



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:37 PM UTC

PDB ID : 6WF0 / pdb_00006wf0
Title : Crystal Structure of Broadly Neutralizing Antibody 3I14 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 : 3.46 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

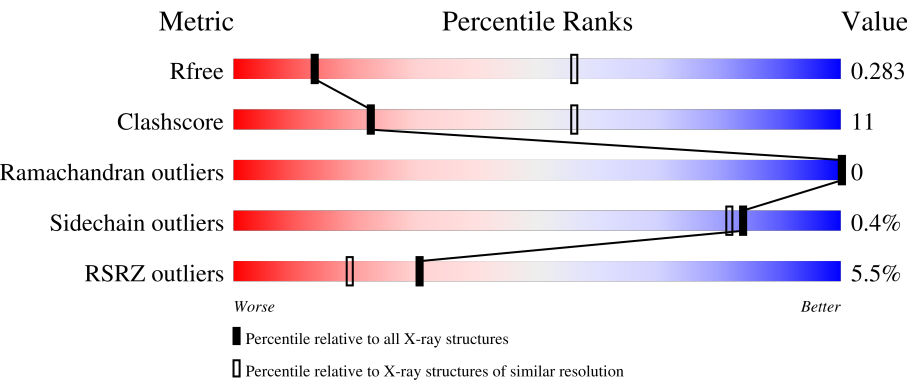
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.46 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.



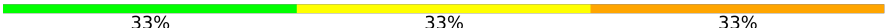
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	317	
2	B	163	
3	H	235	
4	L	213	
5	C	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	3	 33% 33% 33%
5	G	3	 67% 33%
5	I	3	 67% 33%
6	D	2	 50% 50%
6	F	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7170 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	317	Total	C	N	O	S	0	0	0
			2475	1551	441	471	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
2	B	163	Total	C	N	O	S	0	0	0
			1328	821	236	265	6			

- Molecule 3 is a protein called heavy chain.

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

- Molecule 4 is a protein called light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total	C	N	O	S	0	0	0
			1468	916	246	301	5			

- 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
5	C	3	Total	C	N	O	0	0	0
			38	22	2	14			
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	G	3	Total	C	N	O	0	0	0
			39	22	2	15			
5	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

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

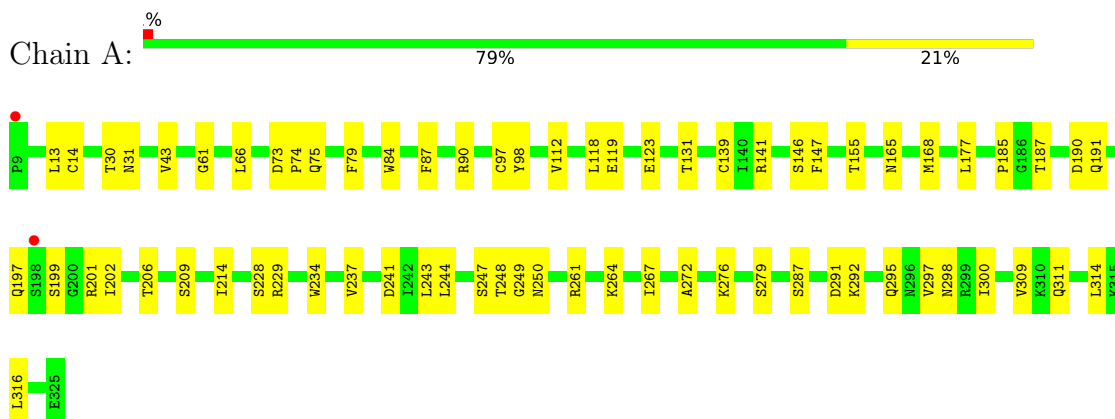


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

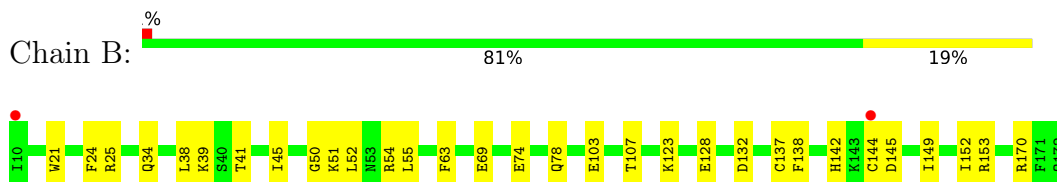
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

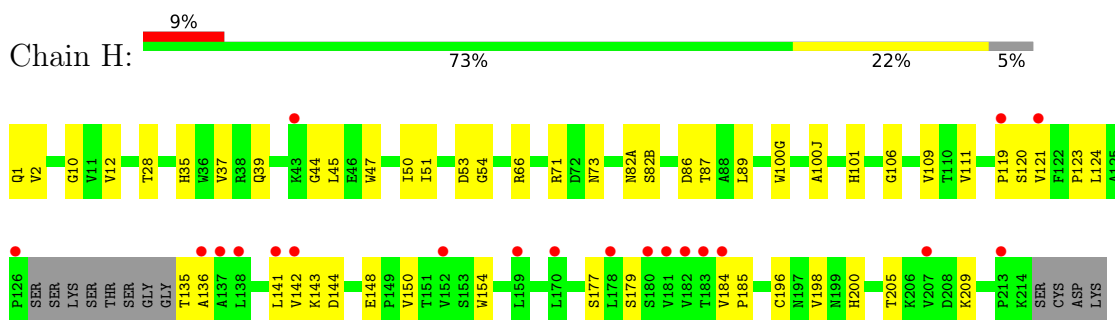
- Molecule 1: Hemagglutinin



- Molecule 2: Hemagglutinin

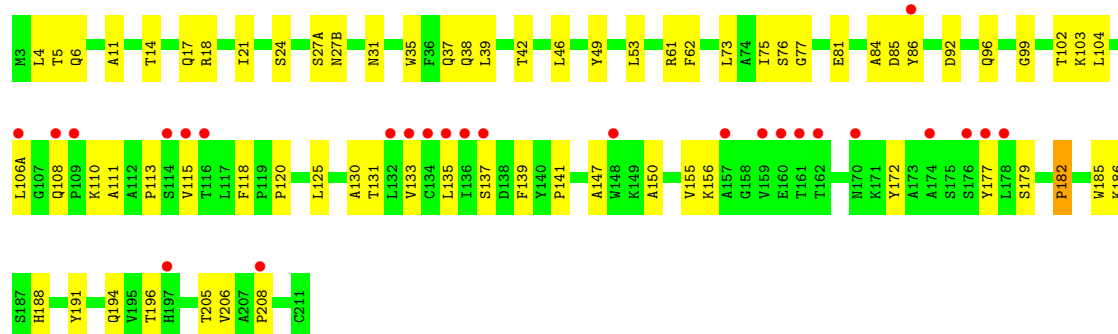


- Molecule 3: heavy chain



- Molecule 4: light chain



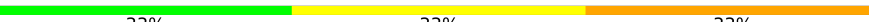


- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:  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 E:  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 G:  67% 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 I:  67% 33%



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

Chain D:  50% 50%



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

Chain F:

100%

M61
M62

4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	130.32Å 130.32Å 188.55Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.66 – 3.46 42.66 – 3.46	Depositor EDS
% Data completeness (in resolution range)	99.1 (42.66-3.46) 99.2 (42.66-3.46)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.231 , 0.282 0.233 , 0.283	Depositor DCC
R_{free} test set	1989 reflections (8.35%)	wwPDB-VP
Wilson B-factor (Å ²)	94.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7170	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.17	0/2532	0.38	0/3443
2	B	0.11	0/1350	0.31	0/1812
3	H	0.14	0/1734	0.43	0/2363
4	L	0.15	0/1498	0.39	0/2039
All	All	0.15	0/7114	0.38	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	47	0
2	B	1328	0	1255	26	0
3	H	1688	0	1656	40	0
4	L	1468	0	1301	47	0
5	C	38	0	31	0	0
5	E	39	0	34	1	0
5	G	39	0	34	0	0
5	I	39	0	34	1	0
6	D	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	F	28	0	25	0	0
All	All	7170	0	6818	147	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 11.

All (147) 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	1.59	1.00
3:H:136:ALA:HB3	3:H:184:VAL:O	1.76	0.86
4:L:115:VAL:HA	4:L:135:LEU:O	1.78	0.83
1:A:87:PHE:HB3	1:A:267:ILE:HG13	1.68	0.76
1:A:97:CYS:SG	1:A:98:TYR:N	2.59	0.74
3:H:66:ARG:NH2	3:H:86:ASP:OD2	2.24	0.70
3:H:66:ARG:NH1	3:H:82(A):ASN:O	2.25	0.70
4:L:120:PRO:HB3	4:L:131:THR:H	1.57	0.69
1:A:191:GLN:OE1	1:A:250:ASN:ND2	2.25	0.68
1:A:197:GLN:NE2	1:A:199:SER:O	2.29	0.66
4:L:14:THR:HG22	4:L:106(A):LEU:HB2	1.77	0.66
2:B:74:GLU:HB2	2:B:78:GLN:HB2	1.77	0.66
3:H:71:ARG:NH1	3:H:73:ASN:OD1	2.29	0.66
4:L:6:GLN:NE2	4:L:86:TYR:O	2.29	0.65
1:A:131:THR:HB	1:A:155:THR:HG23	1.79	0.63
4:L:111:ALA:O	4:L:113:PRO:HD3	1.99	0.63
2:B:128:GLU:O	2:B:170:ARG:NH1	2.32	0.62
3:H:89:LEU:HD22	3:H:106:GLY:HA3	1.82	0.62
1:A:295:GLN:NE2	1:A:298:ASN:O	2.34	0.61
1:A:123:GLU:HB3	1:A:168:MET:HE2	1.83	0.61
4:L:125:LEU:HD11	4:L:130:ALA:HB2	1.82	0.60
1:A:13:LEU:HD11	2:B:24:PHE:HB3	1.82	0.60
1:A:206:THR:OG1	1:A:209:SER:OG	2.20	0.59
3:H:143:LYS:HG2	3:H:144:ASP:H	1.67	0.59
1:A:119:GLU:OE1	1:A:261:ARG:NH2	2.36	0.58
1:A:228:SER:O	1:A:229:ARG:NH1	2.31	0.58
1:A:237:VAL:HG13	1:A:241:ASP:HB3	1.84	0.58
1:A:185:PRO:HA	1:A:228:SER:HB3	1.86	0.58
4:L:185:TRP:HB2	4:L:188:HIS:CE1	2.37	0.58
3:H:124:LEU:HD23	4:L:118:PHE:HB3	1.86	0.58
3:H:12:VAL:HG13	3:H:111:VAL:HG12	1.86	0.58
2:B:21:TRP:H	2:B:41:THR:HG21	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:155:VAL:HG12	4:L:156:LYS:H	1.69	0.57
4:L:11:ALA:HB3	4:L:104:LEU:HB3	1.86	0.57
1:A:311:GLN:HG2	1:A:314:LEU:HD21	1.87	0.56
3:H:47:TRP:HZ2	3:H:50:ILE:HG22	1.70	0.56
4:L:182:PRO:O	4:L:186:LYS:N	2.39	0.56
4:L:130:ALA:O	4:L:179:SER:HA	2.05	0.56
1:A:30:THR:OG1	1:A:31:ASN:OD1	2.23	0.55
1:A:201:ARG:HD3	5:I:1:NAG:C8	2.37	0.55
1:A:187:THR:OG1	1:A:190:ASP:OD1	2.23	0.55
1:A:90:ARG:NH1	1:A:272:ALA:O	2.30	0.54
3:H:143:LYS:HG3	3:H:177:SER:HB2	1.88	0.54
4:L:61:ARG:NH1	4:L:77:GLY:O	2.41	0.54
1:A:295:GLN:OE1	1:A:297:VAL:N	2.41	0.54
3:H:124:LEU:HB3	4:L:118:PHE:HD2	1.74	0.53
2:B:123:LYS:NZ	2:B:132:ASP:OD2	2.39	0.53
1:A:14:CYS:HA	2:B:137:CYS:HA	1.91	0.53
1:A:61:GLY:HA2	1:A:79:PHE:CZ	2.43	0.53
3:H:35:HIS:NE2	4:L:96:GLN:OE1	2.43	0.53
4:L:113:PRO:HB2	4:L:115:VAL:HG23	1.92	0.52
3:H:119:PRO:HD2	3:H:205:THR:HG21	1.92	0.52
4:L:113:PRO:HA	4:L:137:SER:O	2.09	0.51
1:A:141:ARG:NH1	1:A:146:SER:OG	2.43	0.51
4:L:5:THR:OG1	4:L:24:SER:HB3	2.10	0.51
1:A:291:ASP:OD1	1:A:292:LYS:N	2.44	0.51
3:H:121:VAL:HG22	3:H:142:VAL:HG13	1.91	0.51
4:L:205:THR:HG22	4:L:206:VAL:H	1.74	0.51
3:H:101:HIS:ND1	4:L:46:LEU:HB3	2.27	0.50
1:A:300:ILE:HD11	2:B:69:GLU:HG3	1.94	0.50
3:H:37:VAL:HG13	3:H:47:TRP:HA	1.92	0.50
1:A:201:ARG:HG3	1:A:214:ILE:HD11	1.92	0.50
2:B:51:LYS:NZ	2:B:107:THR:OG1	2.41	0.50
3:H:123:PRO:HD3	3:H:209:LYS:HG2	1.94	0.50
1:A:197:GLN:OE1	1:A:248:THR:OG1	2.30	0.49
1:A:264:LYS:HB3	2:B:63:PHE:CD2	2.47	0.49
2:B:45:ILE:HD13	3:H:100(G):TRP:HB3	1.95	0.49
2:B:142:HIS:CE1	2:B:144:CYS:HB2	2.46	0.49
4:L:27(B):ASN:OD1	4:L:27(B):ASN:N	2.43	0.49
1:A:206:THR:HG21	1:A:237:VAL:HG22	1.94	0.49
4:L:14:THR:N	4:L:17:GLN:OE1	2.46	0.49
4:L:133:VAL:HG13	4:L:177:TYR:HB3	1.94	0.49
4:L:139:PHE:O	4:L:172:TYR:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:135:THR:HA	3:H:185:PRO:HA	1.94	0.48
4:L:21:ILE:HD13	4:L:102:THR:HG21	1.94	0.48
1:A:316:LEU:HD22	2:B:55:LEU:HD12	1.96	0.48
4:L:27(A):SER:OG	4:L:92:ASP:OD2	2.31	0.48
1:A:84:TRP:HZ3	1:A:118:LEU:HG	1.78	0.47
3:H:142:VAL:HG11	3:H:198:VAL:HG11	1.95	0.47
4:L:150:ALA:HA	4:L:191:TYR:HB3	1.95	0.47
2:B:149:ILE:O	2:B:153:ARG:HG3	2.14	0.47
1:A:165:ASN:OD1	1:A:244:LEU:HD11	2.14	0.47
1:A:74:PRO:HB3	1:A:141:ARG:HB2	1.96	0.47
1:A:177:LEU:HD11	1:A:234:TRP:HB2	1.96	0.47
2:B:52:LEU:HB3	3:H:100(J):ALA:HB2	1.96	0.47
1:A:237:VAL:HG21	1:A:243:LEU:HB2	1.96	0.47
5:E:1:NAG:H61	5:E:2:NAG:N2	2.30	0.46
3:H:148:GLU:O	3:H:150:VAL:N	2.49	0.46
1:A:43:VAL:HG23	1:A:314:LEU:HB2	1.97	0.45
2:B:50:GLY:HA2	4:L:53:LEU:HD21	1.98	0.45
4:L:81:GLU:OE1	4:L:81:GLU:N	2.46	0.45
4:L:5:THR:OG1	4:L:5:THR:O	2.33	0.45
2:B:51:LYS:HE3	2:B:51:LYS:HB2	1.73	0.45
2:B:123:LYS:HB2	2:B:138:PHE:HZ	1.81	0.45
3:H:120:SER:OG	3:H:144:ASP:OD2	2.23	0.45
2:B:25:ARG:NE	2:B:34:GLN:OE1	2.39	0.45
3:H:200:HIS:HB3	3:H:205:THR:HB	1.98	0.45
4:L:4:LEU:HD11	4:L:27(B):ASN:ND2	2.31	0.45
2:B:24:PHE:CD1	2:B:153:ARG:HD2	2.50	0.45
3:H:51:ILE:HD13	3:H:71:ARG:HB3	1.99	0.45
1:A:202:ILE:HD11	1:A:249:GLY:O	2.17	0.45
1:A:191:GLN:CD	1:A:250:ASN:HD21	2.22	0.45
4:L:85:ASP:OD2	4:L:103:LYS:NZ	2.50	0.44
4:L:147:ALA:HB3	4:L:194:GLN:HB3	1.97	0.44
4:L:108:GLN:O	4:L:110:LYS:N	2.44	0.44
1:A:214:ILE:HD13	1:A:214:ILE:HA	1.84	0.44
3:H:66:ARG:HH11	3:H:82(B):SER:HG	1.65	0.44
3:H:39:GLN:HG3	3:H:44:GLY:O	2.17	0.44
3:H:87:THR:OG1	3:H:111:VAL:HG22	2.17	0.44
3:H:143:LYS:HG2	3:H:144:ASP:N	2.31	0.44
4:L:4:LEU:HB2	4:L:99:GLY:HA2	1.99	0.43
3:H:28:THR:OG1	3:H:28:THR:O	2.35	0.43
2:B:39:LYS:HD3	2:B:39:LYS:HA	1.71	0.43
4:L:139:PHE:HD2	4:L:141:PRO:HD2	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:87:THR:OG1	3:H:111:VAL:N	2.52	0.42
4:L:18:ARG:HG3	4:L:76:SER:HA	2.01	0.42
4:L:37:GLN:NE2	4:L:39:LEU:HD21	2.34	0.42
4:L:49:TYR:O	4:L:53:LEU:HB2	2.20	0.42
1:A:279:SER:HB3	1:A:287:SER:HB3	2.01	0.42
2:B:54:ARG:NH2	2:B:103:GLU:OE2	2.52	0.42
3:H:53:ASP:OD1	3:H:54:GLY:N	2.53	0.42
4:L:39:LEU:O	4:L:42:THR:OG1	2.29	0.42
1:A:309:VAL:HG23	1:A:311:GLN:H	1.85	0.42
1:A:276:LYS:HE2	1:A:276:LYS:HB2	1.87	0.42
1:A:66:LEU:HD21	1:A:112:VAL:HG12	2.01	0.42
2:B:149:ILE:O	2:B:152:ILE:HB	2.20	0.42
1:A:247:SER:OG	1:A:248:THR:N	2.52	0.42
3:H:1:GLN:HG2	3:H:2:VAL:H	1.83	0.42
2:B:21:TRP:H	2:B:41:THR:CG2	2.31	0.42
4:L:38:GLN:O	4:L:84:ALA:HB1	2.19	0.41
1:A:73:ASP:OD1	1:A:75:GLN:HG2	2.20	0.41
3:H:10:GLY:O	3:H:109:VAL:HA	2.20	0.41
2:B:38:LEU:O	2:B:41:THR:OG1	2.36	0.41
3:H:141:LEU:HD13	3:H:179:SER:HB3	2.01	0.41
2:B:39:LYS:NZ	4:L:31:ASN:OD1	2.38	0.41
4:L:62:PHE:HD1	4:L:75:ILE:HG12	1.85	0.41
3:H:39:GLN:HE22	4:L:38:GLN:HE22	1.69	0.41
3:H:66:ARG:NH1	3:H:82(B):SER:OG	2.50	0.41
3:H:45:LEU:HD23	3:H:45:LEU:HA	1.77	0.41
3:H:154:TRP:CZ3	3:H:196:CYS:HB3	2.56	0.41
1:A:30:THR:OG1	1:A:31:ASN:N	2.53	0.41
2:B:145:ASP:OD1	2:B:145:ASP:N	2.46	0.41
4:L:35:TRP:CE2	4:L:73:LEU:HB2	2.56	0.41
3:H:143:LYS:HG3	3:H:177:SER:CB	2.50	0.40
1:A:146:SER:OG	1:A:147:PHE:N	2.55	0.40
1:A:139:CYS:HB3	1:A:146:SER:O	2.20	0.40
4:L:6:GLN:HE21	4:L:102:THR:CB	2.33	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	315/317 (99%)	301 (96%)	14 (4%)	0	100	100
2	B	161/163 (99%)	152 (94%)	9 (6%)	0	100	100
3	H	219/235 (93%)	204 (93%)	15 (7%)	0	100	100
4	L	211/213 (99%)	178 (84%)	33 (16%)	0	100	100
All	All	906/928 (98%)	835 (92%)	71 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/280 (100%)	280 (100%)	0	100	100
2	B	141/141 (100%)	141 (100%)	0	100	100
3	H	187/198 (94%)	187 (100%)	0	100	100
4	L	148/177 (84%)	145 (98%)	3 (2%)	48	67
All	All	756/796 (95%)	753 (100%)	3 (0%)	84	81

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	182	PRO
4	L	196	THR
4	L	208	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	191	GLN
1	A	250	ASN
2	B	65	GLN
3	H	39	GLN
4	L	38	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 ⓘ

16 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	1,5	14,14,15	0.20	0	17,19,21	0.55	0
5	NAG	C	2	5	14,14,15	0.19	0	17,19,21	0.60	0
5	BMA	C	3	5	10,10,12	0.75	0	14,14,17	0.69	0
6	NAG	D	1	6,1	14,14,15	0.71	1 (7%)	17,19,21	0.47	0
6	NAG	D	2	6	14,14,15	0.30	0	17,19,21	0.42	0
5	NAG	E	1	1,5	14,14,15	0.35	0	17,19,21	0.72	1 (5%)
5	NAG	E	2	5	14,14,15	0.66	0	17,19,21	0.57	0
5	BMA	E	3	5	11,11,12	0.62	0	15,15,17	0.70	0
6	NAG	F	1	6,1	14,14,15	0.26	0	17,19,21	0.46	0
6	NAG	F	2	6	14,14,15	0.30	0	17,19,21	0.58	0
5	NAG	G	1	1,5	14,14,15	0.39	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	2	5	14,14,15	0.30	0	17,19,21	0.45	0
5	BMA	G	3	5	11,11,12	0.76	0	15,15,17	0.91	1 (6%)
5	NAG	I	1	1,5	14,14,15	0.61	0	17,19,21	0.87	0
5	NAG	I	2	5	14,14,15	0.32	0	17,19,21	0.49	0
5	BMA	I	3	5	11,11,12	0.55	0	15,15,17	0.78	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	1,5	-	0/6/23/26	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	6,1	-	2/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
6	NAG	F	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
5	NAG	G	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	BMA	G	3	5	-	1/2/19/22	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	BMA	I	3	5	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	1	NAG	O5-C1	-2.52	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1	NAG	C1-O5-C5	2.47	115.49	112.19
5	G	3	BMA	C1-O5-C5	2.42	115.42	112.19

There are no chirality outliers.

All (20) torsion outliers are listed below:

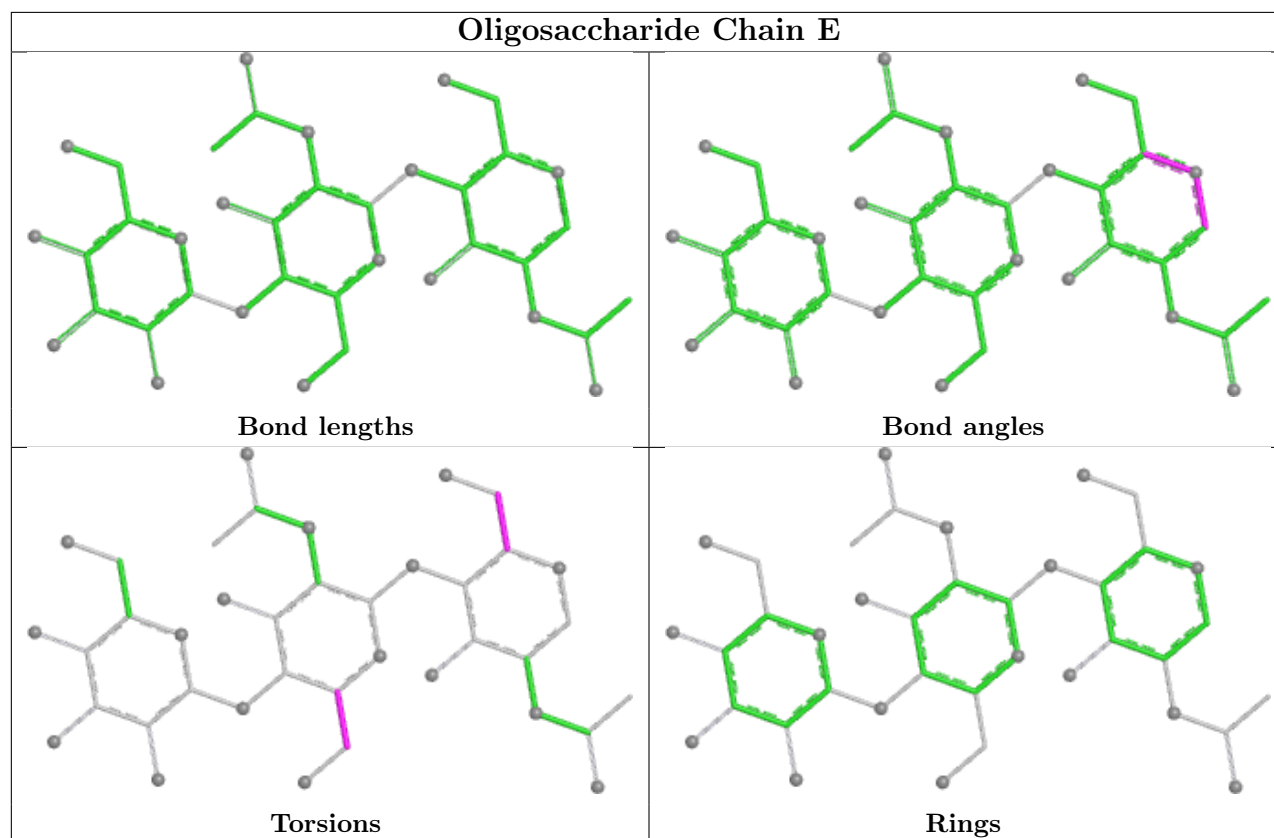
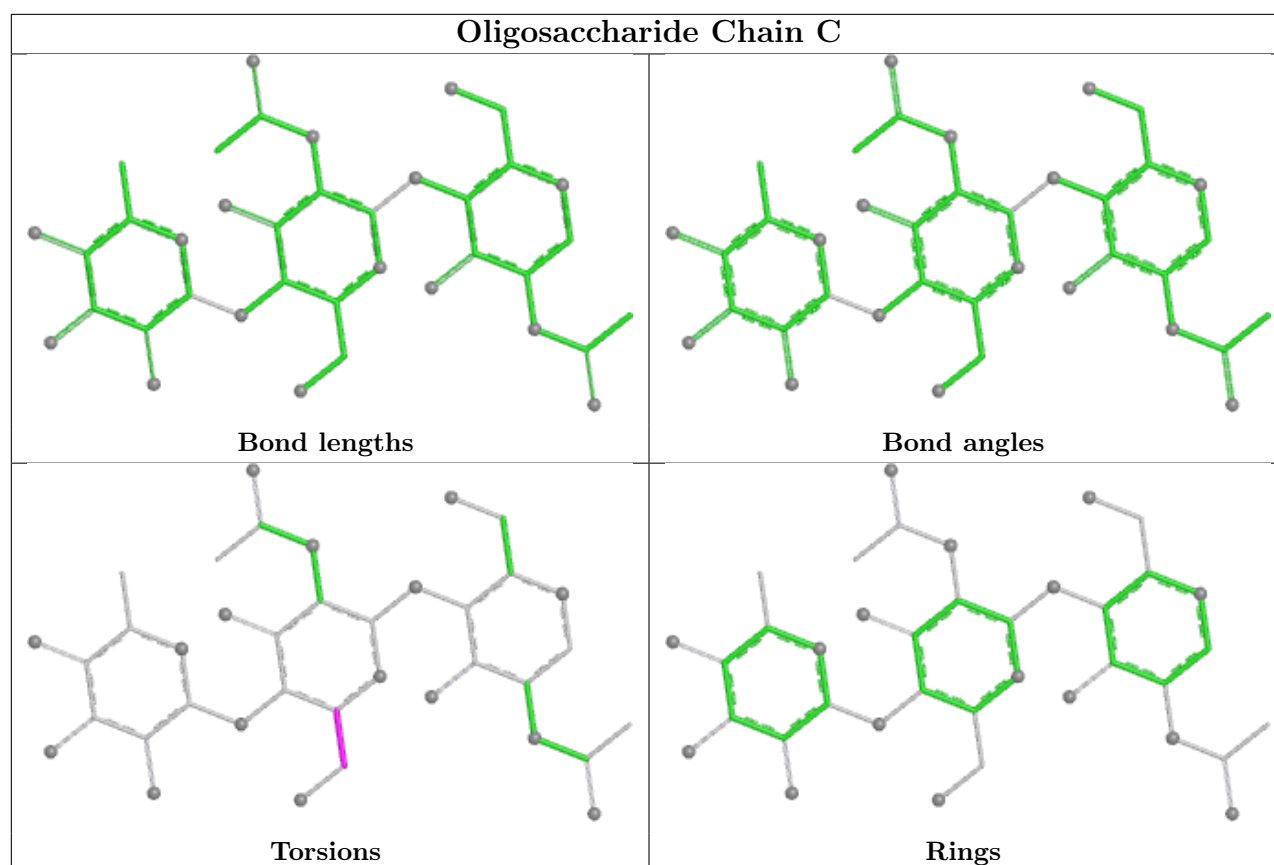
Mol	Chain	Res	Type	Atoms
5	I	1	NAG	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
6	F	1	NAG	O5-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
6	D	1	NAG	O5-C5-C6-O6
6	D	1	NAG	C4-C5-C6-O6
6	F	1	NAG	C4-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	C	2	NAG	O5-C5-C6-O6
6	D	2	NAG	C4-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6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

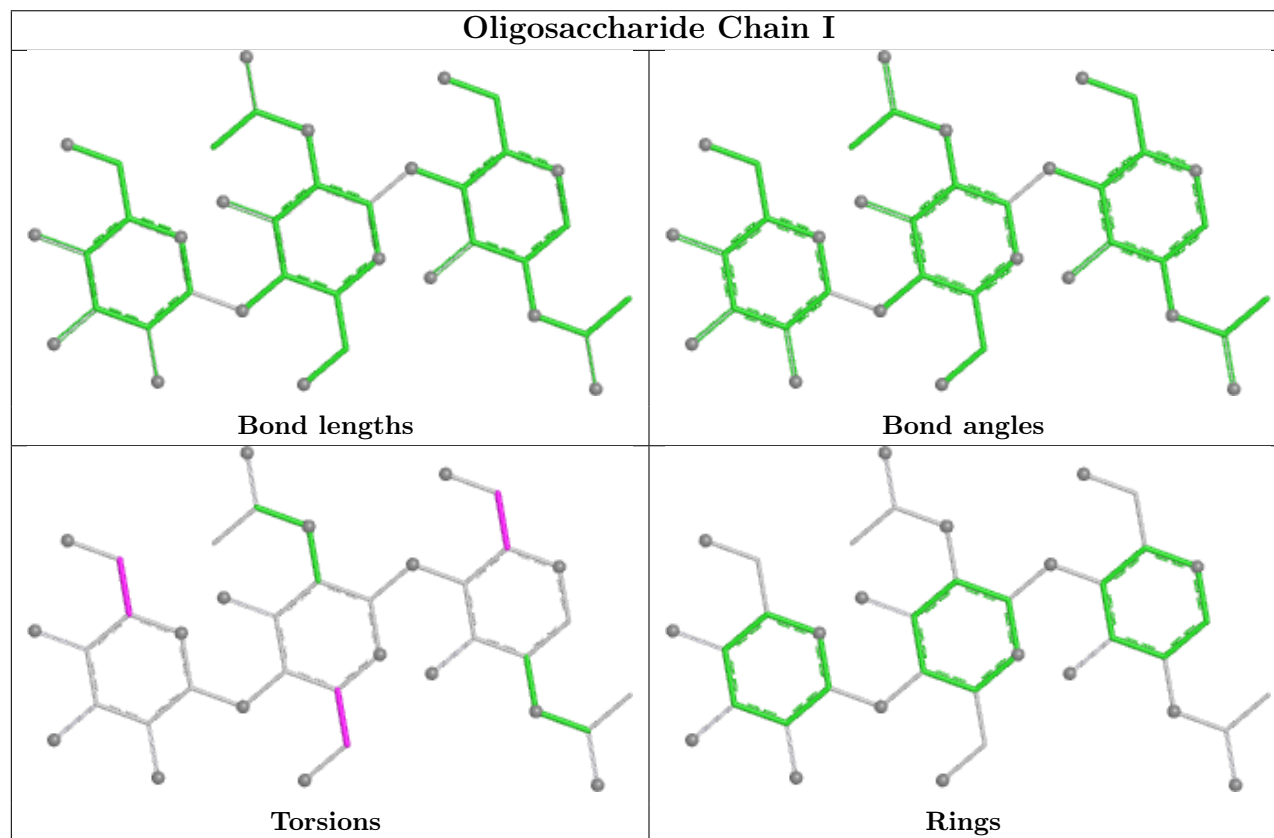
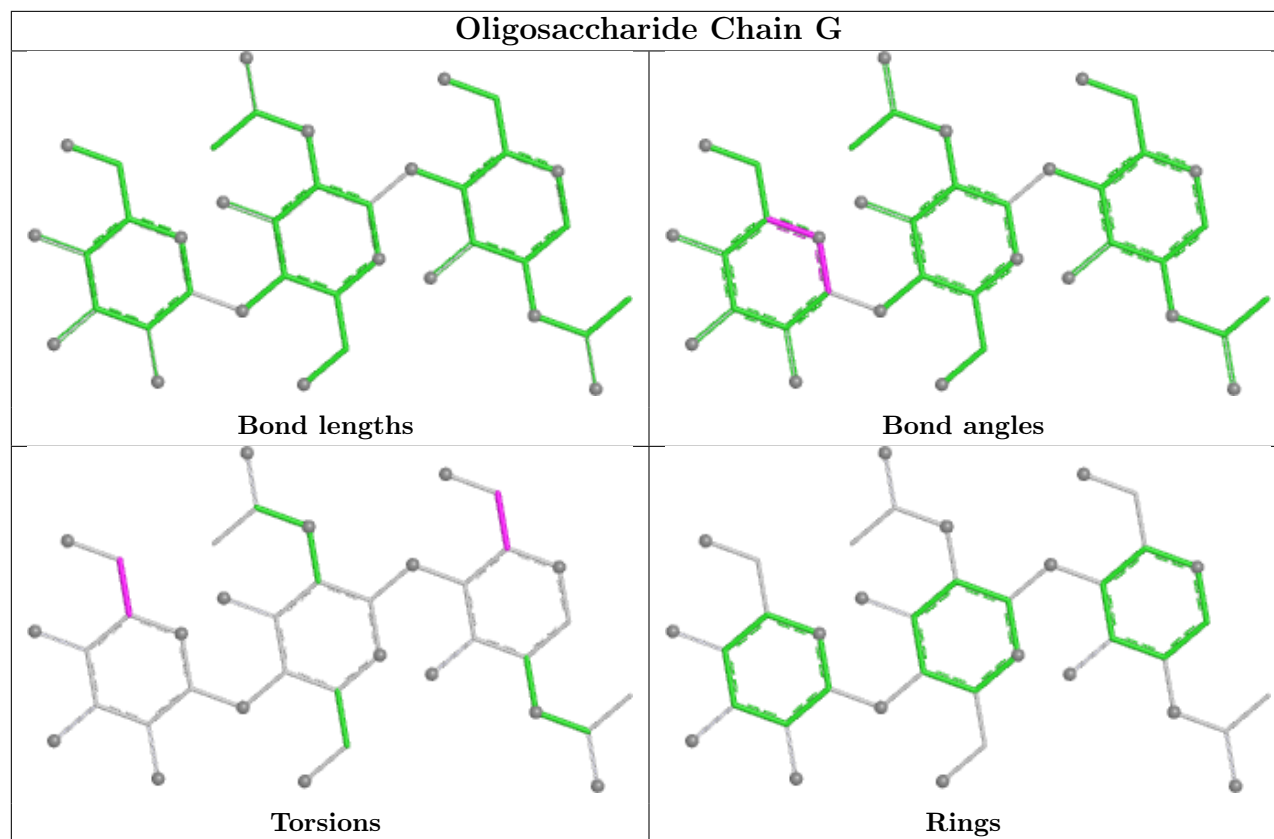
There are no ring outliers.

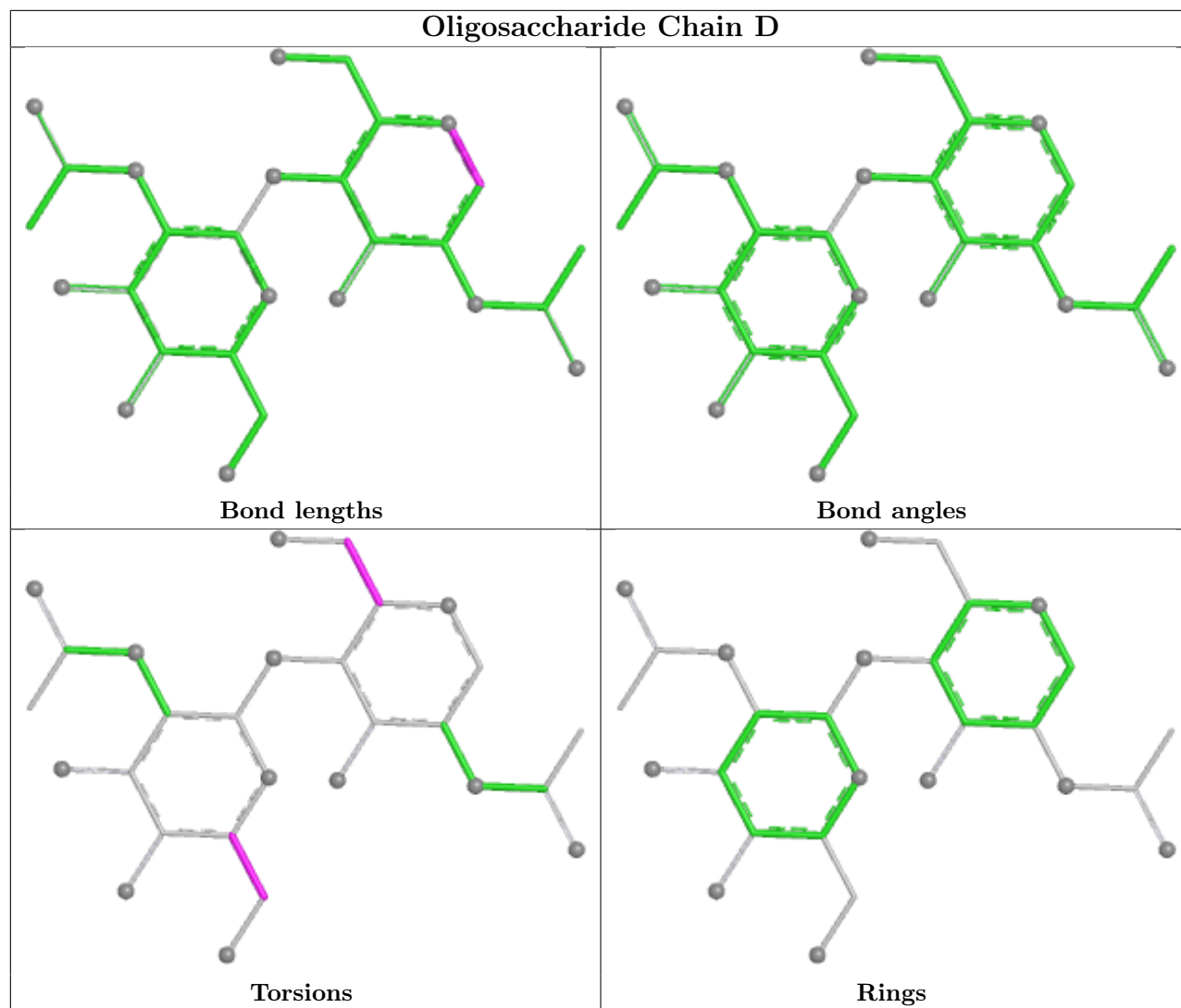
3 monomers are involved in 2 short contacts:

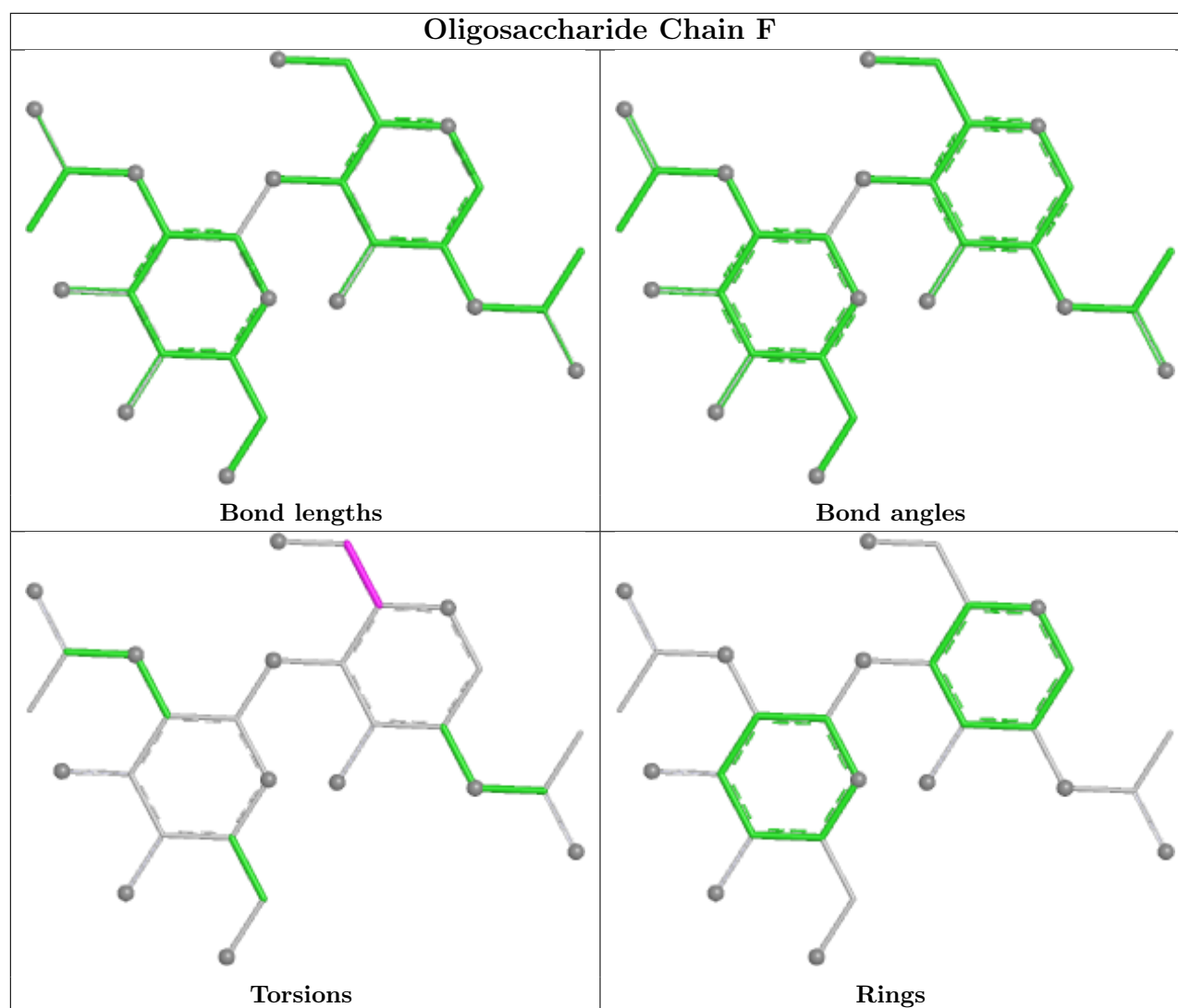
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	1	NAG	1	0
5	E	2	NAG	1	0
5	E	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	317/317 (100%)	-0.10	2 (0%) 85 66	48, 73, 100, 132	0
2	B	163/163 (100%)	-0.02	2 (1%) 76 53	45, 88, 117, 140	0
3	H	223/235 (94%)	0.49	20 (8%) 15 11	57, 103, 190, 205	0
4	L	213/213 (100%)	0.77	26 (12%) 8 7	62, 127, 188, 202	0
All	All	916/928 (98%)	0.26	50 (5%) 30 19	45, 88, 185, 205	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	138	LEU	5.4
4	L	178	LEU	5.1
4	L	134	CYS	4.9
1	A	9	PRO	4.7
4	L	135	LEU	4.6
3	H	137	ALA	4.6
3	H	182	VAL	4.4
4	L	115	VAL	3.9
4	L	160	GLU	3.9
3	H	181	VAL	3.8
4	L	176	SER	3.7
4	L	177	TYR	3.6
3	H	207	VAL	3.5
4	L	86	TYR	3.5
4	L	106(A)	LEU	3.5
4	L	162	THR	3.4
3	H	180	SER	3.2
4	L	133	VAL	3.1
3	H	119	PRO	3.1
2	B	10	ILE	2.9
4	L	208	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	L	174	ALA	2.8
3	H	184	VAL	2.8
4	L	109	PRO	2.8
4	L	136	ILE	2.7
4	L	170	ASN	2.7
4	L	116	THR	2.6
3	H	126	PRO	2.6
3	H	43	LYS	2.6
3	H	170	LEU	2.5
3	H	159	LEU	2.5
3	H	141	LEU	2.5
4	L	137	SER	2.4
4	L	157	ALA	2.4
4	L	148	TRP	2.4
4	L	159	VAL	2.3
4	L	114	SER	2.3
3	H	121	VAL	2.3
3	H	178	LEU	2.3
4	L	132	LEU	2.2
3	H	136	ALA	2.2
1	A	198	SER	2.2
3	H	142	VAL	2.2
4	L	108	GLN	2.2
3	H	183	THR	2.1
3	H	152	VAL	2.1
2	B	144	CYS	2.1
4	L	161	THR	2.1
3	H	213	PRO	2.1
4	L	197	HIS	2.0

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

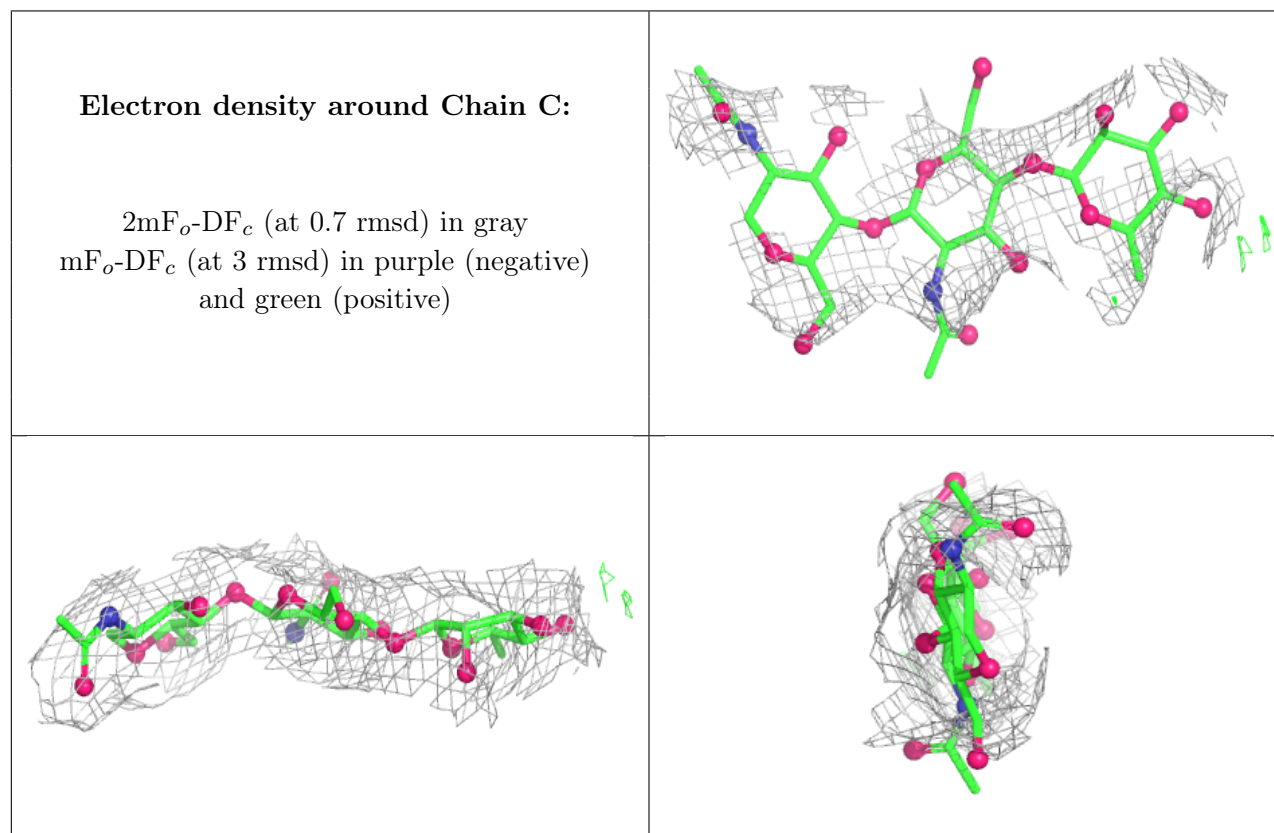
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

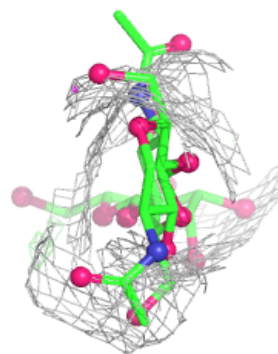
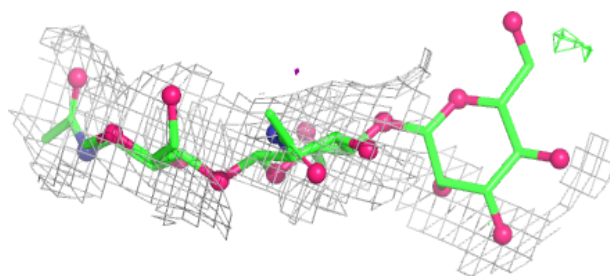
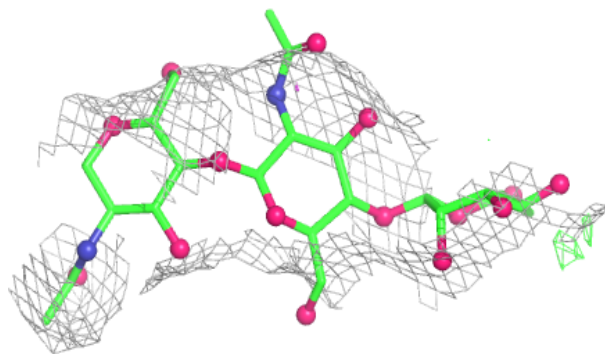
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	C	1	14/15	-	-	85,105,123,132	0
5	NAG	C	2	14/15	-	-	129,150,167,168	0
5	BMA	C	3	10/12	-	-	144,167,194,206	0
5	BMA	E	3	11/12	0.30	0.14	140,173,181,184	0
5	BMA	G	3	11/12	0.48	0.13	85,94,101,107	0
5	NAG	E	2	14/15	0.67	0.12	147,161,175,177	0
5	NAG	G	1	14/15	0.71	0.12	61,72,93,96	0
6	NAG	F	2	14/15	0.74	0.10	104,135,150,153	0
5	NAG	G	2	14/15	0.77	0.10	71,85,99,108	0
6	NAG	F	1	14/15	0.78	0.12	75,104,132,132	0
5	BMA	I	3	11/12	0.78	0.08	124,139,148,151	0
5	NAG	E	1	14/15	0.90	0.09	98,124,138,141	0
6	NAG	D	1	14/15	-	-	91,113,138,144	0
6	NAG	D	2	14/15	-	-	108,130,141,154	0
5	NAG	I	2	14/15	0.91	0.10	90,107,137,147	0
5	NAG	I	1	14/15	0.95	0.08	77,83,104,112	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.

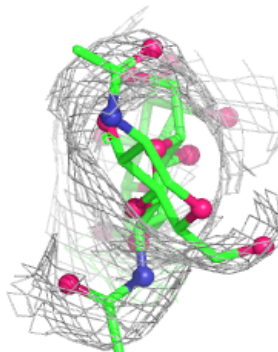
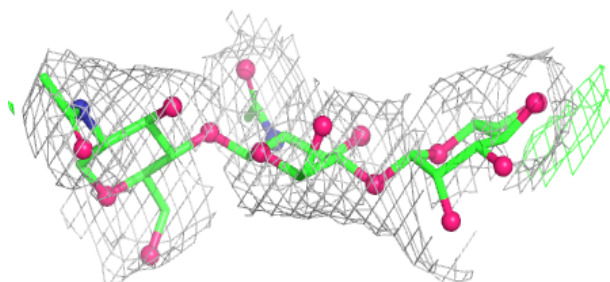
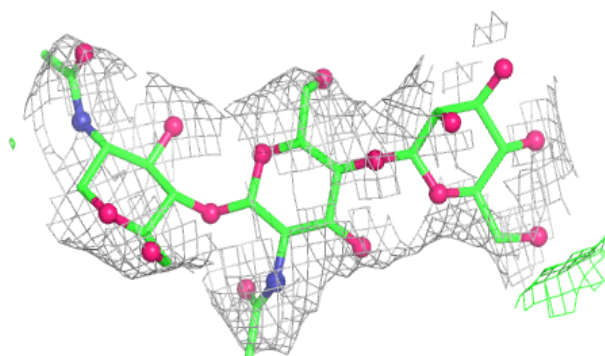


Electron density around Chain E:

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

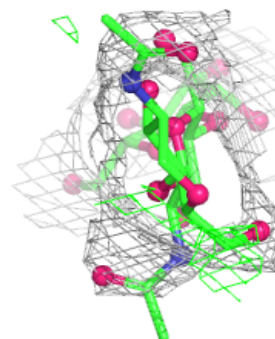
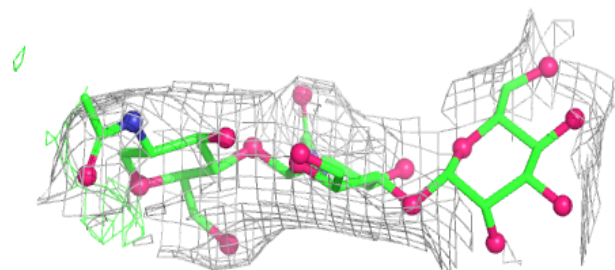
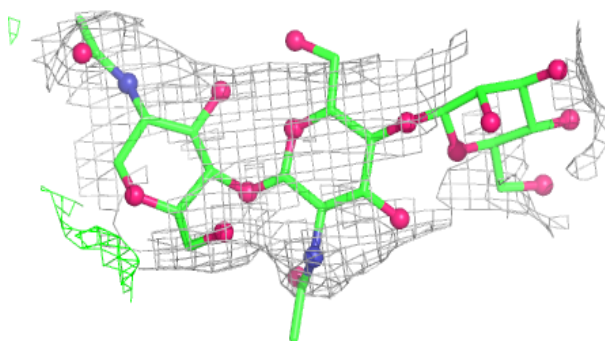
**Electron density around Chain G:**

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

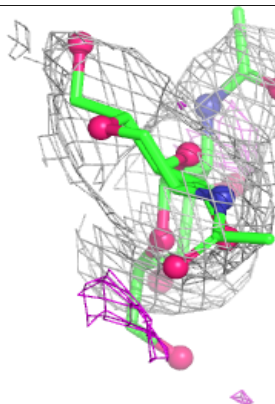
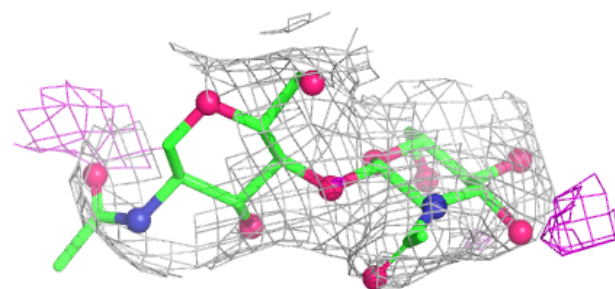
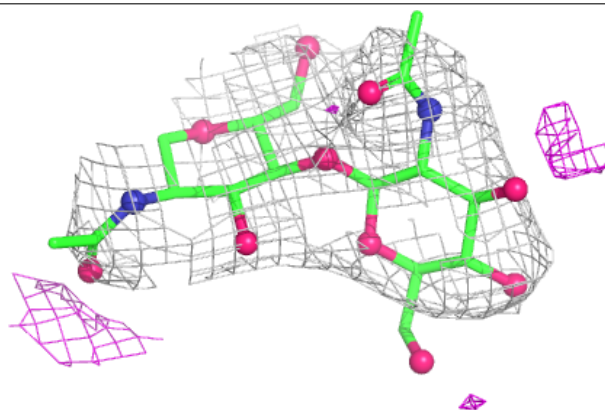


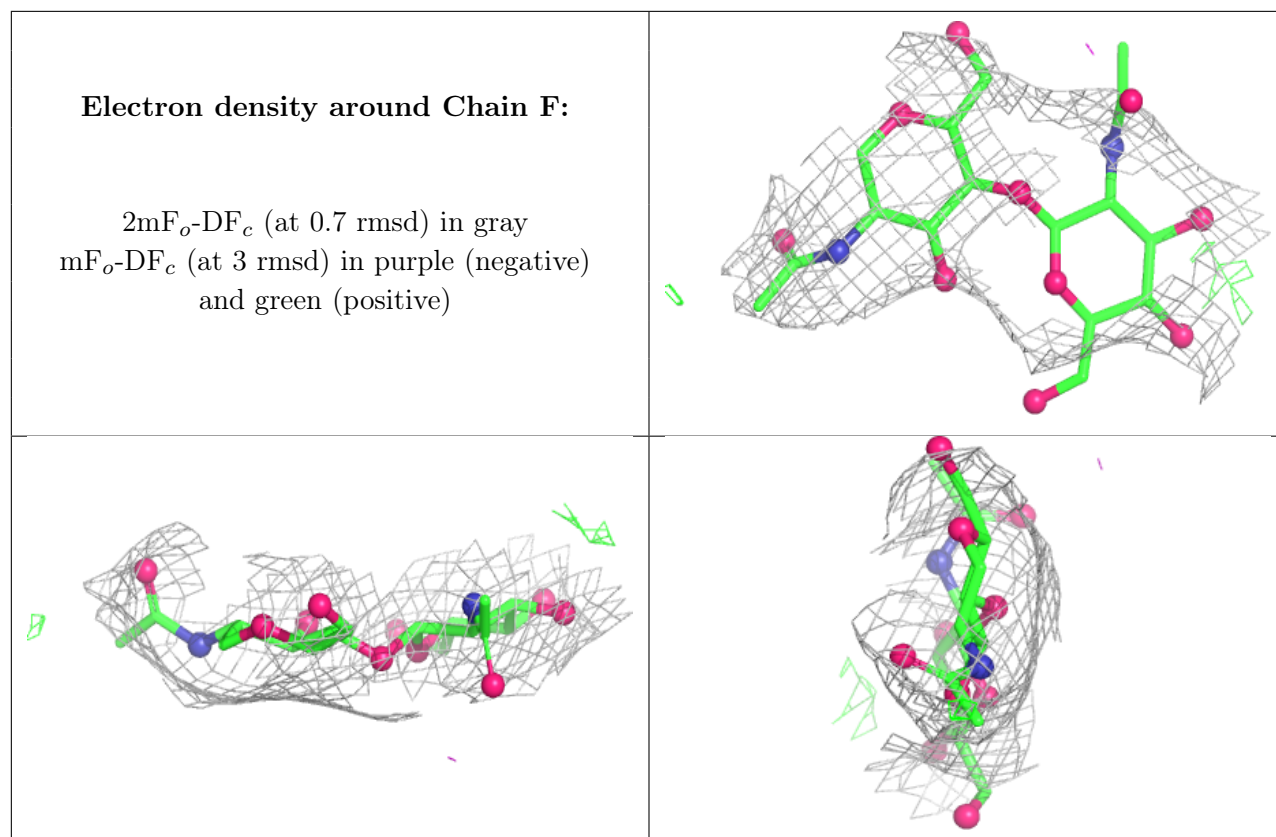
Electron density around Chain I:

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

**Electron density around Chain D:**

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





6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.