



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2021 – 10:07 AM EDT

PDB ID : 6XQ0
Title : Human antibody S8V2-18 in complex with the influenza hemagglutinin head domain of A/California/7/2009(NYMC-X181)(H1N1)
Authors : McCarthy, K.R.; Harrison, S.C.
Deposited on : 2020-07-09
Resolution : 2.30 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 : 2.18
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) : 2.18

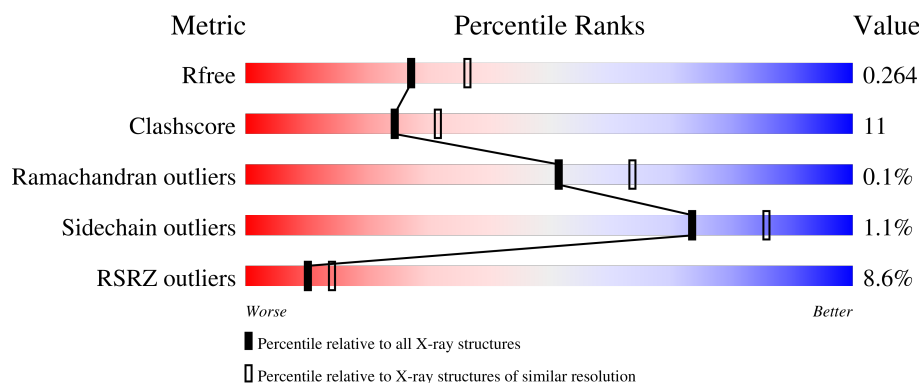
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 ≥ 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	225	<div> <div>4%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	D	225	<div> <div>2%</div> <div>80%</div> <div>16%</div> <div>.</div> </div>
2	C	215	<div> <div>7%</div> <div>80%</div> <div>19%</div> <div>..</div> </div>
2	F	215	<div> <div>23%</div> <div>78%</div> <div>21%</div> <div>.</div> </div>
3	B	240	<div> <div>7%</div> <div>78%</div> <div>16%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	240	<div><div></div><div>8%</div><div>75%</div><div>19%</div><div></div><div></div></div>
4	G	5	<div><div></div><div>60%</div><div>20%</div><div>20%</div></div>
4	H	5	<div><div></div><div>20%</div><div>80%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10954 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	216	Total	C	N	O	S	0	0	0
			1711	1090	289	326	6			
1	A	219	Total	C	N	O	S	0	0	0
			1729	1101	292	330	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	54	ALA	-	expression tag	UNP I6T519
D	55	SER	-	expression tag	UNP I6T519
D	268	LEU	-	expression tag	UNP I6T519
D	269	GLU	-	expression tag	UNP I6T519
D	270	VAL	-	expression tag	UNP I6T519
D	271	LEU	-	expression tag	UNP I6T519
D	272	PHE	-	expression tag	UNP I6T519
D	273	GLN	-	expression tag	UNP I6T519
A	54	ALA	-	expression tag	UNP I6T519
A	55	SER	-	expression tag	UNP I6T519
A	268	LEU	-	expression tag	UNP I6T519
A	269	GLU	-	expression tag	UNP I6T519
A	270	VAL	-	expression tag	UNP I6T519
A	271	LEU	-	expression tag	UNP I6T519
A	272	PHE	-	expression tag	UNP I6T519
A	273	GLN	-	expression tag	UNP I6T519

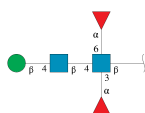
- Molecule 2 is a protein called antibody S8V2-18 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	213	Total	C	N	O	S	0	0	0
			1645	1032	281	328	4			
2	F	213	Total	C	N	O	S	0	0	0
			1645	1032	281	328	4			

- Molecule 3 is a protein called antibody S8V2-18 heavy chain.

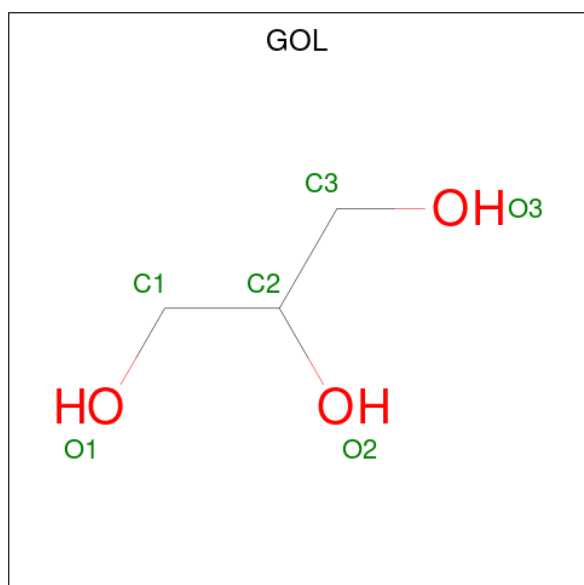
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	230	Total	C	N	O	S	0	0	0
			1729	1090	302	328	9			
3	E	230	Total	C	N	O	S	0	0	0
			1729	1090	302	328	9			

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



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

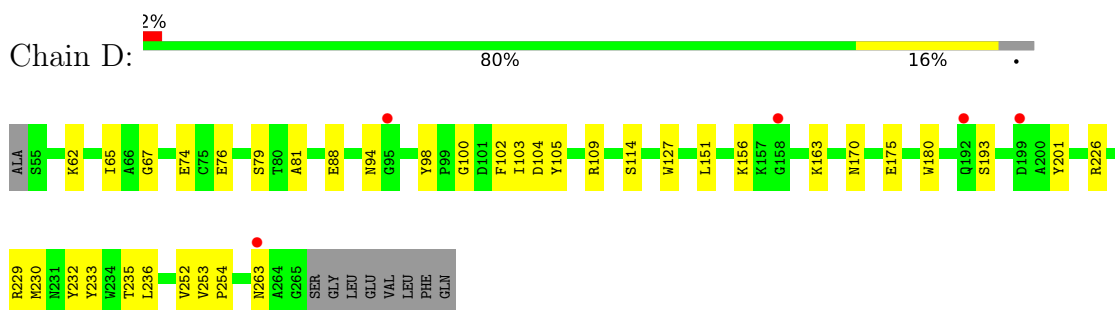
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	132	Total 132	O 132	0	0
6	A	127	Total 127	O 127	0	0
6	C	86	Total 86	O 86	0	0
6	B	114	Total 114	O 114	0	0
6	E	114	Total 114	O 114	0	0
6	F	69	Total 69	O 69	0	0

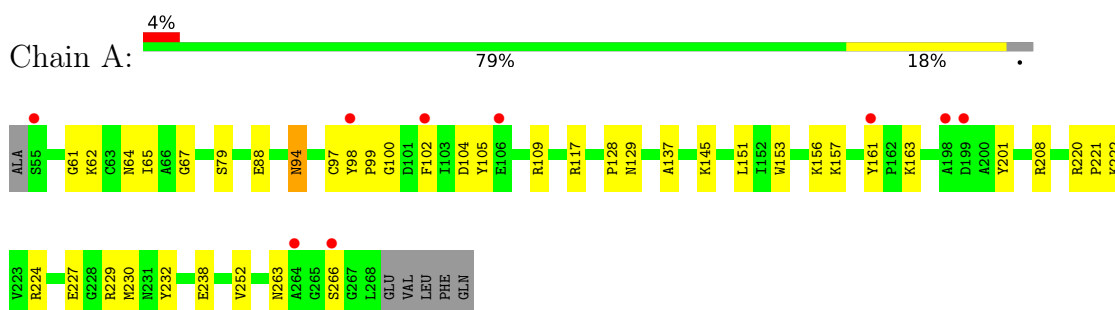
3 Residue-property plots [i](#)

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.

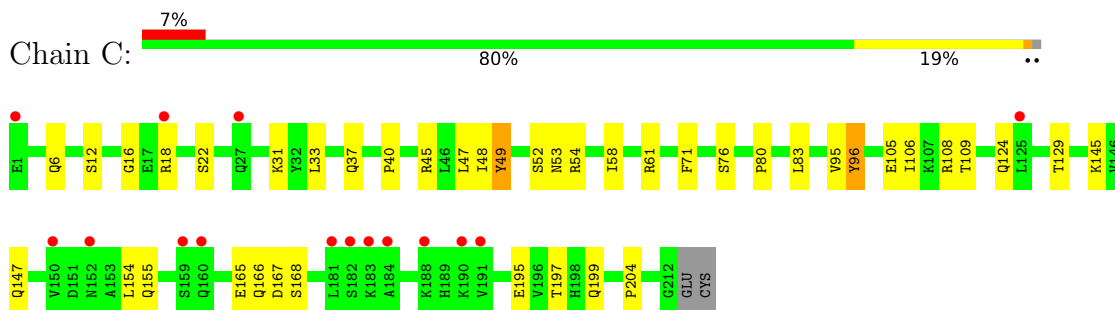
- Molecule 1: Hemagglutinin



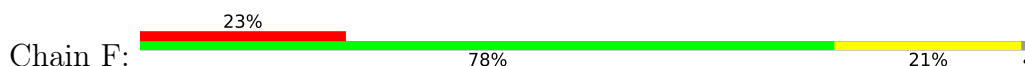
- Molecule 1: Hemagglutinin

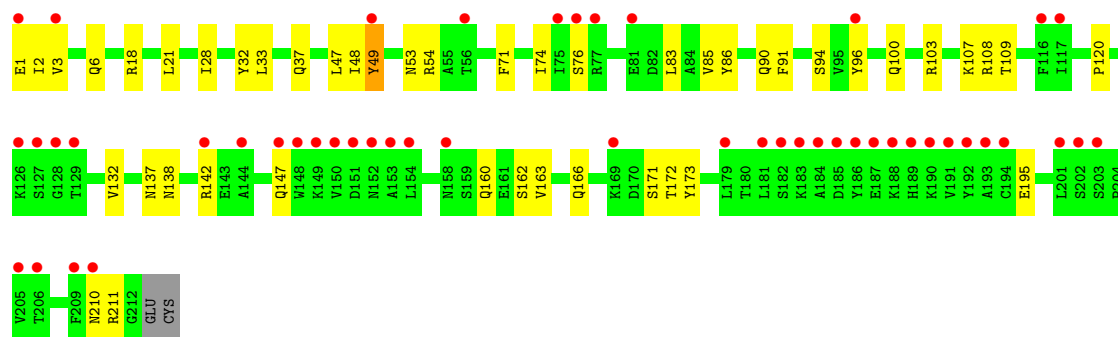


- Molecule 2: antibody S8V2-18 light chain

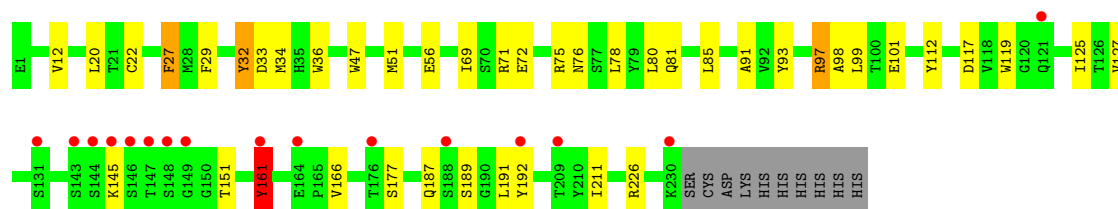
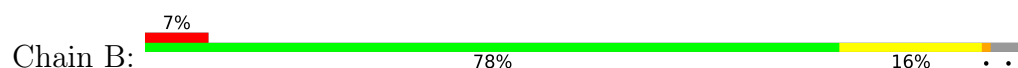


- Molecule 2: antibody S8V2-18 light chain

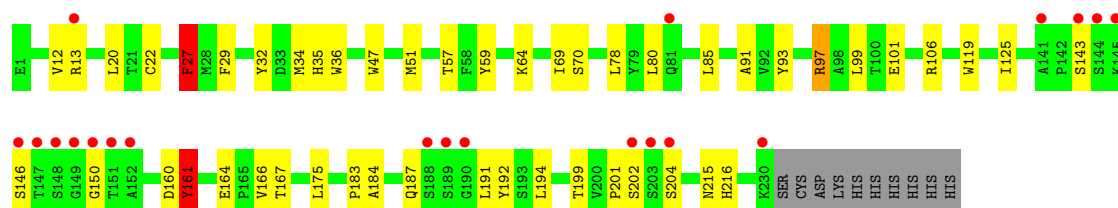
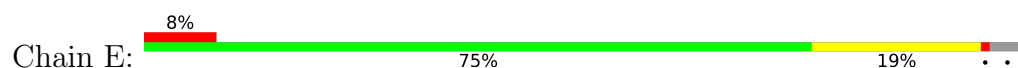




• Molecule 3: antibody S8V2-18 heavy chain



• Molecule 3: antibody S8V2-18 heavy chain



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	160.20Å 55.26Å 168.00Å 90.00° 95.02° 90.00°	Depositor
Resolution (Å)	44.88 – 2.30 44.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.3 (44.88-2.30) 95.3 (44.88-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.222 , 0.268 0.221 , 0.264	Depositor DCC
R_{free} test set	3042 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10954	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.73 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6264e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, GOL, FUC, 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	0/1779	0.51	0/2415
1	D	0.31	0/1761	0.53	0/2391
2	C	0.30	0/1679	0.59	0/2278
2	F	0.30	0/1679	0.57	0/2278
3	B	0.31	0/1772	0.62	1/2405 (0.0%)
3	E	0.30	0/1772	0.62	2/2405 (0.1%)
All	All	0.30	0/10442	0.58	3/14172 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	161	TYR	CA-CB-CG	5.20	123.28	113.40
3	E	27	PHE	CB-CG-CD2	-5.17	117.18	120.80
3	B	161	TYR	CA-CB-CG	5.03	122.95	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1729	0	1658	38	1
1	D	1711	0	1639	28	1
2	C	1645	0	1614	40	0
2	F	1645	0	1614	41	0
3	B	1729	0	1690	37	0
3	E	1729	0	1690	49	0
4	G	59	0	52	3	0
4	H	59	0	52	3	0
5	A	6	0	8	3	0
6	A	127	0	0	9	1
6	B	114	0	0	5	1
6	C	86	0	0	7	0
6	D	132	0	0	5	0
6	E	114	0	0	9	1
6	F	69	0	0	3	0
All	All	10954	0	10017	221	4

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 11.

All (221) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:ASN:O	6:D:301:HOH:O	1.80	0.98
2:C:22:SER:O	6:C:301:HOH:O	1.80	0.97
3:E:57:THR:OG1	6:E:301:HOH:O	1.83	0.95
1:A:102:PHE:HD1	1:A:232:TYR:HB2	1.34	0.92
3:E:204:SER:OG	6:E:303:HOH:O	1.88	0.92
1:A:62:LYS:HD2	4:H:5:FUC:H62	1.52	0.89
1:D:88:GLU:OE2	6:D:302:HOH:O	1.91	0.88
3:E:161:TYR:OH	6:E:302:HOH:O	1.85	0.88
2:F:1:GLU:O	6:F:301:HOH:O	1.93	0.86
1:D:127:TRP:CZ2	1:D:253:VAL:HG11	2.11	0.85
1:A:98:TYR:HD1	1:A:99:PRO:HD2	1.43	0.84
3:E:106:ARG:NH1	6:E:307:HOH:O	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:161:TYR:CE1	3:E:192:TYR:HB2	2.13	0.83
2:C:147:GLN:HE21	2:C:154:LEU:HD11	1.45	0.81
3:B:145:LYS:NZ	3:B:151:THR:O	2.15	0.80
2:F:172:THR:OG1	6:F:302:HOH:O	2.01	0.79
3:E:20:LEU:HD11	3:E:125:ILE:HD11	1.66	0.78
1:A:266:SER:O	6:A:401:HOH:O	2.01	0.78
3:E:119:TRP:O	6:E:304:HOH:O	1.99	0.78
1:A:102:PHE:CD1	1:A:232:TYR:HB2	2.18	0.77
3:B:161:TYR:CE1	3:B:192:TYR:HB2	2.20	0.77
2:C:31:LYS:O	6:C:303:HOH:O	2.03	0.76
3:B:119:TRP:O	6:B:302:HOH:O	2.04	0.75
1:A:229:ARG:NE	3:B:101:GLU:OE2	2.19	0.75
1:D:229:ARG:NE	3:E:101:GLU:OE2	2.15	0.75
2:C:52:SER:OG	6:C:302:HOH:O	2.03	0.74
1:D:76:GLU:O	6:D:303:HOH:O	2.04	0.74
1:A:98:TYR:HH	5:A:300:GOL:HO2	1.32	0.74
1:A:227:GLU:OE1	6:A:402:HOH:O	2.06	0.73
3:E:22:CYS:HB3	3:E:78:LEU:HB3	1.71	0.72
3:E:143:SER:O	6:E:305:HOH:O	2.07	0.72
3:B:189:SER:O	6:B:303:HOH:O	2.08	0.71
2:C:45:ARG:HD2	6:C:374:HOH:O	1.91	0.71
2:F:83:LEU:HD11	2:F:166:GLN:HB3	1.71	0.70
3:B:20:LEU:HD11	3:B:125:ILE:HD11	1.74	0.70
3:E:175:LEU:O	6:E:306:HOH:O	2.10	0.69
2:F:37:GLN:HG3	2:F:86:TYR:HE1	1.58	0.69
6:A:527:HOH:O	4:H:3:BMA:O3	2.09	0.69
1:A:208:ARG:HH21	1:A:238:GLU:HB3	1.57	0.69
2:F:210:ASN:O	2:F:211:ARG:HG3	1.93	0.69
1:D:62:LYS:HE3	1:D:94:ASN:OD1	1.93	0.68
1:A:220:ARG:HG2	3:B:99:LEU:HD21	1.74	0.68
1:A:208:ARG:NH1	6:A:409:HOH:O	2.27	0.68
2:F:108:ARG:HG2	2:F:109:THR:N	2.12	0.65
2:F:49:TYR:CD1	2:F:53:ASN:HB2	2.33	0.64
3:E:13:ARG:HG2	6:E:377:HOH:O	1.97	0.63
2:C:49:TYR:CE1	2:C:53:ASN:HB2	2.32	0.63
3:B:27:PHE:HD2	3:B:97:ARG:NH1	1.97	0.63
2:C:49:TYR:CD1	2:C:53:ASN:HB2	2.34	0.62
3:E:164:GLU:HG3	6:E:302:HOH:O	1.99	0.62
2:C:83:LEU:HB2	2:C:106:ILE:HD12	1.80	0.62
6:D:428:HOH:O	4:G:4:FUC:O5	2.16	0.62
2:C:145:LYS:HB3	2:C:197:THR:OG1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:35:HIS:CE1	2:F:96:TYR:HE2	2.19	0.61
3:B:29:PHE:HB2	3:B:76:ASN:OD1	2.01	0.60
3:B:22:CYS:HB3	3:B:78:LEU:HB3	1.83	0.60
3:E:150:GLY:O	3:E:202:SER:N	2.29	0.60
2:F:85:VAL:HG22	2:F:103:ARG:HD2	1.83	0.60
2:F:37:GLN:HG3	2:F:86:TYR:CE1	2.36	0.59
1:A:79:SER:HB3	1:A:117:ARG:HH21	1.66	0.59
2:F:91:PHE:HB2	2:F:96:TYR:HE1	1.67	0.59
1:D:103:ILE:HG13	1:D:233:TYR:CE1	2.37	0.59
1:A:98:TYR:OH	5:A:300:GOL:O2	2.11	0.59
3:B:161:TYR:CD1	3:B:192:TYR:HB2	2.38	0.59
1:D:62:LYS:NZ	1:D:74:GLU:OE1	2.26	0.58
1:A:153:TRP:HH2	5:A:300:GOL:H31	1.69	0.57
3:B:177:SER:O	6:B:304:HOH:O	2.17	0.57
3:E:27:PHE:HD2	3:E:97:ARG:NH1	2.02	0.57
3:E:51:MET:HG3	3:E:57:THR:HG22	1.85	0.57
1:D:62:LYS:HD2	4:G:5:FUC:H62	1.88	0.56
2:C:95:VAL:HG23	3:B:47:TRP:CZ3	2.40	0.56
1:A:97:CYS:HA	1:A:224:ARG:NH1	2.20	0.56
2:C:37:GLN:OE1	2:C:45:ARG:HD3	2.05	0.56
3:B:34:MET:HB3	3:B:78:LEU:HD22	1.87	0.56
3:E:187:GLN:HG2	3:E:191:LEU:O	2.06	0.56
2:F:33:LEU:HD22	2:F:71:PHE:CG	2.41	0.56
3:B:97:ARG:HE	3:B:117:ASP:HB3	1.71	0.56
1:A:128:PRO:O	1:A:157:LYS:NZ	2.25	0.56
3:B:51:MET:HE2	3:B:69:ILE:HG12	1.87	0.55
2:F:18:ARG:HG3	2:F:76:SER:HA	1.88	0.55
1:A:109:ARG:NH1	6:A:418:HOH:O	2.38	0.55
2:C:199:GLN:HG2	6:C:317:HOH:O	2.06	0.55
2:F:49:TYR:CE1	2:F:53:ASN:HB2	2.42	0.55
1:D:163:LYS:NZ	1:D:201:TYR:OH	2.39	0.55
1:D:81:ALA:HB3	6:D:319:HOH:O	2.06	0.55
3:B:56:GLU:HG2	6:B:373:HOH:O	2.07	0.54
1:D:102:PHE:HD2	1:D:105:TYR:HB2	1.73	0.54
2:F:120:PRO:HD3	2:F:132:VAL:HG22	1.90	0.54
1:D:62:LYS:HD2	4:G:5:FUC:C6	2.38	0.54
2:C:33:LEU:HD22	2:C:71:PHE:CG	2.42	0.54
2:F:2:ILE:HG21	2:F:28:ILE:HD11	1.89	0.54
2:C:105:GLU:HG2	6:C:356:HOH:O	2.06	0.54
2:C:197:THR:HG22	2:C:204:PRO:HB3	1.90	0.53
1:A:222:LYS:NZ	6:A:420:HOH:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:27:PHE:HE1	3:E:29:PHE:HD1	1.56	0.53
3:E:199:THR:HG21	2:F:137:ASN:ND2	2.23	0.53
2:C:49:TYR:HD1	2:C:49:TYR:O	1.91	0.53
3:B:187:GLN:HG3	3:B:191:LEU:O	2.08	0.53
1:A:102:PHE:CE2	1:A:105:TYR:HD1	2.26	0.52
3:E:161:TYR:CD1	3:E:192:TYR:HB2	2.43	0.52
1:A:163:LYS:NZ	1:A:201:TYR:OH	2.42	0.52
2:F:138:ASN:ND2	6:F:312:HOH:O	2.42	0.52
2:C:16:GLY:O	2:F:1:GLU:HB2	2.10	0.52
1:A:98:TYR:CD1	1:A:99:PRO:HD2	2.35	0.52
3:B:91:ALA:HB3	3:B:93:TYR:HE1	1.75	0.52
3:B:211:ILE:CD1	3:B:226:ARG:HG2	2.39	0.52
3:E:51:MET:HE2	3:E:69:ILE:HG12	1.91	0.52
2:F:147:GLN:HB3	2:F:195:GLU:HB3	1.92	0.51
1:D:98:TYR:HE1	1:D:226:ARG:HD3	1.74	0.51
1:A:97:CYS:O	1:A:224:ARG:HD2	2.11	0.51
3:E:161:TYR:HD1	3:E:161:TYR:O	1.93	0.51
2:F:49:TYR:O	2:F:49:TYR:HD1	1.93	0.51
1:A:102:PHE:HE2	1:A:105:TYR:HD1	1.57	0.51
1:A:137:ALA:HA	1:A:145:LYS:HG2	1.92	0.51
3:B:33:ASP:OD1	6:B:305:HOH:O	2.19	0.51
3:B:97:ARG:NH2	3:B:117:ASP:OD2	2.37	0.51
2:C:61:ARG:HD2	2:C:76:SER:O	2.11	0.51
2:F:107:LYS:NZ	4:H:2:NAG:H83	2.26	0.51
3:E:201:PRO:HG2	3:E:204:SER:OG	2.11	0.51
3:E:51:MET:HE1	3:E:70:SER:C	2.31	0.50
2:C:106:ILE:O	2:C:166:GLN:NE2	2.41	0.50
1:A:98:TYR:HD1	1:A:99:PRO:CD	2.20	0.50
3:B:12:VAL:HG11	3:B:85:LEU:HD13	1.94	0.50
3:B:211:ILE:HD12	3:B:226:ARG:HG2	1.92	0.50
3:E:51:MET:CE	3:E:69:ILE:HG12	2.41	0.50
3:E:183:PRO:HG2	2:F:162:SER:HB2	1.94	0.50
3:E:150:GLY:O	3:E:201:PRO:HA	2.12	0.49
2:C:18:ARG:NE	2:F:3:VAL:HG22	2.27	0.49
1:D:98:TYR:CD2	1:D:230:MET:HB2	2.48	0.49
2:C:76:SER:HB3	2:F:3:VAL:HG21	1.95	0.49
1:D:114:SER:OG	1:D:263:ASN:HB3	2.12	0.49
3:B:161:TYR:HE2	3:B:166:VAL:HG22	1.78	0.49
1:D:253:VAL:HG12	1:D:254:PRO:O	2.12	0.48
1:A:64:ASN:HA	1:A:88:GLU:HG3	1.94	0.48
3:E:161:TYR:HE2	3:E:166:VAL:HG22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:GLN:HE21	2:F:171:SER:HB3	1.77	0.48
3:E:27:PHE:CD2	3:E:97:ARG:NH1	2.81	0.48
2:F:6:GLN:O	2:F:100:GLN:NE2	2.46	0.48
1:A:102:PHE:HD2	1:A:105:TYR:HB2	1.78	0.48
3:E:12:VAL:HG11	3:E:85:LEU:HD13	1.96	0.48
2:C:80:PRO:HA	2:C:106:ILE:HD13	1.95	0.47
3:B:51:MET:HE1	3:B:71:ARG:HB3	1.95	0.47
3:E:47:TRP:CG	2:F:96:TYR:HB2	2.49	0.47
3:E:36:TRP:NE1	3:E:80:LEU:HB2	2.30	0.47
3:B:161:TYR:HD1	3:B:161:TYR:O	1.97	0.47
2:F:49:TYR:HD1	2:F:49:TYR:C	2.18	0.47
2:C:49:TYR:CD1	2:C:49:TYR:C	2.88	0.47
2:F:49:TYR:CD1	2:F:49:TYR:C	2.88	0.47
2:C:108:ARG:HG2	2:C:109:THR:O	2.15	0.47
1:A:129:ASN:ND2	6:A:417:HOH:O	2.35	0.47
3:B:72:GLU:OE1	3:B:75:ARG:HD2	2.15	0.47
3:E:32:TYR:CE1	3:E:99:LEU:HG	2.50	0.46
1:A:62:LYS:NZ	1:A:94:ASN:OD1	2.49	0.46
2:C:96:TYR:HD1	2:C:96:TYR:N	2.13	0.46
3:E:187:GLN:HA	2:F:160:GLN:HE22	1.81	0.46
2:C:95:VAL:HG23	3:B:47:TRP:HZ3	1.81	0.46
3:E:59:TYR:HB2	3:E:64:LYS:HG2	1.98	0.46
2:C:96:TYR:N	2:C:96:TYR:CD1	2.84	0.46
3:E:51:MET:HE2	3:E:69:ILE:HG23	1.97	0.46
2:C:48:ILE:HD13	2:C:54:ARG:HA	1.98	0.46
1:A:151:LEU:HB3	1:A:252:VAL:HG12	1.97	0.45
3:B:32:TYR:HB3	3:B:98:ALA:O	2.15	0.45
1:A:263:ASN:ND2	6:A:430:HOH:O	2.49	0.45
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.99	0.45
2:F:142:ARG:HH21	2:F:163:VAL:HB	1.82	0.45
2:C:49:TYR:HD1	2:C:49:TYR:C	2.20	0.45
3:E:161:TYR:CD1	3:E:161:TYR:C	2.90	0.45
1:D:65:ILE:HD12	1:D:109:ARG:HG2	1.98	0.45
2:C:154:LEU:HD12	2:C:155:GLN:H	1.81	0.45
2:F:142:ARG:HB2	2:F:173:TYR:CE2	2.52	0.45
1:D:98:TYR:HD2	1:D:230:MET:CB	2.29	0.45
1:A:102:PHE:CE2	1:A:105:TYR:CD1	3.04	0.45
3:B:91:ALA:HB3	3:B:93:TYR:CE1	2.51	0.44
3:E:91:ALA:HB3	3:E:93:TYR:HE1	1.83	0.44
3:B:161:TYR:CD1	3:B:161:TYR:C	2.91	0.44
2:C:12:SER:HA	2:C:105:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:LYS:HE2	1:D:193:SER:O	2.18	0.44
1:A:221:PRO:HB3	2:C:49:TYR:OH	2.18	0.44
3:B:161:TYR:CE2	3:B:166:VAL:HG13	2.52	0.44
1:D:102:PHE:CD1	1:D:232:TYR:HB2	2.53	0.44
3:B:32:TYR:CD2	3:B:97:ARG:HD3	2.53	0.44
1:D:98:TYR:CE1	1:D:226:ARG:HD3	2.53	0.43
2:C:83:LEU:HD11	2:C:166:GLN:HB3	2.00	0.43
3:E:167:THR:OG1	3:E:215:ASN:HB2	2.18	0.43
1:D:67:GLY:HA3	1:D:94:ASN:O	2.18	0.43
1:A:65:ILE:HD12	1:A:109:ARG:HG2	1.99	0.43
1:A:100:GLY:HA3	1:A:230:MET:O	2.18	0.43
2:C:147:GLN:HB3	2:C:195:GLU:HB3	2.00	0.43
3:E:34:MET:HB3	3:E:78:LEU:HD22	2.01	0.43
3:B:36:TRP:NE1	3:B:80:LEU:HB2	2.34	0.43
2:F:18:ARG:HE	2:F:74:ILE:CG2	2.32	0.43
3:B:12:VAL:O	3:B:127:VAL:HA	2.19	0.43
1:D:180:TRP:HZ3	1:D:235:THR:HG22	1.84	0.43
2:C:6:GLN:HG2	6:C:301:HOH:O	2.19	0.42
1:D:102:PHE:CE2	1:D:105:TYR:HD1	2.37	0.42
2:C:40:PRO:HB3	2:C:165:GLU:OE1	2.19	0.42
3:E:27:PHE:HE1	3:E:29:PHE:CD1	2.38	0.42
2:F:48:ILE:HD13	2:F:54:ARG:HA	2.02	0.42
2:F:91:PHE:CD1	2:F:96:TYR:CE1	3.08	0.42
1:D:100:GLY:HA3	1:D:230:MET:O	2.20	0.42
3:B:27:PHE:CD2	3:B:97:ARG:NH1	2.84	0.41
1:A:156:LYS:HA	1:A:161:TYR:HD1	1.85	0.41
3:E:160:ASP:OD1	3:E:187:GLN:NE2	2.53	0.41
3:E:161:TYR:CE2	3:E:166:VAL:HG13	2.56	0.41
2:F:37:GLN:HB2	2:F:47:LEU:HD11	2.02	0.41
2:F:91:PHE:CE1	2:F:94:SER:HA	2.56	0.41
1:A:61:GLY:O	6:A:405:HOH:O	2.22	0.41
2:C:124:GLN:HG2	2:C:129:THR:O	2.20	0.41
3:E:91:ALA:HB3	3:E:93:TYR:CE1	2.56	0.41
2:F:21:LEU:HD21	2:F:86:TYR:HD2	1.85	0.41
1:D:151:LEU:HB3	1:D:252:VAL:HG12	2.03	0.41
2:C:167:ASP:OD1	2:C:168:SER:N	2.54	0.41
3:E:166:VAL:HG12	3:E:216:HIS:HB2	2.03	0.41
2:F:32:TYR:O	2:F:90:GLN:HA	2.21	0.41
1:A:67:GLY:HA3	1:A:94:ASN:O	2.21	0.41
2:F:91:PHE:HE1	2:F:94:SER:HA	1.86	0.41
1:D:175:GLU:OE1	1:D:236:LEU:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:45:ARG:HH11	2:C:58:ILE:HD13	1.86	0.40
3:E:184:ALA:HA	3:E:194:LEU:HB3	2.04	0.40
3:E:27:PHE:CD1	3:E:27:PHE:C	2.94	0.40
3:E:161:TYR:HD1	3:E:161:TYR:C	2.24	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:503:HOH:O	6:A:515:HOH:O[4_557]	2.06	0.14
1:D:79:SER:OG	1:D:104:ASP:OD1[4_546]	2.14	0.06
6:B:406:HOH:O	6:E:405:HOH:O[3_455]	2.16	0.04
1:A:79:SER:OG	1:A:104:ASP:OD1[4_547]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/225 (96%)	211 (97%)	6 (3%)	0	100	100
1	D	214/225 (95%)	206 (96%)	8 (4%)	0	100	100
2	C	211/215 (98%)	205 (97%)	6 (3%)	0	100	100
2	F	211/215 (98%)	203 (96%)	8 (4%)	0	100	100
3	B	228/240 (95%)	224 (98%)	4 (2%)	0	100	100
3	E	228/240 (95%)	224 (98%)	3 (1%)	1 (0%)	34	42
All	All	1309/1360 (96%)	1273 (97%)	35 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	146	SER

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	188/193 (97%)	188 (100%)	0	100	100
1	D	186/193 (96%)	186 (100%)	0	100	100
2	C	184/186 (99%)	182 (99%)	2 (1%)	73	86
2	F	184/186 (99%)	183 (100%)	1 (0%)	88	95
3	B	185/195 (95%)	179 (97%)	6 (3%)	39	54
3	E	185/195 (95%)	182 (98%)	3 (2%)	62	78
All	All	1112/1148 (97%)	1100 (99%)	12 (1%)	73	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	49	TYR
2	C	96	TYR
3	B	27	PHE
3	B	32	TYR
3	B	81	GLN
3	B	97	ARG
3	B	112	TYR
3	B	161	TYR
3	E	27	PHE
3	E	97	ARG
3	E	161	TYR
2	F	49	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	147	GLN
2	F	53	ASN
2	F	160	GLN

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 ⓘ

10 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	G	1	1,4	14,14,15	0.36	0	17,19,21	0.55	0
4	NAG	G	2	4	14,14,15	0.45	0	17,19,21	0.38	0
4	BMA	G	3	4	11,11,12	0.62	0	15,15,17	0.75	0
4	FUC	G	4	4	10,10,11	0.69	0	14,14,16	0.85	0
4	FUC	G	5	4	10,10,11	0.67	1 (10%)	14,14,16	1.53	3 (21%)
4	NAG	H	1	1,4	14,14,15	0.35	0	17,19,21	0.69	1 (5%)
4	NAG	H	2	4	14,14,15	0.28	0	17,19,21	0.41	0
4	BMA	H	3	4	11,11,12	0.55	0	15,15,17	0.72	0
4	FUC	H	4	4	10,10,11	0.65	0	14,14,16	0.86	0
4	FUC	H	5	4	10,10,11	0.86	0	14,14,16	0.96	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	5	FUC	C1-C2	2.01	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5	FUC	C1-O5-C5	3.22	120.08	112.78
4	G	5	FUC	O5-C5-C6	-2.20	102.59	107.33
4	H	1	NAG	C1-O5-C5	2.12	115.07	112.19
4	G	5	FUC	O5-C5-C4	2.01	113.12	109.52

There are no chirality outliers.

All (6) torsion outliers are listed below:

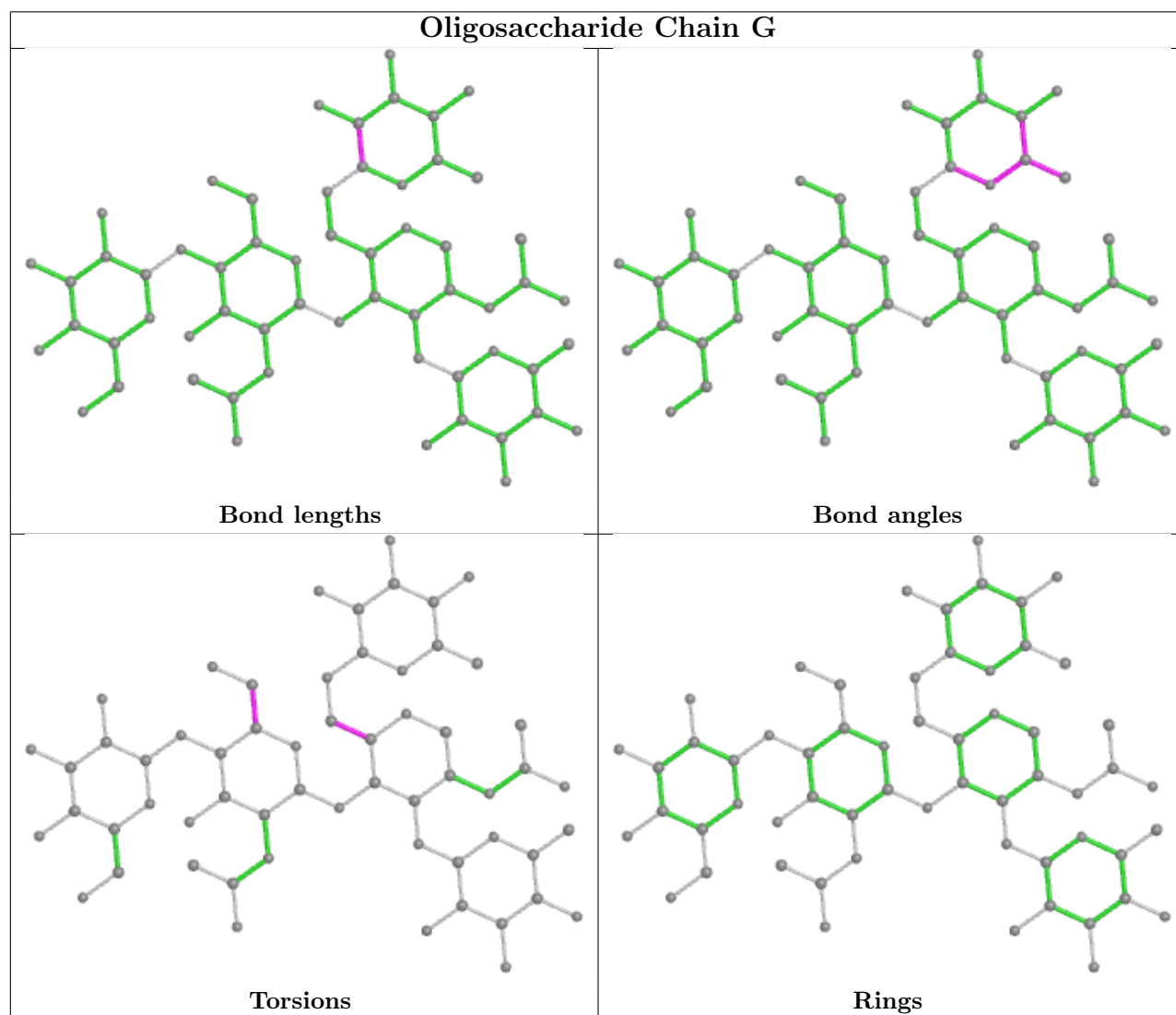
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6

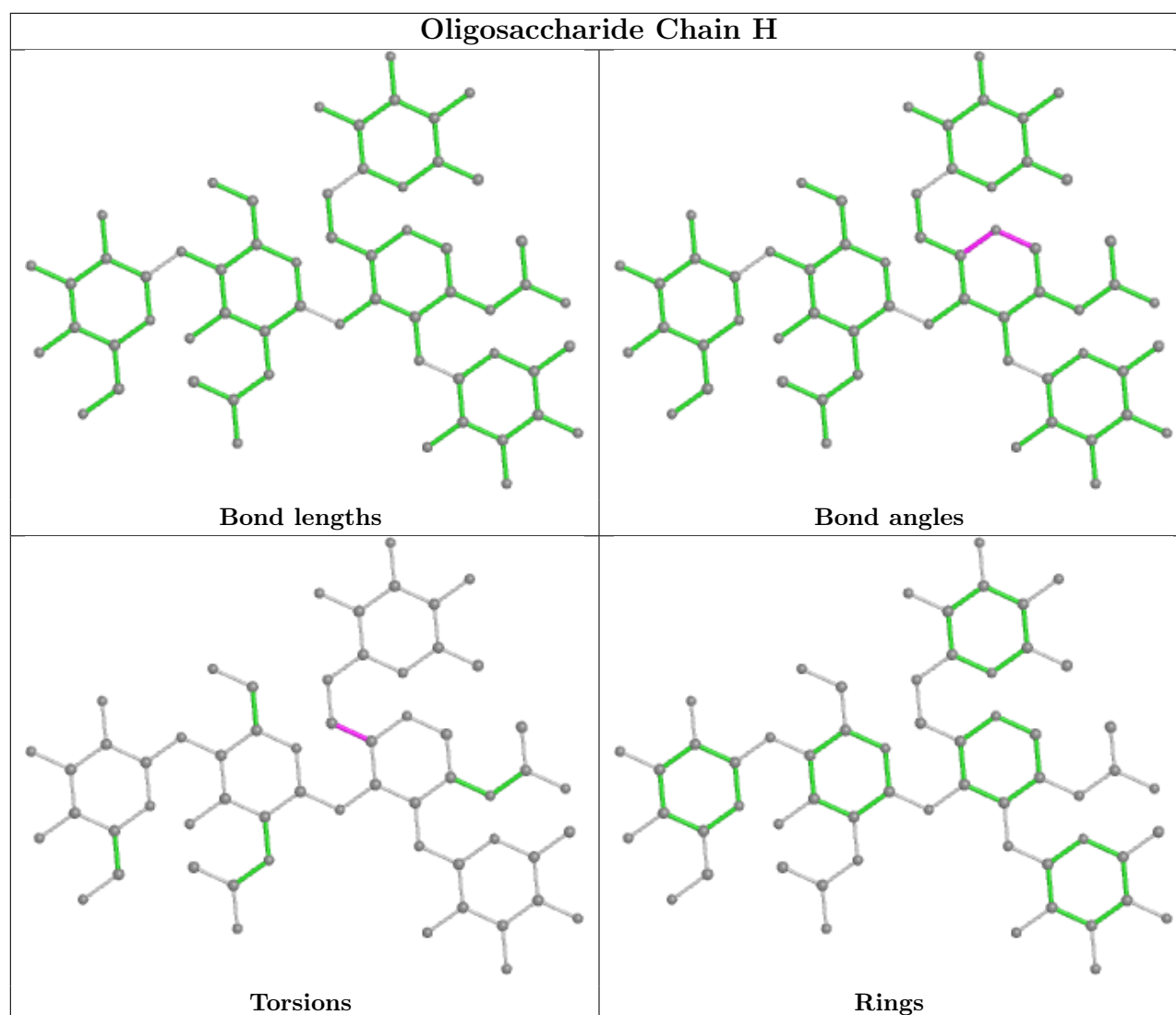
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	5	FUC	1	0
4	H	2	NAG	1	0
4	G	5	FUC	2	0
4	G	4	FUC	1	0
4	H	3	BMA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	GOL	A	300	-	5,5,5	0.91	0	5,5,5	1.24	1 (20%)

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	A	300	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	300	GOL	C3-C2-C1	-2.13	103.44	111.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	300	GOL	O1-C1-C2-C3
5	A	300	GOL	C1-C2-C3-O3
5	A	300	GOL	O2-C2-C3-O3
5	A	300	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	300	GOL	3	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	219/225 (97%)	0.47	9 (4%) 37 44	24, 34, 55, 76	0
1	D	216/225 (96%)	0.50	5 (2%) 60 67	19, 32, 48, 71	0
2	C	213/215 (99%)	0.62	15 (7%) 16 21	29, 41, 66, 88	0
2	F	213/215 (99%)	1.15	49 (23%) 0 1	31, 56, 89, 108	0
3	B	230/240 (95%)	0.75	16 (6%) 16 21	24, 38, 70, 186	0
3	E	230/240 (95%)	0.92	20 (8%) 10 14	26, 42, 70, 195	0
All	All	1321/1360 (97%)	0.73	114 (8%) 10 14	19, 39, 74, 195	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	149	GLY	24.7
3	B	146	SER	13.9
3	B	147	THR	13.4
3	E	148	SER	10.9
3	E	146	SER	7.6
3	E	143	SER	7.6
3	B	148	SER	7.0
3	E	147	THR	6.7
3	E	150	GLY	6.7
3	B	145	LYS	6.3
2	C	190	LYS	6.2
2	F	194	CYS	6.2
2	F	150	VAL	6.1
2	F	188	LYS	5.7
3	B	149	GLY	5.6
3	E	145	LYS	5.6
2	F	153	ALA	5.5
2	C	191	VAL	5.2
3	E	144	SER	5.1

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Mol	Chain	Res	Type	RSRZ
2	F	203	SER	5.1
2	F	187	GLU	4.7
2	F	127	SER	4.6
1	A	266	SER	4.6
2	F	129	THR	4.4
3	B	188	SER	4.4
3	E	151	THR	4.4
3	E	230	LYS	4.2
3	E	203	SER	4.1
3	E	190	GLY	4.1
3	E	188	SER	4.1
2	F	191	VAL	4.1
2	F	126	LYS	4.0
2	F	151	ASP	3.9
2	F	210	ASN	3.8
2	F	184	ALA	3.8
2	F	209	PHE	3.6
1	A	198	ALA	3.5
2	F	128	GLY	3.5
2	F	202	SER	3.5
3	E	202	SER	3.4
3	B	176	THR	3.3
3	B	230	LYS	3.3
2	C	181	LEU	3.3
1	D	199	ASP	3.2
3	B	143	SER	3.1
2	F	76	SER	3.1
2	F	147	GLN	3.1
3	E	13	ARG	3.1
2	F	49	TYR	3.0
2	F	158	ASN	3.0
3	B	131	SER	3.0
2	C	1	GLU	2.9
2	C	184	ALA	2.9
2	F	192	TYR	2.9
2	F	201	LEU	2.9
2	F	183	LYS	2.8
2	F	1	GLU	2.8
3	E	204	SER	2.8
2	F	81	GLU	2.8
1	D	263	ASN	2.8
2	C	27	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	141	ALA	2.7
2	F	144	ALA	2.7
2	F	190	LYS	2.7
1	D	192	GLN	2.6
2	C	182	SER	2.5
1	A	98	TYR	2.5
3	B	144	SER	2.5
2	C	183	LYS	2.5
2	F	189	HIS	2.5
2	F	116	PHE	2.5
1	D	95	GLY	2.5
2	F	117	ILE	2.4
3	E	81	GLN	2.4
2	F	149	LYS	2.4
2	C	152	ASN	2.4
1	A	199	ASP	2.4
2	F	185	ASP	2.4
3	B	192	TYR	2.4
2	C	188	LYS	2.4
2	C	159	SER	2.3
1	A	55	SER	2.3
1	A	102	PHE	2.3
2	C	160	GLN	2.3
2	F	205	VAL	2.3
2	F	152	ASN	2.3
2	F	182	SER	2.3
1	A	161	TYR	2.3
2	F	142	ARG	2.2
3	B	161	TYR	2.2
3	E	189	SER	2.2
3	B	164	GLU	2.2
2	F	186	TYR	2.2
2	C	150	VAL	2.2
1	A	106	GLU	2.2
2	F	56	THR	2.2
2	F	148	TRP	2.2
1	A	264	ALA	2.2
3	B	209	THR	2.1
3	E	152	ALA	2.1
3	B	121	GLN	2.1
2	C	125	LEU	2.1
2	F	181	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	158	GLY	2.1
2	F	169	LYS	2.1
2	C	18	ARG	2.1
2	F	75	ILE	2.1
2	F	3	VAL	2.1
2	F	77	ARG	2.1
2	F	179	LEU	2.1
2	F	96	TYR	2.1
2	F	193	ALA	2.0
2	F	154	LEU	2.0
2	F	206	THR	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](#)

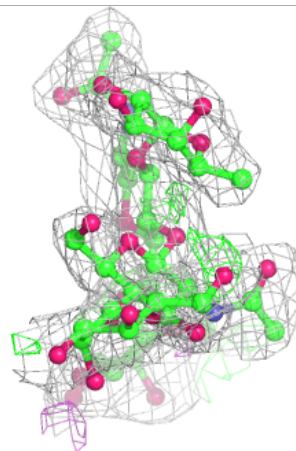
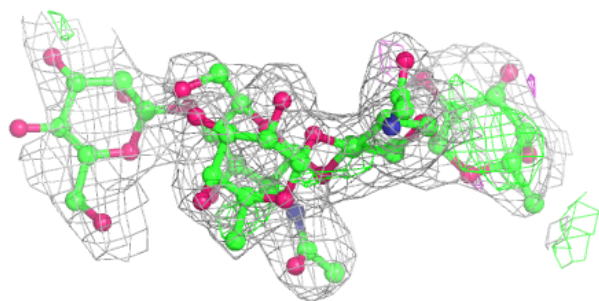
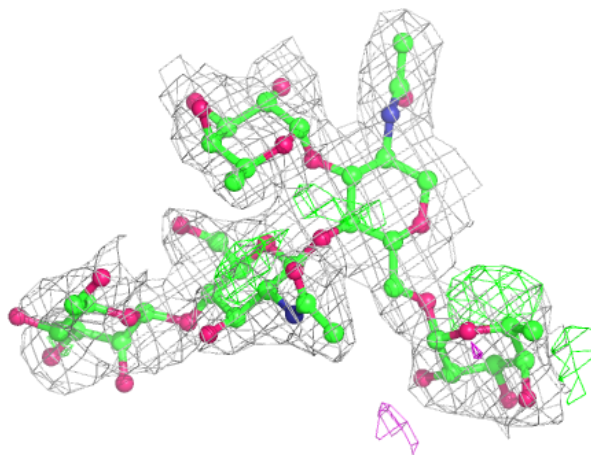
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

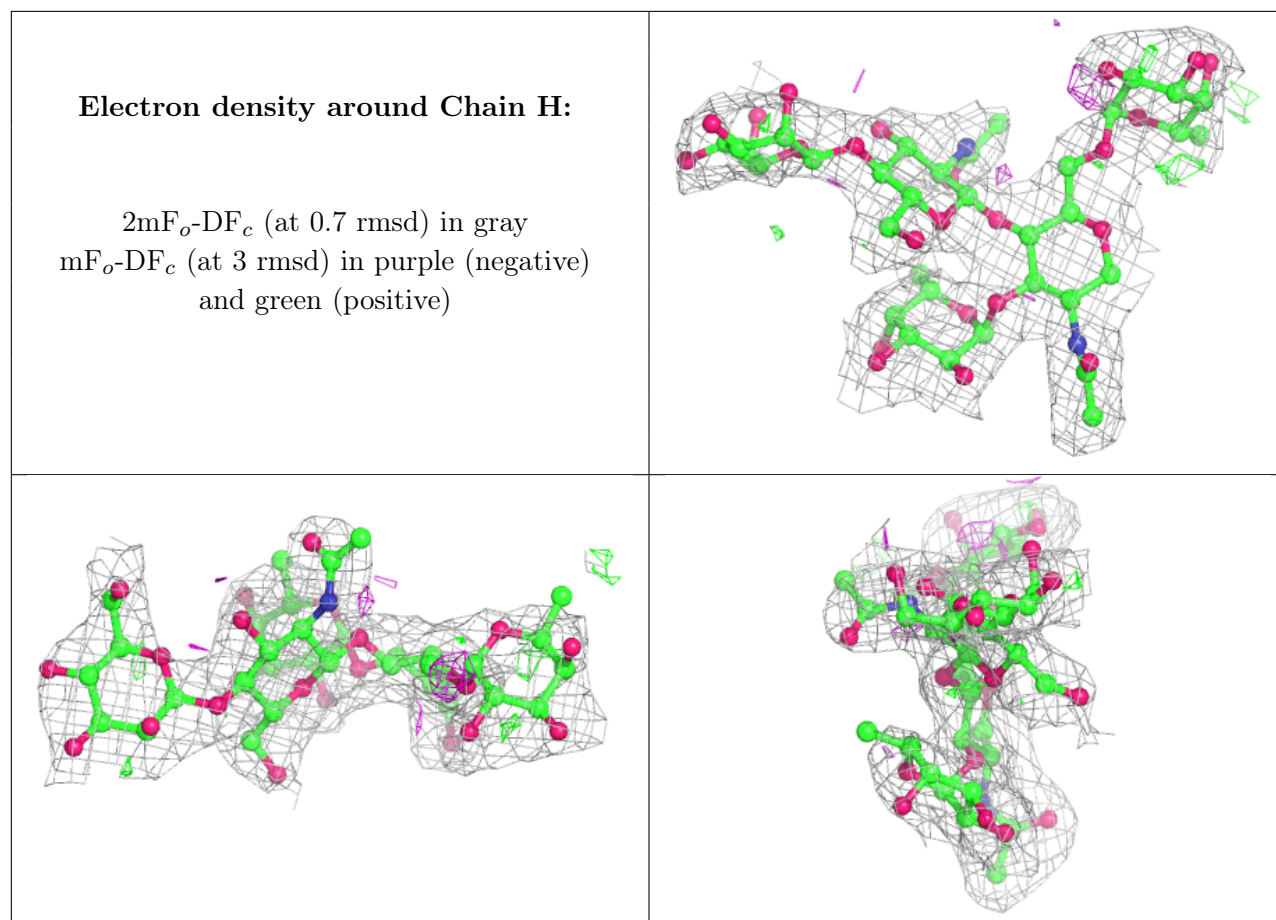
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FUC	H	5	10/11	0.69	0.26	53,57,61,64	0
4	BMA	G	3	11/12	0.72	0.23	66,69,73,76	0
4	FUC	G	5	10/11	0.74	0.26	43,48,55,62	0
4	BMA	H	3	11/12	0.78	0.20	61,66,68,69	0
4	FUC	G	4	10/11	0.79	0.17	40,48,50,52	0
4	NAG	G	2	14/15	0.81	0.18	40,49,58,62	0
4	NAG	H	1	14/15	0.85	0.18	24,33,44,53	0
4	FUC	H	4	10/11	0.85	0.22	44,49,52,52	0
4	NAG	H	2	14/15	0.85	0.17	43,50,55,56	0
4	NAG	G	1	14/15	0.88	0.19	27,36,45,45	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain G:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





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
5	GOL	A	300	6/6	0.88	0.29	40,53,54,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.