Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 07:09 PM EDT

PDB ID	:	4MA1
Title	:	Unliganded 3 crystal structure of S25-26 Fab
Authors	:	Haji-Ghassemi, O.; Evans, S.V.
Deposited on	:	2013-08-15
Resolution	:	2.32 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

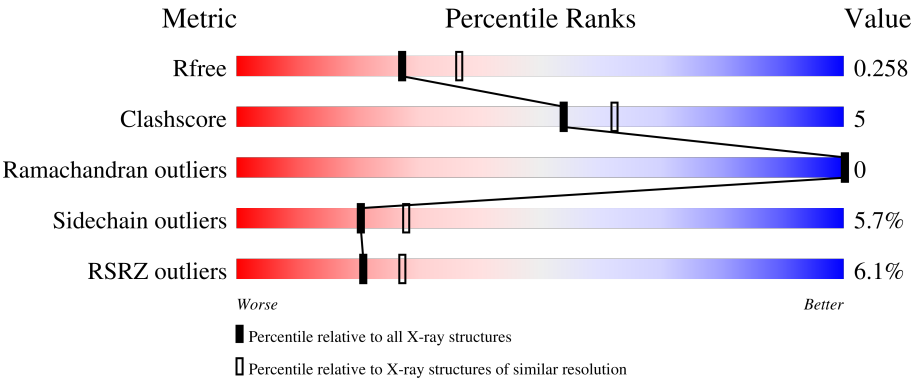
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.32 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.



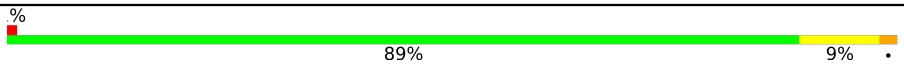
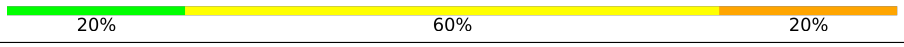
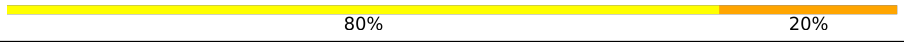
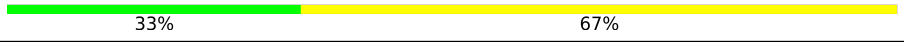
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 <=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	B	219	3% 86% 11%
1	E	219	25% 79% 16%
1	H	219	2% 87% 11%
2	C	219	2% 90% 9%
2	F	219	4% 89% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	L	219	
3	A	5	
4	D	5	
5	G	9	

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
3	MAN	A	4	-	-	-	X
4	BMA	D	3	-	-	-	X
4	MAN	D	4	-	-	-	X
5	GAL	G	6	-	-	-	X
5	GLA	G	7	-	-	-	X
5	MAN	G	8	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10552 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.

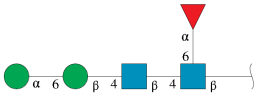
- Molecule 1 is a protein called S25-26 Fab (IgG1k) heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	218	Total	C	N	O	S	0	0	0
			1647	1050	273	317	7			
1	E	216	Total	C	N	O	S	0	0	0
			1631	1039	270	315	7			
1	H	218	Total	C	N	O	S	0	1	0
			1653	1053	274	318	8			

- Molecule 2 is a protein called S25-26 Fab (IgG1k) light chain.

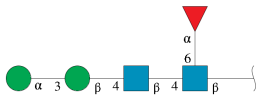
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	219	Total	C	N	O	S	0	0	0
			1712	1072	291	342	7			
2	F	219	Total	C	N	O	S	0	0	0
			1712	1072	291	342	7			
2	L	219	Total	C	N	O	S	0	0	0
			1712	1072	291	342	7			

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



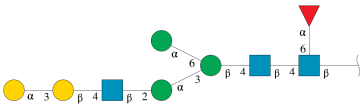
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	5	Total	C	N	O	0	0	0
			60	34	2	24			

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



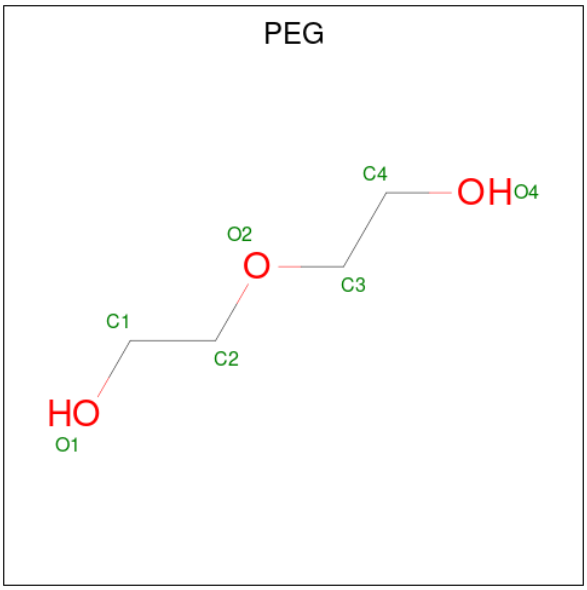
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	D	5	60	34	2	24	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-galactopyranose-(1-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-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
			Total	C	N	O			
5	G	9	107	60	3	44	0	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	7	4	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C O 7 4 3	0	0

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total K 1 1	0	0

- Molecule 8 is water.

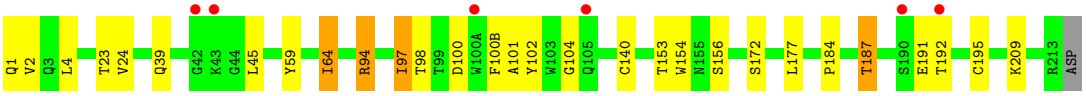
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	38	Total O 38 38	0	0
8	E	16	Total O 16 16	0	0
8	H	62	Total O 62 62	0	0
8	C	34	Total O 34 34	0	0
8	F	47	Total O 47 47	0	0
8	L	46	Total O 46 46	0	0

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.

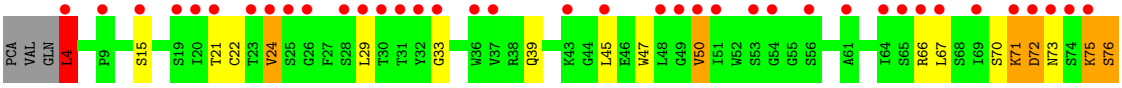
• Molecule 1: S25-26 Fab (IgG1k) heavy chain

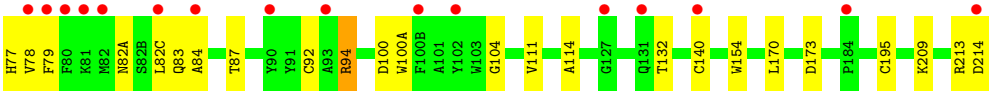
Chain B:



• Molecule 1: S25-26 Fab (IgG1k) heavy chain

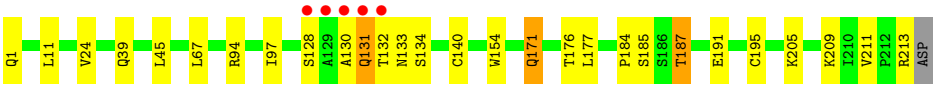
Chain E:





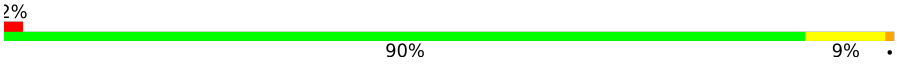
• Molecule 1: S25-26 Fab (IgG1k) heavy chain

Chain H:



• Molecule 2: S25-26 Fab (IgG1k) light chain

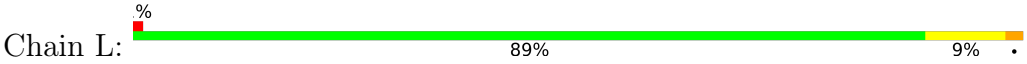
Chain C:

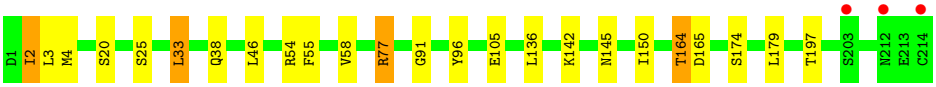


• Molecule 2: S25-26 Fab (IgG1k) light chain

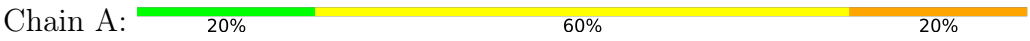
Chain F:

• Molecule 2: S25-26 Fab (IgG1k) light chain

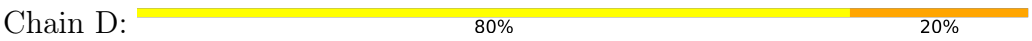




• Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



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



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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.26Å 66.51Å 122.08Å 90.00° 113.46° 90.00°	Depositor
Resolution (Å)	29.93 – 2.32 29.91 – 2.32	Depositor EDS
% Data completeness (in resolution range)	81.4 (29.93-2.32) 81.4 (29.91-2.32)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.12 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.229 , 0.260 0.230 , 0.258	Depositor DCC
R_{free} test set	2621 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10552	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, K, PEG, GLA, FUC, GAL, NAG, MAN, PCA

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	B	0.47	0/1686	0.67	1/2311 (0.0%)
1	E	0.41	0/1677	0.71	4/2297 (0.2%)
1	H	0.49	0/1692	0.71	0/2319
2	C	0.47	0/1752	0.66	0/2376
2	F	0.51	0/1752	0.72	1/2376 (0.0%)
2	L	0.50	0/1752	0.70	1/2376 (0.0%)
All	All	0.47	0/10311	0.70	7/14055 (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	B	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	108	ARG	CB-CA-C	-8.07	94.25	110.40
1	E	82(A)	ASN	N-CA-C	5.98	127.14	111.00
1	E	50	VAL	CB-CA-C	-5.69	100.59	111.40
1	B	140	CYS	CA-CB-SG	5.68	124.22	114.00
1	E	4	LEU	CB-CG-CD2	-5.40	101.81	111.00
2	L	33	LEU	CA-CB-CG	-5.22	103.30	115.30
1	E	71	LYS	N-CA-C	5.09	124.75	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	100	ASP	Peptide

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	B	1647	0	1618	12	0
1	E	1631	0	1598	40	0
1	H	1653	0	1621	12	0
2	C	1712	0	1649	14	0
2	F	1712	0	1649	12	0
2	L	1712	0	1648	15	0
3	A	60	0	52	3	0
4	D	60	0	52	4	0
5	G	107	0	91	0	0
6	B	7	0	10	0	0
6	H	7	0	10	0	0
7	L	1	0	0	0	0
8	B	38	0	0	1	0
8	C	34	0	0	2	0
8	E	16	0	0	0	0
8	F	47	0	0	0	0
8	H	62	0	0	0	0
8	L	46	0	0	1	0
All	All	10552	0	9998	107	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 5.

All (107) 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:A:2:NAG:H82	3:A:5:FUC:O2	1.45	1.15
4:D:1:NAG:H62	4:D:5:FUC:H5	1.27	1.08
3:A:2:NAG:H82	3:A:5:FUC:HO2	1.33	0.91
4:D:1:NAG:H62	4:D:5:FUC:C5	2.07	0.82
1:E:71:LYS:HE3	1:E:73:ASN:OD1	1.82	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:47:TRP:HZ2	1:E:50:VAL:CG2	1.98	0.76
1:E:4:LEU:CD2	1:E:22:CYS:SG	2.77	0.73
1:E:29:LEU:HD13	1:E:72:ASP:HB3	1.71	0.72
1:E:77:HIS:HB3	1:E:79:PHE:HE1	1.54	0.71
1:H:39:GLN:OE1	2:L:38:GLN:NE2	2.20	0.70
1:E:71:LYS:HE3	1:E:73:ASN:ND2	2.06	0.70
1:E:78:VAL:C	1:E:79:PHE:HD1	1.95	0.70
2:C:2:ILE:HD13	2:C:93:HIS:HB2	1.76	0.68
3:A:2:NAG:C8	3:A:5:FUC:O2	2.33	0.67
1:E:4:LEU:HD22	1:E:92:CYS:SG	2.35	0.67
2:F:210:ASN:N	2:F:210:ASN:OD1	2.28	0.67
1:E:71:LYS:HE3	1:E:73:ASN:CG	2.16	0.66
1:E:33:GLY:O	1:E:94:ARG:NH1	2.28	0.66
2:F:2:ILE:HD13	2:F:93:HIS:HB2	1.77	0.65
1:E:77:HIS:HB3	1:E:79:PHE:CE1	2.32	0.65
1:E:71:LYS:CE	1:E:73:ASN:HD21	2.09	0.65
2:C:164:THR:HG23	2:C:165:ASP:O	1.97	0.64
1:E:47:TRP:HZ2	1:E:50:VAL:HG23	1.62	0.64
1:E:71:LYS:HE3	1:E:73:ASN:HD21	1.61	0.64
2:L:164:THR:HG23	2:L:165:ASP:O	2.00	0.62
2:L:2:ILE:HD11	2:L:4:MET:SD	2.40	0.62
1:E:24:VAL:O	1:E:76:SER:HB2	2.00	0.60
2:L:77:ARG:O	2:L:77:ARG:HG2	2.02	0.59
2:C:60:ASP:N	2:C:60:ASP:OD1	2.36	0.59
1:E:71:LYS:NZ	1:E:73:ASN:HD21	2.00	0.58
2:C:30:ASN:OD1	2:C:50:LYS:HE3	2.03	0.58
1:E:4:LEU:HD21	1:E:22:CYS:SG	2.44	0.57
1:E:83:GLN:O	1:E:111:VAL:HG21	2.05	0.57
1:B:154:TRP:CZ3	1:B:195:CYS:HB3	2.40	0.56
1:B:97:ILE:HD11	2:C:49:TYR:CG	2.40	0.56
1:H:131:GLN:HE21	1:H:131:GLN:HA	1.70	0.56
1:E:154:TRP:CZ3	1:E:195:CYS:HB3	2.40	0.56
1:E:82(C):LEU:HB3	1:E:111:VAL:HG11	1.88	0.55
1:B:94:ARG:NH2	1:B:100(B):PHE:O	2.39	0.54
2:C:67:SER:HB3	8:C:308:HOH:O	2.07	0.54
1:E:213:ARG:NH1	2:F:120:PRO:O	2.36	0.54
1:H:128:SER:O	1:H:130:ALA:N	2.41	0.54
2:L:145:ASN:HB3	2:L:197:THR:CG2	2.37	0.54
2:F:164:THR:HG23	2:F:165:ASP:O	2.06	0.54
4:D:1:NAG:C6	4:D:5:FUC:H5	2.19	0.52
2:C:24:ARG:HG2	2:C:70:ASP:OD1	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:LEU:O	1:B:104:GLY:HA2	2.10	0.52
1:E:47:TRP:CZ2	1:E:50:VAL:HG23	2.42	0.52
1:H:154:TRP:CZ3	1:H:195:CYS:HB3	2.45	0.52
1:H:171:GLN:NE2	1:H:176:THR:OG1	2.43	0.51
2:L:77:ARG:O	2:L:77:ARG:CG	2.58	0.51
1:B:59:TYR:HB2	1:B:64:ILE:HG13	1.93	0.51
1:E:114:ALA:HB2	1:E:173:ASP:HB3	1.92	0.50
1:E:87:THR:OG1	1:E:111:VAL:HG22	2.11	0.50
1:H:133:ASN:O	1:H:185:SER:HB2	2.11	0.50
2:L:2:ILE:HG23	8:L:401:HOH:O	2.11	0.50
2:L:2:ILE:HD13	2:L:25:SER:HB2	1.94	0.50
1:H:39:GLN:HB2	1:H:45:LEU:HD23	1.93	0.50
2:L:150:ILE:HD11	2:L:179:LEU:HD21	1.94	0.49
1:E:75:LYS:HB2	1:E:77:HIS:CE1	2.48	0.49
1:B:39:GLN:HB2	1:B:45:LEU:HD23	1.95	0.48
1:E:84:ALA:HA	1:E:111:VAL:HG23	1.94	0.48
1:E:39:GLN:HB2	1:E:45:LEU:HD23	1.94	0.48
2:C:46:LEU:HD23	2:C:55:PHE:CD1	2.48	0.48
1:E:21:THR:HG23	1:E:79:PHE:CE1	2.49	0.48
2:F:46:LEU:HD23	2:F:55:PHE:CD1	2.49	0.47
1:E:24:VAL:O	1:E:76:SER:CB	2.61	0.47
2:C:49:TYR:O	2:C:53:ASN:HB2	2.15	0.47
2:F:150:ILE:HD11	2:F:179:LEU:HD21	1.96	0.47
1:E:71:LYS:CE	1:E:73:ASN:ND2	2.73	0.47
1:E:100:ASP:HB2	1:E:100(A):TRP:CE3	2.50	0.47
1:H:184:PRO:O	1:H:187:THR:HG22	2.15	0.46
1:E:79:PHE:CD1	1:E:79:PHE:N	2.83	0.46
2:C:150:ILE:HD11	2:C:179:LEU:HD21	1.97	0.46
2:F:16:GLY:HA2	2:F:77:ARG:HG2	1.96	0.45
1:E:47:TRP:HZ2	1:E:50:VAL:HG22	1.78	0.45
1:B:154:TRP:CH2	1:B:195:CYS:HB3	2.52	0.44
1:H:39:GLN:NE2	2:L:38:GLN:OE1	2.40	0.44
4:D:1:NAG:C6	4:D:5:FUC:C5	2.86	0.44
2:F:2:ILE:HD12	2:F:2:ILE:N	2.33	0.44
2:L:54:ARG:HD3	2:L:58:VAL:O	2.17	0.44
1:B:2:VAL:HG21	1:B:100(B):PHE:HA	1.98	0.44
1:B:177:LEU:C	1:B:177:LEU:HD12	2.38	0.44
8:B:511:HOH:O	2:F:212:ASN:HB3	2.18	0.44
2:L:46:LEU:HD23	2:L:55:PHE:CD1	2.52	0.44
1:B:153:THR:HB	1:B:156:SER:O	2.17	0.43
2:C:164:THR:HG22	2:C:174:SER:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:67:SER:CB	8:C:308:HOH:O	2.65	0.43
1:E:29:LEU:CD1	1:E:72:ASP:HB3	2.44	0.42
1:B:184:PRO:O	1:B:187:THR:HG22	2.19	0.42
2:F:170:ASP:OD1	2:F:170:ASP:C	2.58	0.42
2:F:164:THR:HG22	2:F:174:SER:H	1.85	0.42
1:B:101:ALA:HB3	2:C:55:PHE:CE1	2.54	0.42
1:E:154:TRP:CH2	1:E:195:CYS:HB3	2.55	0.42
1:E:4:LEU:HD22	1:E:22:CYS:SG	2.59	0.42
2:L:91:GLY:HA2	2:L:96:TYR:CD1	2.55	0.42
2:L:164:THR:HG22	2:L:174:SER:H	1.85	0.42
1:E:4:LEU:HB3	1:E:104:GLY:HA2	2.02	0.41
1:E:47:TRP:CZ2	1:E:50:VAL:CG2	2.89	0.41
2:C:2:ILE:HD12	2:C:2:ILE:N	2.34	0.41
1:E:79:PHE:HD1	1:E:79:PHE:N	2.17	0.41
1:H:187:THR:OG1	1:H:191:GLU:HG3	2.22	0.40
1:H:133:ASN:CG	1:H:134:SER:N	2.75	0.40
1:E:78:VAL:C	1:E:79:PHE:CD1	2.85	0.40
2:F:27(D):HIS:O	2:F:27(E):ARG:HD2	2.21	0.40
2:L:136:LEU:N	2:L:136:LEU:HD12	2.36	0.40
1:H:177:LEU:C	1:H:177:LEU:HD12	2.41	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	B	216/219 (99%)	212 (98%)	4 (2%)	0	100	100
1	E	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
1	H	217/219 (99%)	213 (98%)	4 (2%)	0	100	100
2	C	217/219 (99%)	214 (99%)	3 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	217/219 (99%)	214 (99%)	3 (1%)	0	100	100
2	L	217/219 (99%)	214 (99%)	3 (1%)	0	100	100
All	All	1298/1314 (99%)	1272 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	B	187/188 (100%)	175 (94%)	12 (6%)	17	23
1	E	186/188 (99%)	171 (92%)	15 (8%)	11	14
1	H	188/188 (100%)	173 (92%)	15 (8%)	12	15
2	C	196/196 (100%)	188 (96%)	8 (4%)	30	43
2	F	196/196 (100%)	188 (96%)	8 (4%)	30	43
2	L	196/196 (100%)	188 (96%)	8 (4%)	30	43
All	All	1149/1152 (100%)	1083 (94%)	66 (6%)	20	28

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	23	THR
1	B	24	VAL
1	B	64	ILE
1	B	94	ARG
1	B	97	ILE
1	B	98	THR
1	B	102	TYR
1	B	172	SER
1	B	187	THR
1	B	191	GLU
1	B	192	THR
1	B	209	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	4	LEU
1	E	15	SER
1	E	24	VAL
1	E	66	ARG
1	E	67	LEU
1	E	70	SER
1	E	72	ASP
1	E	75	LYS
1	E	76	SER
1	E	94	ARG
1	E	132	THR
1	E	140	CYS
1	E	170	LEU
1	E	209	LYS
1	E	214	ASP
1	H	11	LEU
1	H	24	VAL
1	H	67	LEU
1	H	94	ARG
1	H	97	ILE
1	H	131	GLN
1	H	132	THR
1	H	140[A]	CYS
1	H	140[B]	CYS
1	H	171	GLN
1	H	187	THR
1	H	205	LYS
1	H	209	LYS
1	H	211	VAL
1	H	213	ARG
2	C	31	THR
2	C	50	LYS
2	C	54	ARG
2	C	60	ASP
2	C	106	LEU
2	C	142	LYS
2	C	164	THR
2	C	168	SER
2	F	18	GLN
2	F	20	SER
2	F	31	THR
2	F	52	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	106	LEU
2	F	164	THR
2	F	188	ARG
2	F	210	ASN
2	L	2	ILE
2	L	3	LEU
2	L	20	SER
2	L	33	LEU
2	L	77	ARG
2	L	105	GLU
2	L	142	LYS
2	L	164	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	73	ASN
1	E	77	HIS
1	H	13	GLN
1	H	39	GLN
1	H	131	GLN
1	H	171	GLN
2	F	18	GLN
2	L	38	GLN
2	L	156	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	PCA	B	1	1	7,8,9	0.53	0	9,10,12	1.12	1 (11%)
1	PCA	H	1	1	7,8,9	0.51	0	9,10,12	1.45	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	1	PCA	CB-CA-C	-3.19	108.31	112.70
1	B	1	PCA	OE-CD-CG	-2.22	122.89	126.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

19 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	$\#\|Z\|>2$
3	NAG	A	1	3,1	14,14,15	0.70	0	17,19,21	1.38	3 (17%)
3	NAG	A	2	3	14,14,15	0.62	0	17,19,21	2.66	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	A	3	3	11,11,12	0.40	0	15,15,17	0.92	0
3	MAN	A	4	3	11,11,12	0.47	0	15,15,17	2.49	2 (13%)
3	FUC	A	5	3	10,10,11	0.30	0	14,14,16	0.62	0
4	NAG	D	1	4,1	14,14,15	0.55	0	17,19,21	1.62	3 (17%)
4	NAG	D	2	4	14,14,15	0.49	0	17,19,21	2.23	3 (17%)
4	BMA	D	3	4	11,11,12	0.30	0	15,15,17	1.99	3 (20%)
4	MAN	D	4	4	11,11,12	0.57	0	15,15,17	1.06	1 (6%)
4	FUC	D	5	4	10,10,11	0.32	0	14,14,16	0.81	0
5	NAG	G	1	5,1	14,14,15	0.29	0	17,19,21	0.61	0
5	NAG	G	2	5	14,14,15	1.37	1 (7%)	17,19,21	2.20	3 (17%)
5	BMA	G	3	5	11,11,12	0.45	0	15,15,17	2.23	3 (20%)
5	MAN	G	4	5	11,11,12	0.51	0	15,15,17	1.36	1 (6%)
5	NAG	G	5	5	14,14,15	0.50	0	17,19,21	0.83	0
5	GAL	G	6	5	11,11,12	0.72	0	15,15,17	2.13	4 (26%)
5	GLA	G	7	5	11,11,12	0.42	0	15,15,17	1.09	2 (13%)
5	MAN	G	8	5	11,11,12	0.26	0	15,15,17	0.63	0
5	FUC	G	9	5	10,10,11	0.45	0	14,14,16	1.24	2 (14%)

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
3	NAG	A	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	1/6/23/26	0/1/1/1
3	BMA	A	3	3	-	2/2/19/22	0/1/1/1
3	MAN	A	4	3	-	2/2/19/22	0/1/1/1
3	FUC	A	5	3	-	-	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
4	FUC	D	5	4	-	-	0/1/1/1
5	NAG	G	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	5/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	5	5	-	2/6/23/26	0/1/1/1
5	GAL	G	6	5	-	0/2/19/22	0/1/1/1
5	GLA	G	7	5	-	1/2/19/22	0/1/1/1
5	MAN	G	8	5	-	2/2/19/22	0/1/1/1
5	FUC	G	9	5	-	-	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	2	NAG	O4-C4	-4.47	1.32	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2	NAG	O5-C1-C2	8.67	124.97	111.29
3	A	4	MAN	C1-O5-C5	8.61	123.86	112.19
4	D	2	NAG	C1-O5-C5	7.69	122.61	112.19
5	G	2	NAG	C4-C3-C2	-6.99	100.77	111.02
5	G	3	BMA	C1-O5-C5	6.73	121.31	112.19
4	D	3	BMA	C1-C2-C3	5.80	116.79	109.67
5	G	6	GAL	C1-O5-C5	5.46	119.59	112.19
5	G	4	MAN	C1-O5-C5	4.48	118.27	112.19
5	G	2	NAG	C1-O5-C5	4.47	118.25	112.19
3	A	2	NAG	C4-C3-C2	4.21	117.19	111.02
5	G	6	GAL	O3-C3-C2	-4.21	101.93	109.99
3	A	2	NAG	C3-C4-C5	3.93	117.25	110.24
4	D	1	NAG	O5-C1-C2	-3.62	105.57	111.29
5	G	3	BMA	C2-C3-C4	-3.41	105.00	110.89
4	D	2	NAG	O5-C5-C4	3.28	118.81	110.83
4	D	1	NAG	C1-O5-C5	3.24	116.58	112.19
3	A	1	NAG	O6-C6-C5	-3.04	100.86	111.29
3	A	4	MAN	O5-C5-C4	3.03	118.19	110.83
5	G	6	GAL	C2-C3-C4	-3.02	105.67	110.89
4	D	3	BMA	O5-C1-C2	2.81	115.10	110.77
3	A	1	NAG	O5-C5-C4	-2.57	104.58	110.83
3	A	1	NAG	C3-C4-C5	-2.45	105.86	110.24
5	G	7	GLA	O2-C2-C1	-2.44	104.16	109.15
5	G	9	FUC	O2-C2-C1	2.42	114.11	109.15
4	D	1	NAG	O7-C7-C8	-2.39	117.63	122.06
5	G	7	GLA	O5-C5-C6	2.36	110.90	107.20
5	G	9	FUC	C2-C3-C4	-2.34	106.85	110.89
4	D	4	MAN	C1-C2-C3	2.29	112.48	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2	NAG	C3-C4-C5	2.27	114.29	110.24
4	D	3	BMA	O3-C3-C2	-2.25	105.69	109.99
5	G	3	BMA	O5-C1-C2	-2.24	107.31	110.77
5	G	2	NAG	O4-C4-C3	2.16	115.34	110.35
5	G	6	GAL	C1-C2-C3	-2.14	107.03	109.67

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	C4-C5-C6-O6
3	A	3	BMA	O5-C5-C6-O6
3	A	4	MAN	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
3	A	3	BMA	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
5	G	5	NAG	O5-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
5	G	2	NAG	C8-C7-N2-C2
5	G	5	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
5	G	8	MAN	C4-C5-C6-O6
5	G	4	MAN	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	G	2	NAG	O7-C7-N2-C2
5	G	7	GLA	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
5	G	8	MAN	O5-C5-C6-O6
3	A	4	MAN	C4-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	G	2	NAG	C3-C2-N2-C7
4	D	4	MAN	C4-C5-C6-O6
3	A	2	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

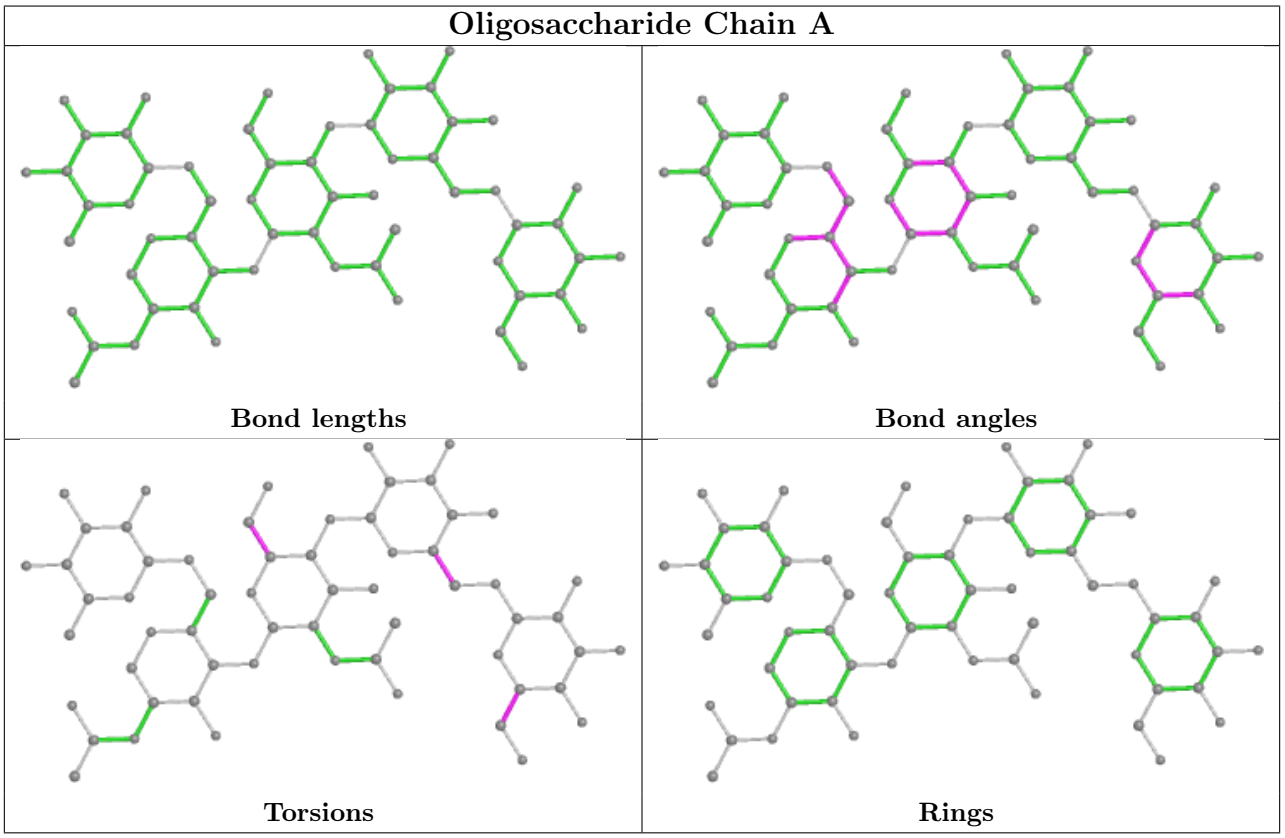
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5	FUC	3	0
4	D	1	NAG	4	0

Continued on next page...

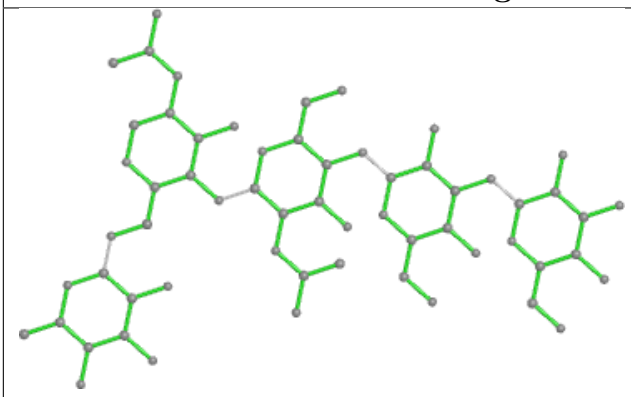
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	NAG	3	0
4	D	5	FUC	4	0

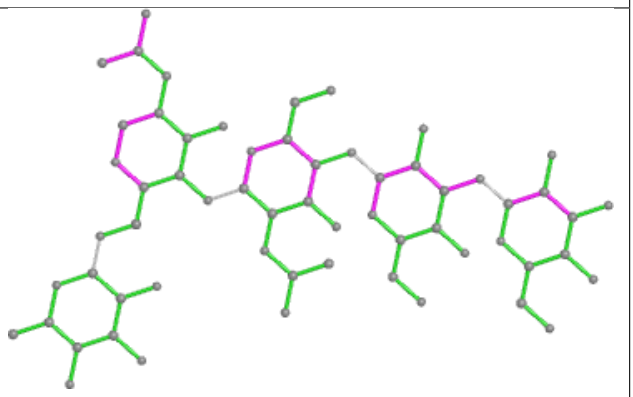
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



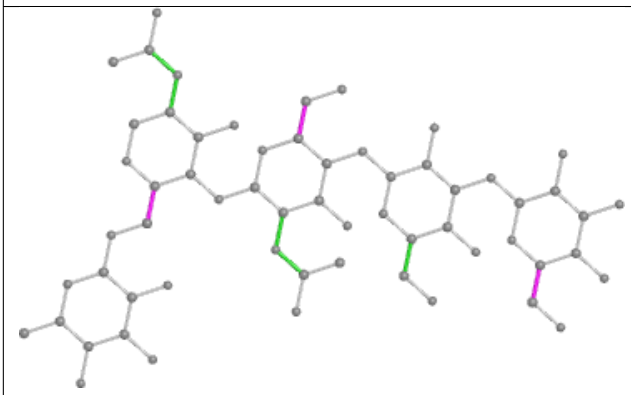
Oligosaccharide Chain D



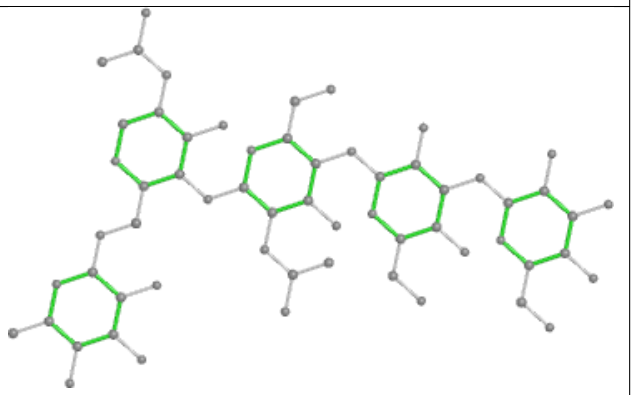
Bond lengths



Bond angles

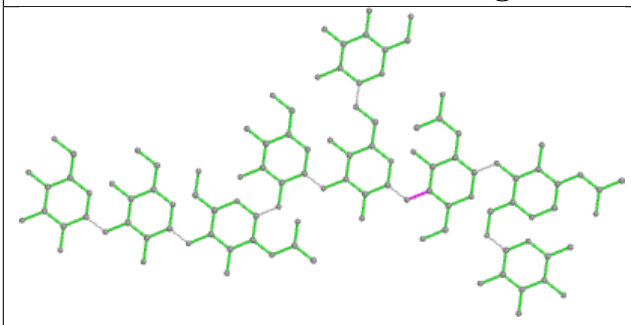


Torsions

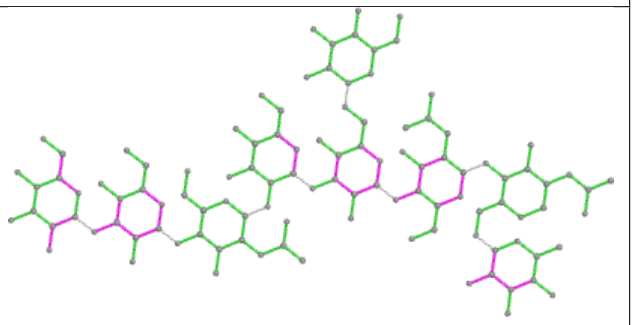


Rings

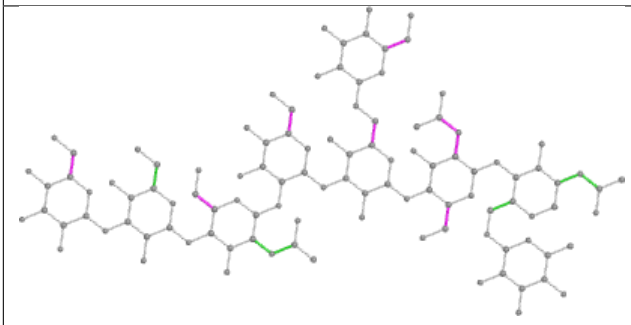
Oligosaccharide Chain G



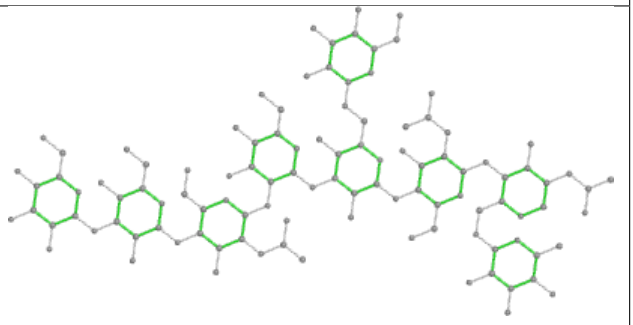
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PEG	B	406	-	6,6,6	0.55	0	5,5,5	0.28	0
6	PEG	H	410	-	6,6,6	0.44	0	5,5,5	0.34	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	PEG	B	406	-	-	3/4/4/4	-
6	PEG	H	410	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	406	PEG	O1-C1-C2-O2
6	H	410	PEG	O2-C3-C4-O4
6	B	406	PEG	O2-C3-C4-O4
6	H	410	PEG	O1-C1-C2-O2
6	B	406	PEG	C4-C3-O2-C2
6	H	410	PEG	C1-C2-O2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	B	217/219 (99%)	0.16	6 (2%) 53 60	25, 45, 68, 75	0
1	E	216/219 (98%)	1.38	54 (25%) 0 1	36, 70, 134, 182	0
1	H	217/219 (99%)	0.14	5 (2%) 60 67	17, 33, 58, 105	0
2	C	219/219 (100%)	0.22	4 (1%) 68 75	30, 48, 71, 85	0
2	F	219/219 (100%)	0.15	8 (3%) 41 48	26, 39, 60, 79	0
2	L	219/219 (100%)	-0.00	3 (1%) 75 80	14, 37, 58, 78	0
All	All	1307/1314 (99%)	0.34	80 (6%) 21 27	14, 43, 89, 182	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	30	THR	10.8
1	E	29	LEU	7.7
1	E	32	TYR	7.2
1	E	71	LYS	5.9
1	E	51	ILE	5.8
1	H	131	GLN	5.6
1	H	129	ALA	5.1
1	E	65	SER	5.0
1	E	73	ASN	4.9
1	E	31	THR	4.8
1	E	61	ALA	4.6
1	E	33	GLY	4.4
1	E	72	ASP	4.4
1	E	28	SER	4.3
2	F	214	CYS	4.1
1	H	128	SER	3.9
1	H	132	THR	3.9
2	C	214	CYS	3.8
1	E	75	LYS	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	79	PHE	3.7
1	E	56	SER	3.6
1	E	54	GLY	3.5
1	E	100(B)	PHE	3.5
1	E	36	TRP	3.4
1	E	93	ALA	3.4
1	E	23	THR	3.3
1	E	26	GLY	3.2
1	E	69	ILE	3.2
1	E	37	VAL	3.2
1	E	78	VAL	3.2
2	F	210	ASN	3.2
1	E	131	GLN	3.1
1	E	102	TYR	3.1
1	B	43	LYS	3.0
2	C	212	ASN	2.9
2	L	203	SER	2.9
1	E	9	PRO	2.9
1	E	24	VAL	2.9
1	E	53	SER	2.8
1	E	15	SER	2.8
1	E	20	ILE	2.8
2	L	214	CYS	2.8
1	E	81	LYS	2.8
1	E	19	SER	2.8
2	F	169	LYS	2.8
1	E	80	PHE	2.7
1	E	82	MET	2.7
1	E	48	LEU	2.7
1	E	84	ALA	2.6
2	F	212	ASN	2.6
1	E	184	PRO	2.6
1	E	64	ILE	2.6
1	E	45	LEU	2.5
1	B	100(A)	TRP	2.5
2	F	42	GLN	2.5
1	B	105	GLN	2.5
2	C	77	ARG	2.4
1	E	67	LEU	2.4
1	E	90	TYR	2.4
1	B	190	SER	2.4
1	E	25	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	74	SER	2.3
1	E	49	GLY	2.3
1	E	82(C)	LEU	2.3
1	H	130	ALA	2.3
2	F	2	ILE	2.3
1	B	42	GLY	2.2
1	E	66	ARG	2.2
1	E	214	ASP	2.2
2	F	3	LEU	2.2
2	L	212	ASN	2.2
1	E	21	THR	2.2
1	B	192	THR	2.2
1	E	127	GLY	2.1
1	E	140	CYS	2.1
2	F	163	TRP	2.1
1	E	43	LYS	2.1
1	E	4	LEU	2.0
1	E	50	VAL	2.0
2	C	157	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
1	PCA	B	1	8/9	0.75	0.39	58,69,74,78	0
1	PCA	H	1	8/9	0.95	0.18	47,50,52,54	0

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, 95^{th} 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
3	MAN	A	4	11/12	0.41	0.56	108,119,121,122	0
3	NAG	A	2	14/15	0.49	0.34	85,91,98,101	0

Continued on next page...

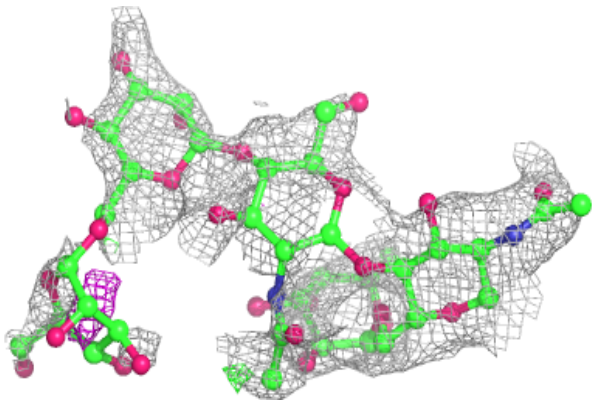
Continued from previous page...

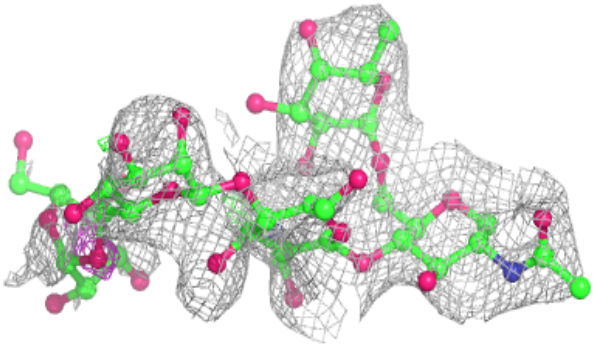
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GLA	G	7	11/12	0.52	0.51	86,92,93,94	0
5	FUC	G	9	10/11	0.54	0.37	79,85,91,91	0
4	NAG	D	2	14/15	0.62	0.38	104,110,114,115	0
5	MAN	G	4	11/12	0.62	0.39	97,105,108,111	0
4	MAN	D	4	11/12	0.63	0.42	77,92,99,101	0
5	BMA	G	3	11/12	0.64	0.33	84,93,98,100	0
5	GAL	G	6	11/12	0.66	0.47	89,100,103,105	0
4	FUC	D	5	10/11	0.67	0.39	95,104,107,109	0
4	NAG	D	1	14/15	0.68	0.30	59,71,101,105	0
3	BMA	A	3	11/12	0.72	0.37	92,99,108,115	0
5	NAG	G	5	14/15	0.75	0.37	104,107,109,113	0
3	FUC	A	5	10/11	0.75	0.35	90,93,96,97	0
4	BMA	D	3	11/12	0.78	0.45	97,105,109,109	0
5	NAG	G	2	14/15	0.78	0.23	60,64,70,80	0
5	MAN	G	8	11/12	0.79	0.43	92,97,99,100	0
3	NAG	A	1	14/15	0.85	0.18	56,69,80,84	0
5	NAG	G	1	14/15	0.88	0.27	41,50,62,74	0

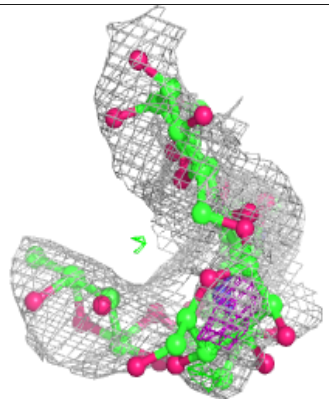
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain A:

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

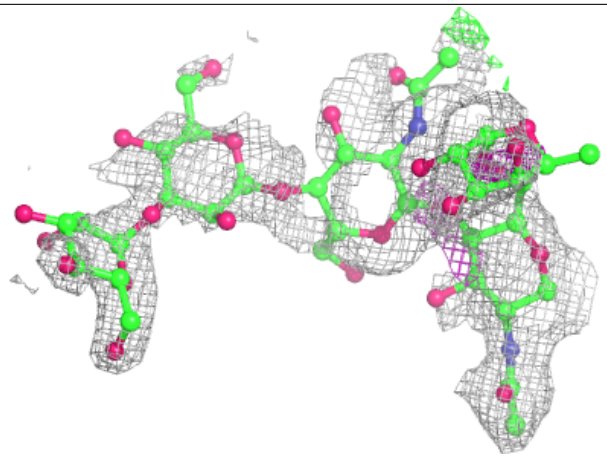


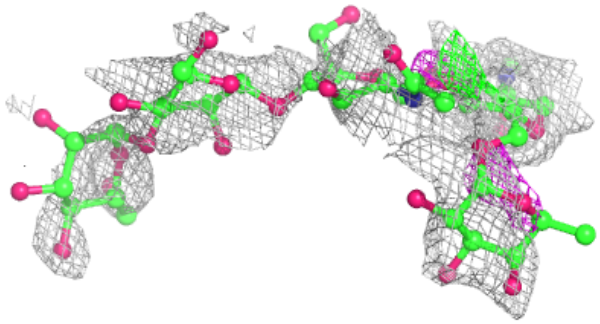


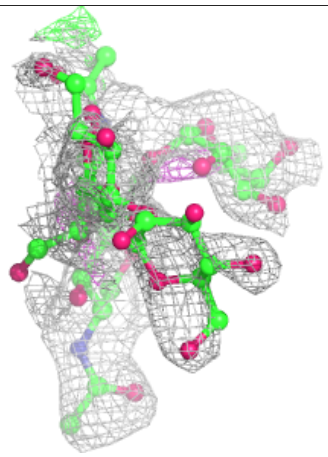


Electron density around Chain D:

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

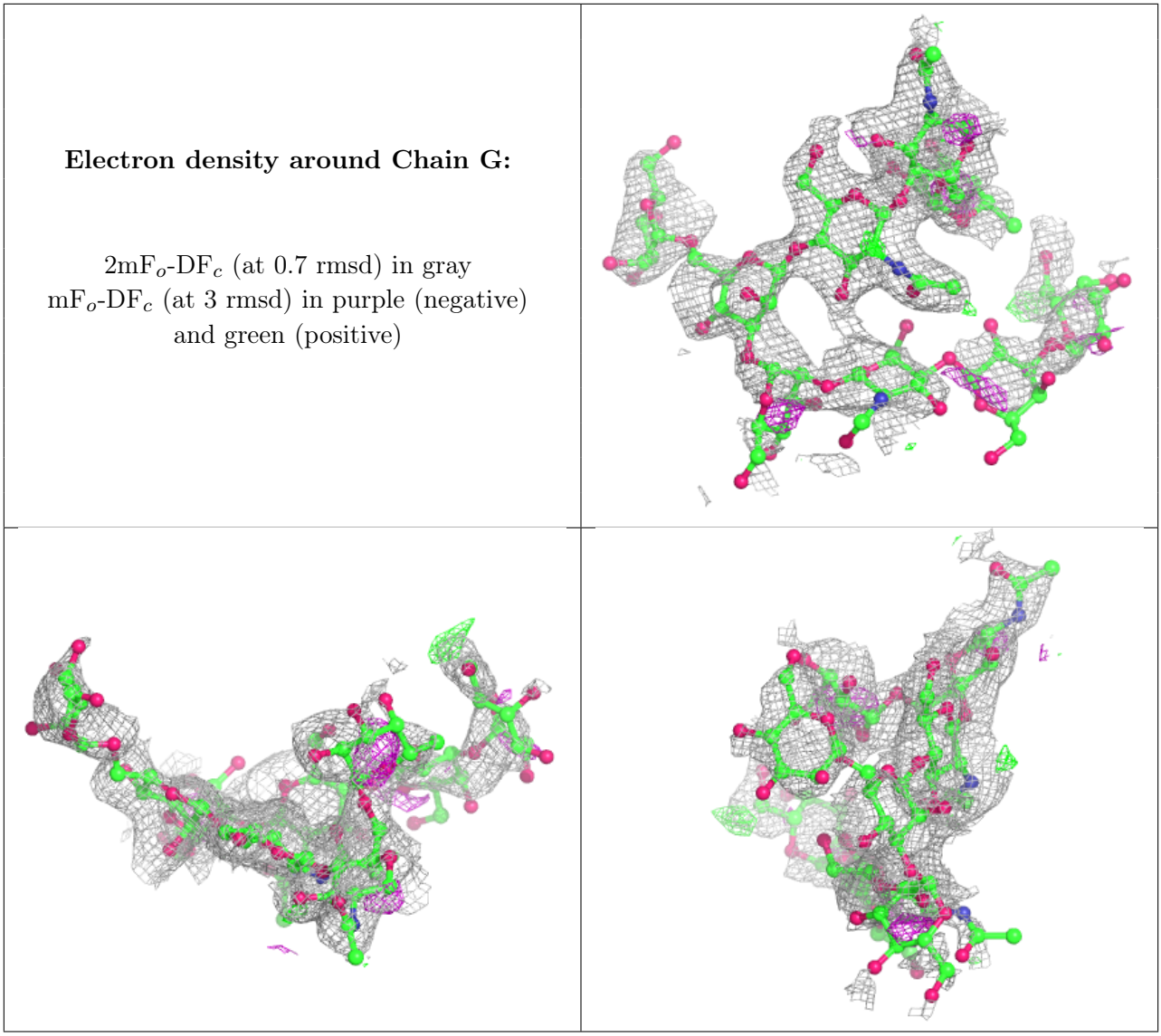






Electron density around Chain G:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	PEG	B	406	7/7	0.84	0.14	44,46,48,48	0
6	PEG	H	410	7/7	0.86	0.14	54,56,59,61	0
7	K	L	301	1/1	0.97	0.05	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.