



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 01:36 AM BST

PDB ID : 6E62
Title : Crystal structure of malaria transmission-blocking antigen Pfs48/45 6C in complex with antibody 85RF45.1
Authors : Kundu, P.; Semesi, A.; Julien, J.P.
Deposited on : 2018-07-23
Resolution : 2.70 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 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 : 2.13.1
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

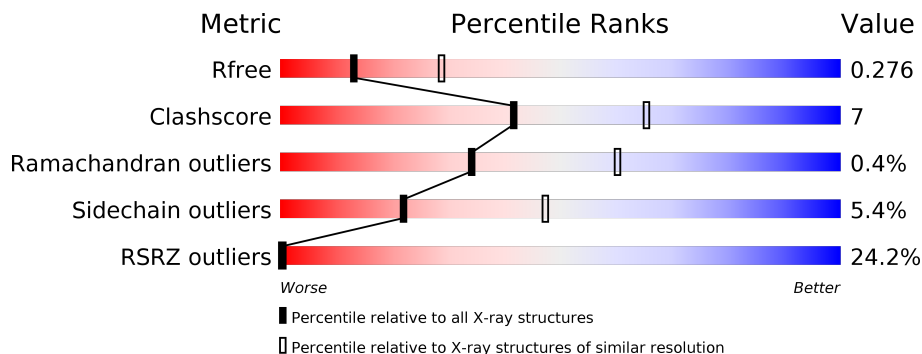
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 ≥ 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	139	 2% 76% 21% ..
1	P	139	 68% 28% ..
2	B	222	 26% 86% 10% ..
2	H	222	 37% 83% 13% ..
3	C	216	 28% 76% 19% ..
3	L	216	 32% 82% 15% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8799 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 Pf48/45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	P	137	1059	667	167	218	7	0	0	0
1	A	137	1059	667	167	218	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	429	GLY	-	expression tag	UNP A8QVT1
A	429	GLY	-	expression tag	UNP A8QVT1

- Molecule 2 is a protein called 85RF45.1 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	217	1650	1045	275	322	8	0	0	0
2	B	217	1650	1045	275	322	8	0	0	0

- Molecule 3 is a protein called 85RF45.1 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	213	1625	1013	277	329	6	0	0	0
3	C	213	1625	1013	277	329	6	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	H	1	6	3	3	0	0
5	B	1	6	3	3	0	0

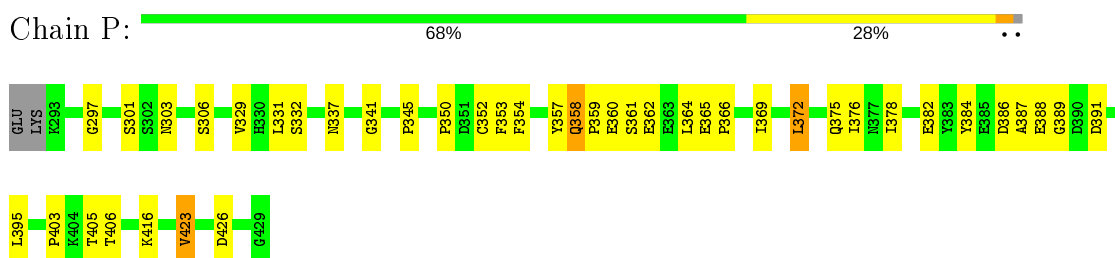
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	20	Total 20	O 20	0	0
6	H	9	Total 9	O 9	0	0
6	L	9	Total 9	O 9	0	0
6	A	26	Total 26	O 26	0	0
6	B	17	Total 17	O 17	0	0
6	C	10	Total 10	O 10	0	0

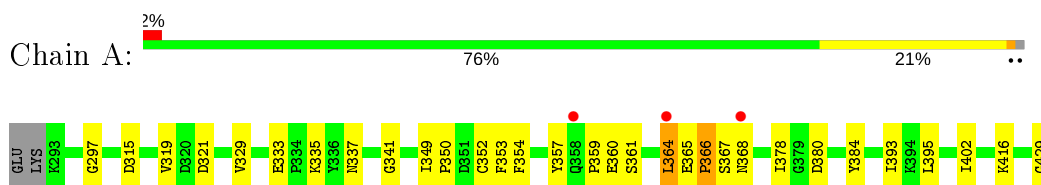
3 Residue-property plots [i](#)

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.

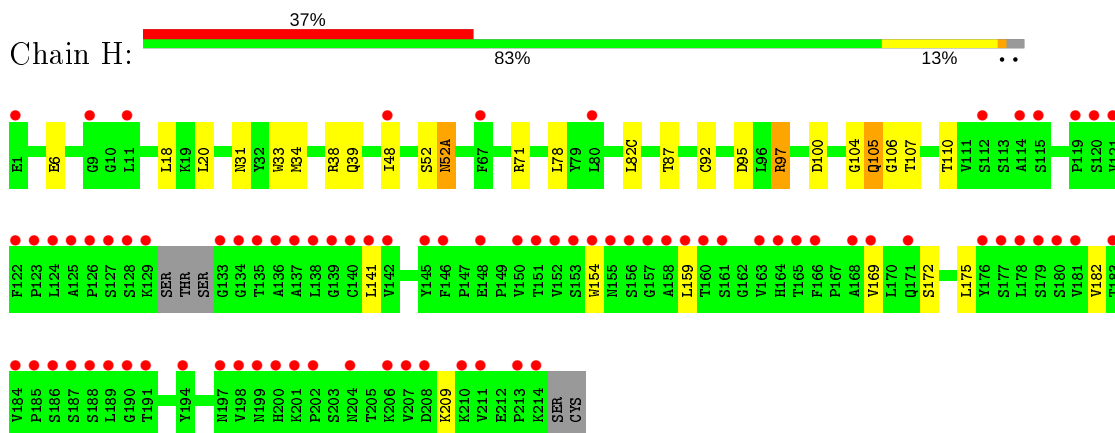
- Molecule 1: Pf48/45



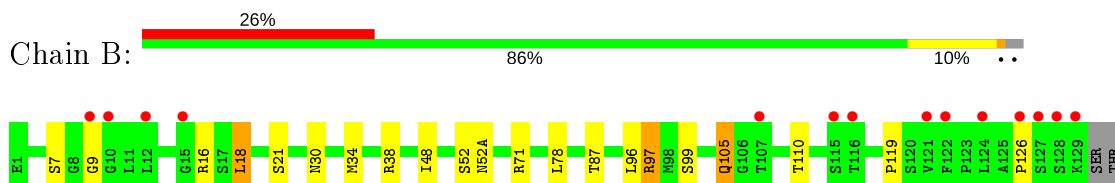
- Molecule 1: Pf48/45

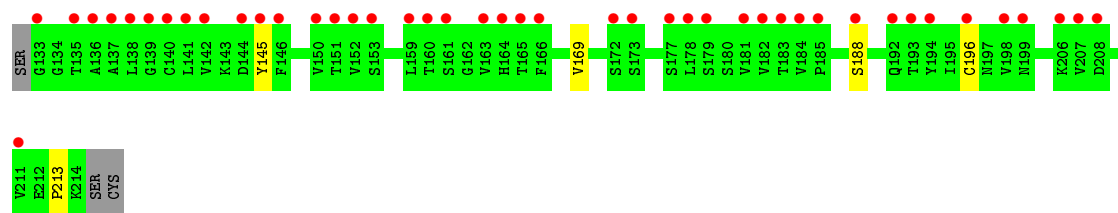


- Molecule 2: 85RF45.1 Fab heavy chain

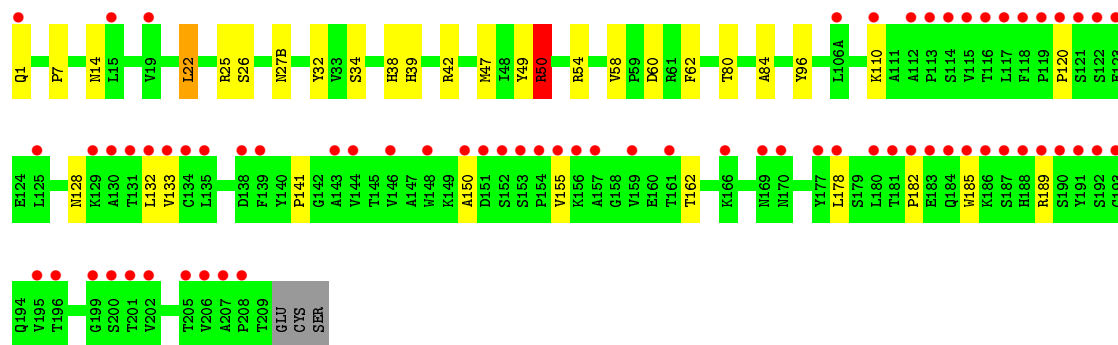
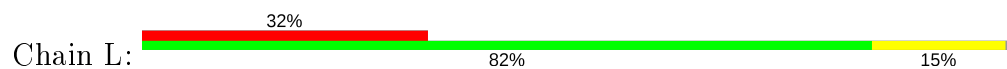


- Molecule 2: 85RF45.1 Fab heavy chain

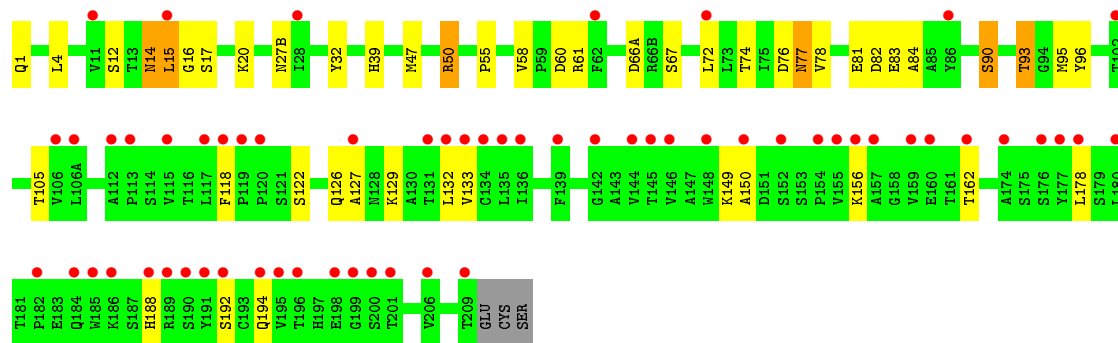
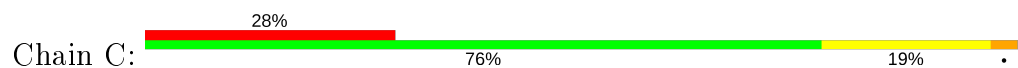




- Molecule 3: 85RF45.1 Fab light chain



- Molecule 3: 85RF45.1 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	54.51Å 74.45Å 321.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.70 48.70 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.70-2.70) 100.0 (48.70-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.246 , 0.276 0.246 , 0.276	Depositor DCC
R_{free} test set	1858 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtrriage
Anisotropy	0.252	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8799	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: GOL, 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	0.29	0/1081	0.51	0/1466
1	P	0.28	0/1081	0.46	0/1466
2	B	0.26	0/1690	0.48	0/2299
2	H	0.25	0/1690	0.46	0/2299
3	C	0.26	0/1664	0.46	1/2268 (0.0%)
3	L	0.25	0/1664	0.46	0/2268
All	All	0.26	0/8870	0.47	1/12066 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	15	LEU	CA-CB-CG	5.07	126.97	115.30

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	1059	0	1008	23	0
1	P	1059	0	1008	20	0
2	B	1650	0	1616	17	0
2	H	1650	0	1616	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1625	0	1567	27	0
3	L	1625	0	1567	23	0
4	A	14	0	13	0	0
4	P	14	0	13	1	0
5	B	6	0	8	2	0
5	H	6	0	8	2	0
6	A	26	0	0	4	0
6	B	17	0	0	0	0
6	C	10	0	0	1	0
6	H	9	0	0	1	0
6	L	9	0	0	3	0
6	P	20	0	0	2	0
All	All	8799	0	8424	120	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 7.

All (120) 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)
3:L:96:TYR:OH	6:L:301:HOH:O	1.92	0.86
2:B:97:ARG:NH2	3:C:96:TYR:OH	2.14	0.80
1:P:301:SER:O	6:P:601:HOH:O	2.00	0.79
3:C:83:GLU:HG3	3:C:105:THR:HA	1.64	0.78
3:L:54:ARG:NH2	3:L:62:PHE:O	2.18	0.77
1:A:429:GLY:O	6:A:601:HOH:O	2.04	0.75
1:P:303:ASN:OD1	6:P:602:HOH:O	2.06	0.72
2:H:100:ASP:O	6:H:401:HOH:O	2.09	0.69
1:P:384:TYR:HB2	1:P:395:LEU:HB2	1.75	0.68
1:A:384:TYR:HB2	1:A:395:LEU:HB2	1.75	0.67
2:H:31:ASN:O	5:H:301:GOL:O2	2.14	0.65
2:H:97:ARG:NH1	2:H:100:ASP:OD1	2.30	0.64
1:A:378:ILE:HG22	1:A:380:ASP:H	1.62	0.63
3:L:1:GLN:N	6:L:303:HOH:O	2.34	0.61
3:L:25:ARG:NH2	3:L:27(B):ASN:O	2.34	0.61
3:L:26:SER:O	6:L:302:HOH:O	2.16	0.60
1:A:367:SER:O	6:A:602:HOH:O	2.17	0.58
2:H:87:THR:HG23	2:H:110:THR:HA	1.84	0.58
2:B:52:SER:O	2:B:71:ARG:NH1	2.36	0.58
3:C:20:LYS:NZ	6:C:302:HOH:O	2.37	0.57
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52(A):ASN:OD1	2:H:52(A):ASN:N	2.38	0.56
3:L:128:ASN:HA	3:L:182:PRO:HG2	1.87	0.56
3:L:39:HIS:CG	3:L:42:ARG:HH21	2.24	0.56
3:C:61:ARG:NH1	3:C:77:ASN:O	2.39	0.56
3:C:150:ALA:HB1	3:C:188:HIS:CD2	2.40	0.56
1:A:315:ASP:OD1	6:A:603:HOH:O	2.18	0.56
2:H:154:TRP:HB3	2:H:159:LEU:HD23	1.88	0.56
2:B:97:ARG:HD3	2:B:97:ARG:O	2.06	0.55
1:A:366:PRO:HD2	5:B:301:GOL:H32	1.88	0.55
2:B:38:ARG:HB3	2:B:48:ILE:HD11	1.88	0.55
3:L:132:LEU:HD12	3:L:178:LEU:HD23	1.89	0.55
1:P:416:LYS:HE2	3:L:32:TYR:CD1	2.42	0.55
2:H:141:LEU:HD21	3:L:133:VAL:HG21	1.88	0.54
2:B:87:THR:HG23	2:B:110:THR:HA	1.89	0.54
3:C:14:ASN:ND2	3:C:17:SER:OG	2.40	0.54
3:L:150:ALA:H	3:L:155:VAL:HG23	1.73	0.54
3:L:110:LYS:HD3	3:L:141:PRO:HD3	1.90	0.54
3:C:15:LEU:HD22	3:C:78:VAL:O	2.08	0.54
3:L:80:THR:HB	3:C:156:LYS:HE3	1.91	0.53
3:C:20:LYS:HB3	3:C:72:LEU:HD23	1.91	0.53
3:L:150:ALA:H	3:L:155:VAL:CG2	2.22	0.52
1:A:335:LYS:NZ	6:A:605:HOH:O	2.36	0.52
2:H:52:SER:O	2:H:71:ARG:NH1	2.42	0.52
1:P:341:GLY:HA2	1:P:353:PHE:CE2	2.45	0.52
3:C:132:LEU:HD12	3:C:178:LEU:HD23	1.92	0.52
1:A:365:GLU:OE1	5:B:301:GOL:O3	2.19	0.51
1:P:350:PRO:HB3	1:P:369:ILE:HD13	1.92	0.51
2:B:34:MET:HB3	2:B:78:LEU:HD22	1.92	0.51
1:P:358:GLN:HG3	1:P:375:GLN:NE2	2.25	0.51
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.91	0.51
2:H:38:ARG:HD3	2:H:48:ILE:HD11	1.93	0.50
2:H:6:GLU:OE1	2:H:106:GLY:N	2.38	0.50
2:B:7:SER:HB3	2:B:21:SER:HB2	1.93	0.50
2:B:30:ASN:O	2:B:52(A):ASN:HB3	2.12	0.49
3:C:82:ASP:OD1	3:C:82:ASP:N	2.45	0.49
1:A:341:GLY:HA3	1:A:395:LEU:HD23	1.94	0.49
2:B:126:PRO:HD2	2:B:213:PRO:HA	1.95	0.49
3:C:4:LEU:HD11	3:C:90:SER:HB2	1.94	0.49
1:A:341:GLY:HA2	1:A:353:PHE:CE2	2.47	0.49
1:P:332:SER:HA	1:P:426:ASP:HB2	1.94	0.49
1:A:364:LEU:HG	3:C:50:ARG:NH2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:49:TYR:HD2	3:L:50:ARG:HG2	1.77	0.49
2:B:38:ARG:HD3	2:B:48:ILE:HD11	1.94	0.48
2:H:33:TRP:CZ2	2:H:97:ARG:HD2	2.48	0.48
2:B:9:GLY:HA2	2:B:18:LEU:HD11	1.95	0.48
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.95	0.48
3:C:66(A):ASP:OD1	3:C:67:SER:OG	2.26	0.48
1:A:297:GLY:HA2	1:A:329:VAL:HG21	1.94	0.47
3:L:54:ARG:HG3	3:L:58:VAL:HB	1.96	0.47
3:C:127:ALA:O	3:C:129:LYS:HG2	2.14	0.47
1:P:297:GLY:HA2	1:P:329:VAL:HG21	1.97	0.47
1:P:365:GLU:OE2	5:H:301:GOL:O3	2.30	0.47
1:P:372:LEU:HD22	1:P:376:ILE:HG13	1.97	0.47
2:H:33:TRP:HB2	2:H:95:ASP:HB2	1.97	0.47
3:C:122:SER:OG	3:C:126:GLN:NE2	2.38	0.47
1:P:388:GLU:HB3	1:P:391:ASP:HB2	1.95	0.47
2:H:105:GLN:HG3	2:H:105:GLN:H	1.53	0.46
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.98	0.46
2:B:169:VAL:HB	3:C:162:THR:HG22	1.97	0.46
3:C:77:ASN:C	3:C:77:ASN:HD22	2.20	0.45
3:C:55:PRO:HD2	3:C:58:VAL:HG21	1.99	0.45
2:B:105:GLN:HB2	2:B:105:GLN:HE21	1.61	0.45
3:C:15:LEU:HD13	3:C:16:GLY:N	2.33	0.44
3:L:132:LEU:HD21	3:L:185:TRP:CZ3	2.52	0.44
1:A:321:ASP:OD1	1:A:321:ASP:N	2.48	0.44
2:B:105:GLN:H	2:B:105:GLN:HG3	1.55	0.44
3:L:120:PRO:HD2	3:L:185:TRP:CZ2	2.53	0.44
2:H:39:GLN:OE1	3:L:38:HIS:NE2	2.51	0.44
1:A:365:GLU:OE2	2:B:99:SER:OG	2.25	0.44
1:P:329:VAL:O	1:P:423:VAL:HA	2.17	0.44
3:C:149:LYS:HD3	3:C:194:GLN:OE1	2.17	0.44
3:C:39:HIS:HE1	3:C:81:GLU:O	2.01	0.43
2:H:20:LEU:HD13	2:H:107:THR:HG21	1.99	0.43
2:H:169:VAL:HB	3:L:162:THR:HG22	2.00	0.43
1:A:360:GLU:HG2	1:A:368:ASN:OD1	2.18	0.43
3:L:132:LEU:HB2	3:L:178:LEU:HB3	2.01	0.43
1:A:365:GLU:HG3	2:B:96:LEU:HD23	2.01	0.43
1:A:357:TYR:CZ	1:A:359:PRO:HB3	2.54	0.42
2:H:209:LYS:HD3	2:H:209:LYS:HA	1.74	0.42
1:A:349:ILE:HA	1:A:350:PRO:HA	1.89	0.42
1:P:386:ASP:OD1	1:P:387:ALA:N	2.52	0.42
3:L:39:HIS:CE1	3:L:84:ALA:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:CYS:HA	1:A:353:PHE:HA	1.73	0.42
1:P:352:CYS:HA	1:P:353:PHE:HA	1.70	0.42
3:C:82:ASP:O	3:C:84:ALA:N	2.47	0.42
1:A:378:ILE:HG22	1:A:380:ASP:N	2.30	0.42
1:P:297:GLY:HA3	1:P:341:GLY:O	2.19	0.42
3:L:7:PRO:HD3	3:L:22:LEU:HG	2.01	0.41
1:P:389:GLY:HA3	4:P:501:NAG:H4	2.03	0.41
1:A:297:GLY:HA3	1:A:341:GLY:O	2.21	0.41
3:C:149:LYS:HB2	3:C:192:SER:OG	2.21	0.41
3:C:61:ARG:HB3	3:C:76:ASP:O	2.21	0.41
2:H:92:CYS:O	2:H:104:GLY:N	2.54	0.41
1:P:357:TYR:CZ	1:P:359:PRO:HB3	2.56	0.41
1:A:378:ILE:HD11	1:A:402:ILE:HG22	2.02	0.40
3:C:118:PHE:HB2	3:C:133:VAL:HB	2.03	0.40
1:A:416:LYS:HE2	3:C:32:TYR:CD1	2.57	0.40
1:P:301:SER:HA	1:P:345:PRO:HG3	2.04	0.40
1:P:372:LEU:HD23	1:P:372:LEU:HA	1.91	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	135/139 (97%)	122 (90%)	12 (9%)	1 (1%)	22	46
1	P	135/139 (97%)	123 (91%)	10 (7%)	2 (2%)	10	26
2	B	213/222 (96%)	208 (98%)	5 (2%)	0	100	100
2	H	213/222 (96%)	209 (98%)	4 (2%)	0	100	100
3	C	211/216 (98%)	194 (92%)	16 (8%)	1 (0%)	29	54
3	L	211/216 (98%)	198 (94%)	12 (6%)	1 (0%)	29	54
All	All	1118/1154 (97%)	1054 (94%)	59 (5%)	5 (0%)	34	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	366	PRO
3	L	50	ARG
1	A	366	PRO
3	C	93	THR
1	P	403	PRO

5.3.2 Protein sidechains [i](#)

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	125/127 (98%)	118 (94%)	7 (6%)	21	45
1	P	125/127 (98%)	110 (88%)	15 (12%)	5	11
2	B	186/191 (97%)	180 (97%)	6 (3%)	39	68
2	H	186/191 (97%)	179 (96%)	7 (4%)	33	62
3	C	185/188 (98%)	173 (94%)	12 (6%)	17	38
3	L	185/188 (98%)	178 (96%)	7 (4%)	33	62
All	All	992/1012 (98%)	938 (95%)	54 (5%)	22	47

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	306	SER
1	P	331	LEU
1	P	337	ASN
1	P	354	PHE
1	P	358	GLN
1	P	360	GLU
1	P	361	SER
1	P	362	GLU
1	P	364	LEU
1	P	372	LEU
1	P	378	ILE
1	P	382	GLU

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Mol	Chain	Res	Type
1	P	405	THR
1	P	406	THR
1	P	423	VAL
2	H	18	LEU
2	H	52(A)	ASN
2	H	82(C)	LEU
2	H	97	ARG
2	H	105	GLN
2	H	172	SER
2	H	175	LEU
3	L	14	ASN
3	L	22	LEU
3	L	34	SER
3	L	47	MET
3	L	50	ARG
3	L	60	ASP
3	L	189	ARG
1	A	319	VAL
1	A	333	GLU
1	A	337	ASN
1	A	354	PHE
1	A	361	SER
1	A	364	LEU
1	A	393	ILE
2	B	16	ARG
2	B	18	LEU
2	B	97	ARG
2	B	105	GLN
2	B	188	SER
2	B	196	CYS
3	C	1	GLN
3	C	12	SER
3	C	14	ASN
3	C	27(B)	ASN
3	C	47	MET
3	C	50	ARG
3	C	60	ASP
3	C	74	THR
3	C	77	ASN
3	C	90	SER
3	C	93	THR
3	C	95	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	337	ASN
1	P	358	GLN
1	P	368	ASN
1	P	377	ASN
2	H	31	ASN
2	H	39	GLN
2	H	81	GLN
1	A	296	HIS
1	A	337	ASN
2	B	3	GLN
2	B	30	ASN
3	C	14	ASN
3	C	39	HIS
3	C	77	ASN
3	C	108	GLN
3	C	126	GLN
3	C	188	HIS

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$
5	GOL	H	301	-	5,5,5	1.06	0	5,5,5	0.72	0
4	NAG	A	501	1	14,14,15	0.29	0	17,19,21	0.50	0
5	GOL	B	301	-	5,5,5	0.93	0	5,5,5	0.93	0
4	NAG	P	501	1	14,14,15	0.33	0	17,19,21	0.58	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
5	GOL	H	301	-	-	2/4/4/4	-
4	NAG	A	501	1	-	2/6/23/26	0/1/1/1
5	GOL	B	301	-	-	2/4/4/4	-
4	NAG	P	501	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	301	GOL	O1-C1-C2-O2
5	H	301	GOL	O1-C1-C2-C3
5	B	301	GOL	O1-C1-C2-C3
4	P	501	NAG	O5-C5-C6-O6
4	P	501	NAG	C4-C5-C6-O6
5	B	301	GOL	O1-C1-C2-O2
4	A	501	NAG	C4-C5-C6-O6
4	A	501	NAG	O5-C5-C6-O6
4	P	501	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	301	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301	GOL	2	0
4	P	501	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, 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	137/139 (98%)	0.55	3 (2%) 62 63	34, 51, 114, 146	0
1	P	137/139 (98%)	0.39	0 100 100	38, 57, 107, 129	0
2	B	217/222 (97%)	1.78	58 (26%) 0 0	35, 115, 170, 199	0
2	H	217/222 (97%)	2.33	82 (37%) 0 0	39, 128, 202, 216	0
3	C	213/216 (98%)	1.62	61 (28%) 0 0	45, 127, 190, 206	0
3	L	213/216 (98%)	1.93	70 (32%) 0 0	42, 127, 209, 243	0
All	All	1134/1154 (98%)	1.57	274 (24%) 0 0	34, 97, 195, 243	0

All (274) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	128	SER	19.2
2	H	136	ALA	15.4
2	B	181	VAL	14.9
2	H	123	PRO	14.5
3	L	133	VAL	13.9
2	B	136	ALA	13.5
2	H	129	LYS	13.3
2	H	135	THR	13.1
3	L	131	THR	11.6
3	L	157	ALA	11.6
2	B	129	LYS	11.4
2	H	138	LEU	10.5
3	L	118	PHE	10.4
2	B	127	SER	10.3
2	B	185	PRO	10.1
3	L	130	ALA	9.9
3	L	183	GLU	9.5
3	C	117	LEU	9.5
3	L	206	VAL	9.4

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Mol	Chain	Res	Type	RSRZ
2	H	134	GLY	9.3
2	H	137	ALA	9.2
2	B	159	LEU	9.0
2	H	124	LEU	8.9
2	B	137	ALA	8.9
3	C	196	THR	8.6
2	H	121	VAL	8.5
3	L	117	LEU	8.4
3	C	157	ALA	8.3
2	H	186	SER	8.2
2	H	194	TYR	8.2
2	B	183	THR	8.0
2	B	152	VAL	8.0
2	H	141	LEU	7.9
2	H	190	GLY	7.9
2	H	126	PRO	7.8
2	H	202	PRO	7.8
2	H	120	SER	7.7
3	C	156	LYS	7.6
3	C	154	PRO	7.6
2	H	198	VAL	7.5
2	H	191	THR	7.5
2	B	144	ASP	7.3
3	C	188	HIS	7.2
3	L	177	TYR	7.1
3	L	156	LYS	6.9
2	H	133	GLY	6.8
2	B	166	PHE	6.7
2	H	159	LEU	6.6
3	L	181	THR	6.6
2	H	146	PHE	6.5
2	H	183	THR	6.5
2	H	125	ALA	6.5
2	H	211	VAL	6.5
3	L	185	TRP	6.4
3	C	148	TRP	6.3
2	H	185	PRO	6.2
3	L	202	VAL	6.2
2	H	207	VAL	6.1
2	H	9	GLY	6.1
2	H	114	ALA	6.0
3	L	119	PRO	6.0

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Mol	Chain	Res	Type	RSRZ
2	B	141	LEU	6.0
2	H	180	SER	5.9
2	B	179	SER	5.9
2	H	142	VAL	5.8
3	L	207	ALA	5.8
3	L	178	LEU	5.8
3	L	205	THR	5.7
3	L	166	LYS	5.7
3	L	182	PRO	5.7
2	H	200	HIS	5.6
2	H	201	LYS	5.6
2	H	214	LYS	5.4
3	L	132	LEU	5.3
2	H	154	TRP	5.3
3	C	209	THR	5.3
2	H	176	TYR	5.2
2	H	158	ALA	5.2
2	H	161	SER	5.1
3	L	116	THR	5.1
3	C	191	TYR	5.1
2	B	193	THR	5.0
3	C	139	PHE	5.0
2	B	211	VAL	5.0
3	L	186	LYS	5.0
2	H	165	THR	5.0
2	B	138	LEU	5.0
2	B	122	PHE	4.9
2	B	133	GLY	4.9
2	B	206	LYS	4.9
3	L	200	SER	4.9
3	C	136	ILE	4.9
3	L	148	TRP	4.9
3	C	178	LEU	4.9
3	L	115	VAL	4.8
2	H	157	GLY	4.8
3	C	155	VAL	4.8
3	L	180	LEU	4.8
2	B	163	VAL	4.8
2	H	187	SER	4.8
2	B	10	GLY	4.7
2	B	151	THR	4.7
2	H	188	SER	4.7

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Mol	Chain	Res	Type	RSRZ
3	C	184	GLN	4.6
2	B	121	VAL	4.6
3	L	120	PRO	4.5
2	B	150	VAL	4.5
2	H	213	PRO	4.5
2	H	166	PHE	4.5
2	H	152	VAL	4.4
3	C	177	TYR	4.4
3	L	146	VAL	4.4
2	B	161	SER	4.3
3	C	112	ALA	4.3
3	C	182	PRO	4.2
3	C	150	ALA	4.2
3	L	129	LYS	4.2
2	B	188	SER	4.1
3	L	169	ASN	4.1
2	H	210	LYS	4.1
3	L	135	LEU	4.1
3	C	186	LYS	4.1
3	C	132	LEU	4.0
2	H	208	ASP	4.0
2	H	199	ASN	4.0
3	L	144	VAL	3.9
2	B	194	TYR	3.9
2	B	184	VAL	3.9
3	C	146	VAL	3.9
2	B	165	THR	3.9
2	H	145	TYR	3.9
2	B	208	ASP	3.9
1	A	364	LEU	3.8
3	C	185	TRP	3.8
3	L	121	SER	3.8
2	B	139	GLY	3.8
3	L	170	ASN	3.7
3	C	135	LEU	3.7
3	L	208	PRO	3.7
2	H	184	VAL	3.7
3	C	106(A)	LEU	3.6
3	C	142	GLY	3.6
3	C	115	VAL	3.6
3	C	190	SER	3.6
3	C	11	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	12	LEU	3.5
3	L	191	TYR	3.5
3	L	187	SER	3.5
2	H	150	VAL	3.5
3	L	196	THR	3.5
2	H	197	ASN	3.5
2	H	148	GLU	3.5
2	H	119	PRO	3.4
2	H	151	THR	3.4
2	B	140	CYS	3.4
2	B	182	VAL	3.4
3	L	195	VAL	3.4
3	L	189	ARG	3.4
3	C	160	GLU	3.3
3	L	190	SER	3.3
2	H	11	LEU	3.3
2	H	163	VAL	3.3
3	C	159	VAL	3.3
3	C	119	PRO	3.3
3	C	206	VAL	3.3
3	C	189	ARG	3.3
3	C	106	VAL	3.2
3	L	138	ASP	3.2
3	L	201	THR	3.2
2	H	122	PHE	3.2
3	C	145	THR	3.2
2	H	153	SER	3.2
3	L	151	ASP	3.1
3	L	113	PRO	3.1
2	B	196	CYS	3.1
3	L	155	VAL	3.1
2	B	178	LEU	3.1
3	L	15	LEU	3.1
3	L	199	GLY	3.1
2	H	115	SER	3.0
2	H	1	GLU	3.0
2	B	164	HIS	3.0
3	C	200	SER	3.0
2	H	140	CYS	3.0
2	B	207	VAL	3.0
3	C	176	SER	3.0
2	B	192	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	189	LEU	3.0
2	H	67	PHE	2.9
3	C	199	GLY	2.9
2	H	171	GLN	2.9
2	B	160	THR	2.9
2	B	177	SER	2.9
3	C	131	THR	2.9
3	C	174	ALA	2.9
3	C	194	GLN	2.8
3	C	198	GLU	2.8
2	B	146	PHE	2.8
2	H	168	ALA	2.8
2	H	128	SER	2.8
3	C	162	THR	2.8
3	L	1	GLN	2.7
3	L	110	LYS	2.7
2	B	15	GLY	2.7
3	L	134	CYS	2.7
3	L	161	THR	2.7
3	C	28	ILE	2.6
3	L	112	ALA	2.6
3	L	150	ALA	2.6
3	L	19	VAL	2.6
3	L	193	CYS	2.6
2	B	172	SER	2.6
2	B	153	SER	2.6
2	B	173	SER	2.5
2	H	164	HIS	2.5
2	H	169	VAL	2.5
2	B	198	VAL	2.5
1	A	358	GLN	2.5
3	L	143	ALA	2.5
3	C	195	VAL	2.5
3	L	152	SER	2.5
3	L	192	SER	2.5
3	L	125	LEU	2.4
3	C	180	LEU	2.4
3	L	153	SER	2.4
2	H	204	ASN	2.4
3	L	154	PRO	2.4
3	L	122	SER	2.4
2	B	142	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
3	L	184	GLN	2.3
3	C	127	ALA	2.3
3	C	201	THR	2.3
2	H	139	GLY	2.3
2	H	112	SER	2.3
2	H	177	SER	2.3
2	B	9	GLY	2.3
3	L	139	PHE	2.3
3	L	159	VAL	2.3
2	H	178	LEU	2.3
2	B	107	THR	2.3
2	H	80	LEU	2.3
2	B	116	THR	2.3
2	H	179	SER	2.3
3	L	106(A)	LEU	2.3
3	L	114	SER	2.3
2	B	126	PRO	2.3
2	H	181	VAL	2.3
2	B	115	SER	2.2
2	H	48	ILE	2.2
3	C	133	VAL	2.2
3	C	134	CYS	2.2
3	C	192	SER	2.2
3	C	72	LEU	2.2
3	C	120	PRO	2.2
3	C	144	VAL	2.2
3	L	188	HIS	2.2
3	C	113	PRO	2.2
2	B	199	ASN	2.2
2	B	124	LEU	2.2
2	H	156	SER	2.1
3	C	62	PHE	2.1
2	B	135	THR	2.1
3	C	118	PHE	2.1
3	C	15	LEU	2.1
3	C	86	TYR	2.1
3	L	123	GLU	2.1
2	H	127	SER	2.1
2	H	160	THR	2.1
2	H	206	LYS	2.0
2	H	155	ASN	2.0
3	C	102	THR	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	152	SER	2.0
1	A	368	ASN	2.0
2	B	145	TYR	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(Å ²)	Q<0.9
5	GOL	H	301	6/6	0.83	0.28	63,75,84,90	0
4	NAG	P	501	14/15	0.86	0.28	85,100,114,119	0
5	GOL	B	301	6/6	0.89	0.24	70,75,76,78	0
4	NAG	A	501	14/15	0.92	0.15	62,68,74,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.