



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2022 – 02:14 PM EST

PDB ID : 7SX6  
Title : Crystal structure of broadly neutralizing antibody N49P9.3 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 : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.31.2  
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

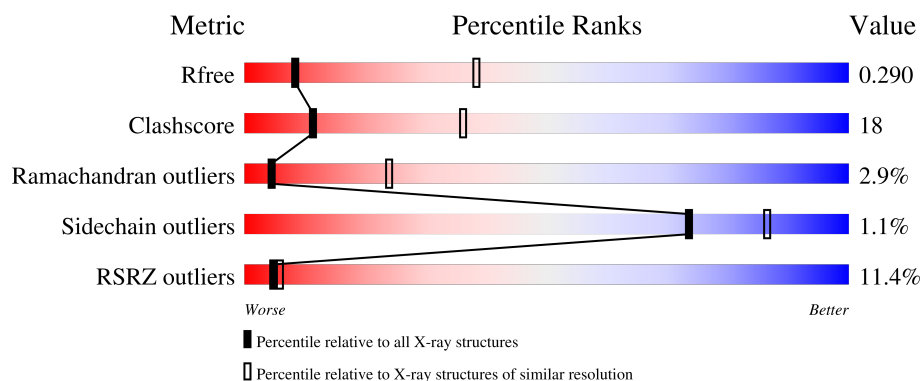
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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  $\geq 3$ , 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	A	355	<div> <div>8%</div> <div>68%</div> <div>29%</div> <div>.</div> </div>
1	G	355	<div> <div>6%</div> <div>68%</div> <div>30%</div> <div>.</div> </div>
2	B	223	<div> <div>12%</div> <div>52%</div> <div>40%</div> <div>.</div> </div>
2	H	223	<div> <div>16%</div> <div>56%</div> <div>37%</div> <div>.</div> </div>
3	C	203	<div> <div>12%</div> <div>57%</div> <div>37%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	203	

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	A	503	-	-	-	X
4	NAG	G	501	-	-	-	X
4	NAG	G	505	-	-	-	X
6	MG	A	513	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11995 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	346	Total	C	N	O	S	0	0	0
			2706	1695	469	519	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 ANTIBODY FAB HEAVY CHAIN.

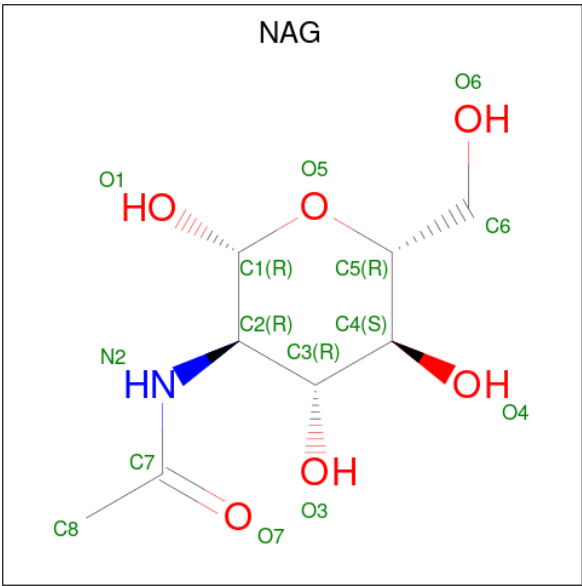
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	0	0
			1646	1048	283	305	10			
2	B	213	Total	C	N	O	S	0	0	0
			1646	1048	283	305	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	199	Total	C	N	O	S	0	0	0
			1503	947	253	298	5			
3	C	199	Total	C	N	O	S	0	0	0
			1503	947	253	298	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		
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		

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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		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

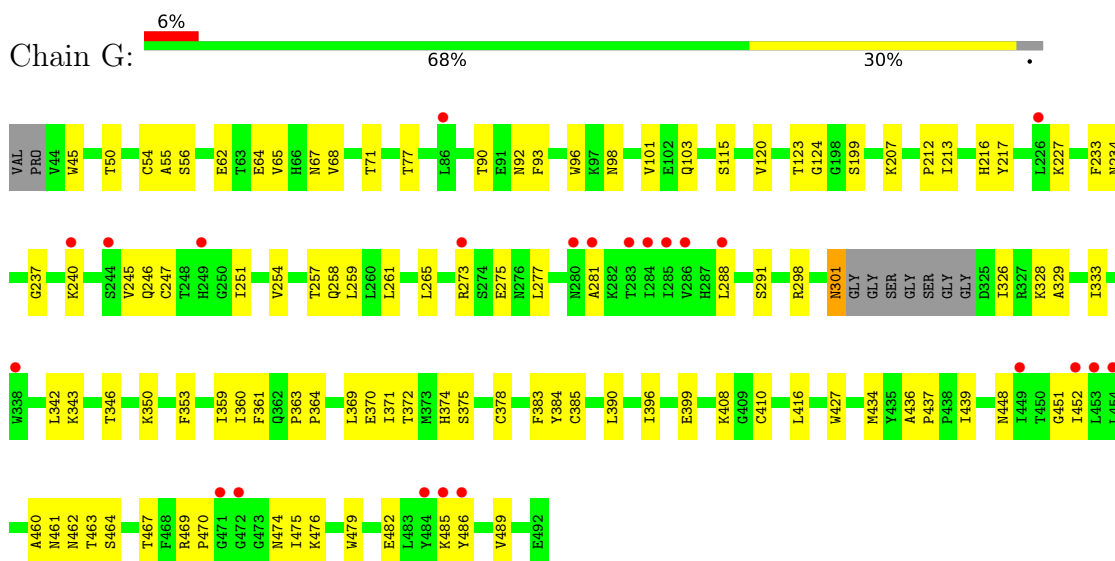
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Mg	0	0
			1	1		
6	A	2	Total	Mg	0	0
			2	2		

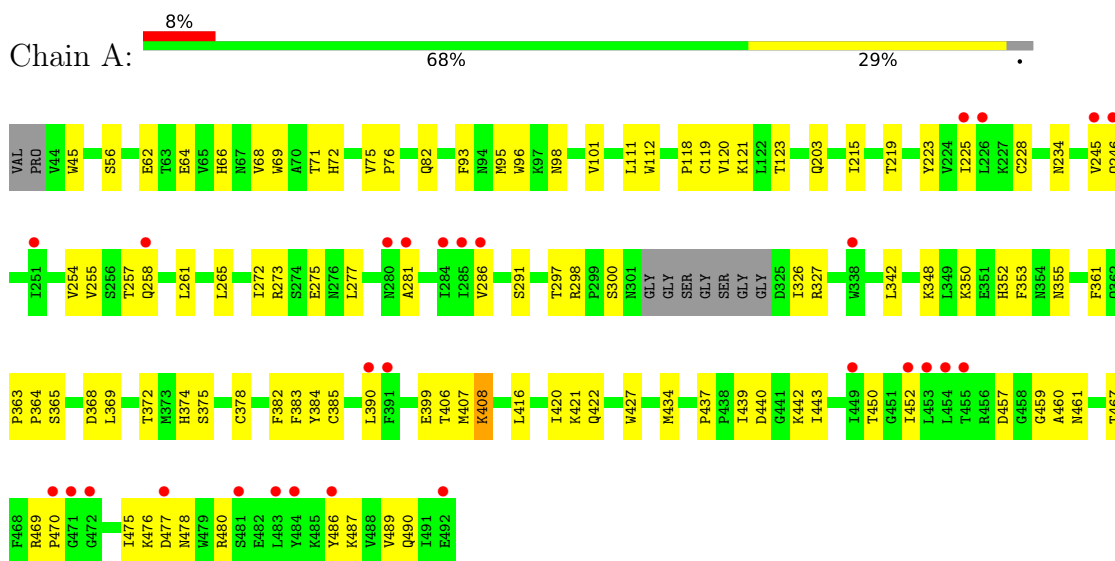
### 3 Residue-property plots

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

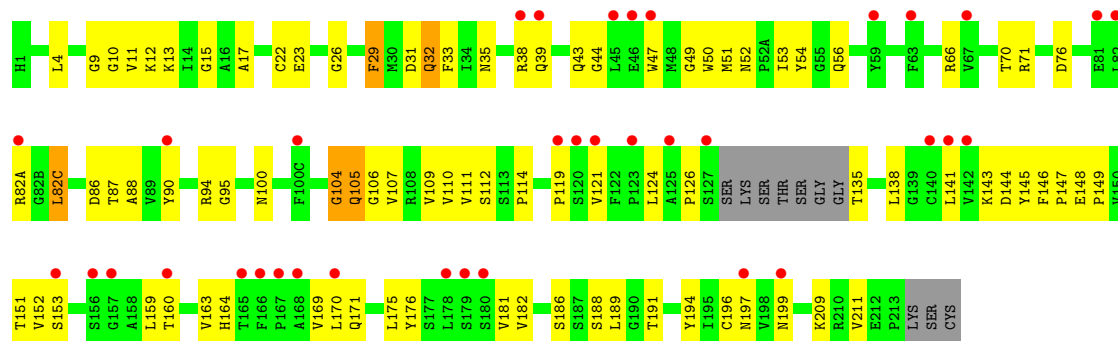


- Molecule 1: clade A/E 93TH057 HIV-1 gp120 core



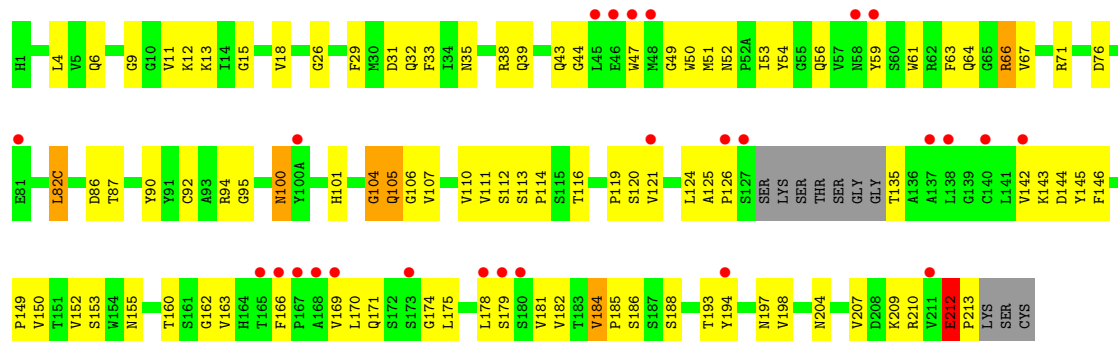
- Molecule 2: N49P9.3 ANTIBODY FAB HEAVY CHAIN

Chain H: 16% 56% 37%



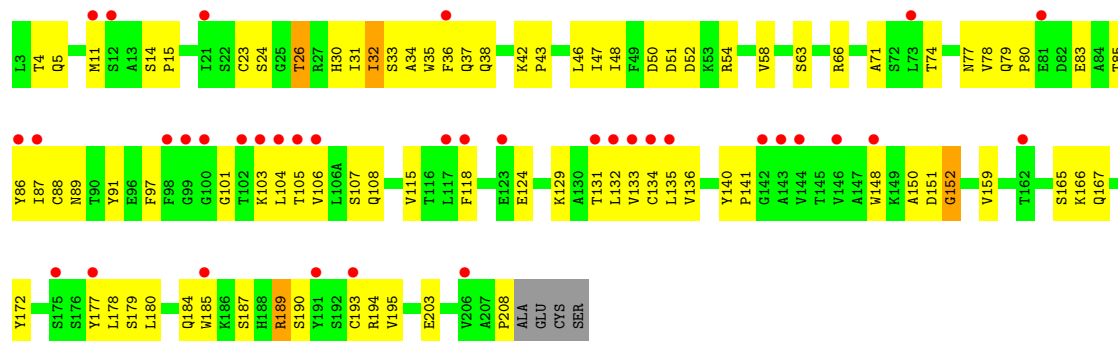
• Molecule 2: N49P9.3 ANTIBODY FAB HEAVY CHAIN

Chain B: 12% 52% 40%



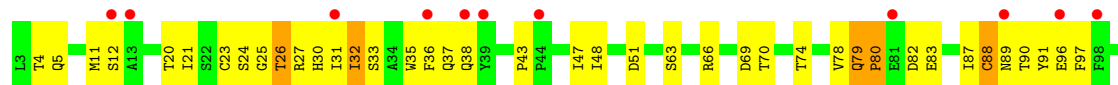
• Molecule 3: N49P9.3 ANTIBODY FAB LIGHT CHAIN

Chain L: 18% 56% 40%

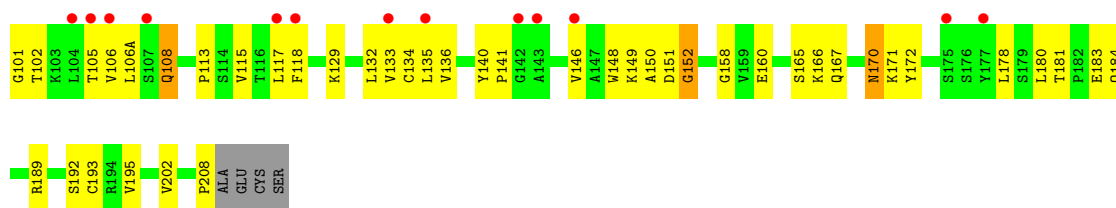


• Molecule 3: N49P9.3 ANTIBODY FAB LIGHT CHAIN

Chain C: 12% 57% 37%







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.21Å 68.21Å 115.06Å 90.26° 102.35° 90.38°	Depositor
Resolution (Å)	35.46 – 3.40 49.23 – 3.36	Depositor EDS
% Data completeness (in resolution range)	94.9 (35.46-3.40) 94.9 (49.23-3.36)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.03 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.234 , 0.287 0.236 , 0.290	Depositor DCC
$R_{free}$ test set	1274 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	129.8	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 116.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.438 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11995	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, MG

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	0.28	0/2762	0.53	0/3748
1	G	0.29	0/2762	0.54	0/3748
2	B	0.33	0/1693	0.61	0/2308
2	H	0.29	0/1693	0.60	0/2308
3	C	0.29	0/1543	0.59	0/2106
3	L	0.29	0/1543	0.59	0/2106
All	All	0.29	0/11996	0.57	0/16324

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	2638	82	0
1	G	2706	0	2638	73	0
2	B	1646	0	1594	94	0
2	H	1646	0	1594	68	0
3	C	1503	0	1473	65	0
3	L	1503	0	1473	65	0
4	A	140	0	130	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	140	0	130	1	0
5	A	1	0	0	1	0
5	G	1	0	0	0	0
6	A	2	0	0	0	0
6	G	1	0	0	0	0
All	All	11995	0	11670	421	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (421) 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:212:GLU:CG	2:B:213:PRO:HD3	1.72	1.20
2:B:184:VAL:HG12	2:B:185:PRO:CD	1.81	1.08
2:B:184:VAL:CG1	2:B:185:PRO:HD3	1.81	1.08
2:B:212:GLU:HB3	2:B:213:PRO:CD	1.81	1.06
2:B:212:GLU:HG3	2:B:213:PRO:HD3	1.26	1.05
1:A:399:GLU:HG3	1:A:408:LYS:HG3	1.41	1.01
2:B:212:GLU:HB3	2:B:213:PRO:HD2	1.44	0.99
2:B:32:GLN:HG3	2:B:94:ARG:HH21	1.27	0.97
2:B:212:GLU:CB	2:B:213:PRO:CD	2.41	0.96
2:B:184:VAL:HG12	2:B:185:PRO:HD3	0.95	0.95
2:B:185:PRO:HG2	2:B:188:SER:HB2	1.50	0.93
2:B:212:GLU:CB	2:B:213:PRO:HD3	2.00	0.91
2:H:32:GLN:HG3	2:H:94:ARG:HH21	1.38	0.87
2:B:184:VAL:CG1	2:B:185:PRO:CD	2.48	0.86
3:C:26:THR:HG23	3:C:30:HIS:H	1.41	0.84
2:B:184:VAL:HB	2:B:185:PRO:HD2	1.59	0.84
1:G:369:LEU:HA	1:G:372:THR:HG22	1.58	0.83
2:B:152:VAL:HG12	2:B:198:VAL:HG12	1.60	0.83
2:B:38:ARG:HH22	2:B:86:ASP:HA	1.44	0.81
1:A:298:ARG:HH21	1:A:326:ILE:HB	1.43	0.81
2:H:11:VAL:HG12	2:H:110:VAL:HB	1.63	0.81
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.62	0.80
2:H:138:LEU:HD13	2:H:211:VAL:HG11	1.65	0.79
3:L:35:TRP:HD1	3:L:48:ILE:HD11	1.46	0.79
3:L:32:ILE:HG22	3:L:33:SER:H	1.45	0.78
1:G:101:VAL:HG23	1:G:479:TRP:HB2	1.66	0.78
1:A:348:LYS:HE3	1:A:352:HIS:HE1	1.49	0.78
2:B:35:ASN:ND2	2:B:50:TRP:HB3	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:VAL:CB	2:B:185:PRO:CD	2.62	0.78
2:B:121:VAL:HG22	2:B:142:VAL:HG12	1.64	0.77
1:A:342:LEU:HD11	1:A:361:PHE:HE2	1.49	0.77
1:G:463:THR:HG22	1:G:464:SER:H	1.49	0.76
1:A:62:GLU:HG3	1:A:64:GLU:H	1.50	0.76
3:C:170:ASN:O	3:C:170:ASN:ND2	2.19	0.76
1:A:327:ARG:NH2	5:A:511:CL:CL	2.56	0.75
1:A:277:LEU:HD13	1:A:353:PHE:HE1	1.51	0.75
2:B:105:GLN:HA	3:C:43:PRO:HG3	1.68	0.74
3:C:32:ILE:HG22	3:C:33:SER:H	1.53	0.74
2:B:150:VAL:HG11	2:B:178:LEU:CD2	2.18	0.74
2:B:150:VAL:HG11	2:B:178:LEU:HD23	1.70	0.74
2:B:184:VAL:HB	2:B:185:PRO:CD	2.18	0.74
2:B:185:PRO:HG2	2:B:188:SER:CB	2.18	0.73
3:C:20:THR:HG22	3:C:74:THR:HG22	1.71	0.72
3:L:189:ARG:NH1	3:L:190:SER:OG	2.23	0.72
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.71	0.71
1:A:369:LEU:HA	1:A:372:THR:HG22	1.72	0.71
3:L:26:THR:HG23	3:L:30:HIS:H	1.55	0.71
2:B:43:GLN:HG2	2:B:44:GLY:H	1.55	0.71
2:H:153:SER:HB2	2:H:197:ASN:HB2	1.71	0.71
2:B:153:SER:HB3	2:B:197:ASN:HB2	1.72	0.71
1:G:277:LEU:HD13	1:G:353:PHE:HE1	1.55	0.70
2:H:163:VAL:HG12	2:H:182:VAL:HB	1.73	0.70
1:A:45:TRP:CD1	1:A:489:VAL:HG21	2.27	0.70
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.74	0.69
3:C:146:VAL:HG12	3:C:195:VAL:HG22	1.73	0.69
3:L:178:LEU:HD13	3:L:180:LEU:HD13	1.74	0.69
1:A:272:ILE:HG22	1:A:286:VAL:HG12	1.73	0.69
2:B:66:ARG:NH2	2:B:86:ASP:OD2	2.25	0.69
2:B:178:LEU:C	2:B:178:LEU:HD12	2.14	0.69
3:C:136:VAL:HG11	3:C:195:VAL:HG21	1.75	0.69
1:A:363:PRO:O	1:A:469:ARG:NH1	2.26	0.68
1:G:281:ALA:HB1	2:H:33:PHE:HE2	1.58	0.68
2:B:212:GLU:HG3	2:B:213:PRO:CD	2.16	0.68
2:H:87:THR:HG23	2:H:110:VAL:HA	1.76	0.68
1:G:62:GLU:HG3	1:G:64:GLU:H	1.57	0.68
2:H:194:TYR:HB2	2:H:211:VAL:HB	1.75	0.68
2:B:135:THR:HB	2:B:186:SER:HB3	1.75	0.67
1:G:207:LYS:NZ	1:G:437:PRO:O	2.27	0.67
2:H:90:TYR:O	2:H:106:GLY:HA2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LEU:HD21	1:A:291:SER:HB3	1.77	0.66
2:B:87:THR:HG23	2:B:110:VAL:HA	1.75	0.66
3:L:132:LEU:HD11	3:L:185:TRP:CD1	2.30	0.66
3:L:194:ARG:HG3	3:L:203:GLU:HG2	1.78	0.66
2:B:124:LEU:HB3	3:C:118:PHE:CD2	2.30	0.66
3:C:181:THR:HG22	3:C:183:GLU:H	1.61	0.65
1:G:298:ARG:NH2	1:G:439:ILE:O	2.29	0.65
1:A:69:TRP:HA	1:A:72:HIS:CE1	2.31	0.65
1:A:378:CYS:HB3	1:A:383:PHE:CE2	2.30	0.65
1:A:457:ASP:HB2	1:A:467:THR:HB	1.77	0.65
2:B:90:TYR:O	2:B:106:GLY:HA2	1.96	0.65
3:L:132:LEU:HD13	3:L:178:LEU:HD11	1.79	0.65
2:H:163:VAL:HA	2:H:181:VAL:O	1.98	0.64
2:H:105:GLN:HA	3:L:43:PRO:HG3	1.80	0.64
3:C:24:SER:HA	3:C:70:THR:HA	1.79	0.64
1:A:120:VAL:HG12	1:A:434:MET:HB3	1.79	0.64
1:G:364:PRO:HG3	1:G:372:THR:HA	1.80	0.64
3:L:79:GLN:HB3	3:L:80:PRO:HD2	1.80	0.63
3:C:115:VAL:HG22	3:C:136:VAL:HG12	1.80	0.63
3:C:132:LEU:HB2	3:C:178:LEU:HB3	1.80	0.63
3:L:11:MET:HB2	3:L:104:LEU:HD12	1.82	0.62
2:H:43:GLN:HG2	2:H:44:GLY:H	1.62	0.62
3:L:134:CYS:HB2	3:L:148:TRP:CH2	2.34	0.62
1:A:281:ALA:HB1	2:B:33:PHE:HE2	1.64	0.62
2:H:141:LEU:HD12	3:L:133:VAL:HG21	1.82	0.61
1:A:93:PHE:CE2	1:A:228:CYS:HB2	2.35	0.61
2:B:184:VAL:CB	2:B:185:PRO:HD2	2.28	0.61
1:A:460:ALA:H	3:C:97:PHE:HE1	1.48	0.61
3:L:36:PHE:HE2	3:L:89:ASN:HD22	1.47	0.61
3:L:38:GLN:NE2	3:L:42:LYS:O	2.33	0.61
2:H:151:THR:HB	2:H:199:ASN:HB3	1.83	0.61
2:B:155:ASN:HD21	2:B:194:TYR:HD1	1.48	0.61
3:C:180:LEU:HB3	3:C:184:GLN:HB2	1.82	0.60
2:H:47:TRP:HZ2	2:H:50:TRP:HD1	1.49	0.60
3:L:47:ILE:HD12	3:L:48:ILE:HG23	1.84	0.60
3:L:63:SER:HB2	3:L:74:THR:HB	1.83	0.60
1:A:75:VAL:HG22	1:A:76:PRO:HD2	1.82	0.60
1:G:378:CYS:HB3	1:G:383:PHE:CE2	2.37	0.59
3:L:42:LYS:HB3	3:L:43:PRO:HD2	1.84	0.59
3:C:36:PHE:HE2	3:C:89:ASN:HD22	1.49	0.59
3:L:83:GLU:HG3	3:L:105:THR:HA	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:136:VAL:HG11	3:L:195:VAL:HG11	1.84	0.59
1:A:254:VAL:O	1:A:478:ASN:ND2	2.35	0.59
1:G:371:ILE:HD13	2:H:56:GLN:HG3	1.85	0.59
2:H:95:GLY:HA3	2:H:100:ASN:O	2.03	0.59
2:B:144:ASP:HB3	2:B:175:LEU:HD23	1.84	0.58
1:G:374:HIS:HB3	1:G:385:CYS:HB2	1.84	0.58
2:H:146:PHE:CD1	2:H:147:PRO:HA	2.39	0.58
4:A:505:NAG:H61	3:C:32:ILE:HG12	1.86	0.58
3:L:150:ALA:O	3:L:152:GLY:N	2.36	0.57
1:A:118:PRO:O	1:A:203:GLN:HB2	2.04	0.57
2:H:152:VAL:HA	2:H:197:ASN:O	2.05	0.57
1:G:120:VAL:HG12	1:G:434:MET:HB3	1.86	0.57
3:L:131:THR:HG22	3:L:179:SER:HA	1.85	0.57
2:H:164:HIS:CD2	3:L:167:GLN:HA	2.40	0.57
3:L:34:ALA:HB3	3:L:89:ASN:HB3	1.87	0.57
1:A:258:GLN:HG2	1:A:470:PRO:HB2	1.87	0.57
2:H:35:ASN:OD1	2:H:50:TRP:HB3	2.04	0.57
3:C:21:ILE:HD12	3:C:102:THR:HG21	1.86	0.57
1:G:65:VAL:HB	1:G:115:SER:HB2	1.86	0.56
3:L:132:LEU:HB2	3:L:178:LEU:HG	1.87	0.56
2:B:193:THR:OG1	2:B:210:ARG:NE	2.38	0.56
3:L:140:TYR:CD1	3:L:141:PRO:HA	2.41	0.56
1:A:298:ARG:HD3	1:A:443:ILE:HD12	1.88	0.56
3:C:150:ALA:O	3:C:152:GLY:N	2.37	0.56
2:B:82(C):LEU:HD22	2:B:111:VAL:HG22	1.87	0.56
3:C:134:CYS:HB2	3:C:148:TRP:CH2	2.40	0.56
1:A:406:THR:O	1:A:408:LYS:N	2.38	0.56
3:C:83:GLU:HG3	3:C:105:THR:HA	1.88	0.56
1:G:50:THR:O	1:G:103:GLN:NE2	2.36	0.55
1:G:346:THR:HG23	1:G:359:ILE:HB	1.88	0.55
3:L:77:ASN:OD1	3:L:79:GLN:NE2	2.38	0.55
1:A:342:LEU:HD11	1:A:361:PHE:CE2	2.35	0.55
2:B:63:PHE:HB3	2:B:67:VAL:HG12	1.88	0.55
3:L:54:ARG:HH11	3:L:58:VAL:HG23	1.69	0.55
2:B:95:GLY:HA3	2:B:100:ASN:O	2.07	0.55
3:L:66:ARG:HG3	3:L:71:ALA:HB2	1.87	0.55
3:C:35:TRP:HB2	3:C:48:ILE:HB	1.88	0.55
1:G:227:LYS:HA	1:G:485:LYS:O	2.07	0.55
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.88	0.55
1:G:460:ALA:HA	3:L:97:PHE:HE1	1.72	0.55
3:C:166:LYS:HG2	3:C:167:GLN:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:TYR:CD1	3:C:141:PRO:HA	2.42	0.55
3:C:181:THR:HB	3:C:184:GLN:HG2	1.88	0.54
1:G:363:PRO:O	1:G:469:ARG:NH1	2.36	0.54
2:H:70:THR:HG22	2:H:71:ARG:H	1.71	0.54
2:H:38:ARG:NH1	2:H:86:ASP:HA	2.22	0.54
1:A:300:SER:HB2	1:A:442:LYS:N	2.22	0.54
2:B:121:VAL:HG21	2:B:198:VAL:HG21	1.89	0.54
1:G:298:ARG:NH1	1:G:326:ILE:O	2.40	0.54
2:H:124:LEU:HB3	3:L:118:PHE:CD2	2.43	0.54
2:B:32:GLN:HG3	2:B:94:ARG:NH2	2.10	0.54
1:G:90:THR:HG22	1:G:240:LYS:HA	1.89	0.54
3:L:148:TRP:CE3	3:L:178:LEU:HD23	2.42	0.54
3:L:35:TRP:HB2	3:L:48:ILE:HG13	1.88	0.54
1:A:399:GLU:HG3	1:A:408:LYS:CG	2.26	0.54
3:C:149:LYS:HB3	3:C:192:SER:HB2	1.90	0.54
1:A:257:THR:OG1	1:A:375:SER:N	2.29	0.53
1:A:281:ALA:HB1	2:B:33:PHE:CE2	2.42	0.53
1:A:422:GLN:HE21	1:A:437:PRO:HA	1.72	0.53
2:B:125:ALA:HB1	2:B:126:PRO:HD2	1.90	0.53
1:A:82:GLN:N	1:A:82:GLN:OE1	2.41	0.53
2:B:198:VAL:CG2	2:B:207:VAL:HB	2.39	0.53
3:L:184:GLN:HA	3:L:187:SER:HB2	1.90	0.53
1:A:364:PRO:HG3	1:A:372:THR:HA	1.91	0.53
1:G:474:ASN:OD1	1:G:476:LYS:HB2	2.09	0.53
2:B:38:ARG:NH2	2:B:86:ASP:HA	2.19	0.52
1:G:93:PHE:HB2	1:G:233:PHE:HZ	1.74	0.52
1:G:343:LYS:HD3	1:G:396:ILE:HB	1.90	0.52
1:A:475:ILE:O	1:A:478:ASN:N	2.38	0.52
2:H:135:THR:HB	2:H:186:SER:HB2	1.91	0.52
3:L:54:ARG:NH1	3:L:58:VAL:O	2.43	0.52
1:G:212:PRO:HG2	1:G:254:VAL:HG12	1.92	0.52
2:H:188:SER:O	2:H:191:THR:OG1	2.28	0.52
2:H:126:PRO:HG3	2:H:138:LEU:HB3	1.91	0.51
2:B:170:LEU:HD12	2:B:170:LEU:O	2.10	0.51
2:B:112:SER:HB2	2:B:146:PHE:CE1	2.46	0.51
3:C:113:PRO:HG2	3:C:202:VAL:HG21	1.92	0.51
3:C:170:ASN:HD22	3:C:170:ASN:C	2.14	0.51
2:H:38:ARG:HH12	2:H:86:ASP:HA	1.73	0.51
3:L:185:TRP:CH2	3:L:208:PRO:HA	2.45	0.51
1:A:68:VAL:O	1:A:71:THR:HG22	2.10	0.51
2:B:33:PHE:HB2	2:B:100:ASN:OD1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASN:ND2	1:A:486:TYR:O	2.43	0.51
3:C:79:GLN:HB3	3:C:80:PRO:HD3	1.94	0.50
1:A:327:ARG:HH21	1:A:421:LYS:HG2	1.76	0.50
2:H:47:TRP:CH2	2:H:49:GLY:HA2	2.47	0.50
2:H:82(C):LEU:HD22	2:H:111:VAL:HG22	1.94	0.50
1:A:66:HIS:CD2	1:A:111:LEU:HD21	2.46	0.50
3:C:5:GLN:NE2	3:C:88:CYS:H	2.10	0.50
1:G:98:ASN:O	1:G:101:VAL:HG12	2.10	0.50
2:B:4:LEU:HD12	2:B:104:GLY:HA2	1.94	0.50
1:G:98:ASN:ND2	1:G:486:TYR:O	2.44	0.50
3:C:32:ILE:HG22	3:C:33:SER:N	2.23	0.50
1:G:55:ALA:N	1:G:216:HIS:O	2.32	0.50
3:L:166:LYS:HG2	3:L:167:GLN:O	2.12	0.49
1:A:439:ILE:HD12	1:A:440:ASP:O	2.11	0.49
3:L:23:CYS:HB2	3:L:35:TRP:CH2	2.47	0.49
2:B:47:TRP:CH2	2:B:49:GLY:HA2	2.47	0.49
1:G:56:SER:O	1:G:77:THR:N	2.45	0.49
1:G:227:LYS:HB2	1:G:486:TYR:CE1	2.48	0.49
1:G:463:THR:HG22	1:G:464:SER:N	2.24	0.49
1:A:64:GLU:OE2	1:A:66:HIS:ND1	2.42	0.49
1:A:121:LYS:NZ	1:A:123:THR:OG1	2.45	0.49
2:B:82(C):LEU:HD13	2:B:111:VAL:HG13	1.94	0.49
3:L:159:VAL:HA	3:L:177:TYR:O	2.12	0.49
1:G:254:VAL:HG21	1:G:261:LEU:O	2.13	0.49
2:H:70:THR:HG22	2:H:71:ARG:N	2.28	0.49
1:A:254:VAL:HG21	1:A:261:LEU:O	2.13	0.49
3:C:165:SER:O	3:C:172:TYR:HA	2.13	0.49
2:B:143:LYS:HZ3	3:C:129:LYS:HD3	1.78	0.49
3:L:87:ILE:HG13	3:L:101:GLY:HA2	1.94	0.49
3:C:117:LEU:HD12	3:C:193:CYS:HB2	1.94	0.49
3:L:15:PRO:HA	3:L:78:VAL:HB	1.95	0.48
2:B:61:TRP:HA	2:B:64:GLN:HG2	1.94	0.48
2:B:169:VAL:HG21	3:C:160:GLU:HB3	1.95	0.48
1:A:93:PHE:HE2	1:A:228:CYS:HB2	1.78	0.48
1:A:234:ASN:O	1:A:273:ARG:HG2	2.13	0.48
3:C:79:GLN:CB	3:C:80:PRO:HD3	2.42	0.48
2:H:144:ASP:HB3	2:H:175:LEU:HD13	1.95	0.48
1:A:75:VAL:CG2	1:A:76:PRO:HD2	2.44	0.48
1:A:298:ARG:NH2	1:A:326:ILE:HB	2.22	0.48
2:B:51:MET:HE3	2:B:71:ARG:HB3	1.93	0.48
2:H:4:LEU:HA	2:H:23:GLU:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:85:THR:HG22	3:L:103:LYS:HA	1.95	0.48
3:C:78:VAL:HG13	3:C:82:ASP:HB2	1.95	0.48
1:G:92:ASN:HA	1:G:237:GLY:O	2.13	0.48
1:G:370:GLU:HG3	1:G:384:TYR:HE1	1.77	0.48
1:A:427:TRP:CE3	1:A:475:ILE:HG13	2.48	0.48
1:G:45:TRP:CD1	1:G:489:VAL:HG11	2.49	0.48
2:H:169:VAL:O	2:H:176:TYR:HA	2.13	0.48
3:C:87:ILE:HG13	3:C:101:GLY:HA2	1.95	0.48
1:G:333:ILE:HD13	1:G:390:LEU:HD11	1.97	0.47
1:A:384:TYR:CE2	1:A:421:LYS:HD3	2.49	0.47
1:G:251:ILE:HG23	1:G:482:GLU:OE1	2.15	0.47
1:G:257:THR:HG21	1:G:370:GLU:O	2.13	0.47
1:G:328:LYS:HD2	1:G:329:ALA:H	1.80	0.47
2:H:121:VAL:HG13	2:H:209:LYS:HD3	1.97	0.47
2:H:143:LYS:HE2	2:H:171:GLN:HE22	1.80	0.47
2:H:144:ASP:HA	2:H:175:LEU:HB3	1.97	0.47
3:C:167:GLN:NE2	3:C:171:LYS:HB2	2.30	0.47
1:G:258:GLN:HE21	1:G:470:PRO:CB	2.28	0.47
2:H:181:VAL:HG11	3:L:135:LEU:HD11	1.96	0.47
2:H:196:CYS:SG	2:H:209:LYS:HB3	2.54	0.47
1:G:234:ASN:O	1:G:273:ARG:HG2	2.15	0.47
2:B:4:LEU:CD1	2:B:104:GLY:HA2	2.44	0.47
3:C:26:THR:HG22	3:C:69:ASP:HA	1.96	0.46
2:B:47:TRP:HZ2	2:B:50:TRP:HD1	1.63	0.46
1:G:342:LEU:HD11	1:G:361:PHE:CE2	2.50	0.46
3:L:148:TRP:CD2	3:L:178:LEU:HD23	2.51	0.46
2:B:181:VAL:HG11	3:C:135:LEU:HD11	1.96	0.46
1:G:245:VAL:HG22	1:G:246:GLN:H	1.81	0.46
1:A:286:VAL:CG2	1:A:452:ILE:HB	2.45	0.46
2:B:50:TRP:HZ3	2:B:52:ASN:HB2	1.81	0.46
1:G:68:VAL:O	1:G:71:THR:HG22	2.16	0.46
3:C:158:GLY:O	3:C:178:LEU:HA	2.15	0.46
1:G:281:ALA:HB1	2:H:33:PHE:CE2	2.45	0.46
1:G:123:THR:HB	1:G:199:SER:HB2	1.97	0.46
1:A:459:GLY:HA2	3:C:96:GLU:HG3	1.97	0.46
1:G:207:LYS:HZ3	1:G:436:ALA:HB3	1.80	0.46
2:H:31:ASP:O	2:H:32:GLN:HB2	2.16	0.46
2:H:160:THR:O	2:H:163:VAL:HG22	2.16	0.46
2:B:207:VAL:HG13	2:B:209:LYS:HE2	1.98	0.46
2:H:29:PHE:HB2	2:H:76:ASP:OD1	2.15	0.45
1:G:227:LYS:HB2	1:G:486:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:82(C):LEU:HD13	2:H:111:VAL:HG13	1.99	0.45
2:H:4:LEU:HD12	2:H:104:GLY:HA2	1.97	0.45
2:H:126:PRO:HG2	2:H:189:LEU:CD2	2.47	0.45
2:B:35:ASN:ND2	2:B:47:TRP:HE1	2.15	0.45
1:G:54:CYS:HA	1:G:217:TYR:HA	1.98	0.45
3:L:79:GLN:HB3	3:L:80:PRO:CD	2.45	0.45
2:B:178:LEU:HD12	2:B:179:SER:N	2.32	0.45
3:C:25:GLY:O	3:C:27:ARG:N	2.50	0.45
2:H:148:GLU:CG	2:H:149:PRO:HA	2.47	0.45
3:L:50:ASP:O	3:L:52:ASP:N	2.49	0.45
1:A:265:LEU:HG	1:A:450:THR:OG1	2.17	0.45
1:G:291:SER:HB2	1:G:448:ASN:HB3	1.98	0.45
1:A:56:SER:HB3	1:A:215:ILE:HG22	1.98	0.45
1:A:297:THR:HG21	4:A:507:NAG:H62	1.98	0.45
1:A:350:LYS:CG	1:A:355:ASN:HA	2.46	0.45
3:C:118:PHE:HB2	3:C:133:VAL:CG1	2.47	0.45
1:G:301:ASN:O	1:G:301:ASN:ND2	2.38	0.45
3:L:83:GLU:HG3	3:L:105:THR:HG22	1.99	0.45
3:C:11:MET:HG3	3:C:12:SER:N	2.32	0.45
1:A:368:ASP:OD2	2:B:71:ARG:NH2	2.50	0.45
3:C:63:SER:HB3	3:C:74:THR:OG1	2.17	0.45
3:C:189:ARG:O	3:C:208:PRO:HD2	2.17	0.45
1:G:363:PRO:HB2	1:G:364:PRO:HD2	1.98	0.44
3:L:4:THR:O	3:L:23:CYS:HA	2.17	0.44
3:L:35:TRP:O	3:L:47:ILE:HG13	2.17	0.44
3:C:5:GLN:HE22	3:C:87:ILE:HA	1.81	0.44
2:H:10:GLY:O	2:H:109:VAL:HA	2.18	0.44
2:B:9:GLY:H	2:B:107:VAL:HG21	1.83	0.44
2:B:163:VAL:HA	2:B:181:VAL:O	2.16	0.44
1:G:463:THR:CG2	1:G:464:SER:H	2.26	0.44
1:A:374:HIS:HB3	1:A:385:CYS:HB2	1.99	0.44
1:G:265:LEU:HD11	1:G:291:SER:HB3	2.00	0.44
1:G:265:LEU:HD21	1:G:291:SER:H	1.81	0.44
2:H:54:TYR:HB2	2:H:56:GLN:HE22	1.82	0.44
3:L:37:GLN:NE2	3:L:86:TYR:OH	2.51	0.44
2:B:35:ASN:HD21	2:B:50:TRP:HB3	1.81	0.44
1:G:93:PHE:HB2	1:G:233:PHE:CZ	2.53	0.44
1:G:346:THR:O	1:G:350:LYS:HG3	2.17	0.44
2:H:143:LYS:HZ3	2:H:144:ASP:CG	2.20	0.44
4:G:505:NAG:H62	3:L:32:ILE:HG12	2.00	0.44
1:G:399:GLU:HG3	1:G:408:LYS:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:VAL:CG1	2:B:185:PRO:HD2	2.41	0.44
3:C:31:ILE:HD13	3:C:91:TYR:CD2	2.53	0.44
1:A:112:TRP:CZ2	1:A:255:VAL:HG21	2.53	0.43
2:B:43:GLN:CG	2:B:44:GLY:H	2.29	0.43
3:C:31:ILE:HD12	3:C:31:ILE:O	2.17	0.43
3:L:165:SER:O	3:L:172:TYR:HA	2.19	0.43
1:G:288:LEU:HD13	1:G:451:GLY:HA2	2.00	0.43
1:G:399:GLU:O	1:G:408:LYS:HG2	2.18	0.43
3:C:33:SER:HB3	3:C:66:ARG:HD3	1.99	0.43
3:L:134:CYS:HB2	3:L:148:TRP:CZ2	2.53	0.43
1:A:223:TYR:CE1	1:A:490:GLN:HB2	2.53	0.43
1:G:240:LYS:HB2	1:G:240:LYS:HE2	1.82	0.43
1:A:96:TRP:CD2	1:A:275:GLU:HB2	2.54	0.43
2:B:171:GLN:HB3	3:C:160:GLU:HG3	2.00	0.43
3:L:133:VAL:HG22	3:L:177:TYR:CD1	2.54	0.43
2:H:66:ARG:HG3	2:H:82(A):ARG:O	2.18	0.43
1:A:257:THR:O	1:A:258:GLN:HB2	2.19	0.43
1:G:399:GLU:HG3	1:G:399:GLU:O	2.19	0.43
2:H:52:ASN:HB3	2:H:56:GLN:HB2	2.00	0.43
3:L:132:LEU:HB2	3:L:178:LEU:CG	2.48	0.43
2:H:153:SER:O	2:H:196:CYS:HA	2.18	0.43
2:B:124:LEU:HB3	3:C:118:PHE:HD2	1.78	0.43
1:G:67:ASN:HD21	1:G:213:ILE:HG21	1.83	0.42
1:G:298:ARG:HD2	1:G:298:ARG:C	2.39	0.42
1:G:375:SER:HA	1:G:383:PHE:O	2.19	0.42
1:G:427:TRP:CE3	1:G:475:ILE:HD13	2.54	0.42
2:B:11:VAL:HG12	2:B:110:VAL:CG1	2.49	0.42
2:B:160:THR:O	2:B:163:VAL:HG12	2.19	0.42
3:C:4:THR:O	3:C:23:CYS:HA	2.19	0.42
2:H:51:MET:HE3	2:H:71:ARG:HB3	2.00	0.42
2:H:54:TYR:HB2	2:H:56:GLN:NE2	2.33	0.42
3:L:124:GLU:HG2	3:L:129:LYS:O	2.19	0.42
1:A:219:THR:HG23	1:A:225:ILE:HG12	2.02	0.42
2:B:4:LEU:HD13	2:B:92:CYS:SG	2.59	0.42
1:A:406:THR:O	1:A:406:THR:HG23	2.20	0.42
1:A:477:ASP:OD1	1:A:480:ARG:NH1	2.52	0.42
3:C:37:GLN:HB2	3:C:47:ILE:HG13	2.00	0.42
1:G:259:LEU:HD22	1:G:452:ILE:HD12	2.01	0.42
1:A:297:THR:HA	1:A:443:ILE:O	2.18	0.42
1:A:378:CYS:HB3	1:A:383:PHE:HE2	1.77	0.42
3:C:106(A):LEU:HD23	3:C:106(A):LEU:HA	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:141:LEU:CD2	2:H:143:LYS:HB2	2.49	0.42
2:B:166:PHE:HE2	3:C:135:LEU:HG	1.84	0.42
2:H:112:SER:HB3	2:H:146:PHE:CE1	2.54	0.42
2:B:12:LYS:HG3	2:B:18:VAL:HB	2.00	0.42
2:B:113:SER:HB3	2:B:174:GLY:HA3	2.01	0.42
2:B:150:VAL:HG21	2:B:178:LEU:HD21	2.01	0.42
2:H:170:LEU:HB2	2:H:176:TYR:CE1	2.55	0.42
3:L:115:VAL:HA	3:L:135:LEU:O	2.20	0.42
3:L:131:THR:HA	3:L:178:LEU:O	2.20	0.42
3:L:148:TRP:CZ3	3:L:193:CYS:HB2	2.54	0.41
1:A:350:LYS:HG3	1:A:355:ASN:HA	2.01	0.41
2:B:162:GLY:C	2:B:182:VAL:HG23	2.40	0.41
1:A:327:ARG:NH2	1:A:421:LYS:HG2	2.35	0.41
2:H:4:LEU:CD1	2:H:104:GLY:HA2	2.50	0.41
1:A:68:VAL:O	1:A:72:HIS:ND1	2.53	0.41
2:B:142:VAL:HG11	2:B:198:VAL:HG11	2.02	0.41
2:H:170:LEU:HD13	2:H:176:TYR:CZ	2.55	0.41
3:L:5:GLN:NE2	3:L:86:TYR:O	2.53	0.41
1:G:360:ILE:HB	1:G:467:THR:HG22	2.03	0.41
2:H:39:GLN:O	2:H:88:ALA:HB1	2.21	0.41
2:B:54:TYR:HB2	2:B:56:GLN:HE22	1.85	0.41
2:H:9:GLY:H	2:H:107:VAL:HG21	1.84	0.41
1:A:272:ILE:HD11	1:A:352:HIS:CD2	2.55	0.41
2:B:39:GLN:NE2	3:C:38:GLN:OE1	2.46	0.41
3:C:132:LEU:HD22	3:C:178:LEU:HD22	2.03	0.41
1:A:245:VAL:HG22	1:A:246:GLN:H	1.86	0.41
1:A:365:SER:HB3	2:B:59:TYR:CE1	2.56	0.41
2:B:31:ASP:O	2:B:32:GLN:HB2	2.20	0.41
1:G:96:TRP:CD2	1:G:275:GLU:HB2	2.56	0.41
1:G:385:CYS:HB3	1:G:416:LEU:CD1	2.51	0.41
2:H:12:LYS:HE2	2:H:17:ALA:O	2.21	0.41
2:H:47:TRP:CZ2	2:H:50:TRP:HD1	2.34	0.41
1:A:365:SER:HB3	2:B:59:TYR:HE1	1.85	0.41
1:A:368:ASP:CG	2:B:71:ARG:HH22	2.24	0.41
1:A:382:PHE:O	1:A:420:ILE:HA	2.20	0.41
1:A:390:LEU:HD13	1:A:416:LEU:HD23	2.03	0.41
2:B:6:GLN:HE21	2:B:6:GLN:HB3	1.68	0.41
2:B:178:LEU:C	2:B:178:LEU:CD1	2.86	0.41
3:C:23:CYS:HB2	3:C:35:TRP:CH2	2.56	0.41
3:C:89:ASN:OD1	3:C:90:THR:N	2.54	0.41
1:G:257:THR:O	1:G:259:LEU:N	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:36:PHE:CE1	3:L:46:LEU:HB2	2.55	0.41
1:A:93:PHE:CD2	1:A:228:CYS:HB2	2.55	0.41
2:B:116:THR:HA	2:B:146:PHE:O	2.21	0.41
2:B:120:SER:O	2:B:142:VAL:HA	2.21	0.41
2:H:148:GLU:HG3	2:H:149:PRO:HA	2.01	0.40
3:L:107:SER:O	3:L:108:GLN:HB2	2.21	0.40
1:A:245:VAL:HG22	1:A:246:GLN:N	2.36	0.40
3:L:4:THR:HB	3:L:24:SER:HB3	2.03	0.40
1:A:93:PHE:CE1	1:A:487:LYS:HE2	2.57	0.40
1:A:95:MET:SD	1:A:273:ARG:HD3	2.61	0.40
1:A:119:CYS:N	1:A:434:MET:O	2.53	0.40
2:B:212:GLU:CD	2:B:213:PRO:HD3	2.37	0.40
3:C:11:MET:CG	3:C:12:SER:N	2.84	0.40
3:L:31:ILE:HG21	3:L:91:TYR:CE2	2.57	0.40
3:L:32:ILE:HD12	3:L:32:ILE:HG23	1.88	0.40
2:B:4:LEU:HD12	2:B:4:LEU:O	2.21	0.40
2:B:185:PRO:CG	2:B:188:SER:HB2	2.37	0.40
3:C:178:LEU:HD23	3:C:180:LEU:HG	2.03	0.40
1:G:217:TYR:O	1:G:247:CYS:HA	2.22	0.40
1:G:342:LEU:HD11	1:G:361:PHE:HE2	1.86	0.40
2:H:43:GLN:CG	2:H:44:GLY:H	2.32	0.40
1:A:390:LEU:CD1	1:A:416:LEU:HD23	2.52	0.40
3:C:108:GLN:NE2	3:C:171:LYS:HD3	2.36	0.40
3:C:180:LEU:HB3	3:C:184:GLN:CB	2.51	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%)	17 (5%)	4 (1%)	<b>13</b> 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	342/355 (96%)	314 (92%)	24 (7%)	4 (1%)	13	41
2	B	209/223 (94%)	172 (82%)	25 (12%)	12 (6%)	1	12
2	H	209/223 (94%)	181 (87%)	20 (10%)	8 (4%)	3	19
3	C	197/203 (97%)	174 (88%)	14 (7%)	9 (5%)	2	15
3	L	197/203 (97%)	174 (88%)	17 (9%)	6 (3%)	4	23
All	All	1496/1562 (96%)	1336 (89%)	117 (8%)	43 (3%)	4	24

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	462	ASN
2	H	105	GLN
3	L	26	THR
2	B	100	ASN
2	B	105	GLN
2	B	149	PRO
2	B	184	VAL
2	B	212	GLU
3	C	26	THR
3	C	32	ILE
3	C	79	GLN
3	C	80	PRO
1	G	124	GLY
1	G	461	ASN
2	H	13	LYS
2	H	15	GLY
3	L	32	ILE
3	L	51	ASP
1	A	407	MET
1	A	461	ASN
2	B	13	LYS
2	B	114	PRO
3	C	151	ASP
2	H	32	GLN
2	H	104	GLY
2	H	114	PRO
2	B	15	GLY
2	B	53	ILE
2	B	104	GLY
2	H	53	ILE

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Mol	Chain	Res	Type
3	L	151	ASP
1	A	408	LYS
1	A	476	LYS
3	C	51	ASP
3	C	106	VAL
1	G	410	CYS
2	B	26	GLY
2	B	204	ASN
3	L	106	VAL
3	C	108	GLN
3	L	152	GLY
2	H	26	GLY
3	C	152	GLY

### 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%)	309 (100%)	0	100	100
1	G	309/313 (99%)	308 (100%)	1 (0%)	92	97
2	B	181/189 (96%)	175 (97%)	6 (3%)	38	66
2	H	181/189 (96%)	178 (98%)	3 (2%)	60	80
3	C	171/174 (98%)	169 (99%)	2 (1%)	71	85
3	L	171/174 (98%)	168 (98%)	3 (2%)	59	79
All	All	1322/1352 (98%)	1307 (99%)	15 (1%)	73	86

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	301	ASN
2	H	22	CYS
2	H	29	PHE
2	H	82(C)	LEU
3	L	14	SER

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Mol	Chain	Res	Type
3	L	88	CYS
3	L	189	ARG
2	B	29	PHE
2	B	66	ARG
2	B	76	ASP
2	B	82(C)	LEU
2	B	101	HIS
2	B	212	GLU
3	C	88	CYS
3	C	170	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	101	HIS
2	H	171	GLN
1	A	352	HIS
2	B	35	ASN
3	C	5	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](#)

Of 25 ligands modelled in this entry, 5 are monoatomic - leaving 20 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	A	508	1	14,14,15	0.36	0	17,19,21	0.42	0
4	NAG	G	507	1	14,14,15	0.20	0	17,19,21	0.40	0
4	NAG	A	507	1	14,14,15	0.24	0	17,19,21	0.38	0
4	NAG	G	503	1	14,14,15	0.25	0	17,19,21	0.46	0
4	NAG	G	509	1	14,14,15	0.40	0	17,19,21	0.40	0
4	NAG	A	510	1	14,14,15	0.22	0	17,19,21	0.38	0
4	NAG	A	505	1	14,14,15	0.46	0	17,19,21	0.35	0
4	NAG	A	503	1	14,14,15	0.29	0	17,19,21	0.44	0
4	NAG	A	502	1	14,14,15	0.18	0	17,19,21	0.33	0
4	NAG	A	509	1	14,14,15	0.27	0	17,19,21	0.41	0
4	NAG	G	505	1	14,14,15	0.49	0	17,19,21	0.36	0
4	NAG	G	506	1	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	A	506	1	14,14,15	0.21	0	17,19,21	0.51	0
4	NAG	A	504	1	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	G	504	1	14,14,15	0.29	0	17,19,21	0.45	0
4	NAG	A	501	1	14,14,15	0.19	0	17,19,21	0.40	0
4	NAG	G	510	1	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	G	501	1	14,14,15	0.25	0	17,19,21	0.35	0
4	NAG	G	502	1	14,14,15	0.23	0	17,19,21	0.30	0
4	NAG	G	508	1	14,14,15	0.43	0	17,19,21	0.48	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	508	1	-	0/6/23/26	0/1/1/1
4	NAG	G	507	1	-	2/6/23/26	0/1/1/1
4	NAG	A	507	1	-	2/6/23/26	0/1/1/1
4	NAG	G	503	1	-	2/6/23/26	0/1/1/1
4	NAG	G	509	1	-	2/6/23/26	0/1/1/1
4	NAG	A	510	1	-	2/6/23/26	0/1/1/1
4	NAG	A	505	1	-	2/6/23/26	0/1/1/1
4	NAG	A	503	1	-	2/6/23/26	0/1/1/1
4	NAG	A	502	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	509	1	-	0/6/23/26	0/1/1/1
4	NAG	G	505	1	-	1/6/23/26	0/1/1/1
4	NAG	G	506	1	-	0/6/23/26	0/1/1/1
4	NAG	A	506	1	-	1/6/23/26	0/1/1/1
4	NAG	A	504	1	-	2/6/23/26	0/1/1/1
4	NAG	G	504	1	-	2/6/23/26	0/1/1/1
4	NAG	A	501	1	-	1/6/23/26	0/1/1/1
4	NAG	G	510	1	-	2/6/23/26	0/1/1/1
4	NAG	G	501	1	-	0/6/23/26	0/1/1/1
4	NAG	G	502	1	-	2/6/23/26	0/1/1/1
4	NAG	G	508	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	NAG	O5-C5-C6-O6
4	A	510	NAG	O5-C5-C6-O6
4	G	510	NAG	O5-C5-C6-O6
4	A	504	NAG	O5-C5-C6-O6
4	A	505	NAG	O5-C5-C6-O6
4	G	504	NAG	O5-C5-C6-O6
4	A	505	NAG	C4-C5-C6-O6
4	A	504	NAG	C4-C5-C6-O6
4	G	503	NAG	O5-C5-C6-O6
4	G	504	NAG	C4-C5-C6-O6
4	A	503	NAG	C4-C5-C6-O6
4	G	507	NAG	O5-C5-C6-O6
4	A	510	NAG	C4-C5-C6-O6
4	G	510	NAG	C4-C5-C6-O6
4	G	507	NAG	C4-C5-C6-O6
4	G	503	NAG	C4-C5-C6-O6
4	G	502	NAG	O5-C5-C6-O6
4	G	509	NAG	O5-C5-C6-O6
4	A	507	NAG	O5-C5-C6-O6
4	A	507	NAG	C4-C5-C6-O6
4	G	509	NAG	C4-C5-C6-O6
4	G	505	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	G	502	NAG	C4-C5-C6-O6
4	A	502	NAG	O5-C5-C6-O6
4	A	501	NAG	O5-C5-C6-O6
4	A	506	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	507	NAG	1	0
4	A	505	NAG	1	0
4	G	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

### 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	A	346/355 (97%)	0.27	28 (8%) 12 13	86, 133, 183, 222	0
1	G	346/355 (97%)	0.22	23 (6%) 18 20	87, 130, 180, 220	0
2	B	213/223 (95%)	0.60	26 (12%) 4 5	88, 145, 214, 242	0
2	H	213/223 (95%)	0.82	36 (16%) 1 2	90, 149, 228, 260	0
3	C	199/203 (98%)	0.33	24 (12%) 4 5	141, 188, 252, 278	0
3	L	199/203 (98%)	0.74	36 (18%) 1 1	130, 201, 260, 294	0
All	All	1516/1562 (97%)	0.45	173 (11%) 5 6	86, 151, 233, 294	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	179	SER	12.9
2	H	165	THR	9.9
2	H	179	SER	9.9
2	B	168	ALA	9.0
2	H	167	PRO	8.8
1	A	471	GLY	8.5
3	L	133	VAL	8.1
2	H	178	LEU	8.0
2	H	140	CYS	7.9
1	A	472	GLY	7.4
2	H	166	PHE	7.1
2	H	142	VAL	6.9
2	H	46	GLU	6.8
2	B	180	SER	6.7
2	H	121	VAL	6.6
2	B	178	LEU	6.6
2	B	127	SER	6.5
2	B	140	CYS	6.4
2	H	168	ALA	6.3

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Mol	Chain	Res	Type	RSRZ
3	L	11	MET	6.2
3	L	104	LEU	6.1
2	H	180	SER	5.9
3	L	86	TYR	5.9
3	C	81	GLU	5.8
2	B	167	PRO	5.8
3	L	81	GLU	5.5
3	L	118	PHE	5.4
3	L	193	CYS	5.3
3	L	12	SER	5.1
3	L	206	VAL	4.7
2	B	137	ALA	4.7
3	L	131	THR	4.6
3	C	133	VAL	4.5
1	A	454	LEU	4.5
1	G	338	TRP	4.5
3	C	104	LEU	4.5
3	L	98	PHE	4.5
1	G	285	ILE	4.5
2	B	165	THR	4.4
3	L	21	ILE	4.4
3	L	135	LEU	4.4
3	L	117	LEU	4.4
3	C	96	GLU	4.4
1	A	452	ILE	4.4
3	L	36	PHE	4.4
2	H	45	LEU	4.3
1	G	452	ILE	4.3
3	L	103	LYS	4.2
3	L	134	CYS	4.2
2	H	141	LEU	4.1
2	B	166	PHE	4.1
3	L	177	TYR	4.1
1	A	453	LEU	4.0
3	C	106	VAL	4.0
1	G	484	TYR	4.0
3	C	98	PHE	4.0
3	L	142	GLY	4.0
2	B	142	VAL	3.9
2	B	47	TRP	3.9
3	L	105	THR	3.8
1	A	281	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
3	L	144	VAL	3.8
2	H	39	GLN	3.7
3	C	177	TYR	3.7
3	L	175	SER	3.7
3	L	132	LEU	3.7
2	H	38	ARG	3.7
2	B	46	GLU	3.7
1	G	286	VAL	3.6
1	A	226	LEU	3.6
3	C	89	ASN	3.6
1	A	338	TRP	3.5
1	G	472	GLY	3.5
3	C	118	PHE	3.5
1	A	470	PRO	3.4
3	C	105	THR	3.4
3	L	73	LEU	3.4
1	G	454	LEU	3.4
1	A	285	ILE	3.4
1	A	280	ASN	3.3
1	A	286	VAL	3.3
1	G	486	TYR	3.3
2	B	194	TYR	3.3
1	G	284	ILE	3.3
1	G	240	LYS	3.3
1	G	283	THR	3.3
3	L	162	THR	3.2
2	H	82	LEU	3.1
3	C	143	ALA	3.1
2	H	127	SER	3.1
2	B	45	LEU	3.1
3	L	106	VAL	3.1
1	G	485	LYS	3.1
2	B	59	TYR	3.0
1	G	453	LEU	3.0
1	A	492	GLU	2.9
3	L	99	GLY	2.8
2	H	82(A)	ARG	2.8
1	A	483	LEU	2.8
1	G	249	HIS	2.8
1	A	258	GLN	2.8
1	G	226	LEU	2.8
1	G	471	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	81	GLU	2.8
3	C	13	ALA	2.7
2	H	123	PRO	2.7
1	A	390	LEU	2.7
2	B	126	PRO	2.7
2	H	90	TYR	2.7
2	B	81	GLU	2.7
1	A	284	ILE	2.7
3	C	31	ILE	2.7
1	A	484	TYR	2.6
3	L	143	ALA	2.6
2	H	157	GLY	2.6
2	H	197	ASN	2.6
3	L	87	ILE	2.6
3	C	107	SER	2.6
1	A	449	ILE	2.6
2	B	138	LEU	2.5
2	B	48	MET	2.5
3	L	185	TRP	2.5
2	B	211	VAL	2.5
1	G	288	LEU	2.5
2	H	160	THR	2.5
3	C	36	PHE	2.5
1	G	244	SER	2.5
3	L	123	GLU	2.5
2	H	63	PHE	2.5
1	G	280	ASN	2.4
3	L	102	THR	2.4
2	B	58	ASN	2.4
3	L	191	TYR	2.4
2	H	153	SER	2.4
3	L	148	TRP	2.4
1	A	455	THR	2.4
3	L	100	GLY	2.3
1	A	246	GLN	2.3
1	A	477	ASP	2.3
2	H	170	LEU	2.3
1	G	273	ARG	2.3
2	H	47	TRP	2.3
1	G	449	ILE	2.3
2	H	125	ALA	2.3
3	C	135	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	173	SER	2.3
3	C	12	SER	2.3
1	A	245	VAL	2.3
2	H	67	VAL	2.3
1	A	391	PHE	2.2
3	C	146	VAL	2.2
2	B	100(A)	TYR	2.2
2	H	100(C)	PHE	2.2
2	H	59	TYR	2.2
3	C	117	LEU	2.2
2	H	156	SER	2.2
3	C	175	SER	2.1
1	A	251	ILE	2.1
1	G	281	ALA	2.1
3	C	44	PRO	2.1
2	H	199	ASN	2.1
3	C	38	GLN	2.1
1	A	481	SER	2.1
3	L	146	VAL	2.1
1	A	486	TYR	2.1
2	B	169	VAL	2.1
1	G	86	LEU	2.1
2	B	121	VAL	2.0
3	C	39	TYR	2.0
2	H	119	PRO	2.0
3	C	142	GLY	2.0
1	A	225	ILE	2.0
2	H	120	SER	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, 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(Å <sup>2</sup> )	Q<0.9
4	NAG	G	505	14/15	0.69	0.59	164,201,229,238	0
6	MG	G	512	1/1	0.71	0.31	90,90,90,90	0
4	NAG	G	501	14/15	0.76	0.41	202,220,239,245	0
6	MG	A	513	1/1	0.78	0.67	108,108,108,108	0
4	NAG	A	503	14/15	0.80	0.55	177,193,208,210	0
4	NAG	G	507	14/15	0.81	0.34	93,144,177,178	0
4	NAG	A	507	14/15	0.82	0.27	84,142,181,181	0
4	NAG	A	501	14/15	0.82	0.42	197,216,239,250	0
4	NAG	G	508	14/15	0.82	0.36	145,183,206,215	0
4	NAG	A	505	14/15	0.83	0.44	161,199,214,227	0
5	CL	G	511	1/1	0.84	0.26	100,100,100,100	0
4	NAG	A	509	14/15	0.86	0.24	124,141,165,183	0
4	NAG	G	503	14/15	0.86	0.32	162,178,189,192	0
4	NAG	G	510	14/15	0.87	0.17	149,194,208,211	0
4	NAG	A	508	14/15	0.88	0.26	159,183,197,204	0
4	NAG	A	510	14/15	0.89	0.18	153,195,209,220	0
4	NAG	A	502	14/15	0.90	0.20	141,163,177,181	0
4	NAG	G	506	14/15	0.91	0.17	117,141,158,161	0
4	NAG	G	509	14/15	0.91	0.18	119,139,172,176	0
4	NAG	G	502	14/15	0.92	0.20	133,156,167,178	0
6	MG	A	512	1/1	0.94	0.29	73,73,73,73	0
4	NAG	G	504	14/15	0.95	0.16	100,120,137,139	0
4	NAG	A	504	14/15	0.95	0.21	102,121,136,137	0
5	CL	A	511	1/1	0.95	0.28	84,84,84,84	0
4	NAG	A	506	14/15	0.96	0.11	140,155,170,176	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.