Supplementary Materials for

Crystal Structure of a Soluble Cleaved HIV-1 Envelope Trimer

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Materials and Methods

**Fab expression and purification**

Recombinant Fabs for co-crystallization experiments were expressed using a protocol similar to that previously described (23). Briefly, the heavy and light chain genes were co-transfected using 293Fectin (Invitrogen) into human embryonic kidney (HEK) 293F cells in a 2:1 ratio to minimize formation of light chain homodimers. Secreted Fabs were isolated from the expression media 6-days post-transfection by affinity purification via an anti-human λ/κ light chain affinity matrix (CaptureSelect Fab λ/κ; BAC), followed by cation exchange and gel filtration chromatography.

**SOSIP gp140 expression and purification**

To increase the probability of successful crystallization and structure determination, several soluble, cleaved trimers of the SOSIP.664 gp140 design were expressed and purified as described elsewhere (17, 18, 23, 64). Crystallization candidates based on env genes from HIV-1 isolates KNH1144, ADA, 1182.6.1D2, BG505 and 208.9.C10 were selected from an initial panel
of 20, based on their expression and trimer-formation properties, as assessed by SDS-PAGE and BN-PAGE. Notably, for isolates that did not naturally contain residue N332, a point substitution was made to introduce it, thereby creating the 2G12 epitope to facilitate affinity purification. The Env constructs were co-transfected with the furin protease in HEK 293S GnTI−/− cells, which lack N-acetylglucosaminyltransferase I and, therefore, produce glycoproteins bearing only high-mannose (Man5,6) glycans. Secreted SOSIP.664 Env proteins were harvested from supernatants and affinity purified using a 2G12 MAb affinity column. Following a high salt elution process, trimers were purified to size homogeneity using a Superose 6 size exclusion chromatography (SEC) matrix (GE Healthcare).

Sample preparation and crystal screening

Purified SOSIP.664 gp140 trimers were tested for crystallizability either alone or as complexes with one or more ligands from the following list: soluble CD4, Fabs: PGT121, PGT122, PGT123, PGT127, PGT128, PGT135, PG9, PG16, PGT145, PGV04, 17b. In addition, purified trimers and complexes were in some cases treated with the following glycosidases, alone or in combination, for 3 h at temperatures ranging between 20-37°C: EndoH (New England Biolabs), EndoD (VWR), Endo F1 (EMD Chemicals) or α1,2,3,6 mannosidase (QA-Bio). The monodispersity of the resulting samples was measured by SDS-PAGE, BN-PAGE and SEC coupled in-line with multi-angle light scattering (SEC-MALS) using the following layout: a Superose 6 10/30 SEC column (GE Healthcare) operated on an AKTA Avant FPLC system (GE Healthcare) with the following calibrated detectors: 1) HP1 1050 Hewlett-Packard UV detector (Norwalk, CT); 2) MiniDawn Treos multi-angle light scattering (MALS) detector (Wyatt Corporation, CA); 3) quasi-elastic light scattering (QELS) detector (Wyatt Corporation, CA); and 4) Optilab T-reX refractive index (RI) detector (Wyatt Corporation, CA). The purified
complexes were concentrated to approximately 2-6 mg/ml and subjected to extensive crystallization trials using either: 1) the Oryx8 crystallization robot (Douglas Instruments) with 96 different crystallization conditions at 16°C; or 2) the automated IAVI/JCSG/TRSI CrystalMation robotic system (Rigaku) at the Joint Center for Structural Genomics (www.jcsg.org), where 384 different crystallization conditions were tested at 4°C and 22°C.

In the above trials, only the partially deglycosylated SOSIP.664 gp140 trimers from various isolates in complex with antibodies of the PGT121-family (PGT121, PGT122 and PGT123) resulted in crystal hits. Surprisingly, for these complexes, hits were obtained from approximately 10% of the crystallization conditions, but the majority of crystals tested (>600) only diffracted to 8 Å or worse at various synchrotron sources (APS, SSRL, and CLS). Several pre- and post-crystallization strategies were explored in an effort to improve the x-ray diffraction properties of these crystals: however, the use of single-chain Fv instead of Fab, limited in-situ proteolysis, varying temperature of crystal growth, additives screening, crystal cross-linking, dehydration, and annealing all met with limited success. In addition, we attempted use of a SOSIP construct further truncated to gp41 position 650. Although crystals could be obtained with the trimer in complex with PGT122 Fab, these did not show improved diffraction properties compared to the majority of SOSIP.664-containing crystals.

X-ray data collection, structure solution and model building

Ultimately, only the thermostable BG505 SOSIP.664 trimers (18, 23) allowed us to achieve higher resolution x-ray diffraction. Two crystals obtained from crystallization condition 0.1 M CAPS, 2 M ammonium sulfate, 0.2 M lithium sulfate, pH 10.5, with the EndoH-treated, SEC-purified PGT122 Fab plus BG505 SOSIP.664 trimer complex showed a maximum visible
diffraction of up to 3.7 Å along the c-axis at the Advanced Photon Source (APS) beamline 23-ID-D (fig. S1). However, these crystals showed severe anisotropic diffraction and diffracted to a maximum of only ~5 Å and ~6 Å along the a- and b-axes, respectively. In addition, due to radiation damage during data collection, it was necessary to merge the data from two crystals to obtain a dataset with sufficient redundancy and completeness. Integration and scaling were performed using the program XDS (65), and output files were subsequently corrected for anisotropy using the UCLA MBI — Diffraction Anisotropy Server (http://services.mbi.ucla.edu/anisoscale/anisoscale_xds/) (66), with truncations at 4.5 Å, 5.5 Å and 4.0 Å along the a, b and c axes, respectively. The overall data were then truncated to 4.7 Å based on an I/σ >2 criteria in the highest resolution shell. Only few higher resolution reflections to 3.7 Å met these I/σ >2 criteria and their inclusion in the dataset did not subsequently improve the quality of maps. Data statistics are reported in table S1.

Molecular replacement was performed using Phaser (67) with a composite search model comprised of: 1) the variable domain of PGT122 at 1.8 Å (PDB ID: 4JY5); 2) CD4-bound gp120 core at 2.6 Å (PDB ID: 3JWD); and 3) these components docked in a trimeric arrangement using the previously reported ~14 Å EM reconstruction of the PGT122 Fab in complex with the BG505 SOSIP.664 trimer (EMDB: 5624). The molecular replacement solution indicated only one copy of the trimer-antibody complex was present in the asymmetric unit with a TFZ=6.2 and an LLG=1,344 (resulting in an ~82% solvent content (V_m= 6.87 A^3/Da) based on a molecular weight of ~400 kDa for the partially deglycosylated complex (68)). Additional components, such as the PGT122 Fab constant domain, gp120 V1/V2/V3, and gp41 helices were added manually based on clear electron density for these elements in the initial maps (fig. S3). Rigid-body, grouped-B-factor, XYZ, real-space and TLS refinements were carried out in PHENIX using
NCS-restraints, as well as secondary structure and reference model restraints imposed from high-resolution structures (69). Model building was performed using Coot (70). Secondary structure was determined using STRIDE (71). Slightly higher crystallographic R-values for the trimer structure compared to the mean reported for other structures to the same resolution (72) likely results from the relatively poor diffraction properties of the crystals and the anisotropy of the resulting data. We also note that ~20% of the trimer is not modeled (N-terminus of gp120, V2, V4, C-terminus of gp120, N-terminus of gp41, gp41 disulfide loop region, N-terminus of gp41 HR2), which also contributes to higher R-values. BG505 SOSIP.664 trimer elements included in the deposited model are summarized in table S2. Structure validation was performed using Molprobity (73) and refinement statistics are reported in table S1.

_Pseudovirus production and neutralization assay_

The BG505 _env_ gene used to make Env-pseudoviruses lacks the N332 glycosylation site, but the viruses are still neutralized by antibodies of the PGT121 family. To assess the importance of specific glycosylation sites on neutralization by these antibodies, site-directed mutations were introduced into the _env_ gene using QuikChange according to the manufacturer’s protocol (Stratagene, La Jolla, CA). Mutants were verified by DNA sequence analysis (Eton Bioscience, San Diego, CA). Pseudoviruses were generated by transfection of 293T cells for 72 h with an Env-expressing plasmid and an Env-deficient genomic backbone plasmid (pSG3ΔEnv) in a 1:2 ratio, using Fugene 6 (Promega). A single-cycle neutralization assay with TZM-bl target cells was performed as described previously (74). Briefly, TZM-bl cells were seeded in a 96-well flat bottom plate at a concentration of 20,000 cells/well. Pseudoviruses were preincubated with serial dilutions of antibody for 1 h at 37°C before infection of the cells. Luciferase reporter gene expression was quantified 48 h after infection by cell lysis and the addition of Luciferase
substrate (Promega). To determine IC$_{50}$ values, dose-response curves were fitted using nonlinear regression.
Fig. S1. Complex formation, crystallization and x-ray diffraction experiments. (A) SEC purification of PGT122 Fab in complex with partially deglycosylated BG505 SOSIP.664 trimers in the presence of excess Fab. (B) Non-reducing SDS-PAGE analysis of the SEC-purified complex. (C) Crystals of the Env trimer-Fab complex from a condition containing 0.1 M CAPS, 2 M ammonium sulfate, 0.2 M lithium sulfate, pH 10.5. (D) X-ray diffraction image at APS beamline 23-ID-B of one of the crystals in (C), illustrating that the best diffraction was observed along the c-axis. The 3D-profile of a reflection at 3.7 Å along the c-axis shows that its intensity is significantly above background.
**Fig. S2. Crystal packing of the Env trimer-PGT122 complex.** (A) Details of the Env trimer crystal packing with C2 symmetry, with the unit cell shown in pink. (B) The soluble Env trimers pack tail-to-tail with their HR2 helices forming crystal contacts. Therefore, crystal lattice interactions for gp41 HR2 might lead to some slight change in orientation of this helix. (C) Crystal packing interactions mediated by PGT122 constant domains influence the flexible Fab elbow angle, which differs from that observed in the high resolution crystal structure (PDB ID: 4JY5) and the ~14 Å negative-stain EM reconstruction (fig. S8). In (B) and (C), symmetry-related molecules are shown in gray.
Fig. S3. Unbiased Fo-Fc electron density around regions in the Env trimer that were not present in the molecular replacement search model. Fo-Fc maps, contoured at 1.25 $\sigma$, were calculated immediately after molecular replacement and rigid body refinement. The search model composed of the PGT122 variable domain (blue) and core gp120 (yellow) is shown as cartoons. Strong and unambiguous electron density for new features that were not present in the MR model is shown as a mesh and colored by elements: gp41 HR1 (green), gp41 HR1 (dark green), gp120 V1/V2 (orange), and gp120 V3 (red). The gp120 $\alpha_1$ helix is longer in the SOSIP gp140 structure compared to gp120 core monomeric structures, as revealed by unbiased Fo-Fc density (magenta). (A) Side-view and (B) view down the trimer axis. By protein mass, the search model used for molecular replacement represents 53% of the final deposited model.
Fig. S4. Comparison between (A) the maps/reconstruction and (B) the Env trimer models derived from the X-ray and EM data. (A) The EM reconstruction of the BG505 SOSIP.664 Env trimer (25) is shown on the left and the X-ray electron density for the BG505 SOSIP.664 Env trimer is shown on the right in a gray 2Fo-Fc map contoured at 1.0 σ. (B) A comparison of the EM and x-ray BG505 SOSIP.664 trimer structures are shown according to secondary structure elements. For one protomer, gp120 and gp41 elements are colored yellow and green, respectively, whereas the other two protomers are colored gray. The trimer structures derived using these independent techniques are very similar, as indicated by a Ca rmsd of 1.5 Å after aligning gp120 protomers.
Fig. S5. Comparison of PGT122 Fab and V3 structures with the soluble Env trimer structure. (A) PGT122 Fab variable domain from the high-resolution crystal structure (PDB ID: 4JY5, pale green) superimposed on the variable domain of PGT122 Fab in the co-crystal structure (blue). Electron density around the PGT122 Fab variable domain is shown in a gray 2Fo-Fc map contoured at 1.0 σ. (B) V3 peptide from the high-resolution NMR structure (PDB ID: 2ESX, pale green) superimposed on the V3 loop in the Env trimer structure (red). Electron density around N301, marking the beginning of the N-terminal V3 β-strand, is shown in a gray 2Fo-Fc map contoured at 1.0 σ. (C) Superimposition of V3 from a gp120-V3-containing structure (PDB ID: 2B4C, pale blue) on the V3 loop in the trimer structure. V3 adopts an anti-
parallel β-hairpin in the gp120 structure that agrees overall with its conformation in our trimer structure. However, the orientation of V3 in the crystal structure of the gp120 core plus V3, in complex with CD4 and CD4i antibody X5, significantly differs from the one in the trimer structure (D) that probably reflects more flexibility in the free monomer versus its restricted conformation in the trimer or a different conformation when CD4 and CD4i antibodies (or co-receptor) bind.
Fig. S6. The conformation of gp120 β2-β3-β21-β22 elements in the Env trimer structure significantly differs from the bridging sheet conformation observed in core gp120 monomer structures. (A) Cartoon rendering according to secondary structure for gp120 of a single protomer in the SOSIP gp140 trimer crystal structure. The gp120 elements are colored differently: core (yellow), V1/V2 (orange), V3 (red), β2-β3 (blue) and β21-β22 (magenta). In the SOSIP gp140 trimer structure, β2-β3 strands are inverted compared to the bridging sheet conformation observed in several core monomeric gp120 structures (B-E). The β21-β22 strands, however, are in a similar conformation to the bridging sheet and, therefore, form the previously defined binding pocket for the small molecule inhibitor of HIV-1 entry, BMS806, a known marker of the Env pre-fusion closed conformation. However, it is not yet known whether BMS806 can bind to the BG505 virus, as this compound has a limited range of specificity (75). (B) In the unliganded core monomeric gp120 structure (PDB ID: 3TGT), where V1/V2 elements
have been truncated, β2-β3-β21-β22 elements adopt the bridging sheet conformation. The same is also true for core monomeric gp120 in complex with (C) soluble CD4 and 17b Fab (PDB ID: 1GC1), (D) VRC01 Fab (PDB ID: 3NGB), and (E) NIH45/46 (PDB ID: 3U7Y). In structures of core monomeric gp120 in complex with (F) b12 Fab (PDB ID: 2NY7), (G) b13 Fab (PDB ID: 3IDX) and (H) F105 Fab (PDB ID: 3HI1), β2-β3-β21-β22 elements differ in conformation from both the bridging sheet structures in (B-E) and the arrangement observed in the trimer structure (A).
Fig. S7. Electron density for gp41 N-terminus and HR1 and for the gp41-gp120 interacting region around gp120 C1 and C5. (A) Whereas the gp41 central HR1 has a strong electron density that can be fitted by a helix, the connection to the FP at the N-terminus of the helix has much weaker density, which suggests the lack of any significant secondary structure and probably a loop conformation, akin to that seen in Influenza HA (Fig. 3). (B) Connecting electron density is observed between gp41 HR1 and HR2, attributable to the gp41 disulfide loop (DSL) region. In the same region, electron density also emanates from gp120 C1 (N-terminus) and C5 (C-terminus), implying a close interaction between the gp41 DSL region and the extended structure of the gp120 termini (5, 48). Electron density around gp41 and selected gp120 elements is shown in a gray 2Fo-Fc map contoured at 1.0 σ. The gp120 and gp41 subunits are
shown as yellow and green elements rendered according to their secondary structure, respectively.
Fig. S8. Comparison of the soluble Env trimer crystal structure at 4.7 Å and the equivalent ~14 Å negative-stain EM reconstruction. (A) The crystal structure agrees well with the negative-stain EM reconstruction (gray surface) of the same complex, except for the PGT122 Fab constant domain, which can rotate around the flexible elbow region. The gp41, gp120 and PGT122 Fab components are shown as green, yellow and gray secondary structure elements, respectively. Glycans are represented as sticks. The figure was generated with UCSF Chimera (76). (B) Difference in the flexible Fab elbow angle between PGT122 in the Env trimer structure (blue) and the high-resolution unliganded structure (PDB ID: 4JY5, pale green). The variable domains are in the same orientation to highlight the difference in the elbow angle. Differences in
Fab elbow angle can probably be attributed to inherent flexibility and crystal packing interactions.
Fig. S9. Complete structural definition of the PGT122 epitope in stereo view. (A) In addition to the N332 glycan (yellow), antibody PGT122 recognizes both protein and glycan elements near the base of gp120 V1 (orange) and V3 (red) to mediate broad and potent HIV-1 neutralization. Heavy and light chain CDRs are shown as dark and light blue tubes, respectively. Electron density for oligomannose glycans (spheres) surrounding the PGT122 epitope is shown as a 2Fo-Fc gray mesh contoured at 1.0 σ.
Fig. S10. Effect of mutating glycosylation sites in BG505 HIV-1 Env on pseudovirus neutralization by antibodies of the PGT121 family. (A) PGT121. (B) PGT123. (C) PGV04. Antibodies of the PGT121 family differ slightly in their dependency on glycans surrounding the PGT122 epitope, showing that their epitopes are similar but not identical. PGV04, a bnAb against the CD4bs, serves as a comparator antibody; it is not affected by any of the sequence changes tested.
Table S1. X-ray Crystallographic Data and Refinement Statistics

<table>
<thead>
<tr>
<th><strong>Data Collection</strong></th>
<th><strong>APS 23-ID-B</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td>Wavelength, Å</td>
<td>1.0332</td>
</tr>
<tr>
<td>No. of crystals used</td>
<td>2</td>
</tr>
<tr>
<td>Space group</td>
<td>C2</td>
</tr>
<tr>
<td>Unit cell a, b, c (Å)</td>
<td>152.2, 260.1, 282.8</td>
</tr>
<tr>
<td>α, β, γ (°)</td>
<td>90.0, 99.6, 90.0</td>
</tr>
<tr>
<td>Resolution (Å)</td>
<td>40.0 – 4.7 (4.8 – 4.7)</td>
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<tr>
<td>Completeness</td>
<td>91.0 (59.4)</td>
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<tr>
<td>Redundancy</td>
<td>4.0 (2.7)</td>
</tr>
<tr>
<td>No. total reflections</td>
<td>228,125</td>
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<tr>
<td>No. unique reflections</td>
<td>51,575</td>
</tr>
<tr>
<td>I/σᵣ</td>
<td>4.9 (2.0)</td>
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<tr>
<td>R&lt;sub&gt;merge&lt;/sub&gt;</td>
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</tr>
<tr>
<td>R&lt;sub&gt;free&lt;/sub&gt;</td>
<td>0.16 (0.41)</td>
</tr>
<tr>
<td>CC₁₂&lt;sup&gt;₂&lt;/sup&gt;</td>
<td>96.2 (56.6)</td>
</tr>
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</table>

**Refinement statistics**

| Resolution (Å) | 40.0 – 4.7 |
| No. reflections total/R<sub>free</sub> | 48,915/2,620 |
| R<sub>cryst</sub>/R<sub>free</sub> | 37.5/38.9 |
| RMSD bond length (Å) | 0.006 |
| RMSD bond angles (°) | 1.4 |
| Protein atoms/glycan atoms | 20,274/1,797 |
| Wilson B-value (Å<sup>²</sup>) | 140 |
| Ramachandran Preferred % | 90.7 |
| Allowed % | 98.3 |
| MolProbity all-atom clashscore | 24.5 |
| PDB ID | 4NCO |
Values in parentheses are for the highest resolution shell.

† $R_{	ext{merge}} = \Sigma |I-<I>|/\Sigma <I>$, where $I$ is the observed intensity, and $<I>$ is the average intensity of multiple observations of related reflections.

‡ $R_{\text{pim}} = \Sigma_{hkl} (1/(n-1))^{1/2} \Sigma_i |I_{hkl,i} - <I_{hkl}>| / \Sigma_{hkl} \Sigma_i I_{hkl,i}$, where $I_{hkl,i}$ is the scaled intensity of the $i^{th}$ measurement of reflection h, k, l, $<I_{hkl}>$ is the average intensity for that reflection, and $n$ is the redundancy.

§ $CC_{1/2} =$ correlation coefficient of half-datasets (77)

‡ $R_{\text{cryst}} = \Sigma_{hkl} |F_{\text{obs}}|-|F_{\text{calc}}|/\Sigma_{hkl}|F_{\text{obs}}|$

‡ $R_{\text{free}}$ calculated as for $R_{\text{cryst}}$ but for 5% of the reflections excluded from refinement

Table S2. BG505 SOSIP.664 elements modeled in the deposited Env trimer structure

<table>
<thead>
<tr>
<th>gp140 elements</th>
<th>Modeled in deposited structure</th>
</tr>
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<tbody>
<tr>
<td>gp120</td>
<td>44-493</td>
</tr>
<tr>
<td></td>
<td>(V2 residues 178-190 disordered)</td>
</tr>
<tr>
<td></td>
<td>(V4 residues 402-410 disordered)</td>
</tr>
<tr>
<td>gp41 HR1</td>
<td>37 residues</td>
</tr>
<tr>
<td>gp41 HR2</td>
<td>625-664</td>
</tr>
<tr>
<td>PGT122 Fab</td>
<td>Heavy and light chain residues</td>
</tr>
<tr>
<td></td>
<td>entirely modeled</td>
</tr>
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</table>
References and Notes


The BG505 SOSIP.664 trimer possesses most, if not all, of the characteristics associated with the pre-fusion closed Env trimer conformation: the presence of a V1V2/V3 cap assembled at the membrane-distal apex; antigenic reactivity with antibodies of quaternary epitopes; the likely inability of gp41 to bind to free HR2 peptides; a coherent binding site for residues associated with binding of the small molecule inhibitor of HIV-1 entry, BMS806; and many residues of the inner domain previously analyzed by mutational substitution for which we can now explain their mutational phenotypes.


29. A hole was also reported in cleaved trimer structures determined by EM ([11]), but seems to result from the low resolution of the reconstructions [see discussion in (25)].


44. Stronger electron density reappears for a loop prior to the N terminus of the gp41 HR1 central helix, near the gp120/gp41 interface. We assign this electron density to the gp41 fusion peptide proximal region (FPPR) elements. Indeed, gp41 and gp120 elements in this region (gp120 residues 73-84, glycans at gp120 N88 and gp41 N625, and the C-terminal HR2 helix from an adjacent protomer) are particularly hydrophobic and could easily interact with and occlude the hydrophobic gp41 FP. In addition, this ascribed FP region is in close relative proximity to the C terminus of gp120 C5, to which it was connected in the uncleaved gp160 precursor prior to furin cleavage.


51. A slight difference in HR2 helix orientation is observed between the trimer crystal structure and the cryo-EM structure reported in the accompanying manuscript (25). Crystal packing interactions at the gp41 C terminus probably account for this small shift (fig. S2).


58. The complex biantennary glycan observed in the PGT121 paratope in crystal structures (23, 55) is fortuitous, as the glycan comes from a symmetry-related PGT121 Fab molecule in the crystal. Indeed, Fab PGT121 is glycosylated and was expressed in mammalian cells. PGT121 also reacts on the glycan array with complex biantennary glycans possessing α1-6 sialylated ends (23), which make substantial contacts with the paratope in the crystal structures. Although the N137 glycoform remains uncharacterized on virus-derived HIV-1 Env, PGT121 reactivity with the glycan array, and the liganded crystal structures, suggest that N137 is probably a biantennary complex glycan. The relatively weaker electron density for the oligomannose N137 glycan in the trimer structure also suggests that, when it is not an α1-6 sialylated complex carbohydrate, the N137 glycan lacks significant putative sites of interaction with PGT122. Hence, it might not be fully protected from glycosidase treatment, or it may be slightly disordered.

60. The PGT122 and PGT128 bnAbs appear to recognize a closely related N332-dependent epitope, but they approach gp120 with an inverted disposition of their light and heavy chains. Indeed, while the PGT128 heavy chain predominantly interacts with the gp120 V3 base, PGT122 recognizes this region mainly through its light chain. Conversely, N137 is recognized by the PGT122 heavy chain, but is putatively contacted by the PGT128 light chain.


63. The PyMOL Molecular Graphics System, Version 1.6.0.0 Schrödinger, LLC.


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