



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2017 – 08:29 PM EDT

PDB ID : 4DVT
Title : Crystal structure of clade A/E 93TH057 HIV-1 gp120 core in complex with AS-II-37
Authors : Kwon, Y.D.; Kwong, P.D.
Deposited on : 2012-02-23
Resolution : 2.40 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029077

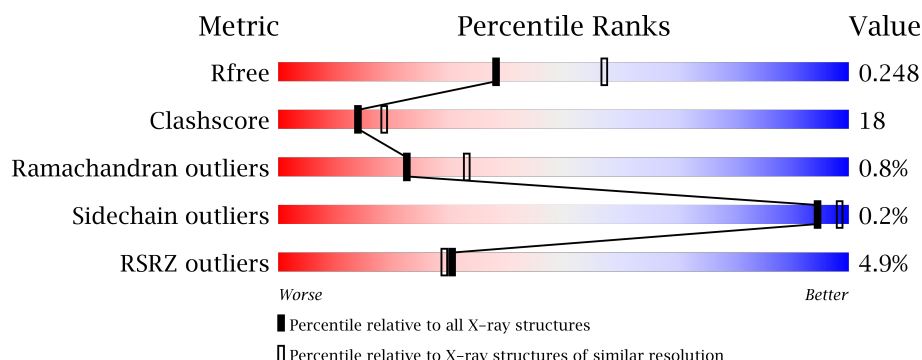
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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>3%</div> <div>69%</div> <div>27%</div> <div>••</div> </div>
1	B	353	<div> <div>7%</div> <div>61%</div> <div>34%</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	505	-	-	-	X
2	NAG	A	506	-	-	-	X
2	NAG	A	507	-	-	-	X
2	NAG	A	509	X	-	-	-
2	NAG	A	510	-	-	-	X
2	NAG	A	511	-	-	-	X
2	NAG	B	510	-	-	-	X
2	NAG	B	511	-	-	-	X
3	0LZ	A	512	-	-	-	X
3	0LZ	B	512	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5837 atoms, of which 34 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.

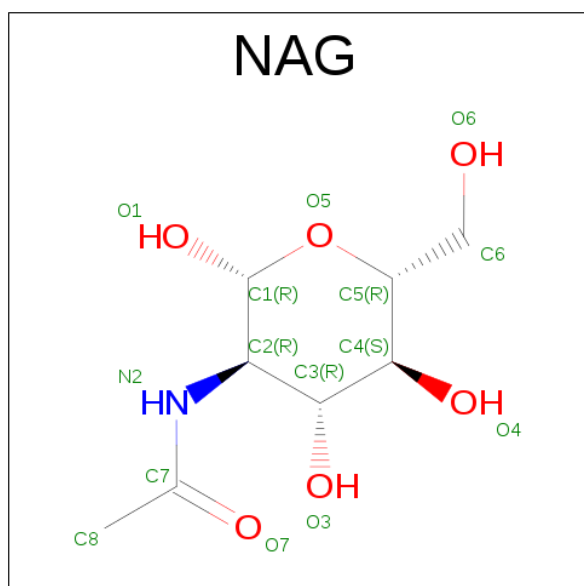
- Molecule 1 is a protein called clade A/E 93TH057 HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2654	1666	460	507	21			
1	B	339	Total	C	N	O	S	0	0	0
			2654	1666	460	507	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9
B	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



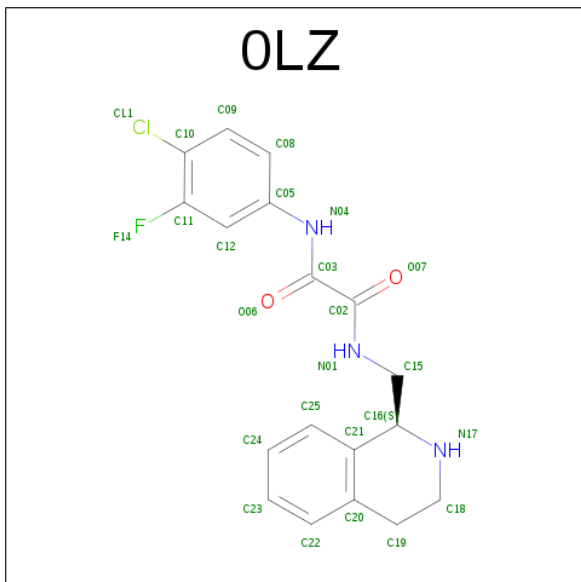
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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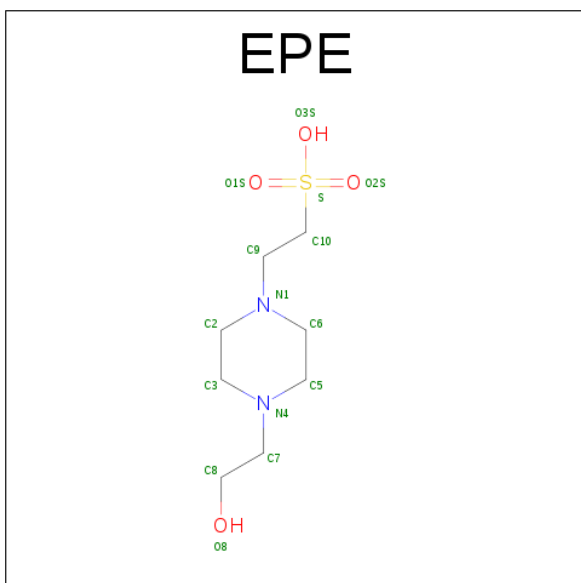
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1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

- Molecule 3 is N-(4-chloro-3-fluorophenyl)-N'-[(1S)-1,2,3,4-tetrahydroisoquinolin-1-ylmethyl]ethanediamide (three-letter code: 0LZ) (formula: $C_{18}H_{17}ClFN_3O_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	H	N	O	0	0
			42	18	1	1	17	3	2		
3	B	1	Total	C	Cl	F	H	N	O	0	0
			42	18	1	1	17	3	2		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

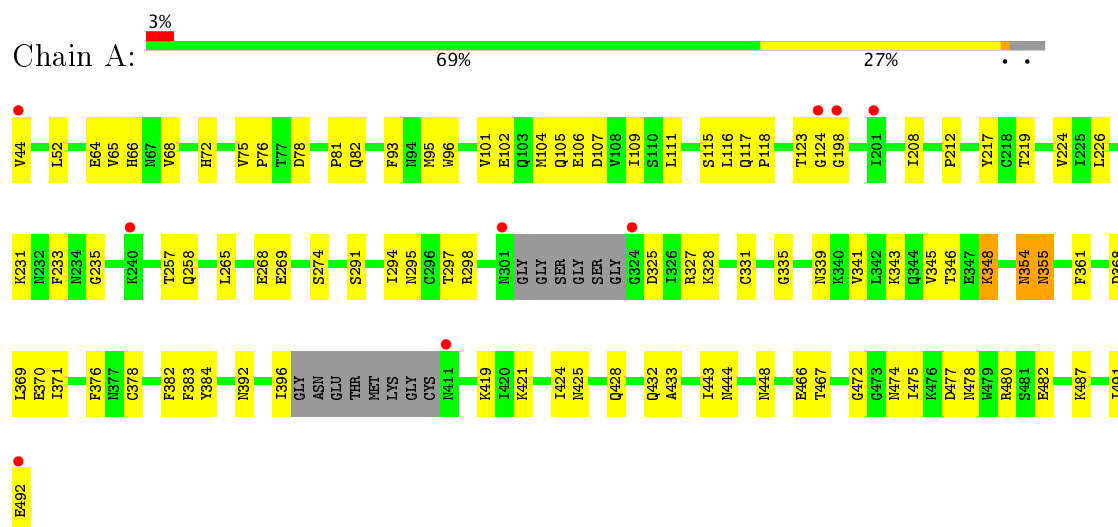
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	72	Total	O	0	0
			72	72		
5	B	35	Total	O	0	0
			35	35		

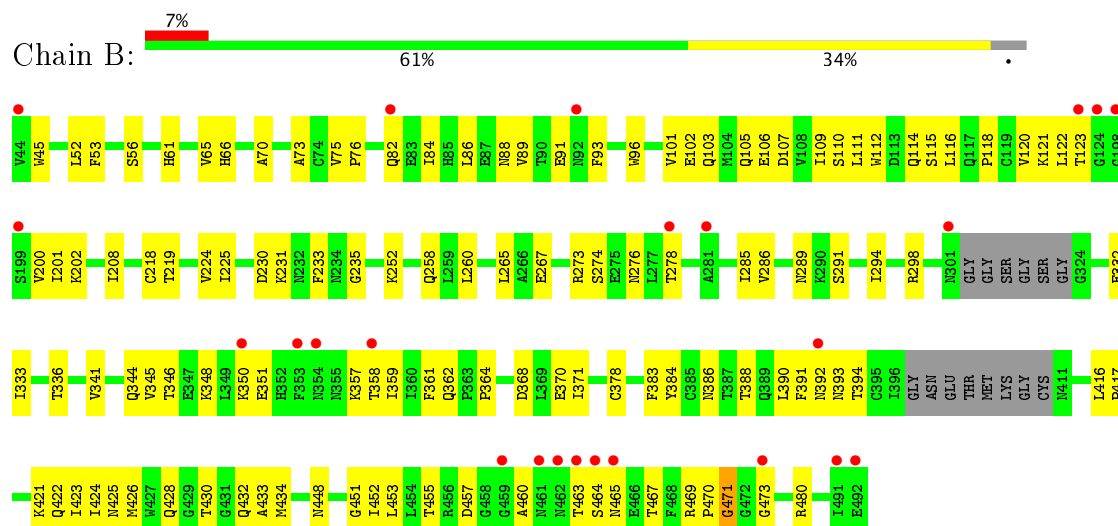
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 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: 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	64.81Å 68.40Å 93.99Å 90.00° 91.94° 90.00°	Depositor
Resolution (Å)	28.19 – 2.40 46.97 – 2.43	Depositor EDS
% Data completeness (in resolution range)	87.2 (28.19-2.40) 84.3 (46.97-2.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.196 , 0.248 0.187 , 0.248	Depositor DCC
R_{free} test set	1265 reflections (4.83%)	DCC
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5837	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% 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, NAG, 0LZ

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	0.24	1/2709 (0.0%)	0.39	1/3678 (0.0%)
1	B	0.20	0/2709	0.37	0/3678
All	All	0.22	1/5418 (0.0%)	0.38	1/7356 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	ASN	C-N	-6.39	1.19	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	ASN	O-C-N	5.03	130.75	122.70

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	0	2588	89	0
1	B	2654	0	2588	108	0
2	A	154	0	143	9	0
2	B	154	0	143	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	25	17	17	2	0
3	B	25	17	17	1	0
4	A	15	0	17	3	0
4	B	15	0	17	3	0
5	A	72	0	0	4	0
5	B	35	0	0	4	0
All	All	5803	34	5530	197	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 18.

All (197) 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:224:VAL:HG22	1:A:491:ILE:HD11	1.45	0.96
1:A:480:ARG:NH2	5:A:619:HOH:O	1.98	0.94
1:A:65:VAL:HG11	1:A:208:ILE:HD12	1.51	0.92
1:B:289:ASN:O	5:B:631:HOH:O	1.92	0.88
1:A:343:LYS:HD3	1:A:396:ILE:HG23	1.61	0.83
1:B:378:CYS:HB3	1:B:383:PHE:CE1	2.13	0.83
1:B:423:ILE:C	1:B:424:ILE:HD12	2.08	0.74
1:B:428:GLN:N	1:B:428:GLN:OE1	2.21	0.73
1:A:82:GLN:OE1	1:A:82:GLN:N	2.23	0.72
2:A:508:NAG:H82	1:B:252:LYS:HE3	1.72	0.71
1:B:426:MET:HE3	1:B:433:ALA:HB2	1.72	0.70
1:A:477:ASP:OD1	1:A:480:ARG:NH1	2.24	0.70
1:A:231:LYS:HD3	1:A:268:GLU:OE2	1.92	0.70
1:A:65:VAL:CG1	1:A:208:ILE:HD12	2.20	0.70
1:B:122:LEU:HD22	1:B:200:VAL:HG22	1.72	0.69
1:B:260:LEU:HD12	1:B:451:GLY:HA3	1.73	0.69
1:A:428:GLN:OE1	1:A:428:GLN:N	2.24	0.69
1:B:201:ILE:HD12	1:B:201:ILE:N	2.10	0.67
1:B:332:GLU:C	1:B:333:ILE:HD12	2.15	0.67
1:B:103:GLN:HB3	4:B:513:EPE:O8	1.95	0.67
1:A:384:TYR:OH	1:A:424:ILE:HG23	1.95	0.65
1:B:107:ASP:OD2	4:B:513:EPE:H72	1.95	0.65
1:B:425:ASN:OD1	1:B:432:GLN:HG2	1.96	0.65
1:A:65:VAL:CG1	1:A:115:SER:HB2	2.27	0.65
1:A:107:ASP:OD1	4:A:513:EPE:H51	1.98	0.64
1:A:448:ASN:HD22	2:A:511:NAG:H83	1.62	0.63
1:A:354:ASN:OD1	2:A:508:NAG:H81	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:LEU:HD11	1:B:416:LEU:HD11	1.80	0.62
1:A:52:LEU:CD2	1:A:219:THR:HG22	2.30	0.62
1:B:333:ILE:HD12	1:B:333:ILE:N	2.15	0.62
1:A:224:VAL:CG2	1:A:491:ILE:HD11	2.26	0.62
1:A:355:ASN:ND2	2:A:508:NAG:H83	2.15	0.61
1:B:111:LEU:HD23	1:B:111:LEU:O	2.01	0.61
1:B:82:GLN:NE2	1:B:84:ILE:HD11	2.16	0.61
1:B:233:PHE:CE2	1:B:235:GLY:HA2	2.35	0.61
1:B:116:LEU:CD2	1:B:208:ILE:HD11	2.29	0.61
1:B:45:TRP:NE1	1:B:91:GLU:OE2	2.33	0.61
1:A:111:LEU:HD23	1:A:111:LEU:C	2.21	0.60
1:B:101:VAL:HG21	1:B:480:ARG:HG2	1.83	0.60
1:A:369:LEU:HD12	1:A:421:LYS:HE3	1.82	0.60
2:A:508:NAG:C8	1:B:252:LYS:HE3	2.32	0.59
1:B:426:MET:CE	1:B:433:ALA:HB2	2.32	0.59
1:A:116:LEU:HD21	1:A:208:ILE:HD11	1.84	0.59
1:B:378:CYS:HB3	1:B:383:PHE:CD1	2.38	0.59
1:B:88:ASN:ND2	5:B:634:HOH:O	2.35	0.58
1:A:482:GLU:OE2	5:A:635:HOH:O	2.16	0.58
1:A:432:GLN:OE1	1:A:432:GLN:N	2.37	0.58
1:B:86:LEU:HB3	1:B:89:VAL:HG21	1.85	0.58
1:B:105:GLN:O	1:B:109:ILE:HG13	2.03	0.58
1:B:116:LEU:HD21	1:B:208:ILE:HD11	1.84	0.58
1:B:53:PHE:CZ	1:B:218:CYS:HB2	2.39	0.57
1:B:73:ALA:O	5:B:623:HOH:O	2.17	0.57
1:A:382:PHE:CG	1:A:424:ILE:CD1	2.88	0.57
1:B:453:LEU:O	1:B:471:GLY:N	2.34	0.57
1:A:68:VAL:O	1:A:72:HIS:ND1	2.38	0.56
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.87	0.56
1:A:123:THR:O	1:A:198:GLY:N	2.34	0.56
1:A:335:GLY:O	1:A:339:ASN:ND2	2.38	0.56
1:B:219:THR:HG23	1:B:225:ILE:CG1	2.36	0.56
1:A:346:THR:CG2	1:A:361:PHE:HE2	2.19	0.55
1:B:102:GLU:O	1:B:106:GLU:HG3	2.06	0.55
1:B:265:LEU:HD11	1:B:291:SER:OG	2.07	0.55
1:B:364:PRO:HG3	1:B:470:PRO:HG2	1.86	0.55
2:A:504:NAG:HN2	1:B:61:HIS:CG	2.24	0.55
1:A:265:LEU:HD11	1:A:291:SER:OG	2.06	0.55
1:B:370:GLU:N	1:B:370:GLU:OE1	2.35	0.55
1:A:111:LEU:HD23	1:A:111:LEU:O	2.07	0.55
1:B:386:ASN:HD22	2:B:509:NAG:H83	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:VAL:HG12	1:A:115:SER:HB2	1.88	0.55
1:B:65:VAL:CG1	1:B:115:SER:HB2	2.37	0.55
1:B:122:LEU:CD2	1:B:200:VAL:HG22	2.37	0.55
1:B:286:VAL:HB	1:B:452:ILE:HB	1.89	0.54
1:B:344:GLN:NE2	2:B:505:NAG:H5	2.21	0.54
1:B:386:ASN:HD22	2:B:509:NAG:C8	2.20	0.54
1:B:358:THR:OG1	1:B:465:ASN:OD1	2.24	0.54
1:B:424:ILE:HD12	1:B:424:ILE:N	2.23	0.54
2:A:508:NAG:C8	1:B:252:LYS:CE	2.86	0.54
1:B:457:ASP:OD2	1:B:467:THR:OG1	2.24	0.53
1:A:295:ASN:O	1:A:331:CYS:HA	2.08	0.53
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.73	0.53
1:B:230:ASP:HB2	1:B:233:PHE:HB2	1.90	0.53
1:B:358:THR:OG1	1:B:464:SER:O	2.26	0.53
1:A:348:LYS:HB2	1:A:348:LYS:NZ	2.23	0.53
1:A:341:VAL:O	1:A:345:VAL:HG23	2.09	0.52
1:A:44:VAL:HG13	1:A:492:GLU:HB3	1.92	0.52
1:A:269:GLU:HG2	2:A:505:NAG:H61	1.92	0.52
1:B:384:TYR:CE1	1:B:421:LYS:HB2	2.45	0.52
1:A:117:GLN:OE1	1:A:117:GLN:HA	2.10	0.52
1:B:65:VAL:HG23	1:B:66:HIS:N	2.24	0.52
1:A:224:VAL:HG22	1:A:491:ILE:CD1	2.29	0.51
1:A:466:GLU:HA	5:A:604:HOH:O	2.11	0.51
1:A:107:ASP:OD2	4:A:513:EPE:H82	2.10	0.51
1:B:111:LEU:HD23	1:B:111:LEU:C	2.31	0.51
1:B:291:SER:HB3	1:B:448:ASN:HB3	1.91	0.51
1:B:357:LYS:HE3	1:B:463:THR:O	2.11	0.51
1:B:425:ASN:HB2	5:B:633:HOH:O	2.11	0.50
1:A:104:MET:HG3	1:A:217:TYR:OH	2.10	0.50
1:A:325:ASP:HB3	1:A:328:LYS:HG3	1.91	0.50
1:A:475:ILE:O	1:A:478:ASN:HB2	2.11	0.50
1:A:325:ASP:CG	1:A:328:LYS:HG3	2.32	0.50
1:B:294:ILE:O	1:B:294:ILE:HG23	2.11	0.49
1:B:93:PHE:HB2	1:B:233:PHE:HZ	1.77	0.49
1:A:378:CYS:HB3	1:A:383:PHE:CE1	2.48	0.49
1:A:491:ILE:HD12	1:A:491:ILE:N	2.27	0.49
1:A:327:ARG:O	1:A:419:LYS:HA	2.13	0.48
1:B:473:GLY:HA3	3:B:512:OLZ:H13	1.96	0.48
1:A:424:ILE:HG22	1:A:425:ASN:N	2.28	0.48
1:B:219:THR:HG23	1:B:225:ILE:HG13	1.94	0.48
1:B:112:TRP:CE3	1:B:116:LEU:HD13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:LYS:HG2	1:B:123:THR:HG23	1.95	0.48
1:B:348:LYS:HD3	1:B:351:GLU:OE2	2.13	0.48
1:A:65:VAL:HB	1:A:115:SER:OG	2.14	0.48
1:A:64:GLU:OE1	1:A:66:HIS:N	2.47	0.48
1:B:358:THR:N	1:B:464:SER:O	2.46	0.48
1:B:341:VAL:O	1:B:345:VAL:HG23	2.14	0.48
1:A:102:GLU:O	1:A:106:GLU:HG3	2.14	0.48
1:B:276:ASN:OD1	1:B:278:THR:OG1	2.25	0.47
1:A:369:LEU:CD1	1:A:421:LYS:HE3	2.44	0.47
1:B:364:PRO:HD3	1:B:470:PRO:CG	2.45	0.47
1:B:358:THR:OG1	1:B:465:ASN:HA	2.14	0.47
1:A:346:THR:HG22	1:A:361:PHE:HE2	1.80	0.47
1:B:200:VAL:C	1:B:201:ILE:HD12	2.34	0.47
1:A:105:GLN:O	1:A:109:ILE:HG13	2.15	0.47
1:B:118:PRO:HG3	1:B:433:ALA:HB1	1.96	0.47
1:B:75:VAL:HB	1:B:76:PRO:HD2	1.96	0.47
1:A:64:GLU:OE2	1:A:66:HIS:ND1	2.39	0.47
1:B:346:THR:HG23	1:B:359:ILE:HB	1.97	0.46
1:A:116:LEU:CD2	1:A:208:ILE:HD11	2.43	0.46
1:B:231:LYS:HE3	1:B:267:GLU:OE1	2.15	0.46
1:A:348:LYS:HZ2	1:A:348:LYS:HB2	1.79	0.46
1:B:110:SER:O	1:B:114:GLN:HG3	2.15	0.46
1:B:96:TRP:CZ2	1:B:274:SER:HA	2.51	0.46
1:A:75:VAL:HB	1:A:76:PRO:HD2	1.98	0.46
1:B:386:ASN:HB3	1:B:417:PRO:HG2	1.98	0.46
1:B:350:LYS:HG2	1:B:357:LYS:O	2.15	0.45
1:B:350:LYS:HZ2	1:B:359:ILE:HG12	1.81	0.45
1:B:56:SER:OG	1:B:70:ALA:HB1	2.16	0.45
1:A:368:ASP:HB3	1:A:370:GLU:OE1	2.16	0.45
1:A:78:ASP:O	1:A:81:PRO:HD3	2.17	0.45
1:B:368:ASP:O	1:B:371:ILE:HG22	2.17	0.45
1:A:66:HIS:CD2	1:A:212:PRO:HA	2.52	0.45
1:A:297:THR:HA	1:A:443:ILE:O	2.17	0.45
1:B:112:TRP:CD2	1:B:116:LEU:HD12	2.51	0.45
1:B:448:ASN:HD22	2:B:511:NAG:H83	1.81	0.45
1:A:474:ASN:HB2	3:A:512:OLZ:H16	1.98	0.45
1:A:96:TRP:CZ2	1:A:274:SER:HA	2.52	0.45
1:A:118:PRO:HG3	1:A:433:ALA:HB1	1.98	0.44
1:A:257:THR:O	1:A:258:GLN:HB2	2.17	0.44
1:A:343:LYS:O	1:A:346:THR:OG1	2.30	0.44
1:B:258:GLN:HG2	1:B:470:PRO:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:THR:HG22	2:B:507:NAG:H61	2.00	0.44
1:B:424:ILE:HG22	1:B:425:ASN:N	2.32	0.44
1:B:103:GLN:OE1	4:B:513:EPE:O8	2.18	0.44
1:A:346:THR:HG22	1:A:361:PHE:CE2	2.53	0.44
1:A:233:PHE:CE2	1:A:235:GLY:HA2	2.53	0.44
1:B:65:VAL:HG12	1:B:115:SER:HB2	1.98	0.44
1:A:64:GLU:OE1	1:A:66:HIS:HB2	2.18	0.44
1:B:392:ASN:C	1:B:394:THR:H	2.20	0.44
1:A:376:PHE:HA	3:A:512:OLZ:CL1	2.55	0.43
1:B:294:ILE:HG13	1:B:333:ILE:HD11	2.00	0.43
1:A:371:ILE:HD12	1:A:472:GLY:O	2.18	0.43
1:A:467:THR:N	5:A:604:HOH:O	2.18	0.43
1:B:273:ARG:HB2	1:B:285:ILE:HB	1.99	0.43
1:B:364:PRO:CG	1:B:470:PRO:HG2	2.48	0.43
1:A:325:ASP:CB	1:A:328:LYS:HG3	2.47	0.43
1:B:52:LEU:CD2	1:B:219:THR:HG22	2.49	0.43
1:B:116:LEU:HD23	1:B:208:ILE:HD11	1.98	0.42
1:A:298:ARG:C	1:A:298:ARG:HD2	2.40	0.42
1:B:86:LEU:HB3	1:B:89:VAL:CG2	2.48	0.42
1:A:226:LEU:HD12	1:A:487:LYS:HE3	2.02	0.42
1:A:44:VAL:CG1	1:A:492:GLU:HB3	2.49	0.42
1:B:422:GLN:O	1:B:434:MET:HA	2.18	0.42
1:B:120:VAL:HG22	1:B:202:LYS:HG2	2.02	0.42
1:A:294:ILE:O	1:A:294:ILE:HG23	2.20	0.42
1:A:382:PHE:CB	1:A:424:ILE:HD11	2.49	0.42
1:B:361:PHE:HB3	1:B:391:PHE:HB3	2.01	0.42
1:B:455:THR:HG23	1:B:471:GLY:HA3	2.01	0.42
1:A:297:THR:HG22	1:A:444:ASN:CG	2.41	0.41
1:B:392:ASN:OD1	1:B:394:THR:HG23	2.20	0.41
1:B:224:VAL:HG12	1:B:225:ILE:N	2.35	0.41
1:A:95:MET:SD	1:A:235:GLY:HA3	2.60	0.41
1:A:392:ASN:HD22	2:A:510:NAG:H83	1.85	0.41
1:B:112:TRP:CE3	1:B:116:LEU:CD1	3.03	0.41
1:B:65:VAL:HG11	1:B:115:SER:HB2	2.03	0.41
1:B:362:GLN:HB3	1:B:469:ARG:NH1	2.36	0.41
1:A:297:THR:HG22	1:A:444:ASN:OD1	2.21	0.41
1:A:325:ASP:HB3	1:A:328:LYS:CG	2.50	0.41
1:B:298:ARG:C	1:B:298:ARG:HD2	2.41	0.41
1:A:52:LEU:HD21	1:A:219:THR:HG22	2.03	0.41
1:B:258:GLN:CG	1:B:470:PRO:HB2	2.51	0.41
1:A:65:VAL:HG23	1:A:66:HIS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:VAL:HG23	1:B:66:HIS:H	1.86	0.40
1:A:297:THR:HG22	1:A:444:ASN:CB	2.51	0.40
1:B:116:LEU:HD23	1:B:208:ILE:CD1	2.51	0.40
1:B:392:ASN:O	1:B:394:THR:N	2.55	0.40
1:A:107:ASP:CG	4:A:513:EPE:H51	2.42	0.40
1:B:388:THR:HG21	2:B:509:NAG:H62	2.03	0.40

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%)	314 (94%)	18 (5%)	1 (0%)	44	60
1	B	333/353 (94%)	306 (92%)	23 (7%)	4 (1%)	15	21
All	All	666/706 (94%)	620 (93%)	41 (6%)	5 (1%)	22	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	430	THR
1	A	124	GLY
1	B	460	ALA
1	B	393	ASN
1	B	471	GLY

5.3.2 Protein sidechains [i](#)

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	98
1	B	303/311 (97%)	303 (100%)	0	100	100
All	All	606/622 (97%)	605 (100%)	1 (0%)	94	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	465	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	0.53	0	15,19,21	0.51	0
2	NAG	A	502	1	14,14,15	0.53	0	15,19,21	0.58	0
2	NAG	A	503	1	14,14,15	0.52	0	15,19,21	0.62	0
2	NAG	A	504	1	14,14,15	0.51	0	15,19,21	0.56	0
2	NAG	A	505	1	14,14,15	0.51	0	15,19,21	0.58	0
2	NAG	A	506	1	14,14,15	0.54	0	15,19,21	0.56	0
2	NAG	A	507	1	14,14,15	0.53	0	15,19,21	0.57	0
2	NAG	A	508	1	14,14,15	0.56	0	15,19,21	0.50	0
2	NAG	A	509	1	14,14,15	0.54	0	15,19,21	0.55	0
2	NAG	A	510	1	14,14,15	0.53	0	15,19,21	0.56	0
2	NAG	A	511	1	14,14,15	0.50	0	15,19,21	0.71	0
3	0LZ	A	512	-	25,27,27	1.51	5 (20%)	31,37,37	1.92	5 (16%)
4	EPE	A	513	-	15,15,15	0.79	1 (6%)	18,20,20	1.98	6 (33%)
2	NAG	B	501	1	14,14,15	0.52	0	15,19,21	0.61	0
2	NAG	B	502	1	14,14,15	0.51	0	15,19,21	0.71	0
2	NAG	B	503	1	14,14,15	0.49	0	15,19,21	0.79	0
2	NAG	B	504	1	14,14,15	0.50	0	15,19,21	0.62	0
2	NAG	B	505	1	14,14,15	0.52	0	15,19,21	0.54	0
2	NAG	B	506	1	14,14,15	0.54	0	15,19,21	0.60	0
2	NAG	B	507	1	14,14,15	0.51	0	15,19,21	0.59	0
2	NAG	B	508	1	14,14,15	0.53	0	15,19,21	0.58	0
2	NAG	B	509	1	14,14,15	0.51	0	15,19,21	0.62	0
2	NAG	B	510	1	14,14,15	0.52	0	15,19,21	0.65	0
2	NAG	B	511	1	14,14,15	0.51	0	15,19,21	0.71	0
3	0LZ	B	512	-	25,27,27	1.53	5 (20%)	31,37,37	1.93	5 (16%)
4	EPE	B	513	-	15,15,15	0.80	1 (6%)	18,20,20	2.02	6 (33%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1/1/5/7	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	0LZ	A	512	-	-	0/13/23/23	0/3/3/3
4	EPE	A	513	-	-	0/9/19/19	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1
2	NAG	B	503	1	-	0/6/23/26	0/1/1/1
2	NAG	B	504	1	-	0/6/23/26	0/1/1/1
2	NAG	B	505	1	-	0/6/23/26	0/1/1/1
2	NAG	B	506	1	-	0/6/23/26	0/1/1/1
2	NAG	B	507	1	-	0/6/23/26	0/1/1/1
2	NAG	B	508	1	-	0/6/23/26	0/1/1/1
2	NAG	B	509	1	-	0/6/23/26	0/1/1/1
2	NAG	B	510	1	-	0/6/23/26	0/1/1/1
2	NAG	B	511	1	-	0/6/23/26	0/1/1/1
3	0LZ	B	512	-	-	0/13/23/23	0/3/3/3
4	EPE	B	513	-	-	0/9/19/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	512	0LZ	C12-C11	2.05	1.41	1.37
3	B	512	0LZ	C12-C11	2.08	1.41	1.37
3	A	512	0LZ	C21-C16	2.48	1.54	1.52
4	A	513	EPE	C10-S	2.59	1.81	1.77
3	B	512	0LZ	C21-C16	2.60	1.54	1.52
4	B	513	EPE	C10-S	2.63	1.81	1.77
3	A	512	0LZ	C03-N04	2.91	1.42	1.35
3	B	512	0LZ	C03-N04	2.95	1.42	1.35
3	A	512	0LZ	C02-N01	3.38	1.39	1.33
3	A	512	0LZ	C03-C02	3.39	1.58	1.53
3	B	512	0LZ	C03-C02	3.41	1.58	1.53
3	B	512	0LZ	C02-N01	3.46	1.39	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	512	0LZ	O06-C03-C02	-3.77	116.77	121.31
3	B	512	0LZ	O06-C03-C02	-3.74	116.80	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	512	0LZ	C08-C05-C12	-2.38	116.86	119.66
3	B	512	0LZ	C08-C05-C12	-2.37	116.88	119.66
3	B	512	0LZ	O07-C02-C03	-2.15	118.72	121.31
3	A	512	0LZ	O07-C02-C03	-2.10	118.78	121.31
4	A	513	EPE	O1S-S-C10	2.62	109.04	106.79
4	B	513	EPE	O2S-S-C10	2.83	109.23	106.79
4	B	513	EPE	O1S-S-C10	2.88	109.27	106.79
4	B	513	EPE	O3S-S-C10	2.97	109.71	106.06
4	A	513	EPE	O3S-S-C10	3.00	109.74	106.06
4	A	513	EPE	C7-N4-C3	3.14	119.30	111.26
4	A	513	EPE	O2S-S-C10	3.16	109.51	106.79
4	B	513	EPE	C7-N4-C5	3.22	119.52	111.26
4	A	513	EPE	C7-N4-C5	3.39	119.94	111.26
4	B	513	EPE	C7-N4-C3	3.52	120.28	111.26
4	A	513	EPE	C5-N4-C3	4.02	117.97	108.87
4	B	513	EPE	C5-N4-C3	4.29	118.58	108.87
3	A	512	0LZ	C03-C02-N01	5.14	119.71	113.51
3	B	512	0LZ	C03-C02-N01	5.14	119.72	113.51
3	A	512	0LZ	C02-C03-N04	5.97	121.17	112.20
3	B	512	0LZ	C02-C03-N04	6.00	121.22	112.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	509	NAG	C1

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	NAG	1	0
2	A	505	NAG	1	0
2	A	508	NAG	5	0
2	A	510	NAG	1	0
2	A	511	NAG	1	0
3	A	512	0LZ	2	0
4	A	513	EPE	3	0
2	B	505	NAG	1	0
2	B	507	NAG	1	0
2	B	509	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	511	NAG	1	0
3	B	512	0LZ	1	0
4	B	513	EPE	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	355:ASN	C	357:LYS	N	1.19

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%)	-0.01	9 (2%) 55 52	45, 63, 105, 137	0
1	B	339/353 (96%)	0.44	24 (7%) 17 15	49, 80, 129, 190	0
All	All	678/706 (96%)	0.22	33 (4%) 30 29	45, 71, 120, 190	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	350	LYS	6.1
1	B	124	GLY	5.7
1	B	492	GLU	4.8
1	B	462	ASN	4.7
1	B	44	VAL	4.7
1	B	392	ASN	4.5
1	B	301	ASN	4.1
1	B	461	ASN	4.0
1	B	198	GLY	3.9
1	B	278	THR	3.7
1	A	492	GLU	3.5
1	A	198	GLY	3.5
1	B	463	THR	3.4
1	A	301	ASN	3.3
1	B	358	THR	3.1
1	B	123	THR	3.1
1	A	411	ASN	3.1
1	B	82	GLN	3.0
1	B	459	GLY	3.0
1	B	465	ASN	2.9
1	B	199	SER	2.9
1	A	124	GLY	2.9
1	A	44	VAL	2.7
1	B	473	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	354	ASN	2.4
1	A	324	GLY	2.3
1	B	464	SER	2.2
1	B	353	PHE	2.2
1	B	92	ASN	2.2
1	B	281	ALA	2.1
1	A	201	ILE	2.1
1	B	491	ILE	2.1
1	A	240	LYS	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(Å ²)	Q<0.9
2	NAG	A	510	14/15	0.60	0.44	7.83	117,161,177,181	0
2	NAG	A	506	14/15	0.89	0.25	5.29	74,89,97,99	0
3	0LZ	B	512	25/25	0.77	0.42	4.97	89,127,199,202	0
2	NAG	A	511	14/15	0.73	0.28	4.61	84,105,110,113	0
2	NAG	B	510	14/15	0.76	0.58	3.04	178,194,202,206	0
3	0LZ	A	512	25/25	0.89	0.23	2.76	64,98,152,156	0
2	NAG	A	507	14/15	0.86	0.24	2.51	76,97,122,132	0
2	NAG	B	511	14/15	0.81	0.25	2.27	92,101,106,112	0
2	NAG	A	505	14/15	0.92	0.19	2.24	58,69,92,99	0
2	NAG	B	501	14/15	0.83	0.24	1.26	87,93,100,100	0
4	EPE	A	513	15/15	0.95	0.21	1.26	49,62,81,97	0
2	NAG	B	506	14/15	0.88	0.17	1.19	66,88,101,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	EPE	B	513	15/15	0.96	0.18	0.52	42,70,84,99	0
2	NAG	A	501	14/15	0.91	0.15	0.14	69,83,95,97	0
2	NAG	A	508	14/15	0.91	0.16	-0.00	54,59,72,86	0
2	NAG	B	505	14/15	0.87	0.15	-0.66	79,104,114,115	0
2	NAG	B	503	14/15	0.94	0.14	-1.26	49,54,63,64	0
2	NAG	A	503	14/15	0.96	0.13	-1.46	46,62,67,68	0
2	NAG	A	509	14/15	0.87	0.16	-	76,94,99,99	0
2	NAG	A	504	14/15	0.91	0.14	-	70,84,92,94	0
2	NAG	B	504	14/15	0.75	0.45	-	100,108,117,118	0
2	NAG	B	507	14/15	0.73	0.32	-	69,112,127,128	0
2	NAG	B	508	14/15	0.59	0.69	-	132,147,157,158	0
2	NAG	B	509	14/15	0.79	0.21	-	86,103,111,119	0
2	NAG	B	502	14/15	0.76	0.40	-	115,125,147,147	0
2	NAG	A	502	14/15	0.62	0.56	-	120,130,137,139	0

6.5 Other polymers [i](#)

There are no such residues in this entry.