



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2023 – 04:05 PM EDT

PDB ID : 8F9Z
Title : Crystal structure of clade A/E 93TH057 HIV-1 gp120 core in complex with NBD-14204, an HIV-1 gp120 antagonist
Authors : Kwon, Y.D.; Kwong, P.D.
Deposited on : 2022-11-25
Resolution : 1.94 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

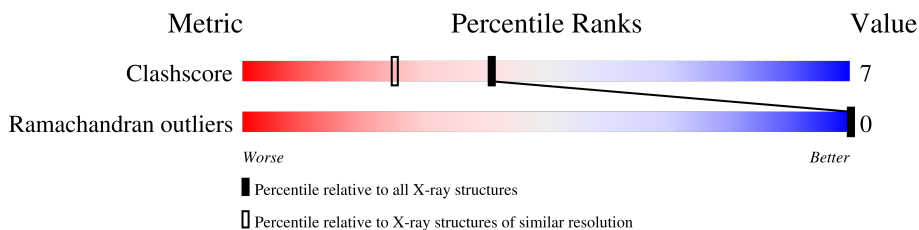
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 Å.


Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	353	 84% 12% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5763 atoms, of which 2705 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

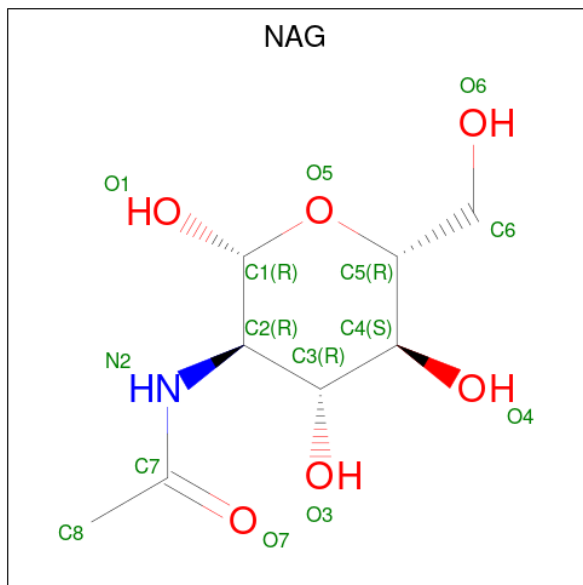
- Molecule 1 is a protein called HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	339	5248	1666	2594	460	507	21	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	SER	HIS	engineered mutation	UNP A0A0M3KKW8

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



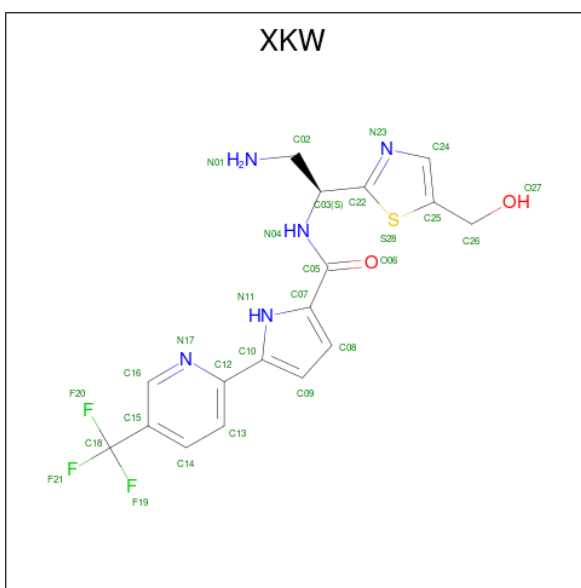
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	27	8	13	1	5	0	0
2	A	1	27	8	13	1	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
2	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 3 is (5M)-N-{(1S)-2-amino-1-[5-(hydroxymethyl)-1,3-thiazol-2-yl]ethyl}-5-[5-(trifluoromethyl)pyridin-2-yl]-1H-pyrrole-2-carboxamide (three-letter code: XKW) (formula: C₁₇H₁₆F₃N₅O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
3	A	1	Total	C	F	H	N	O	S	0	0
			44	17	3	16	5	2	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
4	A	1	32	8	17	2	4	1	0	0

- Molecule 5 is water.

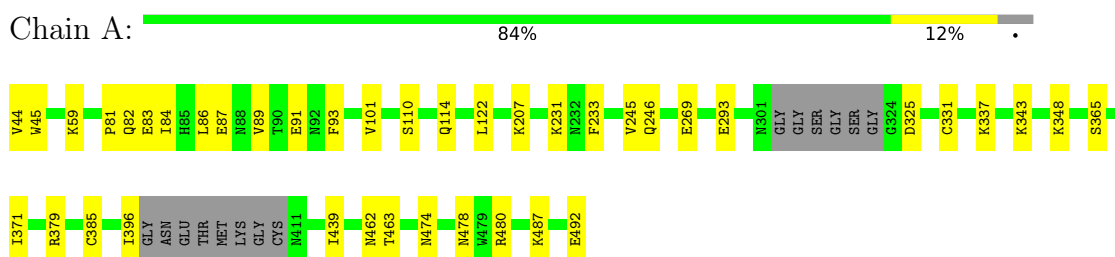
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	277	Total	O	0	0
			277	277		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS failed to run properly.

- Molecule 1: HIV-1 gp120 core



4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.20Å 67.59Å 87.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.44 – 1.94	Depositor
% Data completeness (in resolution range)	84.2 (36.44-1.94)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.95Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.183 , 0.216	Depositor
Wilson B-factor (Å ²)	18.6	Xtrriage
Anisotropy	0.113	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.024 for k,h,-l	Xtrriage
Total number of atoms	5763	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, XKW, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/2709	0.54	0/3678

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2654	2594	2594	36	0
2	A	84	78	78	2	0
3	A	28	16	0	2	0
4	A	15	17	17	0	0
5	A	277	0	0	21	0
All	All	3058	2705	2689	39	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 39 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLN:NE2	5:A:602:HOH:O	1.83	1.12
1:A:337:LYS:NZ	5:A:604:HOH:O	1.95	0.97
1:A:59:LYS:NZ	5:A:601:HOH:O	1.82	0.95
1:A:59:LYS:NZ	5:A:608:HOH:O	2.11	0.82
1:A:365:SER:O	5:A:605:HOH:O	2.00	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	333/353 (94%)	325 (98%)	8 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	XKW	A	507	-	27,30,30	1.71	5 (18%)	25,43,43	2.28	8 (32%)
2	NAG	A	504	1	14,14,15	0.53	0	17,19,21	0.46	0
2	NAG	A	503	1	14,14,15	0.29	0	17,19,21	0.53	0
2	NAG	A	505	1	14,14,15	0.26	0	17,19,21	0.45	0
4	EPE	A	508	-	15,15,15	0.86	1 (6%)	18,20,20	2.34	8 (44%)
2	NAG	A	506	1	14,14,15	0.34	0	17,19,21	0.50	0
2	NAG	A	501	1	14,14,15	0.35	0	17,19,21	0.32	0
2	NAG	A	502	1	14,14,15	0.57	0	17,19,21	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	XKW	A	507	-	-	3/14/26/26	0/3/3/3
2	NAG	A	504	1	-	1/6/23/26	0/1/1/1
2	NAG	A	503	1	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1	-	2/6/23/26	0/1/1/1
4	EPE	A	508	-	-	5/9/19/19	0/1/1/1
2	NAG	A	506	1	-	2/6/23/26	0/1/1/1
2	NAG	A	501	1	-	2/6/23/26	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	507	XKW	C24-N23	5.09	1.43	1.36
3	A	507	XKW	C05-N04	4.14	1.43	1.34
4	A	508	EPE	C10-S	2.77	1.81	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	507	XKW	C12-C10	2.35	1.54	1.49
3	A	507	XKW	C12-N17	2.21	1.39	1.35

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	507	XKW	C24-C25-S28	-6.29	105.75	112.00
3	A	507	XKW	C07-C05-N04	4.83	124.17	115.20
4	A	508	EPE	C5-N4-C3	4.67	119.33	108.83
4	A	508	EPE	C7-N4-C5	4.12	121.78	111.23
3	A	507	XKW	C13-C12-N17	-3.81	116.59	122.26

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

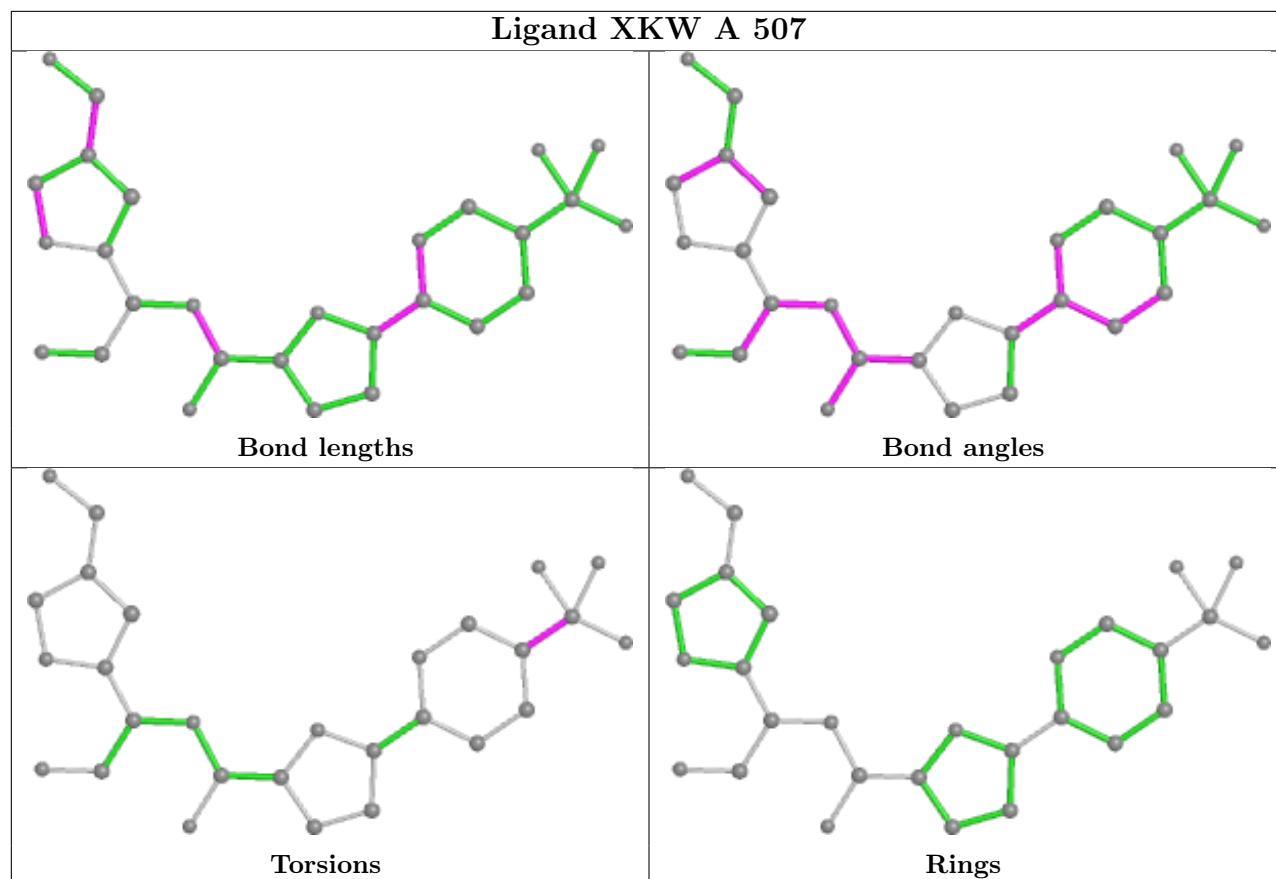
Mol	Chain	Res	Type	Atoms
4	A	508	EPE	C8-C7-N4-C5
4	A	508	EPE	C9-C10-S-O2S
2	A	506	NAG	O5-C5-C6-O6
2	A	506	NAG	C4-C5-C6-O6
4	A	508	EPE	C9-C10-S-O3S

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	507	XKW	2	0
2	A	504	NAG	1	0
2	A	505	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.