



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2022 – 02:15 PM EST

PDB ID : 7SX7
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:

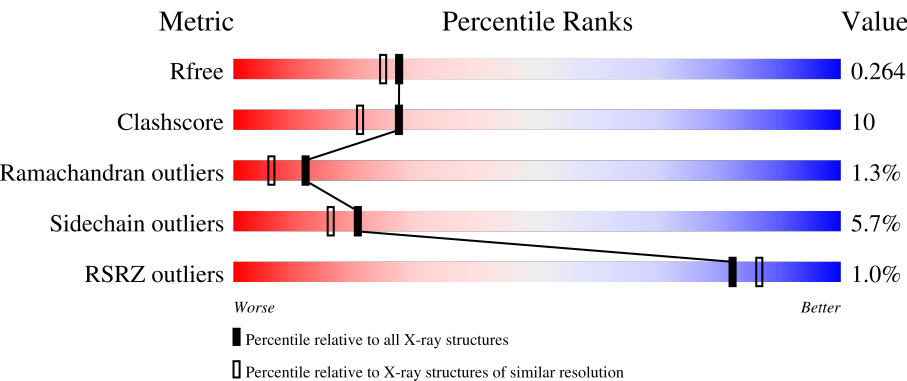
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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	<div><div>%</div><div><div></div><div>73%</div><div>21%</div><div></div></div><div></div></div>
1	G	355	<div><div>2%</div><div><div></div><div>75%</div><div>20%</div><div></div></div><div></div></div>
2	B	230	<div><div></div><div><div></div><div>74%</div><div>22%</div><div></div></div><div></div></div>
2	H	230	<div><div></div><div><div></div><div>72%</div><div>24%</div><div></div></div><div></div></div>
3	C	203	<div><div>%</div><div><div></div><div>70%</div><div>26%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
3	L	203	 71%26%.

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.

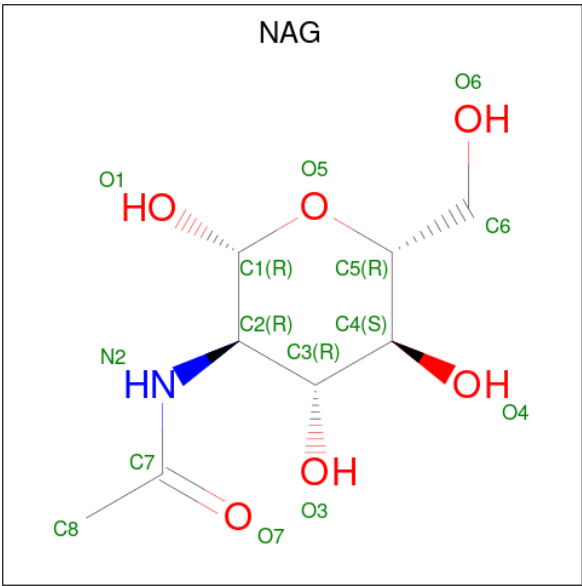
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	223	Total	C	N	O	S	0	0	0
			1720	1092	297	321	10			
2	B	224	Total	C	N	O	S	0	0	0
			1724	1094	298	322	10			

- 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 (three-letter code: NAG) (formula:

C₈H₁₅NO₆).



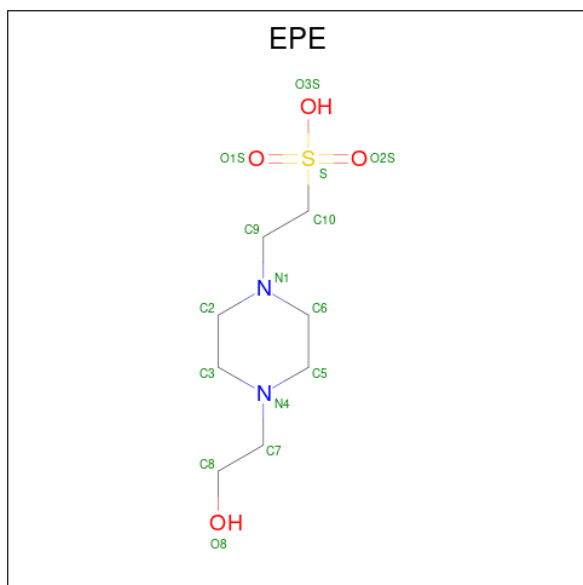
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	Total	C	N	O	0	0
			14	8	1	5		
4	G	1	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 (three-letter code: 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		

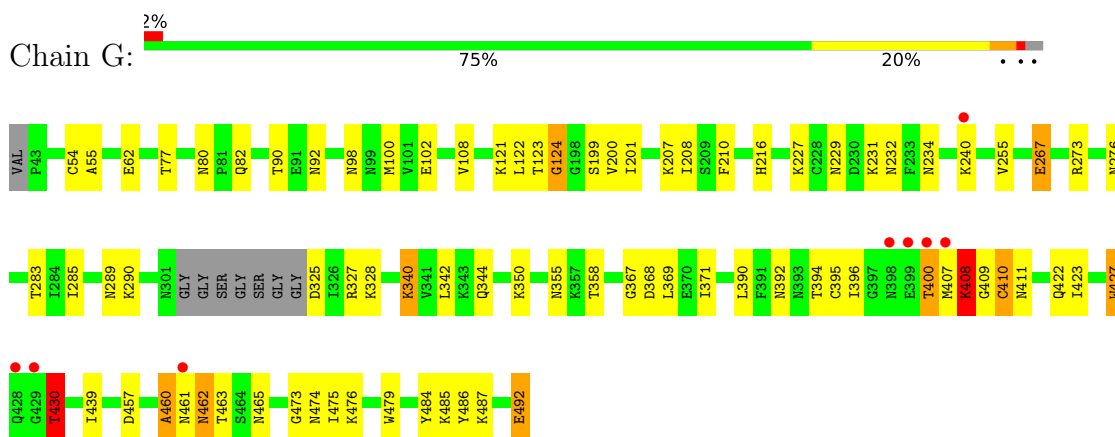
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	124	Total	O	0	0
			124	124		
6	H	60	Total	O	0	0
			60	60		
6	L	41	Total	O	0	0
			41	41		
6	A	121	Total	O	0	0
			121	121		
6	B	59	Total	O	0	0
			59	59		
6	C	38	Total	O	0	0
			38	38		

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



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 1.19.1_4122	Depositor
R, R_{free}	0.209 , 0.266 0.208 , 0.264	Depositor DCC
R_{free} test set	3644 reflections (4.94%)	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)	0.29 , 22.7	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	0.95	EDS
Total number of atoms	12727	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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: EPE, 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	0.36	0/2762	0.56	0/3748
1	G	0.38	0/2778	0.58	0/3770
2	B	0.36	0/1774	0.60	0/2419
2	H	0.37	0/1770	0.62	0/2414
3	C	0.36	0/1563	0.60	0/2133
3	L	0.35	0/1563	0.57	0/2133
All	All	0.36	0/12210	0.59	0/16617

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2706	0	2635	61	0
1	G	2721	0	2650	61	0
2	B	1724	0	1661	30	0
2	H	1720	0	1658	36	0
3	C	1523	0	1488	39	0
3	L	1523	0	1488	34	0
4	A	168	0	156	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	154	0	143	0	0
5	A	30	0	34	7	0
5	G	15	0	17	0	0
6	A	121	0	0	6	0
6	B	59	0	0	1	0
6	C	38	0	0	1	0
6	G	124	0	0	2	0
6	H	60	0	0	4	0
6	L	41	0	0	0	0
All	All	12727	0	11930	245	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 10.

All (245) 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:G:492:GLU:OE1	1:G:492:GLU:OXT	1.76	1.04
3:L:163:LYS:HD2	3:L:164:PRO:HD2	1.53	0.90
2:B:143:LYS:HE3	3:C:131:THR:HG21	1.62	0.82
1:G:350:LYS:HG2	1:G:355:ASN:HA	1.63	0.79
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.66	0.78
1:G:492:GLU:OXT	1:G:492:GLU:CG	2.31	0.78
3:C:26:THR:HG22	3:C:30:HIS:H	1.47	0.77
3:C:196:THR:HB	3:C:201:THR:HG22	1.66	0.77
1:G:492:GLU:OXT	1:G:492:GLU:CD	2.22	0.77
2:B:198:VAL:HB	2:B:207:VAL:HG23	1.65	0.75
1:G:411:ASN:ND2	6:G:601:HOH:O	2.21	0.73
1:A:283:THR:HG21	1:A:472:GLY:O	1.88	0.73
2:H:76(C):ASP:N	2:H:76(D):PRO:HD2	2.04	0.72
1:G:462:ASN:O	1:G:463:THR:HG23	1.90	0.71
2:H:126:PRO:HG3	2:H:138:LEU:HB3	1.70	0.71
1:A:473:GLY:HA2	2:B:56:GLN:NE2	2.05	0.71
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.75	0.69
3:L:4:THR:HG1	3:L:24:SER:HG	1.40	0.69
3:C:117:LEU:HD12	3:C:193:CYS:HB3	1.75	0.69
3:C:6:PRO:O	3:C:102:THR:HG22	1.93	0.68
2:H:76(C):ASP:O	2:H:76(E):ASP:N	2.28	0.67
2:B:126:PRO:HG3	2:B:138:LEU:HB3	1.77	0.67
3:C:161:THR:HB	3:C:176:SER:HB2	1.77	0.65
1:G:283:THR:HG21	1:G:473:GLY:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:LEU:C	2:B:178:LEU:HD12	2.17	0.65
2:B:210:ARG:HD2	2:B:212:GLU:HG3	1.79	0.64
3:C:35:TRP:HB2	3:C:48:ILE:HB	1.79	0.64
1:A:342:LEU:HD23	1:A:396:ILE:HG21	1.79	0.63
2:B:38:ARG:HH21	2:B:62:ARG:HH22	1.46	0.63
2:H:13:LYS:HG2	2:H:114:PRO:HA	1.80	0.63
1:A:116:LEU:HD23	1:A:382:PHE:HZ	1.64	0.63
3:L:25:GLY:O	3:L:27:ARG:N	2.29	0.62
1:A:400:THR:HG22	1:A:407:MET:H	1.63	0.62
1:A:327:ARG:HD2	1:A:422:GLN:HE22	1.65	0.62
1:G:121:LYS:HB2	1:G:201:ILE:HG12	1.82	0.61
1:G:427:TRP:HZ3	1:G:475:ILE:HG21	1.66	0.60
3:C:61:ARG:NH2	3:C:82:ASP:OD2	2.35	0.60
1:G:492:GLU:OXT	1:G:492:GLU:HG2	1.99	0.60
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.84	0.60
1:A:325:ASP:N	6:A:606:HOH:O	2.33	0.60
3:L:50:ASP:HB3	3:L:53:LYS:HD2	1.83	0.60
1:A:327:ARG:HH12	5:A:514:EPE:H101	1.65	0.60
1:G:367:GLY:HA3	1:G:371:ILE:HD11	1.83	0.59
3:L:26:THR:HG22	3:L:30:HIS:H	1.67	0.59
1:A:340:LYS:HD3	1:A:340:LYS:O	2.03	0.59
1:G:325:ASP:HB3	1:G:328:LYS:HG3	1.85	0.59
1:G:408:LYS:O	1:G:410:CYS:N	2.36	0.59
2:H:195:ILE:HG12	2:H:210:ARG:HA	1.84	0.59
3:L:52:ASP:OD1	3:L:53:LYS:NZ	2.36	0.58
1:A:473:GLY:HA2	2:B:56:GLN:HE21	1.69	0.57
1:A:294:ILE:HG13	1:A:333:ILE:HD11	1.86	0.57
2:H:42:GLY:HA3	3:L:163:LYS:HD3	1.87	0.57
3:L:55:PRO:HD2	3:L:58:VAL:HG21	1.86	0.57
1:G:207:LYS:HG3	1:G:439:ILE:HG23	1.85	0.57
1:A:219:THR:HG23	1:A:225:ILE:HG13	1.85	0.57
1:A:67:ASN:O	1:A:71:THR:HG23	2.05	0.56
1:G:55:ALA:HB1	1:G:77:THR:HA	1.87	0.56
1:A:327:ARG:NH1	5:A:514:EPE:H101	2.21	0.56
2:B:36:TRP:CE2	2:B:80:MET:HB2	2.41	0.56
3:L:26:THR:HG21	3:L:66:ARG:HD2	1.88	0.56
1:A:473:GLY:O	1:A:474:ASN:HB2	2.07	0.55
1:G:122:LEU:HD22	1:G:200:VAL:HG22	1.89	0.55
3:L:61:ARG:HB3	3:L:76:SER:O	2.06	0.55
1:A:88:ASN:N	1:A:88:ASN:OD1	2.40	0.55
3:L:105:THR:HG21	3:L:141:PRO:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:342:LEU:HD23	1:G:396:ILE:HG21	1.88	0.55
3:C:54:ARG:NH1	3:C:62:PHE:O	2.39	0.55
2:B:144:ASP:HB3	2:B:175:LEU:HD13	1.87	0.55
1:G:124:GLY:HA2	2:H:75:GLN:HG3	1.87	0.55
3:C:120:PRO:HD3	3:C:132:LEU:CD2	2.36	0.55
2:H:126:PRO:HD2	2:H:213:PRO:HA	1.89	0.54
2:H:189:LEU:HD23	2:H:213:PRO:HB3	1.89	0.54
1:A:422:GLN:N	5:A:514:EPE:O1S	2.32	0.54
1:G:283:THR:HG21	1:G:473:GLY:H	1.73	0.54
2:H:215:SER:OG	2:H:216:CYS:N	2.41	0.54
3:C:103:LYS:NZ	6:C:307:HOH:O	2.40	0.54
1:A:117:GLN:HE21	1:A:117:GLN:HA	1.72	0.54
2:H:47:TRP:CG	3:L:96:GLU:HB2	2.43	0.54
1:A:199:SER:N	6:A:607:HOH:O	2.37	0.54
3:C:117:LEU:CD1	3:C:193:CYS:HB3	2.38	0.53
3:L:61:ARG:NH2	3:L:82:ASP:OD1	2.41	0.53
2:H:43:GLN:NE2	6:H:301:HOH:O	2.23	0.53
1:A:298:ARG:NH2	1:A:439:ILE:O	2.41	0.53
1:G:108:VAL:HG21	1:G:479:TRP:CZ2	2.43	0.53
2:H:143:LYS:HE2	3:L:131:THR:HG21	1.90	0.53
2:B:54:TYR:HB2	2:B:56:GLN:NE2	2.23	0.53
3:L:21:ILE:HG12	3:L:102:THR:HG21	1.90	0.53
1:G:92:ASN:O	1:G:487:LYS:NZ	2.32	0.52
3:L:115:VAL:O	3:L:204:LYS:NZ	2.28	0.52
1:A:327:ARG:NH1	1:A:422:GLN:OE1	2.41	0.52
2:B:12:LYS:HE3	2:B:18:VAL:HG23	1.92	0.52
2:B:121:VAL:HG21	2:B:207:VAL:HG21	1.91	0.52
1:A:357:LYS:NZ	6:A:610:HOH:O	2.39	0.51
1:G:234:ASN:O	1:G:273:ARG:HG2	2.11	0.51
1:A:108:VAL:HG21	1:A:479:TRP:CZ2	2.46	0.51
2:B:200:HIS:CE1	2:B:202:PRO:HG2	2.45	0.51
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.46	0.51
1:A:407:MET:O	1:A:408:LYS:HB2	2.11	0.51
1:G:90:THR:OG1	1:G:240:LYS:NZ	2.39	0.50
1:G:80:ASN:HB2	1:G:82:GLN:NE2	2.27	0.50
2:H:101:HIS:CD2	3:L:46:LEU:HD13	2.47	0.50
3:C:3:LEU:CD1	3:C:26:THR:H	2.24	0.50
1:G:227:LYS:HG2	1:G:229:ASN:OD1	2.12	0.50
3:L:26:THR:HG22	3:L:30:HIS:N	2.27	0.50
2:B:33:PHE:HB2	2:B:100:ASN:OD1	2.11	0.50
1:G:427:TRP:CZ3	1:G:475:ILE:HG21	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:117:LEU:HD23	3:L:206:VAL:HG13	1.94	0.49
3:C:26:THR:HG22	3:C:30:HIS:N	2.23	0.49
3:L:150:ALA:HB1	3:L:188:HIS:ND1	2.28	0.49
1:A:298:ARG:HB3	1:A:443:ILE:HB	1.95	0.49
3:L:54:ARG:CZ	3:L:60:SER:HA	2.42	0.48
2:H:163:VAL:HG22	2:H:182:VAL:CG1	2.43	0.48
2:B:47:TRP:CG	3:C:96:GLU:HB2	2.48	0.48
1:G:98:ASN:OD1	1:G:100:MET:HG3	2.14	0.48
2:B:123:PRO:HD3	2:B:209:LYS:HD2	1.95	0.48
1:G:255:VAL:HG13	1:G:475:ILE:HD11	1.95	0.48
1:G:368:ASP:O	1:G:371:ILE:HG13	2.13	0.48
3:L:62:PHE:CD1	3:L:75:ILE:HG12	2.49	0.48
3:L:66:ARG:HG3	3:L:71:ALA:HB2	1.96	0.48
1:G:255:VAL:HG13	1:G:475:ILE:CD1	2.43	0.48
3:L:113:PRO:HB3	3:L:139:PHE:HB3	1.95	0.48
3:L:149:LYS:HD3	3:L:194:ARG:HD2	1.94	0.48
1:G:430:THR:HG21	2:H:73:LEU:HD13	1.95	0.47
2:H:163:VAL:HG22	2:H:182:VAL:HG12	1.96	0.47
2:B:28:ASN:HA	2:B:76(E):ASP:HB2	1.96	0.47
1:G:227:LYS:HE3	1:G:485:LYS:HE2	1.95	0.47
2:H:135:THR:N	6:H:316:HOH:O	2.48	0.47
1:A:384:TYR:CG	1:A:421:LYS:HD3	2.49	0.47
1:G:392:ASN:OD1	1:G:394:THR:OG1	2.20	0.47
2:H:83:ARG:NH2	6:H:314:HOH:O	2.46	0.47
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.79	0.47
1:A:327:ARG:HG3	1:A:420:ILE:O	2.14	0.47
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.50	0.47
2:B:76:ASP:OD2	2:B:76(B):ASP:HB2	2.14	0.47
3:L:25:GLY:C	3:L:27:ARG:H	2.16	0.47
1:A:208:ILE:CD1	1:A:210:PHE:HB2	2.45	0.47
2:H:29:PHE:CG	2:H:76(G):GLY:HA3	2.49	0.46
2:B:169:VAL:HG11	3:C:160:GLU:HB3	1.98	0.46
2:B:216:CYS:C	3:C:211:CYS:HA	2.36	0.46
3:C:61:ARG:HB3	3:C:76:SER:O	2.14	0.46
1:A:343:LYS:HE3	1:A:347:GLU:HG2	1.96	0.46
1:A:231:LYS:HG2	1:A:267:GLU:OE2	2.15	0.46
3:C:210:GLU:HG3	3:C:211:CYS:N	2.30	0.46
2:H:15:GLY:O	2:H:82(C):LEU:HB2	2.15	0.46
2:B:32:GLN:HG3	2:B:94:ARG:CZ	2.46	0.46
2:H:52(A):PRO:O	2:H:71:ARG:NE	2.39	0.46
1:A:116:LEU:HD23	1:A:382:PHE:CZ	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:430:THR:O	1:G:430:THR:OG1	2.31	0.46
2:H:33:PHE:HB2	2:H:100:ASN:OD1	2.16	0.46
1:G:327:ARG:NH2	1:G:422:GLN:OE1	2.43	0.46
2:H:182:VAL:HG23	2:H:184:VAL:HG13	1.97	0.46
3:L:123:GLU:H	3:L:123:GLU:HG2	1.49	0.46
1:A:47:ASP:OD2	1:A:487:LYS:NZ	2.48	0.46
3:C:124:GLU:OE1	3:C:129:LYS:HB2	2.15	0.46
3:C:169:ASN:C	3:C:171:LYS:H	2.18	0.46
1:A:219:THR:CG2	1:A:225:ILE:HG13	2.46	0.46
1:A:64:GLU:HA	1:A:209:SER:HB3	1.98	0.45
1:A:388:THR:HG22	4:A:510:NAG:H81	1.97	0.45
1:A:421:LYS:HG2	5:A:514:EPE:O2S	2.16	0.45
3:C:62:PHE:CD2	3:C:75:ILE:HG12	2.50	0.45
3:C:181:THR:HG23	3:C:184:GLN:NE2	2.31	0.45
1:G:400:THR:HG22	1:G:407:MET:H	1.81	0.45
1:A:348:LYS:HA	1:A:348:LYS:HD3	1.56	0.45
1:G:121:LYS:HB2	1:G:201:ILE:CG1	2.45	0.45
1:G:208:ILE:CD1	1:G:210:PHE:HB2	2.46	0.45
1:A:118:PRO:HG2	1:A:121:LYS:HG3	1.98	0.45
1:G:232[B]:ASN:H	1:G:232[B]:ASN:ND2	2.14	0.45
2:B:138:LEU:HD13	2:B:211:VAL:HG21	1.98	0.45
3:C:169:ASN:O	3:C:171:LYS:N	2.49	0.45
3:L:150:ALA:HB1	3:L:188:HIS:CE1	2.51	0.45
1:A:407:MET:SD	1:A:407:MET:N	2.90	0.45
1:A:60:ALA:HA	1:A:71:THR:HG21	1.99	0.44
2:B:178:LEU:C	2:B:178:LEU:CD1	2.83	0.44
1:G:273:ARG:HB2	1:G:285:ILE:HB	1.99	0.44
1:G:427:TRP:CZ3	1:G:475:ILE:HD13	2.52	0.44
1:A:56:SER:HB3	1:A:215:ILE:HD13	1.98	0.44
3:L:20:THR:HG22	3:L:74:THR:HB	1.99	0.44
2:H:76:ASP:HA	2:H:76(A):PRO:HD3	1.85	0.44
2:H:216:CYS:C	3:L:211:CYS:HA	2.38	0.44
3:C:204:LYS:HA	3:C:204:LYS:HD2	1.75	0.44
3:C:13:ALA:HB2	3:C:19:VAL:HG13	1.99	0.44
1:G:484:TYR:CE1	1:G:485:LYS:HG3	2.52	0.44
2:H:66:ARG:HD2	2:H:82(A):ARG:O	2.17	0.44
2:H:78:ALA:HB1	6:H:335:HOH:O	2.17	0.43
2:B:171:GLN:HG2	3:C:160:GLU:OE1	2.18	0.43
1:G:427:TRP:HZ3	1:G:475:ILE:HD13	1.84	0.43
2:B:201:LYS:HG3	6:B:348:HOH:O	2.17	0.43
1:G:231:LYS:HD3	1:G:267:GLU:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:340:LYS:O	1:G:344:GLN:HG3	2.19	0.43
1:G:227:LYS:HD2	1:G:486:TYR:CE1	2.53	0.43
1:G:123:THR:HG23	1:G:124:GLY:H	1.83	0.43
1:G:460:ALA:O	1:G:462:ASN:N	2.52	0.43
1:A:265:LEU:HD11	1:A:291:SER:OG	2.19	0.43
1:G:80:ASN:HB2	1:G:82:GLN:HE21	1.84	0.43
2:H:121:VAL:HB	2:H:207:VAL:HG11	2.01	0.43
1:A:369:LEU:HA	1:A:372:THR:HG22	2.01	0.43
1:G:395:CYS:HB3	1:G:410:CYS:HB3	1.96	0.43
3:L:179:SER:O	3:L:180:LEU:HD23	2.18	0.43
2:H:122:PHE:CD1	3:L:124:GLU:HB2	2.54	0.43
3:C:115:VAL:O	3:C:204:LYS:NZ	2.51	0.43
3:C:122:SER:O	3:C:126:GLN:HB3	2.19	0.43
3:C:196:THR:HA	3:C:201:THR:HA	2.01	0.42
1:A:484:TYR:CE2	1:A:485:LYS:HG3	2.54	0.42
1:A:64:GLU:OE1	1:A:66:HIS:HB2	2.19	0.42
3:C:37:GLN:HB2	3:C:47:ILE:HD13	2.02	0.42
2:H:47:TRP:CD2	3:L:96:GLU:HB2	2.55	0.42
1:A:342:LEU:O	1:A:346:THR:HG23	2.19	0.42
3:C:21:ILE:HG23	3:C:102:THR:HG21	2.01	0.42
1:A:92:ASN:ND2	6:A:621:HOH:O	2.52	0.42
1:A:462:ASN:HA	6:A:612:HOH:O	2.19	0.42
3:C:13:ALA:HB2	3:C:19:VAL:CG1	2.50	0.42
1:G:289:ASN:O	1:G:290:LYS:HE2	2.20	0.42
2:H:76(C):ASP:H	2:H:76(D):PRO:HD2	1.81	0.42
2:H:53:ILE:HG22	2:H:54:TYR:CD2	2.55	0.42
1:G:474:ASN:OD1	1:G:476:LYS:HB2	2.20	0.42
1:A:389:GLN:NE2	1:A:415:THR:O	2.53	0.41
3:C:17:GLN:O	3:C:78:VAL:HG13	2.19	0.41
3:C:130:ALA:HB3	3:C:180:LEU:HD12	2.02	0.41
1:A:353:PHE:O	1:A:357:LYS:HB2	2.20	0.41
1:A:410:CYS:SG	4:A:510:NAG:O6	2.77	0.41
3:C:145:THR:O	3:C:195:VAL:HA	2.19	0.41
1:G:369:LEU:HD12	1:G:369:LEU:HA	1.86	0.41
1:G:423:ILE:HD12	5:A:513:EPE:O1S	2.20	0.41
1:A:104:MET:O	1:A:108:VAL:HG23	2.20	0.41
1:G:102:GLU:HG3	1:G:476:LYS:CE	2.50	0.41
1:A:110:SER:O	1:A:114:GLN:HG3	2.20	0.41
1:A:390:LEU:HD23	1:A:390:LEU:HA	1.88	0.41
1:G:122:LEU:HD13	1:A:76:PRO:HD2	2.02	0.41
1:G:358:THR:O	1:G:465:ASN:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:390:LEU:HD23	1:G:390:LEU:HA	1.78	0.41
5:A:513:EPE:H51	5:A:513:EPE:H82	1.60	0.41
1:A:103:GLN:HB3	5:A:513:EPE:H81	2.03	0.41
3:C:180:LEU:HD11	3:C:185:TRP:HB2	2.03	0.41
1:A:202:LYS:H	1:A:202:LYS:HG2	1.64	0.41
1:A:290:LYS:CE	1:A:337:LYS:HE3	2.51	0.41
1:G:290:LYS:HD3	6:G:602:HOH:O	2.21	0.41
1:A:243:SER:HB3	6:A:654:HOH:O	2.20	0.41
2:B:32:GLN:OE1	2:B:97:SER:HA	2.20	0.41
1:G:102:GLU:HG3	1:G:476:LYS:HE2	2.03	0.40
2:B:163:VAL:HG22	2:B:182:VAL:HB	2.03	0.40
3:C:62:PHE:CE2	3:C:75:ILE:HG12	2.56	0.40
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.56	0.40
1:A:477:ASP:HA	1:A:480:ARG:HG3	2.03	0.40
3:C:156:LYS:O	3:C:159:VAL:HG13	2.21	0.40
1:G:54:CYS:HA	1:G:216:HIS:O	2.22	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%)	319 (93%)	20 (6%)	3 (1%)	17	11
1	G	344/355 (97%)	319 (93%)	17 (5%)	8 (2%)	6	1
2	B	220/230 (96%)	209 (95%)	11 (5%)	0	100	100
2	H	219/230 (95%)	210 (96%)	6 (3%)	3 (1%)	11	5
3	C	200/203 (98%)	188 (94%)	8 (4%)	4 (2%)	7	2
3	L	200/203 (98%)	183 (92%)	15 (8%)	2 (1%)	15	9
All	All	1525/1576 (97%)	1428 (94%)	77 (5%)	20 (1%)	12	6

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	409	GLY
1	G	430	THR
1	G	461	ASN
2	H	76(D)	PRO
1	A	474	ASN
1	A	430	THR
1	G	124	GLY
1	A	408	LYS
3	C	24	SER
1	G	408	LYS
1	G	457	ASP
1	G	460	ALA
1	G	462	ASN
2	H	136	ALA
3	C	32	ILE
3	C	168	SER
3	C	170	ASN
3	L	151	ASP
2	H	214	LYS
3	L	67	PRO

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%)	290 (94%)	19 (6%)	18	14
1	G	311/313 (99%)	300 (96%)	11 (4%)	36	34
2	B	190/195 (97%)	175 (92%)	15 (8%)	12	7
2	H	190/195 (97%)	180 (95%)	10 (5%)	22	19
3	C	173/174 (99%)	162 (94%)	11 (6%)	17	12
3	L	173/174 (99%)	162 (94%)	11 (6%)	17	12
All	All	1346/1364 (99%)	1269 (94%)	77 (6%)	20	16

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	62	GLU
1	G	199	SER
1	G	267	GLU
1	G	276	ASN
1	G	340	LYS
1	G	400	THR
1	G	408	LYS
1	G	410	CYS
1	G	427	TRP
1	G	430	THR
1	G	492	GLU
2	H	1	HIS
2	H	68	THR
2	H	76	ASP
2	H	83	ARG
2	H	97	SER
2	H	113	SER
2	H	159	LEU
2	H	161	SER
2	H	186	SER
2	H	199	ASN
3	L	12	SER
3	L	18	SER
3	L	23	CYS
3	L	24	SER
3	L	61	ARG
3	L	74	THR
3	L	114	SER
3	L	123	GLU
3	L	129	LYS
3	L	145	THR
3	L	155	VAL
1	A	88	ASN
1	A	202	LYS
1	A	207	LYS
1	A	209	SER
1	A	290	LYS
1	A	327	ARG
1	A	328	LYS
1	A	340	LYS
1	A	347	GLU
1	A	348	LYS

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Mol	Chain	Res	Type
1	A	357	LYS
1	A	407	MET
1	A	413	THR
1	A	419	LYS
1	A	422	GLN
1	A	426	MET
1	A	427	TRP
1	A	465	ASN
1	A	489	VAL
2	B	7	SER
2	B	24	VAL
2	B	60	SER
2	B	71	ARG
2	B	76(E)	ASP
2	B	83	ARG
2	B	113	SER
2	B	115	SER
2	B	153	SER
2	B	177	SER
2	B	178	LEU
2	B	191	THR
2	B	207	VAL
2	B	209	LYS
2	B	215	SER
3	C	3	LEU
3	C	22	SER
3	C	122	SER
3	C	161	THR
3	C	162	THR
3	C	163	LYS
3	C	168	SER
3	C	193	CYS
3	C	196	THR
3	C	200	SER
3	C	204	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	114	GLN
1	G	461	ASN
1	A	114	GLN

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Mol	Chain	Res	Type
1	A	117	GLN
1	A	229	ASN
2	B	101	HIS
2	B	171	GLN
2	B	199	ASN
3	C	184	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [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	G	504	1	14,14,15	0.27	0	17,19,21	1.23	1 (5%)
4	NAG	A	505	1	14,14,15	0.46	0	17,19,21	0.53	0
4	NAG	A	504	1	14,14,15	0.31	0	17,19,21	0.52	0
4	NAG	A	507	1	14,14,15	0.41	0	17,19,21	0.48	0
4	NAG	A	502	1	14,14,15	0.34	0	17,19,21	0.53	0
5	EPE	G	512	-	15,15,15	0.72	1 (6%)	18,20,20	1.73	4 (22%)
4	NAG	G	503	1	14,14,15	0.69	1 (7%)	17,19,21	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	502	1	14,14,15	0.28	0	17,19,21	0.35	0
4	NAG	G	506	1	14,14,15	0.25	0	17,19,21	0.62	1 (5%)
5	EPE	A	514	-	15,15,15	0.72	1 (6%)	18,20,20	1.77	4 (22%)
4	NAG	G	510	1	14,14,15	0.53	0	17,19,21	0.57	0
4	NAG	A	512	1	14,14,15	0.92	1 (7%)	17,19,21	1.38	3 (17%)
4	NAG	G	511	1	14,14,15	0.38	0	17,19,21	0.60	1 (5%)
4	NAG	G	508	1	14,14,15	0.55	0	17,19,21	0.51	0
4	NAG	A	503	1	14,14,15	0.42	0	17,19,21	0.69	1 (5%)
5	EPE	A	513	-	15,15,15	0.76	1 (6%)	18,20,20	1.97	7 (38%)
4	NAG	A	501	1	14,14,15	0.33	0	17,19,21	0.69	0
4	NAG	G	507	1	14,14,15	0.25	0	17,19,21	0.55	0
4	NAG	G	509	1	14,14,15	0.28	0	17,19,21	0.66	1 (5%)
4	NAG	G	505	1	14,14,15	0.22	0	17,19,21	0.37	0
4	NAG	A	508	1	14,14,15	0.28	0	17,19,21	0.84	1 (5%)
4	NAG	A	506	1	14,14,15	0.33	0	17,19,21	0.51	0
4	NAG	G	501	1	14,14,15	1.18	2 (14%)	17,19,21	1.46	3 (17%)
4	NAG	A	510	1	14,14,15	0.29	0	17,19,21	0.49	0
4	NAG	A	511	1	14,14,15	0.36	0	17,19,21	0.70	0
4	NAG	A	509	1	14,14,15	0.38	0	17,19,21	0.53	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	G	504	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	504	1	-	2/6/23/26	0/1/1/1
4	NAG	A	507	1	-	0/6/23/26	0/1/1/1
4	NAG	A	502	1	-	2/6/23/26	0/1/1/1
5	EPE	G	512	-	-	6/9/19/19	0/1/1/1
4	NAG	G	503	1	-	2/6/23/26	0/1/1/1
4	NAG	G	502	1	-	0/6/23/26	0/1/1/1
4	NAG	G	506	1	-	0/6/23/26	0/1/1/1
5	EPE	A	514	-	-	6/9/19/19	0/1/1/1
4	NAG	G	510	1	-	0/6/23/26	0/1/1/1
4	NAG	A	512	1	-	0/6/23/26	0/1/1/1
4	NAG	G	511	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	G	508	1	-	2/6/23/26	0/1/1/1
4	NAG	A	503	1	-	0/6/23/26	0/1/1/1
5	EPE	A	513	-	-	4/9/19/19	0/1/1/1
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	NAG	G	507	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	505	1	-	0/6/23/26	0/1/1/1
4	NAG	A	508	1	-	1/6/23/26	0/1/1/1
4	NAG	A	506	1	-	2/6/23/26	0/1/1/1
4	NAG	G	501	1	-	1/6/23/26	0/1/1/1
4	NAG	A	510	1	-	1/6/23/26	0/1/1/1
4	NAG	A	511	1	-	2/6/23/26	0/1/1/1
4	NAG	A	509	1	-	2/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	501	NAG	O5-C1	3.43	1.49	1.43
4	A	512	NAG	O5-C1	2.99	1.48	1.43
4	G	501	NAG	C1-C2	2.67	1.56	1.52
5	A	513	EPE	C10-S	2.36	1.80	1.77
5	G	512	EPE	C10-S	2.33	1.80	1.77
4	G	503	NAG	O5-C1	2.23	1.47	1.43
5	A	514	EPE	C10-S	2.21	1.80	1.77

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	504	NAG	C1-O5-C5	4.48	118.26	112.19
4	G	501	NAG	C1-O5-C5	4.47	118.25	112.19
5	G	512	EPE	C5-N4-C3	4.28	118.46	108.83
5	A	513	EPE	C5-N4-C3	3.91	117.64	108.83
5	A	514	EPE	C5-N4-C3	3.89	117.58	108.83
4	A	512	NAG	C1-O5-C5	3.58	117.05	112.19
5	A	514	EPE	C7-N4-C5	3.38	119.87	111.23
5	A	514	EPE	O3S-S-C10	3.30	111.11	105.77
5	G	512	EPE	C7-N4-C5	3.29	119.64	111.23
5	A	513	EPE	C7-N4-C3	3.25	119.54	111.23
5	A	513	EPE	C7-N4-C5	2.93	118.73	111.23
5	G	512	EPE	C7-N4-C3	2.80	118.40	111.23
4	A	508	NAG	C1-O5-C5	2.79	115.97	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	514	EPE	C6-N1-C2	2.73	114.98	108.83
5	G	512	EPE	O3S-S-C10	2.71	110.15	105.77
4	A	503	NAG	C1-O5-C5	2.44	115.49	112.19
5	A	513	EPE	O3S-S-C10	2.42	109.67	105.77
5	A	513	EPE	C9-N1-C2	-2.40	105.11	111.23
4	G	509	NAG	C1-O5-C5	2.32	115.34	112.19
5	A	513	EPE	O1S-S-C10	2.24	109.62	106.92
4	A	512	NAG	C4-C3-C2	-2.18	107.83	111.02
5	A	513	EPE	C9-N1-C6	-2.12	105.81	111.23
4	A	512	NAG	C3-C4-C5	-2.11	106.48	110.24
4	G	501	NAG	C3-C4-C5	-2.05	106.59	110.24
4	G	506	NAG	C1-O5-C5	2.03	114.94	112.19
4	G	511	NAG	C1-O5-C5	2.02	114.93	112.19
4	G	501	NAG	C2-N2-C7	2.01	125.77	122.90

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	512	EPE	C8-C7-N4-C3
5	G	512	EPE	C9-C10-S-O2S
5	A	513	EPE	C8-C7-N4-C5
5	A	514	EPE	S-C10-C9-N1
5	A	514	EPE	C9-C10-S-O1S
5	A	514	EPE	C9-C10-S-O2S
5	A	514	EPE	C9-C10-S-O3S
4	A	511	NAG	O5-C5-C6-O6
4	A	504	NAG	O5-C5-C6-O6
4	G	503	NAG	C4-C5-C6-O6
4	A	509	NAG	O5-C5-C6-O6
4	A	509	NAG	C4-C5-C6-O6
4	A	511	NAG	C4-C5-C6-O6
4	A	504	NAG	C4-C5-C6-O6
4	G	503	NAG	O5-C5-C6-O6
4	A	502	NAG	O5-C5-C6-O6
5	G	512	EPE	C9-C10-S-O3S
4	A	506	NAG	O5-C5-C6-O6
4	G	501	NAG	C1-C2-N2-C7
4	A	510	NAG	O5-C5-C6-O6
5	A	513	EPE	N4-C7-C8-O8
4	A	502	NAG	C4-C5-C6-O6
5	G	512	EPE	C10-C9-N1-C6

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Mol	Chain	Res	Type	Atoms
5	A	513	EPE	C10-C9-N1-C2
5	A	513	EPE	C10-C9-N1-C6
5	G	512	EPE	C9-C10-S-O1S
4	A	506	NAG	C4-C5-C6-O6
5	A	514	EPE	N4-C7-C8-O8
5	G	512	EPE	C10-C9-N1-C2
4	G	508	NAG	O5-C5-C6-O6
4	A	508	NAG	C4-C5-C6-O6
5	A	514	EPE	C8-C7-N4-C3
4	G	508	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	514	EPE	4	0
5	A	513	EPE	3	0
4	A	510	NAG	2	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	346/355 (97%)	-0.28	3 (0%) 84 88	31, 45, 73, 89	0
1	G	347/355 (97%)	-0.19	8 (2%) 60 68	32, 45, 73, 91	0
2	B	224/230 (97%)	-0.28	1 (0%) 92 94	29, 46, 74, 90	0
2	H	223/230 (96%)	-0.34	1 (0%) 92 94	29, 45, 72, 88	0
3	C	202/203 (99%)	-0.09	2 (0%) 82 86	37, 53, 66, 92	0
3	L	202/203 (99%)	-0.24	1 (0%) 91 93	36, 54, 65, 91	0
All	All	1544/1576 (97%)	-0.24	16 (1%) 82 86	29, 48, 72, 92	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	211	CYS	6.5
1	A	398	ASN	3.5
1	A	397	GLY	3.5
1	G	399	GLU	3.3
1	A	200	VAL	3.3
1	G	461	ASN	3.2
1	G	428	GLN	3.1
2	B	216	CYS	2.5
1	G	400	THR	2.4
3	L	211	CYS	2.4
1	G	407	MET	2.3
2	H	215	SER	2.2
1	G	429	GLY	2.1
1	G	240	LYS	2.1
1	G	398	ASN	2.0
3	C	129	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 monosaccharides 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(\AA^2)	Q<0.9
4	NAG	G	505	14/15	0.70	0.22	60,73,84,85	0
4	NAG	G	501	14/15	0.76	0.26	75,92,100,105	0
4	NAG	A	501	14/15	0.82	0.30	79,88,94,97	0
4	NAG	A	505	14/15	0.83	0.25	66,74,85,86	0
4	NAG	A	509	14/15	0.85	0.20	51,66,71,76	0
4	NAG	A	512	14/15	0.87	0.20	54,73,80,96	0
4	NAG	A	511	14/15	0.88	0.23	54,66,87,94	0
4	NAG	A	503	14/15	0.88	0.27	63,79,89,90	0
5	EPE	G	512	15/15	0.88	0.18	70,82,114,124	0
4	NAG	G	511	14/15	0.90	0.15	54,68,78,80	0
4	NAG	A	506	14/15	0.90	0.12	45,52,59,62	0
4	NAG	G	503	14/15	0.91	0.14	69,89,97,97	0
4	NAG	G	510	14/15	0.91	0.14	53,69,77,77	0
4	NAG	A	510	14/15	0.91	0.16	66,74,79,83	0
4	NAG	G	509	14/15	0.93	0.15	48,58,65,72	0
4	NAG	G	506	14/15	0.93	0.11	46,52,58,64	0
4	NAG	A	507	14/15	0.94	0.12	38,51,57,61	0
4	NAG	A	502	14/15	0.94	0.13	40,44,54,63	0
5	EPE	A	514	15/15	0.94	0.13	53,60,105,107	0
4	NAG	G	502	14/15	0.95	0.09	38,49,53,56	0
4	NAG	G	507	14/15	0.95	0.09	41,50,57,57	0
4	NAG	A	504	14/15	0.95	0.10	29,39,47,48	0
4	NAG	G	504	14/15	0.96	0.11	31,37,43,50	0
4	NAG	G	508	14/15	0.96	0.10	34,48,56,57	0
5	EPE	A	513	15/15	0.96	0.18	41,52,65,74	0
4	NAG	A	508	14/15	0.96	0.07	40,49,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.