



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2022 – 09:54 AM EDT

PDB ID : 7S07
Title : Crystal structure of Epstein-Barr virus glycoprotein gH/gL/gp42-peptide in complex with human neutralizing antibodies 769B10 and 769C2
Authors : Chen, W.-H.; Kanekiyo, M.; Cohen, J.I.; Joyce, M.G.
Deposited on : 2021-08-30
Resolution : 3.29 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

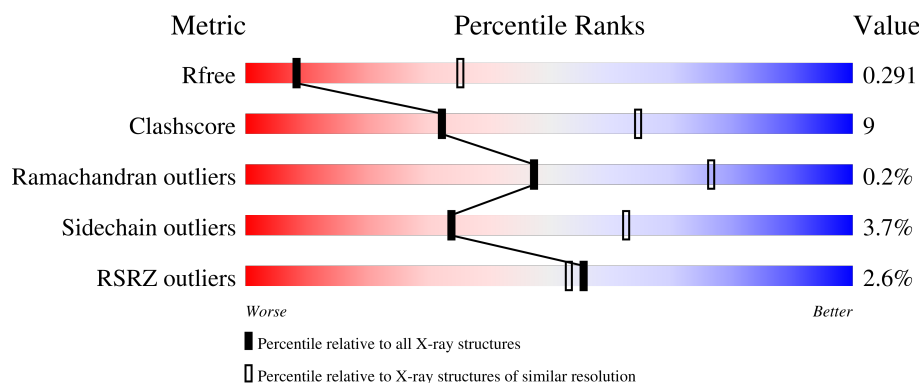
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	657	<div> <div>0%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
2	B	98	<div> <div>5%</div> <div>69%</div> <div>29%</div> <div>.</div> </div>
3	C	33	<div> <div>3%</div> <div>94%</div> <div>6%</div> <div>.</div> </div>
4	X	225	<div> <div>2%</div> <div>69%</div> <div>24%</div> <div>.</div> <div>.</div> </div>
5	Y	215	<div> <div>7%</div> <div>71%</div> <div>25%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
6	H	234	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>78%</div><div>20%</div><div></div></div></div>
7	L	214	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>78%</div><div>19%</div><div></div></div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12693 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			5082	3256	840	955	31			

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			744	469	126	145	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	35	ALA	ARG	conflict	UNP P03212

- Molecule 3 is a protein called Soluble gp42.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	33	Total	C	N	O	0	0	0
			266	173	42	51			

- Molecule 4 is a protein called 769C2 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	215	Total	C	N	O	S	0	0	0
			1609	1016	271	315	7			

- Molecule 5 is a protein called 769C2 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Y	212	Total	C	N	O	S	0	0	0
			1576	983	260	328	5			

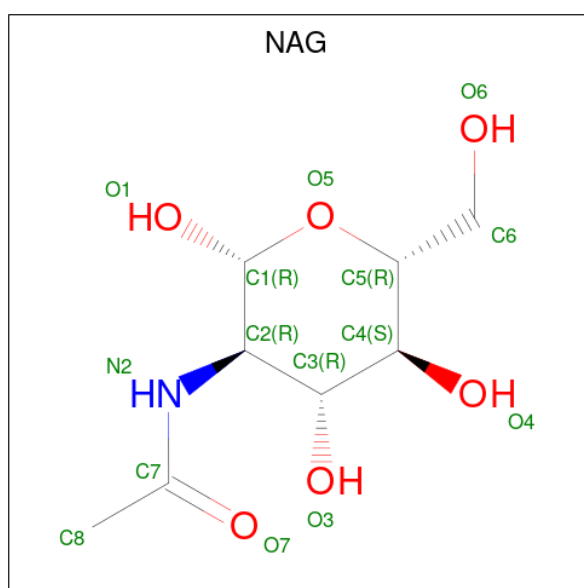
- Molecule 6 is a protein called 769B10 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	230	Total	C	N	O	S	0	0	0
			1748	1100	303	339	6			

- Molecule 7 is a protein called 769B10 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	209	Total	C	N	O	S	0	0	0
			1612	1013	267	325	7			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

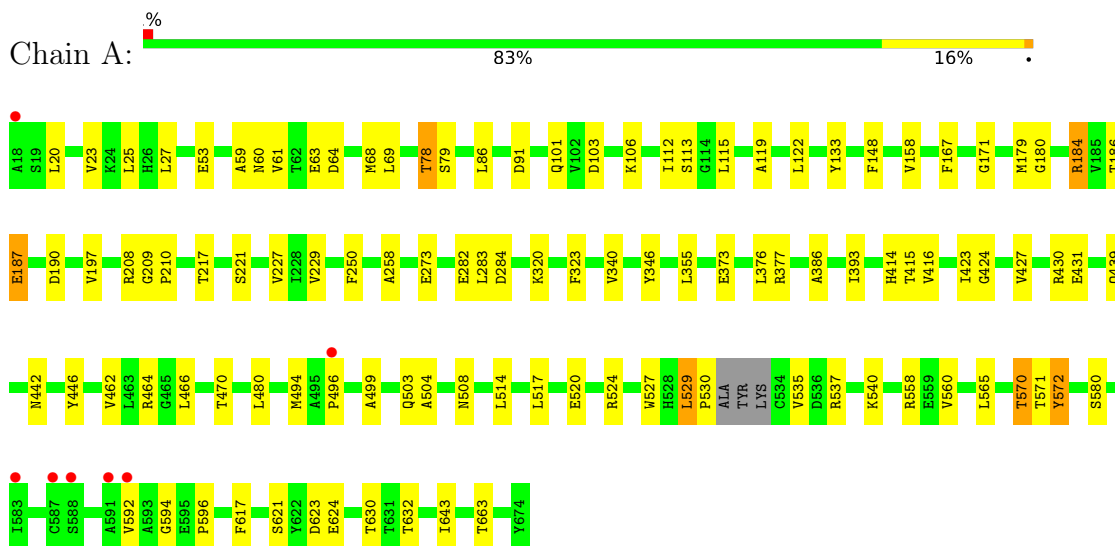


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	A	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		
8	B	1	Total	C	N	O	0	0
			14	8	1	5		

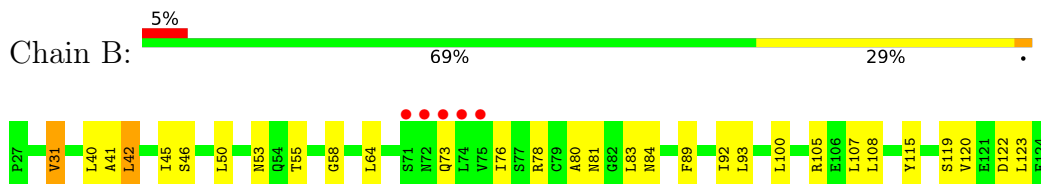
3 Residue-property plots [i](#)

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.

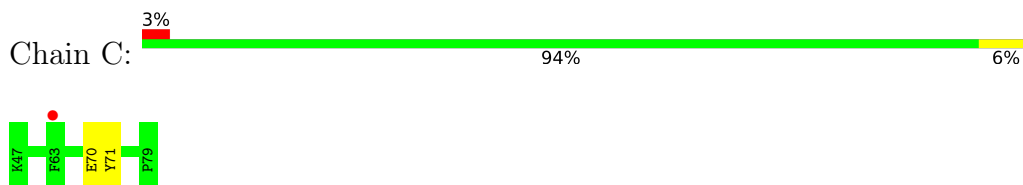
- Molecule 1: Envelope glycoprotein H



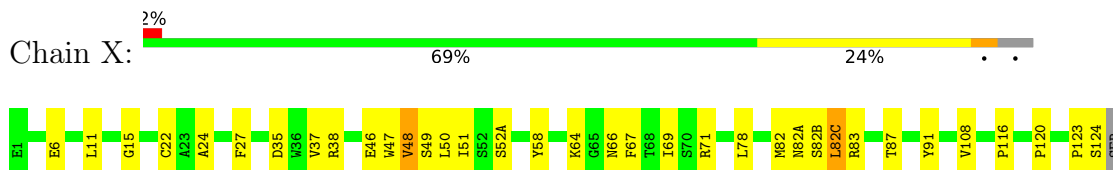
- Molecule 2: Envelope glycoprotein L



- Molecule 3: Soluble gp42

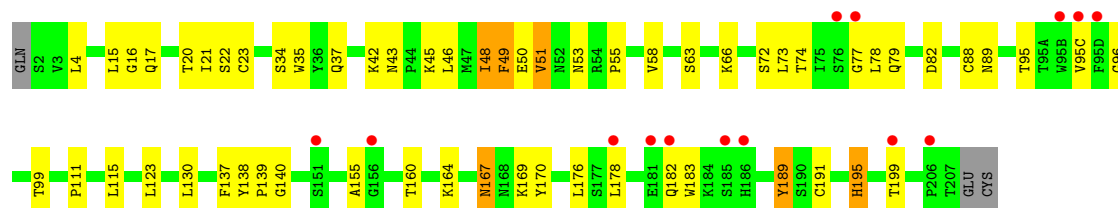


- Molecule 4: 769C2 Fab Heavy chain

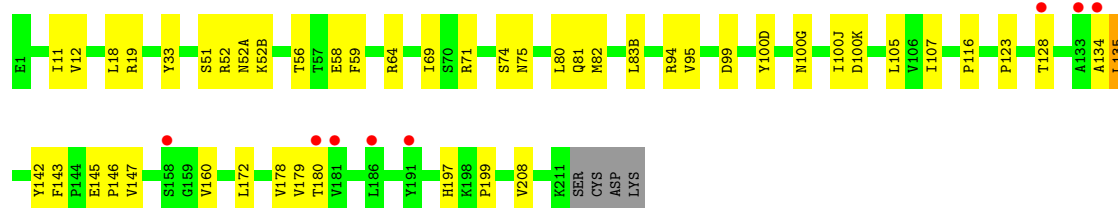
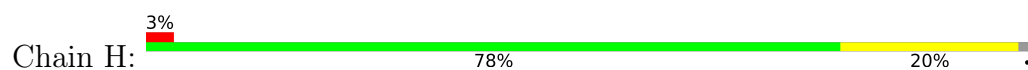




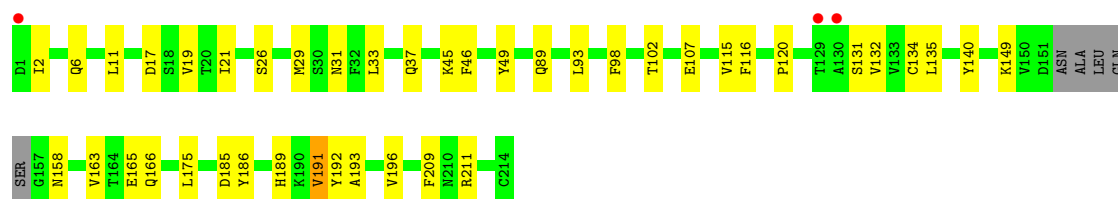
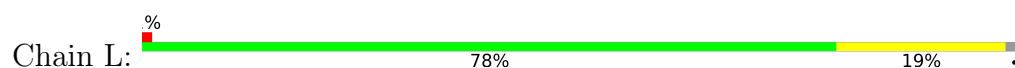
• Molecule 5: 769C2 Fab Light chain



• Molecule 6: 769B10 Fab heavy chain



• Molecule 7: 769B10 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.69Å 130.37Å 93.61Å 90.00° 104.59° 90.00°	Depositor
Resolution (Å)	48.58 – 3.29 48.58 – 3.29	Depositor EDS
% Data completeness (in resolution range)	54.7 (48.58-3.29) 65.0 (48.58-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.243 , 0.291 0.244 , 0.291	Depositor DCC
R_{free} test set	1998 reflections (8.83%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , -14.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.037 for l,-k,h	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	12693	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0/5189	0.47	0/7042
2	B	0.27	0/755	0.46	0/1024
3	C	0.26	0/276	0.40	0/380
4	X	0.28	0/1647	0.56	0/2239
5	Y	0.30	0/1614	0.55	0/2206
6	H	0.27	0/1791	0.47	0/2437
7	L	0.27	0/1648	0.47	0/2234
All	All	0.28	0/12920	0.49	0/17562

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	5082	0	5095	74	0
2	B	744	0	740	23	0
3	C	266	0	257	2	0
4	X	1609	0	1573	40	0
5	Y	1576	0	1512	51	0
6	H	1748	0	1703	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	1612	0	1554	23	0
8	A	28	0	26	2	0
8	B	28	0	26	0	0
All	All	12693	0	12486	222	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 9.

All (222) 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)
5:Y:35:TRP:HB2	5:Y:48:ILE:HG22	1.14	1.08
5:Y:35:TRP:HB2	5:Y:48:ILE:CG2	1.89	1.01
1:A:60:ASN:HB3	1:A:63:GLU:HB2	1.59	0.83
5:Y:17:GLN:CA	5:Y:77:GLY:HA2	2.10	0.81
2:B:119:SER:HB2	2:B:122:ASP:HB3	1.65	0.79
5:Y:17:GLN:HA	5:Y:77:GLY:HA2	1.67	0.77
4:X:82(C):LEU:O	4:X:82(C):LEU:HG	1.84	0.75
1:A:499:ALA:O	1:A:503:GLN:NE2	2.21	0.74
5:Y:46:LEU:HD21	5:Y:49:PHE:HB3	1.69	0.73
1:A:217:THR:HG22	1:A:227:VAL:HG22	1.71	0.73
1:A:208:ARG:NH2	8:A:701:NAG:H82	2.06	0.70
5:Y:16:GLY:O	5:Y:78:LEU:N	2.25	0.70
1:A:208:ARG:HH22	8:A:701:NAG:H82	1.55	0.69
5:Y:111:PRO:HB3	5:Y:137:PHE:HB3	1.77	0.67
1:A:514:LEU:HD13	1:A:517:LEU:HD12	1.77	0.67
2:B:81:ASN:ND2	2:B:84:ASN:OD1	2.26	0.67
5:Y:35:TRP:CB	5:Y:48:ILE:HG22	2.09	0.67
1:A:25:LEU:HD23	2:B:107:LEU:HD11	1.78	0.65
7:L:2:ILE:HG13	7:L:93:LEU:HD11	1.77	0.65
5:Y:16:GLY:O	5:Y:77:GLY:C	2.34	0.65
1:A:558:ARG:HH21	1:A:592:VAL:HG23	1.62	0.64
5:Y:17:GLN:HB3	5:Y:77:GLY:HA2	1.81	0.63
7:L:186:TYR:HE1	7:L:211:ARG:HD3	1.62	0.63
6:H:123:PRO:HD3	6:H:208:VAL:HG12	1.81	0.62
1:A:504:ALA:O	1:A:508:ASN:ND2	2.28	0.62
1:A:167:PHE:HD2	1:A:184:ARG:HB2	1.65	0.61
5:Y:17:GLN:HB3	5:Y:77:GLY:CA	2.31	0.61
5:Y:88:CYS:O	5:Y:96:GLY:N	2.31	0.61
4:X:211:LYS:H	4:X:211:LYS:HD3	1.66	0.61
5:Y:35:TRP:CB	5:Y:48:ILE:CG2	2.74	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:12:VAL:HG21	6:H:18:LEU:HB2	1.83	0.60
1:A:439:GLN:HG3	1:A:442:ASN:HB2	1.83	0.60
1:A:79:SER:O	6:H:52:ARG:NH1	2.35	0.60
4:X:197:HIS:HD2	4:X:199:PRO:HD2	1.67	0.60
1:A:103:ASP:OD2	1:A:106:LYS:NZ	2.35	0.59
2:B:64:LEU:HB2	2:B:78:ARG:HB3	1.84	0.59
5:Y:35:TRP:CD1	5:Y:48:ILE:CG2	2.85	0.59
1:A:23:VAL:HG23	2:B:46:SER:HA	1.85	0.59
4:X:38:ARG:NH2	4:X:46:GLU:OE1	2.36	0.58
1:A:623:ASP:OD1	1:A:624:GLU:N	2.37	0.58
4:X:47:TRP:HZ2	4:X:50:LEU:HB2	1.69	0.58
1:A:520:GLU:HG3	1:A:527:TRP:CD1	2.38	0.58
1:A:186:THR:HG23	1:A:186:THR:O	2.03	0.58
4:X:15:GLY:HA2	4:X:83:ARG:HG2	1.84	0.58
5:Y:17:GLN:CB	5:Y:77:GLY:HA2	2.33	0.57
4:X:120:PRO:HD3	4:X:206:LYS:HG2	1.85	0.57
1:A:617:PHE:HE1	1:A:663:THR:HG22	1.70	0.57
5:Y:15:LEU:HD23	5:Y:15:LEU:N	2.19	0.57
1:A:386:ALA:HB2	1:A:430:ARG:HB3	1.87	0.56
1:A:571:THR:OG1	1:A:572:TYR:N	2.38	0.56
6:H:52(A):ASN:OD1	6:H:52(B):LYS:N	2.39	0.56
1:A:59:ALA:HA	1:A:208:ARG:HE	1.70	0.56
1:A:537:ARG:HG3	1:A:540:LYS:HB2	1.87	0.56
1:A:112:ILE:HD11	1:A:119:ALA:HB2	1.88	0.55
4:X:87:THR:HG21	4:X:108:VAL:H	1.71	0.55
6:H:99:ASP:O	6:H:100(G):ASN:ND2	2.38	0.55
2:B:100:LEU:HD23	2:B:105:ARG:HE	1.71	0.55
6:H:94:ARG:NH2	6:H:100(K):ASP:OD2	2.34	0.55
1:A:184:ARG:HH11	1:A:283:LEU:HD22	1.71	0.55
7:L:2:ILE:HG23	7:L:26:SER:HB3	1.88	0.55
1:A:167:PHE:CD2	1:A:184:ARG:HB2	2.42	0.55
1:A:535:VAL:HG12	1:A:560:VAL:HG13	1.89	0.54
6:H:123:PRO:HG3	6:H:135:LEU:HB3	1.89	0.54
5:Y:15:LEU:HA	5:Y:79:GLN:HB3	1.89	0.54
7:L:120:PRO:HD3	7:L:132:VAL:HG22	1.88	0.54
4:X:15:GLY:CA	4:X:83:ARG:HG2	2.37	0.54
1:A:446:TYR:HE2	1:A:480:LEU:HD13	1.72	0.54
1:A:464:ARG:HB2	1:A:496:PRO:HB3	1.89	0.54
6:H:59:PHE:HB2	6:H:64:ARG:HA	1.89	0.53
7:L:191:VAL:HG13	7:L:192:TYR:H	1.73	0.53
7:L:186:TYR:CE1	7:L:211:ARG:HD3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:22:CYS:HB3	4:X:78:LEU:HB3	1.89	0.53
5:Y:130:LEU:HD13	5:Y:176:LEU:HD23	1.91	0.53
1:A:179:MET:HG3	1:A:197:VAL:HG22	1.90	0.52
7:L:163:VAL:HG22	7:L:175:LEU:HD13	1.91	0.52
6:H:145:GLU:HB2	6:H:146:PRO:HD3	1.91	0.52
5:Y:111:PRO:HD3	5:Y:195:HIS:HD2	1.74	0.52
5:Y:49:PHE:CD1	5:Y:49:PHE:C	2.83	0.52
1:A:221:SER:HB3	1:A:250:PHE:HE2	1.74	0.52
5:Y:111:PRO:HD3	5:Y:195:HIS:CD2	2.45	0.51
5:Y:48:ILE:HG23	5:Y:48:ILE:O	2.11	0.51
1:A:439:GLN:OE1	1:A:442:ASN:ND2	2.43	0.51
5:Y:164:LYS:HA	5:Y:170:TYR:HA	1.93	0.51
1:A:393:ILE:HD12	1:A:439:GLN:HB3	1.93	0.51
4:X:123:PRO:HG2	4:X:210:PRO:HA	1.92	0.51
4:X:197:HIS:CD2	4:X:199:PRO:HD2	2.46	0.51
6:H:82:MET:HB3	6:H:83(B):LEU:HD21	1.93	0.51
6:H:143:PHE:HB2	6:H:172:LEU:HD22	1.93	0.51
5:Y:22:SER:HA	5:Y:72:SER:HA	1.91	0.51
5:Y:35:TRP:CE2	5:Y:73:LEU:HB2	2.47	0.50
1:A:68:MET:SD	2:B:81:ASN:ND2	2.70	0.50
1:A:171:GLY:HA2	1:A:180:GLY:HA2	1.92	0.50
6:H:11:ILE:HA	6:H:107:ILE:HG23	1.94	0.50
7:L:11:LEU:HD21	7:L:19:VAL:HB	1.94	0.50
5:Y:63:SER:N	5:Y:74:THR:O	2.43	0.50
4:X:158:SER:H	4:X:160:VAL:HG23	1.77	0.49
7:L:185:ASP:O	7:L:189:HIS:ND1	2.45	0.49
6:H:69:ILE:HG12	6:H:80:LEU:HD12	1.94	0.49
1:A:64:ASP:HA	2:B:31:VAL:HB	1.95	0.48
6:H:147:VAL:HG22	6:H:197:HIS:CD2	2.48	0.48
1:A:346:TYR:HB3	3:C:70:GLU:HG2	1.95	0.48
7:L:116:PHE:CE1	7:L:135:LEU:HD23	2.48	0.48
4:X:48:VAL:HG12	4:X:49:SER:H	1.79	0.48
7:L:158:ASN:O	7:L:158:ASN:ND2	2.47	0.48
1:A:210:PRO:HB2	2:B:120:VAL:HG13	1.95	0.48
2:B:122:ASP:HA	6:H:64:ARG:HD2	1.95	0.48
1:A:91:ASP:OD2	1:A:258:ALA:N	2.46	0.47
5:Y:63:SER:O	5:Y:73:LEU:HD12	2.14	0.47
1:A:376:LEU:HD13	1:A:424:GLY:HA3	1.96	0.47
4:X:124:SER:HB2	4:X:211:LYS:HD2	1.96	0.47
5:Y:35:TRP:CD1	5:Y:48:ILE:HG21	2.48	0.47
1:A:558:ARG:NH2	1:A:594:GLY:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:LEU:HD23	1:A:596:PRO:HB3	1.96	0.47
4:X:49:SER:HB2	4:X:69:ILE:HD12	1.97	0.47
5:Y:49:PHE:O	5:Y:53:ASN:O	2.33	0.47
6:H:134:ALA:HA	6:H:180:THR:HA	1.95	0.47
4:X:82(B):SER:O	4:X:83:ARG:N	2.47	0.47
6:H:95:VAL:HG22	6:H:100(J):ILE:HG12	1.96	0.47
1:A:78:THR:OG1	6:H:100(D):TYR:O	2.26	0.47
4:X:24:ALA:HB1	4:X:27:PHE:CZ	2.50	0.46
4:X:153:SER:OG	4:X:194:ASN:ND2	2.48	0.46
4:X:15:GLY:HA2	4:X:83:ARG:CG	2.46	0.46
5:Y:4:LEU:HB2	5:Y:96:GLY:HA2	1.98	0.46
6:H:59:PHE:HE1	6:H:69:ILE:HG13	1.80	0.46
6:H:178:VAL:HG11	7:L:135:LEU:HD21	1.96	0.46
1:A:20:LEU:HD11	1:A:53:GLU:HG3	1.96	0.46
1:A:115:LEU:HD23	1:A:355:LEU:HD22	1.98	0.46
2:B:93:LEU:HB2	2:B:108:LEU:HD13	1.97	0.46
4:X:51:ILE:HG21	4:X:78:LEU:HD11	1.97	0.46
5:Y:4:LEU:HD11	5:Y:95(C):VAL:HG13	1.97	0.46
5:Y:48:ILE:HD12	5:Y:53:ASN:O	2.16	0.46
6:H:116:PRO:HB3	6:H:142:TYR:HB3	1.97	0.46
4:X:152:ASN:HB3	4:X:155:ALA:HB2	1.97	0.46
5:Y:155:ALA:HB3	5:Y:178:LEU:HD22	1.97	0.46
4:X:50:LEU:HB3	4:X:58:TYR:HB2	1.98	0.46
6:H:52:ARG:NH2	6:H:58:GLU:OE1	2.49	0.46
1:A:210:PRO:HB3	2:B:83:LEU:HD13	1.98	0.45
5:Y:35:TRP:CD2	5:Y:73:LEU:HB2	2.51	0.45
5:Y:49:PHE:CD1	5:Y:49:PHE:O	2.69	0.45
1:A:101:GLN:HB3	1:A:122:LEU:HD21	1.98	0.45
6:H:33:TYR:HB2	6:H:95:VAL:HB	1.98	0.45
7:L:21:ILE:HG23	7:L:102:THR:HG21	1.98	0.45
1:A:69:LEU:HD11	2:B:123:LEU:HD12	1.98	0.45
2:B:40:LEU:HD23	2:B:40:LEU:HA	1.86	0.45
1:A:184:ARG:NH1	1:A:283:LEU:HD22	2.30	0.45
1:A:133:TYR:OH	3:C:71:TYR:O	2.32	0.45
7:L:115:VAL:HG21	7:L:196:VAL:HG21	1.99	0.45
1:A:320:LYS:HA	1:A:377:ARG:HD3	1.98	0.45
1:A:570:THR:OG1	1:A:571:THR:N	2.50	0.45
4:X:64:LYS:C	4:X:66:ASN:H	2.20	0.45
7:L:46:PHE:HZ	7:L:49:TYR:HB3	1.80	0.45
1:A:148:PHE:CZ	1:A:229:VAL:HG21	2.52	0.45
4:X:47:TRP:CZ2	4:X:50:LEU:HB2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:182:GLN:HG2	5:Y:189:TYR:CE1	2.51	0.45
2:B:40:LEU:HD11	2:B:78:ARG:HG2	1.97	0.45
4:X:51:ILE:HG12	4:X:71:ARG:HG2	1.98	0.44
4:X:52(A):SER:HA	4:X:71:ARG:NH2	2.31	0.44
7:L:37:GLN:O	7:L:45:LYS:N	2.45	0.44
1:A:393:ILE:HD11	1:A:431:GLU:HG3	1.99	0.44
6:H:75:ASN:OD1	6:H:75:ASN:N	2.48	0.44
4:X:167:LEU:HD23	4:X:167:LEU:H	1.83	0.44
4:X:6:GLU:OE1	4:X:6:GLU:N	2.51	0.44
7:L:165:GLU:HG3	7:L:166:GLN:H	1.83	0.44
5:Y:35:TRP:CG	5:Y:48:ILE:CG2	3.00	0.43
4:X:116:PRO:HB3	4:X:142:TYR:HB3	2.01	0.43
5:Y:167:ASN:ND2	5:Y:169:LYS:HE3	2.34	0.43
2:B:89:PHE:HA	2:B:92:ILE:HG22	2.01	0.43
1:A:621:SER:OG	1:A:630:THR:OG1	2.23	0.43
4:X:87:THR:HG21	4:X:108:VAL:N	2.33	0.43
5:Y:42:LYS:NZ	5:Y:43:ASN:OD1	2.33	0.43
1:A:158:VAL:HG22	1:A:340:VAL:HG22	2.01	0.43
1:A:462:VAL:O	1:A:466:LEU:N	2.51	0.43
4:X:168:GLN:HB3	4:X:172:LEU:O	2.18	0.43
5:Y:115:LEU:HD22	5:Y:191:CYS:HB3	2.01	0.43
1:A:20:LEU:HD21	2:B:42:LEU:HB3	2.00	0.43
5:Y:55:PRO:HD2	5:Y:58:VAL:HG21	2.01	0.43
7:L:29:MET:HE1	7:L:33:LEU:HB2	2.00	0.43
1:A:27:LEU:HD13	2:B:50:LEU:HB2	2.01	0.43
1:A:414:HIS:CD2	1:A:416:VAL:HB	2.54	0.42
4:X:135:LEU:HG	4:X:208:VAL:HG11	2.00	0.42
1:A:414:HIS:ND1	1:A:415:THR:N	2.67	0.42
4:X:143:PHE:HA	4:X:144:PRO:HA	1.84	0.42
1:A:59:ALA:O	2:B:84:ASN:ND2	2.52	0.42
1:A:282:GLU:O	1:A:284:ASP:N	2.52	0.42
7:L:89:GLN:HB2	7:L:98:PHE:CD2	2.54	0.42
1:A:632:THR:HG21	1:A:643:ILE:HD11	2.01	0.42
6:H:19:ARG:NH1	6:H:81:GLN:OE1	2.52	0.42
4:X:166:VAL:HA	5:Y:160:THR:HG22	2.01	0.42
5:Y:22:SER:OG	5:Y:23:CYS:N	2.53	0.42
4:X:37:VAL:O	4:X:91:TYR:N	2.49	0.42
2:B:41:ALA:O	2:B:45:ILE:HD13	2.20	0.42
2:B:53:ASN:HB2	2:B:58:GLY:HA2	2.02	0.42
1:A:323:PHE:CZ	1:A:423:ILE:HG13	2.55	0.42
1:A:424:GLY:O	1:A:427:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:35:ASP:OD1	4:X:50:LEU:HG	2.20	0.42
5:Y:182:GLN:HG2	5:Y:189:TYR:OH	2.20	0.42
6:H:51:SER:OG	6:H:71:ARG:NH1	2.53	0.42
7:L:120:PRO:HB3	7:L:131:SER:H	1.84	0.42
1:A:61:VAL:O	2:B:80:ALA:HB1	2.19	0.42
1:A:209:GLY:O	2:B:115:TYR:OH	2.25	0.42
5:Y:45:LYS:HD3	5:Y:45:LYS:HA	1.79	0.42
7:L:149:LYS:HB2	7:L:193:ALA:HB3	2.02	0.42
5:Y:35:TRP:CD1	5:Y:48:ILE:HG23	2.54	0.41
4:X:87:THR:HG22	4:X:108:VAL:HG23	2.02	0.41
1:A:187:GLU:OE2	1:A:187:GLU:CA	2.68	0.41
5:Y:137:PHE:CE2	5:Y:140:GLY:HA2	2.55	0.41
6:H:197:HIS:CD2	6:H:199:PRO:HD2	2.56	0.41
5:Y:63:SER:HB2	5:Y:74:THR:HB	2.03	0.41
5:Y:138:TYR:CD1	5:Y:139:PRO:HA	2.56	0.41
1:A:187:GLU:N	1:A:187:GLU:CD	2.74	0.41
1:A:529:LEU:N	1:A:530:PRO:HD3	2.35	0.41
4:X:152:ASN:C	4:X:154:GLY:H	2.24	0.41
1:A:373:GLU:O	1:A:377:ARG:HG3	2.20	0.41
6:H:160:VAL:HG22	6:H:179:VAL:HB	2.03	0.41
5:Y:34:SER:HB2	5:Y:89:ASN:OD1	2.22	0.40
5:Y:35:TRP:HD1	5:Y:48:ILE:HG23	1.86	0.40
1:A:524:ARG:HE	1:A:524:ARG:HB3	1.47	0.40
1:A:565:LEU:HD12	1:A:580:SER:HB3	2.04	0.40
7:L:107:GLU:HA	7:L:140:TYR:OH	2.22	0.40
1:A:187:GLU:OE2	1:A:187:GLU:HA	2.22	0.40
4:X:11:LEU:HD13	4:X:144:PRO:HD3	2.04	0.40
7:L:6:GLN:NE2	7:L:102:THR:HG23	2.36	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	650/657 (99%)	606 (93%)	44 (7%)	0	100	100
2	B	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
3	C	31/33 (94%)	29 (94%)	2 (6%)	0	100	100
4	X	211/225 (94%)	190 (90%)	19 (9%)	2 (1%)	17	48
5	Y	210/215 (98%)	176 (84%)	32 (15%)	2 (1%)	15	46
6	H	228/234 (97%)	211 (92%)	17 (8%)	0	100	100
7	L	205/214 (96%)	191 (93%)	14 (7%)	0	100	100
All	All	1631/1676 (97%)	1491 (91%)	136 (8%)	4 (0%)	47	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	X	82(C)	LEU
5	Y	51	VAL
5	Y	50	GLU
4	X	154	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	560/562 (100%)	548 (98%)	12 (2%)	53	75
2	B	87/87 (100%)	82 (94%)	5 (6%)	20	51
3	C	31/31 (100%)	31 (100%)	0	100	100
4	X	181/189 (96%)	171 (94%)	10 (6%)	21	52
5	Y	180/183 (98%)	164 (91%)	16 (9%)	9	32
6	H	196/200 (98%)	191 (97%)	5 (3%)	46	71
7	L	184/188 (98%)	179 (97%)	5 (3%)	44	71
All	All	1419/1440 (98%)	1366 (96%)	53 (4%)	34	63

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	THR
1	A	86	LEU
1	A	113	SER
1	A	184	ARG
1	A	187	GLU
1	A	190	ASP
1	A	273	GLU
1	A	470	THR
1	A	494	MET
1	A	529	LEU
1	A	570	THR
1	A	572	TYR
2	B	31	VAL
2	B	42	LEU
2	B	55	THR
2	B	73	GLN
2	B	76	ILE
4	X	48	VAL
4	X	67	PHE
4	X	82	MET
4	X	82(A)	ASN
4	X	149	VAL
4	X	150	SER
4	X	157	THR
4	X	158	SER
4	X	167	LEU
4	X	211	LYS
5	Y	20	THR
5	Y	21	ILE
5	Y	37	GLN
5	Y	48	ILE
5	Y	49	PHE
5	Y	51	VAL
5	Y	66	LYS
5	Y	82	ASP
5	Y	95	THR
5	Y	99	THR
5	Y	123	LEU
5	Y	167	ASN
5	Y	183	TRP
5	Y	189	TYR
5	Y	195	HIS
5	Y	199	THR

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Mol	Chain	Res	Type
6	H	56	THR
6	H	74	SER
6	H	105	LEU
6	H	128	THR
6	H	135	LEU
7	L	17	ASP
7	L	31	ASN
7	L	134	CYS
7	L	191	VAL
7	L	209	PHE

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

Mol	Chain	Res	Type
7	L	27	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](#)

4 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
8	NAG	B	202	2	14,14,15	0.47	0	17,19,21	0.98	1 (5%)
8	NAG	B	201	2	14,14,15	0.79	1 (7%)	17,19,21	1.05	1 (5%)
8	NAG	A	701	1	14,14,15	1.01	1 (7%)	17,19,21	0.78	1 (5%)
8	NAG	A	702	1	14,14,15	2.50	1 (7%)	17,19,21	2.41	2 (11%)

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
8	NAG	B	202	2	-	3/6/23/26	0/1/1/1
8	NAG	B	201	2	-	0/6/23/26	0/1/1/1
8	NAG	A	701	1	-	2/6/23/26	0/1/1/1
8	NAG	A	702	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	702	NAG	O5-C1	9.13	1.58	1.43
8	A	701	NAG	O5-C1	3.49	1.49	1.43
8	B	201	NAG	O5-C1	2.71	1.48	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	702	NAG	C1-O5-C5	9.10	124.52	112.19
8	B	201	NAG	C1-O5-C5	3.56	117.01	112.19
8	A	701	NAG	C1-O5-C5	2.47	115.53	112.19
8	B	202	NAG	C2-N2-C7	2.24	126.10	122.90
8	A	702	NAG	O3-C3-C2	2.24	114.11	109.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	701	NAG	O5-C5-C6-O6
8	B	202	NAG	O5-C5-C6-O6
8	B	202	NAG	C1-C2-N2-C7
8	A	701	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	B	202	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	701	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	654/657 (99%)	-0.01	7 (1%) 80 81	15, 37, 76, 102	0
2	B	98/98 (100%)	0.13	5 (5%) 28 26	19, 43, 91, 135	0
3	C	33/33 (100%)	0.15	1 (3%) 50 49	30, 53, 76, 108	0
4	X	215/225 (95%)	0.22	5 (2%) 60 59	30, 58, 84, 117	0
5	Y	212/215 (98%)	0.41	14 (6%) 18 18	35, 65, 110, 147	0
6	H	230/234 (98%)	0.22	8 (3%) 44 42	23, 54, 105, 126	0
7	L	209/214 (97%)	-0.03	3 (1%) 75 75	17, 42, 83, 101	0
All	All	1651/1676 (98%)	0.12	43 (2%) 56 53	15, 49, 92, 147	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	72	ASN	6.3
5	Y	182	GLN	5.1
1	A	18	ALA	4.0
7	L	1	ASP	3.9
5	Y	185	SER	3.6
6	H	181	VAL	3.4
6	H	133	ALA	3.4
5	Y	77	GLY	3.3
2	B	73	GLN	3.3
1	A	592	VAL	3.1
2	B	75	VAL	3.1
6	H	134	ALA	2.8
6	H	180	THR	2.8
2	B	74	LEU	2.7
5	Y	156	GLY	2.7
5	Y	181	GLU	2.7
7	L	129	THR	2.7

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Mol	Chain	Res	Type	RSRZ
5	Y	186	HIS	2.7
3	C	63	PHE	2.7
7	L	130	ALA	2.6
5	Y	178	LEU	2.6
4	X	149	VAL	2.6
5	Y	95(D)	PHE	2.6
4	X	204	VAL	2.5
1	A	588	SER	2.5
2	B	71	SER	2.5
5	Y	95(B)	TRP	2.5
5	Y	76	SER	2.5
5	Y	199	THR	2.5
6	H	186	LEU	2.5
4	X	132	THR	2.5
1	A	496	PRO	2.4
1	A	587	CYS	2.4
5	Y	151	SER	2.3
6	H	191	TYR	2.3
6	H	128	THR	2.3
5	Y	206	PRO	2.2
6	H	158	SER	2.2
5	Y	95(C)	VAL	2.2
1	A	583	ILE	2.1
4	X	169	SER	2.1
1	A	591	ALA	2.0
4	X	209	GLU	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
8	NAG	A	702	14/15	0.87	0.26	32,38,49,50	0
8	NAG	A	701	14/15	0.88	0.20	20,33,40,47	0
8	NAG	B	201	14/15	0.89	0.37	25,41,51,54	0
8	NAG	B	202	14/15	0.90	0.18	26,42,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.