Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2020 – 10:11 PM BST

PDB ID	:	6MI2
Title	:	Structure of the human 4-1BB / Utomilumab Fab complex
Authors	:	Kimberlin, C.R.; Chin, S.M.; Roe-Zurz, Z.; Xu, A.; Yang, Y.
Deposited on	:	2018-09-19
Resolution	:	2.72 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

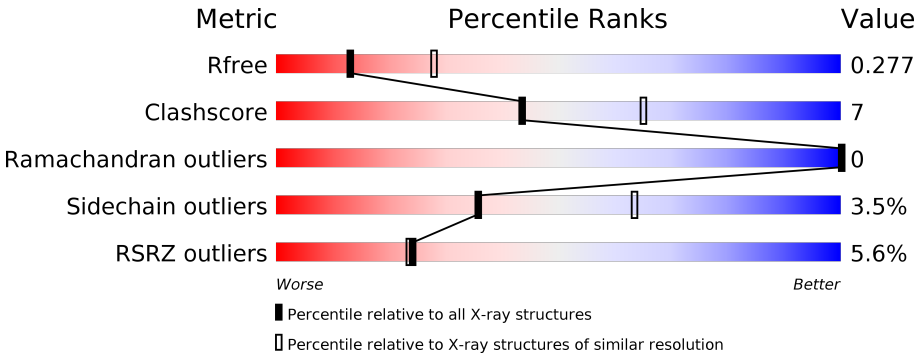
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	230	8% 79% 12% 9%
1	D	230	6% 76% 15% 9%
2	B	214	4% 83% 15%
2	E	214	7% 83% 14%
3	C	145	% 84% 14%
3	F	145	% 65% 26% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	G	2	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8119 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 Utomilumab Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1488	955	244	282	7			
1	D	210	Total	C	N	O	S	0	0	0
			1498	955	244	292	7			

- Molecule 2 is a protein called Utomilumab Fab lambda chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1478	933	244	296	5			
2	E	210	Total	C	N	O	S	0	0	0
			1475	925	246	299	5			

- Molecule 3 is a protein called Tumor necrosis factor receptor superfamily member 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	133	Total	C	N	O	S	0	0	0
			916	538	166	190	22			
3	C	143	Total	C	N	O	S	0	0	0
			1026	611	183	210	22			

There are 14 discrepancies between the modelled and reference sequences:

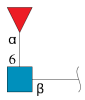
Chain	Residue	Modelled	Actual	Comment	Reference
F	163	GLU	-	expression tag	UNP Q07011
F	164	ASN	-	expression tag	UNP Q07011
F	165	LEU	-	expression tag	UNP Q07011
F	166	TYR	-	expression tag	UNP Q07011
F	167	PHE	-	expression tag	UNP Q07011
F	168	GLN	-	expression tag	UNP Q07011
F	169	GLY	-	expression tag	UNP Q07011
C	163	GLU	-	expression tag	UNP Q07011

Continued on next page...

Continued from previous page...

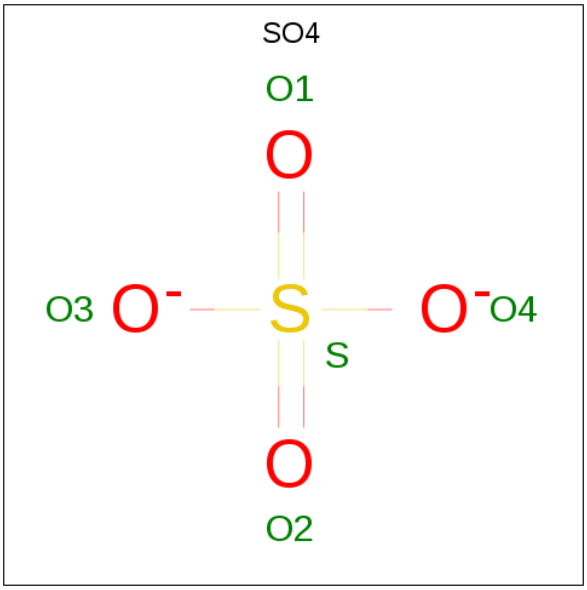
Chain	Residue	Modelled	Actual	Comment	Reference
C	164	ASN	-	expression tag	UNP Q07011
C	165	LEU	-	expression tag	UNP Q07011
C	166	TYR	-	expression tag	UNP Q07011
C	167	PHE	-	expression tag	UNP Q07011
C	168	GLN	-	expression tag	UNP Q07011
C	169	GLY	-	expression tag	UNP Q07011

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	2	Total C N O 24 14 1 9	0	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



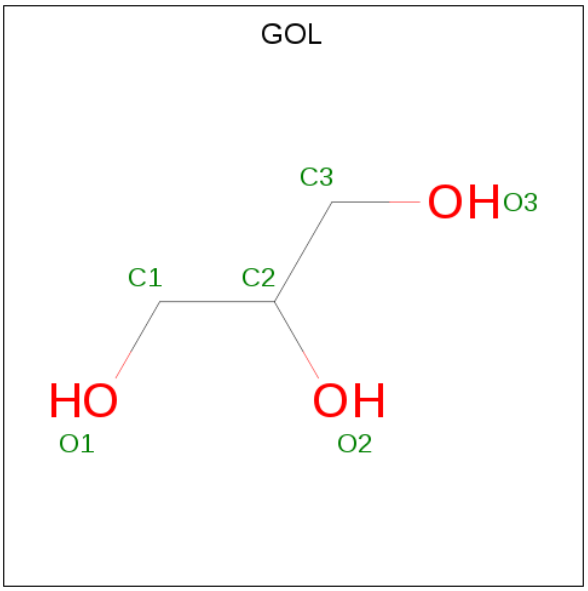
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

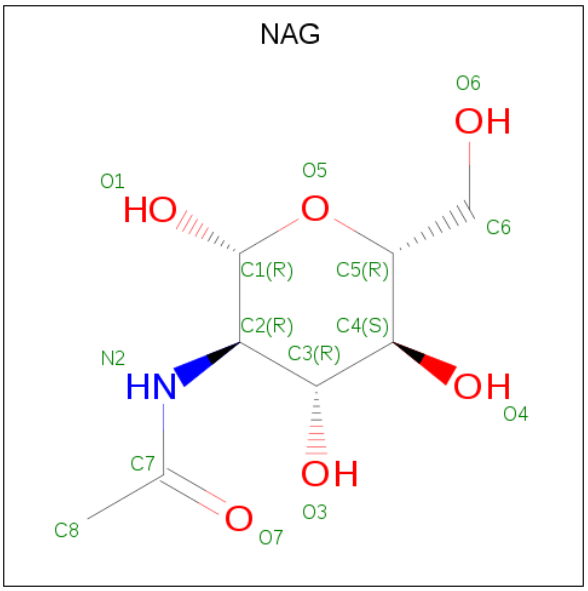
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0

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



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

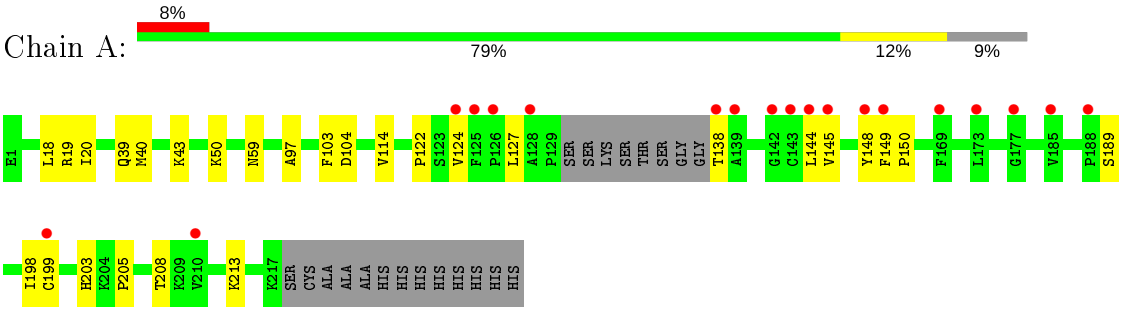
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	6	Total O 6 6	0	0
8	B	12	Total O 12 12	0	0
8	D	3	Total O 3 3	0	0
8	E	9	Total O 9 9	0	0
8	F	9	Total O 9 9	0	0
8	C	7	Total O 7 7	0	0

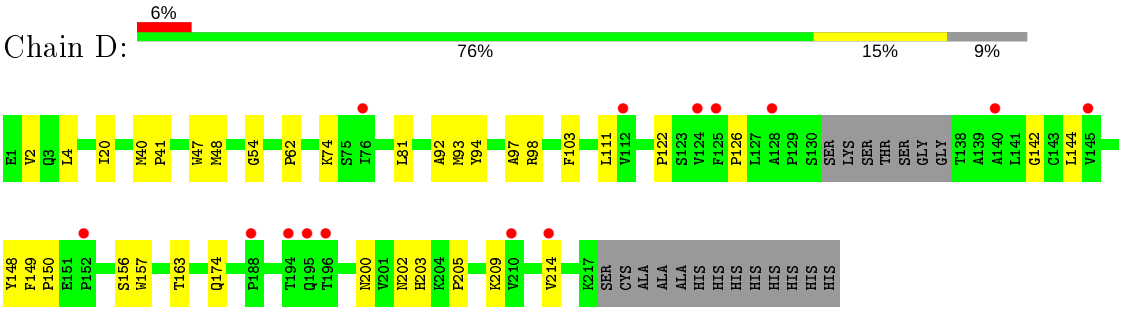
3 Residue-property plots (i)

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.

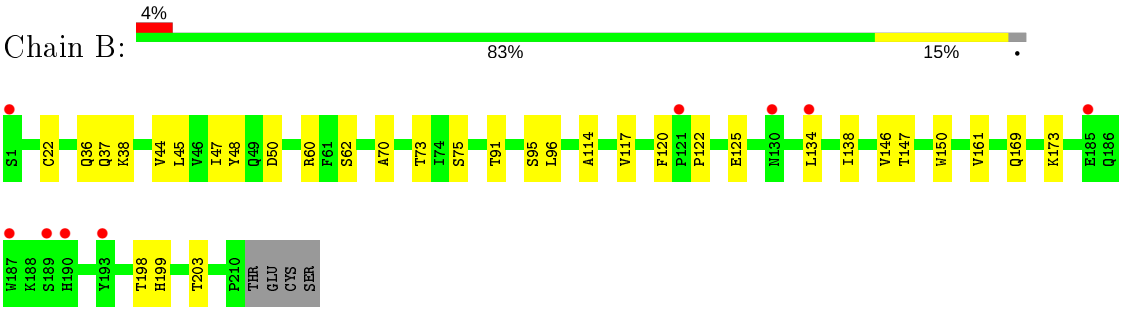
- Molecule 1: Utomilumab Fab heavy chain



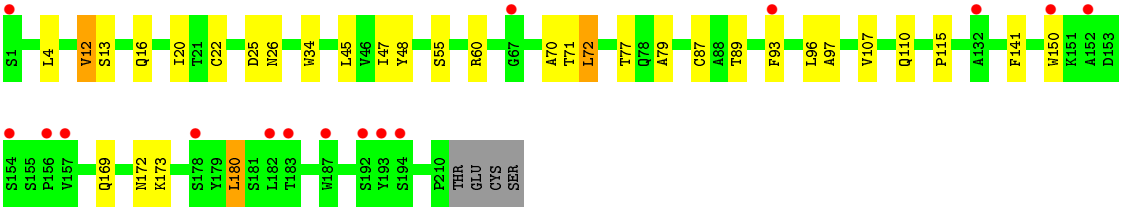
- Molecule 1: Utomilumab Fab heavy chain



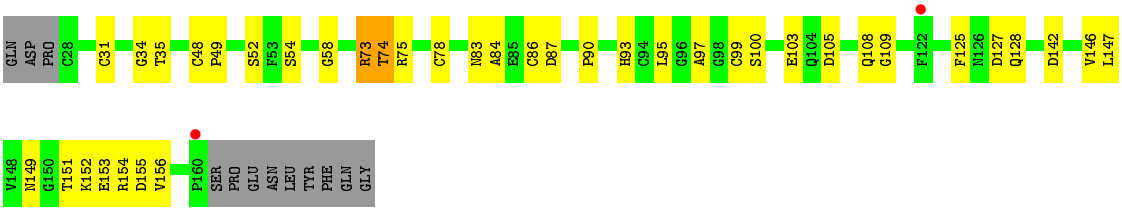
- Molecule 2: Utomilumab Fab lambda chain



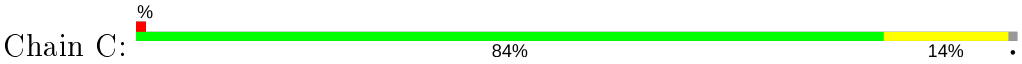
- Molecule 2: Utomilumab Fab lambda chain

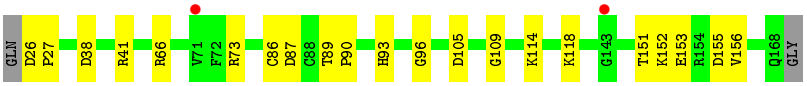


• Molecule 3: Tumor necrosis factor receptor superfamily member 9



• Molecule 3: Tumor necrosis factor receptor superfamily member 9





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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	136.90Å 73.34Å 175.12Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	49.30 – 2.72 49.30 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.30-2.72) 82.6 (49.30-2.72)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.45 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.238 , 0.278 0.239 , 0.277	Depositor DCC
R_{free} test set	2000 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 68.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8119	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: FUC, GOL, SO4, 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	0.25	0/1531	0.45	0/2100
1	D	0.24	0/1541	0.45	0/2117
2	B	0.25	0/1518	0.47	0/2094
2	E	0.25	0/1515	0.47	0/2088
3	C	0.25	0/1045	0.46	0/1414
3	F	0.25	0/931	0.45	0/1262
All	All	0.25	0/8081	0.46	0/11075

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1488	0	1312	21	0
1	D	1498	0	1318	17	0
2	B	1478	0	1305	19	0
2	E	1475	0	1281	19	0
3	C	1026	0	882	11	0
3	F	916	0	757	20	0
4	G	24	0	22	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	15	0	0	0	0
5	B	25	0	0	1	0
5	C	30	0	0	0	0
5	D	10	0	0	0	0
5	E	10	0	0	0	0
5	F	10	0	0	0	0
6	A	6	0	8	0	0
6	B	18	0	24	1	0
6	C	18	0	24	0	0
6	E	12	0	16	1	0
7	C	14	0	13	0	0
8	A	6	0	0	0	0
8	B	12	0	0	0	0
8	C	7	0	0	0	0
8	D	3	0	0	0	0
8	E	9	0	0	1	0
8	F	9	0	0	1	0
All	All	8119	0	6962	100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (100) 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:B:36:GLN:HE22	6:B:308:GOL:H12	1.54	0.72
3:F:149:ASN:HB2	4:G:1:NAG:N2	2.05	0.70
3:F:75:ARG:H	3:F:86:CYS:HA	1.56	0.69
1:A:59:ASN:ND2	2:B:95:SER:O	2.27	0.67
2:E:4:LEU:HD11	2:E:89:THR:HG22	1.77	0.65
1:A:124:VAL:HG22	1:A:145:VAL:HG12	1.80	0.63
3:C:73:ARG:NH2	3:C:87:ASP:OD2	2.30	0.62
1:A:122:PRO:HB3	1:A:148:TYR:HB3	1.83	0.60
3:C:66:ARG:NE	3:C:86:CYS:SG	2.74	0.60
2:E:60:ARG:NH1	8:E:401:HOH:O	2.35	0.60
1:A:138:THR:N	1:A:189:SER:HG	1.99	0.58
3:F:48:CYS:SG	3:F:54:SER:OG	2.61	0.58
4:G:1:NAG:H3	4:G:1:NAG:H83	1.85	0.58
2:E:12:VAL:HG22	2:E:16:GLN:HG3	1.84	0.58
3:F:78:CYS:HB3	3:F:84:ALA:HB2	1.86	0.57
2:B:147:THR:HG1	2:B:198:THR:HG1	1.51	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:LEU:HD11	1:A:20:ILE:HG23	1.88	0.55
2:E:22:CYS:N	2:E:70:ALA:O	2.39	0.55
1:A:203:HIS:HB3	1:A:208:THR:HB	1.89	0.54
2:B:45:LEU:HD21	2:B:48:TYR:HB3	1.89	0.54
1:A:122:PRO:HD3	1:A:203:HIS:CD2	2.44	0.53
2:E:12:VAL:HG11	2:E:77:THR:HG21	1.90	0.53
3:F:151:THR:HG22	3:F:154:ARG:HG2	1.89	0.53
2:E:45:LEU:HD21	2:E:48:TYR:HB3	1.89	0.53
1:D:62:PRO:HD3	2:E:96:LEU:HD11	1.91	0.53
1:A:127:LEU:HD21	1:A:144:LEU:HB2	1.91	0.52
3:F:151:THR:HG23	3:F:153:GLU:H	1.75	0.52
2:E:79:ALA:HA	2:E:107:VAL:HG21	1.92	0.51
3:F:125:PHE:CZ	3:F:155:ASP:HB2	2.45	0.51
1:A:50:LYS:HZ3	1:A:59:ASN:HD22	1.59	0.51
2:B:22:CYS:N	2:B:70:ALA:O	2.42	0.51
1:D:20:ILE:HD11	1:D:81:LEU:HD23	1.91	0.51
1:A:39:GLN:HE22	2:B:37:GLN:HE22	1.59	0.51
3:F:128:GLN:NE2	8:F:302:HOH:O	2.39	0.50
1:A:198:ILE:HA	1:A:213:LYS:HA	1.94	0.49
1:A:97:ALA:HB1	1:A:103:PHE:HB3	1.94	0.49
1:D:142:GLY:HA2	1:D:157:TRP:CZ2	2.47	0.49
2:E:34:TRP:CE3	2:E:72:LEU:HD22	2.48	0.49
3:F:34:GLY:H	3:F:54:SER:HB2	1.77	0.49
3:F:83:ASN:OD1	3:F:84:ALA:N	2.44	0.48
1:D:142:GLY:HA2	1:D:157:TRP:HZ2	1.79	0.48
3:C:38:ASP:HB3	3:C:41:ARG:HD2	1.95	0.48
1:D:156:SER:OG	1:D:200:ASN:HB2	2.14	0.48
3:F:108:GLN:NE2	3:F:127:ASP:O	2.47	0.48
3:C:26:ASP:HB3	3:C:27:PRO:HD3	1.96	0.47
2:E:110:GLN:NE2	2:E:172:ASN:O	2.45	0.47
2:B:169:GLN:HE21	2:B:173:LYS:HB2	1.79	0.47
1:D:54:GLY:O	1:D:74:LYS:NZ	2.37	0.47
1:D:97:ALA:HB1	1:D:103:PHE:HB3	1.96	0.47
1:D:41:PRO:HD3	1:D:92:ALA:HA	1.96	0.47
2:E:150:TRP:CE3	2:E:180:LEU:HD12	2.50	0.46
2:E:34:TRP:CZ3	2:E:87:CYS:HB3	2.50	0.46
3:C:93:HIS:ND1	3:C:105:ASP:OD1	2.40	0.46
1:D:93:MET:HG3	1:D:111:LEU:HA	1.97	0.46
2:B:122:PRO:HD3	2:B:134:LEU:HD23	1.97	0.46
1:D:4:LEU:HD11	1:D:98:ARG:HB2	1.98	0.46
1:D:203:HIS:CD2	1:D:205:PRO:HD2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:115:PRO:HB3	2:E:141:PHE:HB3	1.97	0.46
1:A:127:LEU:HB3	2:B:120:PHE:CD1	2.51	0.46
3:F:97:ALA:O	3:F:100:SER:OG	2.34	0.45
2:B:125:GLU:N	2:B:125:GLU:OE2	2.38	0.45
1:A:39:GLN:HE22	2:B:37:GLN:NE2	2.14	0.45
2:B:50:ASP:OD2	3:C:114:LYS:NZ	2.43	0.45
2:E:169:GLN:HG2	2:E:173:LYS:O	2.17	0.45
2:B:150:TRP:CD1	2:B:161:VAL:HG21	2.52	0.45
1:D:48:MET:HE1	1:D:94:TYR:HD1	1.81	0.45
2:E:34:TRP:HB2	2:E:47:ILE:HB	1.98	0.45
1:A:149:PHE:HA	1:A:150:PRO:HA	1.81	0.45
3:F:87:ASP:HA	3:F:99:CYS:SG	2.58	0.44
1:D:126:PRO:HB3	1:D:214:VAL:HG22	2.00	0.44
3:F:109:GLY:HA2	3:F:152:LYS:O	2.17	0.44
3:C:155:ASP:OD1	3:C:156:VAL:N	2.49	0.43
3:F:146:VAL:HG23	3:F:156:VAL:HG13	2.00	0.43
3:F:73:ARG:NH1	3:F:90:PRO:HD3	2.34	0.43
2:B:60:ARG:HB2	2:B:75:SER:O	2.19	0.43
2:E:13:SER:O	2:E:16:GLN:HG2	2.18	0.43
2:B:114:ALA:N	5:B:304:SO4:O3	2.49	0.43
1:D:149:PHE:HA	1:D:150:PRO:HA	1.77	0.43
1:D:202:ASN:HA	1:D:209:LYS:HA	2.01	0.43
3:F:31:CYS:O	3:F:58:GLY:N	2.51	0.43
1:D:122:PRO:HB3	1:D:148:TYR:HB3	2.00	0.43
2:E:55:SER:HB2	6:E:304:GOL:H12	2.00	0.43
3:C:151:THR:HG23	3:C:153:GLU:H	1.82	0.43
2:E:20:ILE:HB	2:E:72:LEU:HD23	2.01	0.43
1:D:47:TRP:CG	2:E:97:ALA:HB3	2.53	0.42
2:B:117:VAL:HG22	2:B:138:ILE:HG23	2.01	0.42
2:B:62:SER:HB3	2:B:73:THR:HB	2.00	0.42
1:A:203:HIS:CE1	1:A:205:PRO:HD2	2.55	0.42
1:A:40:MET:HB2	1:A:43:LYS:HB2	2.02	0.42
2:B:146:VAL:HG12	2:B:199:HIS:HB2	2.01	0.42
3:F:74:THR:HA	3:F:86:CYS:SG	2.60	0.42
3:F:49:PRO:O	3:F:52:SER:OG	2.32	0.41
1:A:50:LYS:NZ	1:A:59:ASN:HD22	2.17	0.41
3:C:109:GLY:HA2	3:C:152:LYS:O	2.20	0.41
2:B:36:GLN:NE2	2:B:38:LYS:HE3	2.36	0.41
1:A:18:LEU:HD22	1:A:19:ARG:H	1.85	0.41
3:C:89:THR:HB	3:C:90:PRO:HD2	2.02	0.40
1:A:104:ASP:HB2	3:C:96:GLY:HA2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:93:HIS:NE2	3:F:103:GLU:HB3	2.36	0.40
1:A:203:HIS:N	1:A:208:THR:O	2.48	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	205/230 (89%)	193 (94%)	12 (6%)	0	100	100
1	D	206/230 (90%)	195 (95%)	11 (5%)	0	100	100
2	B	208/214 (97%)	196 (94%)	12 (6%)	0	100	100
2	E	208/214 (97%)	201 (97%)	7 (3%)	0	100	100
3	C	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
3	F	131/145 (90%)	126 (96%)	5 (4%)	0	100	100
All	All	1099/1178 (93%)	1050 (96%)	49 (4%)	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	A	138/194 (71%)	136 (99%)	2 (1%)	67	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	144/194 (74%)	139 (96%)	5 (4%)	36 63
2	B	141/179 (79%)	136 (96%)	5 (4%)	36 63
2	E	139/179 (78%)	132 (95%)	7 (5%)	24 49
3	C	113/126 (90%)	112 (99%)	1 (1%)	78 91
3	F	98/126 (78%)	91 (93%)	7 (7%)	14 33
All	All	773/998 (78%)	746 (96%)	27 (4%)	36 63

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	VAL
1	A	199	CYS
2	B	44	VAL
2	B	47	ILE
2	B	91	THR
2	B	96	LEU
2	B	203	THR
1	D	2	VAL
1	D	40	MET
1	D	144	LEU
1	D	163	THR
1	D	174	GLN
2	E	12	VAL
2	E	25	ASP
2	E	26	ASN
2	E	71	THR
2	E	72	LEU
2	E	93	PHE
2	E	180	LEU
3	F	35	THR
3	F	73	ARG
3	F	74	THR
3	F	95	LEU
3	F	105	ASP
3	F	142	ASP
3	F	147	LEU
3	C	118	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	203	HIS
2	B	36	GLN
2	B	37	GLN
2	B	49	GLN
2	B	169	GLN
1	D	3	GLN
1	D	59	ASN
2	E	26	ASN
2	E	41	GLN
2	E	78	GLN
3	F	104	GLN
3	F	128	GLN
3	C	128	GLN
3	C	168	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

2 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	3,4	14,14,15	1.06	2 (14%)	17,19,21	1.41	3 (17%)
4	FUC	G	2	4	10,10,11	0.96	0	14,14,16	1.13	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
4	NAG	G	1	3,4	-	5/6/23/26	0/1/1/1
4	FUC	G	2	4	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	1	NAG	C1-C2	3.22	1.57	1.52
4	G	1	NAG	O5-C1	2.04	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1	NAG	C2-N2-C7	4.27	128.99	122.90
4	G	1	NAG	C1-C2-N2	2.52	114.79	110.49
4	G	1	NAG	C1-O5-C5	2.48	115.56	112.19
4	G	2	FUC	C1-O5-C5	2.23	117.83	112.78
4	G	2	FUC	O5-C5-C4	2.01	113.13	109.52

There are no chirality outliers.

All (5) torsion outliers are listed below:

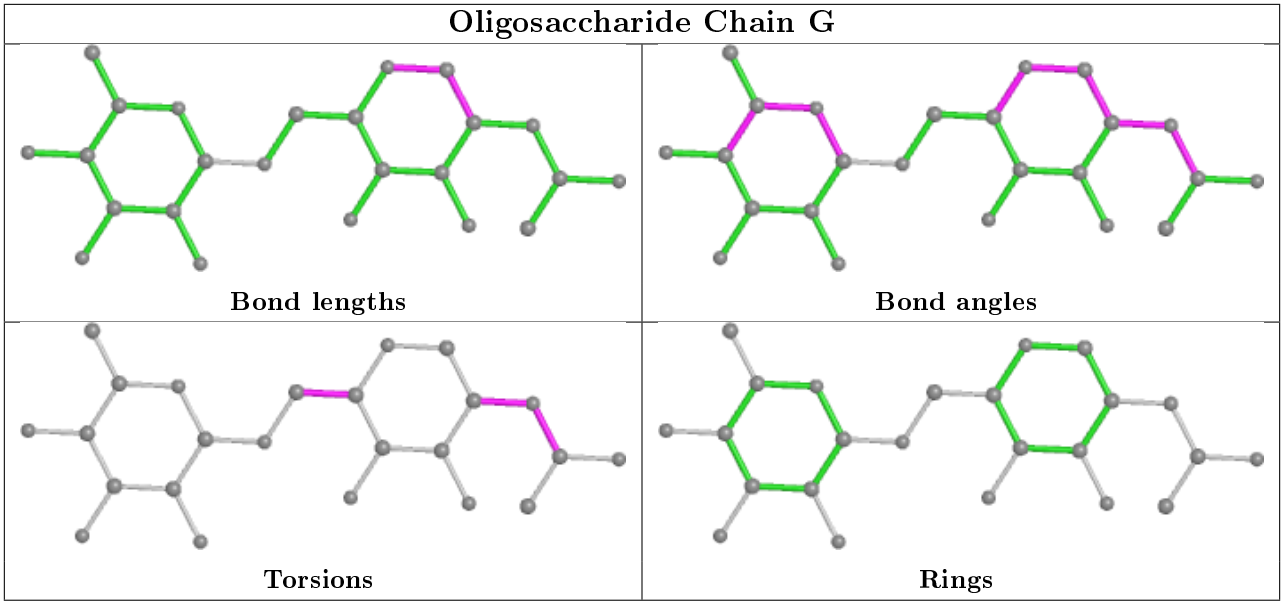
Mol	Chain	Res	Type	Atoms
4	G	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	NAG	2	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)

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	C	205	-	4,4,4	0.14	0	6,6,6	0.05	0
6	GOL	C	209	-	5,5,5	0.90	0	5,5,5	1.00	0
6	GOL	E	303	-	5,5,5	0.91	0	5,5,5	0.99	0
5	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	C	204	-	4,4,4	0.14	0	6,6,6	0.05	0
6	GOL	B	307	-	5,5,5	0.90	0	5,5,5	1.02	0
5	SO4	C	207	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	E	301	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	303	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	304	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	C	206	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	E	302	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	C	202	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	F	203	-	4,4,4	0.13	0	6,6,6	0.04	0
7	NAG	C	201	3	14,14,15	0.35	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	B	306	-	5,5,5	0.89	0	5,5,5	1.03	0
5	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.06	0
6	GOL	B	308	-	5,5,5	0.91	0	5,5,5	0.97	0
6	GOL	A	304	-	5,5,5	0.91	0	5,5,5	0.99	0
5	SO4	B	305	-	4,4,4	0.13	0	6,6,6	0.05	0
5	SO4	D	302	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	D	301	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	C	203	-	4,4,4	0.14	0	6,6,6	0.06	0
6	GOL	C	208	-	5,5,5	0.89	0	5,5,5	1.04	0
5	SO4	B	303	-	4,4,4	0.14	0	6,6,6	0.05	0
6	GOL	C	210	-	5,5,5	0.90	0	5,5,5	1.04	0
6	GOL	E	304	-	5,5,5	0.89	0	5,5,5	1.02	0
5	SO4	F	204	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.05	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	C	210	-	-	0/4/4/4	-
6	GOL	C	209	-	-	2/4/4/4	-
6	GOL	E	304	-	-	1/4/4/4	-
6	GOL	B	306	-	-	0/4/4/4	-
6	GOL	B	308	-	-	2/4/4/4	-
6	GOL	A	304	-	-	1/4/4/4	-
6	GOL	E	303	-	-	3/4/4/4	-
7	NAG	C	201	3	-	0/6/23/26	0/1/1/1
6	GOL	B	307	-	-	1/4/4/4	-
6	GOL	C	208	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	308	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	C	208	GOL	O1-C1-C2-C3
6	E	303	GOL	C1-C2-C3-O3
6	B	308	GOL	O1-C1-C2-O2
6	C	208	GOL	O1-C1-C2-O2
6	E	304	GOL	O1-C1-C2-O2
6	C	209	GOL	O2-C2-C3-O3
6	E	303	GOL	O1-C1-C2-O2
6	A	304	GOL	C1-C2-C3-O3
6	C	209	GOL	C1-C2-C3-O3
6	E	303	GOL	O2-C2-C3-O3
6	C	208	GOL	O2-C2-C3-O3
6	B	307	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	304	SO4	1	0
6	B	308	GOL	1	0
6	E	304	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

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	A	209/230 (90%)	0.39	19 (9%) 9 7	38, 83, 143, 163	0
1	D	210/230 (91%)	0.31	14 (6%) 17 16	46, 99, 147, 160	0
2	B	210/214 (98%)	0.22	9 (4%) 35 34	32, 69, 146, 174	0
2	E	210/214 (98%)	0.39	16 (7%) 13 12	47, 91, 149, 190	0
3	C	143/145 (98%)	0.04	2 (1%) 75 77	33, 68, 94, 118	0
3	F	133/145 (91%)	0.01	2 (1%) 73 76	62, 87, 130, 144	0
All	All	1115/1178 (94%)	0.25	62 (5%) 24 23	32, 81, 143, 190	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	139	ALA	5.2
1	D	145	VAL	4.8
2	E	193	TYR	4.8
2	B	190	HIS	4.6
2	E	187	TRP	4.2
1	A	125	PHE	4.1
2	E	178	SER	4.1
1	A	143	CYS	3.9
2	B	130	ASN	3.7
2	B	134	LEU	3.6
1	A	142	GLY	3.6
1	A	210	VAL	3.5
2	E	132	ALA	3.5
2	E	183	THR	3.5
2	E	194	SER	3.4
2	B	189	SER	3.4
1	D	188	PRO	3.2
1	D	125	PHE	3.2
2	E	192	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	F	160	PRO	3.1
1	A	177	GLY	3.1
1	D	128	ALA	3.1
2	E	157	VAL	3.0
2	E	154	SER	2.9
2	E	152	ALA	2.8
2	E	1	SER	2.8
1	A	144	LEU	2.8
2	B	185	GLU	2.7
1	A	148	TYR	2.7
1	A	173	LEU	2.7
3	F	122	PHE	2.7
2	B	187	TRP	2.7
3	C	71	VAL	2.6
2	B	121	PRO	2.6
1	A	124	VAL	2.6
1	A	145	VAL	2.6
2	E	93	PHE	2.6
1	A	188	PRO	2.5
1	A	149	PHE	2.5
1	A	199	CYS	2.5
2	E	182	LEU	2.5
2	B	1	SER	2.5
1	D	196	THR	2.4
1	D	195	GLN	2.4
2	E	150	TRP	2.4
1	D	194	THR	2.4
1	A	126	PRO	2.4
1	A	138	THR	2.3
2	E	67	GLY	2.3
1	D	152	PRO	2.3
1	A	169	PHE	2.3
1	D	210	VAL	2.3
2	E	156	PRO	2.3
1	D	124	VAL	2.2
1	D	76	ILE	2.2
3	C	143	GLY	2.2
1	D	112	VAL	2.2
1	D	140	ALA	2.1
2	B	193	TYR	2.1
1	D	214	VAL	2.1
1	A	128	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	185	VAL	2.0

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

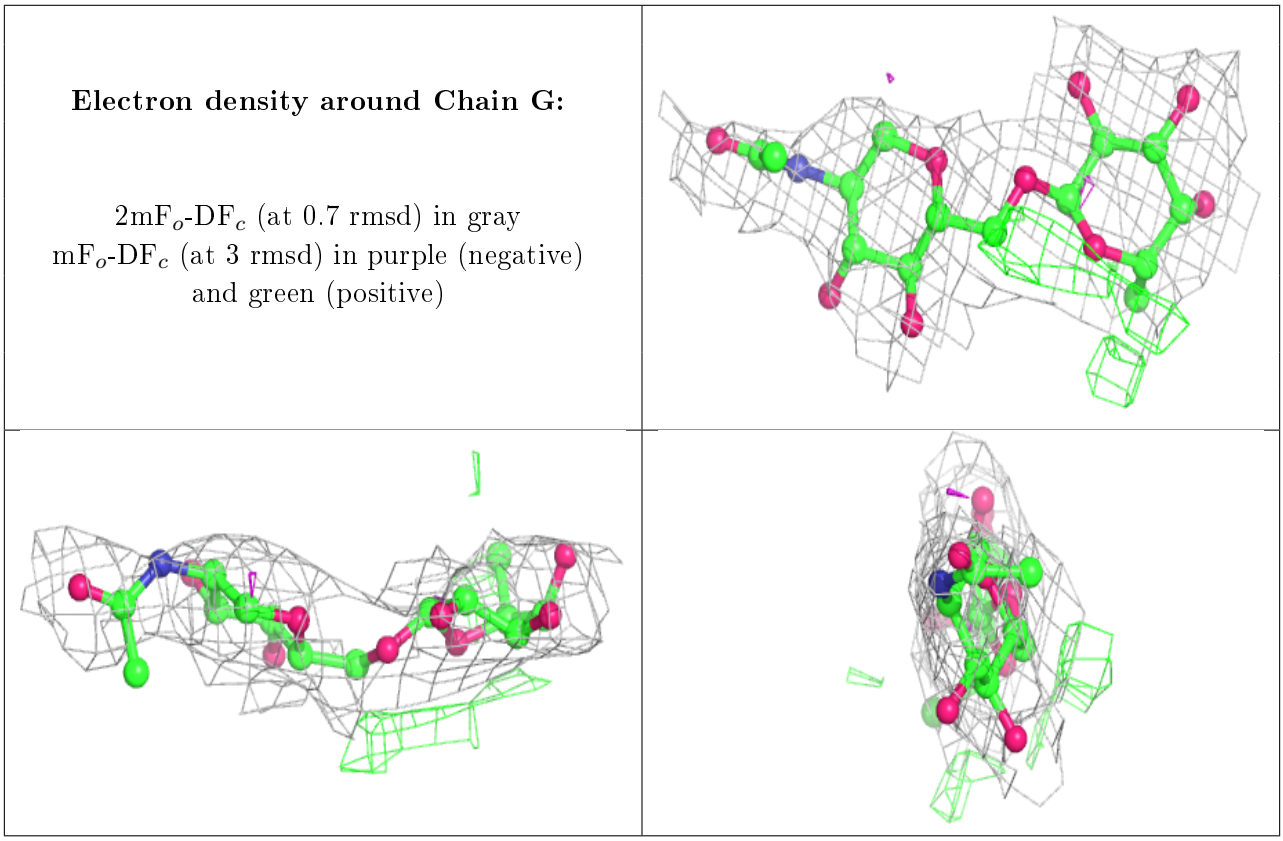
There are no non-standard protein/DNA/RNA residues in this entry.

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, 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
4	NAG	G	1	14/15	0.69	0.29	95,109,119,120	0
4	FUC	G	2	10/11	0.72	0.22	93,111,120,121	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.



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, 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
5	SO4	C	207	5/5	0.59	0.33	153,158,159,162	0
5	SO4	A	302	5/5	0.61	0.25	143,147,149,151	0
5	SO4	B	304	5/5	0.65	0.34	167,168,170,171	0
5	SO4	A	303	5/5	0.66	0.34	160,163,166,168	0
5	SO4	C	206	5/5	0.67	0.36	151,153,156,157	0
6	GOL	E	303	6/6	0.71	0.23	90,90,101,103	0
5	SO4	D	302	5/5	0.71	0.22	124,126,130,136	0
5	SO4	B	303	5/5	0.74	0.30	137,137,145,150	0
6	GOL	B	307	6/6	0.77	0.20	83,89,97,102	0
6	GOL	B	308	6/6	0.79	0.26	64,67,68,72	0
5	SO4	B	305	5/5	0.79	0.29	132,133,136,139	0
5	SO4	B	302	5/5	0.79	0.23	149,151,152,152	0
7	NAG	C	201	14/15	0.80	0.21	89,102,108,115	0
5	SO4	F	204	5/5	0.81	0.15	124,127,129,130	0
6	GOL	C	209	6/6	0.85	0.21	45,62,80,82	0
6	GOL	C	208	6/6	0.87	0.30	73,96,97,105	0
6	GOL	C	210	6/6	0.87	0.15	77,88,90,90	0
5	SO4	F	203	5/5	0.88	0.18	148,150,151,152	0
6	GOL	A	304	6/6	0.88	0.20	67,74,79,80	0
5	SO4	C	205	5/5	0.88	0.17	148,149,150,151	0
5	SO4	E	302	5/5	0.88	0.20	151,151,152,153	0
5	SO4	D	301	5/5	0.88	0.12	113,117,119,120	0
5	SO4	C	203	5/5	0.89	0.19	95,107,107,115	0
6	GOL	E	304	6/6	0.89	0.17	58,70,73,74	0
5	SO4	C	202	5/5	0.92	0.16	92,98,101,112	0
6	GOL	B	306	6/6	0.93	0.26	94,99,104,105	0
5	SO4	E	301	5/5	0.93	0.15	73,90,91,100	0
5	SO4	B	301	5/5	0.94	0.14	98,100,104,108	0
5	SO4	A	301	5/5	0.94	0.18	68,74,88,90	0
5	SO4	C	204	5/5	0.95	0.13	104,111,114,115	0

6.5 Other polymers (i)

There are no such residues in this entry.