Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 08:52 AM EDT

PDB ID	:	6XQ2
Title	:	Human antibody S8V2-37 in complex with the influenza hemagglutinin head domain of A/Texas/50/2012(H3N2)
Authors	:	McCarthy, K.R.; Harrison, S.C.
Deposited on	:	2020-07-09
Resolution	:	3.00 Å(reported)

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

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

The 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:

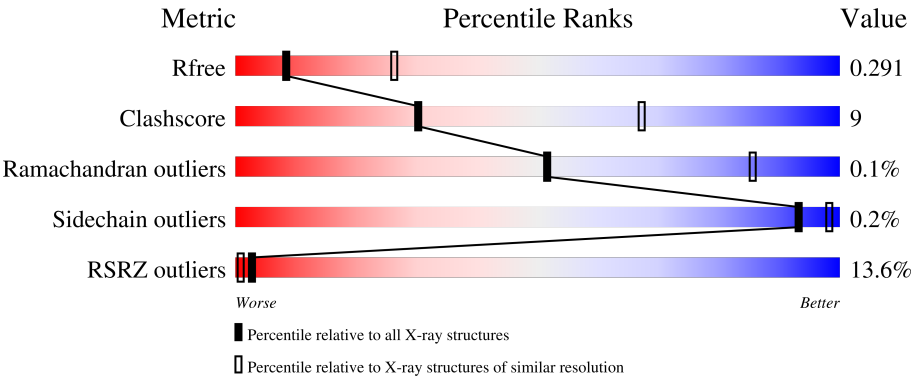
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	A	291	7% 71% 20% 9%
1	D	291	20% 73% 18% 9%
2	C	233	72% 21% 7%
2	F	233	18% 71% 22% 7%
3	B	214	10% 81% 18% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	214	21% 76% 23%
4	G	3	33% 67%
4	I	3	67% 33%
5	H	2	100%

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
4	BMA	I	3	-	-	-	X
5	NAG	H	1	-	-	-	X
5	NAG	H	2	-	-	-	X
6	NAG	D	402	-	-	-	X
6	NAG	D	403	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10890 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	A	265	Total	C	N	O	S	0	0	0
			2104	1327	374	393	10			
1	D	265	Total	C	N	O	S	0	0	0
			2104	1327	374	393	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLY	-	expression tag	UNP R4L1D1
A	321	ALA	-	expression tag	UNP R4L1D1
A	322	LEU	-	expression tag	UNP R4L1D1
A	323	GLU	-	expression tag	UNP R4L1D1
A	324	VAL	-	expression tag	UNP R4L1D1
A	325	LEU	-	expression tag	UNP R4L1D1
A	326	PHE	-	expression tag	UNP R4L1D1
A	327	GLN	-	expression tag	UNP R4L1D1
D	320	GLY	-	expression tag	UNP R4L1D1
D	321	ALA	-	expression tag	UNP R4L1D1
D	322	LEU	-	expression tag	UNP R4L1D1
D	323	GLU	-	expression tag	UNP R4L1D1
D	324	VAL	-	expression tag	UNP R4L1D1
D	325	LEU	-	expression tag	UNP R4L1D1
D	326	PHE	-	expression tag	UNP R4L1D1
D	327	GLN	-	expression tag	UNP R4L1D1

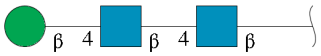
- Molecule 2 is a protein called antibody S8V2-37 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	217	Total	C	N	O	S	0	0	0
			1630	1025	276	322	7			
2	F	217	Total	C	N	O	S	0	0	0
			1630	1025	276	322	7			

- Molecule 3 is a protein called antibody S8V2-37 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	211	Total	C	N	O	S	0	0	0
			1630	1023	275	328	4			
3	E	211	Total	C	N	O	S	0	0	0
			1630	1023	275	328	4			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

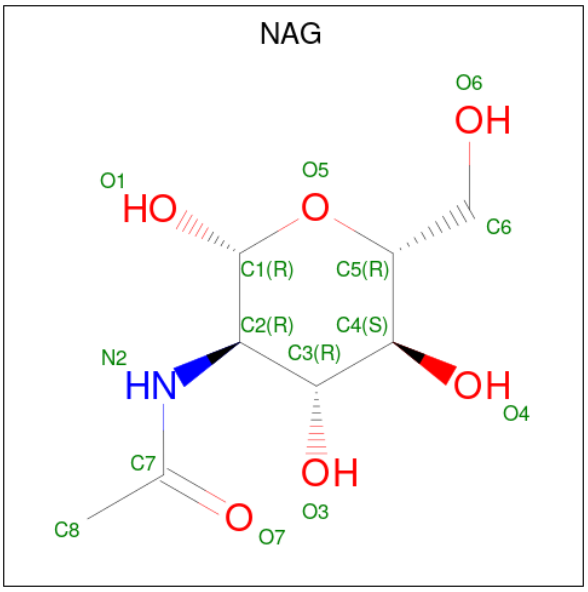


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



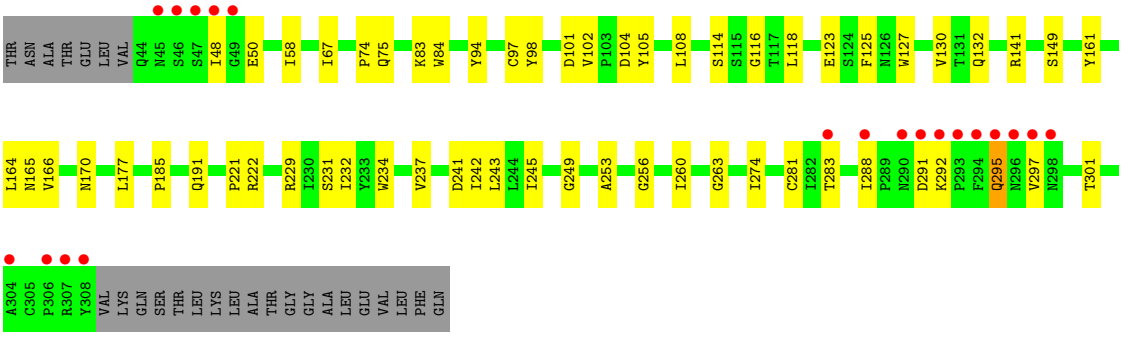
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0
6	D	1	Total C N O 14 8 1 5	0	0

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.

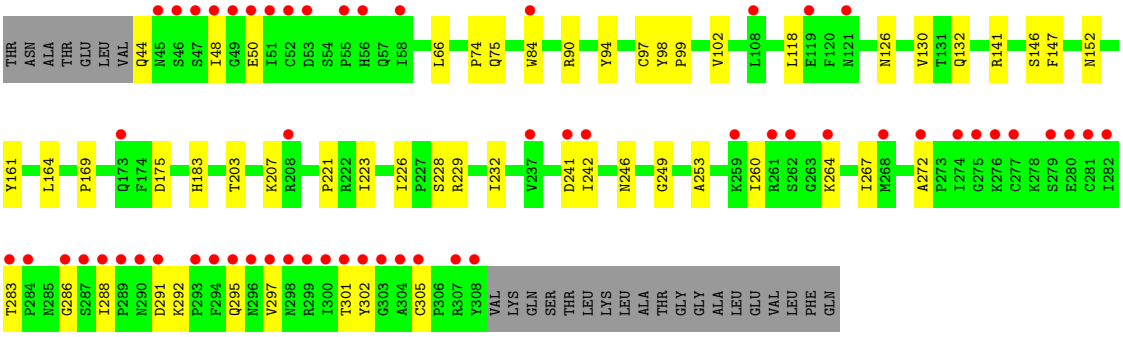
• Molecule 1: Hemagglutinin

Chain A:



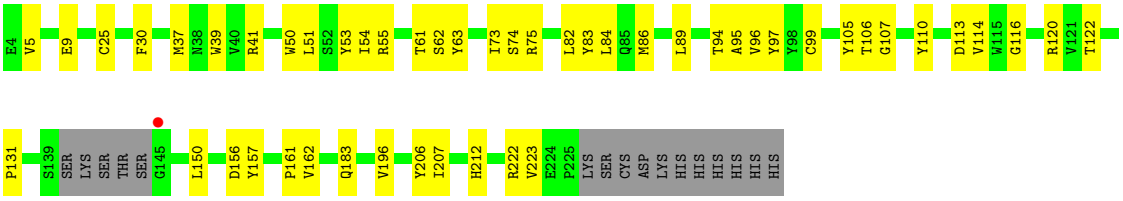
• Molecule 1: Hemagglutinin

Chain D:



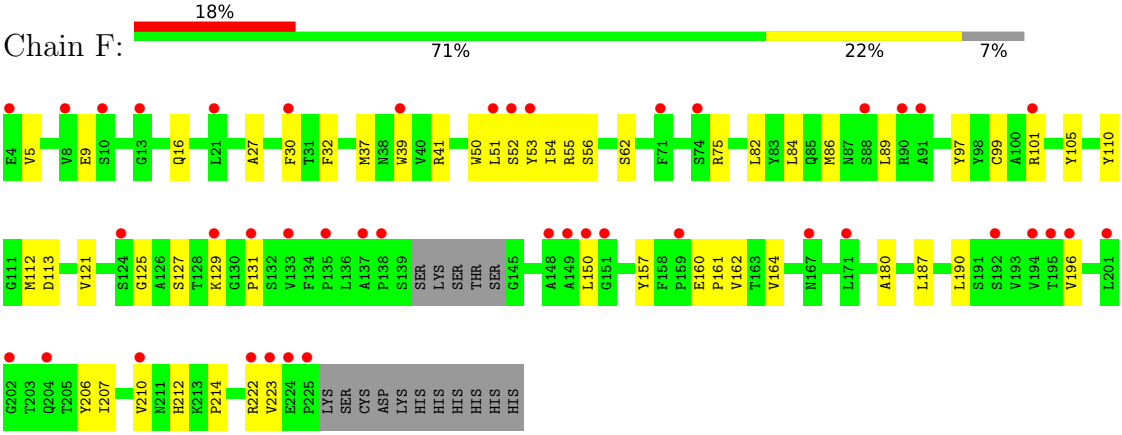
• Molecule 2: antibody S8V2-37 heavy chain

Chain C:



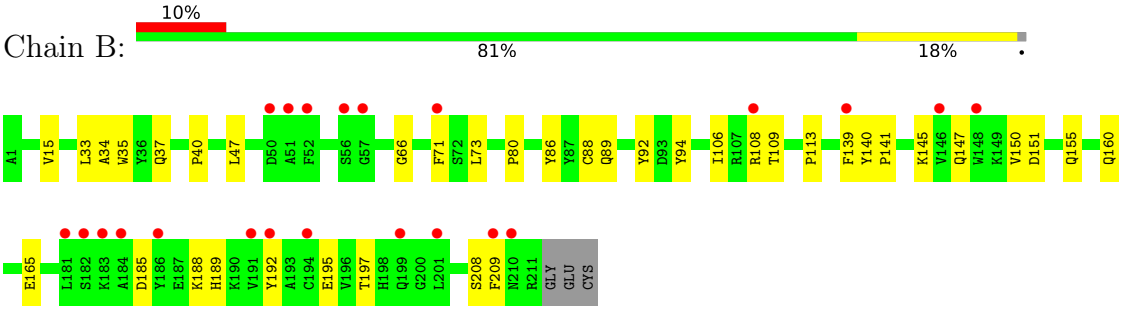
• Molecule 2: antibody S8V2-37 heavy chain

Chain F:



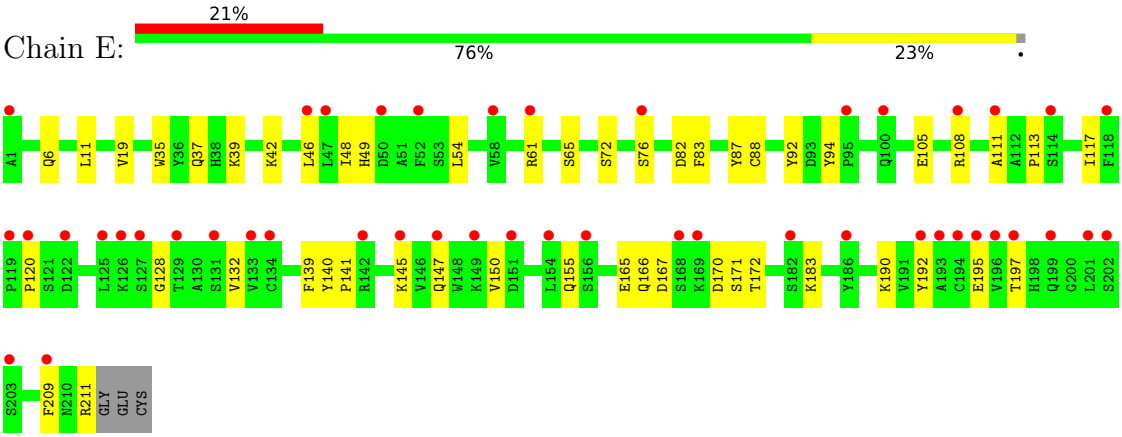
• Molecule 3: antibody S8V2-37 light chain

Chain B:



• Molecule 3: antibody S8V2-37 light chain

Chain E:



• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	294.80Å 42.38Å 155.76Å 90.00° 111.50° 90.00°	Depositor
Resolution (Å)	49.06 – 3.00 49.06 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.06-3.00) 98.6 (49.06-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.247 , 0.290 0.248 , 0.291	Depositor DCC
R_{free} test set	1887 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	88.1	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 85.8	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	0.92	EDS
Total number of atoms	10890	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: NAG, BMA

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	0/2158	0.45	0/2932
1	D	0.25	0/2158	0.43	0/2932
2	C	0.26	0/1667	0.48	0/2269
2	F	0.26	0/1667	0.48	0/2269
3	B	0.25	0/1668	0.48	0/2267
3	E	0.25	0/1668	0.44	0/2267
All	All	0.25	0/10986	0.46	0/14936

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
2	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	160	GLU	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	2104	0	2046	39	0
1	D	2104	0	2046	37	0
2	C	1630	0	1582	34	0
2	F	1630	0	1582	35	0
3	B	1630	0	1581	28	0
3	E	1630	0	1581	33	0
4	G	39	0	34	1	0
4	I	39	0	34	0	0
5	H	28	0	25	0	0
6	A	14	0	13	0	0
6	D	42	0	39	0	0
All	All	10890	0	10563	200	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (200) 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:98:TYR:HE1	1:D:226:ILE:HG21	1.35	0.89
1:D:169:PRO:HA	1:D:242:ILE:HG22	1.66	0.78
3:B:37:GLN:HB2	3:B:47:LEU:HD21	1.67	0.75
1:D:161:TYR:HE2	1:D:249:GLY:HA2	1.52	0.73
2:F:37:MET:HB3	2:F:82:LEU:HD22	1.68	0.73
2:C:96:VAL:HG22	2:C:120:ARG:HG2	1.71	0.73
3:E:108:ARG:HH12	3:E:111:ALA:HB2	1.54	0.73
3:E:61:ARG:NH2	3:E:82:ASP:OD1	2.22	0.72
2:C:53:TYR:HE2	2:C:62:SER:HB3	1.54	0.72
2:C:37:MET:HB3	2:C:82:LEU:HD22	1.74	0.70
3:B:33:LEU:HD13	3:B:71:PHE:CD2	2.26	0.70
2:C:183:GLN:HA	3:B:160:GLN:HE22	1.57	0.70
2:F:54:ILE:HD13	2:F:75:ARG:HG3	1.74	0.69
1:A:161:TYR:CE2	1:A:249:GLY:HA2	2.28	0.68
2:C:86:MET:HB3	2:C:89:LEU:HD21	1.74	0.68
1:A:104:ASP:HB3	1:A:234:TRP:HH2	1.59	0.67
1:D:283:THR:HG22	1:D:301:THR:HG22	1.77	0.67
3:B:80:PRO:HA	3:B:106:ILE:HG12	1.76	0.67
3:B:33:LEU:HD13	3:B:71:PHE:CE2	2.30	0.67
2:C:207:ILE:HG12	2:C:222:ARG:HG2	1.76	0.66
2:F:53:TYR:HE2	2:F:62:SER:HB3	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:50:TRP:HZ2	2:C:53:TYR:HB3	1.61	0.66
1:D:98:TYR:CE1	1:D:226:ILE:HG21	2.25	0.65
2:C:131:PRO:HB3	2:C:157:TYR:HB3	1.79	0.64
3:E:108:ARG:HD3	3:E:171:SER:HB2	1.80	0.64
2:F:16:GLN:HG2	2:F:125:GLY:HA2	1.80	0.64
1:D:130:VAL:HG11	1:D:164:LEU:HD11	1.79	0.63
2:C:156:ASP:OD1	2:C:183:GLN:NE2	2.32	0.63
1:D:102:VAL:HG22	1:D:232:ILE:HB	1.81	0.62
2:C:120:ARG:HD2	2:C:161:PRO:HD3	1.83	0.61
3:B:145:LYS:HB3	3:B:197:THR:HB	1.82	0.61
1:D:175:ASP:HB2	1:D:260:ILE:HG21	1.81	0.61
2:F:131:PRO:HB3	2:F:157:TYR:HB3	1.82	0.61
1:A:97:CYS:SG	1:A:98:TYR:N	2.75	0.60
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.85	0.59
1:A:141:ARG:HH12	1:A:149:SER:HB3	1.67	0.59
2:F:86:MET:HB3	2:F:89:LEU:HD21	1.83	0.59
1:A:283:THR:HG22	1:A:301:THR:HG22	1.85	0.59
1:D:99:PRO:HG3	1:D:223:ILE:HB	1.85	0.59
1:A:104:ASP:HB3	1:A:234:TRP:CH2	2.39	0.58
1:D:203:THR:HB	1:D:246:ASN:HB2	1.84	0.58
2:C:95:ALA:HB3	2:C:97:TYR:HE1	1.68	0.58
1:A:222:ARG:HH21	2:C:55:ARG:HH22	1.51	0.58
1:D:97:CYS:SG	1:D:98:TYR:N	2.76	0.58
3:B:15:VAL:HG22	3:B:106:ILE:HD11	1.85	0.57
2:F:129:LYS:HE3	2:F:187:LEU:HD21	1.86	0.57
2:F:164:VAL:HG22	2:F:210:VAL:HG22	1.86	0.57
1:A:170:ASN:ND2	1:A:237:VAL:O	2.38	0.57
3:E:6:GLN:HE22	3:E:87:TYR:HA	1.70	0.57
1:A:74:PRO:HG3	1:A:141:ARG:HE	1.69	0.57
2:F:27:ALA:HB1	2:F:30:PHE:HE1	1.69	0.57
2:C:94:THR:HG23	2:C:122:THR:HA	1.86	0.57
2:F:180:ALA:HB2	2:F:190:LEU:HD23	1.86	0.57
2:F:41:ARG:HD3	2:F:51:LEU:HD11	1.87	0.56
1:D:74:PRO:HB3	1:D:141:ARG:HB3	1.87	0.56
2:F:27:ALA:HB1	2:F:30:PHE:CE1	2.40	0.56
1:D:295:GLN:HE21	1:D:297:VAL:HB	1.69	0.55
3:B:66:GLY:HA3	3:B:71:PHE:HA	1.88	0.55
3:E:147:GLN:HB3	3:E:195:GLU:HB3	1.88	0.55
1:A:127:TRP:HB2	1:A:132:GLN:HE21	1.72	0.55
3:B:34:ALA:HB3	3:B:89:GLN:HG2	1.87	0.54
3:E:65:SER:OG	3:E:72:SER:OG	2.25	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:53:TYR:CE2	2:C:62:SER:HB3	2.39	0.54
2:F:150:LEU:HB2	2:F:223:VAL:HG11	1.88	0.54
3:E:61:ARG:HB2	3:E:76:SER:H	1.71	0.54
1:A:48:ILE:HG13	1:A:50:GLU:H	1.73	0.54
3:B:192:TYR:HB2	3:B:209:PHE:CE2	2.43	0.53
1:A:83:LYS:HD2	1:A:116:GLY:O	2.07	0.53
2:C:54:ILE:HG22	2:C:61:THR:HG22	1.91	0.53
1:A:161:TYR:HE2	1:A:249:GLY:HA2	1.71	0.53
1:D:161:TYR:CE2	1:D:249:GLY:HA2	2.39	0.53
3:E:150:VAL:HG13	3:E:192:TYR:HE1	1.74	0.53
2:F:127:SER:HB3	2:F:129:LYS:HE2	1.90	0.52
2:C:41:ARG:HD3	2:C:51:LEU:HD11	1.90	0.52
2:C:25:CYS:HB3	2:C:82:LEU:HB3	1.90	0.52
2:F:32:PHE:O	2:F:75:ARG:NH2	2.42	0.52
1:A:123:GLU:HG3	1:A:256:GLY:HA2	1.91	0.51
2:C:63:TYR:HE1	2:C:73:ILE:HG22	1.75	0.51
1:A:241:ASP:OD1	1:A:242:ILE:N	2.44	0.51
3:E:145:LYS:HB3	3:E:197:THR:HB	1.92	0.51
1:A:84:TRP:CZ3	1:A:118:LEU:HG	2.46	0.51
1:A:166:VAL:HG22	1:A:245:ILE:HB	1.93	0.51
2:F:105:TYR:HB3	2:F:110:TYR:CE2	2.47	0.50
2:F:50:TRP:HZ2	2:F:53:TYR:HB3	1.76	0.50
3:B:150:VAL:HG23	3:B:155:GLN:HG3	1.94	0.50
3:E:37:GLN:OE1	3:E:39:LYS:HE3	2.11	0.50
3:E:113:PRO:HB3	3:E:139:PHE:HB3	1.93	0.50
1:A:221:PRO:HG3	3:B:94:TYR:HE1	1.77	0.50
2:C:54:ILE:HD12	2:C:75:ARG:HB2	1.94	0.49
4:G:2:NAG:H62	4:G:3:BMA:H2	1.94	0.49
2:F:53:TYR:CE2	2:F:62:SER:HB3	2.45	0.49
3:B:113:PRO:HB3	3:B:139:PHE:HB3	1.95	0.49
2:F:39:TRP:CE2	2:F:84:LEU:HB2	2.47	0.49
1:D:141:ARG:NH2	1:D:147:PHE:O	2.44	0.49
3:E:166:GLN:NE2	3:E:171:SER:HB3	2.28	0.49
1:A:58:ILE:HG21	1:A:274:ILE:HD12	1.94	0.49
3:B:35:TRP:CZ3	3:B:88:CYS:HB3	2.48	0.49
1:A:84:TRP:HZ3	1:A:118:LEU:HG	1.78	0.48
1:A:237:VAL:HG21	1:A:243:LEU:HB2	1.94	0.48
3:B:47:LEU:HD11	3:B:86:TYR:HD1	1.78	0.48
1:A:127:TRP:HB2	1:A:132:GLN:NE2	2.28	0.48
1:D:146:SER:OG	1:D:147:PHE:N	2.45	0.48
3:E:11:LEU:O	3:E:105:GLU:N	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LEU:HB2	1:A:260:ILE:HD11	1.96	0.48
1:D:84:TRP:CZ3	1:D:118:LEU:HG	2.49	0.48
1:D:132:GLN:HB3	1:D:152:ASN:HD21	1.78	0.48
1:D:84:TRP:HZ3	1:D:118:LEU:HG	1.79	0.48
2:F:30:PHE:CE2	2:F:32:PHE:HA	2.49	0.48
3:E:167:ASP:HB3	3:E:170:ASP:O	2.13	0.48
3:B:150:VAL:HG22	3:B:192:TYR:CD1	2.49	0.48
3:B:147:GLN:HB3	3:B:195:GLU:HB3	1.95	0.48
1:A:75:GLN:NE2	1:A:94:TYR:O	2.48	0.47
3:B:35:TRP:CE2	3:B:73:LEU:HB2	2.49	0.47
3:E:6:GLN:NE2	3:E:88:CYS:H	2.12	0.47
1:D:98:TYR:CD1	1:D:99:PRO:HD2	2.50	0.47
1:D:221:PRO:HG3	3:E:94:TYR:HE1	1.80	0.46
1:D:226:ILE:HG22	1:D:228:SER:H	1.81	0.46
1:D:288:ILE:HG13	1:D:295:GLN:NE2	2.30	0.46
3:E:35:TRP:CZ3	3:E:88:CYS:HB3	2.50	0.46
2:C:105:TYR:HB3	2:C:110:TYR:CE2	2.51	0.46
2:F:101:ARG:O	2:F:112:MET:HA	2.16	0.46
1:D:98:TYR:OH	1:D:183:HIS:NE2	2.47	0.46
1:A:229:ARG:HD2	3:B:92:TYR:CE1	2.51	0.46
2:F:212:HIS:CD2	2:F:214:PRO:HD2	2.51	0.46
1:D:283:THR:OG1	1:D:286:GLY:O	2.28	0.45
2:F:55:ARG:NH1	2:F:56:SER:OG	2.49	0.45
1:A:108:LEU:HD13	1:A:234:TRP:CG	2.51	0.45
1:A:170:ASN:HD22	1:A:237:VAL:HG12	1.82	0.45
3:E:190:LYS:HG3	3:E:211:ARG:H	1.82	0.45
1:A:165:ASN:N	1:A:165:ASN:OD1	2.49	0.45
3:B:47:LEU:HD11	3:B:86:TYR:CD1	2.52	0.45
3:B:185:ASP:HA	3:B:188:LYS:HD3	1.99	0.45
3:E:140:TYR:CG	3:E:141:PRO:HA	2.52	0.45
2:F:162:VAL:HG21	2:F:190:LEU:HD21	1.99	0.45
3:B:40:PRO:HB3	3:B:165:GLU:HG3	2.00	0.44
3:B:140:TYR:CD1	3:B:141:PRO:HA	2.52	0.44
1:D:291:ASP:OD1	1:D:292:LYS:N	2.49	0.44
2:F:9:GLU:OE2	2:F:99:CYS:N	2.50	0.44
2:C:196:VAL:HG11	2:C:206:TYR:CE1	2.53	0.44
3:E:49:HIS:HA	3:E:54:LEU:CD2	2.47	0.44
3:E:150:VAL:HG13	3:E:192:TYR:CE1	2.52	0.44
1:A:67:ILE:HG13	1:A:105:TYR:CE1	2.53	0.44
1:D:152:ASN:O	1:D:253:ALA:N	2.49	0.44
2:C:5:VAL:HG13	2:C:30:PHE:HD1	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:GLN:HG2	1:D:288:ILE:HG23	1.98	0.44
1:D:90:ARG:NH1	1:D:272:ALA:O	2.50	0.44
3:E:117:ILE:HG23	3:E:209:PHE:CE2	2.52	0.44
3:B:151:ASP:OD2	3:B:189:HIS:ND1	2.37	0.43
2:F:113:ASP:HA	3:E:46:LEU:HG	1.99	0.43
3:E:128:GLY:HA2	3:E:183:LYS:HB2	2.00	0.43
3:B:208:SER:OG	3:B:209:PHE:N	2.51	0.43
2:F:37:MET:SD	2:F:101:ARG:HG2	2.58	0.43
2:F:50:TRP:CZ2	2:F:53:TYR:HB3	2.53	0.43
2:C:9:GLU:OE2	2:C:99:CYS:N	2.51	0.43
2:C:162:VAL:HG12	2:C:212:HIS:HD2	1.82	0.43
2:F:97:TYR:HE2	2:F:121:VAL:HB	1.83	0.43
2:C:39:TRP:NE1	2:C:84:LEU:HB2	2.34	0.43
3:B:35:TRP:CD2	3:B:73:LEU:HB2	2.53	0.43
1:A:101:ASP:OD1	1:A:231:SER:HA	2.18	0.43
1:A:114:SER:O	1:A:263:GLY:HA2	2.19	0.43
1:A:295:GLN:HG2	1:A:297:VAL:H	1.84	0.43
3:E:120:PRO:HD3	3:E:132:VAL:HG22	2.00	0.43
1:D:75:GLN:NE2	1:D:94:TYR:O	2.52	0.43
1:D:207:LYS:HB2	1:D:241:ASP:OD1	2.19	0.43
3:E:83:PHE:HE2	3:E:165:GLU:HB3	1.84	0.43
2:C:50:TRP:CZ2	2:C:53:TYR:HB3	2.48	0.43
2:C:54:ILE:HD12	2:C:75:ARG:NE	2.34	0.43
2:C:113:ASP:OD1	2:C:114:VAL:N	2.52	0.42
1:D:48:ILE:HG13	1:D:50:GLU:H	1.84	0.42
1:D:229:ARG:HD2	3:E:92:TYR:CE1	2.54	0.42
2:C:150:LEU:HB2	2:C:223:VAL:HG11	2.01	0.42
2:F:207:ILE:HG12	2:F:222:ARG:HG2	1.99	0.42
1:D:301:THR:HB	1:D:305:CYS:SG	2.59	0.42
2:F:5:VAL:HG11	2:F:101:ARG:HH22	1.85	0.42
3:E:108:ARG:NH2	3:E:172:THR:HG22	2.34	0.42
1:A:127:TRP:CZ2	1:A:253:ALA:HB1	2.54	0.42
2:C:95:ALA:HB3	2:C:97:TYR:CE1	2.51	0.42
2:F:129:LYS:CE	2:F:187:LEU:HD21	2.50	0.42
2:C:106:THR:OG1	2:C:107:GLY:N	2.51	0.42
3:E:150:VAL:HB	3:E:155:GLN:NE2	2.34	0.42
1:A:291:ASP:OD1	1:A:292:LYS:N	2.51	0.41
1:D:66:LEU:HD22	1:D:267:ILE:HD12	2.01	0.41
1:A:185:PRO:HG2	1:A:191:GLN:OE1	2.20	0.41
1:A:281:CYS:HB3	1:A:288:ILE:O	2.20	0.41
1:D:288:ILE:HG13	1:D:295:GLN:HE22	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:PHE:HB2	1:A:127:TRP:NE1	2.36	0.41
1:D:264:LYS:O	1:D:302:TYR:OH	2.36	0.41
3:E:11:LEU:HD21	3:E:19:VAL:HG21	2.02	0.41
2:C:74:SER:OG	2:C:83:TYR:HB2	2.20	0.41
2:C:99:CYS:O	2:C:116:GLY:N	2.50	0.41
2:F:196:VAL:HG11	2:F:206:TYR:CE1	2.56	0.41
3:E:49:HIS:HA	3:E:54:LEU:HD22	2.03	0.41
2:F:56:SER:HA	2:F:75:ARG:NH1	2.36	0.41
3:E:39:LYS:HB2	3:E:42:LYS:HB2	2.03	0.41
3:B:35:TRP:HB3	3:B:47:LEU:HD12	2.02	0.40
2:F:52:SER:OG	2:F:53:TYR:N	2.52	0.40
1:A:130:VAL:HG11	1:A:164:LEU:HD11	2.03	0.40
3:E:48:ILE:HG22	3:E:49:HIS:CD2	2.57	0.40
3:B:108:ARG:HG2	3:B:109:THR:N	2.36	0.40
2:C:39:TRP:CE2	2:C:84:LEU:HB2	2.56	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	263/291 (90%)	250 (95%)	13 (5%)	0	100	100
1	D	263/291 (90%)	249 (95%)	14 (5%)	0	100	100
2	C	213/233 (91%)	207 (97%)	6 (3%)	0	100	100
2	F	213/233 (91%)	197 (92%)	15 (7%)	1 (0%)	29	68
3	B	209/214 (98%)	199 (95%)	10 (5%)	0	100	100
3	E	209/214 (98%)	194 (93%)	15 (7%)	0	100	100
All	All	1370/1476 (93%)	1296 (95%)	73 (5%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	161	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	237/258 (92%)	236 (100%)	1 (0%)	91 97
1	D	237/258 (92%)	236 (100%)	1 (0%)	91 97
2	C	181/197 (92%)	181 (100%)	0	100 100
2	F	181/197 (92%)	181 (100%)	0	100 100
3	B	187/189 (99%)	187 (100%)	0	100 100
3	E	187/189 (99%)	187 (100%)	0	100 100
All	All	1210/1288 (94%)	1208 (100%)	2 (0%)	93 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	295	GLN
1	D	126	ASN

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

Mol	Chain	Res	Type
1	A	132	GLN
3	B	160	GLN
1	D	295	GLN
3	E	6	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)

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

5.5 Carbohydrates (i)

8 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	4,1	14,14,15	0.32	0	17,19,21	0.61	0
4	NAG	G	2	4	14,14,15	0.25	0	17,19,21	0.39	0
4	BMA	G	3	4	11,11,12	0.60	0	15,15,17	0.88	0
5	NAG	H	1	1,5	14,14,15	0.29	0	17,19,21	0.51	0
5	NAG	H	2	5	14,14,15	0.29	0	17,19,21	0.48	0
4	NAG	I	1	4	14,14,15	0.66	1 (7%)	17,19,21	0.65	0
4	NAG	I	2	4	14,14,15	0.22	0	17,19,21	0.62	0
4	BMA	I	3	4	11,11,12	0.52	0	15,15,17	0.89	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	4,1	-	1/6/23/26	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
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
4	NAG	I	1	4	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	1/6/23/26	0/1/1/1
4	BMA	I	3	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1	NAG	O5-C1	-2.35	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
4	I	1	NAG	C4-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	G	1	NAG	C3-C2-N2-C7
5	H	2	NAG	C3-C2-N2-C7
5	H	2	NAG	C1-C2-N2-C7

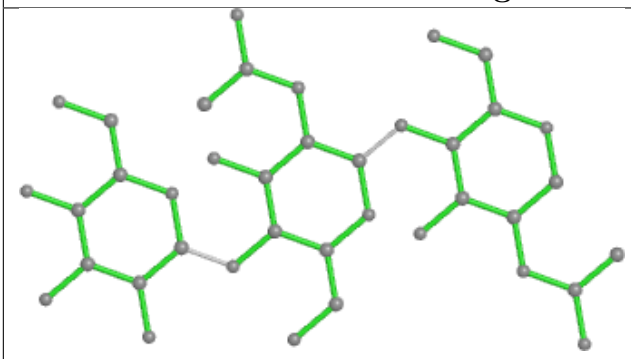
There are no ring outliers.

2 monomers are involved in 1 short contact:

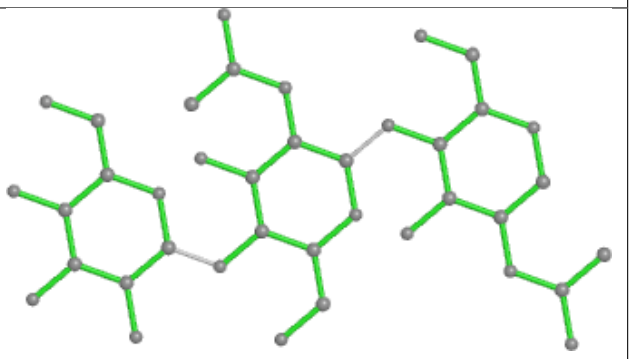
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	1	0
4	G	3	BMA	1	0

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

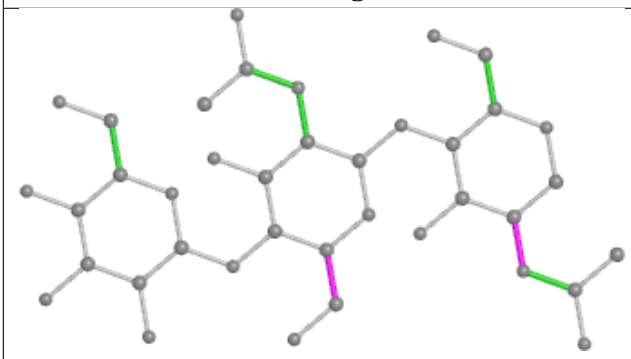
Oligosaccharide Chain G



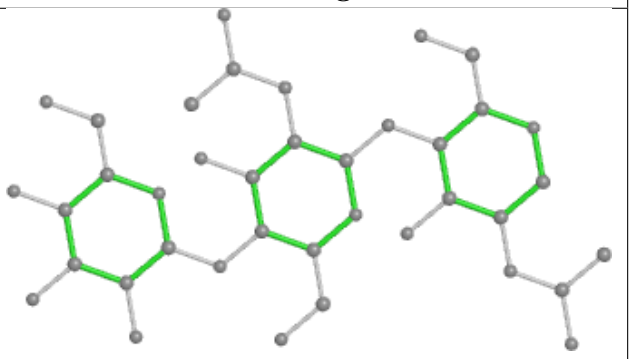
Bond lengths



Bond angles

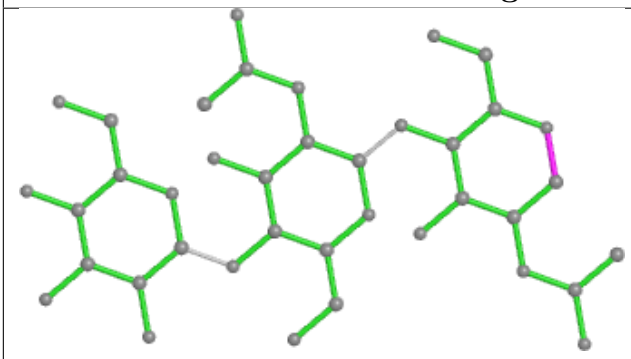


Torsions

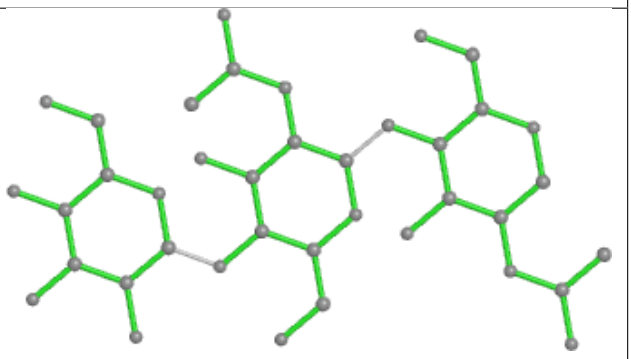


Rings

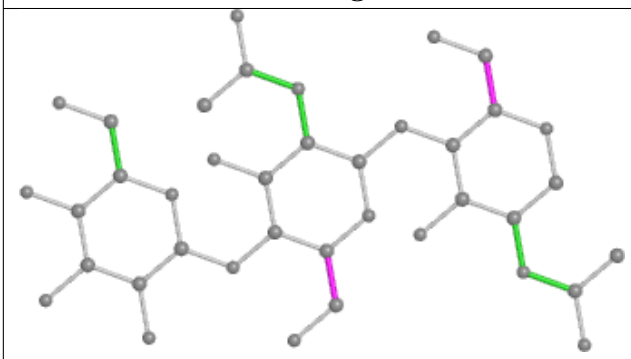
Oligosaccharide Chain I



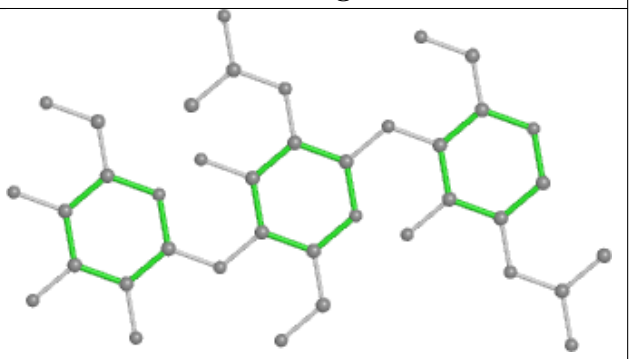
Bond lengths



Bond angles

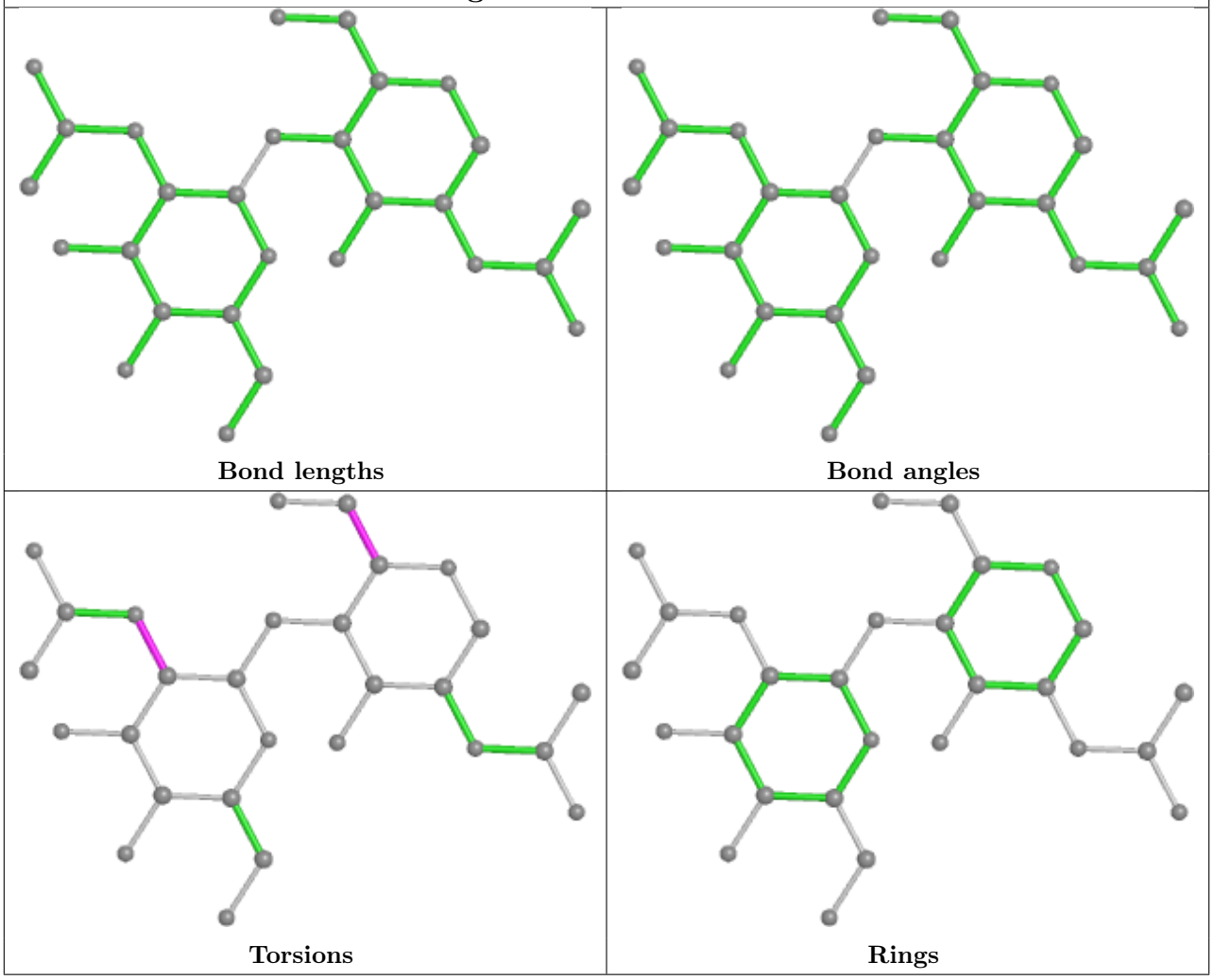


Torsions



Rings

Oligosaccharide Chain H



5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	D	403	1	14,14,15	0.28	0	17,19,21	0.62	0
6	NAG	D	402	1	14,14,15	0.27	0	17,19,21	0.53	0
6	NAG	A	401	1	14,14,15	0.24	0	17,19,21	0.55	0
6	NAG	D	401	1	14,14,15	0.26	0	17,19,21	0.51	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	NAG	D	403	1	-	2/6/23/26	0/1/1/1
6	NAG	D	402	1	-	3/6/23/26	0/1/1/1
6	NAG	A	401	1	-	3/6/23/26	0/1/1/1
6	NAG	D	401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	401	NAG	O5-C5-C6-O6
6	A	401	NAG	C4-C5-C6-O6
6	D	402	NAG	O5-C5-C6-O6
6	D	403	NAG	O5-C5-C6-O6
6	D	402	NAG	C4-C5-C6-O6
6	A	401	NAG	C3-C2-N2-C7
6	D	403	NAG	C3-C2-N2-C7
6	D	402	NAG	C3-C2-N2-C7

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	A	265/291 (91%)	0.62	20 (7%) 14 4	46, 73, 160, 241	0
1	D	265/291 (91%)	1.23	58 (21%) 0 0	71, 148, 227, 265	0
2	C	217/233 (93%)	0.44	1 (0%) 91 75	48, 89, 134, 207	0
2	F	217/233 (93%)	1.12	42 (19%) 1 0	99, 147, 229, 278	0
3	B	211/214 (98%)	0.95	22 (10%) 6 2	48, 121, 189, 298	0
3	E	211/214 (98%)	1.27	46 (21%) 0 0	90, 153, 213, 263	0
All	All	1386/1476 (93%)	0.94	189 (13%) 3 1	46, 122, 208, 298	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	51	ALA	9.5
1	D	46	SER	8.8
2	F	224	GLU	6.9
3	E	76	SER	6.7
1	D	295	GLN	6.6
3	E	120	PRO	6.6
2	F	194	VAL	6.5
3	E	168	SER	6.5
3	E	122	ASP	6.4
1	D	299	ARG	6.3
2	F	196	VAL	6.2
1	D	47	SER	6.0
2	F	137	ALA	6.0
3	B	50	ASP	5.6
1	A	295	GLN	5.6
1	D	287	SER	5.3
1	A	45	ASN	5.2
3	E	52	PHE	4.9
1	D	298	ASN	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	E	108	ARG	4.8
1	D	289	PRO	4.8
1	D	274	ILE	4.7
1	D	290	ASN	4.7
2	F	150	LEU	4.5
1	D	56	HIS	4.5
1	D	302	TYR	4.5
3	E	186	TYR	4.5
1	D	304	ALA	4.4
2	F	223	VAL	4.4
3	E	201	LEU	4.4
3	E	147	GLN	4.3
1	D	275	GLY	4.3
3	E	202	SER	4.2
2	F	148	ALA	4.2
3	E	196	VAL	4.2
1	D	51	ILE	4.2
1	D	282	ILE	4.1
1	D	52	CYS	4.1
3	E	193	ALA	4.1
3	E	50	ASP	4.1
2	F	124	SER	4.0
3	B	184	ALA	4.0
1	D	262	SER	4.0
1	D	84	TRP	4.0
3	B	183	LYS	4.0
1	D	297	VAL	4.0
2	F	171	LEU	4.0
2	F	4	GLU	3.9
3	B	52	PHE	3.9
1	D	268	MET	3.9
2	F	149	ALA	3.9
1	D	296	ASN	3.8
1	D	303	GLY	3.8
3	B	148	TRP	3.8
1	D	294	PHE	3.8
2	F	135	PRO	3.8
1	A	46	SER	3.7
3	E	134	CYS	3.7
1	D	45	ASN	3.7
1	D	301	THR	3.6
2	F	202	GLY	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	264	LYS	3.6
1	D	49	GLY	3.6
1	D	53	ASP	3.5
1	D	48	ILE	3.5
3	E	145	LYS	3.5
1	A	47	SER	3.5
1	D	55	PRO	3.5
3	E	151	ASP	3.5
2	C	145	GLY	3.5
1	D	308	TYR	3.5
1	A	294	PHE	3.4
1	D	288	ILE	3.4
2	F	30	PHE	3.4
1	D	272	ALA	3.3
3	B	181	LEU	3.3
3	E	199	GLN	3.3
3	B	199	GLN	3.2
3	E	209	PHE	3.2
2	F	131	PRO	3.2
2	F	101	ARG	3.2
2	F	204	GLN	3.1
3	E	154	LEU	3.1
2	F	51	LEU	3.1
1	A	291	ASP	3.1
1	D	293	PRO	3.1
1	D	58	ILE	3.1
2	F	88	SER	3.0
1	A	304	ALA	3.0
3	E	197	THR	3.0
1	D	307	ARG	3.0
2	F	10	SER	2.9
3	E	169	LYS	2.9
3	E	127	SER	2.9
1	A	288	ILE	2.9
1	A	48	ILE	2.9
2	F	129	LYS	2.8
2	F	167	ASN	2.8
3	E	118	PHE	2.8
3	B	194	CYS	2.7
2	F	71	PHE	2.7
1	A	290	ASN	2.7
3	E	61	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	192	TYR	2.7
3	E	156	SER	2.7
3	E	149	LYS	2.7
3	E	126	LYS	2.7
1	D	281	CYS	2.7
2	F	52	SER	2.7
2	F	159	PRO	2.7
3	E	1	ALA	2.6
3	E	195	GLU	2.6
1	A	292	LYS	2.6
1	A	307	ARG	2.6
3	B	186	TYR	2.6
1	A	296	ASN	2.6
1	D	261	ARG	2.6
3	E	47	LEU	2.6
1	D	259	LYS	2.6
3	E	125	LEU	2.5
2	F	138	PRO	2.5
3	B	209	PHE	2.5
1	D	277	CYS	2.5
3	B	57	GLY	2.5
1	D	279	SER	2.5
2	F	210	VAL	2.5
3	B	146	VAL	2.5
2	F	225	PRO	2.5
1	D	280	GLU	2.4
2	F	91	ALA	2.4
1	D	305	CYS	2.4
2	F	39	TRP	2.4
2	F	192	SER	2.4
1	D	119	GLU	2.4
2	F	222	ARG	2.4
3	E	131	SER	2.4
3	E	133	VAL	2.4
1	D	173	GLN	2.4
2	F	201	LEU	2.4
1	D	286	GLY	2.3
3	E	100	GLN	2.3
3	E	111	ALA	2.3
1	D	242	ILE	2.3
1	D	276	LYS	2.3
3	E	192	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	121	ASN	2.3
1	D	284	PRO	2.3
1	D	283	THR	2.3
1	A	297	VAL	2.3
1	A	308	TYR	2.3
3	E	114	SER	2.3
1	A	298	ASN	2.2
3	B	201	LEU	2.2
2	F	8	VAL	2.2
2	F	195	THR	2.2
3	E	119	PRO	2.2
2	F	133	VAL	2.2
3	E	142	ARG	2.2
1	D	208	ARG	2.2
1	D	50	GLU	2.2
2	F	53	TYR	2.2
3	E	203	SER	2.2
1	D	291	ASP	2.2
3	B	71	PHE	2.2
3	B	182	SER	2.2
3	E	182	SER	2.1
1	A	306	PRO	2.1
1	D	241	ASP	2.1
1	D	237	VAL	2.1
2	F	13	GLY	2.1
1	A	293	PRO	2.1
1	D	300	ILE	2.1
3	E	129	THR	2.1
1	A	49	GLY	2.1
2	F	90	ARG	2.1
3	E	46	LEU	2.1
3	B	56	SER	2.1
1	D	108	LEU	2.1
2	F	74	SER	2.1
3	B	191	VAL	2.1
2	F	21	LEU	2.1
3	B	139	PHE	2.0
3	B	108	ARG	2.0
3	E	194	CYS	2.0
3	B	210	ASN	2.0
1	A	283	THR	2.0
3	E	58	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	151	GLY	2.0
3	E	95	PRO	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)

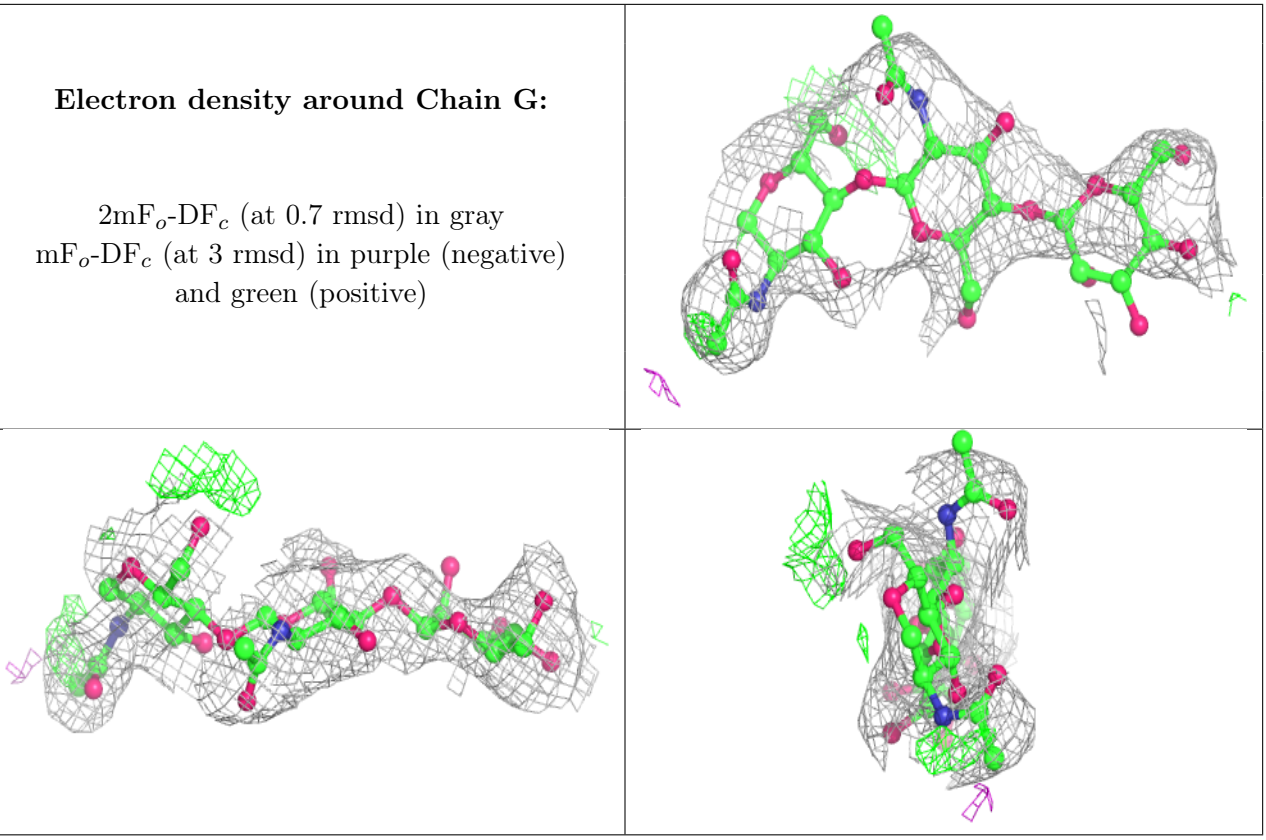
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	NAG	H	1	14/15	0.42	0.62	140,151,164,172	0
5	NAG	H	2	14/15	0.49	1.00	153,172,176,176	0
4	NAG	I	2	14/15	0.60	0.26	142,153,162,167	0
4	BMA	G	3	11/12	0.61	0.39	140,157,166,167	0
4	BMA	I	3	11/12	0.61	0.66	162,166,168,169	0
4	NAG	I	1	14/15	0.69	0.36	143,149,154,154	0
4	NAG	G	1	14/15	0.71	0.27	102,122,135,136	0
4	NAG	G	2	14/15	0.88	0.19	113,136,141,145	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.

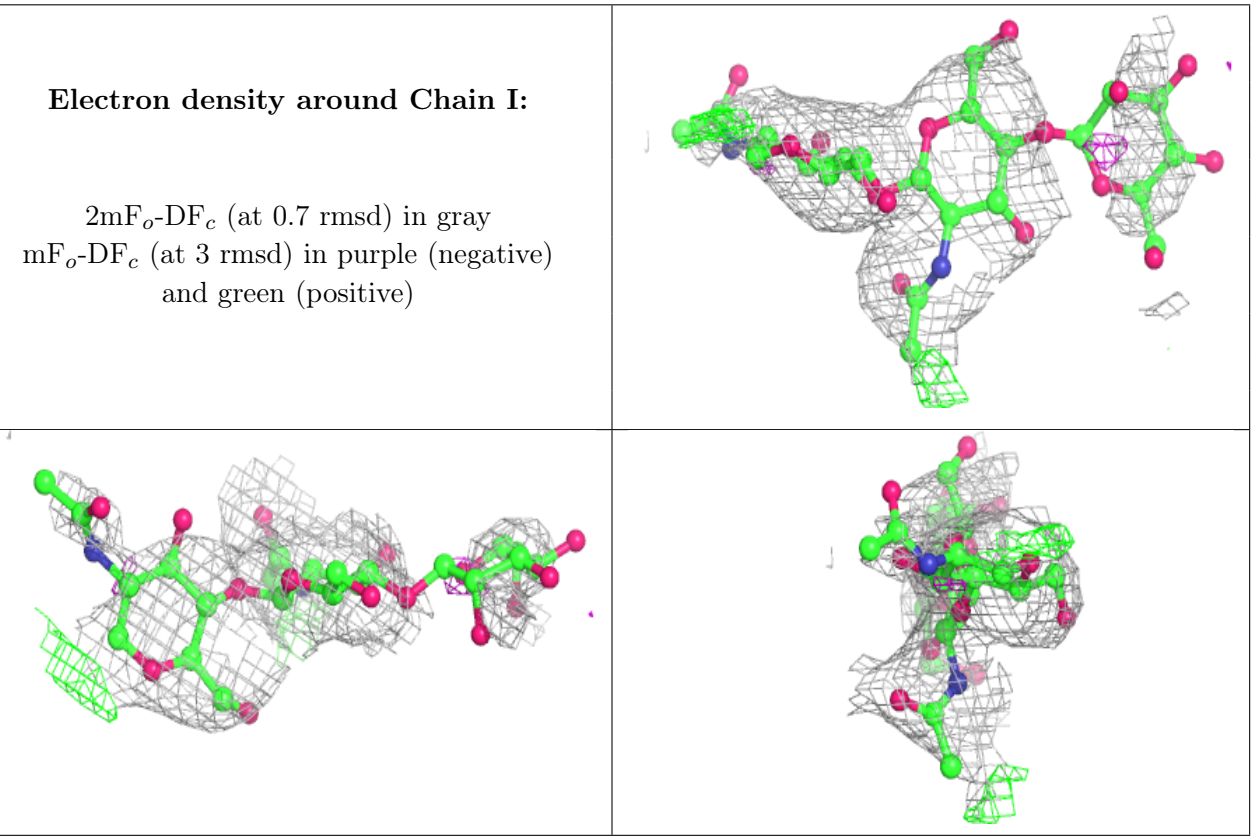
Electron density around Chain G:

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



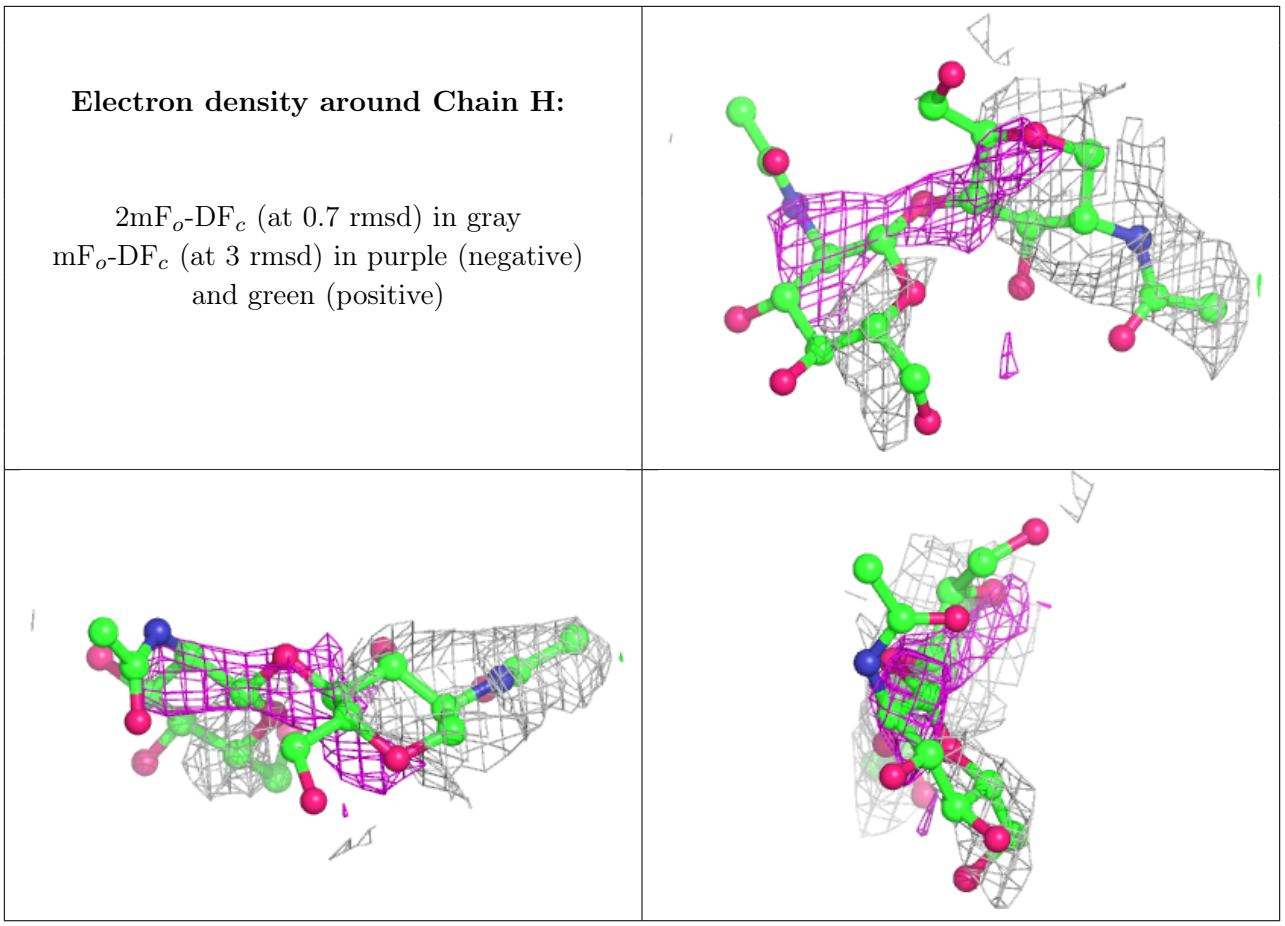
Electron density around Chain I:

$2mF_o$-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 H:

$2mF_o$-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	NAG	D	403	14/15	0.49	0.43	104,134,145,145	0
6	NAG	D	402	14/15	0.78	0.49	112,129,139,145	0
6	NAG	D	401	14/15	0.79	0.17	131,142,152,156	0
6	NAG	A	401	14/15	0.83	0.21	82,89,102,104	0

6.5 Other polymers

There are no such residues in this entry.