



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:28 PM GMT

PDB ID : 4DKR
Title : Crystal structure of clade A/E 93TH057 HIV-1 gp120 core in complex with AWS-I-169
Authors : Kwon, Y.D.; LaLonde, J.M.; Jones, D.M.; Sun, A.W.; Courter, J.R.; Soeta, T.; Kobayashi, T.; Princiotta, A.M.; Wu, X.; Mascola, J.; Schon, A.; Freire, E.; Sodroski, J.; Madani, N.; Smith III, A.B.; Kwong, P.D.
Deposited on : 2012-02-03
Resolution : 1.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

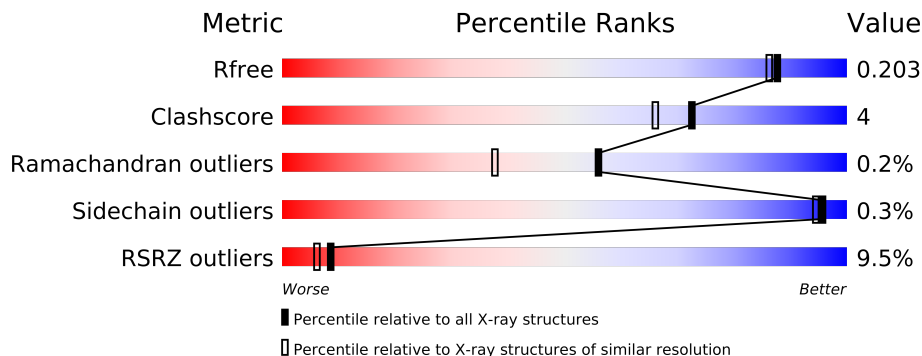
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.80 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))
R_{free}	66092	3513 (1.80-1.80)
Clashscore	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (1.80-1.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	353	
1	C	353	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	A	502	-	X
2	NAG	A	506	-	X
2	NAG	A	510	-	X
2	NAG	A	511	-	X
2	NAG	C	501	-	X
2	NAG	C	504	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	NAG	C	506	-	X
2	NAG	C	507	-	X
2	NAG	C	508	-	X
2	NAG	C	510	-	X
2	NAG	C	511	-	X
4	0LJ	C	513	-	X

2 Entry composition i

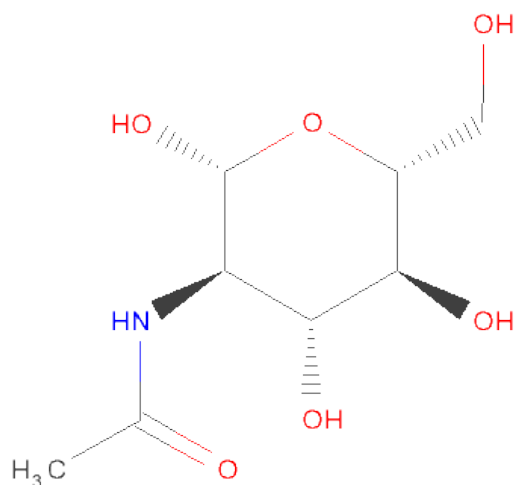
There are 5 unique types of molecules in this entry. The entry contains 6143 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	339	Total	C	N	O	S	0	0	0
			2654	1666	460	507	21			
1	C	339	Total	C	N	O	S	0	0	0
			2654	1666	460	507	21			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



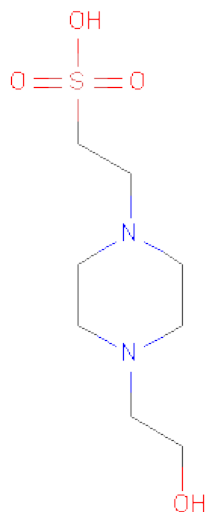
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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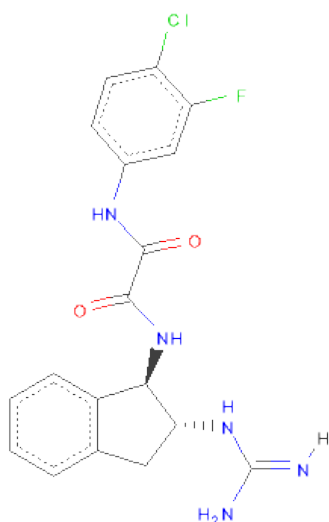
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is N-[(1R,2R)-2-CARBAMIMIDAMIDO-2,3-DIHYDRO-1H-INDEN-1-YL]-N'-(4-CHLORO-3-FLUOROPHENYL)ETHANEDIAMIDE (three-letter code: 0LJ) (formula: C₁₈H₁₇ClFN₅O₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	0	0
			27	18	1	1	5	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	Cl	F	N	O	0	0
			27	18	1	1	5	2		

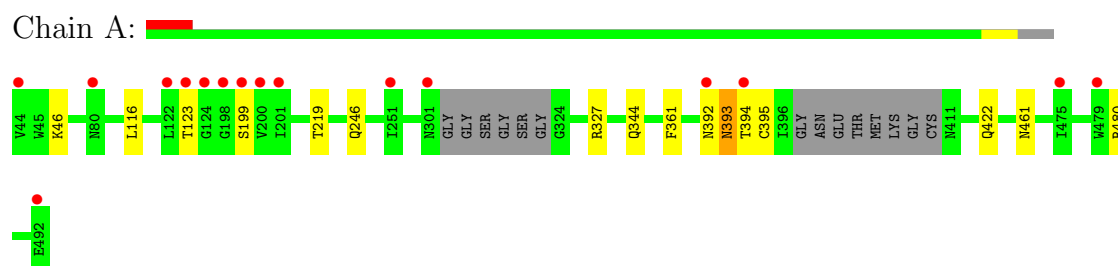
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	298	Total	O	0	0
			298	298		
5	C	145	Total	O	0	0
			145	145		

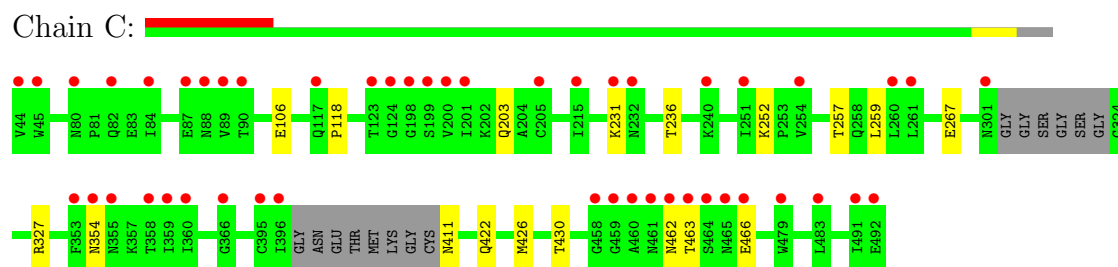
3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

- Molecule 1: HIV-1 gp120 core



- Molecule 1: HIV-1 gp120 core



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.44Å 68.60Å 94.54Å 90.00° 91.38° 90.00°	Depositor
Resolution (Å)	33.74 – 1.80 33.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.5 (33.74-1.80) 79.7 (33.74-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.190 , 0.208 0.189 , 0.203	Depositor DCC
R_{free} test set	3728 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.1	EDS
Estimated twinning fraction	0.015 for -k,-h,-l 0.015 for k,h,-l 0.026 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 77982 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6143	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, NAG, 0LJ

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	0.22	0/2709	0.40	0/3678
1	C	0.24	0/2709	0.40	0/3678
All	All	0.23	0/5418	0.40	0/7356

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2654	0	0	13	0
1	C	2654	0	0	12	0
2	A	154	0	143	1	0
2	C	154	0	143	0	0
3	A	15	0	17	0	0
3	C	15	0	17	0	0
4	A	27	0	16	1	0
4	C	27	0	16	0	0
5	A	298	0	0	6	0
5	C	145	0	0	5	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6143	0	352	26	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (26) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:480:ARG:NH2	5:A:850:HOH:O	2.00	0.92
1:A:461:ASN:ND2	5:A:891:HOH:O	2.10	0.84
1:C:252:LYS:NZ	5:C:606:HOH:O	2.14	0.79
1:A:361:PHE:O	1:A:393:ASN:ND2	2.20	0.75
1:C:106:GLU:OE1	5:C:640:HOH:O	2.08	0.72
1:A:344:GLN:OE1	5:A:657:HOH:O	2.07	0.71
1:C:236:THR:OG1	5:C:722:HOH:O	2.16	0.61
1:A:392:ASN:O	1:A:394:THR:N	2.34	0.60
1:C:118:PRO:O	1:C:203:GLN:NE2	2.35	0.59
1:C:231:LYS:NZ	1:C:267:GLU:OE2	2.40	0.55
1:C:327:ARG:NH2	1:C:422:GLN:OE1	2.41	0.54
1:A:361:PHE:N	1:A:393:ASN:ND2	2.57	0.53
1:A:46:LYS:NZ	5:A:801:HOH:O	2.43	0.51
1:C:354:ASN:ND2	5:C:742:HOH:O	2.42	0.51
1:C:466:GLU:OE1	5:C:733:HOH:O	2.19	0.50
1:A:395:CYS:SG	5:A:636:HOH:O	2.60	0.49
1:C:426:MET:SD	1:C:430:THR:OG1	2.70	0.48
1:A:246:GLN:OE1	5:A:684:HOH:O	2.21	0.46
1:C:462:ASN:OD1	1:C:463:THR:N	2.50	0.45
2:A:508:NAG:H81	1:C:252:LYS:NZ	2.32	0.45
1:A:327:ARG:NH2	1:A:422:GLN:OE1	2.52	0.43
1:A:392:ASN:C	1:A:394:THR:N	2.73	0.42
1:C:257:THR:O	1:C:259:LEU:N	2.52	0.42
1:A:219:THR:O	1:A:246:GLN:NE2	2.53	0.41
1:A:123:THR:OG1	1:A:199:SER:OG	2.38	0.41
4:A:513:OLJ:H8	4:A:513:OLJ:O11	2.21	0.41

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:717:HOH:O	5:C:728:HOH:O[2_545]	1.98	0.22

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	324 (97%)	8 (2%)	1 (0%)	50	31
1	C	333/353 (94%)	323 (97%)	10 (3%)	0	100	100
All	All	666/706 (94%)	647 (97%)	18 (3%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	393	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/311 (97%)	302 (100%)	1 (0%)	96	94
1	C	303/311 (97%)	302 (100%)	1 (0%)	96	94
All	All	606/622 (97%)	604 (100%)	2 (0%)	96	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LEU
1	C	411	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

26 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$
2	NAG	A	501	1	12,14,15	0.70	1 (8%)	15,19,21	0.79	1 (6%)
2	NAG	A	502	1	12,14,15	0.67	0	15,19,21	0.79	1 (6%)
2	NAG	A	503	1	12,14,15	0.63	0	15,19,21	0.91	1 (6%)
2	NAG	A	504	1	12,14,15	0.65	0	15,19,21	0.91	1 (6%)
2	NAG	A	505	1	12,14,15	0.67	0	15,19,21	0.88	1 (6%)
2	NAG	A	506	1	12,14,15	0.64	0	15,19,21	0.81	0
2	NAG	A	507	1	12,14,15	0.65	0	15,19,21	0.94	1 (6%)
2	NAG	A	508	1	12,14,15	0.63	0	15,19,21	1.03	1 (6%)
2	NAG	A	509	1	12,14,15	0.70	1 (8%)	15,19,21	0.90	1 (6%)
2	NAG	A	510	1	12,14,15	0.39	0	15,19,21	0.70	0
2	NAG	A	511	1	12,14,15	0.66	0	15,19,21	1.03	1 (6%)
3	EPE	A	512	-	15,15,15	0.73	1 (6%)	20,20,20	1.85	6 (30%)
4	OLJ	A	513	-	29,29,29	2.86	7 (24%)	41,41,41	2.00	9 (21%)
2	NAG	C	501	1	12,14,15	0.38	0	15,19,21	0.77	1 (6%)
2	NAG	C	502	1	12,14,15	0.66	0	15,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	503	1	12,14,15	0.61	0	15,19,21	0.95	1 (6%)
2	NAG	C	504	1	12,14,15	0.67	0	15,19,21	0.84	1 (6%)
2	NAG	C	505	1	12,14,15	0.64	0	15,19,21	0.85	1 (6%)
2	NAG	C	506	1	12,14,15	0.69	1 (8%)	15,19,21	0.73	0
2	NAG	C	507	1	12,14,15	0.68	1 (8%)	15,19,21	0.93	1 (6%)
2	NAG	C	508	1	12,14,15	0.69	1 (8%)	15,19,21	1.01	1 (6%)
2	NAG	C	509	1	12,14,15	0.66	0	15,19,21	0.85	1 (6%)
2	NAG	C	510	1	12,14,15	0.67	1 (8%)	15,19,21	0.81	1 (6%)
2	NAG	C	511	1	12,14,15	0.65	0	15,19,21	0.79	1 (6%)
3	EPE	C	512	-	15,15,15	0.75	1 (6%)	20,20,20	1.85	7 (35%)
4	OLJ	C	513	-	29,29,29	2.85	7 (24%)	41,41,41	2.14	10 (24%)

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
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1
2	NAG	A	503	1	-	0/6/23/26	0/1/1/1
2	NAG	A	504	1	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1	-	0/6/23/26	0/1/1/1
2	NAG	A	506	1	-	0/6/23/26	0/1/1/1
2	NAG	A	507	1	-	0/6/23/26	0/1/1/1
2	NAG	A	508	1	-	0/6/23/26	0/1/1/1
2	NAG	A	509	1	-	0/6/23/26	0/1/1/1
2	NAG	A	510	1	-	0/6/23/26	0/1/1/1
2	NAG	A	511	1	-	0/6/23/26	0/1/1/1
3	EPE	A	512	-	-	0/9/19/19	0/1/1/1
4	OLJ	A	513	-	-	0/16/28/28	0/1/3/3
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	502	1	-	0/6/23/26	0/1/1/1
2	NAG	C	503	1	-	0/6/23/26	0/1/1/1
2	NAG	C	504	1	-	0/6/23/26	0/1/1/1
2	NAG	C	505	1	-	0/6/23/26	0/1/1/1
2	NAG	C	506	1	-	0/6/23/26	0/1/1/1
2	NAG	C	507	1	-	0/6/23/26	0/1/1/1
2	NAG	C	508	1	-	0/6/23/26	0/1/1/1
2	NAG	C	509	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	510	1	-	0/6/23/26	0/1/1/1
2	NAG	C	511	1	-	0/6/23/26	0/1/1/1
3	EPE	C	512	-	-	0/9/19/19	0/1/1/1
4	0LJ	C	513	-	-	0/16/28/28	0/1/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	513	0LJ	C17-C16	-11.05	1.44	1.54
4	C	513	0LJ	C17-C16	-10.96	1.45	1.54
4	C	513	0LJ	C25-N20	5.16	1.42	1.33
4	A	513	0LJ	C25-N20	5.01	1.42	1.33
4	A	513	0LJ	C15-N13	-4.72	1.39	1.46
4	C	513	0LJ	C12-N13	4.69	1.44	1.34
4	A	513	0LJ	C12-N13	4.53	1.43	1.34
4	C	513	0LJ	C15-N13	-4.48	1.39	1.46
4	C	513	0LJ	C10-N09	4.40	1.44	1.35
4	A	513	0LJ	C10-N09	4.29	1.44	1.35
4	A	513	0LJ	C15-C16	-3.44	1.48	1.54
4	C	513	0LJ	C15-C16	-3.22	1.48	1.54
3	C	512	EPE	C10-S	2.59	1.81	1.77
3	A	512	EPE	C10-S	2.52	1.81	1.77
4	C	513	0LJ	C05-N09	2.24	1.46	1.41
2	A	501	NAG	O5-C5	-2.08	1.41	1.45
2	A	509	NAG	O5-C5	-2.08	1.41	1.45
2	C	508	NAG	O5-C5	-2.06	1.41	1.45
2	C	506	NAG	O5-C5	-2.06	1.41	1.45
4	A	513	0LJ	C05-N09	2.06	1.45	1.41
2	C	507	NAG	O5-C5	-2.03	1.41	1.45
2	C	510	NAG	O5-C5	-2.01	1.41	1.45

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	513	0LJ	C10-C12-N13	6.98	120.05	113.31
4	A	513	0LJ	C10-C12-N13	6.64	119.71	113.31
4	C	513	0LJ	C12-C10-N09	6.45	118.99	112.01
4	A	513	0LJ	C12-C10-N09	5.51	117.97	112.01
4	C	513	0LJ	C19-C15-N13	-4.70	108.05	114.22
4	A	513	0LJ	C19-C15-N13	-4.61	108.17	114.22
3	C	512	EPE	O1S-S-C10	4.24	110.44	106.81
3	A	512	EPE	O1S-S-C10	4.17	110.38	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	512	EPE	C5-N4-C3	4.12	119.09	108.86
3	C	512	EPE	C5-N4-C3	3.91	118.57	108.86
4	A	513	0LJ	C18-C19-C15	-3.83	107.94	110.50
4	C	513	0LJ	C18-C17-C16	3.52	107.57	102.60
4	C	513	0LJ	C19-C15-C16	3.33	106.02	102.84
2	C	508	NAG	O5-C5-C6	2.76	109.88	106.98
4	A	513	0LJ	C17-C18-C19	-2.73	107.98	111.00
2	C	503	NAG	O5-C5-C6	2.69	109.80	106.98
2	C	507	NAG	O5-C5-C6	2.62	109.73	106.98
3	C	512	EPE	O2S-S-C10	2.61	109.05	106.81
4	C	513	0LJ	C18-C19-C15	-2.61	108.75	110.50
2	A	508	NAG	C2-N2-C7	-2.61	118.70	123.09
2	A	507	NAG	O5-C5-C6	2.59	109.70	106.98
2	A	504	NAG	O5-C5-C6	2.59	109.70	106.98
2	A	503	NAG	O5-C5-C6	2.55	109.66	106.98
4	A	513	0LJ	C16-C15-N13	-2.55	110.44	114.49
4	C	513	0LJ	C16-C15-N13	-2.53	110.47	114.49
2	A	509	NAG	O5-C5-C6	2.50	109.61	106.98
3	A	512	EPE	O3S-S-C10	2.44	109.01	105.93
3	A	512	EPE	C5-C6-N1	-2.42	105.84	110.61
2	A	505	NAG	O5-C5-C6	2.41	109.51	106.98
2	C	501	NAG	O5-C5-C6	2.41	109.51	106.98
2	C	504	NAG	O5-C5-C6	2.38	109.48	106.98
2	C	509	NAG	O5-C5-C6	2.36	109.46	106.98
2	C	505	NAG	O5-C5-C6	2.27	109.36	106.98
2	C	510	NAG	O5-C5-C6	2.22	109.31	106.98
3	C	512	EPE	C7-N4-C3	2.21	117.04	111.32
2	C	511	NAG	O5-C5-C6	2.20	109.29	106.98
4	A	513	0LJ	C04-C03-C02	-2.20	120.06	121.75
4	A	513	0LJ	C16-N20-C25	-2.19	120.01	124.00
3	A	512	EPE	C2-C3-N4	2.19	114.92	110.61
3	C	512	EPE	O3S-S-C10	2.18	108.69	105.93
3	A	512	EPE	C7-N4-C3	2.18	116.94	111.32
2	A	501	NAG	O5-C5-C6	2.13	109.22	106.98
4	C	513	0LJ	C17-C18-C19	-2.12	108.66	111.00
2	A	511	NAG	O7-C7-C8	-2.11	117.92	122.04
4	C	513	0LJ	O11-C10-C12	-2.11	119.03	121.31
4	A	513	0LJ	O11-C10-C12	-2.11	119.03	121.31
4	C	513	0LJ	C04-C03-C02	-2.06	120.17	121.75
3	C	512	EPE	C7-N4-C5	2.05	116.61	111.32
2	A	502	NAG	O5-C5-C6	2.03	109.11	106.98
3	C	512	EPE	C5-C6-N1	-2.02	106.64	110.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	339/353 (96%)	0.16	16 (4%) 30 23	20, 32, 62, 97	0
1	C	339/353 (96%)	0.73	48 (14%) 3 2	25, 49, 91, 145	0
All	All	678/706 (96%)	0.45	64 (9%) 8 6	20, 40, 87, 145	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	44	VAL	8.9
1	C	460	ALA	8.5
1	C	492	GLU	7.9
1	A	124	GLY	7.4
1	A	123	THR	6.5
1	C	355	ASN	6.1
1	C	459	GLY	5.8
1	A	198	GLY	5.6
1	C	462	ASN	5.5
1	C	354	ASN	5.3
1	C	466	GLU	5.1
1	A	392	ASN	5.0
1	C	123	THR	5.0
1	C	301	ASN	4.9
1	A	44	VAL	4.9
1	A	492	GLU	4.5
1	C	199	SER	4.5
1	C	458	GLY	4.4
1	C	461	ASN	4.4
1	C	491	ILE	4.4
1	C	124	GLY	4.1
1	C	464	SER	3.9
1	A	301	ASN	3.8
1	C	465	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	359	ILE	3.8
1	A	200	VAL	3.8
1	A	199	SER	3.7
1	A	122	LEU	3.6
1	C	89	VAL	3.5
1	C	240	LYS	3.5
1	C	463	THR	3.3
1	C	358	THR	3.3
1	C	201	ILE	3.1
1	C	88	ASN	3.1
1	C	87	GLU	3.1
1	C	251	ILE	3.1
1	A	394	THR	3.0
1	C	84	ILE	2.8
1	C	82	GLN	2.8
1	C	117	GLN	2.8
1	C	261	LEU	2.8
1	A	201	ILE	2.8
1	A	80	ASN	2.6
1	C	80	ASN	2.6
1	C	200	VAL	2.6
1	C	360	ILE	2.5
1	C	45	TRP	2.5
1	C	198	GLY	2.5
1	C	232	ASN	2.5
1	C	479	TRP	2.4
1	C	353	PHE	2.4
1	C	254	VAL	2.3
1	C	90	THR	2.3
1	A	479	TRP	2.2
1	C	260	LEU	2.2
1	A	251	ILE	2.2
1	C	205	CYS	2.2
1	C	483	LEU	2.2
1	C	395	CYS	2.2
1	C	366	GLY	2.1
1	A	475	ILE	2.1
1	C	396	ILE	2.1
1	C	215	ILE	2.1
1	C	231	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	C	501	14/15	0.58	25.49	57,68,76,77	0
2	NAG	A	502	14/15	0.42	13.96	62,86,97,102	0
2	NAG	A	511	14/15	0.35	6.24	71,82,92,95	0
2	NAG	C	507	14/15	0.26	5.84	55,75,81,82	0
2	NAG	C	508	14/15	0.83	4.04	27,43,67,76	0
4	0LJ	C	513	27/27	0.23	3.45	33,58,89,91	0
2	NAG	A	506	14/15	0.19	3.20	36,55,68,77	0
2	NAG	C	511	14/15	0.21	3.19	30,52,68,76	0
2	NAG	A	510	14/15	0.60	2.83	64,72,75,76	0
2	NAG	C	510	14/15	0.30	2.72	67,79,86,87	0
2	NAG	C	504	14/15	0.28	2.63	63,84,90,92	0
2	NAG	C	506	14/15	0.16	2.14	37,53,70,77	0
2	NAG	A	507	14/15	0.18	1.52	48,53,60,70	0
2	NAG	A	504	14/15	0.16	1.19	31,42,55,60	0
2	NAG	C	505	14/15	0.18	0.84	40,54,59,59	0
3	EPE	A	512	15/15	0.13	0.51	20,26,30,31	0
2	NAG	A	509	14/15	0.10	0.12	38,49,58,64	0
3	EPE	C	512	15/15	0.11	0.11	27,33,41,50	0
2	NAG	A	501	14/15	0.10	0.05	37,56,63,66	0
2	NAG	C	509	14/15	0.13	0.03	48,58,64,67	0
2	NAG	A	505	14/15	0.10	-0.06	29,43,54,64	0
2	NAG	C	502	14/15	0.12	-0.22	60,70,75,80	0
4	0LJ	A	513	27/27	0.11	-0.37	23,38,48,50	0
2	NAG	C	503	14/15	0.11	-0.43	22,26,28,28	0
2	NAG	A	508	14/15	0.17	-0.60	41,48,72,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	503	14/15	0.07	-1.20	22,27,35,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.