



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:29 AM BST

PDB ID : 6UR5
Title : Resurfaced influenza hemagglutinin in complex with a broadly neutralizing antibody
Authors : Bajic, G.; Schmidt, A.G.
Deposited on : 2019-10-22
Resolution : 4.00 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

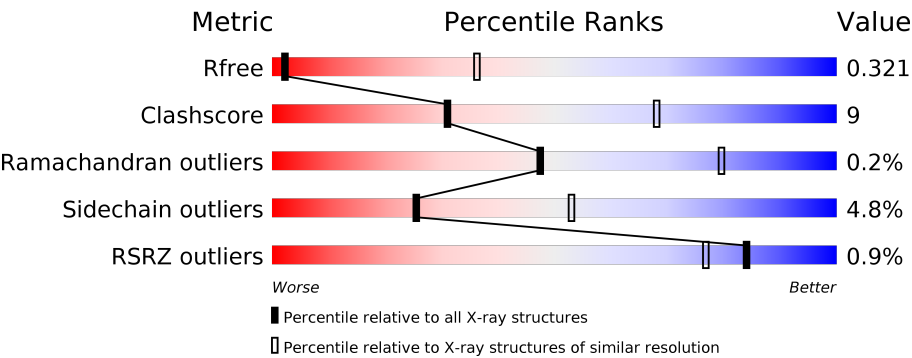
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	246	<div><div></div><div>74%18%5%</div></div>
1	G	246	<div><div></div><div>80%14%5%</div></div>
2	B	216	<div><div>2%</div><div>81%14%</div><div></div></div>
2	H	216	<div><div>%</div><div>83%13%</div><div></div></div>
3	C	295	<div><div></div><div>75%14%11%</div></div>
3	D	295	<div><div>2%</div><div>62%25%11%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
4	E	5	
5	F	6	

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
5	MAN	F	4	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10916 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 Antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1769	1120	297	344	8			
1	G	234	Total	C	N	O	S	0	0	0
			1778	1126	299	345	8			

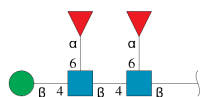
- Molecule 2 is a protein called Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	209	Total	C	N	O	S	0	0	0
			1539	961	255	319	4			
2	H	212	Total	C	N	O	S	0	0	0
			1561	973	258	325	5			

- Molecule 3 is a protein called Influenza hemagglutinin HA1.

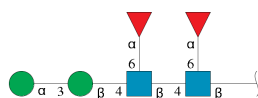
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	264	Total	C	N	O	S	0	0	0
			2067	1302	367	390	8			
3	D	264	Total	C	N	O	S	0	0	0
			2067	1302	367	390	8			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



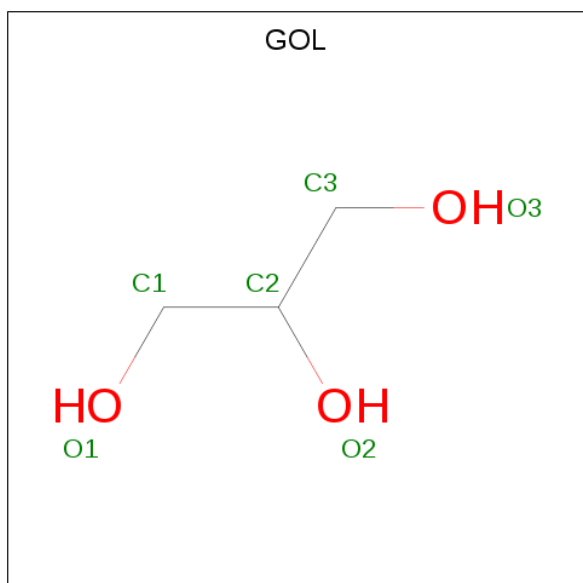
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	5	Total	C	N	O	0	0	0
			59	34	2	23			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	6	Total	C	N	O	0	0	0
			70	40	2	28			

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

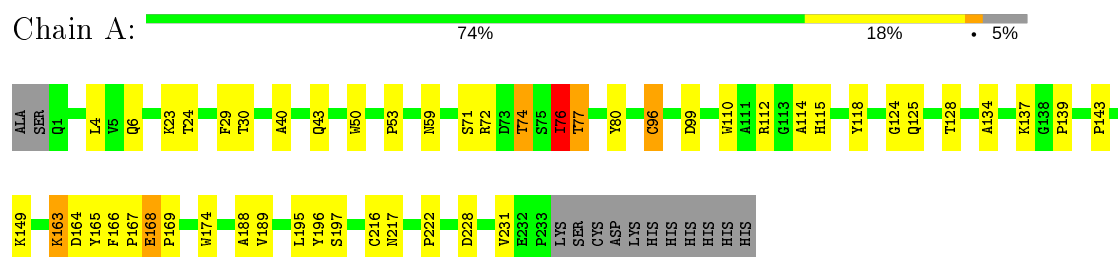


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			6	3	3		

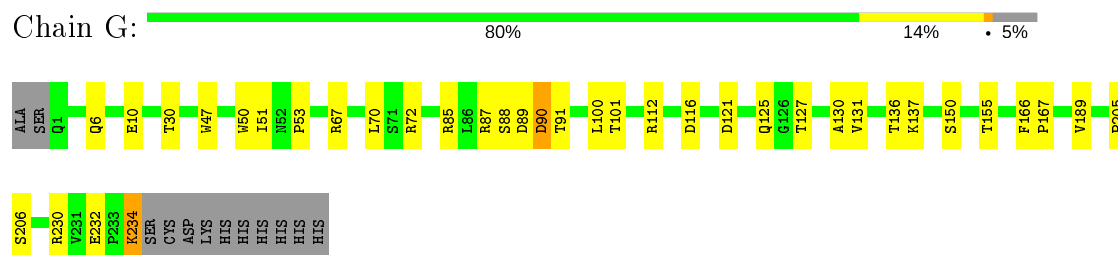
3 Residue-property plots

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.

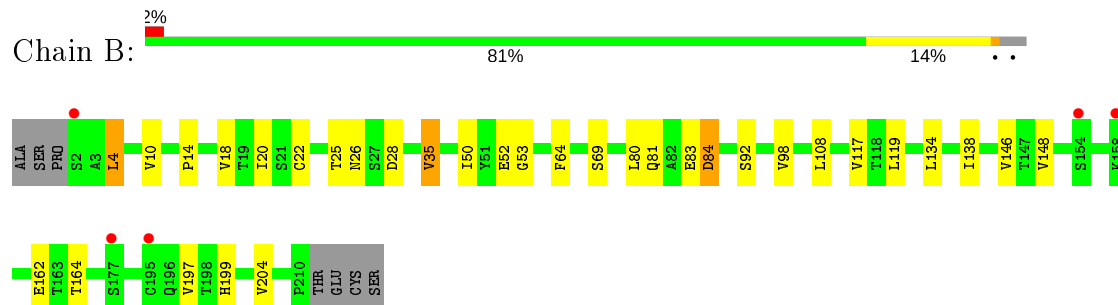
- Molecule 1: Antibody heavy chain



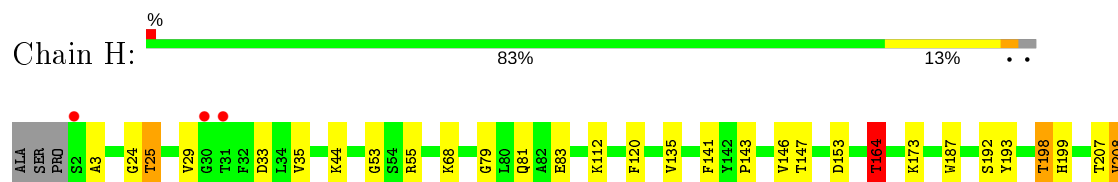
- Molecule 1: Antibody heavy chain



- Molecule 2: Antibody light chain



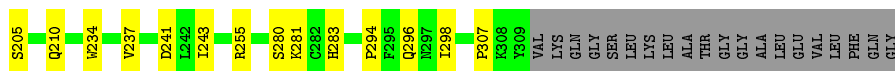
- Molecule 2: Antibody light chain





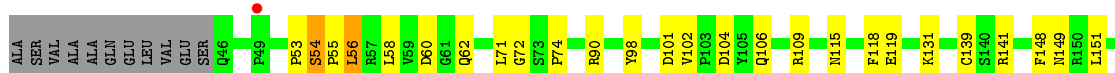
• Molecule 3: Influenza hemagglutinin HA1

Chain C: 75% 14% 11%



• Molecule 3: Influenza hemagglutinin HA1

Chain D: 2% 62% 25% 11%



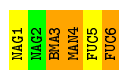
• Molecule 4: beta-D-mannopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 60% 40%



• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 17% 33% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.27Å 141.47Å 166.87Å 90.00° 102.55° 90.00°	Depositor
Resolution (Å)	48.59 – 4.00 48.59 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.59-4.00) 97.6 (48.59-4.00)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.300 , 0.322 0.300 , 0.321	Depositor DCC
R_{free} test set	992 reflections (5.73%)	wwPDB-VP
Wilson B-factor (Å ²)	86.5	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 93.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	10916	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: FUC, GOL, BMA, NAG, MAN

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	0.26	0/1816	0.49	0/2479
1	G	0.27	0/1825	0.47	0/2490
2	B	0.27	0/1575	0.49	0/2148
2	H	0.30	0/1597	0.54	1/2178 (0.0%)
3	C	0.26	0/2119	0.48	0/2888
3	D	0.27	0/2119	0.48	0/2888
All	All	0.27	0/11051	0.49	1/15071 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	164	THR	C-N-CA	6.61	138.23	121.70

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	1769	0	1715	43	0
1	G	1778	0	1728	24	0
2	B	1539	0	1492	20	0
2	H	1561	0	1509	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2067	0	2015	39	0
3	D	2067	0	2015	64	0
4	E	59	0	52	1	0
5	F	70	0	61	2	0
6	H	6	0	8	1	0
All	All	10916	0	10595	195	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 (195) 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:H:79:GLY:O	2:H:81:GLN:NE2	1.58	1.34
3:D:167:THR:CA	3:D:244:VAL:HG23	1.72	1.18
3:D:167:THR:HA	3:D:244:VAL:CG2	1.90	1.01
3:D:167:THR:HA	3:D:244:VAL:HG23	0.99	0.98
3:D:166:LEU:O	3:D:244:VAL:CG2	2.10	0.98
3:D:166:LEU:O	3:D:244:VAL:HG22	1.64	0.96
3:D:166:LEU:C	3:D:244:VAL:CG2	2.36	0.94
3:D:242:LEU:H	3:D:242:LEU:HD12	1.28	0.94
3:D:167:THR:CA	3:D:244:VAL:CG2	2.51	0.86
1:A:118:TYR:OH	3:C:157:LYS:HE3	1.77	0.83
1:A:118:TYR:CZ	3:C:157:LYS:HE3	2.17	0.80
3:D:166:LEU:O	3:D:244:VAL:HG23	1.84	0.79
3:C:78:HIS:HA	3:D:163:LEU:HD12	1.66	0.78
3:D:166:LEU:C	3:D:244:VAL:HG22	2.02	0.78
3:C:55:PRO:HG2	3:C:281:LYS:HG2	1.63	0.77
3:D:237:VAL:HG13	3:D:241:ASP:HB2	1.66	0.77
3:D:237:VAL:CG2	3:D:243:ILE:HD12	2.15	0.77
3:C:160:LEU:HG	3:C:162:PRO:HD3	1.70	0.73
3:C:160:LEU:HA	3:C:196:LYS:HD2	1.70	0.73
3:C:78:HIS:HA	3:D:163:LEU:CD1	2.19	0.72
3:C:160:LEU:O	3:C:160:LEU:HD23	1.90	0.71
3:D:131:LYS:HE3	3:D:157:LYS:HA	1.73	0.70
3:D:53:PRO:HB3	3:D:58:LEU:HG	1.73	0.69
3:D:167:THR:N	3:D:244:VAL:HG23	2.07	0.69
1:A:118:TYR:CE2	3:C:157:LYS:HE3	2.26	0.68
3:D:237:VAL:HG23	3:D:243:ILE:HD12	1.74	0.68
2:B:84:ASP:OD1	2:B:84:ASP:N	2.26	0.68
1:G:189:VAL:HG22	2:H:164:THR:HG23	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:158:ASN:HD21	2:H:55:ARG:HD2	1.57	0.67
1:A:189:VAL:HG22	2:B:164:THR:HB	1.76	0.67
3:D:163:LEU:HD23	3:D:163:LEU:C	2.16	0.67
1:A:24:THR:OG1	1:A:77:THR:OG1	1.89	0.67
1:A:118:TYR:CE2	3:C:157:LYS:CE	2.78	0.66
3:D:167:THR:N	3:D:244:VAL:CG2	2.58	0.66
1:G:6:GLN:H	1:G:125:GLN:HE22	1.42	0.65
2:H:35:VAL:HG22	2:H:53:GLY:HA2	1.77	0.65
2:B:4:LEU:HD12	2:B:98:VAL:HG13	1.78	0.65
3:D:242:LEU:N	3:D:242:LEU:HD12	2.07	0.64
2:B:10:VAL:HG21	2:B:20:ILE:HG12	1.78	0.64
3:D:72:GLY:HA3	3:D:149:ASN:HB3	1.80	0.64
3:D:201:ARG:NH1	3:D:246:ASN:OD1	2.31	0.64
1:A:6:GLN:H	1:A:125:GLN:HE22	1.46	0.63
3:C:148:PHE:HB2	3:C:151:LEU:HB2	1.80	0.62
3:C:205:SER:HB3	3:C:210:GLN:HG3	1.80	0.62
2:H:212:GLU:HG3	2:H:212:GLU:O	1.99	0.61
1:A:76:ILE:O	1:A:76:ILE:HG23	2.00	0.61
3:D:98:TYR:N	3:D:139:CYS:SG	2.72	0.61
1:A:24:THR:CB	1:A:77:THR:HG1	2.14	0.61
3:D:166:LEU:C	3:D:244:VAL:HG23	2.09	0.61
2:H:193:TYR:HB2	2:H:208:VAL:HG12	1.83	0.60
1:A:6:GLN:HE21	1:A:96:CYS:HB3	1.65	0.60
3:D:164:GLN:OE1	3:D:247:THR:O	2.20	0.60
2:B:14:PRO:HD3	2:B:108:LEU:HB3	1.84	0.60
3:D:243:ILE:O	3:D:243:ILE:HG23	2.02	0.60
2:H:143:PRO:HG2	2:H:199:HIS:CE1	2.38	0.59
1:G:88:SER:HA	1:G:131:VAL:HG21	1.85	0.59
3:C:237:VAL:HG21	3:C:243:ILE:HB	1.86	0.58
2:B:18:VAL:CG2	2:B:81:GLN:HE22	2.17	0.58
1:A:118:TYR:HE2	3:C:157:LYS:CE	2.16	0.58
2:H:187:TRP:NE1	2:H:210:PRO:HB3	2.19	0.58
1:G:230:ARG:CZ	1:G:232:GLU:OE2	2.53	0.57
1:G:67:ARG:HD2	1:G:85:ARG:HB2	1.85	0.57
2:H:211:THR:O	2:H:211:THR:HG23	2.05	0.57
3:D:106:GLN:OE1	3:D:109:ARG:NH1	2.37	0.57
3:D:115:ASN:ND2	3:D:259:LYS:O	2.38	0.56
2:B:35:VAL:O	2:B:53:GLY:N	2.38	0.56
3:C:150:ARG:NH1	5:F:6:FUC:O4	2.39	0.56
3:D:54:SER:OG	3:D:280:SER:O	2.24	0.55
3:C:294:PRO:HA	3:C:307:PRO:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:THR:OG1	1:A:77:THR:O	2.23	0.55
2:H:3:ALA:HB3	2:H:25:THR:OG1	2.06	0.55
3:D:177:LEU:HB2	3:D:260:LEU:HD11	1.91	0.53
1:G:53:PRO:O	1:G:72:ARG:NH2	2.40	0.53
1:A:217:ASN:ND2	1:A:228:ASP:OD2	2.36	0.53
1:A:24:THR:HG1	1:A:77:THR:CB	2.18	0.53
1:G:100:LEU:HD21	6:H:301:GOL:H12	1.91	0.53
2:B:18:VAL:HG22	2:B:81:GLN:HE22	1.73	0.53
2:B:148:VAL:HG22	2:B:197:VAL:HG22	1.91	0.52
3:D:270:ASN:N	3:D:270:ASN:OD1	2.41	0.52
3:C:160:LEU:N	3:C:160:LEU:CD2	2.72	0.52
3:D:148:PHE:HB2	3:D:151:LEU:HB2	1.92	0.52
1:G:234:LYS:CB	1:G:234:LYS:NZ	2.73	0.52
3:C:54:SER:OG	3:C:55:PRO:HD3	2.09	0.52
1:A:118:TYR:OH	3:C:157:LYS:CE	2.54	0.51
1:A:189:VAL:HG11	2:B:162:GLU:HB3	1.92	0.51
1:G:155:THR:HG22	1:G:205:PRO:HA	1.93	0.51
1:G:234:LYS:HB3	1:G:234:LYS:NZ	2.25	0.51
1:A:112:ARG:NH1	1:A:114:ALA:O	2.36	0.51
1:G:87:ARG:HG3	1:G:89:ASP:H	1.76	0.51
2:B:25:THR:OG1	2:B:28:ASP:OD2	2.21	0.51
2:B:197:VAL:H	2:B:204:VAL:HG22	1.76	0.51
1:A:72:ARG:NH1	1:A:74:THR:HG23	2.26	0.50
1:A:99:ASP:OD2	1:A:115:HIS:NE2	2.33	0.50
3:C:151:LEU:O	3:C:255:ARG:NE	2.38	0.50
3:C:160:LEU:N	3:C:160:LEU:HD23	2.26	0.50
3:C:296:GLN:HG3	3:C:298:ILE:HG12	1.93	0.50
3:D:55:PRO:HG2	3:D:56:LEU:HG	1.94	0.49
4:E:1:NAG:H62	4:E:2:NAG:C7	2.41	0.49
2:H:81:GLN:NE2	2:H:81:GLN:N	2.60	0.49
2:B:146:VAL:HG22	2:B:199:HIS:HD2	1.78	0.49
3:D:54:SER:HG	3:D:55:PRO:HD3	1.76	0.49
1:A:72:ARG:HH12	1:A:74:THR:HG23	1.76	0.49
3:D:235:THR:HB	3:D:243:ILE:HD11	1.94	0.49
3:D:297:ASN:OD1	3:D:297:ASN:N	2.42	0.49
5:F:3:BMA:H3	5:F:4:MAN:H2	1.55	0.49
1:A:118:TYR:HE2	3:C:157:LYS:HE2	1.77	0.49
3:D:296:GLN:NE2	3:D:307:PRO:HG3	2.29	0.48
1:G:166:PHE:HB3	1:G:167:PRO:HD3	1.95	0.48
1:A:167:PRO:HB2	1:A:222:PRO:HG2	1.95	0.48
3:D:158:ASN:ND2	2:H:55:ARG:HD2	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:VAL:HG22	2:B:81:GLN:NE2	2.28	0.48
1:G:47:TRP:HZ2	1:G:50:TRP:HD1	1.61	0.48
1:A:110:TRP:CE2	3:C:155:THR:HG21	2.48	0.48
3:C:56:LEU:HD12	3:C:283:HIS:CE1	2.49	0.47
3:D:102:VAL:HG22	3:D:232:PHE:HB2	1.95	0.47
1:A:143:PRO:HB3	1:A:231:VAL:HG22	1.97	0.47
2:B:35:VAL:HG23	2:B:92:SER:HB2	1.95	0.47
3:C:53:PRO:HB3	3:C:58:LEU:HG	1.97	0.47
2:B:83:GLU:HG3	2:B:83:GLU:O	2.15	0.47
1:A:139:PRO:HB3	1:A:165:TYR:HB3	1.98	0.46
2:B:119:LEU:HG	2:B:134:LEU:HD11	1.96	0.46
1:G:90:ASP:OD1	1:G:90:ASP:N	2.49	0.46
1:A:4:LEU:HB2	1:A:124:GLY:HA2	1.97	0.46
3:D:203:THR:HA	3:D:211:THR:O	2.16	0.46
3:D:295:PHE:HE1	3:D:308:LYS:HD2	1.81	0.46
1:A:137:LYS:HE2	1:A:164:ASP:O	2.15	0.45
3:D:296:GLN:HG2	3:D:307:PRO:HG3	1.98	0.45
2:H:33:ASP:O	2:H:68:LYS:HE2	2.16	0.45
2:B:50:ILE:HD11	2:B:64:PHE:HB3	1.98	0.45
3:D:197:ASN:ND2	3:D:200:GLY:HA2	2.31	0.45
1:A:166:PHE:HB3	1:A:167:PRO:HD3	1.99	0.45
2:H:187:TRP:HE1	2:H:210:PRO:HB3	1.80	0.45
3:D:60:ASP:OD1	3:D:62:GLN:HG3	2.17	0.45
3:C:54:SER:HG	3:C:280:SER:H	1.62	0.45
1:G:91:THR:HG23	1:G:130:ALA:HA	1.98	0.45
3:D:182:VAL:HG22	3:D:202:VAL:HG11	1.98	0.44
1:A:40:ALA:HB3	1:A:43:GLN:HB2	1.98	0.44
3:D:74:PRO:HA	3:D:141:ARG:HD3	2.00	0.44
3:D:206:THR:HG23	3:D:209:SER:H	1.81	0.44
1:G:150:SER:HB2	1:G:206:SER:HB3	2.00	0.44
2:H:210:PRO:HG2	2:H:210:PRO:O	2.17	0.44
2:H:147:THR:HB	2:H:198:THR:HG23	1.98	0.44
1:A:24:THR:N	1:A:77:THR:OG1	2.50	0.44
3:C:237:VAL:HG13	3:C:241:ASP:HB3	2.00	0.44
2:H:141:PHE:HB2	2:H:199:HIS:CE1	2.53	0.44
3:D:163:LEU:CD2	3:D:163:LEU:C	2.86	0.43
1:G:47:TRP:CZ2	1:G:50:TRP:HD1	2.36	0.43
1:A:165:TYR:CZ	1:A:196:TYR:HB2	2.53	0.43
1:A:134:ALA:HB3	1:A:166:PHE:CE1	2.53	0.43
3:C:102:VAL:HB	3:C:105:TYR:HD2	1.83	0.43
3:D:90:ARG:HH22	3:D:274:PRO:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:THR:OG1	1:A:77:THR:CB	2.64	0.43
2:H:81:GLN:N	2:H:81:GLN:CD	2.72	0.43
3:C:158:ASN:N	3:C:158:ASN:OD1	2.52	0.43
3:D:164:GLN:O	3:D:246:ASN:HA	2.19	0.43
3:D:293:LYS:HB3	3:D:296:GLN:OE1	2.19	0.43
1:A:112:ARG:HE	3:C:131:LYS:NZ	2.16	0.43
3:D:167:THR:HB	3:D:244:VAL:HG21	2.01	0.43
1:A:29:PHE:CG	1:A:77:THR:HB	2.54	0.42
3:C:132:GLN:HB2	3:C:152:ASN:OD1	2.19	0.42
3:D:269:LEU:HD21	3:D:285:ASP:HA	2.01	0.42
3:C:54:SER:HG	3:C:55:PRO:HD3	1.84	0.42
1:A:174:TRP:CH2	1:A:216:CYS:HB3	2.54	0.42
1:G:30:THR:HA	1:G:53:PRO:HB2	2.02	0.42
1:G:121:ASP:OD1	1:G:121:ASP:N	2.35	0.42
1:G:51:ILE:HB	1:G:70:LEU:HD13	2.01	0.42
1:A:50:TRP:CE2	1:A:59:ASN:HB3	2.55	0.42
3:D:220:ARG:HG3	3:D:221:PRO:HD2	2.02	0.42
2:H:112:LYS:NZ	2:H:173:LYS:NZ	2.68	0.42
3:C:78:HIS:HA	3:D:163:LEU:HD13	2.00	0.42
2:B:52:GLU:OE2	3:C:158:ASN:ND2	2.53	0.41
3:D:163:LEU:HD23	3:D:164:GLN:N	2.35	0.41
3:D:201:ARG:HB3	3:D:214:VAL:HG22	2.01	0.41
1:A:71:SER:OG	1:A:80:TYR:HB2	2.20	0.41
3:D:182:VAL:O	3:D:230:ILE:HA	2.20	0.41
3:D:131:LYS:HE2	1:G:112:ARG:HE	1.86	0.41
1:G:67:ARG:NH2	1:G:90:ASP:OD2	2.53	0.41
3:C:188:ILE:HG13	3:C:188:ILE:H	1.71	0.41
3:D:149:ASN:O	3:D:255:ARG:NH2	2.44	0.41
1:G:137:LYS:HD3	1:G:137:LYS:HA	1.58	0.41
3:C:104:ASP:HB3	3:C:234:TRP:CZ3	2.56	0.41
3:D:296:GLN:HG2	3:D:307:PRO:CG	2.51	0.41
3:D:299:SER:OG	3:D:300:ARG:N	2.54	0.41
1:A:168:GLU:HG3	1:A:169:PRO:HD3	2.02	0.41
2:B:117:VAL:HG22	2:B:138:ILE:HG13	2.03	0.41
3:C:104:ASP:HB3	3:C:234:TRP:HZ3	1.86	0.41
1:A:163:LYS:HG2	1:A:197:SER:OG	2.20	0.40
1:A:188:ALA:HB1	1:A:196:TYR:HB3	2.03	0.40
1:A:23:LYS:HA	1:A:77:THR:O	2.22	0.40
3:C:71:LEU:HD22	3:C:151:LEU:HD11	2.03	0.40
2:H:120:PHE:HB2	2:H:135:VAL:HB	2.03	0.40
1:A:30:THR:HA	1:A:53:PRO:HB2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:192:SER:HB2	2:H:207:THR:CG2	2.51	0.40
2:H:24:GLY:O	2:H:29:VAL:HG12	2.22	0.40
1:G:101:THR:HG21	1:G:116:ASP:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	231/246 (94%)	223 (96%)	7 (3%)	1 (0%)	34	71
1	G	232/246 (94%)	227 (98%)	5 (2%)	0	100	100
2	B	207/216 (96%)	193 (93%)	14 (7%)	0	100	100
2	H	210/216 (97%)	184 (88%)	24 (11%)	2 (1%)	15	53
3	C	262/295 (89%)	251 (96%)	11 (4%)	0	100	100
3	D	262/295 (89%)	245 (94%)	17 (6%)	0	100	100
All	All	1404/1514 (93%)	1323 (94%)	78 (6%)	3 (0%)	47	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	83	GLU
2	H	211	THR
1	A	76	ILE

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	194/206 (94%)	185 (95%)	9 (5%)	27	54
1	G	195/206 (95%)	190 (97%)	5 (3%)	46	67
2	B	173/179 (97%)	166 (96%)	7 (4%)	31	57
2	H	176/179 (98%)	169 (96%)	7 (4%)	31	57
3	C	233/255 (91%)	224 (96%)	9 (4%)	32	58
3	D	233/255 (91%)	212 (91%)	21 (9%)	9	34
All	All	1204/1280 (94%)	1146 (95%)	58 (5%)	25	53

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	THR
1	A	76	ILE
1	A	77	THR
1	A	96	CYS
1	A	128	THR
1	A	149	LYS
1	A	163	LYS
1	A	168	GLU
1	A	195	LEU
2	B	4	LEU
2	B	22	CYS
2	B	26	ASN
2	B	35	VAL
2	B	69	SER
2	B	80	LEU
2	B	84	ASP
3	C	54	SER
3	C	62	GLN
3	C	63	THR
3	C	98	TYR
3	C	101	ASP
3	C	118	PHE
3	C	158	ASN
3	C	160	LEU
3	C	163	LEU
3	D	54	SER
3	D	56	LEU

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Mol	Chain	Res	Type
3	D	71	LEU
3	D	101	ASP
3	D	104	ASP
3	D	118	PHE
3	D	119	GLU
3	D	160	LEU
3	D	199	PRO
3	D	205	SER
3	D	217	ILE
3	D	242	LEU
3	D	244	VAL
3	D	270	ASN
3	D	278	CYS
3	D	288	SER
3	D	290	THR
3	D	291	THR
3	D	296	GLN
3	D	306	CYS
3	D	309	TYR
1	G	10	GLU
1	G	90	ASP
1	G	127	THR
1	G	136	THR
1	G	234	LYS
2	H	25	THR
2	H	44	LYS
2	H	146	VAL
2	H	153	ASP
2	H	164	THR
2	H	198	THR
2	H	208	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	81	GLN
3	D	46	GLN
3	D	170	ASN
2	H	199	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

11 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	E	1	3,4	14,14,15	0.79	1 (7%)	17,19,21	1.08	1 (5%)
4	NAG	E	2	4	14,14,15	1.55	1 (7%)	17,19,21	1.31	2 (11%)
4	BMA	E	3	4	11,11,12	0.71	0	15,15,17	1.13	1 (6%)
4	FUC	E	4	4	10,10,11	0.62	0	14,14,16	1.40	2 (14%)
4	FUC	E	5	4	10,10,11	0.52	0	14,14,16	1.18	2 (14%)
5	NAG	F	1	3,5	14,14,15	0.67	1 (7%)	17,19,21	1.41	3 (17%)
5	NAG	F	2	5	14,14,15	0.56	0	17,19,21	0.65	0
5	BMA	F	3	5	11,11,12	0.69	0	15,15,17	1.33	1 (6%)
5	MAN	F	4	5	11,11,12	1.00	1 (9%)	15,15,17	1.11	2 (13%)
5	FUC	F	5	5	10,10,11	0.39	0	14,14,16	1.17	2 (14%)
5	FUC	F	6	5	10,10,11	0.31	0	14,14,16	0.91	1 (7%)

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	E	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	E	3	4	-	1/2/19/22	0/1/1/1
4	FUC	E	4	4	-	-	0/1/1/1
4	FUC	E	5	4	-	-	0/1/1/1
5	NAG	F	1	3,5	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	FUC	F	5	5	-	-	0/1/1/1
5	FUC	F	6	5	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	2	NAG	O5-C1	-5.61	1.34	1.43
4	E	1	NAG	O5-C1	-2.81	1.39	1.43
5	F	4	MAN	C1-C2	2.75	1.58	1.52
5	F	1	NAG	O5-C1	-2.35	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NAG	C4-C3-C2	3.69	116.42	111.02
5	F	1	NAG	C1-O5-C5	-3.57	107.36	112.19
4	E	4	FUC	O5-C1-C2	-3.51	105.36	110.77
5	F	3	BMA	C1-O5-C5	3.50	116.94	112.19
4	E	2	NAG	C3-C4-C5	3.32	116.16	110.24
4	E	5	FUC	O5-C1-C2	-3.06	106.04	110.77
4	E	4	FUC	C1-C2-C3	3.03	113.39	109.67
4	E	1	NAG	C1-O5-C5	2.93	116.16	112.19
4	E	3	BMA	C1-O5-C5	2.93	116.16	112.19
5	F	1	NAG	C4-C3-C2	2.77	115.07	111.02
5	F	6	FUC	O5-C1-C2	-2.72	106.58	110.77
5	F	5	FUC	O5-C1-C2	-2.59	106.77	110.77
5	F	5	FUC	C1-C2-C3	2.50	112.75	109.67
5	F	4	MAN	C1-C2-C3	2.36	112.57	109.67
4	E	5	FUC	C1-C2-C3	2.22	112.39	109.67
5	F	4	MAN	O2-C2-C3	-2.15	105.83	110.14
5	F	1	NAG	O3-C3-C2	-2.12	105.07	109.47

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	2	NAG	C4-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
4	E	1	NAG	C3-C2-N2-C7
5	F	1	NAG	C1-C2-N2-C7
5	F	3	BMA	C4-C5-C6-O6
5	F	1	NAG	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	3	BMA	1	0
4	E	1	NAG	1	0
5	F	6	FUC	1	0
4	E	2	NAG	1	0
5	F	4	MAN	1	0

5.6 Ligand geometry

1 ligand is 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	$\# Z > 2$
6	GOL	H	301	-	5,5,5	0.20	0	5,5,5	0.42	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
6	GOL	H	301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	301	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	233/246 (94%)	-0.11	0	100	100	65, 89, 122, 158	0
1	G	234/246 (95%)	-0.25	0	100	100	60, 83, 115, 159	0
2	B	209/216 (96%)	0.10	5 (2%)	59	49	30, 106, 163, 179	0
2	H	212/216 (98%)	-0.14	3 (1%)	75	65	57, 95, 129, 161	0
3	C	264/295 (89%)	-0.16	0	100	100	56, 91, 136, 150	0
3	D	264/295 (89%)	-0.01	5 (1%)	66	58	64, 95, 151, 176	0
All	All	1416/1514 (93%)	-0.10	13 (0%)	84	77	30, 93, 142, 179	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	158	LYS	4.1
2	H	30	GLY	3.3
2	B	2	SER	3.1
3	D	289	ILE	3.0
2	H	2	SER	3.0
2	B	154	SER	2.7
2	B	177	SER	2.5
2	H	31	THR	2.5
3	D	294	PRO	2.3
3	D	291	THR	2.3
3	D	285	ASP	2.2
3	D	49	PRO	2.1
2	B	195	CYS	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](#)

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
4	BMA	E	3	11/12	0.51	0.31	139,139,139,139	0
5	MAN	F	4	11/12	0.59	0.50	152,152,152,152	0
4	FUC	E	4	10/11	0.66	0.34	130,130,130,130	0
4	NAG	E	2	14/15	0.72	0.24	93,133,145,146	0
5	FUC	F	5	10/11	0.73	0.37	142,142,142,142	0
5	BMA	F	3	11/12	0.73	0.30	140,140,140,140	0
5	NAG	F	2	14/15	0.77	0.24	127,127,127,127	0
5	FUC	F	6	10/11	0.80	0.32	115,115,115,115	0
4	NAG	E	1	14/15	0.81	0.19	90,109,118,127	0
4	FUC	E	5	10/11	0.81	0.32	115,115,115,115	0
5	NAG	F	1	14/15	0.88	0.20	97,106,123,125	0

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
6	GOL	H	301	6/6	0.84	0.31	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.