



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:07 AM UTC

PDB ID : 7SX7 / pdb_00007sx7
Title : Crystal structure of broadly neutralizing antibody N49P9.3-FR3-3 Fab in complex with HIV-1 Clade A/E strain 93TH057 gp120 core
Authors : Tolbert, W.D.; Pazgier, M.
Deposited on : 2021-11-22
Resolution : 2.15 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

<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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

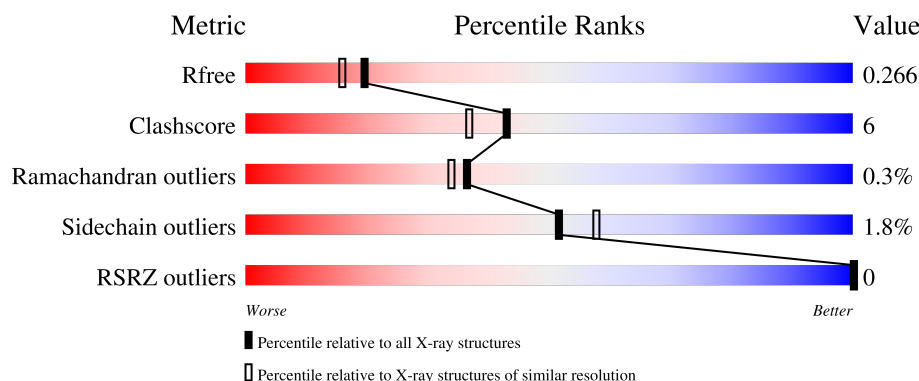
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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 $\leq 5\%$. 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	355	
1	G	355	
2	B	230	
2	H	230	
3	C	203	

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Mol	Chain	Length	Quality of chain
3	L	203	80% 18%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12727 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	G	347	Total	C	N	O	S	0	1	0
			2721	1704	472	522	23			
1	A	346	Total	C	N	O	S	0	0	0
			2706	1695	469	519	23			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	42	VAL	-	expression tag	UNP A0A0M3KKW9
G	43	PRO	-	expression tag	UNP A0A0M3KKW9
G	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9
A	42	VAL	-	expression tag	UNP A0A0M3KKW9
A	43	PRO	-	expression tag	UNP A0A0M3KKW9
A	375	SER	HIS	engineered mutation	UNP A0A0M3KKW9

- Molecule 2 is a protein called N49P9.3-FR3-3 ANTIBODY FAB HEAVY CHAIN.

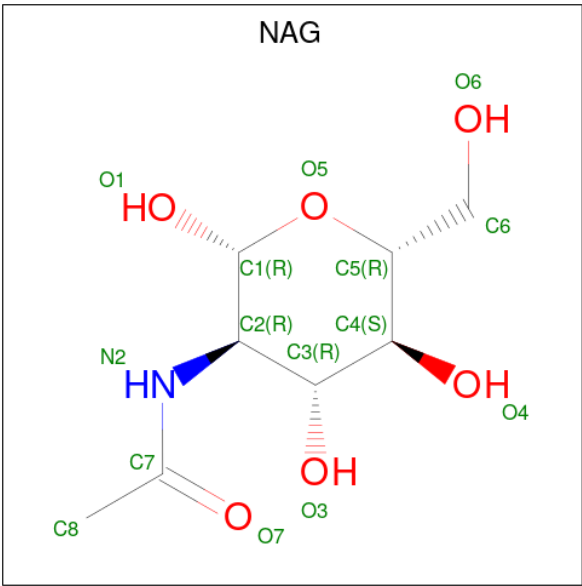
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	223	Total	C	N	O	S	0	0	0
			1720	1092	297	321	10			
2	B	224	Total	C	N	O	S	0	0	0
			1724	1094	298	322	10			

- Molecule 3 is a protein called N49P9.3-FR3-3 ANTIBODY FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	202	Total	C	N	O	S	0	0	0
			1523	958	256	303	6			
3	C	202	Total	C	N	O	S	0	0	0
			1523	958	256	303	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



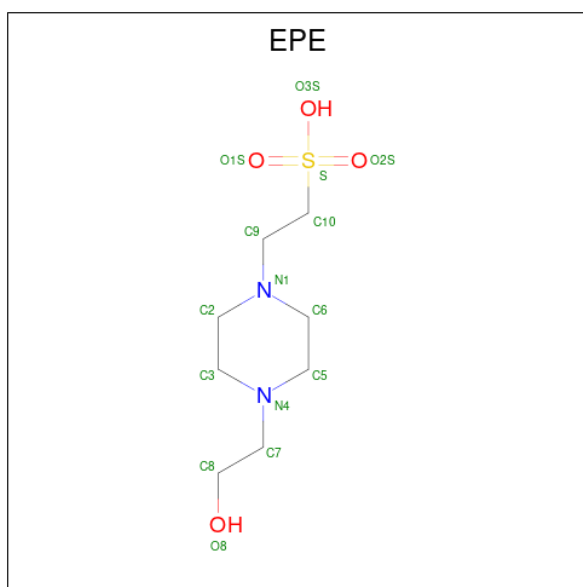
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1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

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

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



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

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

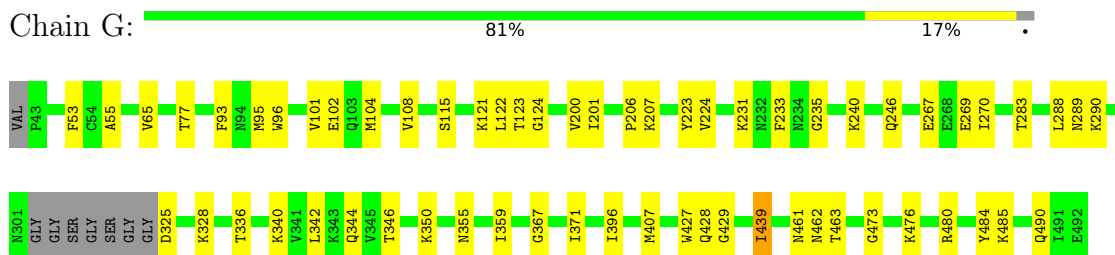
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	121	Total	O	0	0
			121	121		
6	H	60	Total	O	0	0
			60	60		
6	L	42	Total	O	0	0
			42	42		
6	A	124	Total	O	0	0
			124	124		
6	B	57	Total	O	0	0
			57	57		
6	C	39	Total	O	0	0
			39	39		

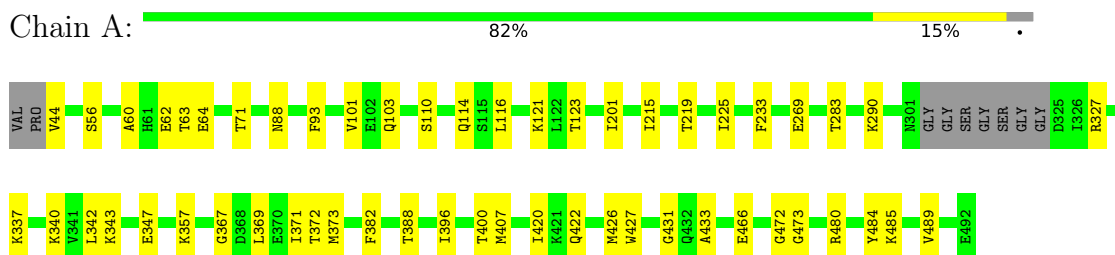
3 Residue-property plots

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 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.

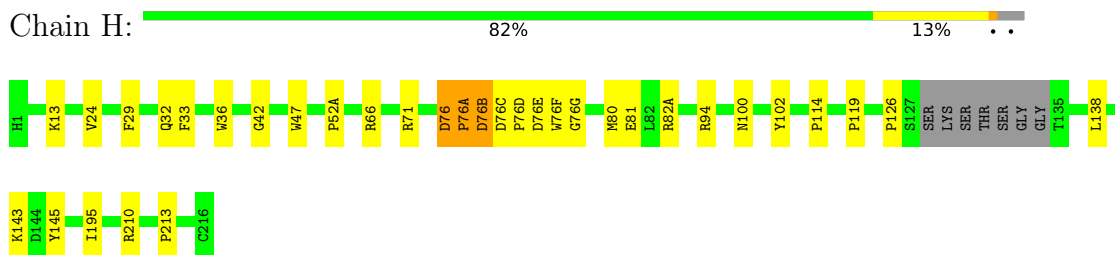
- Molecule 1: clade A/E 93TH057 HIV-1 gp120 core



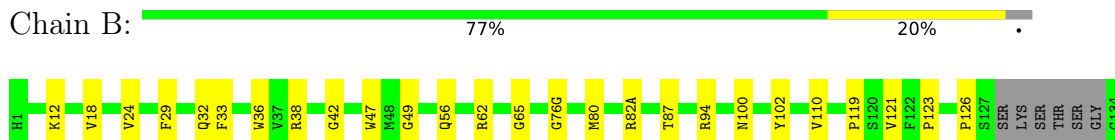
- Molecule 1: clade A/E 93TH057 HIV-1 gp120 core



- Molecule 2: N49P9.3-FR3-3 ANTIBODY FAB HEAVY CHAIN

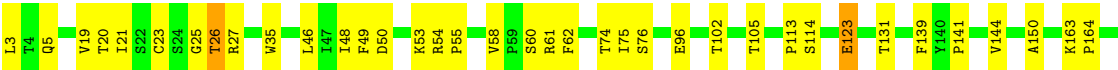
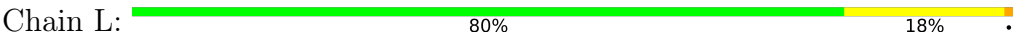


- Molecule 2: N49P9.3-FR3-3 ANTIBODY FAB HEAVY CHAIN

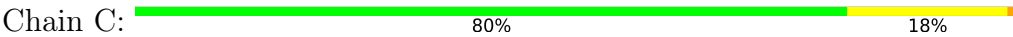




• Molecule 3: N49P9.3-FR3-3 ANTIBODY FAB LIGHT CHAIN



• Molecule 3: N49P9.3-FR3-3 ANTIBODY FAB LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.37Å 65.42Å 112.38Å 90.02° 104.85° 90.02°	Depositor
Resolution (Å)	46.66 – 2.15 46.66 – 2.15	Depositor EDS
% Data completeness (in resolution range)	82.1 (46.66-2.15) 82.1 (46.66-2.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.229 , 0.268 0.228 , 0.266	Depositor DCC
R_{free} test set	3644 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 24.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l 0.427 for -h,k,-l 0.015 for -h,-k,h+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12727	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 5.08% 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: NAG, EPE

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	0.18	0/2762	0.36	0/3748
1	G	0.20	0/2778	0.44	3/3770 (0.1%)
2	B	0.32	0/1774	0.48	0/2419
2	H	0.27	0/1770	0.44	1/2414 (0.0%)
3	C	0.20	0/1563	0.41	0/2133
3	L	0.19	0/1563	0.41	0/2133
All	All	0.23	0/12210	0.42	4/16617 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	407	MET	CB-CA-C	-6.51	108.04	115.79
1	G	206	PRO	CA-C-N	6.28	129.79	120.87
1	G	206	PRO	C-N-CA	6.28	129.79	120.87
2	H	76(B)	ASP	CB-CA-C	6.25	121.13	110.56

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	2706	0	2636	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2721	0	2650	34	0
2	B	1724	0	1661	33	0
2	H	1720	0	1658	17	0
3	C	1523	0	1488	23	0
3	L	1523	0	1488	22	0
4	A	168	0	156	4	0
4	G	154	0	143	1	0
5	A	30	0	36	2	0
5	G	15	0	17	1	0
6	A	124	0	0	0	0
6	B	57	0	0	0	0
6	C	39	0	0	0	0
6	G	121	0	0	1	0
6	H	60	0	0	0	0
6	L	42	0	0	0	0
All	All	12727	0	11933	151	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 6.

All (151) 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)
2:B:198:VAL:HB	2:B:207:VAL:HG23	1.63	0.79
2:B:121:VAL:HG21	2:B:207:VAL:HG21	1.64	0.78
2:B:65:GLY:O	2:B:82(A):ARG:NH2	2.21	0.74
1:G:342:LEU:HD23	1:G:396:ILE:HG21	1.70	0.72
1:A:400:THR:HG22	1:A:407:MET:H	1.55	0.71
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.73	0.71
3:L:163:LYS:HD2	3:L:164:PRO:HD2	1.73	0.71
4:A:505:NAG:H61	3:C:31:ILE:HA	1.72	0.71
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.73	0.70
3:C:159:VAL:HG12	3:C:178:LEU:HD13	1.72	0.70
3:L:55:PRO:HD2	3:L:58:VAL:HG21	1.74	0.69
3:C:117:LEU:HD12	3:C:193:CYS:HB3	1.73	0.69
3:L:50:ASP:HB3	3:L:53:LYS:HD2	1.75	0.67
1:G:231:LYS:HD3	1:G:267:GLU:HG2	1.79	0.65
1:A:342:LEU:HD23	1:A:396:ILE:HG21	1.78	0.65
2:B:198:VAL:HB	2:B:207:VAL:CG2	2.27	0.65
1:A:426:MET:HE3	1:A:433:ALA:HB2	1.77	0.64
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:126:PRO:HG3	2:H:138:LEU:HB3	1.80	0.64
2:B:38:ARG:HH21	2:B:62:ARG:HH22	1.45	0.63
2:H:42:GLY:HA3	3:L:163:LYS:HD3	1.80	0.62
2:H:13:LYS:HG2	2:H:114:PRO:HA	1.81	0.62
2:B:42:GLY:HA3	3:C:163:LYS:HG2	1.81	0.62
1:G:283:THR:HG21	1:G:473:GLY:N	2.14	0.62
1:G:101:VAL:HG21	1:G:480:ARG:HG2	1.82	0.62
2:H:52(A):PRO:HA	2:H:71:ARG:HD2	1.81	0.61
1:A:290:LYS:HE3	1:A:337:LYS:HE3	1.82	0.61
1:A:327:ARG:HD2	1:A:422:GLN:HE22	1.64	0.61
2:B:210:ARG:HD2	2:B:212:GLU:HG2	1.82	0.61
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.81	0.60
1:G:367:GLY:HA3	1:G:371:ILE:HD11	1.83	0.60
1:A:103:GLN:HB3	5:A:513:EPE:H81	1.84	0.60
1:A:123:THR:HG22	1:A:431:GLY:HA3	1.83	0.60
2:B:138:LEU:HD13	2:B:211:VAL:HG21	1.84	0.59
1:G:350:LYS:HG2	1:G:355:ASN:HA	1.85	0.59
2:B:143:LYS:HE3	3:C:131:THR:HG21	1.85	0.59
2:B:126:PRO:HG3	2:B:138:LEU:HB3	1.86	0.58
1:A:283:THR:HG21	1:A:472:GLY:O	2.04	0.58
3:C:35:TRP:HB2	3:C:48:ILE:HB	1.86	0.57
1:G:325:ASP:HB3	1:G:328:LYS:HG3	1.88	0.56
3:C:26:THR:O	3:C:31:ILE:HG12	2.06	0.56
2:H:81:GLU:OE2	1:A:63:THR:HG21	2.07	0.55
3:C:161:THR:HG23	3:C:176:SER:HB2	1.88	0.55
2:B:200:HIS:CE1	2:B:202:PRO:HG2	2.42	0.54
2:B:12:LYS:HE3	2:B:18:VAL:HG23	1.89	0.54
1:G:102:GLU:HG3	1:G:476:LYS:HE2	1.91	0.53
3:L:105:THR:HG21	3:L:141:PRO:HB3	1.90	0.53
1:G:122:LEU:HD22	1:G:200:VAL:HG22	1.89	0.53
2:H:143:LYS:HE2	3:L:131:THR:HG21	1.91	0.53
1:A:60:ALA:HA	1:A:71:THR:HG21	1.90	0.53
2:H:29:PHE:CG	2:H:76(G):GLY:HA3	2.44	0.53
1:A:116:LEU:HD23	1:A:382:PHE:HZ	1.73	0.53
2:B:144:ASP:HB3	2:B:175:LEU:HD13	1.90	0.52
1:G:53:PHE:HB2	6:G:691:HOH:O	2.09	0.52
1:G:207:LYS:HG3	1:G:439:ILE:HG23	1.92	0.51
1:G:336:THR:O	1:G:340:LYS:HG2	2.11	0.51
1:A:427:TRP:H	1:A:427:TRP:CD1	2.28	0.51
3:C:120:PRO:HD3	3:C:132:LEU:HD23	1.92	0.51
3:L:144:VAL:HG22	3:L:197:HIS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LEU:HA	1:A:372:THR:HG22	1.93	0.50
1:A:357:LYS:HD2	1:A:466:GLU:HG2	1.93	0.49
3:C:145:THR:O	3:C:195:VAL:HA	2.12	0.49
1:G:283:THR:HG21	1:G:473:GLY:H	1.79	0.48
2:B:33:PHE:HB2	2:B:100:ASN:OD1	2.14	0.48
2:B:199:ASN:HD21	2:B:206:LYS:NZ	2.11	0.48
1:A:367:GLY:HA3	1:A:371:ILE:HD11	1.95	0.48
1:A:327:ARG:HG3	1:A:420:ILE:O	2.13	0.48
2:B:36:TRP:CE2	2:B:80:MET:HB2	2.49	0.48
3:L:123:GLU:H	3:L:123:GLU:HG2	1.42	0.48
3:L:54:ARG:CZ	3:L:60:SER:HA	2.44	0.48
1:G:95:MET:SD	1:G:235:GLY:HA3	2.54	0.47
3:L:3:LEU:HD23	3:L:26:THR:HG22	1.95	0.47
3:L:21:ILE:HD12	3:L:102:THR:HG21	1.95	0.47
1:A:88:ASN:OD1	4:A:501:NAG:H2	2.13	0.47
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.50	0.47
1:A:110:SER:O	1:A:114:GLN:HG3	2.15	0.46
1:G:121:LYS:HB2	1:G:201:ILE:HG12	1.98	0.46
1:G:427:TRP:CD1	1:G:427:TRP:H	2.34	0.46
3:C:20:THR:OG1	3:C:74:THR:HG22	2.16	0.46
1:G:484:TYR:CE2	1:G:485:LYS:HG3	2.51	0.46
1:A:371:ILE:HD13	2:B:56:GLN:HG3	1.97	0.46
1:G:65:VAL:HB	1:G:115:SER:HB3	1.98	0.46
1:A:327:ARG:HH12	5:A:514:EPE:H101	1.81	0.46
1:G:55:ALA:HB1	1:G:77:THR:HA	1.98	0.46
2:B:29:PHE:CG	2:B:76(G):GLY:HA3	2.51	0.46
3:L:46:LEU:HD21	3:L:49:PHE:HB3	1.98	0.45
1:G:340:LYS:O	1:G:344:GLN:HG3	2.16	0.45
2:H:94:ARG:HG3	2:H:102:TYR:HB2	1.97	0.45
2:B:121:VAL:CG2	2:B:207:VAL:HG21	2.41	0.45
1:G:270:ILE:HD13	1:G:288:LEU:HA	1.98	0.45
3:L:61:ARG:HB3	3:L:76:SER:O	2.16	0.45
1:A:343:LYS:HE3	1:A:347:GLU:HG2	1.99	0.45
2:B:121:VAL:HG21	2:B:207:VAL:CG2	2.42	0.45
2:B:166:PHE:CE2	3:C:135:LEU:HD13	2.52	0.45
2:B:214:LYS:HE3	2:B:214:LYS:HB2	1.73	0.45
1:A:219:THR:HG23	1:A:225:ILE:HG13	1.99	0.44
2:H:66:ARG:HD2	2:H:82(A):ARG:O	2.17	0.44
1:G:223:TYR:CE2	1:G:490:GLN:HB2	2.52	0.44
3:L:25:GLY:C	3:L:27:ARG:H	2.25	0.44
2:H:195:ILE:HG12	2:H:210:ARG:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:20:THR:HG22	3:L:74:THR:HG22	2.00	0.44
2:H:47:TRP:CG	3:L:96:GLU:HB2	2.53	0.44
3:L:5:GLN:HB3	3:L:23:CYS:SG	2.57	0.44
3:C:6:PRO:O	3:C:102:THR:HG22	2.17	0.44
1:A:269:GLU:HG2	4:A:506:NAG:H61	1.99	0.43
1:A:388:THR:HG22	4:A:510:NAG:H81	2.00	0.43
1:G:93:PHE:HB2	1:G:233:PHE:HZ	1.82	0.43
1:G:121:LYS:HB2	1:G:201:ILE:CG1	2.48	0.43
3:C:183:GLU:O	3:C:187:SER:HB3	2.17	0.43
3:C:61:ARG:HB3	3:C:76:SER:O	2.17	0.43
1:G:224:VAL:HG12	1:G:246:GLN:HE21	1.83	0.43
3:L:113:PRO:HB3	3:L:139:PHE:HB3	2.01	0.43
1:A:473:GLY:HA2	2:B:56:GLN:NE2	2.34	0.43
1:A:372:THR:HG23	1:A:373:MET:HG2	2.01	0.43
2:B:169:VAL:HG11	3:C:160:GLU:HB3	2.01	0.42
2:H:33:PHE:HB2	2:H:100:ASN:OD1	2.20	0.42
2:B:216:CYS:C	3:C:211:CYS:HA	2.44	0.42
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.54	0.42
1:G:123:THR:HG23	1:G:124:GLY:H	1.85	0.42
3:C:117:LEU:CD1	3:C:193:CYS:HB3	2.47	0.42
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.84	0.42
1:A:484:TYR:CE2	1:A:485:LYS:HG3	2.54	0.42
1:G:240:LYS:HE2	5:G:512:EPE:H92	2.01	0.42
1:A:121:LYS:HB2	1:A:201:ILE:HB	2.01	0.42
1:G:269:GLU:OE1	4:G:506:NAG:H61	2.20	0.41
1:G:439:ILE:H	1:G:439:ILE:HG13	1.65	0.41
1:G:95:MET:HE2	1:G:96:TRP:CZ2	2.55	0.41
1:A:283:THR:HG21	1:A:472:GLY:C	2.45	0.41
1:A:56:SER:HB3	1:A:215:ILE:HD13	2.02	0.41
1:A:62:GLU:HG3	1:A:64:GLU:H	1.84	0.41
1:G:104:MET:O	1:G:108:VAL:HG23	2.21	0.41
1:G:346:THR:HG23	1:G:359:ILE:HB	2.03	0.41
2:B:209:LYS:HE3	2:B:209:LYS:HB2	1.82	0.41
3:C:11:MET:HE3	3:C:11:MET:HB2	1.70	0.41
3:C:13:ALA:HB2	3:C:19:VAL:CG1	2.51	0.41
2:B:143:LYS:NZ	2:B:171:GLN:HE22	2.19	0.41
1:G:289:ASN:O	1:G:290:LYS:HE2	2.21	0.41
2:H:126:PRO:HD2	2:H:213:PRO:HA	2.03	0.41
1:A:340:LYS:O	1:A:340:LYS:HD3	2.20	0.41
2:B:94:ARG:HG3	2:B:102:TYR:HB2	2.03	0.41
3:C:188:HIS:HB2	3:C:191:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:428:GLN:HG3	1:G:429:GLY:H	1.86	0.40
2:B:87:THR:HG23	2:B:110:VAL:HA	2.02	0.40
3:C:196:THR:HB	3:C:201:THR:HG22	2.03	0.40
2:H:76:ASP:HA	2:H:76(A):PRO:HD3	1.86	0.40
2:B:123:PRO:HD3	2:B:209:LYS:HD3	2.03	0.40
3:L:62:PHE:CD1	3:L:75:ILE:HG12	2.56	0.40
3:L:150:ALA:HB1	3:L:188:HIS:ND1	2.36	0.40
2:H:32:GLN:HG3	2:H:94:ARG:CZ	2.51	0.40
3:L:19:VAL:HG12	3:L:75:ILE:HB	2.02	0.40
2:B:47:TRP:CG	3:C:96:GLU:HB2	2.57	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	342/355 (96%)	321 (94%)	21 (6%)	0	100	100
1	G	344/355 (97%)	329 (96%)	14 (4%)	1 (0%)	36	34
2	B	220/230 (96%)	215 (98%)	3 (1%)	2 (1%)	14	9
2	H	219/230 (95%)	214 (98%)	5 (2%)	0	100	100
3	C	200/203 (98%)	189 (94%)	10 (5%)	1 (0%)	24	20
3	L	200/203 (98%)	186 (93%)	13 (6%)	1 (0%)	24	20
All	All	1525/1576 (97%)	1454 (95%)	66 (4%)	5 (0%)	36	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	26	THR
3	C	32	ILE

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Mol	Chain	Res	Type
1	G	461	ASN
2	B	32	GLN
2	B	155	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	309/313 (99%)	307 (99%)	2 (1%)	78	84
1	G	311/313 (99%)	308 (99%)	3 (1%)	68	75
2	B	190/195 (97%)	189 (100%)	1 (0%)	81	87
2	H	190/195 (97%)	182 (96%)	8 (4%)	26	25
3	C	173/174 (99%)	165 (95%)	8 (5%)	24	22
3	L	173/174 (99%)	171 (99%)	2 (1%)	63	70
All	All	1346/1364 (99%)	1322 (98%)	24 (2%)	51	58

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	439	ILE
1	G	462	ASN
1	G	463	THR
2	H	24	VAL
2	H	76	ASP
2	H	76(A)	PRO
2	H	76(B)	ASP
2	H	76(C)	ASP
2	H	76(D)	PRO
2	H	76(E)	ASP
2	H	76(F)	TRP
3	L	114	SER
3	L	123	GLU
1	A	44	VAL
1	A	489	VAL

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Mol	Chain	Res	Type
2	B	24	VAL
3	C	3	LEU
3	C	19	VAL
3	C	69	ASP
3	C	159	VAL
3	C	162	THR
3	C	180	LEU
3	C	195	VAL
3	C	196	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	246	GLN
1	G	444	ASN
1	G	461	ASN
2	H	64	GLN
2	H	199	ASN
3	L	170	ASN
1	A	114	GLN
1	A	216	HIS
1	A	355	ASN
2	B	39	GLN
2	B	155	ASN
2	B	171	GLN
2	B	199	ASN
3	C	38	GLN
3	C	79	GLN
3	C	184	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	NAG	A	510	1	14,14,15	0.68	0	17,19,21	0.85	0
4	NAG	G	507	1	14,14,15	0.70	0	17,19,21	0.99	1 (5%)
4	NAG	A	509	1	14,14,15	0.71	0	17,19,21	1.09	2 (11%)
4	NAG	A	501	1	14,14,15	0.71	0	17,19,21	2.10	2 (11%)
4	NAG	G	509	1	14,14,15	0.70	0	17,19,21	1.00	1 (5%)
4	NAG	G	508	1	14,14,15	0.78	0	17,19,21	1.00	0
4	NAG	G	502	1	14,14,15	0.67	0	17,19,21	0.78	0
4	NAG	A	512	1	14,14,15	0.79	0	17,19,21	2.29	7 (41%)
4	NAG	A	504	1	14,14,15	0.72	0	17,19,21	1.09	1 (5%)
4	NAG	G	510	1	14,14,15	0.73	0	17,19,21	0.92	0
4	NAG	A	502	1	14,14,15	0.65	0	17,19,21	0.85	1 (5%)
4	NAG	A	503	1	14,14,15	0.76	0	17,19,21	0.88	0
4	NAG	A	508	1	14,14,15	0.77	0	17,19,21	1.21	1 (5%)
4	NAG	A	506	1	14,14,15	0.73	0	17,19,21	0.88	1 (5%)
4	NAG	G	503	1	14,14,15	0.68	0	17,19,21	0.81	0
5	EPE	A	513	-	15,15,15	0.84	1 (6%)	19,20,20	0.75	0
4	NAG	G	501	1	14,14,15	0.80	1 (7%)	17,19,21	1.56	3 (17%)
4	NAG	G	506	1	14,14,15	0.72	0	17,19,21	0.98	0
5	EPE	A	514	-	15,15,15	0.91	1 (6%)	19,20,20	1.28	3 (15%)
4	NAG	G	505	1	14,14,15	0.67	0	17,19,21	0.75	0
5	EPE	G	512	-	15,15,15	1.25	2 (13%)	19,20,20	1.07	1 (5%)
4	NAG	A	507	1	14,14,15	0.72	0	17,19,21	0.92	0
4	NAG	G	504	1	14,14,15	0.72	0	17,19,21	1.08	1 (5%)
4	NAG	G	511	1	14,14,15	0.68	0	17,19,21	0.87	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	505	1	14,14,15	0.72	0	17,19,21	0.84	0
4	NAG	A	511	1	14,14,15	0.68	0	17,19,21	1.09	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
4	NAG	A	510	1	-	0/6/23/26	0/1/1/1
4	NAG	G	507	1	-	0/6/23/26	0/1/1/1
4	NAG	A	509	1	-	2/6/23/26	0/1/1/1
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	NAG	G	509	1	-	0/6/23/26	0/1/1/1
4	NAG	G	508	1	-	2/6/23/26	0/1/1/1
4	NAG	G	502	1	-	0/6/23/26	0/1/1/1
4	NAG	A	512	1	-	0/6/23/26	0/1/1/1
4	NAG	A	504	1	-	2/6/23/26	0/1/1/1
4	NAG	G	510	1	-	0/6/23/26	0/1/1/1
4	NAG	A	502	1	-	0/6/23/26	0/1/1/1
4	NAG	A	503	1	-	0/6/23/26	0/1/1/1
4	NAG	A	508	1	-	0/6/23/26	0/1/1/1
4	NAG	A	506	1	-	1/6/23/26	0/1/1/1
4	NAG	G	503	1	-	2/6/23/26	0/1/1/1
5	EPE	A	513	-	-	4/9/19/19	0/1/1/1
4	NAG	G	501	1	-	2/6/23/26	0/1/1/1
4	NAG	G	506	1	-	1/6/23/26	0/1/1/1
5	EPE	A	514	-	-	5/9/19/19	0/1/1/1
4	NAG	G	505	1	-	0/6/23/26	0/1/1/1
5	EPE	G	512	-	-	0/9/19/19	0/1/1/1
4	NAG	A	507	1	-	0/6/23/26	0/1/1/1
4	NAG	G	504	1	-	1/6/23/26	0/1/1/1
4	NAG	G	511	1	-	0/6/23/26	0/1/1/1
4	NAG	A	505	1	-	0/6/23/26	0/1/1/1
4	NAG	A	511	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	512	EPE	C10-S	3.98	1.83	1.77
5	A	514	EPE	C10-S	2.48	1.81	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	513	EPE	C10-S	2.34	1.80	1.77
5	G	512	EPE	O2S-S	2.25	1.51	1.45
4	G	501	NAG	C1-C2	2.08	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	NAG	C1-O5-C5	7.09	121.69	112.19
4	A	512	NAG	C3-C4-C5	-4.72	101.67	110.23
4	A	512	NAG	C4-C3-C2	-4.67	104.18	111.02
4	A	501	NAG	C4-C3-C2	-3.41	106.02	111.02
4	A	512	NAG	O4-C4-C5	3.31	117.48	109.32
4	G	504	NAG	C1-O5-C5	3.31	116.62	112.19
4	G	501	NAG	C1-O5-C5	3.30	116.61	112.19
4	G	501	NAG	C2-N2-C7	3.07	127.01	122.90
4	G	509	NAG	C1-O5-C5	3.03	116.24	112.19
5	A	514	EPE	C2-C3-N4	3.00	116.70	110.65
4	A	512	NAG	C1-O5-C5	2.96	116.15	112.19
4	A	512	NAG	C6-C5-C4	2.95	120.26	113.02
4	A	504	NAG	C1-O5-C5	2.68	115.78	112.19
4	G	507	NAG	C1-O5-C5	2.51	115.55	112.19
5	G	512	EPE	O2S-S-O1S	2.51	122.00	113.82
4	A	512	NAG	O3-C3-C4	2.50	116.27	110.38
4	A	509	NAG	O4-C4-C3	-2.50	104.49	110.38
5	A	514	EPE	C6-N1-C2	2.42	114.05	108.84
4	A	506	NAG	C1-O5-C5	2.33	115.31	112.19
4	G	501	NAG	C3-C4-C5	-2.24	106.16	110.23
4	A	508	NAG	C2-N2-C7	2.24	125.90	122.90
4	A	509	NAG	O4-C4-C5	2.18	114.69	109.32
4	A	502	NAG	O5-C1-C2	-2.13	108.00	111.29
4	A	512	NAG	C1-C2-N2	2.04	113.65	110.43
4	G	511	NAG	C1-O5-C5	2.03	114.91	112.19
5	A	514	EPE	O2S-S-C10	-2.00	103.70	106.73

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	513	EPE	C8-C7-N4-C5
5	A	513	EPE	C9-C10-S-O2S
5	A	513	EPE	C9-C10-S-O3S
4	A	504	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	509	NAG	C4-C5-C6-O6
4	A	504	NAG	C4-C5-C6-O6
4	A	509	NAG	O5-C5-C6-O6
4	A	506	NAG	O5-C5-C6-O6
4	G	503	NAG	C4-C5-C6-O6
4	G	504	NAG	O5-C5-C6-O6
4	G	508	NAG	O5-C5-C6-O6
4	G	503	NAG	O5-C5-C6-O6
5	A	513	EPE	C9-C10-S-O1S
5	A	514	EPE	C9-C10-S-O1S
5	A	514	EPE	C9-C10-S-O2S
4	G	506	NAG	O5-C5-C6-O6
5	A	514	EPE	N4-C7-C8-O8
5	A	514	EPE	C9-C10-S-O3S
4	G	508	NAG	C4-C5-C6-O6
4	G	501	NAG	C1-C2-N2-C7
4	G	501	NAG	C3-C2-N2-C7
5	A	514	EPE	C10-C9-N1-C6

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	510	NAG	1	0
4	A	501	NAG	1	0
4	A	506	NAG	1	0
5	A	513	EPE	1	0
4	G	506	NAG	1	0
5	A	514	EPE	1	0
5	G	512	EPE	1	0
4	A	505	NAG	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	346/355 (97%)	-1.16	0 100 100	28, 39, 70, 89	0
1	G	347/355 (97%)	-1.14	0 100 100	26, 40, 71, 92	1 (0%)
2	B	224/230 (97%)	-1.14	0 100 100	28, 41, 69, 95	0
2	H	223/230 (96%)	-1.15	0 100 100	27, 42, 68, 86	0
3	C	202/203 (99%)	-1.05	0 100 100	33, 50, 62, 96	0
3	L	202/203 (99%)	-1.09	0 100 100	33, 49, 63, 94	0
All	All	1544/1576 (97%)	-1.13	0 100 100	26, 44, 69, 96	1 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
4	NAG	G	505	14/15	0.95	0.06	57,67,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	G	501	14/15	0.96	0.05	67,80,82,84	0
4	NAG	A	505	14/15	0.96	0.06	57,66,72,74	0
4	NAG	G	510	14/15	0.97	0.05	56,69,75,78	0
4	NAG	G	511	14/15	0.97	0.05	51,60,71,72	0
4	NAG	A	501	14/15	0.97	0.06	80,93,99,99	0
4	NAG	G	503	14/15	0.97	0.05	65,72,78,80	0
4	NAG	A	512	14/15	0.97	0.05	67,69,73,75	0
5	EPE	A	514	15/15	0.97	0.06	54,58,66,67	0
4	NAG	G	508	14/15	0.98	0.04	36,45,51,53	0
4	NAG	A	502	14/15	0.98	0.04	38,41,45,55	0
4	NAG	A	503	14/15	0.98	0.05	56,64,74,75	0
4	NAG	G	509	14/15	0.98	0.04	46,53,58,66	0
4	NAG	A	506	14/15	0.98	0.04	42,47,54,54	0
4	NAG	A	507	14/15	0.98	0.04	43,48,53,54	0
4	NAG	A	508	14/15	0.98	0.03	41,46,49,49	0
4	NAG	A	509	14/15	0.98	0.05	50,58,66,66	0
4	NAG	A	510	14/15	0.98	0.04	64,70,73,75	0
4	NAG	G	504	14/15	0.98	0.04	30,33,38,45	0
5	EPE	G	512	15/15	0.98	0.05	45,54,78,81	0
4	NAG	G	507	14/15	0.98	0.04	39,43,46,48	0
4	NAG	A	511	14/15	0.99	0.04	45,61,70,75	0
4	NAG	G	502	14/15	0.99	0.03	39,46,50,50	0
4	NAG	G	506	14/15	0.99	0.04	45,48,55,55	0
5	EPE	A	513	15/15	0.99	0.05	40,44,52,52	0
4	NAG	A	504	14/15	0.99	0.04	29,33,37,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.