



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:59 PM BST

PDB ID : 6VFR
Title : Crystal structure of human protocadherin 18 EC1-EC4
Authors : Harrison, O.J.; Brasch, J.; Shapiro, L.
Deposited on : 2020-01-06
Resolution : 2.79 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 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 : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

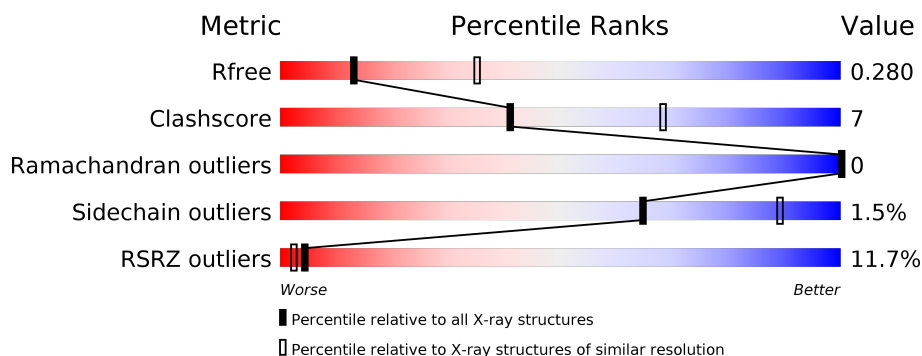
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	436	<div> <div>15%</div> <div> <div></div> <div>81%</div> <div>17%</div> <div></div> </div> </div>
1	B	436	<div> <div>8%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div></div> </div> </div>
2	C	4	<div> <div></div> <div>100%</div> </div>
3	D	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
4	E	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>
5	F	6	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>

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
7	EDO	B	518	-	-	-	X

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 13535 atoms, of which 6487 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.

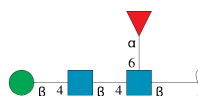
- Molecule 1 is a protein called Protocadherin-18.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total	C	H	N	O	S	0	1	0
			6596	2117	3222	571	678	8			
1	B	428	Total	C	H	N	O	S	0	0	0
			6562	2113	3194	570	677	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	HIS	-	expression tag	UNP Q9HCL0
A	432	HIS	-	expression tag	UNP Q9HCL0
A	433	HIS	-	expression tag	UNP Q9HCL0
A	434	HIS	-	expression tag	UNP Q9HCL0
A	435	HIS	-	expression tag	UNP Q9HCL0
A	436	HIS	-	expression tag	UNP Q9HCL0
B	431	HIS	-	expression tag	UNP Q9HCL0
B	432	HIS	-	expression tag	UNP Q9HCL0
B	433	HIS	-	expression tag	UNP Q9HCL0
B	434	HIS	-	expression tag	UNP Q9HCL0
B	435	HIS	-	expression tag	UNP Q9HCL0
B	436	HIS	-	expression tag	UNP Q9HCL0

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



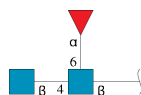
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			49	28	2	19			

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



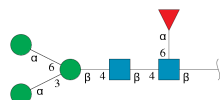
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	3	Total	C	H	N	O	0	0	0
			61	22	23	2	14			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	9	Total	Ca	0	0
			9	9		
6	A	9	Total	Ca	0	0
			9	9		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

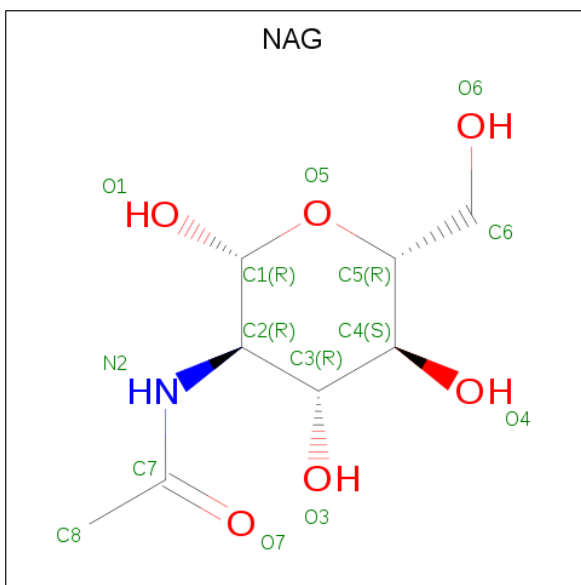


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	A	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		
7	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Na	0	0
			1	1		
8	A	1	Total	Na	0	0
			1	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

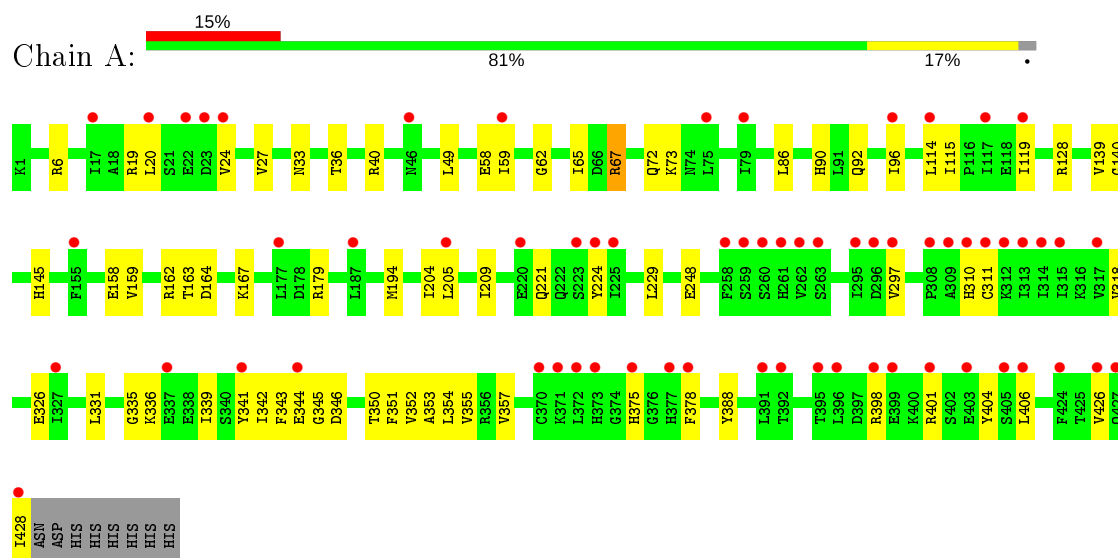
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	26	Total	O	0	0
			26	26		
10	B	18	Total	O	0	0
			18	18		

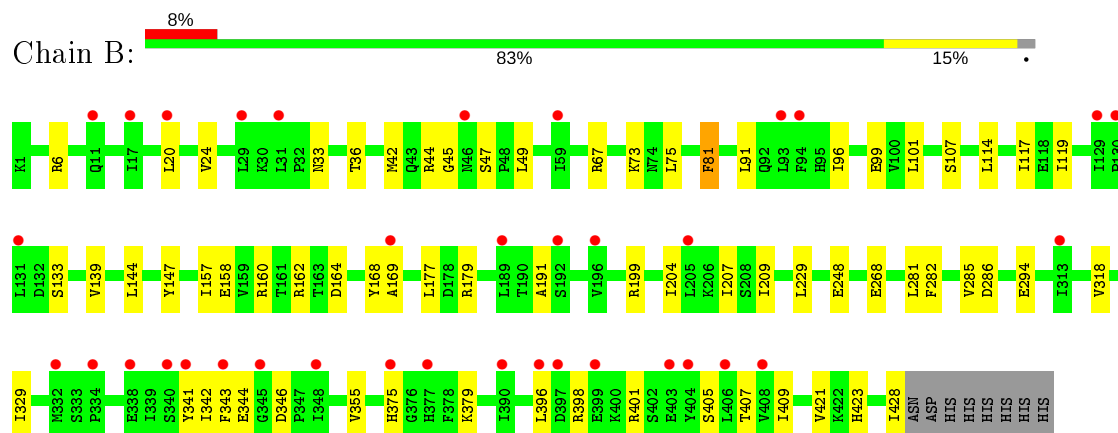
3 Residue-property plots

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: Protocadherin-18



• Molecule 1: Protocadherin-18




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






- Molecule 3: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 



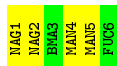
- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 



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

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	126.96 Å 176.94 Å 71.87 Å 90.00° 101.42° 90.00°	Depositor
Resolution (Å)	19.90 – 2.79 38.41 – 2.79	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.90-2.79) 86.9 (38.41-2.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.81 Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.236 , 0.272 0.245 , 0.280	Depositor DCC
R_{free} test set	1912 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	63.7	Xtriage
Anisotropy	0.822	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13535	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NA, CA, EDO, FUC, MAN

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	0.29	0/3433	0.52	0/4656
1	B	0.27	0/3424	0.52	0/4644
All	All	0.28	0/6857	0.52	0/9300

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3374	3222	3346	50	0
1	B	3368	3194	3338	46	0
2	C	49	0	43	0	0
3	D	24	0	22	1	0
4	E	38	23	34	2	0
5	F	71	0	61	3	0
6	A	9	0	0	0	0
6	B	9	0	0	0	0
7	A	20	30	30	0	0
7	B	12	18	18	0	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	1	0	0	0	0
9	B	28	0	26	2	0
10	A	26	0	0	0	0
10	B	18	0	0	0	0
All	All	7048	6487	6918	99	0

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

All (99) 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)
9:B:508:NAG:H82	9:B:508:NAG:O3	1.83	0.78
1:A:115:ILE:HB	1:A:205:LEU:HD23	1.71	0.72
1:A:20:LEU:O	1:A:24:VAL:HG22	1.92	0.69
1:B:162:ARG:NE	1:B:164:ASP:OD2	2.28	0.66
1:A:335:GLY:C	1:A:336:LYS:HG3	2.17	0.64
1:A:128:ARG:NH1	1:A:158:GLU:OE1	2.30	0.63
1:A:354:LEU:HD13	1:B:42:MET:HG3	1.79	0.63
5:F:1:NAG:O4	5:F:2:NAG:H83	2.00	0.62
1:A:404:TYR:HB2	1:A:426:VAL:HB	1.82	0.61
1:B:114:LEU:HD23	1:B:204:ILE:CG2	2.31	0.60
1:B:20:LEU:O	1:B:24:VAL:HG22	2.02	0.60
1:B:158:GLU:OE2	1:B:160:ARG:NH2	2.36	0.58
1:A:339:ILE:HG23	1:A:426:VAL:HA	1.86	0.58
1:A:145:HIS:CG	1:A:194:MET:HG2	2.39	0.57
1:A:145:HIS:CB	1:A:194:MET:HG2	2.35	0.57
1:B:6:ARG:HD2	1:B:99:GLU:HB3	1.88	0.56
1:A:19:ARG:NH2	1:A:58:GLU:OE2	2.39	0.55
1:A:49:LEU:HD23	1:A:65:ILE:HG12	1.89	0.54
1:A:162:ARG:NH1	1:A:164:ASP:OD2	2.39	0.54
5:F:1:NAG:H3	5:F:1:NAG:O7	2.06	0.54
1:A:40:ARG:HB2	1:A:86:LEU:HD21	1.91	0.53
1:A:229:LEU:HD23	1:A:318:VAL:CG2	2.39	0.52
1:B:342:ILE:HB	1:B:346:ASP:OD2	2.09	0.52
1:A:115:ILE:CB	1:A:205:LEU:HD23	2.38	0.51
1:A:179:ARG:NH2	1:A:248:GLU:HB2	2.26	0.50
3:D:1:NAG:O4	3:D:2:FUC:O5	2.26	0.50
1:B:401:ARG:O	1:B:428:ILE:HD11	2.12	0.50
1:B:396:LEU:HD21	1:B:428:ILE:HB	1.94	0.49
1:A:33:ASN:O	1:A:36:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:PHE:O	1:A:398:ARG:HD3	2.13	0.49
1:B:177:LEU:HD23	1:B:209:ILE:HD12	1.95	0.48
1:B:341:TYR:CE2	1:B:396:LEU:HD22	2.48	0.48
1:B:343:PHE:CD1	1:B:344:GLU:HG3	2.48	0.48
1:A:354:LEU:CD1	1:B:42:MET:HG3	2.43	0.48
1:A:297:VAL:CG1	1:A:311:CYS:SG	3.01	0.48
1:B:409:ILE:HD13	1:B:421:VAL:HG12	1.96	0.48
1:A:378:PHE:CD2	1:A:406:LEU:HD11	2.49	0.48
1:B:144:LEU:HD13	1:B:191:ALA:HB1	1.96	0.48
1:B:375:HIS:HE1	1:B:405:SER:OG	1.97	0.47
1:B:81:PHE:CE2	1:B:96:ILE:HB	2.50	0.47
1:B:157:ILE:HD11	1:B:169:ALA:HB1	1.97	0.46
1:A:339:ILE:HG21	1:A:426:VAL:HG22	1.97	0.46
1:B:343:PHE:CE1	1:B:344:GLU:HG3	2.50	0.46
1:A:139:VAL:HG12	1:A:140:GLY:N	2.30	0.46
1:B:6:ARG:HH21	1:B:101:LEU:HD21	1.80	0.46
1:A:351:PHE:CB	1:B:91:LEU:HD21	2.46	0.46
1:B:91:LEU:C	1:B:91:LEU:HD12	2.36	0.46
1:A:119:ILE:O	1:A:209:ILE:HA	2.17	0.45
1:A:331:LEU:HD21	1:A:353:ALA:HB2	1.98	0.44
1:A:145:HIS:CG	1:A:194:MET:CG	3.01	0.44
1:B:329:ILE:HG12	1:B:355:VAL:HG12	2.00	0.44
1:A:145:HIS:O	1:A:167:LYS:HD2	2.18	0.44
4:E:1:NAG:O3	4:E:2:NAG:O5	2.31	0.44
1:A:345:GLY:O	1:A:346:ASP:OD1	2.37	0.43
1:A:86:LEU:N	1:A:86:LEU:HD22	2.34	0.43
1:B:285:VAL:HG12	1:B:286:ASP:N	2.33	0.43
1:B:343:PHE:O	1:B:398:ARG:HD3	2.17	0.43
1:B:73:LYS:HG2	1:B:73:LYS:O	2.18	0.43
1:A:343:PHE:CD1	1:A:344:GLU:HG3	2.54	0.43
1:B:117:ILE:HD11	1:B:207:ILE:HG12	2.01	0.43
5:F:1:NAG:H61	5:F:2:NAG:C7	2.48	0.43
1:A:375:HIS:N	1:A:375:HIS:CD2	2.87	0.42
1:A:139:VAL:CG1	1:A:140:GLY:N	2.81	0.42
1:A:27:VAL:CG1	1:A:92:GLN:HG3	2.50	0.42
1:B:407:THR:HG22	1:B:423:HIS:ND1	2.34	0.42
1:A:67:ARG:NH1	1:A:72:GLN:O	2.53	0.42
1:B:162:ARG:CZ	1:B:164:ASP:OD2	2.67	0.42
4:E:1:NAG:H62	4:E:3:FUC:O2	2.19	0.42
1:B:133:SER:OG	1:B:168:TYR:HB3	2.20	0.42
1:B:341:TYR:CE2	1:B:346:ASP:OD2	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:GLU:O	1:B:282:PHE:HD2	2.03	0.42
9:B:508:NAG:H82	9:B:508:NAG:HO3	1.84	0.42
1:B:107:SER:OG	1:B:199:ARG:HD3	2.19	0.41
1:B:33:ASN:O	1:B:36:THR:HG22	2.20	0.41
1:B:344:GLU:HA	1:B:398:ARG:NH1	2.35	0.41
1:B:75:LEU:HD23	1:B:139:VAL:CG1	2.50	0.41
1:B:91:LEU:HD12	1:B:91:LEU:O	2.20	0.41
1:A:339:ILE:HG12	1:A:352:VAL:HG13	2.02	0.41
1:A:355:VAL:CG2	1:A:388:TYR:HB2	2.50	0.41
1:A:49:LEU:O	1:A:62:GLY:N	2.42	0.41
1:A:40:ARG:CB	1:A:86:LEU:HD21	2.51	0.41
1:B:119:ILE:O	1:B:209:ILE:HA	2.20	0.41
1:B:229:LEU:HD23	1:B:318:VAL:HG21	2.03	0.41
1:A:114:LEU:HD23	1:A:204:ILE:HG23	2.03	0.41
1:A:342:ILE:HD12	1:A:346:ASP:OD1	2.21	0.41
1:A:326:GLU:O	1:A:357:VAL:HA	2.20	0.41
1:A:351:PHE:CG	1:B:91:LEU:HD21	2.56	0.41
1:A:355:VAL:HG22	1:A:388:TYR:O	2.21	0.41
1:A:59:ILE:HD13	1:A:96:ILE:HD13	2.02	0.41
1:B:47:SER:HB2	1:B:49:LEU:CD1	2.51	0.41
1:A:59:ILE:CD1	1:A:96:ILE:HD13	2.51	0.41
1:B:179:ARG:NH2	1:B:248:GLU:HB2	2.36	0.41
1:B:396:LEU:HD11	1:B:428:ILE:HD13	2.02	0.41
1:B:144:LEU:HD21	1:B:147:TYR:OH	2.21	0.41
1:B:44:ARG:HD2	1:B:45:GLY:H	1.86	0.41
1:A:221:GLN:HG3	1:A:224:TYR:CZ	2.57	0.40
1:A:401:ARG:O	1:A:428:ILE:HD11	2.21	0.40
1:A:342:ILE:HB	1:A:346:ASP:OD1	2.20	0.40
1:A:163:THR:OG1	1:B:294:GLU:OE1	2.39	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	427/436 (98%)	417 (98%)	10 (2%)	0	100	100
1	B	426/436 (98%)	416 (98%)	10 (2%)	0	100	100
All	All	853/872 (98%)	833 (98%)	20 (2%)	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	389/396 (98%)	381 (98%)	8 (2%)	53	84
1	B	388/396 (98%)	384 (99%)	4 (1%)	76	93
All	All	777/792 (98%)	765 (98%)	12 (2%)	65	89

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	67	ARG
1	A	73	LYS
1	A	90	HIS
1	A	159	VAL
1	A	310	HIS
1	A	341	TYR
1	A	350	THR
1	B	67	ARG
1	B	81	PHE
1	B	281	LEU
1	B	379	LYS

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

Mol	Chain	Res	Type
1	A	43	GLN

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Mol	Chain	Res	Type
1	A	373	HIS
1	A	375	HIS
1	B	278	HIS
1	B	373	HIS
1	B	375	HIS

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 ⓘ

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	$\# Z > 2$
2	NAG	C	1	1,2	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	C	2	2	14,14,15	0.37	0	17,19,21	0.47	0
2	BMA	C	3	2	11,11,12	0.77	0	15,15,17	0.80	0
2	FUC	C	4	2	10,10,11	0.69	0	14,14,16	0.83	0
3	NAG	D	1	1,3	14,14,15	0.38	0	17,19,21	0.36	0
3	FUC	D	2	3	10,10,11	0.87	0	14,14,16	1.27	2 (14%)
4	NAG	E	1	1,4	14,14,15	0.40	0	17,19,21	0.56	0
4	NAG	E	2	4	14,14,15	0.52	0	17,19,21	0.42	0
4	FUC	E	3	4	10,10,11	1.01	1 (10%)	14,14,16	0.99	1 (7%)
5	NAG	F	1	1,5	14,14,15	0.45	0	17,19,21	0.83	0
5	NAG	F	2	5	14,14,15	0.26	0	17,19,21	0.55	0
5	BMA	F	3	5	11,11,12	0.64	0	15,15,17	0.72	0
5	MAN	F	4	5	11,11,12	0.69	0	15,15,17	1.09	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MAN	F	5	5	11,11,12	0.77	1 (9%)	15,15,17	1.10	2 (13%)
5	FUC	F	6	5	10,10,11	0.85	0	14,14,16	0.98	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
2	NAG	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	FUC	C	4	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	FUC	E	3	4	-	-	0/1/1/1
5	NAG	F	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	4/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	FUC	F	6	5	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3	FUC	C1-C2	2.30	1.57	1.52
5	F	5	MAN	C1-C2	2.26	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	FUC	C1-O5-C5	2.84	119.22	112.78
5	F	4	MAN	C1-O5-C5	2.82	116.02	112.19
3	D	2	FUC	O5-C5-C4	2.81	114.56	109.52
5	F	5	MAN	C1-O5-C5	2.46	115.52	112.19
4	E	3	FUC	O2-C2-C1	2.37	114.00	109.15
5	F	5	MAN	O2-C2-C3	-2.16	105.80	110.14
5	F	4	MAN	O2-C2-C3	-2.11	105.92	110.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

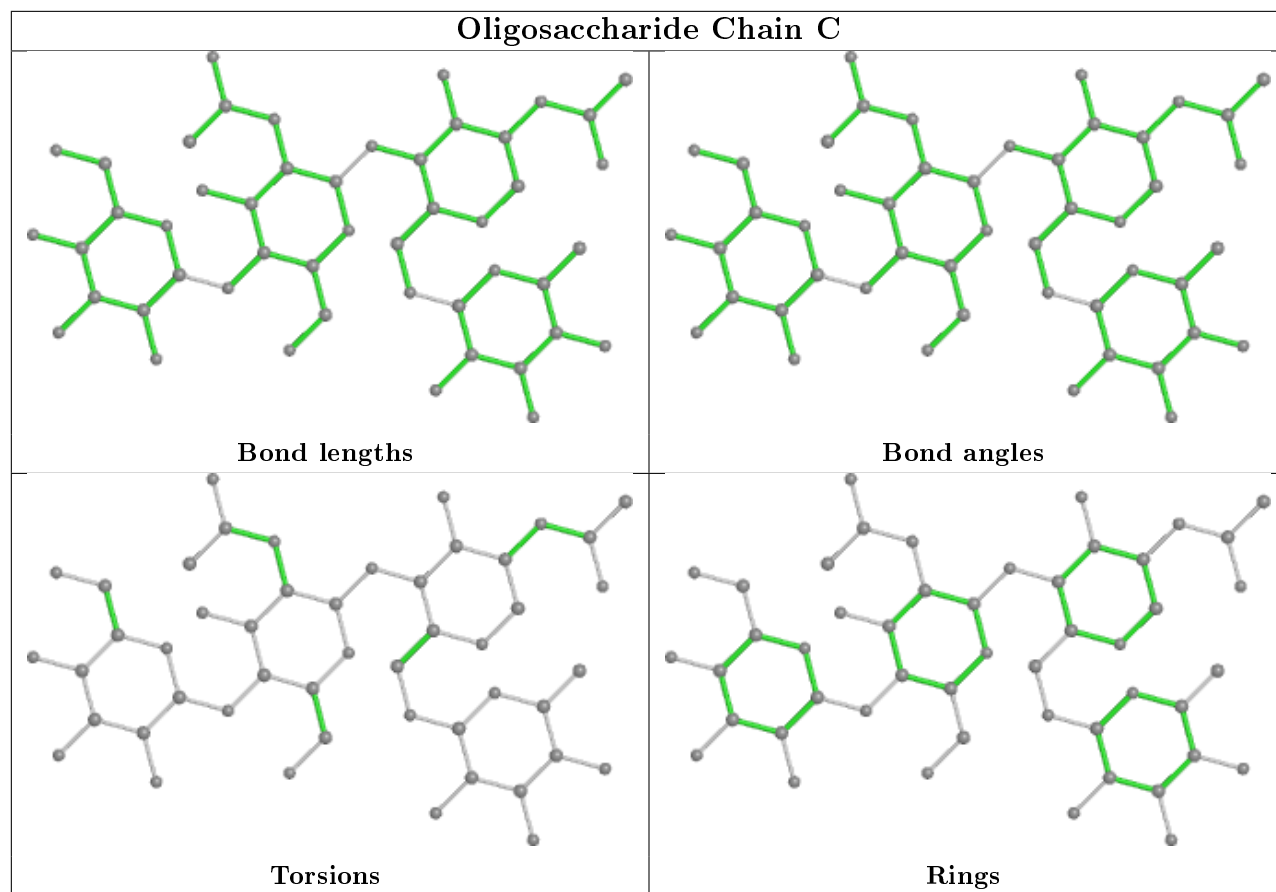
Mol	Chain	Res	Type	Atoms
5	F	1	NAG	C3-C2-N2-C7
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
5	F	2	NAG	C8-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
4	E	1	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6

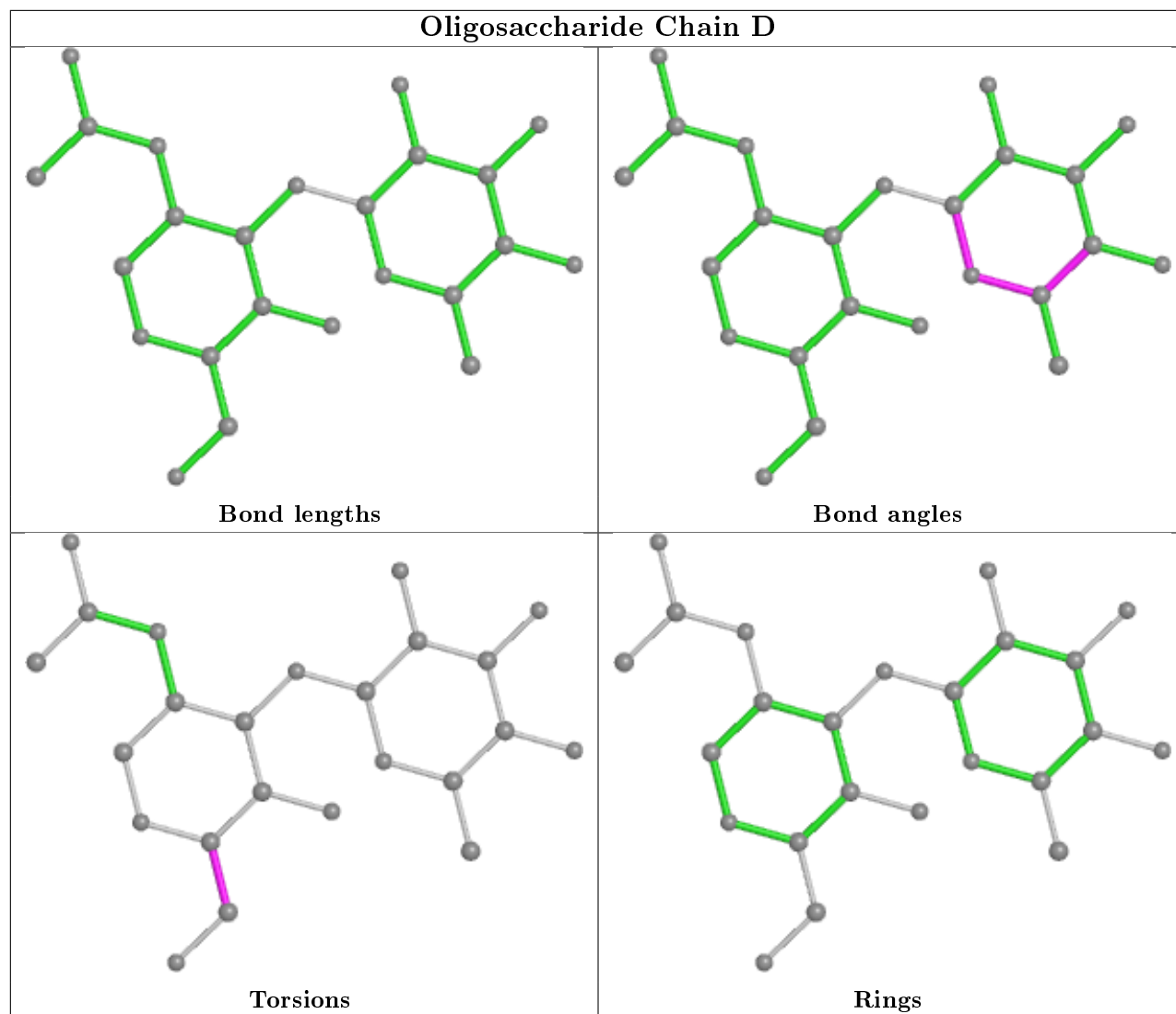
There are no ring outliers.

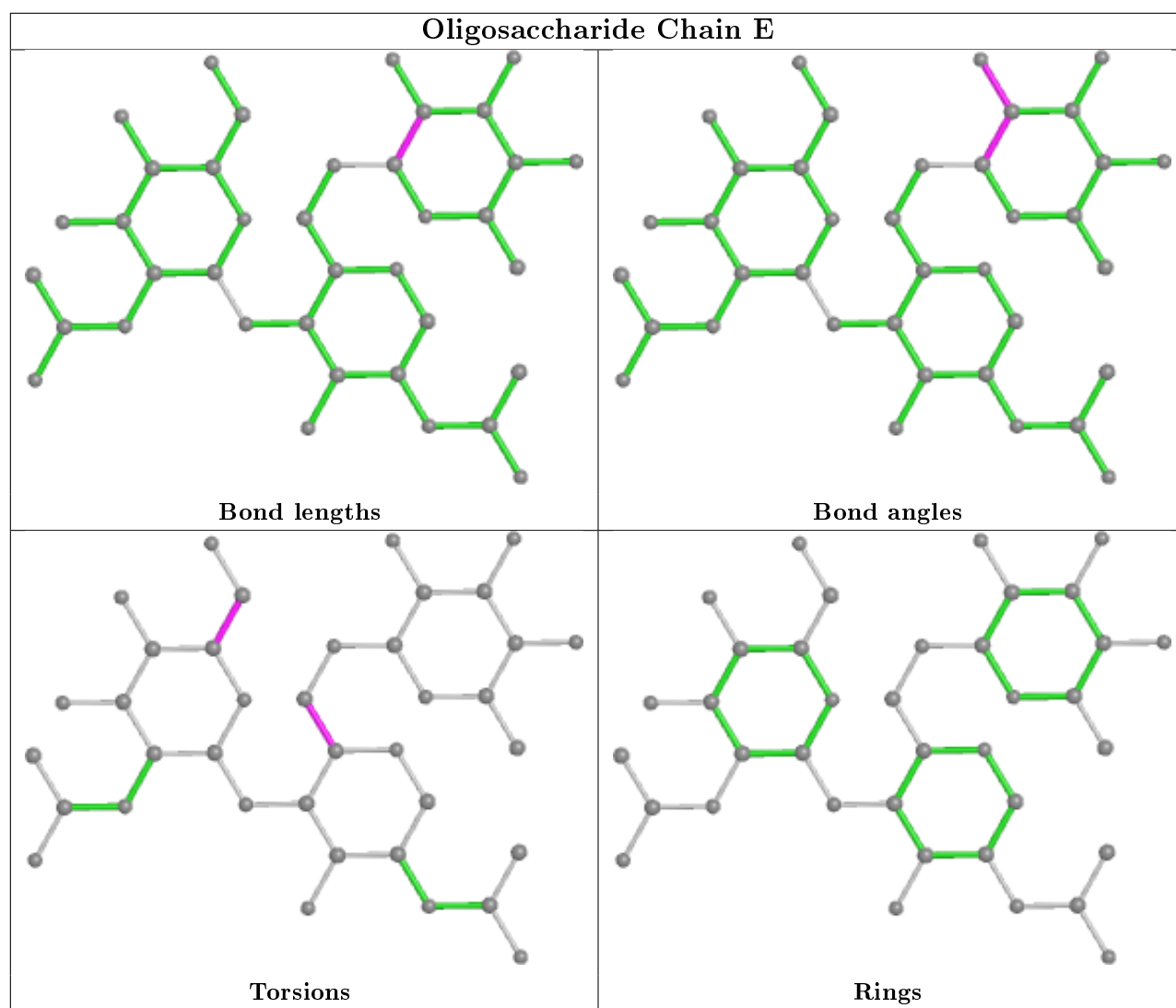
7 monomers are involved in 6 short contacts:

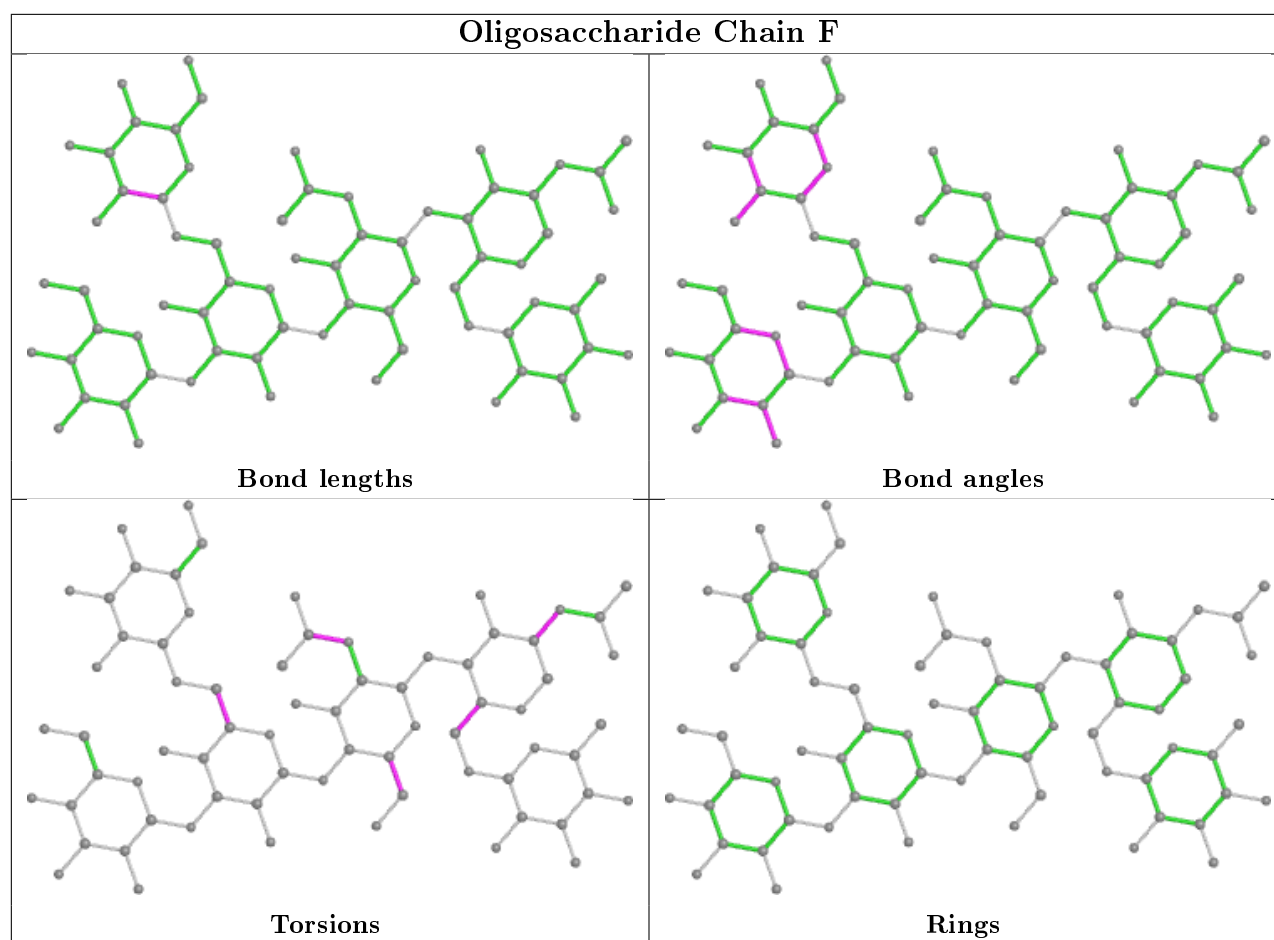
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	1	0
4	E	3	FUC	1	0
3	D	2	FUC	1	0
5	F	2	NAG	2	0
3	D	1	NAG	1	0
5	F	1	NAG	3	0
4	E	1	NAG	2	0

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









5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 20 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	EDO	A	520	-	3,3,3	0.42	0	2,2,2	0.31	0
7	EDO	A	519	-	3,3,3	0.45	0	2,2,2	0.34	0
9	NAG	B	508	1	14,14,15	0.81	1 (7%)	17,19,21	0.67	0
7	EDO	A	523	-	3,3,3	0.40	0	2,2,2	0.24	0
9	NAG	B	501	1	14,14,15	0.27	0	17,19,21	0.33	0
7	EDO	A	522	-	3,3,3	0.47	0	2,2,2	0.27	0
7	EDO	B	520	-	3,3,3	0.50	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	B	519	-	3,3,3	0.46	0	2,2,2	0.31	0
7	EDO	A	521	-	3,3,3	0.45	0	2,2,2	0.27	0
7	EDO	B	518	-	3,3,3	0.41	0	2,2,2	0.28	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	EDO	A	520	-	-	0/1/1/1	-
7	EDO	A	519	-	-	0/1/1/1	-
9	NAG	B	508	1	-	4/6/23/26	0/1/1/1
7	EDO	A	523	-	-	1/1/1/1	-
9	NAG	B	501	1	-	4/6/23/26	0/1/1/1
7	EDO	A	522	-	-	1/1/1/1	-
7	EDO	B	520	-	-	1/1/1/1	-
7	EDO	B	519	-	-	0/1/1/1	-
7	EDO	A	521	-	-	0/1/1/1	-
7	EDO	B	518	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	508	NAG	C1-C2	2.11	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	501	NAG	C4-C5-C6-O6
9	B	501	NAG	O5-C5-C6-O6
9	B	508	NAG	C8-C7-N2-C2
9	B	508	NAG	O7-C7-N2-C2
7	A	523	EDO	O1-C1-C2-O2
9	B	501	NAG	C1-C2-N2-C7
7	B	520	EDO	O1-C1-C2-O2
7	A	522	EDO	O1-C1-C2-O2
9	B	508	NAG	C4-C5-C6-O6
9	B	508	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	B	501	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	508	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	428/436 (98%)	0.68	64 (14%) 2 1	76, 101, 163, 197	0
1	B	428/436 (98%)	0.57	36 (8%) 11 5	78, 107, 150, 200	0
All	All	856/872 (98%)	0.63	100 (11%) 4 2	76, 104, 161, 200	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	TYR	8.1
1	A	341	TYR	6.6
1	B	396	LEU	6.3
1	A	344	GLU	5.1
1	A	375	HIS	4.8
1	A	311	CYS	4.6
1	A	396	LEU	4.5
1	B	397	ASP	4.2
1	B	196	VAL	3.9
1	B	343	PHE	3.8
1	B	345	GLY	3.6
1	A	313	ILE	3.5
1	A	424	PHE	3.3
1	A	395	THR	3.3
1	A	399	GLU	3.3
1	B	205	LEU	3.3
1	A	46	ASN	3.2
1	A	310	HIS	3.2
1	A	295	ILE	3.2
1	A	296	ASP	3.2
1	B	375	HIS	3.1
1	B	20	LEU	3.1
1	A	297	VAL	3.0
1	A	398	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	261	HIS	3.0
1	A	17	ILE	2.9
1	B	377	HIS	2.9
1	A	401	ARG	2.9
1	B	332	MET	2.9
1	A	308	PRO	2.9
1	A	406	LEU	2.8
1	B	403	GLU	2.8
1	B	131	LEU	2.8
1	B	334	PRO	2.8
1	A	427	GLN	2.8
1	A	24	VAL	2.8
1	B	404	TYR	2.8
1	A	177	LEU	2.8
1	A	262	VAL	2.7
1	A	314	ILE	2.7
1	A	155	PHE	2.7
1	A	260	SER	2.7
1	A	403	GLU	2.7
1	B	11	GLN	2.6
1	B	59	ILE	2.6
1	B	46	ASN	2.6
1	A	205	LEU	2.6
1	A	392	THR	2.6
1	A	119	ILE	2.5
1	B	93	LEU	2.5
1	A	59	ILE	2.5
1	A	22	GLU	2.4
1	B	94	PHE	2.4
1	A	258	PHE	2.4
1	A	373	HIS	2.4
1	A	20	LEU	2.4
1	A	391	LEU	2.4
1	B	406	LEU	2.4
1	A	317	VAL	2.4
1	A	327	ILE	2.4
1	A	23	ASP	2.3
1	A	114	LEU	2.3
1	B	17	ILE	2.3
1	A	259	SER	2.3
1	B	189	LEU	2.3
1	B	338	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	426	VAL	2.3
1	A	378	PHE	2.3
1	B	399	GLU	2.3
1	A	312	LYS	2.3
1	A	337	GLU	2.2
1	A	117	ILE	2.2
1	B	192	SER	2.2
1	B	31	LEU	2.2
1	A	315	ILE	2.2
1	A	223	SER	2.2
1	A	75	LEU	2.2
1	A	96	ILE	2.2
1	B	348	ILE	2.2
1	A	370	CYS	2.2
1	A	224	TYR	2.2
1	B	313	ILE	2.2
1	B	340	SER	2.1
1	B	169	ALA	2.1
1	A	220	GLU	2.1
1	B	29	LEU	2.1
1	A	79	ILE	2.1
1	A	428	ILE	2.1
1	A	225	ILE	2.1
1	B	408	VAL	2.1
1	A	371	LYS	2.1
1	A	405	SER	2.1
1	A	377	HIS	2.0
1	B	129	ILE	2.0
1	B	130	PRO	2.0
1	A	263	SER	2.0
1	A	187	LEU	2.0
1	A	372	LEU	2.0
1	A	309	ALA	2.0
1	B	390	ILE	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 ⓘ

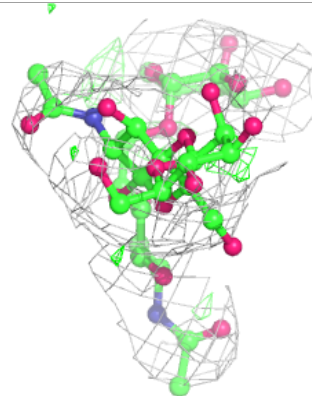
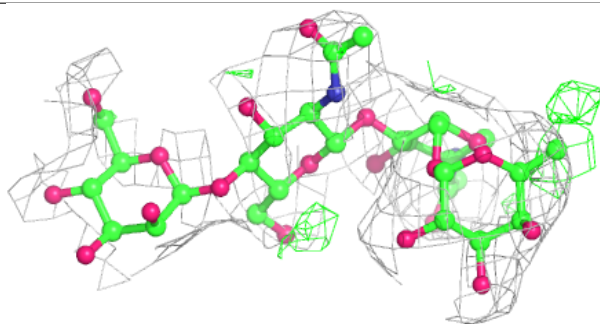
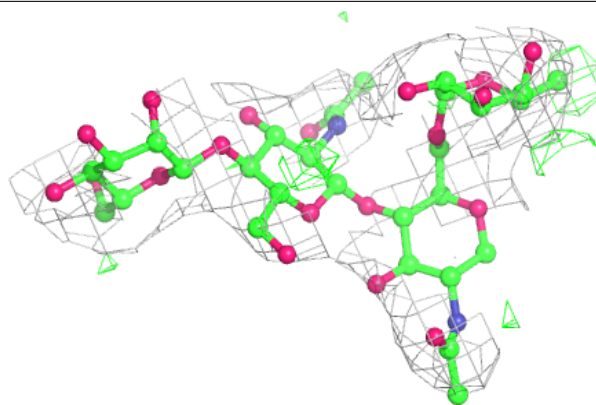
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	BMA	F	3	11/12	0.64	0.22	182,194,197,205	0
5	MAN	F	5	11/12	0.68	0.38	169,191,198,199	0
2	BMA	C	3	11/12	0.69	0.17	136,159,170,171	0
4	FUC	E	3	10/11	0.72	0.36	147,163,176,177	0
3	NAG	D	1	14/15	0.72	0.30	169,192,208,213	0
5	MAN	F	4	11/12	0.74	0.37	165,188,203,203	0
3	FUC	D	2	10/11	0.79	0.34	193,200,212,213	0
4	NAG	E	1	14/15	0.84	0.30	117,164,207,212	0
4	NAG	E	2	14/15	0.86	0.33	164,186,216,218	0
5	NAG	F	2	14/15	0.87	0.18	122,145,168,181	0
5	NAG	F	1	14/15	0.87	0.10	89,121,138,140	0
5	FUC	F	6	10/11	0.89	0.25	106,126,137,142	0
2	NAG	C	2	14/15	0.90	0.16	128,148,160,162	0
2	NAG	C	1	14/15	0.92	0.11	92,119,132,138	0
2	FUC	C	4	10/11	0.93	0.12	108,137,140,145	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.

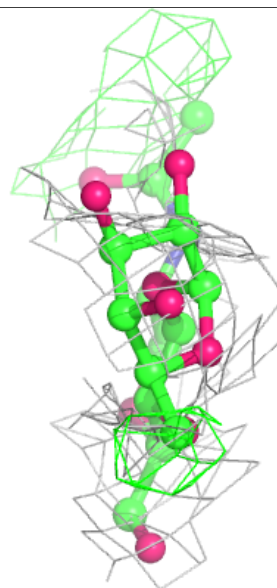
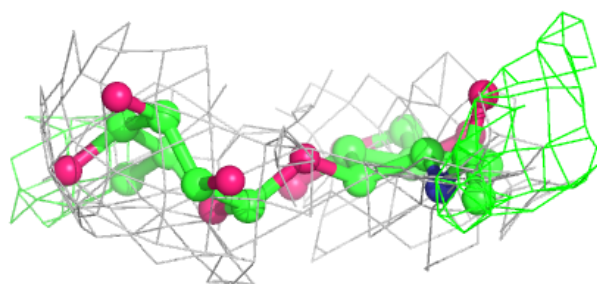
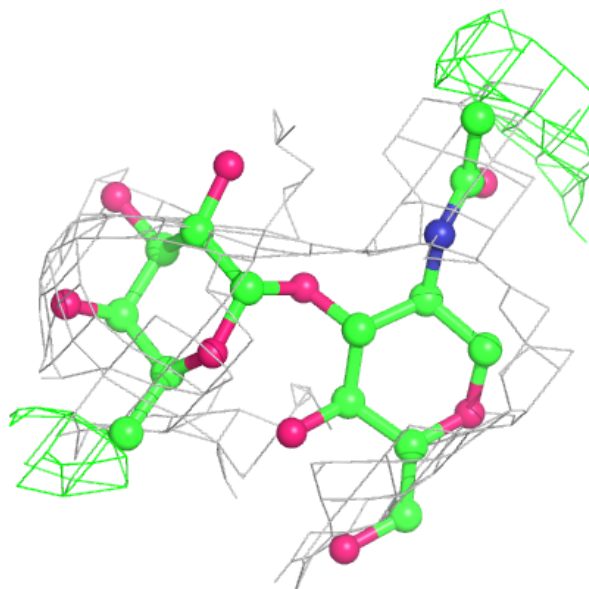
Electron density around Chain C:

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



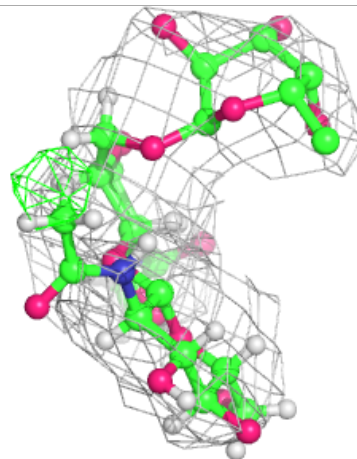
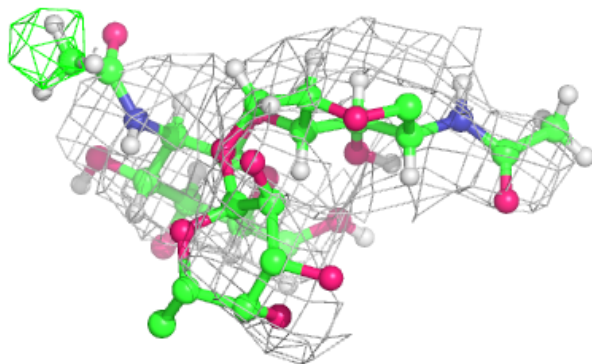
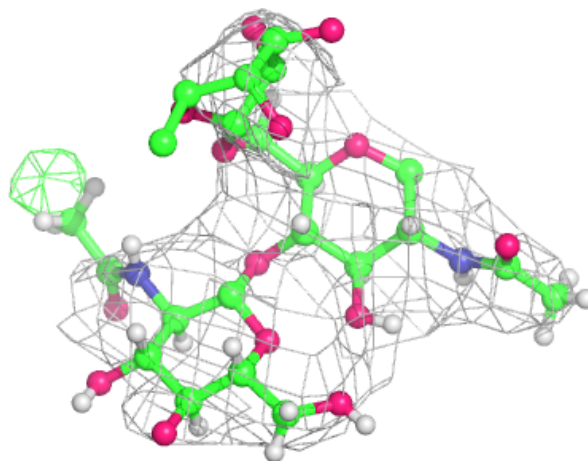
Electron density around Chain D:

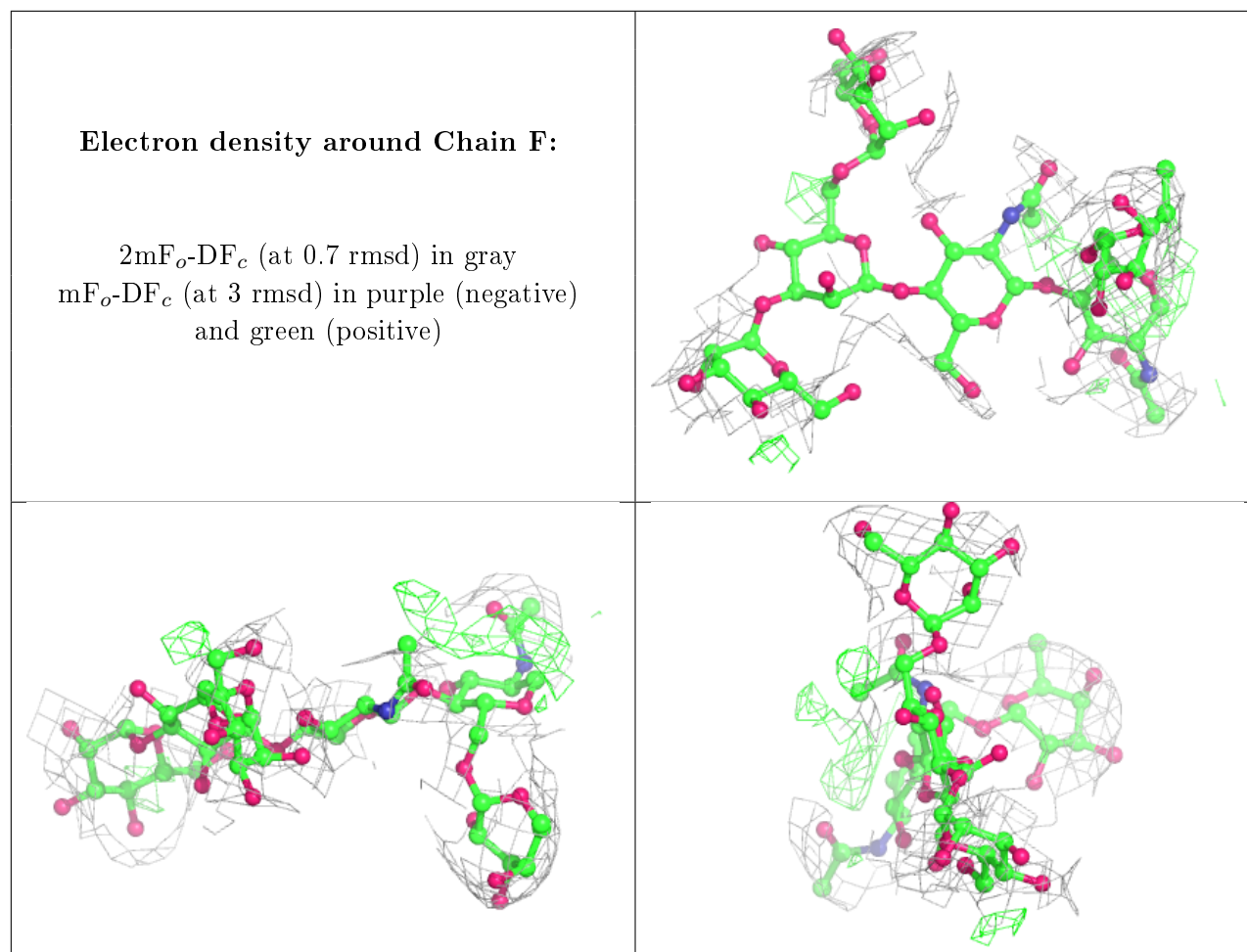
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





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
6	CA	A	513	1/1	0.45	0.35	173,173,173,173	0
7	EDO	B	519	4/4	0.70	0.20	107,129,141,152	0
7	EDO	B	518	4/4	0.76	0.43	114,137,147,147	0
9	NAG	B	501	14/15	0.77	0.24	155,162,171,189	0
9	NAG	B	508	14/15	0.77	0.28	142,161,170,170	0
6	CA	B	513	1/1	0.81	0.17	92,92,92,92	0
6	CA	A	511	1/1	0.82	0.28	138,138,138,138	0
7	EDO	A	520	4/4	0.84	0.60	94,113,123,126	0
7	EDO	A	523	4/4	0.88	0.18	60,88,111,132	0
7	EDO	B	520	4/4	0.88	0.49	85,102,110,132	0
6	CA	B	510	1/1	0.89	0.08	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	EDO	A	519	4/4	0.89	0.30	102,124,130,149	0
6	CA	A	517	1/1	0.89	0.17	100,100,100,100	0
6	CA	A	512	1/1	0.90	0.16	89,89,89,89	0
8	NA	A	524	1/1	0.90	0.20	77,77,77,77	0
6	CA	B	509	1/1	0.91	0.11	94,94,94,94	0
6	CA	B	511	1/1	0.91	0.13	110,110,110,110	0
6	CA	A	518	1/1	0.92	0.14	96,96,96,96	0
7	EDO	A	522	4/4	0.92	0.32	100,126,157,157	0
6	CA	B	515	1/1	0.92	0.21	103,103,103,103	0
6	CA	A	515	1/1	0.92	0.25	96,96,96,96	0
6	CA	B	512	1/1	0.93	0.23	108,108,108,108	0
7	EDO	A	521	4/4	0.93	0.20	82,98,117,120	0
6	CA	B	514	1/1	0.95	0.19	80,80,80,80	0
8	NA	B	521	1/1	0.96	0.15	76,76,76,76	0
6	CA	A	514	1/1	0.96	0.20	88,88,88,88	0
6	CA	B	516	1/1	0.96	0.21	90,90,90,90	0
6	CA	A	516	1/1	0.98	0.13	91,91,91,91	0
6	CA	B	517	1/1	0.99	0.20	93,93,93,93	0
6	CA	A	510	1/1	0.99	0.17	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.