



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:49 PM GMT

PDB ID : 4DKP
Title : Crystal structure of clade A/E 93TH057 HIV-1 gp120 core in complex with AWS-I-50
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Deposited on : 2012-02-03
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

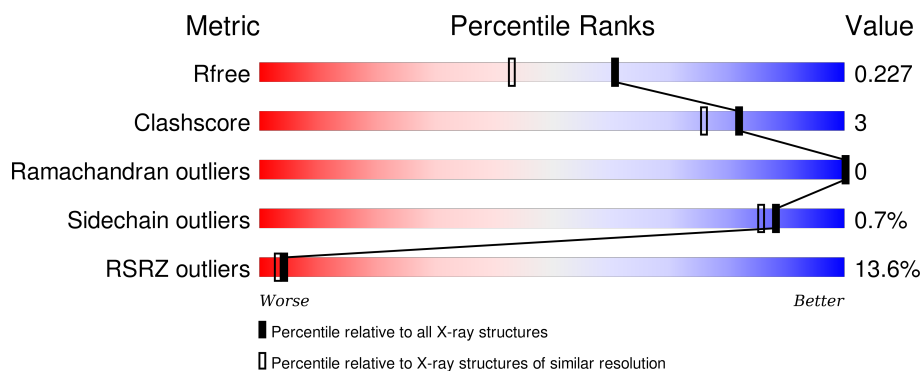
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (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. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	353	<div> <div>9%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>
1	C	353	<div> <div>17%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	506	-	-	-	X
2	NAG	A	507	-	-	-	X
2	NAG	C	511	-	-	-	X
3	EPE	C	512	-	-	-	X
4	OLL	A	513	-	-	-	X
4	OLL	C	513	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6171 atoms, of which 0 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 clade A/E 93TH057 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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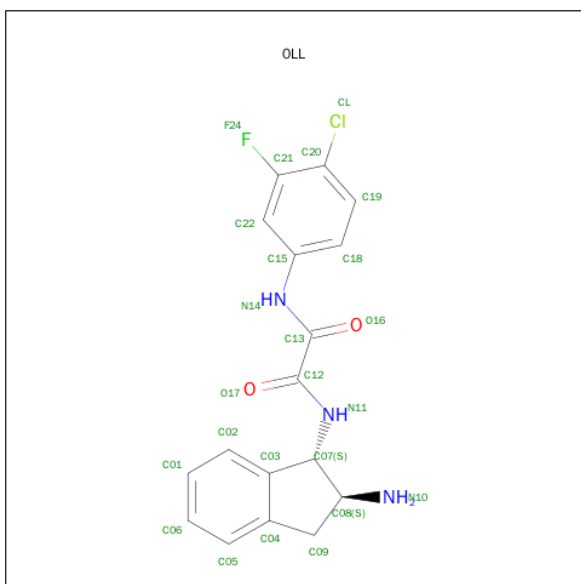
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	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-PIPERAZINE ETHANESULFONIC 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
			13	8	2	2	1		

- Molecule 4 is N-[(1S,2S)-2-AMINO-2,3-DIHYDRO-1H-INDEN-1-YL]-N'-(4-CHLORO-3-FLUOROPHENYL)ETHANEDIAMIDE (three-letter code: 0LL) (formula: C₁₇H₁₅ClFN₃O₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	0	0
			24	17	1	1	3	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	C	1	Total	C	Cl	F	N	O	0	0
			24	17	1	1	3	2		

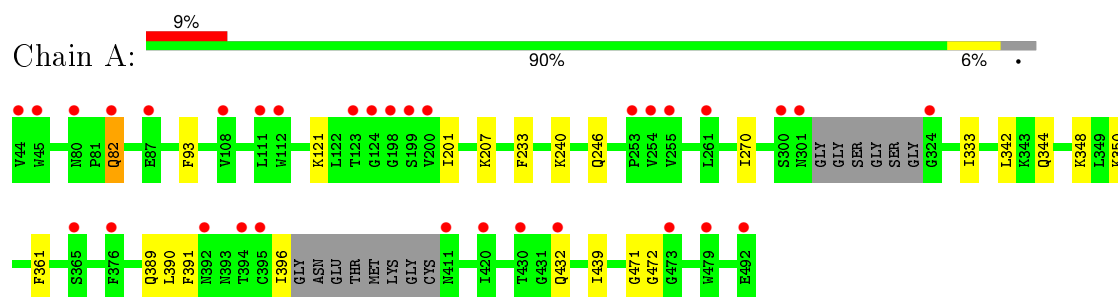
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	296	Total	O	0	0
			296	296		
5	C	183	Total	O	0	0
			183	183		

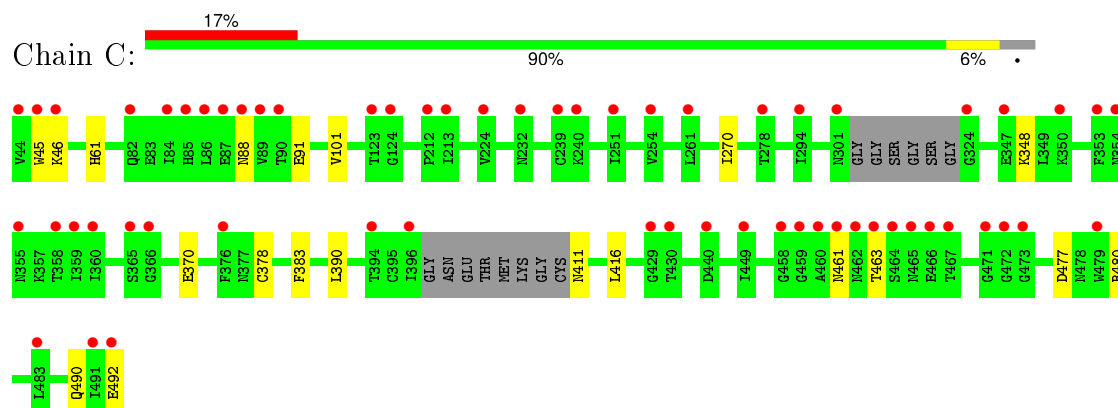
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: clade A/E 93TH057 HIV-1 gp120 core



- Molecule 1: clade A/E 93TH057 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	64.67Å 68.48Å 94.75Å 90.00° 91.60° 90.00°	Depositor
Resolution (Å)	33.70 – 1.80 37.70 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.3 (33.70-1.80) 89.9 (37.70-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.199 , 0.225 0.197 , 0.227	Depositor DCC
R_{free} test set	3784 reflections (5.76%)	DCC
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.2	EDS
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 74245 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6171	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, OLL, 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	0.22	0/2709	0.40	0/3678
1	C	0.21	0/2709	0.39	0/3678
All	All	0.21	0/5418	0.39	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 Too-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 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	0	2589	20	0
1	C	2654	0	2589	13	0
2	A	154	0	143	3	0
2	C	154	0	143	1	0
3	A	15	0	17	0	0
3	C	13	0	17	0	0
4	A	24	0	15	1	0
4	C	24	0	15	1	0
5	A	296	0	0	13	0
5	C	183	0	0	4	0
All	All	6171	0	5528	36	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 3.

All (36) 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:471:GLY:O	5:A:659:HOH:O	1.94	0.85
1:A:350:LYS:NZ	5:A:622:HOH:O	2.17	0.76
1:A:246:GLN:OE1	5:A:681:HOH:O	2.05	0.74
1:A:389:GLN:HG2	2:A:510:NAG:H81	1.70	0.72
1:A:240:LYS:O	5:A:766:HOH:O	2.11	0.68
1:A:344:GLN:OE1	5:A:682:HOH:O	2.12	0.67
4:A:513:OLL:H3	5:A:868:HOH:O	1.94	0.66
2:A:508:NAG:O6	5:A:874:HOH:O	2.14	0.66
1:C:270:ILE:O	1:C:348:LYS:NZ	2.31	0.63
1:A:432:GLN:OE1	5:A:886:HOH:O	2.15	0.63
1:A:333:ILE:HD13	1:A:390:LEU:HD21	1.82	0.62
1:A:342:LEU:HD23	1:A:396:ILE:HD11	1.83	0.60
1:A:121:LYS:HB2	1:A:201:ILE:HB	1.85	0.59
1:A:389:GLN:HG3	5:A:610:HOH:O	2.04	0.58
2:C:506:NAG:H5	5:C:742:HOH:O	2.04	0.57
1:A:270:ILE:HB	1:A:348:LYS:HG3	1.87	0.55
1:C:88:ASN:ND2	5:C:782:HOH:O	2.40	0.55
1:A:472:GLY:N	5:A:850:HOH:O	2.29	0.55
1:A:82:GLN:HE22	1:A:246:GLN:HG2	1.72	0.54
1:C:477:ASP:OD1	5:C:780:HOH:O	2.19	0.54
1:A:391:PHE:O	5:A:698:HOH:O	2.19	0.52
1:C:348:LYS:NZ	5:C:720:HOH:O	2.34	0.51
1:C:101:VAL:HG21	1:C:480:ARG:HG2	1.98	0.46
1:C:492:GLU:OE1	1:C:492:GLU:N	2.48	0.46
1:C:45:TRP:NE1	1:C:91:GLU:OE2	2.45	0.45
2:A:504:NAG:HN2	1:C:61:HIS:CG	2.37	0.43
1:A:348:LYS:HG2	5:A:801:HOH:O	2.18	0.43
1:C:46:LYS:NZ	1:C:490:GLN:OE1	2.51	0.43
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.82	0.43
1:C:378:CYS:HB3	1:C:383:PHE:CE1	2.55	0.42
1:C:390:LEU:HG	1:C:416:LEU:HD11	2.01	0.42
1:A:207:LYS:HD2	1:A:439:ILE:HG23	2.03	0.41
1:C:370:GLU:HG2	4:C:513:OLL:N14	2.36	0.40
1:A:472:GLY:HA3	5:A:659:HOH:O	2.21	0.40
1:A:361:PHE:HB3	1:A:391:PHE:HB3	2.02	0.40
1:C:390:LEU:HA	1:C:390:LEU:HD23	1.94	0.40

There are no symmetry-related clashes.

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%)	326 (98%)	7 (2%)	0	100	100
1	C	333/353 (94%)	321 (96%)	12 (4%)	0	100	100
All	All	666/706 (94%)	647 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	94	94
1	C	303/311 (97%)	300 (99%)	3 (1%)	82	77
All	All	606/622 (97%)	602 (99%)	4 (1%)	88	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	C	411	ASN
1	C	461	ASN
1	C	463	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	344	GLN
1	C	61	HIS
1	C	80	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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	14,14,15	0.48	0	15,19,21	0.77	0
2	NAG	A	502	1	14,14,15	0.49	0	15,19,21	0.69	0
2	NAG	A	503	1	14,14,15	0.46	0	15,19,21	0.86	0
2	NAG	A	504	1	14,14,15	0.50	0	15,19,21	0.60	0
2	NAG	A	505	1	14,14,15	0.50	0	15,19,21	0.81	0
2	NAG	A	506	1	14,14,15	0.47	0	15,19,21	0.86	0
2	NAG	A	507	1	14,14,15	0.51	0	15,19,21	0.83	1 (6%)
2	NAG	A	508	1	14,14,15	0.54	0	15,19,21	0.79	0
2	NAG	A	509	1	14,14,15	0.49	0	15,19,21	0.70	0
2	NAG	A	510	1	14,14,15	0.46	0	15,19,21	0.85	0
2	NAG	A	511	1	14,14,15	0.48	0	15,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EPE	A	512	-	14,15,15	0.34	0	18,20,20	1.89	5 (27%)
4	0LL	A	513	-	25,26,26	1.30	5 (20%)	32,37,37	2.71	10 (31%)
2	NAG	C	501	1	14,14,15	0.47	0	15,19,21	0.78	1 (6%)
2	NAG	C	502	1	14,14,15	0.51	0	15,19,21	0.70	0
2	NAG	C	503	1	14,14,15	0.43	0	15,19,21	0.97	1 (6%)
2	NAG	C	504	1	14,14,15	0.51	0	15,19,21	0.73	0
2	NAG	C	505	1	14,14,15	0.46	0	15,19,21	0.79	0
2	NAG	C	506	1	14,14,15	0.48	0	15,19,21	0.67	0
2	NAG	C	507	1	14,14,15	0.50	0	15,19,21	0.65	0
2	NAG	C	508	1	14,14,15	0.48	0	15,19,21	0.94	1 (6%)
2	NAG	C	509	1	14,14,15	0.49	0	15,19,21	0.74	0
2	NAG	C	510	1	14,14,15	0.51	0	15,19,21	0.62	0
2	NAG	C	511	1	14,14,15	0.49	0	15,19,21	0.63	0
3	EPE	C	512	-	11,13,15	0.39	0	14,15,20	1.65	4 (28%)
4	0LL	C	513	-	25,26,26	1.40	6 (24%)	32,37,37	2.63	9 (28%)

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	0LL	A	513	-	-	0/12/24/24	0/3/3/3
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-	-	0/6/17/19	0/1/1/1
4	OLL	C	513	-	-	0/12/24/24	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	513	OLL	C18-C15	2.00	1.42	1.39
4	C	513	OLL	C15-N14	2.03	1.45	1.41
4	A	513	OLL	C18-C15	2.09	1.42	1.39
4	A	513	OLL	C13-C12	2.10	1.56	1.53
4	A	513	OLL	C12-N11	2.12	1.38	1.34
4	A	513	OLL	C03-C07	2.12	1.53	1.51
4	C	513	OLL	C03-C07	2.22	1.53	1.51
4	C	513	OLL	C13-N14	2.50	1.41	1.35
4	C	513	OLL	C12-N11	2.50	1.39	1.34
4	A	513	OLL	C13-N14	2.62	1.41	1.35
4	C	513	OLL	C13-C12	2.70	1.57	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	513	OLL	C08-C07-N11	-5.70	106.41	114.20
4	A	513	OLL	O16-C13-C12	-5.44	114.38	121.31
4	C	513	OLL	O16-C13-C12	-5.40	114.43	121.31
4	C	513	OLL	C08-C07-N11	-3.51	109.42	114.20
4	C	513	OLL	O17-C12-C13	-2.78	117.76	121.31
4	A	513	OLL	O17-C12-C13	-2.76	117.79	121.31
4	C	513	OLL	C18-C15-C22	-2.64	116.53	119.69
3	A	512	EPE	C5-C6-N1	-2.51	106.14	110.63
4	A	513	OLL	C18-C15-C22	-2.45	116.75	119.69
4	A	513	OLL	C02-C03-C04	-2.14	118.04	120.78
4	C	513	OLL	C02-C03-C04	-2.10	118.09	120.78
3	C	512	EPE	C5-C6-N1	-2.07	106.91	110.63
2	C	501	NAG	C1-O5-C5	2.00	114.79	112.25
2	C	508	NAG	C1-O5-C5	2.10	114.91	112.25
2	C	503	NAG	C1-O5-C5	2.11	114.92	112.25
3	A	512	EPE	C7-N4-C5	2.15	116.77	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	513	0LL	C03-C07-N11	2.22	117.44	114.36
4	C	513	0LL	C04-C03-C07	2.23	112.09	110.39
3	A	512	EPE	C7-N4-C3	2.28	117.12	111.27
3	C	512	EPE	C7-N4-C3	2.30	117.17	111.27
3	C	512	EPE	C7-N4-C5	2.30	117.17	111.27
2	A	507	NAG	C1-O5-C5	2.31	115.17	112.25
4	A	513	0LL	C15-C22-C21	2.31	120.53	118.82
4	A	513	0LL	C07-N11-C12	2.48	126.09	122.05
4	C	513	0LL	C07-N11-C12	3.80	128.26	122.05
3	A	512	EPE	O1S-S-C10	3.81	110.15	106.91
3	C	512	EPE	C5-N4-C3	4.21	118.03	108.90
3	A	512	EPE	C5-N4-C3	4.62	118.91	108.90
4	C	513	0LL	C13-C12-N11	7.49	119.87	113.34
4	A	513	0LL	C13-C12-N11	7.73	120.08	113.34
4	A	513	0LL	C12-C13-N14	7.79	125.00	112.30
4	C	513	0LL	C12-C13-N14	8.06	125.44	112.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	NAG	1	0
2	A	508	NAG	1	0
2	A	510	NAG	1	0
4	A	513	0LL	1	0
2	C	506	NAG	1	0
4	C	513	0LL	1	0

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

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%)	0.62	32 (9%)	11 8	17, 29, 61, 90	0
1	C	339/353 (96%)	1.05	60 (17%)	2 1	21, 43, 83, 111	0
All	All	678/706 (96%)	0.83	92 (13%)	4 3	17, 35, 75, 111	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	44	VAL	9.5
1	A	124	GLY	8.9
1	C	492	GLU	8.3
1	C	460	ALA	8.0
1	C	89	VAL	7.2
1	A	492	GLU	6.6
1	A	44	VAL	6.4
1	C	462	ASN	6.3
1	A	301	ASN	6.0
1	A	198	GLY	5.9
1	A	199	SER	5.8
1	C	491	ILE	5.7
1	C	396	ILE	5.5
1	C	45	TRP	5.3
1	A	123	THR	5.3
1	C	465	ASN	5.2
1	C	458	GLY	5.1
1	C	301	ASN	5.1
1	C	464	SER	4.9
1	C	354	ASN	4.7
1	C	461	ASN	4.7
1	C	355	ASN	4.7
1	C	86	LEU	4.3
1	C	87	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	84	ILE	4.3
1	C	123	THR	4.2
1	A	394	THR	4.1
1	C	261	LEU	4.1
1	A	430	THR	3.9
1	C	358	THR	3.9
1	C	466	GLU	3.8
1	C	459	GLY	3.8
1	C	85	HIS	3.8
1	C	82	GLN	3.7
1	A	255	VAL	3.6
1	C	88	ASN	3.6
1	C	90	THR	3.5
1	A	395	CYS	3.5
1	A	392	ASN	3.4
1	A	200	VAL	3.4
1	C	359	ILE	3.4
1	A	479	TRP	3.3
1	A	254	VAL	3.3
1	C	463	THR	3.3
1	C	254	VAL	3.3
1	A	473	GLY	3.2
1	C	124	GLY	3.2
1	A	45	TRP	3.1
1	C	360	ILE	3.1
1	A	108	VAL	3.1
1	C	430	THR	3.0
1	C	429	GLY	3.0
1	A	365	SER	3.0
1	C	251	ILE	2.9
1	A	80	ASN	2.9
1	C	471	GLY	2.8
1	C	278	THR	2.8
1	C	324	GLY	2.8
1	C	473	GLY	2.8
1	A	253	PRO	2.7
1	A	411	ASN	2.7
1	C	239	CYS	2.6
1	C	394	THR	2.6
1	C	353	PHE	2.6
1	C	347	GLU	2.5
1	C	472	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	261	LEU	2.5
1	C	213	ILE	2.5
1	C	350	LYS	2.5
1	A	324	GLY	2.4
1	C	483	LEU	2.4
1	C	240	LYS	2.4
1	C	224	VAL	2.3
1	A	111	LEU	2.3
1	C	212	PRO	2.3
1	A	87	GLU	2.3
1	A	82	GLN	2.3
1	C	366	GLY	2.2
1	C	46	LYS	2.2
1	C	365	SER	2.2
1	C	467	THR	2.2
1	A	300	SER	2.2
1	C	232	ASN	2.1
1	A	376	PHE	2.1
1	A	112	TRP	2.1
1	C	449	ILE	2.1
1	A	432	GLN	2.0
1	C	376	PHE	2.0
1	C	479	TRP	2.0
1	A	420	ILE	2.0
1	C	294	ILE	2.0
1	C	440	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	OLL	C	513	24/24	0.74	0.33	4.04	32,77,83,86	0
2	NAG	A	506	14/15	0.93	0.14	3.48	31,46,60,61	0
2	NAG	A	507	14/15	0.75	0.29	3.23	45,60,74,83	0
3	EPE	C	512	13/15	0.94	0.14	3.21	23,25,32,37	0
4	OLL	A	513	24/24	0.77	0.27	2.92	37,57,74,78	0
2	NAG	C	511	14/15	0.76	0.21	2.22	37,53,63,69	0
2	NAG	C	506	14/15	0.90	0.14	1.87	34,50,63,64	0
2	NAG	C	501	14/15	0.91	0.19	1.61	48,61,71,74	0
2	NAG	A	505	14/15	0.91	0.15	1.20	28,40,50,58	0
2	NAG	C	505	14/15	0.84	0.19	1.10	34,45,49,50	0
3	EPE	A	512	15/15	0.97	0.16	0.71	19,22,27,33	0
2	NAG	C	503	14/15	0.97	0.15	-0.12	19,23,27,27	0
2	NAG	A	508	14/15	0.87	0.14	-0.35	26,44,60,70	0
2	NAG	A	501	14/15	0.91	0.08	-0.94	34,45,54,57	0
2	NAG	A	503	14/15	0.94	0.10	-0.96	19,26,30,36	0
2	NAG	A	511	14/15	0.47	0.42	-	73,84,96,97	0
2	NAG	C	509	14/15	0.89	0.18	-	41,50,61,64	0
2	NAG	C	504	14/15	0.71	0.24	-	63,75,81,82	0
2	NAG	A	504	14/15	0.92	0.15	-	22,40,49,49	0
2	NAG	C	502	14/15	0.55	0.49	-	79,100,108,108	0
2	NAG	A	509	14/15	0.93	0.10	-	33,47,52,62	0
2	NAG	C	508	14/15	0.63	0.68	-	82,89,100,105	0
2	NAG	C	507	14/15	0.78	0.38	-	63,83,94,96	0
2	NAG	C	510	14/15	0.64	0.34	-	70,80,92,98	0
2	NAG	A	510	14/15	0.72	0.50	-	93,99,107,108	0
2	NAG	A	502	14/15	0.66	0.35	-	48,69,79,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.