Full wwPDB X-ray Structure Validation Report (i)

Jun 26, 2024 – 10:28 AM EDT

PDB ID	:	6WEZ
Title	:	Crystal Structure of Broadly Neutralizing Antibody 3I14-D93N Mutant Bound to the Influenza A H3 Hemagglutinin
Authors	:	Harshbarger, W.D.; Lockbaum, G.J.; Deming, D.T.; Attatippaholkun, N.; Schiffer, C.A.; Marasco, W.A.
Deposited on	:	2020-04-03
Resolution	:	3.21 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

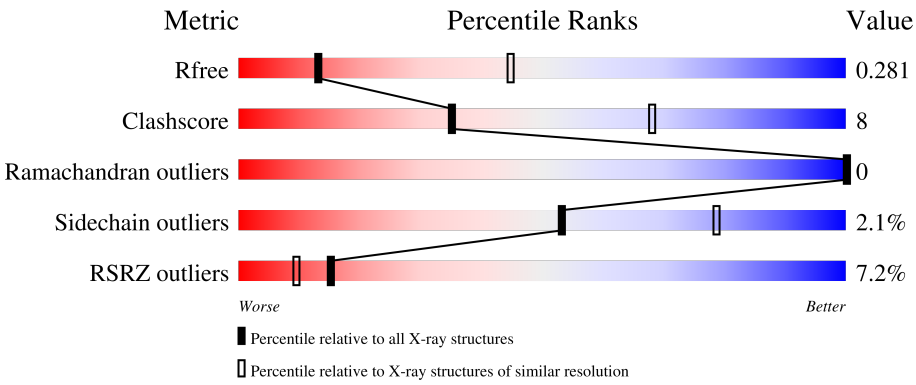
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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	319	80% 19% •
2	B	176	% 82% 11% 7%
3	H	235	15% 72% 21% • 5%
4	L	213	14% 73% 25% •
5	C	3	33% 33% 33%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	3	100%
5	G	3	67% 33%
6	D	2	100%
6	E	2	100%
6	I	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7165 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
			Total	C	N	O	S			
1	A	317	2475	1551	441	471	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	expression tag	UNP A0A5P1MU07
A	8	ASP	-	expression tag	UNP A0A5P1MU07
A	9	PRO	-	expression tag	UNP A0A5P1MU07
A	10	GLY	-	expression tag	UNP A0A5P1MU07

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	163	1328	821	236	265	6	0	0	0

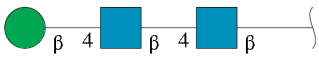
- Molecule 3 is a protein called heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	223	1688	1079	285	318	6	0	0	0

- Molecule 4 is a protein called light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	213	1468	916	247	300	5	0	0	0

- Molecule 5 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.

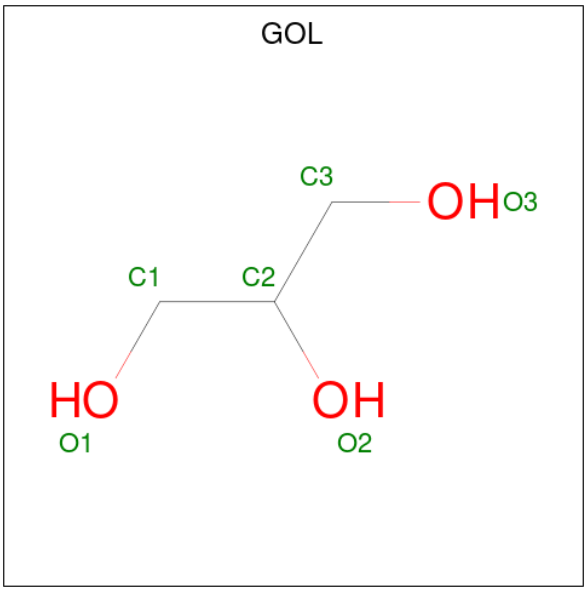


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	C	3	38	22	2	14	0	0	0
5	F	3	39	22	2	15	0	0	0
5	G	3	39	22	2	15	0	0	0

- Molecule 6 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
			Total	C	N	O			
6	D	2	28	16	2	10	0	0	0
6	E	2	28	16	2	10	0	0	0
6	I	2	28	16	2	10	0	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



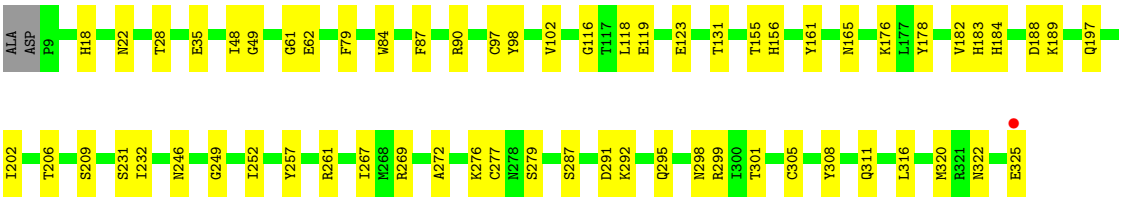
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	6	3	3	0	0

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.

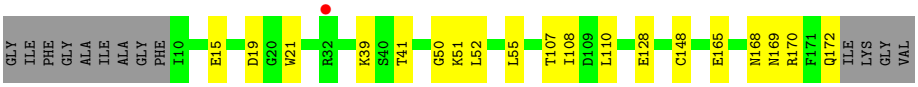
• Molecule 1: Hemagglutinin

Chain A: 80% 19%



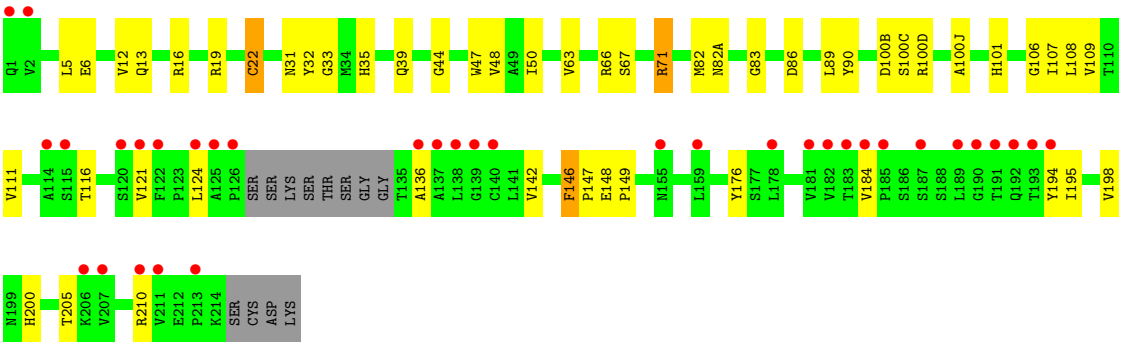
• Molecule 2: Hemagglutinin

Chain B: % 82% 11% 7%



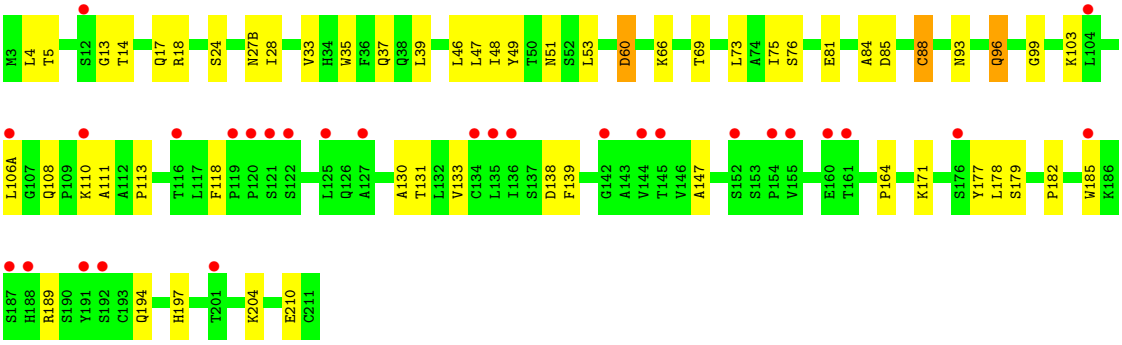
• Molecule 3: heavy chain

Chain H: 15% 72% 21% 5%



• Molecule 4: light chain

Chain L: 14% 73% 25%



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

Chain C: 33% 33% 33%

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

Chain F: 100%

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

Chain G: 67% 33%

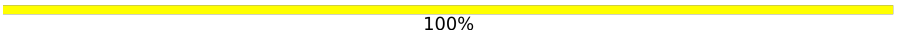
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 100%

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

Chain E: 100%

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

Chain I: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	130.84Å 130.84Å 189.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.42 – 3.21 45.42 – 3.21	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.42-3.21) 98.9 (45.42-3.21)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.233 , 0.281 0.233 , 0.281	Depositor DCC
R_{free} test set	2000 reflections (6.72%)	wwPDB-VP
Wilson B-factor (Å^2)	84.8	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.040 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7165	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, GOL

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	0.27	0/2532	0.48	0/3443
2	B	0.27	0/1350	0.42	0/1812
3	H	0.29	0/1734	0.52	0/2363
4	L	0.27	0/1498	0.51	0/2039
All	All	0.28	0/7114	0.49	0/9657

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2475	0	2423	34	0
2	B	1328	0	1255	14	0
3	H	1688	0	1656	37	0
4	L	1468	0	1303	38	0
5	C	38	0	31	1	0
5	F	39	0	34	0	0
5	G	39	0	34	2	0
6	D	28	0	25	0	0
6	E	28	0	25	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	I	28	0	25	2	0
7	A	6	0	8	0	0
All	All	7165	0	6819	115	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 8.

All (115) 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)
4:L:18:ARG:HA	4:L:75:ILE:O	1.65	0.95
6:I:1:NAG:H61	6:I:2:NAG:HN2	1.48	0.79
3:H:147:PRO:HB2	3:H:149:PRO:HD2	1.65	0.78
2:B:21:TRP:H	2:B:41:THR:HG21	1.53	0.74
4:L:138:ASP:HA	4:L:171:LYS:HB3	1.73	0.69
3:H:116:THR:HB	3:H:147:PRO:HD3	1.76	0.68
2:B:52:LEU:HB3	3:H:100(J):ALA:HB2	1.73	0.68
3:H:136:ALA:HB3	3:H:184:VAL:O	1.95	0.66
2:B:168:ASN:OD1	2:B:172:GLN:NE2	2.29	0.65
2:B:165:GLU:O	2:B:169:ASN:ND2	2.28	0.65
1:A:182:VAL:HG22	1:A:202:ILE:HD13	1.80	0.64
1:A:131:THR:HB	1:A:155:THR:HG23	1.79	0.63
3:H:12:VAL:HG13	3:H:111:VAL:HG12	1.82	0.62
1:A:206:THR:HG1	1:A:209:SER:HG	1.49	0.60
1:A:35:GLU:OE2	1:A:322:ASN:ND2	2.35	0.60
2:B:50:GLY:HA2	4:L:53:LEU:HD21	1.84	0.60
3:H:89:LEU:HD22	3:H:106:GLY:HA3	1.82	0.59
4:L:182:PRO:HA	4:L:185:TRP:HB3	1.84	0.59
1:A:325:GLU:HB3	2:B:15:GLU:HG3	1.85	0.59
1:A:87:PHE:HB3	1:A:267:ILE:HG13	1.84	0.58
3:H:142:VAL:HG21	3:H:198:VAL:HG21	1.85	0.58
1:A:102:VAL:HG22	1:A:232:ILE:HB	1.85	0.58
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.86	0.57
4:L:108:GLN:O	4:L:110:LYS:N	2.34	0.57
3:H:6:GLU:HB3	3:H:107:ILE:HD11	1.86	0.56
3:H:66:ARG:NH1	3:H:82(A):ASN:O	2.38	0.55
3:H:31:ASN:HB2	3:H:100(C):SER:HB3	1.86	0.55
3:H:146:PHE:CD1	3:H:147:PRO:HA	2.42	0.55
4:L:60:ASP:N	4:L:60:ASP:OD1	2.37	0.55
1:A:316:LEU:HD22	2:B:55:LEU:HD12	1.89	0.55
1:A:320:MET:HE1	2:B:21:TRP:HB3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:LYS:NZ	4:L:93:ASN:OD1	2.39	0.55
3:H:124:LEU:HD21	4:L:133:VAL:HG21	1.89	0.55
3:H:6:GLU:HG2	3:H:22:CYS:HB2	1.89	0.53
4:L:4:LEU:HD11	4:L:27(B):ASN:ND2	2.23	0.53
4:L:111:ALA:HB1	4:L:197:HIS:HE1	1.72	0.53
4:L:51:ASN:ND2	4:L:66:LYS:HD3	2.24	0.53
3:H:39:GLN:HG3	3:H:44:GLY:O	2.09	0.52
4:L:14:THR:N	4:L:17:GLN:OE1	2.37	0.52
4:L:81:GLU:N	4:L:81:GLU:OE1	2.42	0.52
3:H:116:THR:HG22	3:H:146:PHE:CE2	2.45	0.51
3:H:100(C):SER:OG	3:H:100(D):ARG:N	2.44	0.51
3:H:67:SER:HB3	3:H:82:MET:HG3	1.93	0.51
2:B:128:GLU:O	2:B:170:ARG:NH1	2.44	0.51
1:A:61:GLY:HA2	1:A:79:PHE:CZ	2.46	0.50
3:H:33:GLY:N	3:H:100(B):ASP:OD1	2.41	0.50
3:H:147:PRO:CB	3:H:149:PRO:HD2	2.40	0.50
4:L:33:VAL:N	4:L:51:ASN:OD1	2.29	0.50
4:L:111:ALA:HA	4:L:139:PHE:HA	1.93	0.50
1:A:246:ASN:HD22	5:G:1:NAG:C7	2.24	0.50
1:A:97:CYS:SG	1:A:98:TYR:N	2.84	0.50
4:L:85:ASP:OD1	4:L:103:LYS:HG2	2.12	0.49
1:A:84:TRP:HZ3	1:A:118:LEU:HG	1.78	0.48
3:H:195:ILE:HA	3:H:210:ARG:HA	1.95	0.48
4:L:133:VAL:HG13	4:L:177:TYR:HB3	1.96	0.48
1:A:22:ASN:N	1:A:22:ASN:OD1	2.46	0.48
4:L:5:THR:OG1	4:L:24:SER:HB3	2.13	0.48
1:A:291:ASP:OD1	1:A:292:LYS:N	2.46	0.48
3:H:200:HIS:HB3	3:H:205:THR:HB	1.96	0.48
3:H:148:GLU:HB2	3:H:176:TYR:CE2	2.49	0.48
1:A:279:SER:HB3	1:A:287:SER:HB3	1.95	0.47
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.95	0.47
4:L:35:TRP:CE2	4:L:73:LEU:HB2	2.49	0.47
3:H:124:LEU:HG	4:L:118:PHE:HB3	1.96	0.46
5:C:2:NAG:H4	5:C:3:BMA:H2	1.65	0.46
1:A:176:LYS:HG2	1:A:257:TYR:CD1	2.51	0.46
1:A:311:GLN:OE1	1:A:311:GLN:N	2.46	0.46
1:A:165:ASN:HB2	5:G:1:NAG:H62	1.98	0.45
3:H:12:VAL:O	3:H:111:VAL:HA	2.15	0.45
4:L:18:ARG:HG3	4:L:76:SER:HA	1.97	0.45
1:A:90:ARG:NH1	1:A:272:ALA:O	2.39	0.45
3:H:121:VAL:HG13	3:H:142:VAL:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASN:OD1	1:A:299:ARG:N	2.50	0.45
2:B:51:LYS:HE3	2:B:51:LYS:HB2	1.77	0.45
4:L:27(B):ASN:N	4:L:27(B):ASN:OD1	2.49	0.45
4:L:39:LEU:HD23	4:L:84:ALA:HB2	1.99	0.45
1:A:184:HIS:NE2	1:A:231:SER:OG	2.42	0.44
1:A:301:THR:HB	1:A:305:CYS:SG	2.57	0.44
1:A:48:ILE:HG13	1:A:49:GLY:H	1.82	0.44
1:A:119:GLU:OE1	1:A:261:ARG:NH2	2.47	0.44
3:H:48:VAL:HG13	3:H:63:VAL:HG21	2.00	0.44
6:I:1:NAG:H61	6:I:2:NAG:N2	2.26	0.44
3:H:35:HIS:NE2	4:L:96:GLN:OE1	2.49	0.43
4:L:13:GLY:O	4:L:106(A):LEU:N	2.50	0.43
1:A:155:THR:OG1	1:A:156:HIS:N	2.52	0.43
4:L:111:ALA:O	4:L:113:PRO:HD3	2.18	0.43
4:L:131:THR:HA	4:L:178:LEU:O	2.19	0.43
3:H:101:HIS:ND1	4:L:46:LEU:HB3	2.34	0.43
4:L:69:THR:O	4:L:69:THR:OG1	2.33	0.43
4:L:147:ALA:HB3	4:L:194:GLN:HB3	2.00	0.43
4:L:49:TYR:O	4:L:53:LEU:HB2	2.19	0.43
3:H:90:TYR:HE1	3:H:109:VAL:HG22	1.84	0.42
3:H:83:GLY:O	3:H:111:VAL:HG21	2.19	0.42
1:A:84:TRP:CE2	1:A:116:GLY:HA2	2.54	0.42
3:H:47:TRP:HZ2	3:H:50:ILE:HG22	1.85	0.42
4:L:35:TRP:HB2	4:L:48:ILE:HB	2.02	0.42
2:B:107:THR:O	2:B:110:LEU:HG	2.21	0.41
4:L:194:GLN:HA	4:L:204:LYS:O	2.20	0.41
1:A:28:THR:HG21	2:B:108:ILE:HD12	2.01	0.41
2:B:19:ASP:OD1	2:B:19:ASP:N	2.45	0.41
3:H:32:TYR:O	3:H:71:ARG:NH2	2.52	0.41
3:H:13:GLN:HB2	3:H:16:ARG:HD2	2.01	0.41
4:L:130:ALA:O	4:L:179:SER:HA	2.20	0.41
3:H:66:ARG:NH2	3:H:86:ASP:OD2	2.34	0.41
3:H:108:LEU:CD2	3:H:149:PRO:HD3	2.51	0.41
4:L:88:CYS:O	4:L:99:GLY:N	2.54	0.41
1:A:62:GLU:HA	1:A:90:ARG:CG	2.51	0.41
1:A:123:GLU:OE1	1:A:178:TYR:OH	2.26	0.41
4:L:28:ILE:O	4:L:66:LYS:NZ	2.34	0.41
1:A:161:TYR:CZ	1:A:249:GLY:HA2	2.55	0.41
3:H:121:VAL:HG22	3:H:142:VAL:HG13	2.03	0.41
4:L:189:ARG:O	4:L:210:GLU:N	2.54	0.41
1:A:295:GLN:O	1:A:308:TYR:HA	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:184:VAL:HG21	3:H:194:TYR:CE2	2.56	0.40
1:A:276:LYS:HE2	1:A:276:LYS:HB2	1.89	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	315/319 (99%)	306 (97%)	9 (3%)	0	100	100
2	B	161/176 (92%)	156 (97%)	5 (3%)	0	100	100
3	H	219/235 (93%)	209 (95%)	10 (5%)	0	100	100
4	L	211/213 (99%)	190 (90%)	21 (10%)	0	100	100
All	All	906/943 (96%)	861 (95%)	45 (5%)	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	280/281 (100%)	274 (98%)	6 (2%)	53	79
2	B	141/148 (95%)	140 (99%)	1 (1%)	84	93
3	H	187/198 (94%)	182 (97%)	5 (3%)	44	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	L	147/177 (83%)	143 (97%)	4 (3%)	44 74
All	All	755/804 (94%)	739 (98%)	16 (2%)	53 79

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	188	ASP
1	A	189	LYS
1	A	197	GLN
1	A	269	ARG
1	A	277	CYS
2	B	148	CYS
3	H	5	LEU
3	H	19	ARG
3	H	22	CYS
3	H	71	ARG
3	H	146	PHE
4	L	60	ASP
4	L	88	CYS
4	L	96	GLN
4	L	164	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
2	B	172	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)

15 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	$\#\|Z\| > 2$
5	NAG	C	1	5,1	14,14,15	0.27	0	17,19,21	0.41	0
5	NAG	C	2	5	14,14,15	0.20	0	17,19,21	0.46	0
5	BMA	C	3	5	10,10,12	0.88	1 (10%)	14,14,17	0.76	0
6	NAG	D	1	1,6	14,14,15	0.43	0	17,19,21	0.52	0
6	NAG	D	2	6	14,14,15	0.17	0	17,19,21	0.53	0
6	NAG	E	1	1,6	14,14,15	0.30	0	17,19,21	0.41	0
6	NAG	E	2	6	14,14,15	0.30	0	17,19,21	0.48	0
5	NAG	F	1	5,1	14,14,15	0.31	0	17,19,21	0.46	0
5	NAG	F	2	5	14,14,15	0.29	0	17,19,21	0.35	0
5	BMA	F	3	5	11,11,12	0.73	0	15,15,17	0.77	0
5	NAG	G	1	5,1	14,14,15	0.68	1 (7%)	17,19,21	0.58	0
5	NAG	G	2	5	14,14,15	0.22	0	17,19,21	0.48	0
5	BMA	G	3	5	11,11,12	0.60	0	15,15,17	0.93	0
6	NAG	I	1	1,6	14,14,15	0.56	0	17,19,21	0.64	0
6	NAG	I	2	6	14,14,15	0.24	0	17,19,21	0.49	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
5	NAG	C	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1
5	BMA	C	3	5	-	-	0/1/1/1
6	NAG	D	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	NAG	E	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	E	2	6	-	2/6/23/26	0/1/1/1
5	NAG	F	1	5,1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3	BMA	C1-C2	2.38	1.57	1.52
5	G	1	NAG	O5-C1	-2.34	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	I	2	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
6	D	2	NAG	C4-C5-C6-O6
5	C	2	NAG	O5-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
6	I	1	NAG	O5-C5-C6-O6
6	E	2	NAG	O5-C5-C6-O6
6	I	1	NAG	C4-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
6	D	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	G	3	BMA	O5-C5-C6-O6
6	E	1	NAG	O5-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
6	E	2	NAG	C4-C5-C6-O6

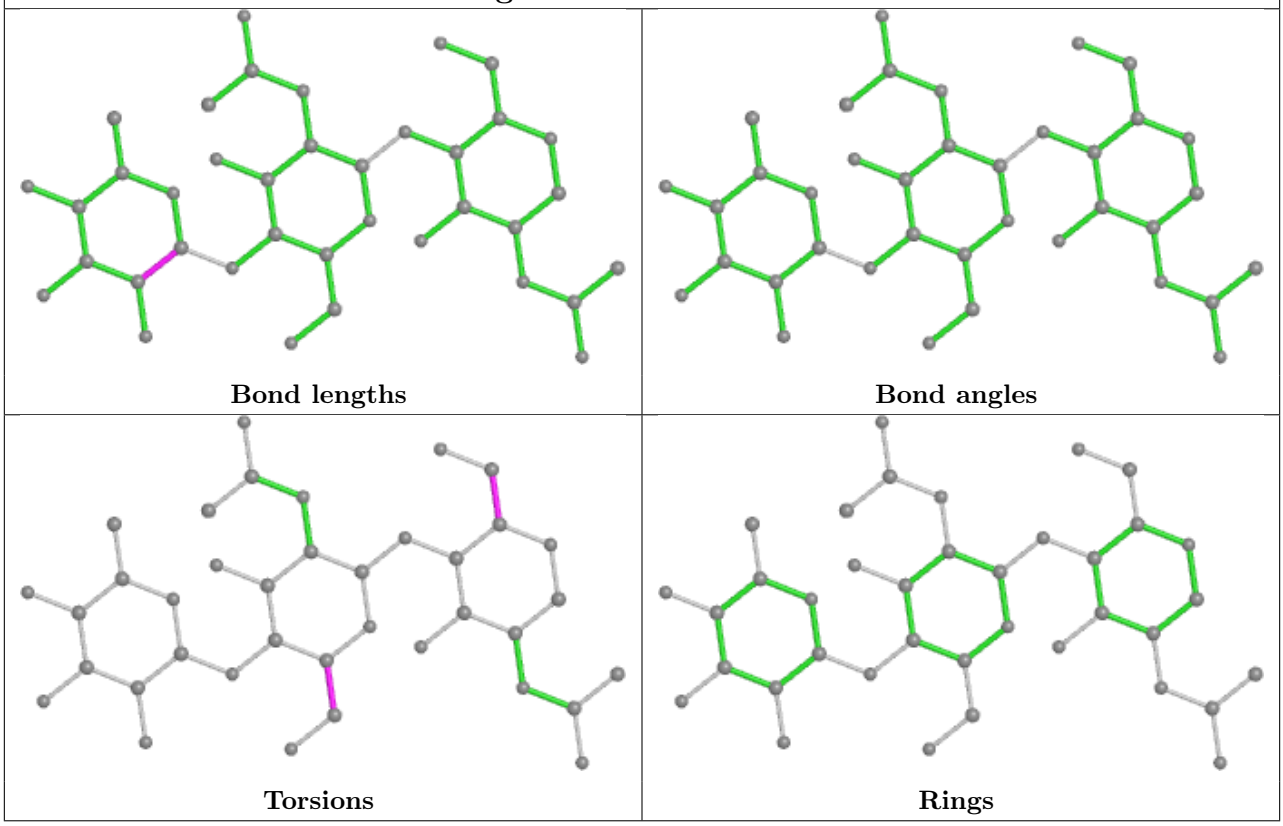
There are no ring outliers.

5 monomers are involved in 5 short contacts:

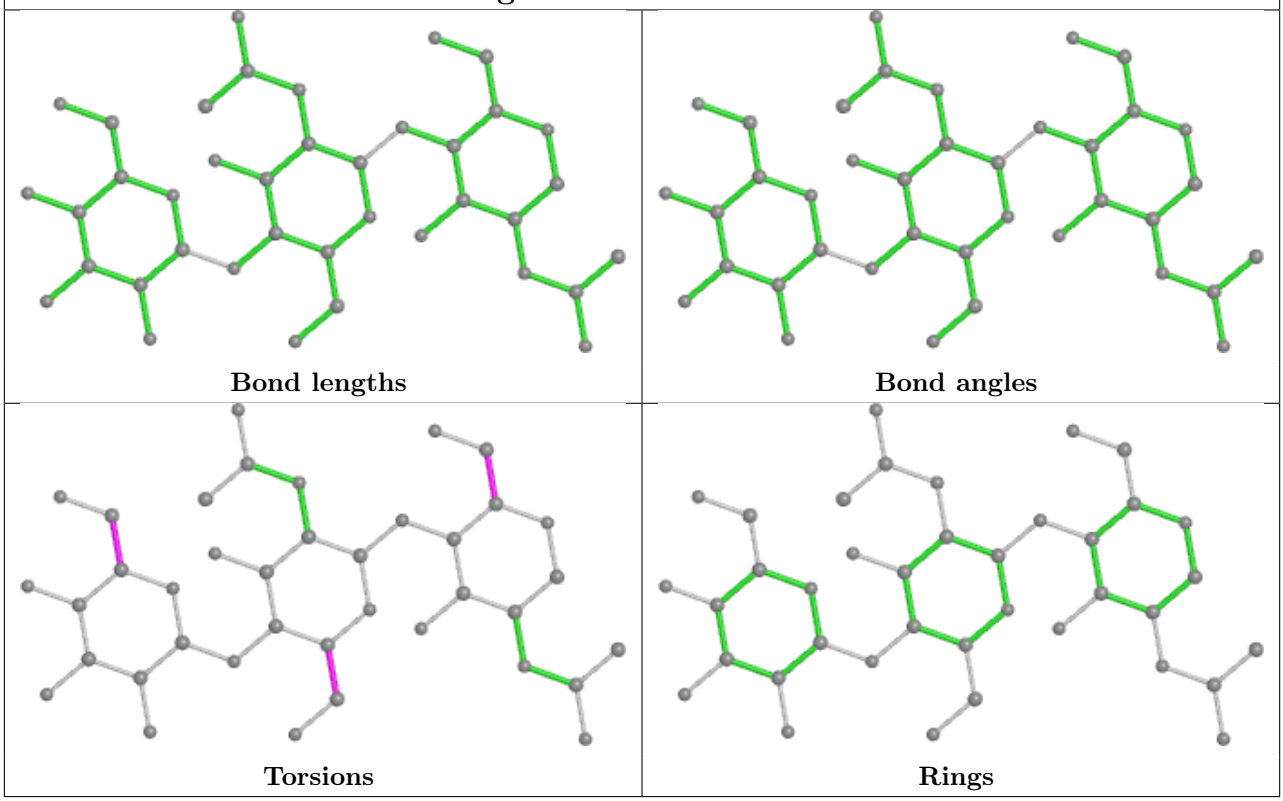
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	2	NAG	2	0
5	C	2	NAG	1	0
5	G	1	NAG	2	0
6	I	1	NAG	2	0
5	C	3	BMA	1	0

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

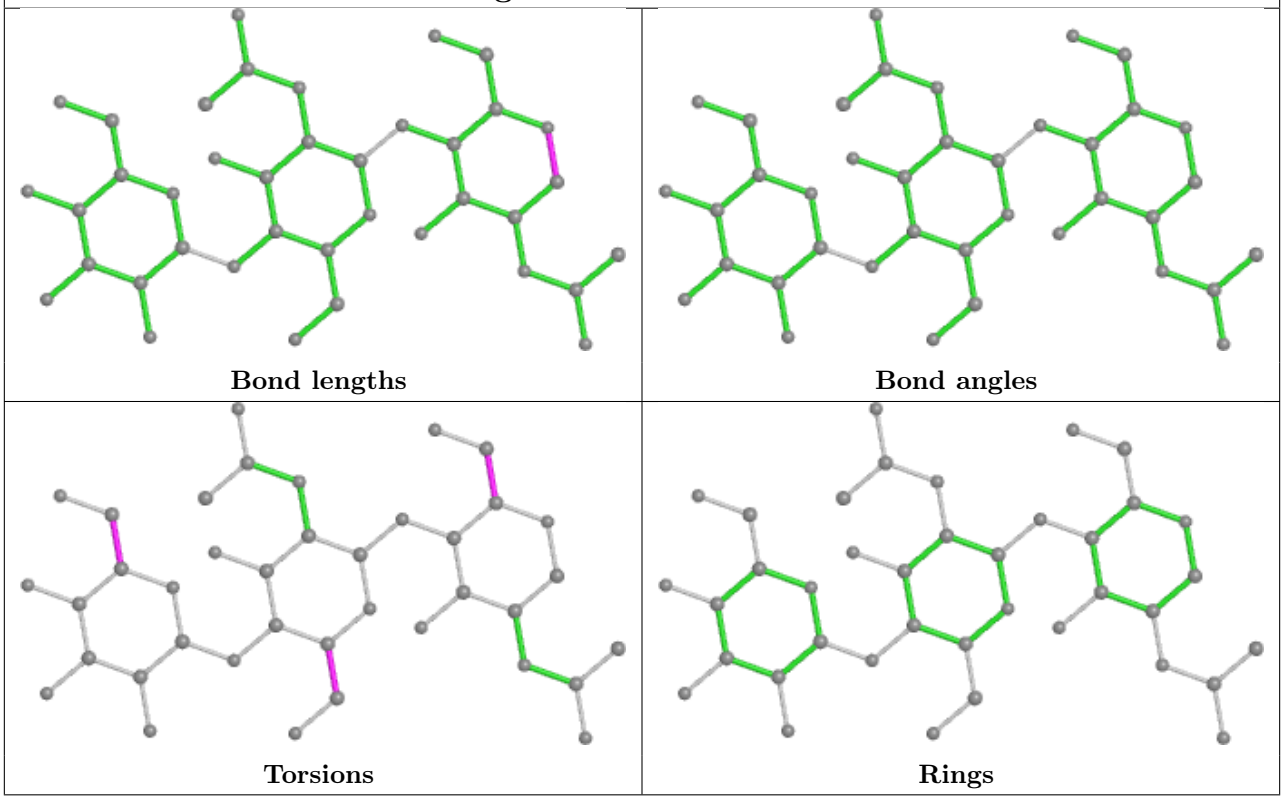
Oligosaccharide Chain C



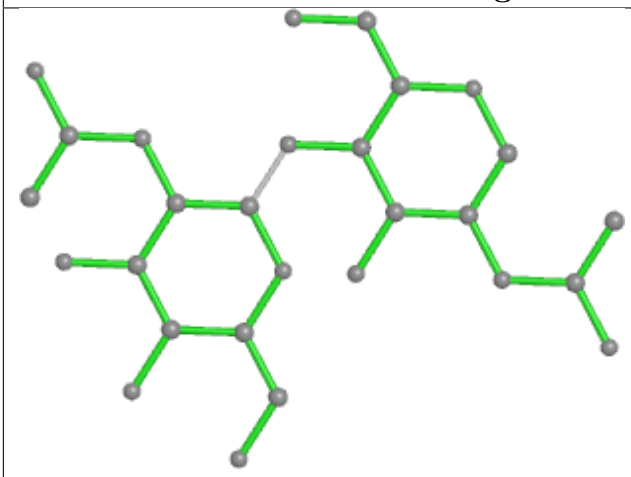
Oligosaccharide Chain F



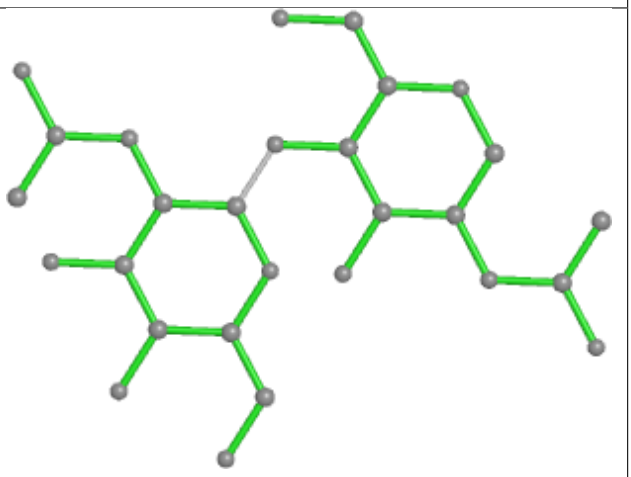
Oligosaccharide Chain G



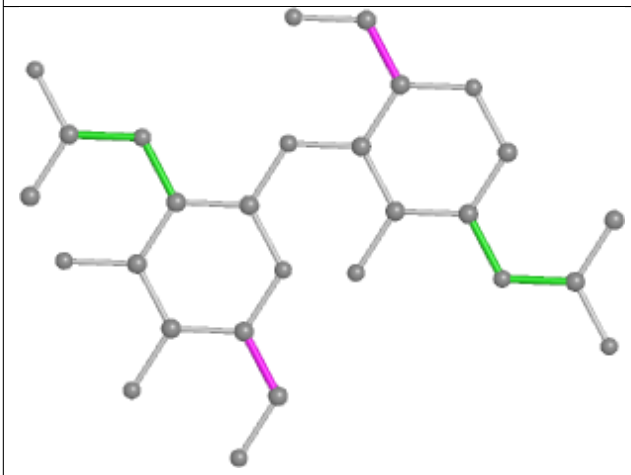
Oligosaccharide Chain D



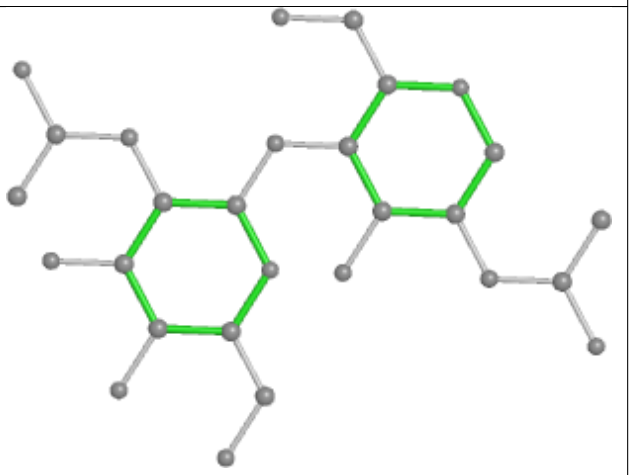
Bond lengths



Bond angles

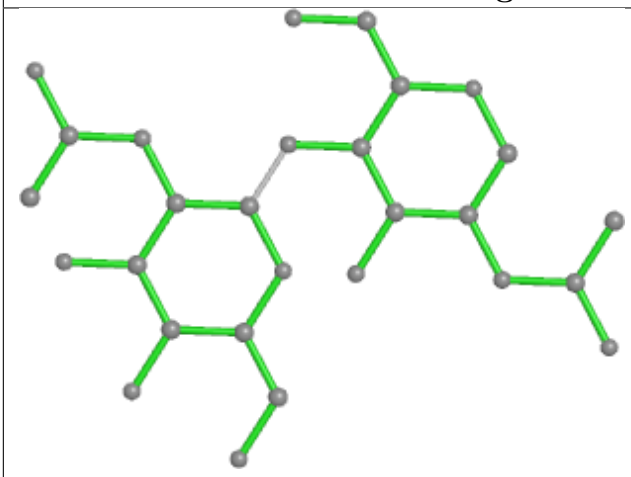


Torsions

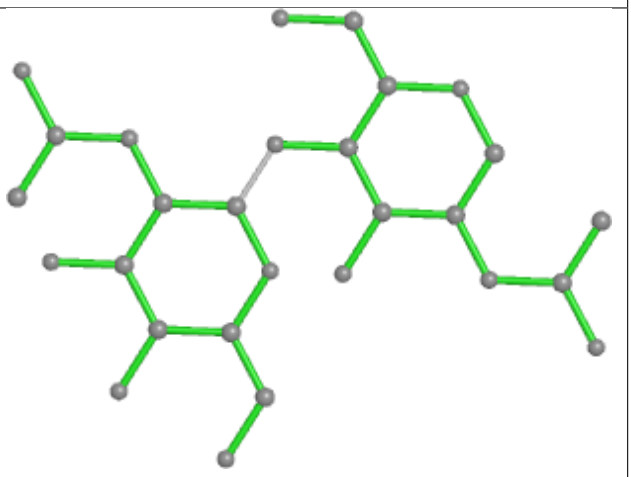


Rings

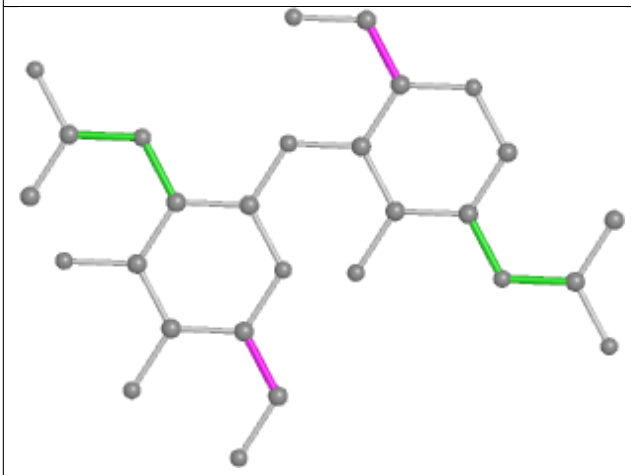
Oligosaccharide Chain E



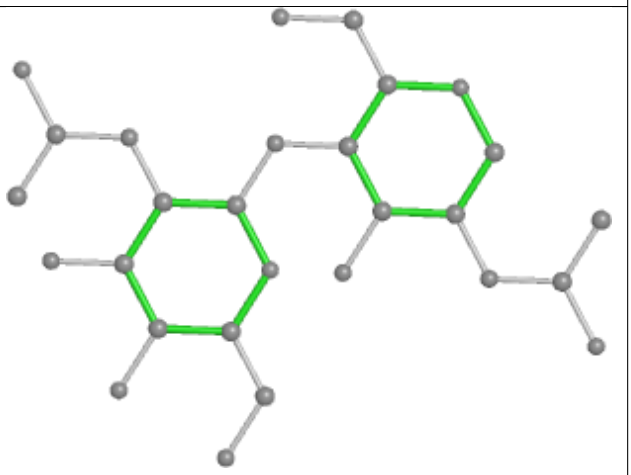
Bond lengths



Bond angles

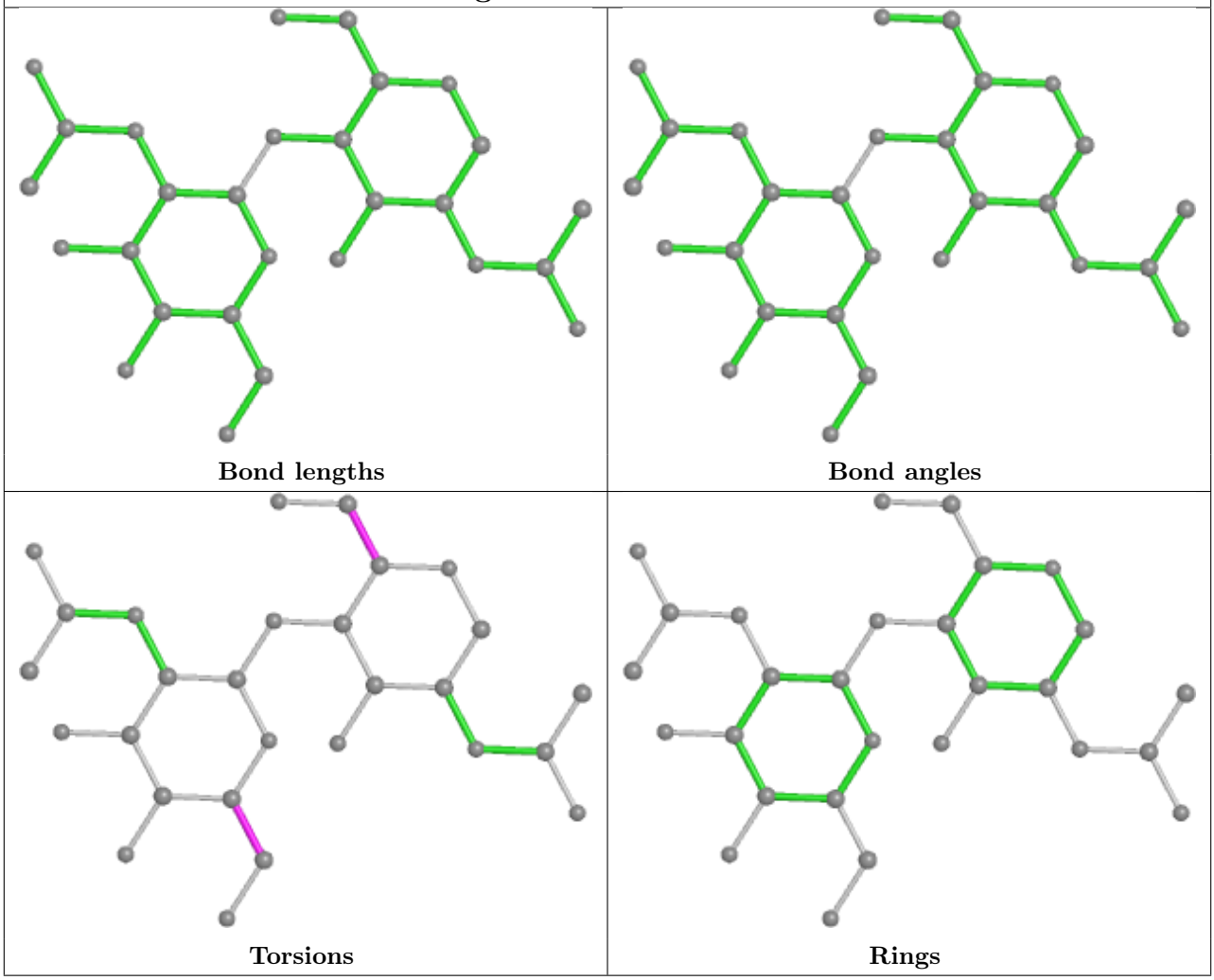


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	GOL	A	416	-	5,5,5	0.86	0	5,5,5	1.01	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
7	GOL	A	416	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	317/319 (99%)	-0.09	1 (0%)	94	92	45, 68, 94, 118	0
2	B	163/176 (92%)	0.07	1 (0%)	89	84	39, 80, 114, 135	0
3	H	223/235 (94%)	0.59	35 (15%)	2	1	51, 92, 193, 206	0
4	L	213/213 (100%)	0.57	29 (13%)	3	2	57, 127, 192, 207	0
All	All	916/943 (97%)	0.26	66 (7%)	15	9	39, 81, 186, 207	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	182	VAL	7.3
3	H	126	PRO	6.7
3	H	137	ALA	5.9
3	H	138	LEU	5.7
3	H	1	GLN	5.6
3	H	181	VAL	5.1
4	L	134	CYS	5.0
4	L	187	SER	4.8
4	L	120	PRO	4.7
3	H	184	VAL	4.7
4	L	152	SER	4.5
3	H	136	ALA	4.5
4	L	119	PRO	4.3
4	L	135	LEU	4.1
3	H	194	TYR	4.0
3	H	183	THR	4.0
4	L	116	THR	3.9
4	L	122	SER	3.8
3	H	206	LYS	3.7
4	L	191	TYR	3.6
3	H	191	THR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	L	188	HIS	3.5
3	H	210	ARG	3.4
3	H	121	VAL	3.3
3	H	207	VAL	3.2
4	L	155	VAL	3.2
4	L	136	ILE	3.1
4	L	201	THR	3.1
3	H	139	GLY	3.0
3	H	190	GLY	3.0
3	H	185	PRO	3.0
3	H	115	SER	2.9
3	H	125	ALA	2.9
3	H	187	SER	2.9
4	L	12	SER	2.9
4	L	127	ALA	2.9
2	B	32	ARG	2.8
4	L	106(A)	LEU	2.8
4	L	160	GLU	2.7
3	H	193	THR	2.7
4	L	176	SER	2.7
3	H	213	PRO	2.7
4	L	161	THR	2.6
3	H	192	GLN	2.5
4	L	144	VAL	2.5
4	L	154	PRO	2.5
4	L	110	LYS	2.4
4	L	192	SER	2.4
3	H	155	ASN	2.4
3	H	211	VAL	2.4
4	L	125	LEU	2.4
3	H	124	LEU	2.3
4	L	121	SER	2.3
3	H	2	VAL	2.2
4	L	145	THR	2.2
3	H	114	ALA	2.2
3	H	159	LEU	2.2
3	H	140	CYS	2.2
1	A	325	GLU	2.1
3	H	122	PHE	2.1
3	H	178	LEU	2.1
3	H	120	SER	2.1
4	L	142	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	L	185	TRP	2.1
4	L	104	LEU	2.1
3	H	189	LEU	2.0

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

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

6.3 Carbohydrates (i)

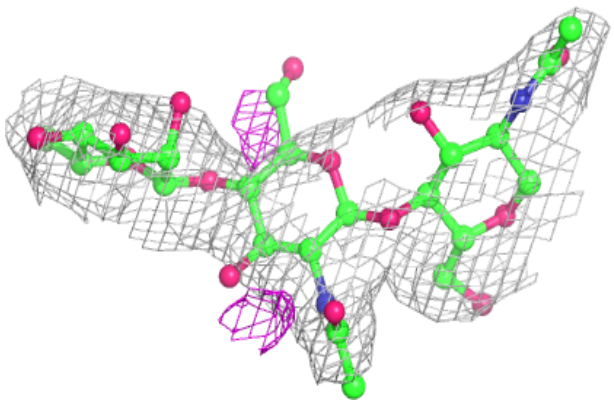
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

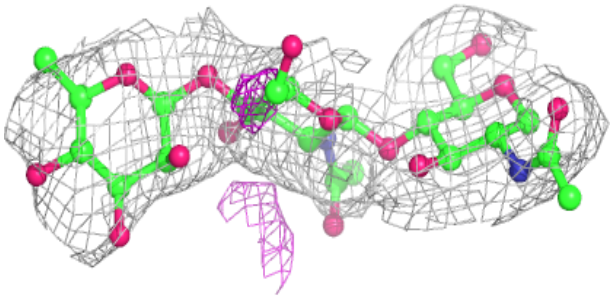
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	I	1	14/15	0.77	0.20	113,127,135,137	0
6	NAG	E	2	14/15	0.81	0.25	99,130,152,154	0
6	NAG	I	2	14/15	0.82	0.32	117,148,161,164	0
6	NAG	D	2	14/15	0.85	0.23	82,118,136,137	0
5	NAG	C	2	14/15	0.85	0.34	93,132,151,154	0
5	BMA	F	3	11/12	0.86	0.12	84,101,105,106	0
5	BMA	G	3	11/12	0.86	0.16	124,136,147,148	0
6	NAG	E	1	14/15	0.88	0.18	69,88,117,136	0
5	BMA	C	3	10/12	0.88	0.26	127,146,151,152	0
5	NAG	G	2	14/15	0.90	0.20	74,98,111,119	0
5	NAG	C	1	14/15	0.91	0.17	79,94,113,131	0
6	NAG	D	1	14/15	0.92	0.17	85,95,126,126	0
5	NAG	F	2	14/15	0.94	0.20	77,90,103,104	0
5	NAG	F	1	14/15	0.94	0.25	59,78,86,93	0
5	NAG	G	1	14/15	0.96	0.15	70,84,101,103	0

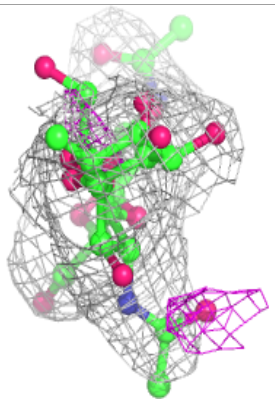
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

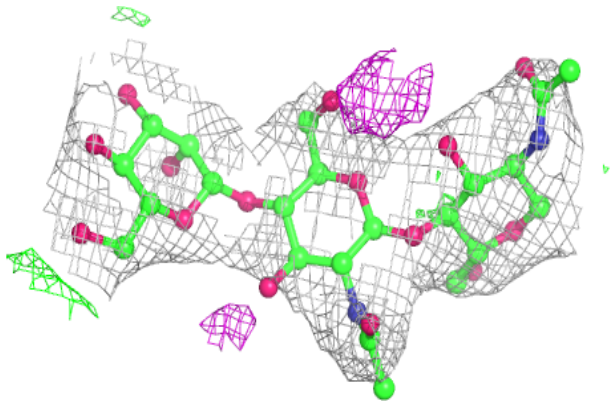


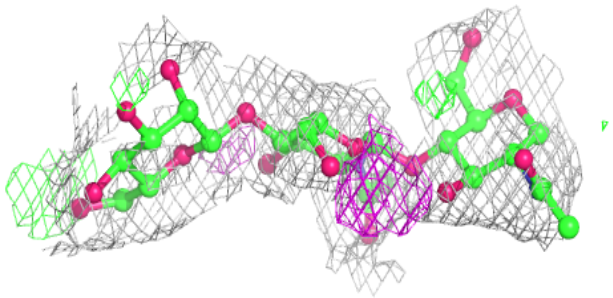


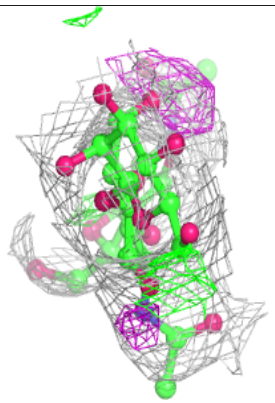


Electron density around Chain F:

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

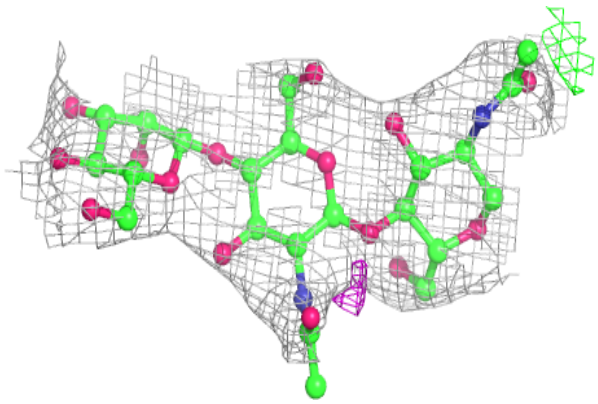


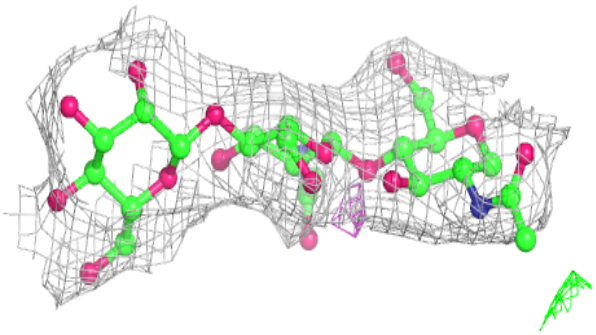


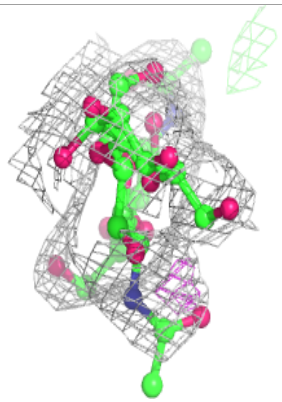


Electron density around Chain G:

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

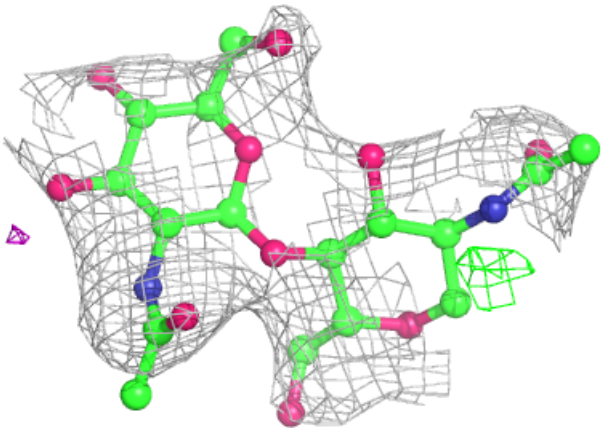


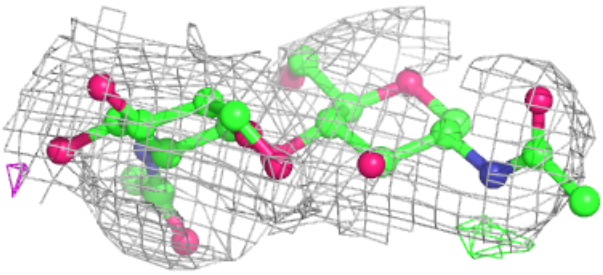


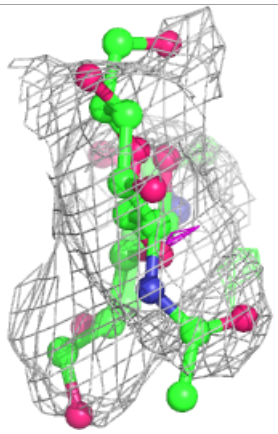


Electron density around Chain D:

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

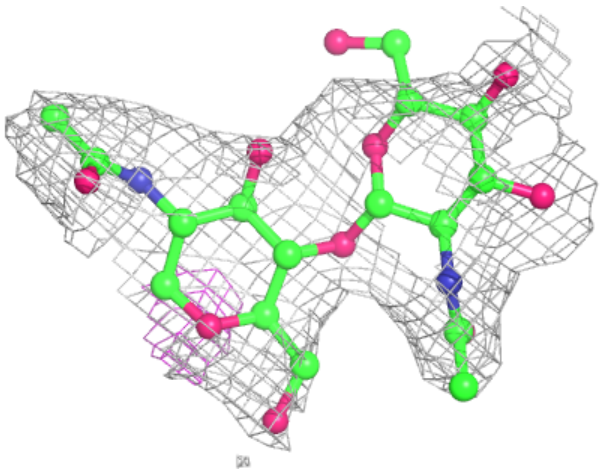


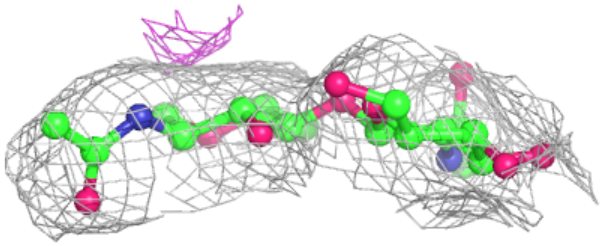


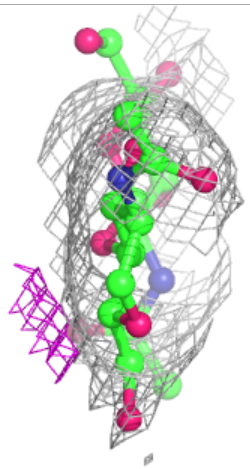


Electron density around Chain E:

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

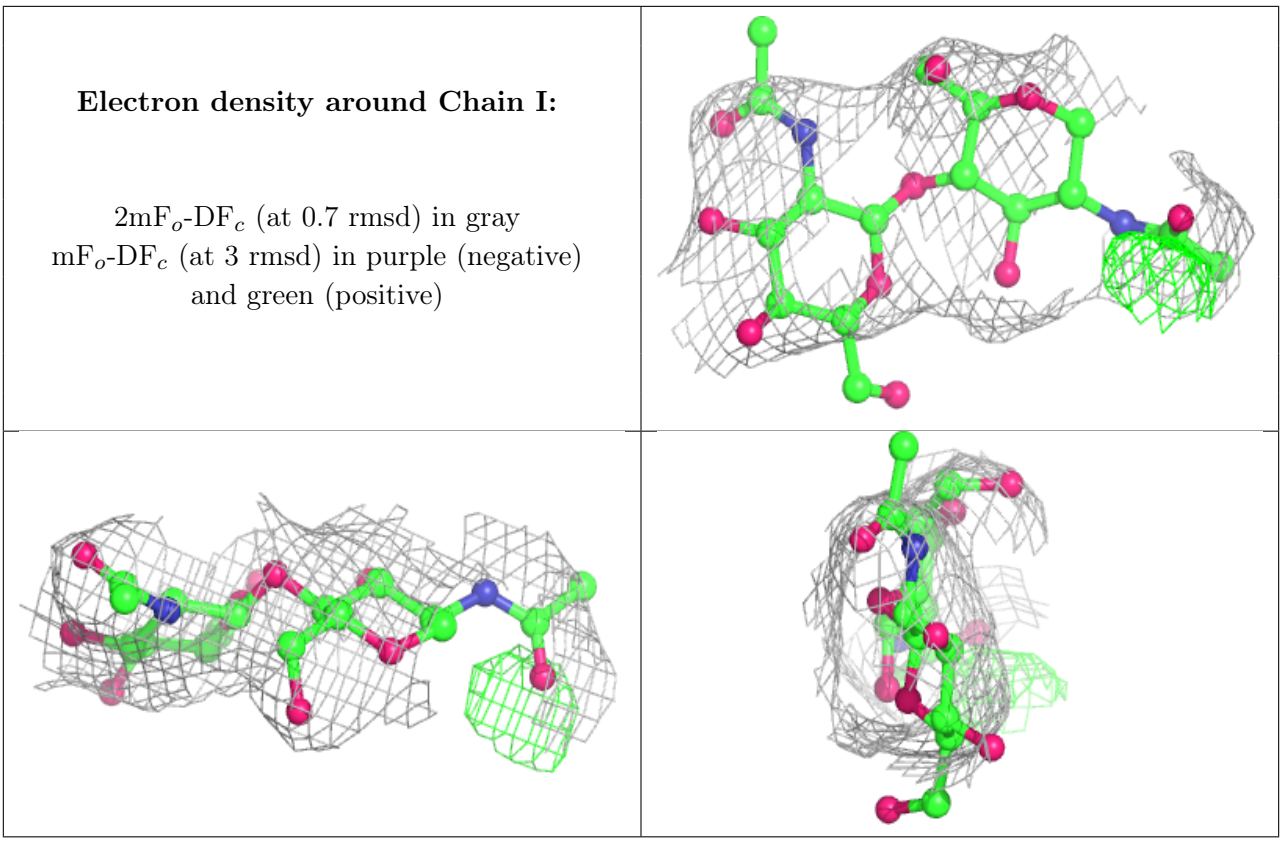






Electron density around Chain I:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	GOL	A	416	6/6	0.83	0.32	67,83,98,103	0

6.5 Other polymers (i)

There are no such residues in this entry.