05	O
HETATM	1134	O	HOH	S	73	−11.337	14.501	2.400	1.00	50.53	O

TABLE 8-continued

Atomic coordinates and structure factors for human apo-PD-1$^{T76P\ A132V}$ (based on a PDB file).

HETATM	1135	O	HOH S	74	−32.632	25.721	13.366	1.00	31.98	O
HETATM	1136	O	HOH S	75	−24.586	8.104	30.871	1.00	45.09	O
HETATM	1137	O	HOH S	76	−27.903	7.346	4.005	1.00	41.45	O
HETATM	1138	O	HOH S	77	−34.626	12.432	27.946	1.00	48.67	O
HETATM	1139	O	HOH S	78	−36.301	15.543	11.735	1.00	43.02	O
HETATM	1140	O	HOH S	79	−28.138	14.618	25.444	1.00	51.79	O
HETATM	1141	O	HOH S	80	−22.311	31.191	−7.395	1.00	60.17	O
HETATM	1142	O	HOH S	81	−34.346	−5.046	19.179	1.00	53.46	O
HETATM	1143	O	HOH S	82	−22.182	24.418	19.827	1.00	48.28	O
TER										
END										

SEQUENCE LISTING

<160> NUMBER OF SEQ ID NOS: 4

<210> SEQ ID NO 1
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<212> TYPE: PRT
<213> ORGANISM: Homo sapiens

<400> SEQUENCE: 1

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1               5                  10                  15

Leu Gly Trp Arg Pro Gly Trp Phe Leu Asp Ser Pro Asp Arg Pro Trp
            20                  25                  30

Asn Pro Pro Thr Phe Ser Pro Ala Leu Leu Val Val Thr Glu Gly Asp
        35                  40                  45

Asn Ala Thr Phe Thr Cys Ser Phe Ser Asn Thr Ser Glu Ser Phe Val
    50                  55                  60

Leu Asn Trp Tyr Arg Met Ser Pro Ser Asn Gln Thr Asp Lys Leu Ala
65                  70                  75                  80

Ala Phe Pro Glu Asp Arg Ser Gln Pro Gly Gln Asp Cys Arg Phe Arg
                85                  90                  95

Val Thr Gln Leu Pro Asn Gly Arg Asp Phe His Met Ser Val Val Arg
            100                 105                 110

Ala Arg Arg Asn Asp Ser Gly Thr Tyr Leu Cys Gly Ala Ile Ser Leu
        115                 120                 125

Ala Pro Lys Ala Gln Ile Lys Glu Ser Leu Arg Ala Glu Leu Arg Val
    130                 135                 140

Thr Glu Arg Arg Ala Glu Val Pro Thr Ala His Pro Ser Pro Ser Pro
145                 150                 155                 160

Arg Pro Ala Gly Gln Phe Gln Thr Leu Val Val Gly Val Val Gly Gly
                165                 170                 175

Leu Leu Gly Ser Leu Val Leu Leu Val Trp Val Leu Ala Val Ile Cys
            180                 185                 190

Ser Arg Ala Ala Arg Gly Thr Ile Gly Ala Arg Arg Thr Gly Gln Pro
        195                 200                 205

Leu Lys Glu Asp Pro Ser Ala Val Pro Val Phe Ser Val Asp Tyr Gly
    210                 215                 220

Glu Leu Asp Phe Gln Trp Arg Glu Lys Thr Pro Glu Pro Pro Val Pro
225                 230                 235                 240

Cys Val Pro Glu Gln Thr Glu Tyr Ala Thr Ile Val Phe Pro Ser Gly
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                245                 250                 255

Met Gly Thr Ser Ser Pro Ala Arg Arg Gly Ser Ala Asp Gly Pro Arg
            260                 265                 270

Ser Ala Gln Pro Leu Arg Pro Glu Asp Gly His Cys Ser Trp Pro Leu
        275                 280                 285


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<212> TYPE: PRT
<213> ORGANISM: Artificial Sequence
<220> FEATURE:
<223> OTHER INFORMATION: Synthetic Construct

<400> SEQUENCE: 2

Met Asn Pro Pro Thr Phe Ser Pro Ala Leu Leu Val Val Thr Glu Gly
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Asp Asn Ala Thr Phe Thr Cys Ser Phe Ser Asn Thr Ser Glu Ser Phe
            20                  25                  30

Val Leu Asn Trp Tyr Arg Met Ser Pro Ser Asn Gln Pro Asp Lys Leu
        35                  40                  45

Ala Ala Phe Pro Glu Asp Arg Ser Gln Pro Gly Gln Asp Ser Arg Phe
    50                  55                  60

Arg Val Thr Gln Leu Pro Asn Gly Arg Asp Phe His Met Ser Val Val
65                  70                  75                  80

Arg Ala Arg Arg Asn Asp Ser Gly Thr Tyr Leu Cys Gly Ala Ile Ser
                85                  90                  95

Leu Ala Pro Lys Val Gln Ile Lys Glu Ser Leu Arg Ala Glu Leu Arg
            100                 105                 110

Val Thr Glu Arg Arg Ala Glu Gly Ser Trp Ser His Pro Gln Phe Glu
        115                 120                 125

Lys


<210> SEQ ID NO 3
<211> LENGTH: 140
<212> TYPE: PRT
<213> ORGANISM: Artificial Sequence
<220> FEATURE:
<223> OTHER INFORMATION: Synthetic Construct

<400> SEQUENCE: 3

Met Gly Trp Ser Cys Ile Ile Leu Phe Leu Val Ala Thr Ala Thr Gly
1               5                   10                  15

Val His Ser Asn Pro Pro Thr Phe Ser Pro Ala Leu Leu Val Val Thr
            20                  25                  30

Glu Gly Asp Ser Ala Thr Phe Thr Cys Ser Phe Ser Ser Thr Ser Glu
        35                  40                  45

Ser Phe Val Leu Asn Trp Tyr Arg Met Ser Pro Ser Gly Gln Pro Asp
    50                  55                  60

Lys Leu Ala Ala Phe Pro Glu Asp Arg Ser Gln Pro Gly Gln Asp Ser
65                  70                  75                  80

Arg Phe Arg Val Thr Gln Leu Pro Asn Gly Arg Asp Phe His Met Ser
                85                  90                  95

Val Val Arg Ala Arg Arg Asp Asp Ser Gly Thr Tyr Leu Cys Gly Ala
            100                 105                 110

Ile Ser Leu Ala Pro Lys Val Gln Ile Lys Glu Ser Leu Arg Ala Glu
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        115                 120                 125

Leu Arg Val Thr Glu Arg Arg Ala Glu Pro Glu Ala
    130                 135                 140


<210> SEQ ID NO 4
<211> LENGTH: 123
<212> TYPE: PRT
<213> ORGANISM: Artificial Sequence
<220> FEATURE:
<223> OTHER INFORMATION: Synthetic Construct

<400> SEQ UENCE: 4

Met Ile Phe Leu Leu Leu Met Leu Ser Leu Glu Leu Gln Leu His Gln
1               5                   10                  15

Ile Ala Ala Leu Phe Thr Val Thr Val Pro Lys Glu Leu Tyr Ile Ile
            20                  25                  30

Glu His Gly Ser Asp Val Thr Leu Glu Cys Asn Phe Asp Thr Gly Ser
        35                  40                  45

His Val Asn Leu Gly Ala Ile Thr Ala Ser Leu Gln Lys Val Glu Asp
    50                  55                  60

Asp Thr Ser Pro His Arg Glu Arg Ala Thr Leu Leu Glu Glu Gln Leu
65                  70                  75                  80

Pro Leu Gly Lys Ala Ser Phe His Ile Pro Gln Val Gln Val Arg Asp
                85                  90                  95

Glu Gly Gln Tyr Gln Cys Ile Ile Ile Tyr Gly Val Ala Trp Asp Tyr
            100                 105                 110

Lys Tyr Leu Thr Leu Lys Val Lys Ala Ser Tyr
        115                 120
```

1. An in silico method of identifying a compound that binds to PD-L2 binding pocket of human PD-1, the method comprising:

(a) receiving, by a computer system, information on a three-dimensional structure of PD-L2 binding pocket of human PD-1 comprising a plurality of amino acids;

(b) receiving, by the computer system, information on a three-dimensional structure of a candidate compound;

(c) using the computer system and the information received into the computer system in steps (a) and (b), performing one or more of molecular dynamic simulations, kinetic Monte Carlo (KMC) simulations, direct simulations Monte Carlo (DSMC), or density functional theory (DFT) simulations to determine if the candidate compound binds to the PD-L2 binding pocket of human PD-1, thereby identifying the compound that binds to PD-L2 binding pocket of human PD-1.

2. A protein comprising a ligand binding pocket with a three-dimensional structure corresponding to a structure of PD-L2 binding pocket of a variant of human PD-1 with one or more of amino acid substitutions in residues corresponding to N74, T76 or A132 of SEQ ID NO:1.

3. A variant of human PD-1 comprising one or more of amino acid substitutions in residues corresponding to N74, T76 and A132 of SEQ ID NO:1.

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