



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 03:16 AM BST

PDB ID : 6EPZ
Title : Structure of the periplasmic binding protein MelB (Atu4661) in complex with melibiose from *Agrobacterium fabrum* C58
Authors : Vigouroux, A.; Morera, S.
Deposited on : 2017-10-12
Resolution : 1.80 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

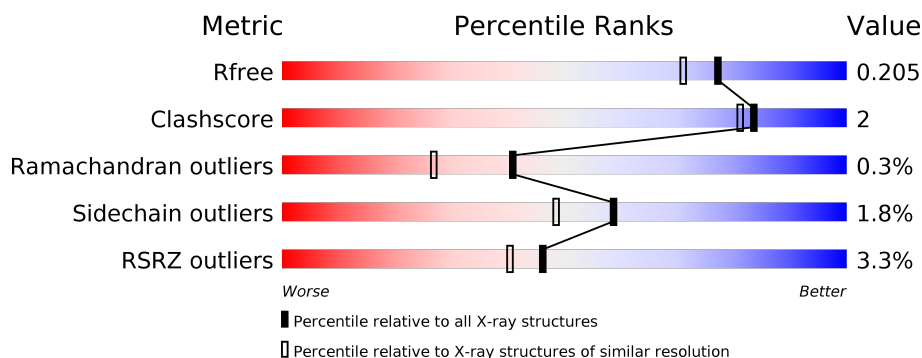
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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.



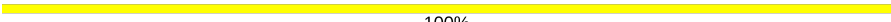
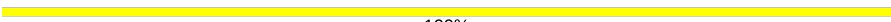
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	683	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> </div> </div>
1	B	683	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>8%</div> </div> </div>
1	C	683	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>8%</div> </div> </div>
1	D	683	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>7%</div> </div> </div>
2	E	2	<div> <div></div> <div>100%</div> </div>
2	F	2	<div> <div></div> <div>100%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22767 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 Periplasmic alpha-galactoside-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	S	0	0	0
			5304	3386	902	1000	16			
1	D	671	Total	C	N	O	S	0	1	0
			5306	3386	903	1001	16			
1	C	673	Total	C	N	O	S	0	0	0
			5313	3390	904	1003	16			
1	B	671	Total	C	N	O	S	0	1	0
			5303	3384	901	1002	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	678	HIS	-	expression tag	UNP A0A083ZM57
A	679	HIS	-	expression tag	UNP A0A083ZM57
A	680	HIS	-	expression tag	UNP A0A083ZM57
A	681	HIS	-	expression tag	UNP A0A083ZM57
A	682	HIS	-	expression tag	UNP A0A083ZM57
A	683	HIS	-	expression tag	UNP A0A083ZM57
D	678	HIS	-	expression tag	UNP A0A083ZM57
D	679	HIS	-	expression tag	UNP A0A083ZM57
D	680	HIS	-	expression tag	UNP A0A083ZM57
D	681	HIS	-	expression tag	UNP A0A083ZM57
D	682	HIS	-	expression tag	UNP A0A083ZM57
D	683	HIS	-	expression tag	UNP A0A083ZM57
C	678	HIS	-	expression tag	UNP A0A083ZM57
C	679	HIS	-	expression tag	UNP A0A083ZM57
C	680	HIS	-	expression tag	UNP A0A083ZM57
C	681	HIS	-	expression tag	UNP A0A083ZM57
C	682	HIS	-	expression tag	UNP A0A083ZM57
C	683	HIS	-	expression tag	UNP A0A083ZM57
B	678	HIS	-	expression tag	UNP A0A083ZM57
B	679	HIS	-	expression tag	UNP A0A083ZM57
B	680	HIS	-	expression tag	UNP A0A083ZM57

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	681	HIS	-	expression tag	UNP A0A083ZM57
B	682	HIS	-	expression tag	UNP A0A083ZM57
B	683	HIS	-	expression tag	UNP A0A083ZM57

- Molecule 2 is an oligosaccharide called alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranoside.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	2	Total	Mg	0	0
			2	2		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	9	Total	Na	0	0
			9	9		
5	A	6	Total	Na	0	0
			6	6		
5	D	4	Total	Na	0	0
			4	4		

Continued on next page...

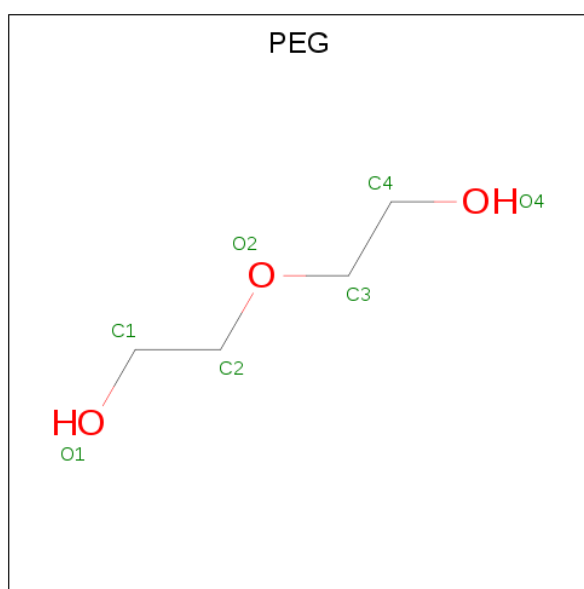
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	9	Total	Na	0	0
			9	9		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	0
			1	1		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			7	4	3		

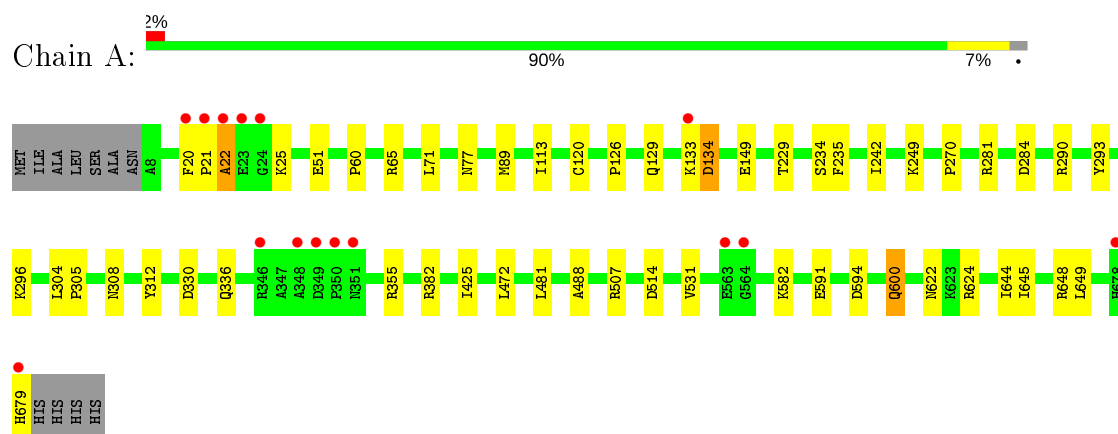
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	369	Total	O	0	0
			369	369		
8	D	332	Total	O	0	0
			332	332		
8	C	384	Total	O	0	0
			384	384		
8	B	287	Total	O	0	0
			287	287		

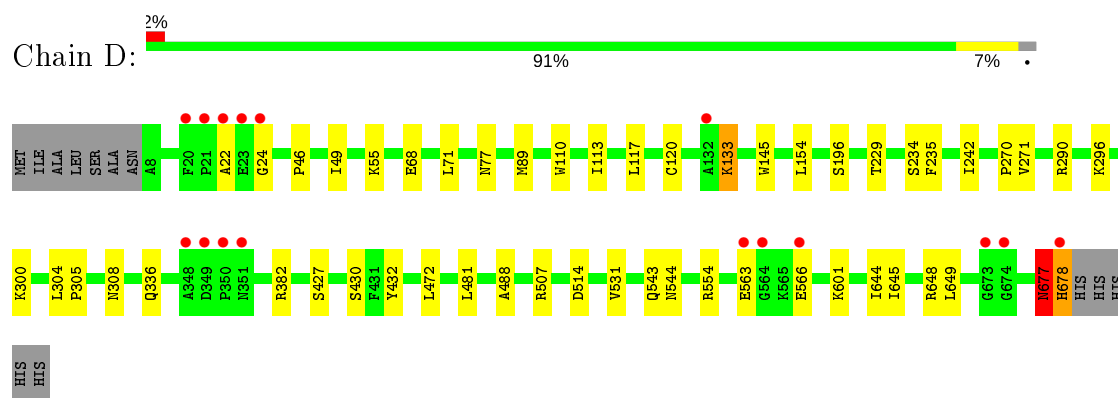
3 Residue-property plots [i](#)

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.

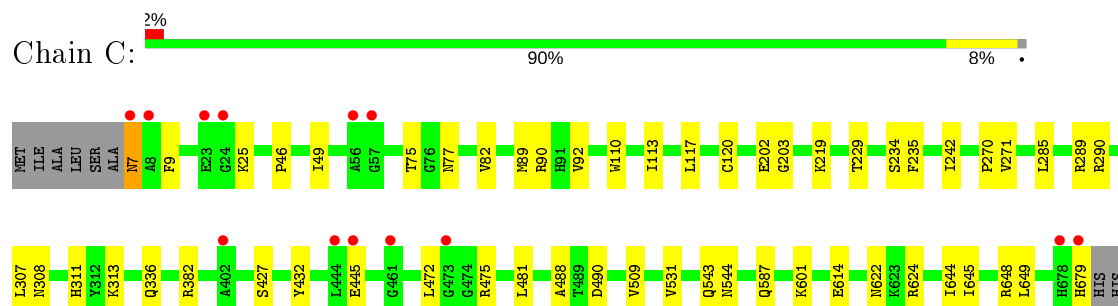
- Molecule 1: Periplasmic alpha-galactoside-binding protein



- Molecule 1: Periplasmic alpha-galactoside-binding protein

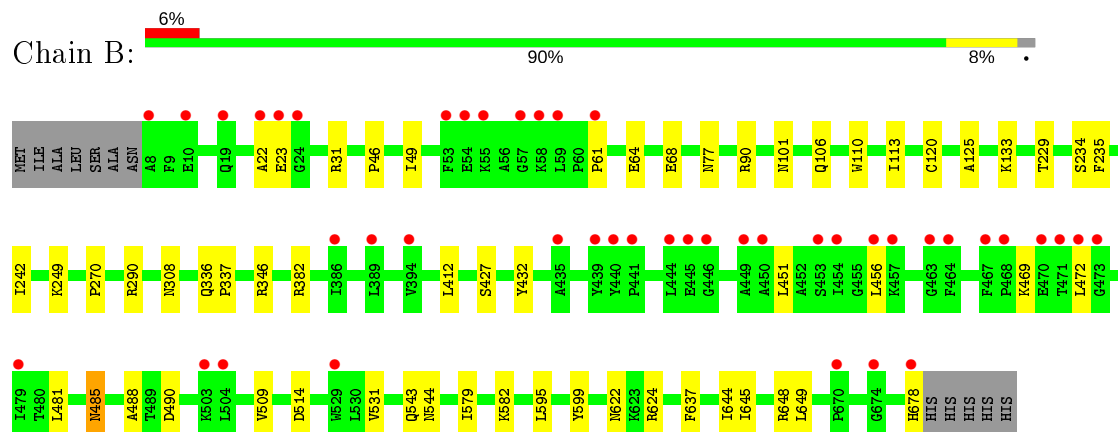


- Molecule 1: Periplasmic alpha-galactoside-binding protein



HIS
HIS

- Molecule 1: Periplasmic alpha-galactoside-binding protein

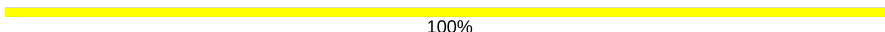


- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose

Chain E: 

GLC1
GLA2

- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose

Chain F: 

GLC1
GLA2

- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose

Chain G: 

GLC1
GLA2

- Molecule 2: alpha-D-galactopyranose-(1-6)-alpha-D-glucopyranose

Chain H: 

GLC1
GLA2

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	351.61Å 73.73Å 107.58Å 90.00° 105.38° 90.00°	Depositor
Resolution (Å)	48.85 – 1.80 48.85 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.85-1.80) 99.5 (48.85-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.79Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.177 , 0.195 0.186 , 0.205	Depositor DCC
R_{free} test set	12316 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.026 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22767	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 56.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8422e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MG, CL, GLA, GLC, EDO, NA, PEG

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	0.52	0/5458	0.62	0/7426
1	B	0.49	0/5456	0.60	0/7424
1	C	0.51	0/5467	0.61	0/7439
1	D	0.50	0/5459	0.61	1/7427 (0.0%)
All	All	0.51	0/21840	0.61	1/29716 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	677	ASN	C-N-CA	5.18	134.65	121.70

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	5304	0	5119	29	0
1	B	5303	0	5117	26	0
1	C	5313	0	5125	26	0
1	D	5306	0	5124	23	0
2	E	23	0	21	0	0
2	F	23	0	21	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	23	0	21	0	0
2	H	23	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	16	0	24	0	0
4	B	8	0	12	1	0
4	C	4	0	6	0	0
4	D	8	0	12	1	0
5	A	6	0	0	0	0
5	B	9	0	0	0	0
5	C	9	0	0	0	0
5	D	4	0	0	0	0
6	D	1	0	0	0	0
7	D	7	0	10	0	0
8	A	369	0	0	0	0
8	B	287	0	0	0	0
8	C	384	0	0	1	0
8	D	332	0	0	0	0
All	All	22767	0	20633	102	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 2.

All (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ILE:H	1:A:600:GLN:HE22	1.18	0.91
1:C:92:VAL:HG22	1:C:313:LYS:HD2	1.67	0.77
1:A:77:ASN:HD22	1:A:648:ARG:HH12	1.36	0.74
1:C:77:ASN:HD22	1:C:648:ARG:HH12	1.37	0.71
1:B:77:ASN:HD22	1:B:648:ARG:HH12	1.37	0.71
1:D:77:ASN:HD22	1:D:648:ARG:HH12	1.40	0.70
1:C:120:CYS:HB3	1:C:235:PHE:O	1.94	0.68
1:D:120:CYS:HB3	1:D:235:PHE:O	1.94	0.68
1:A:120:CYS:HB3	1:A:235:PHE:O	1.95	0.67
1:B:120:CYS:HB3	1:B:235:PHE:O	1.95	0.67
1:B:61:PRO:HG2	1:B:64:GLU:HG3	1.82	0.62
1:A:89:MET:CE	1:A:330:ASP:HB2	2.30	0.61
1:B:101:ASN:H	1:B:106:GLN:HE21	1.47	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASN:ND2	1:A:648:ARG:HH12	1.99	0.59
1:A:113:ILE:HG12	1:A:312:TYR:CD1	2.38	0.58
1:A:242:ILE:HG13	1:A:270:PRO:HG2	1.86	0.57
1:C:313:LYS:HD3	8:C:926:HOH:O	2.04	0.57
1:D:77:ASN:ND2	1:D:648:ARG:HH12	2.01	0.56
1:B:77:ASN:ND2	1:B:648:ARG:HH12	2.01	0.56
1:A:290:ARG:HH11	1:A:308:ASN:HD22	1.52	0.56
1:D:242:ILE:HG13	1:D:270:PRO:HG2	1.86	0.56
1:B:290:ARG:HH11	1:B:308:ASN:HD22	1.54	0.55
1:B:242:ILE:HG13	1:B:270:PRO:HG2	1.88	0.55
1:D:290:ARG:HH11	1:D:308:ASN:HD22	1.52	0.55
1:C:290:ARG:HH11	1:C:308:ASN:HD22	1.53	0.55
1:A:89:MET:CE	1:A:330:ASP:CB	2.85	0.54
1:C:7:ASN:HD22	1:C:9:PHE:H	1.54	0.54
1:B:31:ARG:HH22	4:B:702:EDO:H21	1.74	0.53
1:C:77:ASN:ND2	1:C:648:ARG:HH12	2.03	0.53
1:C:242:ILE:HG13	1:C:270:PRO:HG2	1.90	0.52
1:C:203:GLY:HA3	1:C:219:LYS:HE3	1.92	0.52
1:C:543:GLN:HE21	1:C:544:ASN:ND2	2.08	0.52
1:D:677:ASN:HB2	1:D:678:HIS:HB3	1.90	0.52
1:A:507:ARG:HD2	1:C:509:VAL:HG21	1.93	0.51
1:D:543:GLN:HE21	1:D:544:ASN:ND2	2.09	0.51
1:A:89:MET:HE2	1:A:330:ASP:HB2	1.91	0.51
1:B:382:ARG:HA	1:B:472:LEU:HD11	1.93	0.51
1:D:481:LEU:HD11	1:D:531:VAL:HG23	1.93	0.51
1:B:543:GLN:HE21	1:B:544:ASN:ND2	2.09	0.50
1:A:425:ILE:N	1:A:600:GLN:HE22	1.98	0.49
1:C:472:LEU:O	1:C:475:ARG:HB2	2.12	0.49
1:A:229:THR:O	1:A:234:SER:HB2	2.13	0.49
1:A:600:GLN:HA	1:A:600:GLN:HE21	1.77	0.49
1:D:229:THR:O	1:D:234:SER:HB2	2.12	0.49
1:A:113:ILE:HG12	1:A:312:TYR:CG	2.48	0.48
1:B:110:TRP:O	1:B:113:ILE:HG22	2.13	0.48
1:A:65:ARG:HG2	1:A:293:TYR:CE1	2.49	0.48
1:C:46:PRO:HD2	1:C:49:ILE:HD12	1.95	0.48
1:C:229:THR:O	1:C:234:SER:HB2	2.14	0.48
1:C:89:MET:HB2	1:C:307:LEU:HD13	1.95	0.48
1:B:46:PRO:HD2	1:B:49:ILE:HD12	1.94	0.47
1:B:229:THR:O	1:B:234:SER:HB2	2.15	0.47
1:B:579:ILE:HG21	1:B:599:TYR:HB2	1.97	0.47
1:B:101:ASN:H	1:B:106:GLN:NE2	2.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:TRP:O	1:D:113:ILE:HG22	2.15	0.47
1:B:337:PRO:HB2	1:B:412:LEU:HB3	1.97	0.47
1:B:582:LYS:HD3	1:B:595:LEU:HD21	1.97	0.47
1:C:336:GLN:HE22	1:C:488:ALA:H	1.63	0.46
1:D:507:ARG:HD3	1:B:509:VAL:HG11	1.98	0.46
1:A:133:LYS:HA	1:A:134:ASP:HA	1.62	0.46
1:D:336:GLN:HE22	1:D:488:ALA:H	1.64	0.46
1:A:481:LEU:HD11	1:A:531:VAL:HG23	1.98	0.45
1:C:481:LEU:HD11	1:C:531:VAL:HG23	1.98	0.45
1:D:382:ARG:HA	1:D:472:LEU:HD11	1.97	0.45
1:A:382:ARG:HA	1:A:472:LEU:HD11	1.98	0.45
1:A:622:ASN:HD22	1:A:624:ARG:H	1.64	0.45
1:D:145:TRP:HB2	1:D:154:LEU:HD11	1.99	0.45
1:D:304:LEU:HB3	1:D:305:PRO:HA	1.97	0.45
1:A:20:PHE:C	1:A:22:ALA:H	2.21	0.45
1:A:71:LEU:HB3	1:A:296:LYS:HG2	1.99	0.45
1:A:304:LEU:HB3	1:A:305:PRO:HA	1.99	0.44
1:C:117:LEU:HD22	1:C:271:VAL:HG11	1.99	0.44
1:D:300:LYS:HB3	4:D:703:EDO:H21	1.98	0.44
1:B:427:SER:HA	1:B:432:TYR:CG	2.52	0.44
1:B:451:LEU:HD22	1:B:456:LEU:HD12	1.99	0.44
1:B:481:LEU:HD11	1:B:531:VAL:HG23	1.99	0.44
1:C:427:SER:HA	1:C:432:TYR:CG	2.52	0.44
1:C:622:ASN:HD22	1:C:624:ARG:H	1.66	0.44
1:C:110:TRP:O	1:C:113:ILE:HG22	2.18	0.43
1:C:75:THR:HG22	1:C:82:VAL:HG13	2.00	0.43
1:D:196:SER:HB2	1:D:554:ARG:NH1	2.33	0.43
1:A:336:GLN:HE22	1:A:488:ALA:H	1.65	0.43
1:A:644:ILE:HD12	1:A:649:LEU:HD11	1.99	0.43
1:C:382:ARG:HA	1:C:472:LEU:HD11	2.00	0.43
1:D:46:PRO:HD2	1:D:49:ILE:HD12	2.01	0.43
1:A:126:PRO:O	1:A:129:GLN:HG2	2.18	0.43
1:B:336:GLN:HE22	1:B:488:ALA:H	1.68	0.42
1:A:281:ARG:HD2	1:A:284:ASP:OD2	2.20	0.42
1:D:71:LEU:HB3	1:D:296:LYS:HG2	2.01	0.42
1:A:582:LYS:HE2	1:A:591:GLU:OE2	2.19	0.42
1:B:622:ASN:HD22	1:B:624:ARG:H	1.68	0.42
1:B:644:ILE:HD12	1:B:649:LEU:HD11	2.02	0.42
1:C:285:LEU:HD11	1:C:311:HIS:HB3	2.01	0.41
1:A:60:PRO:HD2	1:A:65:ARG:HD2	2.02	0.41
1:D:117:LEU:HD22	1:D:271:VAL:HG11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ALA:HA	1:B:637:PHE:HB2	2.03	0.41
1:C:644:ILE:HD12	1:C:649:LEU:HD11	2.02	0.41
1:C:289:ARG:HD2	1:C:289:ARG:HA	1.94	0.41
1:D:133:LYS:HG2	1:D:430:SER:OG	2.21	0.41
1:D:427:SER:HA	1:D:432:TYR:CG	2.56	0.41
1:B:485:ASN:ND2	1:B:514:ASP:HA	2.35	0.40
1:D:644:ILE:HD12	1:D:649:LEU:HD11	2.03	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	670/683 (98%)	646 (96%)	21 (3%)	3 (0%)	34	21
1	B	670/683 (98%)	646 (96%)	22 (3%)	2 (0%)	41	27
1	C	671/683 (98%)	650 (97%)	20 (3%)	1 (0%)	51	36
1	D	670/683 (98%)	645 (96%)	22 (3%)	3 (0%)	34	21
All	All	2681/2732 (98%)	2587 (96%)	85 (3%)	9 (0%)	41	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ALA
1	D	22	ALA
1	D	24	GLY
1	B	22	ALA
1	A	21	PRO
1	A	645	ILE
1	C	645	ILE
1	B	645	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	645	ILE

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	558/568 (98%)	548 (98%)	10 (2%)	59	48
1	B	559/568 (98%)	549 (98%)	10 (2%)	59	48
1	C	560/568 (99%)	550 (98%)	10 (2%)	59	48
1	D	559/568 (98%)	549 (98%)	10 (2%)	59	48
All	All	2236/2272 (98%)	2196 (98%)	40 (2%)	59	48

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	51	GLU
1	A	134	ASP
1	A	149	GLU
1	A	249	LYS
1	A	355	ARG
1	A	514	ASP
1	A	594	ASP
1	A	600	GLN
1	A	679	HIS
1	D	55	LYS
1	D	68	GLU
1	D	89	MET
1	D	133	LYS
1	D	514	ASP
1	D	563	GLU
1	D	566	GLU
1	D	601	LYS
1	D	677	ASN
1	D	678	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	7	ASN
1	C	25	LYS
1	C	90	ARG
1	C	202	GLU
1	C	445	GLU
1	C	490	ASP
1	C	587	GLN
1	C	601	LYS
1	C	614	GLU
1	C	679	HIS
1	B	23	GLU
1	B	68	GLU
1	B	90	ARG
1	B	133	LYS
1	B	249	LYS
1	B	346	ARG
1	B	469	LYS
1	B	485	ASN
1	B	490	ASP
1	B	678	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	302	GLN
1	A	308	ASN
1	A	323	GLN
1	A	336	GLN
1	A	339	ASN
1	A	466	ASN
1	A	543	GLN
1	A	544	ASN
1	A	600	GLN
1	A	622	ASN
1	D	77	ASN
1	D	302	GLN
1	D	308	ASN
1	D	323	GLN
1	D	336	GLN
1	D	339	ASN
1	D	368	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	500	GLN
1	D	544	ASN
1	D	547	GLN
1	D	622	ASN
1	D	677	ASN
1	C	7	ASN
1	C	77	ASN
1	C	302	GLN
1	C	303	GLN
1	C	308	ASN
1	C	323	GLN
1	C	336	GLN
1	C	339	ASN
1	C	368	GLN
1	C	544	ASN
1	C	622	ASN
1	C	630	GLN
1	B	77	ASN
1	B	106	GLN
1	B	302	GLN
1	B	303	GLN
1	B	308	ASN
1	B	323	GLN
1	B	336	GLN
1	B	339	ASN
1	B	485	ASN
1	B	544	ASN
1	B	547	GLN
1	B	622	ASN

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 ⓘ

8 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	E	1	2	12,12,12	1.45	2 (16%)	17,17,17	1.84	4 (23%)
2	GLA	E	2	2	11,11,12	1.30	2 (18%)	15,15,17	1.08	1 (6%)
2	GLC	F	1	2	12,12,12	1.22	2 (16%)	17,17,17	1.22	2 (11%)
2	GLA	F	2	2	11,11,12	1.34	1 (9%)	15,15,17	1.25	1 (6%)
2	GLC	G	1	2	12,12,12	1.20	1 (8%)	17,17,17	1.61	3 (17%)
2	GLA	G	2	2	11,11,12	2.09	4 (36%)	15,15,17	1.53	1 (6%)
2	GLC	H	1	2	12,12,12	1.16	1 (8%)	17,17,17	1.77	3 (17%)
2	GLA	H	2	2	11,11,12	1.82	2 (18%)	15,15,17	1.25	1 (6%)

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	GLC	E	1	2	-	0/2/22/22	0/1/1/1
2	GLA	E	2	2	-	0/2/19/22	0/1/1/1
2	GLC	F	1	2	-	0/2/22/22	0/1/1/1
2	GLA	F	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLA	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLA	H	2	2	-	0/2/19/22	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	2	GLA	O5-C1	4.48	1.50	1.43
2	G	2	GLA	O5-C5	4.08	1.51	1.43
2	G	2	GLA	C2-C3	3.40	1.57	1.52
2	G	2	GLA	O5-C1	3.34	1.49	1.43
2	E	1	GLC	C1-C2	3.27	1.60	1.52
2	F	2	GLA	C2-C3	3.10	1.57	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1	GLC	C1-C2	3.00	1.59	1.52
2	H	1	GLC	C1-C2	2.82	1.59	1.52
2	E	2	GLA	C1-C2	2.58	1.58	1.52
2	E	1	GLC	O5-C1	2.38	1.48	1.42
2	E	2	GLA	C2-C3	2.33	1.55	1.52
2	F	1	GLC	C1-C2	2.32	1.57	1.52
2	H	2	GLA	C2-C3	2.24	1.55	1.52
2	G	2	GLA	C4-C3	2.21	1.58	1.52
2	F	1	GLC	O5-C1	2.08	1.48	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	GLA	O5-C5-C6	4.53	114.30	107.20
2	E	1	GLC	C1-O5-C5	4.45	122.05	113.66
2	H	1	GLC	C1-O5-C5	4.35	121.87	113.66
2	H	2	GLA	O5-C5-C6	4.11	113.64	107.20
2	G	1	GLC	C1-O5-C5	3.90	121.02	113.66
2	F	2	GLA	O5-C5-C6	3.74	113.07	107.20
2	F	1	GLC	C1-O5-C5	3.13	119.58	113.66
2	H	1	GLC	O5-C5-C4	2.90	114.96	109.69
2	H	1	GLC	O5-C5-C6	2.81	113.42	106.44
2	E	2	GLA	O5-C5-C6	2.77	111.55	107.20
2	E	1	GLC	O5-C5-C6	2.69	113.12	106.44
2	G	1	GLC	O5-C5-C6	2.63	112.98	106.44
2	E	1	GLC	O5-C5-C4	2.62	114.45	109.69
2	E	1	GLC	O5-C1-C2	2.61	114.95	110.28
2	G	1	GLC	O5-C1-C2	2.44	114.64	110.28
2	F	1	GLC	C6-C5-C4	-2.02	108.28	113.00

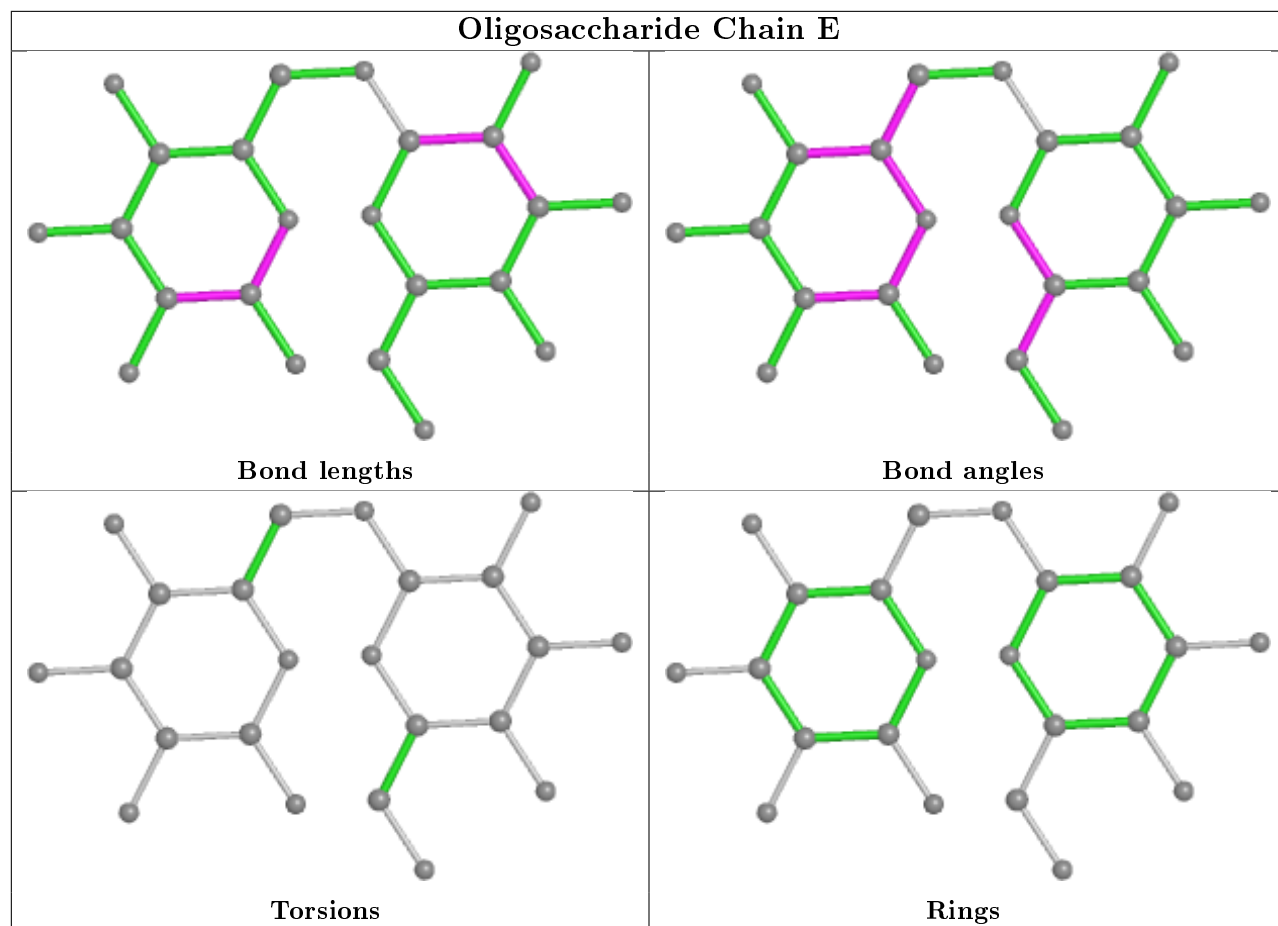
There are no chirality outliers.

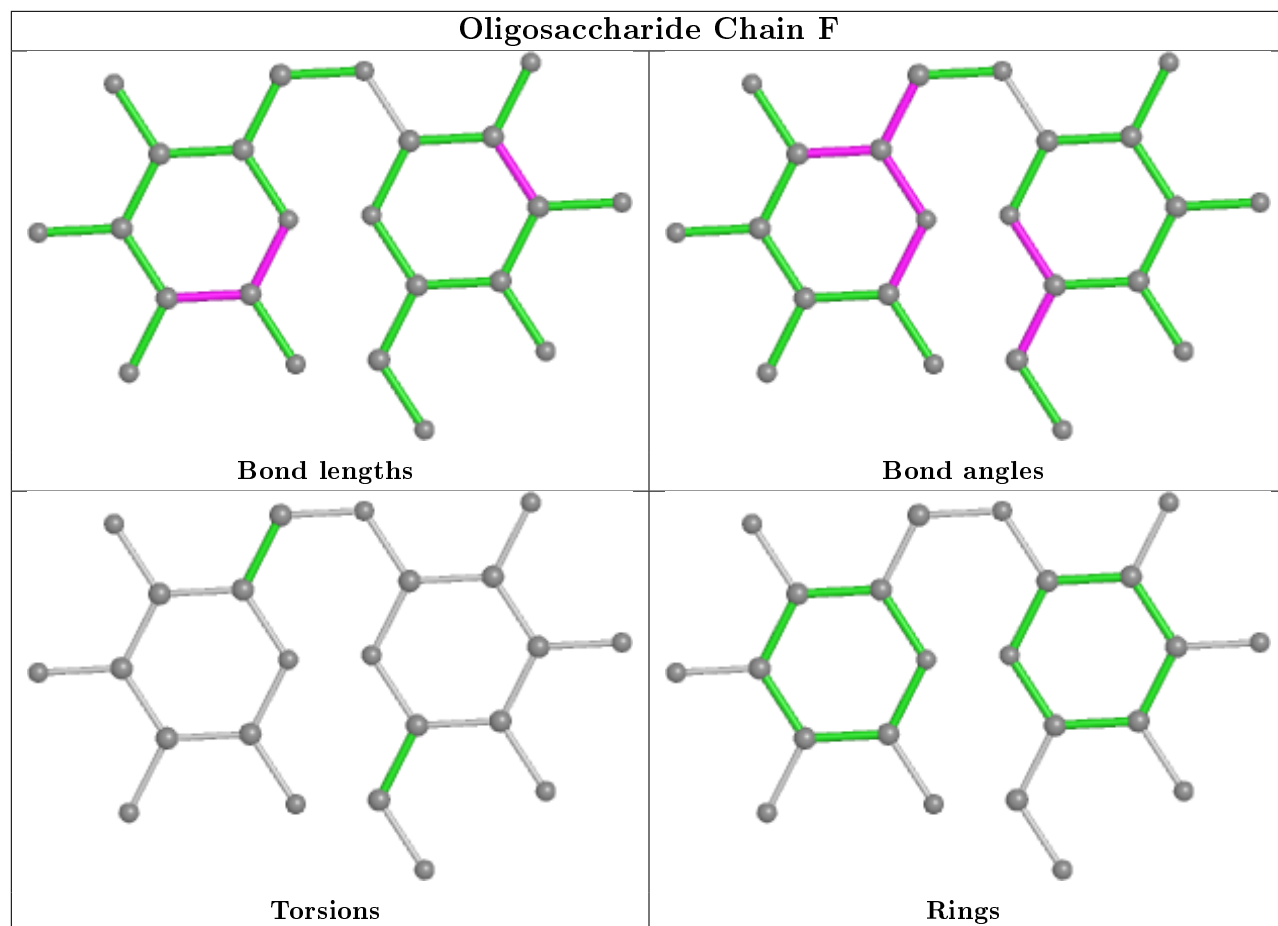
There are no torsion outliers.

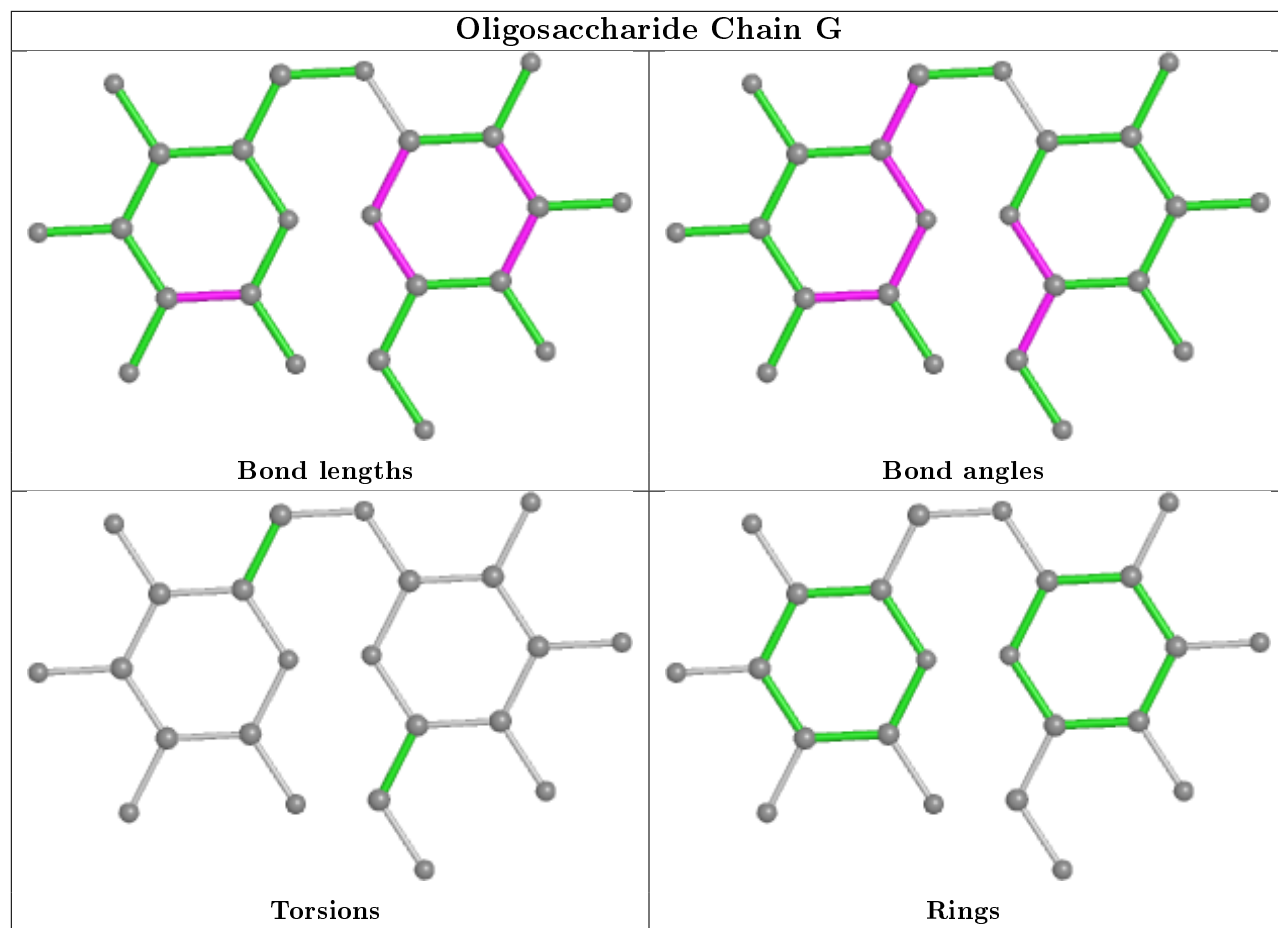
There are no ring outliers.

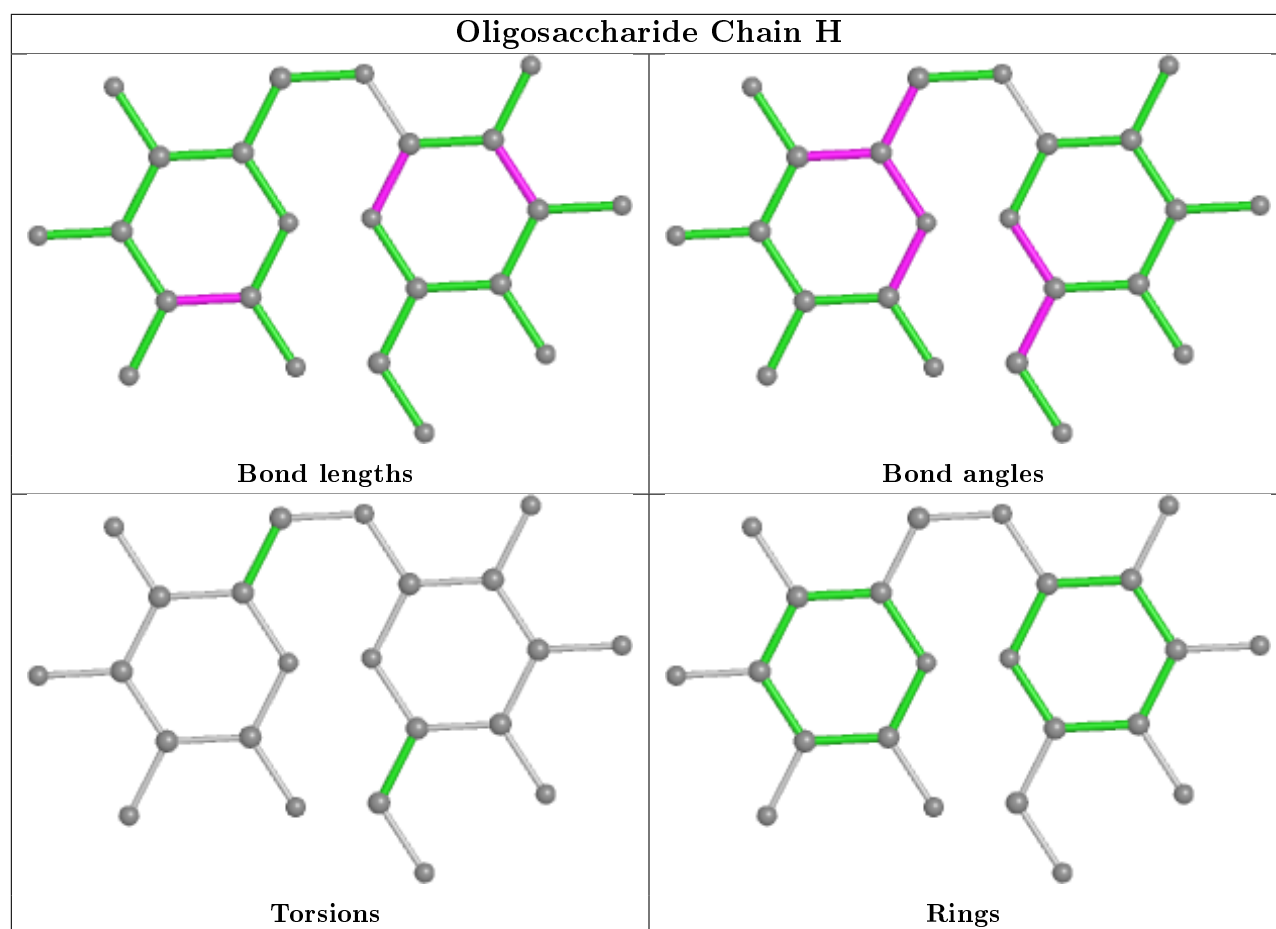
No monomer is involved in short contacts.

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 44 ligands modelled in this entry, 34 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	$\# Z > 2$
4	EDO	D	703	-	3,3,3	0.59	0	2,2,2	0.26	0
4	EDO	A	705	-	3,3,3	0.62	0	2,2,2	0.40	0
4	EDO	B	703	-	3,3,3	0.49	0	2,2,2	0.47	0
4	EDO	D	702	-	3,3,3	0.60	0	2,2,2	0.20	0
4	EDO	C	703	-	3,3,3	0.65	0	2,2,2	0.16	0
4	EDO	A	706	-	3,3,3	0.70	0	2,2,2	0.12	0
4	EDO	B	702	-	3,3,3	0.75	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	703	-	3,3,3	0.68	0	2,2,2	0.31	0
7	PEG	D	710	5	6,6,6	0.23	0	5,5,5	0.34	0
4	EDO	A	704	-	3,3,3	0.53	0	2,2,2	0.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	D	703	-	-	0/1/1/1	-
4	EDO	A	705	-	-	1/1/1/1	-
4	EDO	B	703	-	-	1/1/1/1	-
4	EDO	D	702	-	-	1/1/1/1	-
4	EDO	C	703	-	-	0/1/1/1	-
4	EDO	A	706	-	-	1/1/1/1	-
4	EDO	B	702	-	-	0/1/1/1	-
4	EDO	A	703	-	-	0/1/1/1	-
7	PEG	D	710	5	-	2/4/4/4	-
4	EDO	A	704	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	710	PEG	O2-C3-C4-O4
4	A	705	EDO	O1-C1-C2-O2
4	D	702	EDO	O1-C1-C2-O2
7	D	710	PEG	C4-C3-O2-C2
4	A	706	EDO	O1-C1-C2-O2
4	B	703	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	703	EDO	1	0
4	B	702	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	672/683 (98%)	-0.16	15 (2%) 62 57	18, 29, 53, 102	0
1	B	671/683 (98%)	0.10	44 (6%) 18 14	22, 35, 64, 100	0
1	C	673/683 (98%)	-0.25	13 (1%) 66 63	20, 29, 54, 96	0
1	D	671/683 (98%)	-0.19	16 (2%) 59 54	19, 30, 55, 95	0
All	All	2687/2732 (98%)	-0.13	88 (3%) 46 40	18, 30, 58, 102	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	GLY	10.8
1	D	22	ALA	8.1
1	A	23	GLU	7.7
1	A	21	PRO	7.1
1	A	22	ALA	6.7
1	B	504	LEU	6.0
1	A	679	HIS	6.0
1	D	24	GLY	5.7
1	D	23	GLU	5.5
1	D	21	PRO	5.4
1	B	467	PHE	5.2
1	B	449	ALA	5.1
1	B	8	ALA	4.9
1	B	463	GLY	4.8
1	A	350	PRO	4.7
1	B	445	GLU	4.5
1	D	673	GLY	4.3
1	A	563	GLU	4.1
1	C	23	GLU	3.9
1	B	464	PHE	3.9
1	B	57	GLY	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	350	PRO	3.7
1	A	133	LYS	3.6
1	C	7	ASN	3.5
1	B	479	ILE	3.4
1	A	351	ASN	3.4
1	A	348	ALA	3.3
1	B	678	HIS	3.3
1	D	564	GLY	3.2
1	A	564	GLY	3.2
1	C	8	ALA	3.1
1	B	394	VAL	3.1
1	C	444	LEU	3.1
1	B	453	SER	3.0
1	A	678	HIS	3.0
1	C	678	HIS	3.0
1	D	563	GLU	3.0
1	C	473	GLY	3.0
1	B	670	PRO	2.9
1	C	57	GLY	2.9
1	B	10	GLU	2.9
1	B	389	LEU	2.9
1	B	456	LEU	2.9
1	D	674	GLY	2.9
1	C	679	HIS	2.8
1	B	24	GLY	2.8
1	B	386	ILE	2.8
1	B	457	LYS	2.7
1	B	446	GLY	2.7
1	B	23	GLU	2.7
1	B	470	GLU	2.7
1	B	58	LYS	2.7
1	A	20	PHE	2.6
1	B	55	LYS	2.6
1	D	20	PHE	2.6
1	D	349	ASP	2.6
1	C	445	GLU	2.6
1	B	471	THR	2.6
1	B	454	ILE	2.5
1	B	503	LYS	2.5
1	C	56	ALA	2.5
1	B	450	ALA	2.5
1	B	435	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	461	GLY	2.4
1	B	441	PRO	2.4
1	D	132	ALA	2.3
1	D	351	ASN	2.3
1	B	439	TYR	2.3
1	B	22	ALA	2.3
1	B	674	GLY	2.3
1	B	59	LEU	2.3
1	B	529	TRP	2.2
1	B	53	PHE	2.2
1	B	61	PRO	2.2
1	B	19	GLN	2.2
1	B	440	TYR	2.2
1	A	349	ASP	2.2
1	B	468	PRO	2.1
1	B	444	LEU	2.1
1	D	566	GLU	2.1
1	B	54	GLU	2.1
1	B	472	LEU	2.1
1	C	24	GLY	2.1
1	A	346	ARG	2.1
1	D	348	ALA	2.1
1	D	678	HIS	2.1
1	B	473	GLY	2.1
1	C	402	ALA	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.

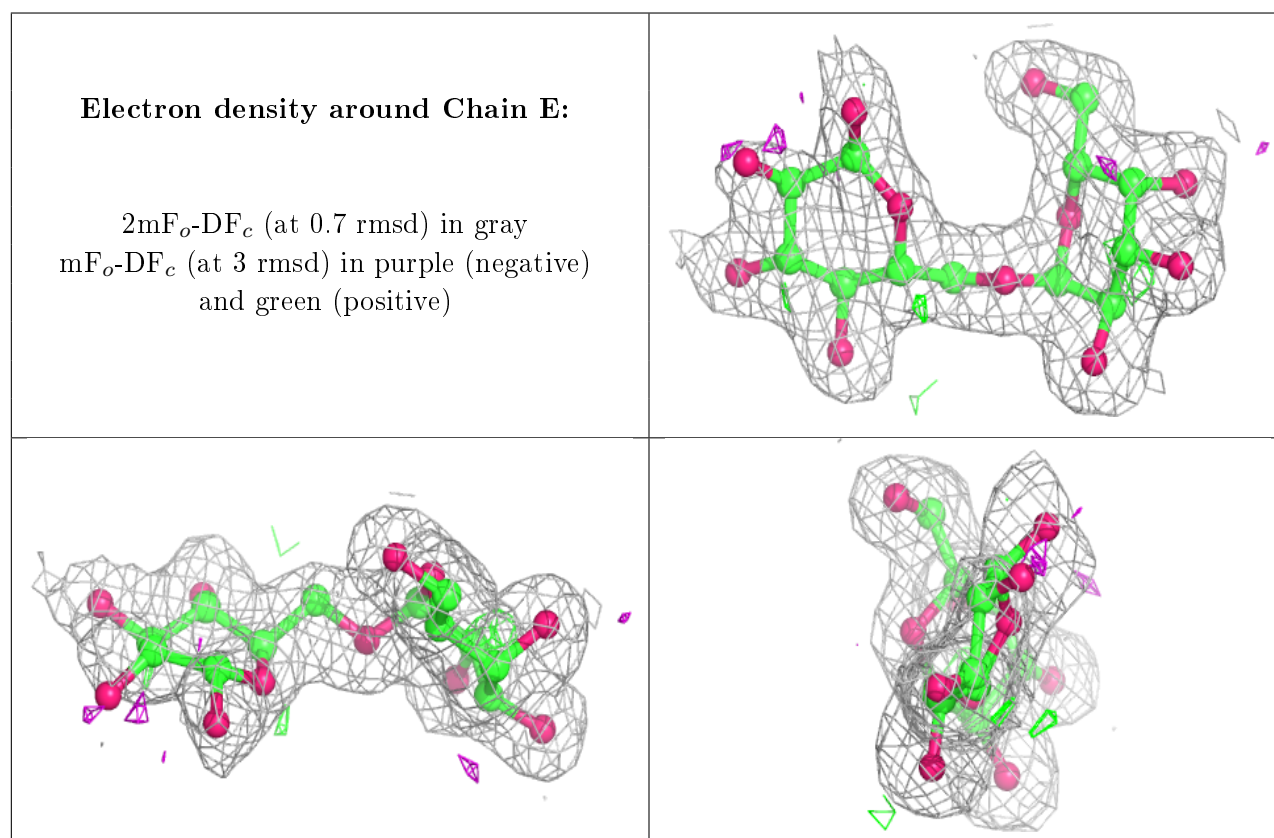
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	H	1	12/12	0.91	0.13	25,40,47,48	0
2	GLC	E	1	12/12	0.92	0.14	23,40,49,53	0
2	GLC	G	1	12/12	0.94	0.10	22,35,44,50	0

Continued on next page...

Continued from previous page...

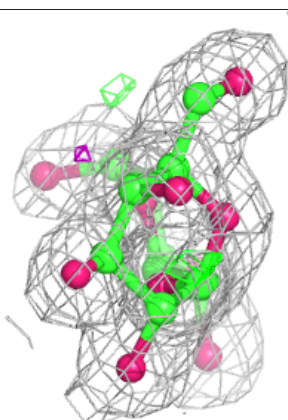
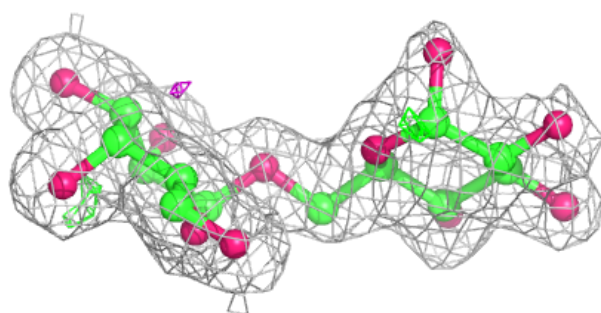
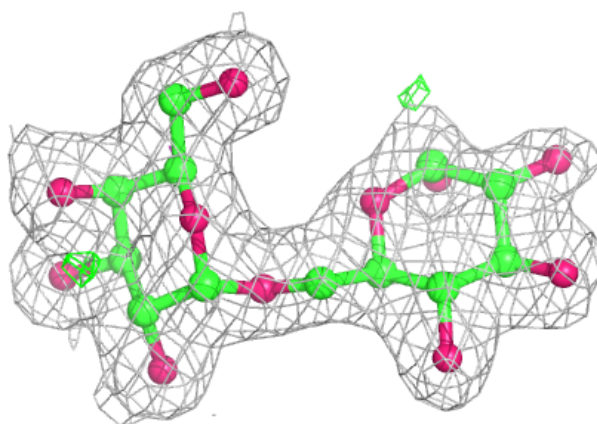
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GLC	F	1	12/12	0.94	0.10	25,37,49,50	0
2	GLA	E	2	11/12	0.96	0.14	18,20,21,22	0
2	GLA	G	2	11/12	0.97	0.14	18,19,22,23	0
2	GLA	H	2	11/12	0.98	0.12	18,23,27,27	0
2	GLA	F	2	11/12	0.98	0.13	20,21,22,24	0

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.

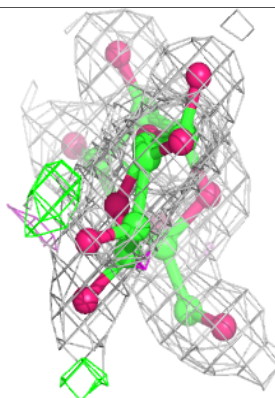
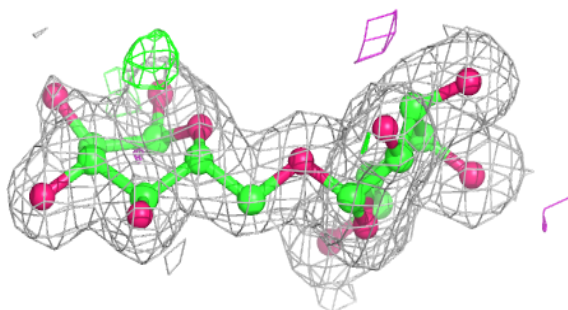
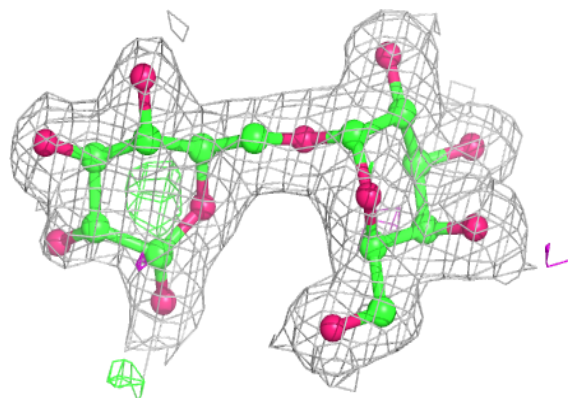


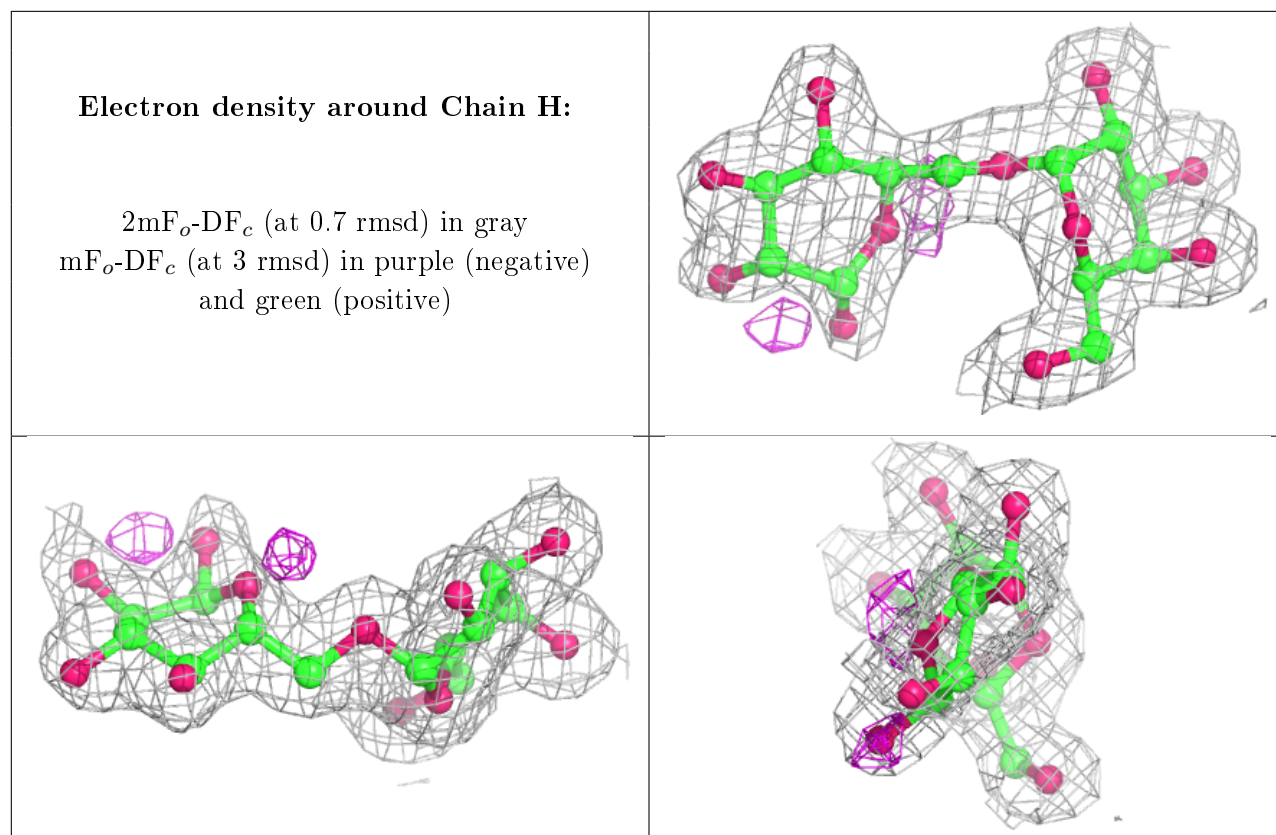
Electron density around Chain F:

$2mF_o-DF_c$ (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)





6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	EDO	A	706	4/4	0.47	0.20	70,70,70,70	0
4	EDO	A	705	4/4	0.66	0.24	62,64,64,65	0
4	EDO	B	702	4/4	0.69	0.15	42,44,45,47	0
4	EDO	A	704	4/4	0.79	0.28	61,61,62,63	0
5	NA	A	712	1/1	0.82	0.06	63,63,63,63	0
7	PEG	D	710	7/7	0.83	0.16	40,42,47,48	0
4	EDO	D	703	4/4	0.84	0.10	65,65,65,66	0
4	EDO	C	703	4/4	0.85	0.13	38,41,43,44	0
5	NA	A	708	1/1	0.85	0.15	55,55,55,55	0
4	EDO	D	702	4/4	0.85	0.23	57,58,59,60	0
4	EDO	B	703	4/4	0.88	0.20	38,47,51,56	0
5	NA	D	707	1/1	0.93	0.11	49,49,49,49	0
5	NA	C	713	1/1	0.94	0.11	41,41,41,41	0
5	NA	B	709	1/1	0.94	0.09	38,38,38,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	NA	C	712	1/1	0.94	0.07	40,40,40,40	0
3	MG	D	701	1/1	0.95	0.04	41,41,41,41	0
5	NA	A	709	1/1	0.95	0.06	51,51,51,51	0
3	MG	B	701	1/1	0.95	0.14	39,39,39,39	0
5	NA	B	713	1/1	0.95	0.11	39,39,39,39	0
4	EDO	A	703	4/4	0.95	0.11	32,34,36,36	0
3	MG	C	701	1/1	0.96	0.05	29,29,29,29	0
5	NA	C	710	1/1	0.96	0.06	47,47,47,47	0
5	NA	C	706	1/1	0.96	0.12	37,37,37,37	0
5	NA	B	710	1/1	0.96	0.14	35,35,35,35	0
5	NA	B	711	1/1	0.96	0.09	37,37,37,37	0
5	NA	B	712	1/1	0.96	0.06	42,42,42,42	0
5	NA	D	705	1/1	0.97	0.15	35,35,35,35	0
5	NA	C	709	1/1	0.97	0.10	42,42,42,42	0
5	NA	B	707	1/1	0.97	0.04	36,36,36,36	0
5	NA	B	706	1/1	0.98	0.10	32,32,32,32	0
5	NA	A	707	1/1	0.98	0.05	27,27,27,27	0
5	NA	A	711	1/1	0.98	0.07	33,33,33,33	0
5	NA	D	706	1/1	0.98	0.10	29,29,29,29	0
3	MG	A	702	1/1	0.98	0.15	28,28,28,28	0
5	NA	C	707	1/1	0.98	0.04	31,31,31,31	0
5	NA	B	705	1/1	0.98	0.11	24,24,24,24	0
5	NA	C	705	1/1	0.99	0.07	25,25,25,25	0
5	NA	C	708	1/1	0.99	0.13	24,24,24,24	0
5	NA	B	708	1/1	0.99	0.12	26,26,26,26	0
5	NA	C	711	1/1	0.99	0.06	27,27,27,27	0
5	NA	D	708	1/1	0.99	0.06	35,35,35,35	0
5	NA	A	710	1/1	0.99	0.08	34,34,34,34	0
3	MG	C	702	1/1	0.99	0.04	36,36,36,36	0
6	CL	D	709	1/1	0.99	0.07	37,37,37,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.