



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:07 AM BST

PDB ID : 6OZ3  
Title : Crystal structure of broadly neutralizing antibody N49P9.1 Fab in complex with HIV-1 Clade A/E strain 93TH057 gp120 core  
Authors : Tolbert, W.D.; Pazgier, M.  
Deposited on : 2019-05-15  
Resolution : 3.15 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](mailto: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.

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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 : 2.13  
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) : 2.13

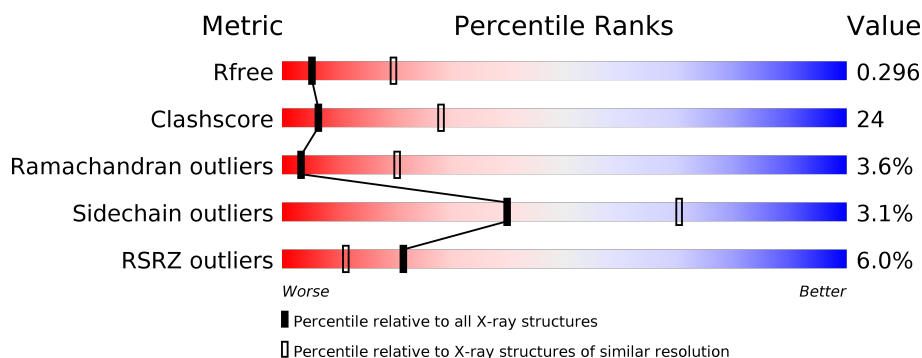
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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  $\geq 3$ , 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	G	355	<div> <div>8%</div> <div> <div></div> <div>50%</div> <div>37%</div> <div>10%</div> </div> </div>
2	H	221	<div> <div>5%</div> <div> <div></div> <div>54%</div> <div>40%</div> <div>6%</div> </div> </div>
3	L	203	<div> <div>2%</div> <div> <div></div> <div>57%</div> <div>35%</div> <div>6%</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
4	NAG	G	502	-	-	X	X
4	NAG	G	507	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5817 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	319	Total	C	N	O	S	0	0	0
			2506	1571	434	481	20			

There are 3 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

- Molecule 2 is a protein called N49P9.1 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1647	1045	283	309	10			

- Molecule 3 is a protein called N49P9.1 antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	200	Total	C	N	O	S	0	0	0
			1509	948	253	303	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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		

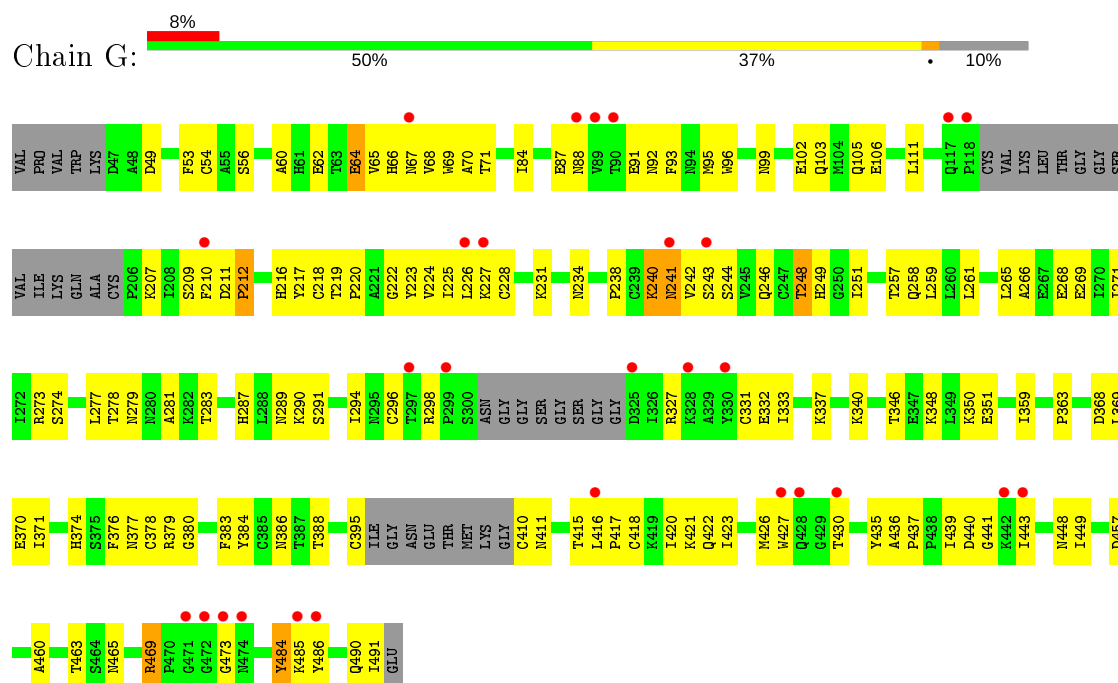
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Na	0	0
			1	1		

### 3 Residue-property plots [i](#)

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.

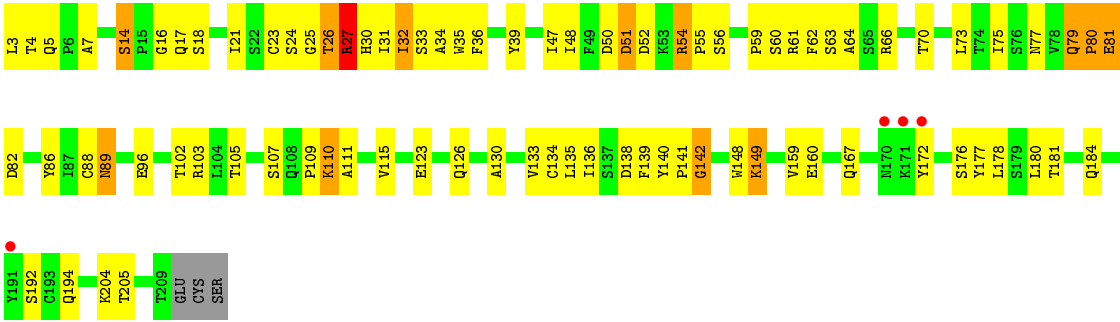
- Molecule 1: clade A/E 93TH057 HIV-1 gp120 core



- Molecule 2: N49P9.1 antibody Fab heavy chain



- Molecule 3: N49P9.1 antibody Fab light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.75Å 110.45Å 152.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.03 – 3.15 35.19 – 3.15	Depositor EDS
% Data completeness (in resolution range)	93.9 (34.03-3.15) 94.0 (35.19-3.15)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, $R_{free}$	0.243 , 0.295 0.243 , 0.296	Depositor DCC
$R_{free}$ test set	734 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	116.1	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 73.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5817	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	G	0.35	0/2558	0.61	0/3472
2	H	0.31	0/1692	0.59	0/2306
3	L	0.34	0/1549	0.59	0/2117
All	All	0.34	0/5799	0.60	0/7895

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2506	0	2429	139	0
2	H	1647	0	1601	75	0
3	L	1509	0	1469	70	0
4	G	154	0	143	13	0
5	H	1	0	0	0	0
All	All	5817	0	5642	275	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 24.

All (275) 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:210:PHE:HZ	1:G:377:ASN:ND2	1.48	1.11
1:G:210:PHE:CE2	1:G:380:GLY:HA2	1.89	1.07
1:G:65:VAL:CG1	1:G:210:PHE:HB3	1.85	1.06
1:G:410:CYS:N	4:G:509:NAG:HO6	1.61	0.97
1:G:427:TRP:HA	2:H:54:TYR:OH	1.65	0.95
1:G:65:VAL:HG22	1:G:210:PHE:HB2	1.48	0.94
1:G:65:VAL:HG13	1:G:210:PHE:HB3	1.53	0.91
1:G:65:VAL:CG2	1:G:210:PHE:HB2	2.01	0.89
1:G:210:PHE:CZ	1:G:380:GLY:HA2	2.08	0.88
1:G:332:GLU:HG2	1:G:415:THR:HG22	1.56	0.88
1:G:210:PHE:CZ	1:G:377:ASN:ND2	2.41	0.88
3:L:3:LEU:HG	3:L:4:THR:HG23	1.59	0.85
3:L:54:ARG:HH22	3:L:60:SER:HA	1.41	0.85
1:G:460:ALA:HB2	2:H:61:TRP:CD1	2.12	0.85
3:L:21:ILE:HD12	3:L:102:THR:HG21	1.58	0.85
1:G:84:ILE:HB	1:G:244:SER:HB3	1.61	0.83
1:G:219:THR:HG23	1:G:246:GLN:HE21	1.42	0.83
1:G:65:VAL:HG11	1:G:210:PHE:HB3	1.61	0.81
1:G:210:PHE:HZ	1:G:377:ASN:HD21	1.28	0.81
1:G:265:LEU:HD11	1:G:291:SER:HB2	1.63	0.77
1:G:240:LYS:HD3	4:G:502:NAG:H81	1.65	0.77
1:G:240:LYS:CD	4:G:502:NAG:H81	2.14	0.77
1:G:226:LEU:O	1:G:486:TYR:HA	1.86	0.76
1:G:395:CYS:SG	1:G:410:CYS:N	2.59	0.76
2:H:6:GLN:O	2:H:105:GLN:NE2	2.21	0.73
1:G:65:VAL:CG2	1:G:210:PHE:CB	2.66	0.73
2:H:87:THR:HG23	2:H:110:VAL:HA	1.70	0.73
1:G:240:LYS:HD3	4:G:502:NAG:C8	2.19	0.71
2:H:95:GLY:HA3	2:H:100:ASN:O	1.91	0.71
1:G:207:LYS:HD3	1:G:439:ILE:HB	1.74	0.70
2:H:139:GLY:HA3	2:H:181:VAL:HG12	1.75	0.69
1:G:220:PRO:O	1:G:246:GLN:NE2	2.25	0.69
3:L:34:ALA:HB3	3:L:89:ASN:HD21	1.58	0.69
2:H:126:PRO:HG3	2:H:138:LEU:HB3	1.74	0.69
1:G:298:ARG:HD3	1:G:443:ILE:HD12	1.73	0.68
1:G:278:THR:HG21	4:G:504:NAG:H61	1.77	0.67
1:G:210:PHE:CE2	1:G:380:GLY:CA	2.74	0.67
3:L:105:THR:HG21	3:L:141:PRO:HB3	1.77	0.66
1:G:274:SER:HB3	1:G:277:LEU:HD12	1.77	0.66
1:G:65:VAL:HG23	1:G:66:HIS:CD2	2.31	0.66
1:G:327:ARG:HD3	1:G:422:GLN:HE22	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:66:ARG:NH2	2:H:86:ASP:OD2	2.27	0.65
2:H:24:VAL:HG21	2:H:29:PHE:HD1	1.62	0.65
1:G:66:HIS:CD2	1:G:111:LEU:HD11	2.32	0.64
2:H:71:ARG:HG2	2:H:71:ARG:HH21	1.61	0.64
3:L:159:VAL:HG22	3:L:178:LEU:HD13	1.77	0.64
1:G:379:ARG:CZ	1:G:439:ILE:HG21	2.28	0.64
1:G:346:THR:HG23	1:G:359:ILE:HB	1.79	0.64
1:G:377:ASN:OD1	1:G:378:CYS:N	2.30	0.64
1:G:241:ASN:N	1:G:241:ASN:OD1	2.31	0.63
2:H:148:GLU:HG2	2:H:149:PRO:HA	1.79	0.63
1:G:219:THR:O	1:G:246:GLN:NE2	2.32	0.63
2:H:54:TYR:O	2:H:71:ARG:NH1	2.33	0.62
1:G:436:ALA:HB1	1:G:437:PRO:HD2	1.82	0.61
1:G:64:GLU:HB2	1:G:67:ASN:HB2	1.82	0.61
2:H:90:TYR:O	2:H:106:GLY:HA2	2.00	0.61
1:G:224:VAL:HG22	1:G:225:ILE:H	1.65	0.61
1:G:266:ALA:H	1:G:289:ASN:HA	1.66	0.61
1:G:440:ASP:OD1	1:G:441:GLY:N	2.33	0.61
3:L:79:GLN:HB2	3:L:80:PRO:CD	2.31	0.61
3:L:148:TRP:HE1	3:L:176:SER:HG	1.46	0.60
3:L:181:THR:HB	3:L:184:GLN:HG3	1.82	0.60
2:H:152:VAL:HG22	2:H:198:VAL:HA	1.82	0.60
2:H:99:GLU:CD	2:H:100:ASN:H	2.05	0.59
2:H:35:ASN:OD1	2:H:50:TRP:HB3	2.01	0.59
2:H:87:THR:HA	2:H:109:VAL:O	2.02	0.59
1:G:95:MET:SD	1:G:273:ARG:HD2	2.42	0.59
3:L:34:ALA:HB3	3:L:89:ASN:ND2	2.18	0.59
1:G:56:SER:CB	1:G:70:ALA:HB1	2.33	0.59
3:L:130:ALA:HB3	3:L:180:LEU:O	2.02	0.58
1:G:66:HIS:ND1	1:G:211:ASP:O	2.36	0.58
3:L:54:ARG:NH2	3:L:59:PRO:O	2.37	0.58
3:L:136:ILE:HD12	3:L:136:ILE:H	1.69	0.58
1:G:223:TYR:HD1	1:G:490:GLN:HA	1.69	0.58
1:G:370:GLU:HG3	1:G:384:TYR:HE1	1.67	0.57
2:H:116:THR:HA	2:H:146:PHE:HD2	1.70	0.57
1:G:49:ASP:OD2	1:G:99:ASN:ND2	2.37	0.57
1:G:102:GLU:O	1:G:106:GLU:HG2	2.05	0.57
1:G:371:ILE:HD13	2:H:56:GLN:HG3	1.87	0.57
1:G:240:LYS:CE	4:G:502:NAG:H81	2.34	0.57
1:G:298:ARG:HD2	1:G:420:ILE:CD1	2.34	0.57
2:H:99:GLU:CG	2:H:100:ASN:H	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:HIS:HD2	1:G:111:LEU:HD11	1.69	0.56
1:G:421:LYS:HE3	1:G:423:ILE:HG13	1.86	0.56
2:H:13:LYS:HD3	2:H:114:PRO:HA	1.86	0.56
3:L:33:SER:N	3:L:51:ASP:OD1	2.38	0.56
3:L:133:VAL:HG22	3:L:177:TYR:CD1	2.41	0.56
3:L:31:ILE:O	3:L:32:ILE:HG13	2.05	0.56
3:L:54:ARG:NH2	3:L:60:SER:HA	2.15	0.56
1:G:65:VAL:HG21	1:G:210:PHE:CB	2.35	0.56
1:G:261:LEU:HD23	1:G:449:ILE:HA	1.88	0.55
1:G:91:GLU:HG2	1:G:92:ASN:N	2.22	0.55
3:L:107:SER:O	3:L:109:PRO:HD3	2.06	0.55
3:L:149:LYS:HD3	3:L:194:GLN:OE1	2.07	0.55
1:G:298:ARG:HB3	1:G:443:ILE:HB	1.89	0.55
1:G:290:LYS:HE3	1:G:337:LYS:HE3	1.89	0.55
1:G:240:LYS:CE	4:G:502:NAG:C8	2.84	0.55
2:H:119:PRO:HB3	2:H:142:VAL:HG23	1.89	0.55
1:G:259:LEU:HB2	1:G:374:HIS:CE1	2.42	0.55
1:G:65:VAL:HG21	1:G:210:PHE:HB2	1.86	0.55
3:L:47:ILE:O	3:L:55:PRO:HD2	2.07	0.55
1:G:289:ASN:OD1	1:G:290:LYS:HG3	2.07	0.55
1:G:207:LYS:HG3	1:G:435:TYR:OH	2.07	0.55
1:G:240:LYS:HE3	4:G:502:NAG:C8	2.38	0.54
3:L:7:ALA:O	3:L:103:ARG:NH1	2.40	0.54
1:G:65:VAL:HG22	1:G:210:PHE:CB	2.27	0.54
3:L:79:GLN:CB	3:L:80:PRO:HD3	2.37	0.54
2:H:172:SER:OG	3:L:160:GLU:OE2	2.23	0.54
3:L:16:GLY:HA2	3:L:77:ASN:OD1	2.07	0.54
1:G:379:ARG:HG2	1:G:443:ILE:HG12	1.89	0.54
3:L:79:GLN:HB2	3:L:80:PRO:HD3	1.89	0.54
2:H:54:TYR:HB2	2:H:56:GLN:OE1	2.08	0.54
1:G:96:TRP:CZ2	1:G:274:SER:HA	2.43	0.53
1:G:469:ARG:HH11	1:G:469:ARG:HG2	1.73	0.53
1:G:257:THR:O	1:G:374:HIS:ND1	2.41	0.53
2:H:19:ARG:CG	2:H:81:GLU:HG2	2.39	0.53
3:L:36:PHE:HE2	3:L:89:ASN:ND2	2.06	0.53
1:G:240:LYS:HE3	4:G:502:NAG:H81	1.90	0.53
1:G:93:PHE:CE2	1:G:228:CYS:HB2	2.43	0.53
1:G:281:ALA:HB3	2:H:99:GLU:OE1	2.08	0.53
3:L:139:PHE:CE1	3:L:142:GLY:HA2	2.44	0.53
2:H:151:THR:HG23	2:H:199:ASN:HB3	1.91	0.53
1:G:222:GLY:HA2	1:G:491:ILE:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:350:LYS:HG2	1:G:359:ILE:HG12	1.92	0.52
3:L:61:ARG:NH2	3:L:82:ASP:OD2	2.31	0.52
2:H:96:PRO:HD2	2:H:100:ASN:O	2.09	0.52
3:L:139:PHE:HE1	3:L:142:GLY:HA2	1.73	0.52
2:H:116:THR:O	2:H:118:GLY:N	2.43	0.52
1:G:273:ARG:HH22	1:G:287:HIS:HB2	1.75	0.51
3:L:133:VAL:HG22	3:L:177:TYR:CE1	2.45	0.51
3:L:80:PRO:HG2	3:L:81:GLU:H	1.75	0.51
2:H:10:GLY:O	2:H:109:VAL:HA	2.09	0.51
3:L:192:SER:OG	3:L:205:THR:HG22	2.10	0.51
1:G:331:CYS:HB2	1:G:418:CYS:SG	2.51	0.51
1:G:386:ASN:O	1:G:416:LEU:HD22	2.11	0.50
1:G:448:ASN:HD22	4:G:510:NAG:H83	1.77	0.50
1:G:91:GLU:O	1:G:238:PRO:HA	2.11	0.50
2:H:150:VAL:HG22	2:H:200:HIS:CD2	2.46	0.50
2:H:137:ALA:HB2	2:H:183:THR:HG22	1.94	0.50
3:L:47:ILE:HD12	3:L:62:PHE:CD1	2.46	0.50
1:G:209:SER:HB3	1:G:379:ARG:CZ	2.41	0.50
2:H:196:CYS:O	2:H:197:ASN:ND2	2.45	0.50
1:G:370:GLU:HG3	1:G:384:TYR:CE1	2.47	0.50
1:G:296:CYS:SG	1:G:376:PHE:HZ	2.35	0.50
1:G:66:HIS:ND1	1:G:212:PRO:HA	2.26	0.50
1:G:279:ASN:ND2	2:H:99:GLU:OE1	2.44	0.50
1:G:240:LYS:CD	4:G:502:NAG:C8	2.84	0.49
1:G:346:THR:O	1:G:350:LYS:HG3	2.12	0.49
3:L:109:PRO:O	3:L:110:LYS:HG2	2.12	0.49
3:L:30:HIS:HA	3:L:66:ARG:HH11	1.78	0.49
1:G:105:GLN:NE2	1:G:427:TRP:HZ3	2.10	0.49
3:L:82:ASP:HA	3:L:86:TYR:OH	2.13	0.49
1:G:337:LYS:HD2	1:G:340:LYS:HE2	1.94	0.49
2:H:66:ARG:HH22	2:H:86:ASP:CG	2.14	0.49
3:L:26:THR:O	3:L:27:ARG:HB2	2.12	0.49
3:L:32:ILE:HD12	3:L:33:SER:N	2.28	0.49
2:H:57:VAL:HG21	2:H:59:TYR:CZ	2.48	0.49
1:G:216:HIS:HD2	1:G:248:THR:O	1.96	0.48
1:G:388:THR:HG21	4:G:508:NAG:H5	1.95	0.48
1:G:227:LYS:HB3	1:G:243:SER:HB3	1.95	0.48
3:L:111:ALA:HB3	3:L:140:TYR:O	2.14	0.48
1:G:222:GLY:O	1:G:491:ILE:N	2.40	0.48
1:G:273:ARG:NH2	1:G:287:HIS:HB2	2.29	0.48
1:G:105:GLN:NE2	1:G:427:TRP:CZ3	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:15:GLY:O	2:H:82(C):LEU:HD12	2.14	0.48
2:H:198:VAL:O	2:H:206:LYS:HA	2.14	0.48
2:H:19:ARG:HG2	2:H:81:GLU:HG2	1.94	0.48
1:G:228:CYS:H	1:G:485:LYS:HB2	1.79	0.48
3:L:136:ILE:HD12	3:L:136:ILE:N	2.28	0.48
1:G:294:ILE:HA	1:G:333:ILE:HG22	1.96	0.48
1:G:386:ASN:HB3	1:G:417:PRO:HG2	1.95	0.48
2:H:85:ASP:OD1	2:H:86:ASP:N	2.47	0.47
3:L:39:TYR:OH	3:L:81:GLU:HG2	2.15	0.47
1:G:421:LYS:HE3	1:G:423:ILE:CG1	2.44	0.47
3:L:61:ARG:HH22	3:L:82:ASP:CG	2.15	0.47
3:L:51:ASP:O	3:L:64:ALA:HB3	2.14	0.47
1:G:348:LYS:NZ	1:G:351:GLU:OE1	2.48	0.47
2:H:6:GLN:H	2:H:105:GLN:NE2	2.12	0.47
2:H:22:CYS:O	2:H:77:THR:OG1	2.29	0.47
1:G:327:ARG:HD3	1:G:422:GLN:NE2	2.27	0.47
1:G:363:PRO:O	1:G:469:ARG:NH1	2.47	0.47
1:G:103:GLN:O	1:G:106:GLU:HB2	2.15	0.47
2:H:168:ALA:HA	2:H:178:LEU:HB3	1.96	0.47
2:H:166:PHE:CD2	3:L:135:LEU:HD22	2.50	0.47
3:L:63:SER:O	3:L:73:LEU:HD12	2.15	0.46
2:H:66:ARG:O	2:H:82(A):ARG:HG2	2.15	0.46
3:L:134:CYS:HB2	3:L:148:TRP:CZ2	2.50	0.46
3:L:79:GLN:CB	3:L:80:PRO:CD	2.92	0.46
1:G:64:GLU:O	1:G:68:VAL:HG22	2.14	0.46
1:G:65:VAL:CG1	1:G:210:PHE:CB	2.77	0.46
2:H:195:ILE:HG22	2:H:196:CYS:O	2.14	0.46
1:G:53:PHE:CE1	1:G:218:CYS:HB2	2.50	0.46
3:L:115:VAL:HG13	3:L:204:LYS:HG3	1.96	0.46
1:G:234:ASN:O	1:G:273:ARG:HG2	2.15	0.46
2:H:23:GLU:HG3	2:H:77:THR:OG1	2.16	0.46
1:G:296:CYS:HB3	1:G:383:PHE:CE2	2.51	0.46
1:G:463:THR:HB	1:G:465:ASN:OD1	2.16	0.46
2:H:24:VAL:HG21	2:H:29:PHE:CD1	2.47	0.46
2:H:47:TRP:CG	3:L:96:GLU:HB2	2.51	0.46
2:H:113:SER:HB2	2:H:174:GLY:O	2.16	0.46
1:G:379:ARG:NH1	1:G:439:ILE:HG21	2.31	0.46
3:L:5:GLN:NE2	3:L:102:THR:OG1	2.49	0.46
1:G:265:LEU:HD21	1:G:291:SER:H	1.81	0.45
1:G:60:ALA:HB2	1:G:71:THR:HG21	1.97	0.45
3:L:142:GLY:HA3	3:L:172:TYR:CG	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.99	0.45
3:L:50:ASP:O	3:L:52:ASP:N	2.47	0.45
2:H:150:VAL:HG12	2:H:152:VAL:HG23	1.98	0.45
2:H:121:VAL:HB	2:H:198:VAL:HG21	1.97	0.45
1:G:62:GLU:O	1:G:64:GLU:N	2.45	0.45
2:H:32:GLN:HA	2:H:32:GLN:NE2	2.32	0.45
2:H:32:GLN:OE1	2:H:97:SER:HA	2.16	0.45
1:G:430:THR:HG22	1:G:430:THR:O	2.17	0.45
2:H:100(C):PHE:N	2:H:100(C):PHE:CD2	2.84	0.45
2:H:99:GLU:CG	2:H:100:ASN:N	2.79	0.44
3:L:14:SER:O	3:L:17:GLN:HB2	2.17	0.44
1:G:298:ARG:HD2	1:G:420:ILE:HD12	1.98	0.44
1:G:249:HIS:HB3	1:G:486:TYR:OH	2.18	0.44
1:G:283:THR:HG21	1:G:473:GLY:HA3	1.98	0.44
2:H:31:ASP:O	2:H:32:GLN:HB2	2.17	0.44
2:H:74:ASP:OD2	2:H:74:ASP:N	2.51	0.44
3:L:80:PRO:CG	3:L:81:GLU:H	2.30	0.44
1:G:368:ASP:OD2	2:H:71:ARG:NH1	2.48	0.44
3:L:24:SER:OG	3:L:25:GLY:N	2.49	0.44
2:H:56:GLN:CD	2:H:56:GLN:H	2.21	0.43
2:H:19:ARG:NE	2:H:81:GLU:OE2	2.51	0.43
3:L:111:ALA:HB2	3:L:140:TYR:HB3	2.00	0.43
3:L:18:SER:HA	3:L:75:ILE:O	2.18	0.43
2:H:32:GLN:HG3	2:H:94:ARG:HH11	1.83	0.43
1:G:54:CYS:HA	1:G:217:TYR:HA	2.00	0.43
1:G:240:LYS:O	1:G:242:VAL:N	2.50	0.43
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.53	0.43
3:L:21:ILE:HD12	3:L:102:THR:CG2	2.40	0.43
2:H:40:ALA:HB3	2:H:43:GLN:HB2	2.00	0.43
2:H:12:LYS:O	2:H:111:VAL:HA	2.19	0.43
1:G:249:HIS:CD2	1:G:251:ILE:HG13	2.54	0.42
1:G:350:LYS:HE3	1:G:350:LYS:HB3	1.58	0.42
2:H:71:ARG:HG2	2:H:71:ARG:NH2	2.30	0.42
1:G:240:LYS:CE	4:G:502:NAG:H82	2.49	0.42
1:G:60:ALA:HB2	1:G:71:THR:OG1	2.19	0.42
3:L:123:GLU:O	3:L:126:GLN:HB3	2.19	0.42
1:G:268:GLU:OE1	1:G:269:GLU:HG3	2.19	0.42
3:L:24:SER:HA	3:L:70:THR:HA	2.02	0.42
1:G:283:THR:HG21	1:G:473:GLY:CA	2.50	0.42
1:G:484:TYR:CE2	1:G:485:LYS:HD3	2.54	0.42
2:H:192:GLN:HG2	2:H:193:THR:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:148:TRP:NE1	3:L:176:SER:OG	2.38	0.42
1:G:91:GLU:HG2	1:G:92:ASN:H	1.84	0.41
3:L:26:THR:HG22	3:L:31:ILE:H	1.85	0.41
3:L:32:ILE:O	3:L:66:ARG:HD3	2.19	0.41
2:H:40:ALA:HB1	2:H:41:PRO:HD2	2.02	0.41
1:G:234:ASN:HA	1:G:271:ILE:HG21	2.01	0.41
1:G:69:TRP:CD1	1:G:111:LEU:HD13	2.55	0.41
3:L:138:ASP:OD1	3:L:167:GLN:NE2	2.44	0.41
1:G:266:ALA:HB1	1:G:271:ILE:HD12	2.01	0.41
1:G:369:LEU:HD12	1:G:421:LYS:HE2	2.03	0.41
2:H:47:TRP:CZ2	2:H:49:GLY:HA2	2.56	0.41
1:G:209:SER:HB3	1:G:379:ARG:NH2	2.35	0.41
1:G:435:TYR:CG	1:G:436:ALA:N	2.89	0.41
1:G:469:ARG:NH1	1:G:469:ARG:HG2	2.34	0.41
1:G:249:HIS:CE1	1:G:485:LYS:HZ1	2.39	0.41
2:H:197:ASN:HA	2:H:208:ASP:HB3	2.02	0.41
2:H:19:ARG:HG3	2:H:81:GLU:HG2	2.01	0.41
2:H:82(A):ARG:HG2	2:H:82(A):ARG:H	1.77	0.41
3:L:134:CYS:HB2	3:L:148:TRP:CH2	2.56	0.41
1:G:457:ASP:OD1	1:G:469:ARG:HD2	2.21	0.41
3:L:80:PRO:O	3:L:81:GLU:C	2.59	0.41
2:H:143:LYS:HA	2:H:177:SER:HB3	2.03	0.40
3:L:139:PHE:CE1	3:L:172:TYR:HB2	2.56	0.40
3:L:3:LEU:HD23	3:L:25:GLY:HA3	2.03	0.40
1:G:261:LEU:HA	1:G:448:ASN:O	2.21	0.40
2:H:144:ASP:HB3	2:H:175:LEU:HD13	2.04	0.40
2:H:197:ASN:ND2	2:H:208:ASP:OD2	2.55	0.40
3:L:79:GLN:HE21	3:L:79:GLN:HB3	1.69	0.40
1:G:384:TYR:O	1:G:418:CYS:HA	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	311/355 (88%)	265 (85%)	36 (12%)	10 (3%)	4	22
2	H	210/221 (95%)	179 (85%)	23 (11%)	8 (4%)	3	19
3	L	198/203 (98%)	166 (84%)	24 (12%)	8 (4%)	3	18
All	All	719/779 (92%)	610 (85%)	83 (12%)	26 (4%)	3	20

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	88	ASN
1	G	240	LYS
1	G	241	ASN
3	L	27	ARG
3	L	79	GLN
3	L	80	PRO
3	L	81	GLU
1	G	231	LYS
1	G	248	THR
1	G	426	MET
2	H	16	ALA
2	H	117	LYS
2	H	204	ASN
3	L	32	ILE
3	L	142	GLY
2	H	53	THR
2	H	104	GLY
2	H	105	GLN
3	L	26	THR
2	H	187	SER
3	L	51	ASP
1	G	87	GLU
1	G	258	GLN
1	G	411	ASN
2	H	115	SER
1	G	212	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	G	287/313 (92%)	284 (99%)	3 (1%)	76	89
2	H	182/187 (97%)	174 (96%)	8 (4%)	28	61
3	L	172/175 (98%)	163 (95%)	9 (5%)	23	55
All	All	641/675 (95%)	621 (97%)	20 (3%)	40	70

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	64	GLU
1	G	469	ARG
1	G	484	TYR
2	H	19	ARG
2	H	22	CYS
2	H	52	ASN
2	H	60	SER
2	H	74	ASP
2	H	92	CYS
2	H	117	LYS
2	H	172	SER
3	L	14	SER
3	L	23	CYS
3	L	27	ARG
3	L	54	ARG
3	L	56	SER
3	L	88	CYS
3	L	89	ASN
3	L	110	LYS
3	L	149	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	99	ASN
1	G	216	HIS
1	G	246	GLN
1	G	339	ASN
2	H	105	GLN
2	H	204	ASN
3	L	30	HIS

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Mol	Chain	Res	Type
3	L	89	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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	507	1	14,14,15	0.89	1 (7%)	17,19,21	0.62	0
4	NAG	G	510	1	14,14,15	0.35	0	17,19,21	0.48	0
4	NAG	G	503	1	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	G	508	1	14,14,15	0.50	0	17,19,21	0.40	0
4	NAG	G	502	1	14,14,15	0.73	0	17,19,21	0.90	1 (5%)
4	NAG	G	505	1	14,14,15	0.33	0	17,19,21	0.39	0
4	NAG	G	501	1	14,14,15	0.29	0	17,19,21	0.35	0
4	NAG	G	506	1	14,14,15	0.22	0	17,19,21	0.58	0
4	NAG	G	504	1	14,14,15	0.42	0	17,19,21	0.38	0
4	NAG	G	509	1	14,14,15	0.55	0	17,19,21	0.77	1 (5%)
4	NAG	G	511	1	14,14,15	0.35	0	17,19,21	0.45	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	507	1	-	0/6/23/26	0/1/1/1
4	NAG	G	510	1	-	4/6/23/26	0/1/1/1
4	NAG	G	503	1	-	2/6/23/26	0/1/1/1
4	NAG	G	508	1	-	4/6/23/26	0/1/1/1
4	NAG	G	502	1	-	2/6/23/26	0/1/1/1
4	NAG	G	505	1	-	2/6/23/26	0/1/1/1
4	NAG	G	501	1	-	2/6/23/26	0/1/1/1
4	NAG	G	506	1	-	0/6/23/26	0/1/1/1
4	NAG	G	504	1	-	2/6/23/26	0/1/1/1
4	NAG	G	509	1	-	4/6/23/26	0/1/1/1
4	NAG	G	511	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	507	NAG	O5-C1	-2.88	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	502	NAG	C1-O5-C5	2.90	116.12	112.19
4	G	509	NAG	C3-C4-C5	2.26	114.27	110.24

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	502	NAG	C4-C5-C6-O6
4	G	505	NAG	O5-C5-C6-O6
4	G	501	NAG	O5-C5-C6-O6
4	G	509	NAG	C4-C5-C6-O6
4	G	504	NAG	O5-C5-C6-O6
4	G	509	NAG	O5-C5-C6-O6
4	G	505	NAG	C4-C5-C6-O6
4	G	510	NAG	C8-C7-N2-C2
4	G	510	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	G	508	NAG	C8-C7-N2-C2
4	G	508	NAG	O7-C7-N2-C2
4	G	509	NAG	C8-C7-N2-C2
4	G	509	NAG	O7-C7-N2-C2
4	G	510	NAG	O5-C5-C6-O6
4	G	501	NAG	C4-C5-C6-O6
4	G	502	NAG	O5-C5-C6-O6
4	G	504	NAG	C4-C5-C6-O6
4	G	510	NAG	C4-C5-C6-O6
4	G	508	NAG	C4-C5-C6-O6
4	G	508	NAG	O5-C5-C6-O6
4	G	511	NAG	O5-C5-C6-O6
4	G	503	NAG	C4-C5-C6-O6
4	G	503	NAG	O5-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	510	NAG	1	0
4	G	508	NAG	1	0
4	G	502	NAG	9	0
4	G	504	NAG	1	0
4	G	509	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	G	319/355 (89%)	0.44	28 (8%) 10 5	81, 140, 184, 220	0
2	H	214/221 (96%)	0.34	12 (5%) 24 13	69, 112, 171, 203	0
3	L	200/203 (98%)	0.03	4 (2%) 65 50	77, 111, 146, 162	0
All	All	733/779 (94%)	0.30	44 (6%) 21 11	69, 121, 176, 220	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	204	ASN	7.3
1	G	325	ASP	7.1
1	G	442	LYS	6.5
1	G	430	THR	5.9
1	G	472	GLY	5.0
1	G	427	TRP	4.9
2	H	191	THR	4.7
1	G	227	LYS	4.7
2	H	205	THR	4.6
1	G	443	ILE	4.3
1	G	328	LYS	4.2
1	G	117	GLN	3.8
2	H	154	TRP	3.6
1	G	90	THR	3.5
1	G	118	PRO	3.4
3	L	170	ASN	3.4
1	G	67	ASN	3.3
1	G	299	PRO	3.3
2	H	119	PRO	3.3
1	G	474	ASN	3.2
1	G	226	LEU	3.2
2	H	206	LYS	3.1
1	G	243	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	184	VAL	2.9
1	G	88	ASN	2.9
1	G	428	GLN	2.8
1	G	89	VAL	2.8
1	G	485	LYS	2.7
1	G	471	GLY	2.6
1	G	297	THR	2.6
3	L	171	LYS	2.6
2	H	199	ASN	2.5
2	H	81	GLU	2.5
3	L	172	TYR	2.4
1	G	486	TYR	2.4
2	H	190	GLY	2.4
1	G	210	PHE	2.3
2	H	126	PRO	2.3
1	G	241	ASN	2.3
2	H	193	THR	2.3
3	L	191	TYR	2.2
1	G	330	TYR	2.1
1	G	473	GLY	2.1
1	G	416	LEU	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	NAG	G	502	14/15	0.66	0.45	138,156,160,162	0
4	NAG	G	509	14/15	0.70	0.33	140,163,168,170	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	G	507	14/15	0.74	0.44	152,167,172,173	0
4	NAG	G	504	14/15	0.86	0.35	117,135,150,150	0
4	NAG	G	511	14/15	0.88	0.29	136,153,157,158	0
4	NAG	G	508	14/15	0.90	0.29	96,122,140,153	0
4	NAG	G	510	14/15	0.90	0.17	105,120,126,130	0
4	NAG	G	506	14/15	0.90	0.34	104,120,130,133	0
4	NAG	G	503	14/15	0.91	0.20	104,120,127,129	0
4	NAG	G	505	14/15	0.94	0.16	90,108,126,130	0
4	NAG	G	501	14/15	0.94	0.13	107,124,132,132	0
5	NA	H	301	1/1	0.96	0.27	54,54,54,54	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.