



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:14 PM UTC

PDB ID : 6BS6 / pdb_00006bs6
Title : SusG with mixed linkage amylosaccharide
Authors : Koropatkin, N.M.; Cockburn, D.W.
Deposited on : 2017-12-01
Resolution : 2.17 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

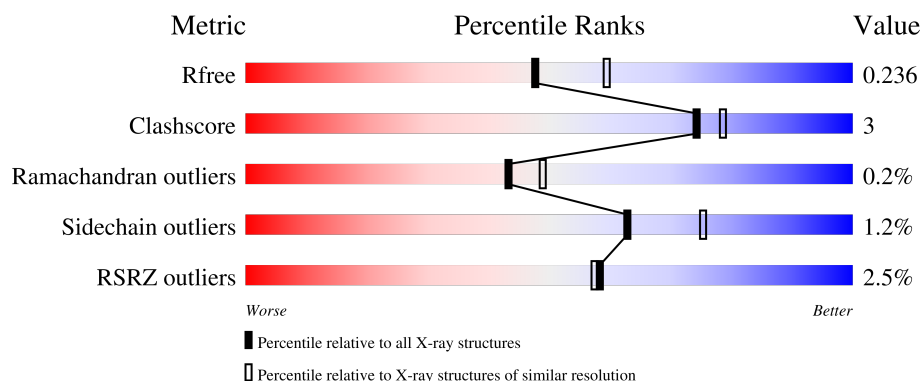
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	670	0% 89% 7% .
1	B	670	3% 89% 8% .
2	C	4	100%
2	H	4	50% 50%
3	D	8	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	6	 50%50%
5	F	3	 100%
6	G	7	 100%

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 11397 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 Alpha-amylase SusG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	648	Total	C	N	O	S	0	0	0
			5164	3286	836	1026	16			
1	B	649	Total	C	N	O	S	0	0	0
			5169	3288	836	1029	16			

There are 4 discrepancies between the modelled and reference sequences:

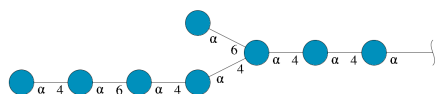
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	GLY	-	expression tag	UNP Q8A1G3
A	498	ASN	ASP	engineered mutation	UNP Q8A1G3
B	23	GLY	-	expression tag	UNP Q8A1G3
B	498	ASN	ASP	engineered mutation	UNP Q8A1G3

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



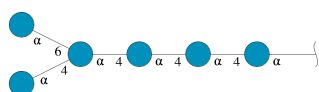
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	4	Total	C	O	0	0	0
			45	24	21			
2	H	4	Total	C	O	0	0	0
			45	24	21			

- Molecule 3 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	8	Total	C	O	0	0	0
			89	48	41			

- Molecule 4 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



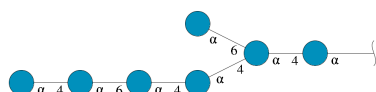
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	E	6	Total	C	O	0	0	0
			67	36	31			

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	F	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 6 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

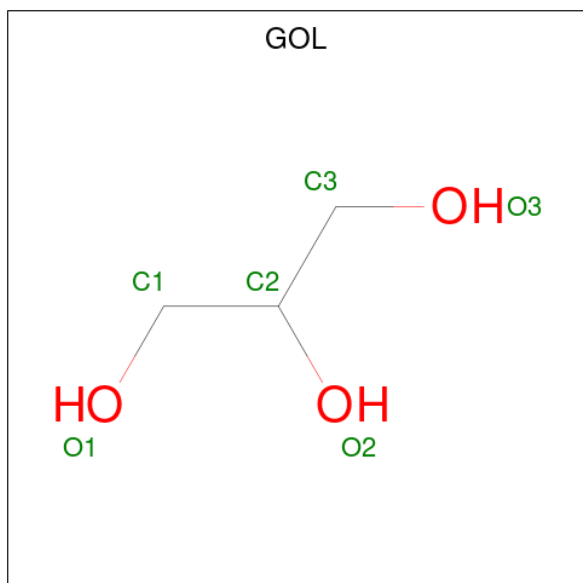


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
6	G	7	Total	C	O	0	0	0
			78	42	36			

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	0	0
			2	2		
7	B	2	Total	Ca	0	0
			2	2		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

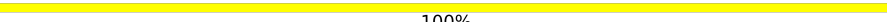
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	467	Total	O	0	0
			467	467		
10	B	225	Total	O	0	0
			225	225		

Chain H:  50% 50%

GLC1
GLC2
GLC3
GLC4

- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:  100%

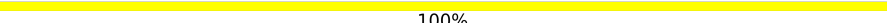
GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7
GLC8

- Molecule 4: alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain E:  50% 50%

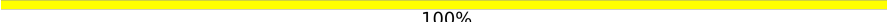
GLC1
GLC2
GLC3
GLC4
GLC5
GLC6

- Molecule 5: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain F:  100%

GLC1
GLC2
GLC3

- Molecule 6: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain G:  100%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7

4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	127.44Å 127.44Å 129.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.40 – 2.17 45.40 – 2.17	Depositor EDS
% Data completeness (in resolution range)	97.1 (45.40-2.17) 82.3 (45.40-2.17)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.89 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.194 , 0.232 0.202 , 0.236	Depositor DCC
R_{free} test set	1977 reflections (1.82%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,-l,-k 0.005 for -h,l,k 0.005 for l,-k,h 0.014 for -l,-k,-h 0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11397	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: GOL, CA, GLC, ACT

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	0.48	0/5302	0.72	0/7204
1	B	0.40	0/5308	0.76	5/7214 (0.1%)
All	All	0.44	0/10610	0.74	5/14418 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ALA	CA-C-N	-13.63	102.80	119.84
1	B	231	ALA	C-N-CA	-13.63	102.80	119.84
1	B	231	ALA	C-N-CD	5.35	146.92	125.00
1	B	601	TYR	CA-C-N	5.04	125.06	119.32
1	B	601	TYR	C-N-CA	5.04	125.06	119.32

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	5164	0	4870	28	0
1	B	5169	0	4872	33	0
2	C	45	0	39	0	0
2	H	45	0	39	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	89	0	75	0	0
4	E	67	0	57	2	0
5	F	34	0	30	0	0
6	G	78	0	66	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
8	A	6	0	8	1	0
9	A	4	0	3	0	0
10	A	467	0	0	3	0
10	B	225	0	0	2	0
All	All	11397	0	10059	64	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 3.

All (64) 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:B:238:VAL:HG21	1:B:314:LEU:HD21	1.64	0.79
1:A:242:THR:O	1:A:243:LYS:HD3	1.93	0.69
1:B:475:LEU:HG	1:B:609:MET:HE3	1.74	0.68
2:H:1:GLC:H62	2:H:2:GLC:H5	1.77	0.67
1:B:615:TYR:HB3	1:B:626:ILE:HD13	1.76	0.67
1:B:359:ASP:OD1	1:B:404:ARG:NH2	2.27	0.67
1:B:596:ARG:O	1:B:600:THR:HG23	1.95	0.67
1:A:271:ASP:OD2	10:A:801:HOH:O	2.13	0.66
1:B:474:ILE:HB	1:B:609:MET:HE1	1.78	0.66
1:A:475:LEU:HG	1:A:609:MET:HE3	1.79	0.66
1:B:54:TRP:CD1	1:B:600:THR:HG22	2.32	0.64
4:E:2:GLC:H61	4:E:3:GLC:H5	1.79	0.64
1:B:666:GLU:HB3	1:B:681:GLY:HA3	1.81	0.63
1:A:61:ASP:OD2	1:A:526:HIS:ND1	2.27	0.62
1:B:109:MET:HE1	1:B:157:THR:HG22	1.83	0.60
1:A:656:LYS:HZ2	1:A:691:GLY:HA3	1.66	0.60
1:B:292:ARG:HD3	1:B:299:TRP:CZ3	2.40	0.56
1:B:678:LEU:HD21	1:B:680:LEU:HG	1.90	0.54
1:B:689:LYS:NZ	10:B:806:HOH:O	2.40	0.52
1:B:68:LEU:HD11	1:B:105:ILE:HG22	1.92	0.51
1:A:172:PRO:HB2	8:A:721:GOL:H32	1.92	0.51
1:A:217:ALA:HB2	1:A:286:THR:HG22	1.93	0.50
1:A:226:LEU:HB2	1:A:277:TYR:HB2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:626:ILE:O	1:B:626:ILE:HD12	2.13	0.49
1:A:47:LEU:HD21	1:A:669:GLN:HB3	1.94	0.49
1:A:238:VAL:HG21	1:A:314:LEU:HD21	1.93	0.48
1:A:469:TYR:OH	1:A:620:GLU:HG3	2.13	0.48
1:A:44:TRP:HB3	1:A:668:GLN:OE1	2.14	0.47
1:B:49:ALA:HA	1:B:660:VAL:HG12	1.98	0.46
1:B:458:LEU:HD13	1:B:519:VAL:HG11	1.96	0.46
1:B:234:PRO:HG2	1:B:322:LEU:HB2	1.98	0.46
1:A:230:ASN:OD1	1:A:232:PRO:HD2	2.14	0.46
1:B:106:HIS:ND1	1:B:119:TYR:HA	2.31	0.46
1:B:54:TRP:CE2	1:B:56:GLU:HA	2.52	0.45
1:A:313:LYS:HE2	1:A:336:GLN:O	2.17	0.45
1:A:71:PHE:HB3	10:A:1023:HOH:O	2.16	0.45
1:A:228:TRP:CE2	1:A:257:LYS:HE3	2.52	0.45
1:B:407:LYS:HB2	1:B:445:GLY:HA2	1.98	0.44
1:B:668:GLN:NE2	1:B:679:LYS:HD3	2.32	0.44
4:E:1:GLC:H62	4:E:2:GLC:H5	1.98	0.44
1:A:129:GLU:OE1	1:A:380:ARG:NH2	2.46	0.44
1:A:633:LYS:NZ	10:A:804:HOH:O	2.37	0.44
1:A:242:THR:OG1	1:A:243:LYS:N	2.48	0.44
1:B:590:ILE:HD13	1:B:590:ILE:HA	1.84	0.43
1:B:623:TYR:HB3	1:B:626:ILE:HG12	2.01	0.43
1:B:224:PHE:O	1:B:278:GLU:HA	2.19	0.43
1:B:101:TRP:CD1	1:B:101:TRP:C	2.96	0.43
1:B:292:ARG:HD2	10:B:870:HOH:O	2.19	0.42
1:B:623:TYR:HB3	1:B:626:ILE:CG1	2.50	0.42
1:A:106:HIS:HB3	1:A:118:ASP:O	2.20	0.42
1:B:106:HIS:CD2	1:B:106:HIS:N	2.88	0.42
1:A:298:PHE:O	1:A:300:PRO:HD3	2.20	0.42
1:A:133:ASP:OD1	1:A:380:ARG:HD2	2.19	0.41
1:B:534:GLU:HA	1:B:591:TYR:CE1	2.55	0.41
1:A:54:TRP:CE2	1:A:56:GLU:HA	2.55	0.41
1:A:101:TRP:C	1:A:101:TRP:CD1	2.98	0.41
1:B:106:HIS:HB3	1:B:118:ASP:O	2.20	0.41
1:B:289:LEU:HG	1:B:331:ILE:HB	2.01	0.41
1:B:292:ARG:HD3	1:B:299:TRP:CH2	2.56	0.41
1:B:514:LYS:NZ	1:B:585:HIS:O	2.41	0.41
1:A:313:LYS:HD3	1:A:334:ASP:HA	2.02	0.40
1:A:417:TYR:CE1	1:A:422:HIS:ND1	2.89	0.40
1:A:671:THR:HA	1:A:675:SER:O	2.22	0.40
1:A:474:ILE:HB	1:A:609:MET:HE1	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	644/670 (96%)	627 (97%)	16 (2%)	1 (0%)	43	49
1	B	647/670 (97%)	621 (96%)	25 (4%)	1 (0%)	43	49
All	All	1291/1340 (96%)	1248 (97%)	41 (3%)	2 (0%)	43	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	THR
1	B	231	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	549/568 (97%)	542 (99%)	7 (1%)	61	74
1	B	550/568 (97%)	544 (99%)	6 (1%)	65	77
All	All	1099/1136 (97%)	1086 (99%)	13 (1%)	63	75

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	115	ASP
1	A	243	LYS
1	A	294	SER
1	A	590	ILE
1	A	620	GLU
1	A	689	LYS
1	B	289	LEU
1	B	294	SER
1	B	423	THR
1	B	433	LEU
1	B	590	ILE
1	B	621	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	342	HIS
1	A	498	ASN
1	B	94	GLN
1	B	317	ASN
1	B	342	HIS
1	B	581	GLN
1	B	668	GLN
1	B	692	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 ⓘ

32 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	C	1	2	12,12,12	1.21	1 (8%)	17,17,17	0.90	0
2	GLC	C	2	2	11,11,12	1.48	2 (18%)	15,15,17	0.73	0
2	GLC	C	3	2	11,11,12	1.51	2 (18%)	15,15,17	0.73	0
2	GLC	C	4	2	11,11,12	1.68	3 (27%)	15,15,17	0.78	0
3	GLC	D	1	3	12,12,12	1.33	1 (8%)	17,17,17	1.11	1 (5%)
3	GLC	D	2	3	11,11,12	1.58	3 (27%)	15,15,17	0.58	0
3	GLC	D	3	3	11,11,12	1.42	2 (18%)	15,15,17	1.02	1 (6%)
3	GLC	D	4	3	11,11,12	1.43	2 (18%)	15,15,17	1.19	2 (13%)
3	GLC	D	5	3	11,11,12	1.57	3 (27%)	15,15,17	0.62	0
3	GLC	D	6	3	11,11,12	1.35	2 (18%)	15,15,17	0.84	1 (6%)
3	GLC	D	7	3	11,11,12	1.57	3 (27%)	15,15,17	0.72	1 (6%)
3	GLC	D	8	3	11,11,12	1.76	3 (27%)	15,15,17	0.54	0
4	GLC	E	1	4	12,12,12	1.25	1 (8%)	17,17,17	1.14	1 (5%)
4	GLC	E	2	4	11,11,12	1.58	2 (18%)	15,15,17	0.48	0
4	GLC	E	3	4	11,11,12	1.51	2 (18%)	15,15,17	0.61	0
4	GLC	E	4	4	11,11,12	1.57	2 (18%)	15,15,17	0.84	0
4	GLC	E	5	4	11,11,12	1.67	3 (27%)	15,15,17	0.80	0
4	GLC	E	6	4	11,11,12	1.72	3 (27%)	15,15,17	0.73	0
5	GLC	F	1	5	12,12,12	1.21	2 (16%)	17,17,17	0.86	0
5	GLC	F	2	5	11,11,12	1.54	2 (18%)	15,15,17	0.62	0
5	GLC	F	3	5	11,11,12	1.63	3 (27%)	15,15,17	1.12	1 (6%)
6	GLC	G	1	6	12,12,12	1.16	1 (8%)	17,17,17	0.68	0
6	GLC	G	2	6	11,11,12	1.53	2 (18%)	15,15,17	0.86	1 (6%)
6	GLC	G	3	6	11,11,12	1.74	3 (27%)	15,15,17	0.88	0
6	GLC	G	4	6	11,11,12	1.60	2 (18%)	15,15,17	0.86	1 (6%)
6	GLC	G	5	6	11,11,12	1.62	2 (18%)	15,15,17	0.56	0
6	GLC	G	6	6	11,11,12	1.66	3 (27%)	15,15,17	0.68	0
6	GLC	G	7	6	11,11,12	1.53	2 (18%)	15,15,17	1.05	0
2	GLC	H	1	2	12,12,12	1.16	1 (8%)	17,17,17	0.82	0
2	GLC	H	2	2	11,11,12	1.54	2 (18%)	15,15,17	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	H	3	2	11,11,12	1.70	3 (27%)	15,15,17	0.63	0
2	GLC	H	4	2	11,11,12	1.63	3 (27%)	15,15,17	0.67	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	GLC	C	1	2	-	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	1/2/19/22	0/1/1/1
2	GLC	C	4	2	-	1/2/19/22	0/1/1/1
3	GLC	D	1	3	-	2/2/22/22	0/1/1/1
3	GLC	D	2	3	-	1/2/19/22	0/1/1/1
3	GLC	D	3	3	-	0/2/19/22	0/1/1/1
3	GLC	D	4	3	-	0/2/19/22	0/1/1/1
3	GLC	D	5	3	-	0/2/19/22	0/1/1/1
3	GLC	D	6	3	-	0/2/19/22	0/1/1/1
3	GLC	D	7	3	-	2/2/19/22	0/1/1/1
3	GLC	D	8	3	-	2/2/19/22	0/1/1/1
4	GLC	E	1	4	-	0/2/22/22	0/1/1/1
4	GLC	E	2	4	-	0/2/19/22	0/1/1/1
4	GLC	E	3	4	-	0/2/19/22	0/1/1/1
4	GLC	E	4	4	-	2/2/19/22	0/1/1/1
4	GLC	E	5	4	-	0/2/19/22	0/1/1/1
4	GLC	E	6	4	-	0/2/19/22	0/1/1/1
5	GLC	F	1	5	-	0/2/22/22	0/1/1/1
5	GLC	F	2	5	-	0/2/19/22	0/1/1/1
5	GLC	F	3	5	-	1/2/19/22	0/1/1/1
6	GLC	G	1	6	-	1/2/22/22	0/1/1/1
6	GLC	G	2	6	-	1/2/19/22	0/1/1/1
6	GLC	G	3	6	-	0/2/19/22	0/1/1/1
6	GLC	G	4	6	-	0/2/19/22	0/1/1/1
6	GLC	G	5	6	-	0/2/19/22	0/1/1/1
6	GLC	G	6	6	-	2/2/19/22	0/1/1/1
6	GLC	G	7	6	-	1/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	2/2/19/22	0/1/1/1
2	GLC	H	3	2	-	0/2/19/22	0/1/1/1
2	GLC	H	4	2	-	2/2/19/22	0/1/1/1

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	6	GLC	O5-C1	4.07	1.50	1.43
3	D	8	GLC	O5-C1	3.96	1.50	1.43
2	H	3	GLC	O5-C1	3.95	1.50	1.43
6	G	5	GLC	O5-C1	3.90	1.50	1.43
2	C	4	GLC	O5-C1	3.84	1.50	1.43
4	E	2	GLC	O5-C1	3.81	1.50	1.43
6	G	3	GLC	O5-C1	3.81	1.50	1.43
4	E	5	GLC	O5-C1	3.77	1.50	1.43
6	G	6	GLC	O5-C1	3.77	1.50	1.43
2	H	4	GLC	O5-C1	3.75	1.50	1.43
5	F	3	GLC	O5-C1	3.72	1.49	1.43
6	G	4	GLC	O5-C1	3.70	1.49	1.43
6	G	2	GLC	O5-C1	3.68	1.49	1.43
2	C	2	GLC	O5-C1	3.54	1.49	1.43
6	G	7	GLC	O5-C1	3.52	1.49	1.43
2	H	2	GLC	O5-C1	3.51	1.49	1.43
3	D	3	GLC	O5-C1	3.50	1.49	1.43
3	D	1	GLC	O5-C1	3.47	1.51	1.42
3	D	7	GLC	O5-C1	3.47	1.49	1.43
2	C	3	GLC	O5-C1	3.46	1.49	1.43
5	F	2	GLC	O5-C1	3.45	1.49	1.43
3	D	2	GLC	O5-C1	3.44	1.49	1.43
3	D	5	GLC	O5-C1	3.37	1.49	1.43
4	E	4	GLC	O5-C1	3.34	1.49	1.43
3	D	8	GLC	C2-C3	-3.27	1.47	1.52
4	E	3	GLC	O5-C1	3.23	1.49	1.43
3	D	4	GLC	O5-C1	3.13	1.48	1.43
4	E	1	GLC	O5-C1	3.11	1.50	1.42
6	G	3	GLC	C2-C3	-3.07	1.47	1.52
2	C	1	GLC	O5-C1	3.06	1.50	1.42
2	H	1	GLC	O5-C1	2.94	1.50	1.42
2	H	3	GLC	C2-C3	-2.91	1.48	1.52
5	F	2	GLC	C2-C3	-2.88	1.48	1.52
2	C	4	GLC	C2-C3	-2.88	1.48	1.52
3	D	5	GLC	C2-C3	-2.86	1.48	1.52
6	G	1	GLC	O5-C1	2.85	1.49	1.42
5	F	1	GLC	O5-C1	2.83	1.49	1.42
4	E	3	GLC	C2-C3	-2.82	1.48	1.52
6	G	6	GLC	C2-C3	-2.81	1.48	1.52
2	C	3	GLC	C2-C3	-2.81	1.48	1.52
3	D	6	GLC	O5-C1	2.77	1.48	1.43
4	E	4	GLC	C2-C3	-2.74	1.48	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	3	GLC	C2-C3	-2.73	1.48	1.52
4	E	5	GLC	C2-C3	-2.73	1.48	1.52
4	E	6	GLC	C2-C3	-2.60	1.48	1.52
2	H	4	GLC	C2-C3	-2.58	1.48	1.52
2	H	2	GLC	C2-C3	-2.57	1.48	1.52
6	G	2	GLC	C2-C3	-2.51	1.48	1.52
3	D	2	GLC	C2-C3	-2.50	1.48	1.52
3	D	6	GLC	C2-C3	-2.48	1.48	1.52
6	G	4	GLC	C2-C3	-2.44	1.48	1.52
6	G	5	GLC	C2-C3	-2.43	1.48	1.52
4	E	6	GLC	O5-C5	2.38	1.48	1.43
3	D	7	GLC	O5-C5	2.33	1.48	1.43
4	E	2	GLC	C2-C3	-2.32	1.48	1.52
3	D	7	GLC	C2-C3	-2.27	1.49	1.52
6	G	3	GLC	O5-C5	2.27	1.47	1.43
6	G	7	GLC	C2-C3	-2.26	1.49	1.52
4	E	5	GLC	O5-C5	2.25	1.47	1.43
2	C	2	GLC	C2-C3	-2.20	1.49	1.52
2	C	4	GLC	O5-C5	2.19	1.47	1.43
3	D	2	GLC	O5-C5	2.18	1.47	1.43
2	H	4	GLC	O5-C5	2.17	1.47	1.43
3	D	3	GLC	C2-C3	-2.15	1.49	1.52
5	F	1	GLC	C3-C2	-2.11	1.46	1.52
6	G	6	GLC	O5-C5	2.11	1.47	1.43
5	F	3	GLC	O5-C5	2.09	1.47	1.43
3	D	4	GLC	C2-C3	-2.09	1.49	1.52
3	D	8	GLC	O5-C5	2.08	1.47	1.43
2	H	3	GLC	O5-C5	2.05	1.47	1.43
3	D	5	GLC	O5-C5	2.04	1.47	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	GLC	O5-C5-C4	2.73	114.62	109.70
3	D	3	GLC	C1-C2-C3	2.68	113.55	109.64
5	F	3	GLC	C3-C4-C5	2.56	114.87	110.23
3	D	4	GLC	O2-C2-C3	2.53	115.40	110.15
3	D	1	GLC	O5-C1-C2	2.34	114.41	110.30
3	D	6	GLC	O2-C2-C1	-2.33	103.89	109.22
3	D	4	GLC	C3-C4-C5	2.25	114.31	110.23
6	G	2	GLC	C1-C2-C3	2.11	112.72	109.64
3	D	7	GLC	C6-C5-C4	-2.01	108.08	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	4	GLC	C6-C5-C4	-2.00	108.11	113.02

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	G	6	GLC	O5-C5-C6-O6
3	D	1	GLC	O5-C5-C6-O6
6	G	6	GLC	C4-C5-C6-O6
3	D	7	GLC	O5-C5-C6-O6
3	D	7	GLC	C4-C5-C6-O6
3	D	8	GLC	O5-C5-C6-O6
3	D	8	GLC	C4-C5-C6-O6
2	H	4	GLC	C4-C5-C6-O6
3	D	1	GLC	C4-C5-C6-O6
2	H	2	GLC	C4-C5-C6-O6
2	H	4	GLC	O5-C5-C6-O6
5	F	3	GLC	O5-C5-C6-O6
2	C	3	GLC	O5-C5-C6-O6
4	E	4	GLC	C4-C5-C6-O6
2	H	2	GLC	O5-C5-C6-O6
6	G	1	GLC	C4-C5-C6-O6
6	G	7	GLC	O5-C5-C6-O6
3	D	2	GLC	C4-C5-C6-O6
6	G	2	GLC	C4-C5-C6-O6
4	E	4	GLC	O5-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6

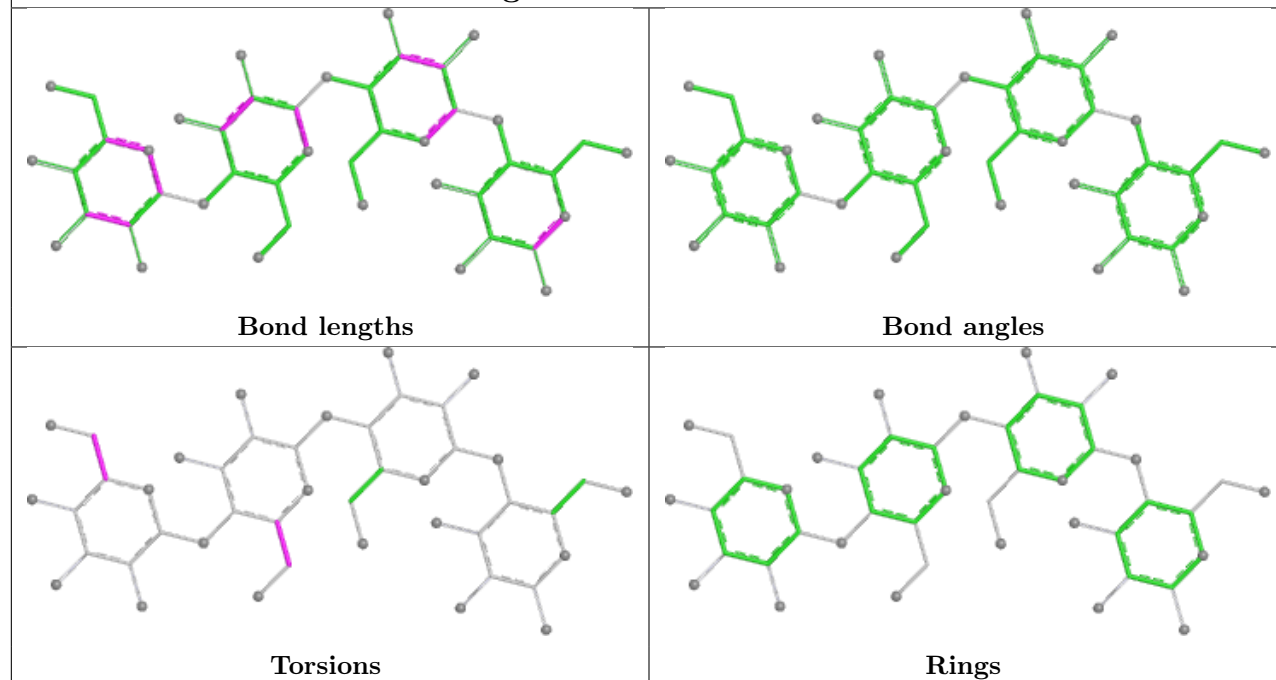
There are no ring outliers.

5 monomers are involved in 3 short contacts:

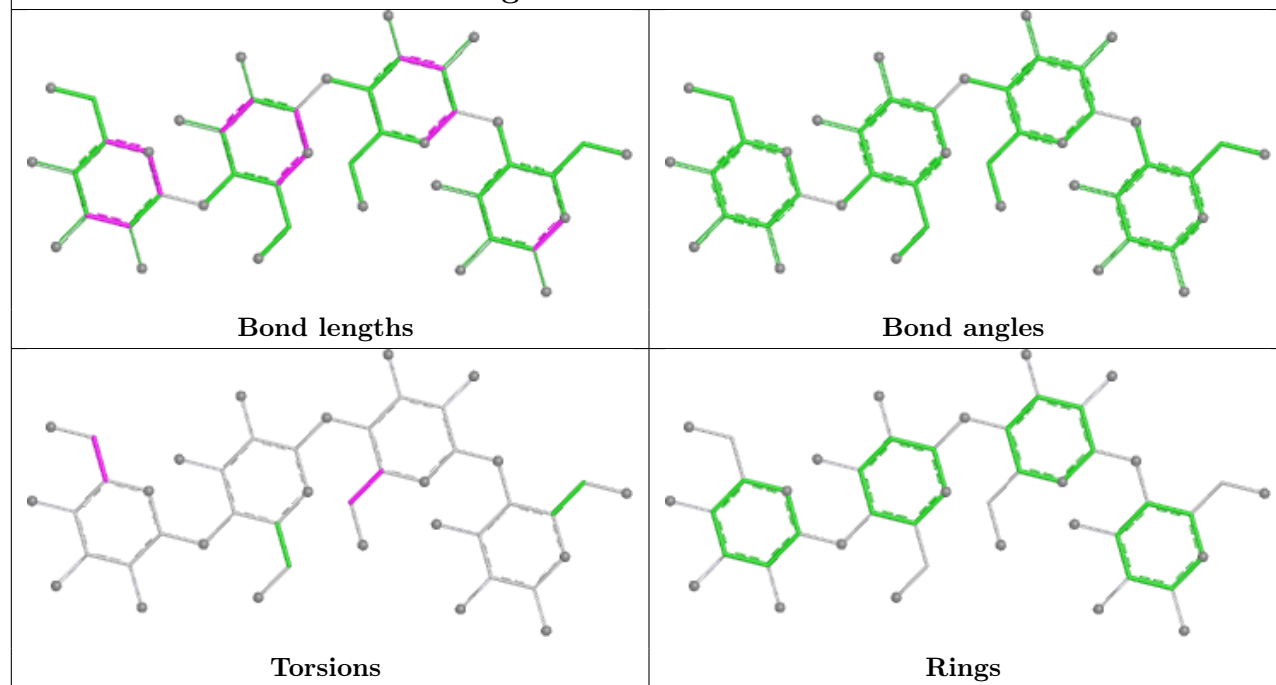
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	3	GLC	1	0
4	E	2	GLC	2	0
4	E	1	GLC	1	0
2	H	2	GLC	1	0
2	H	1	GLC	1	0

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

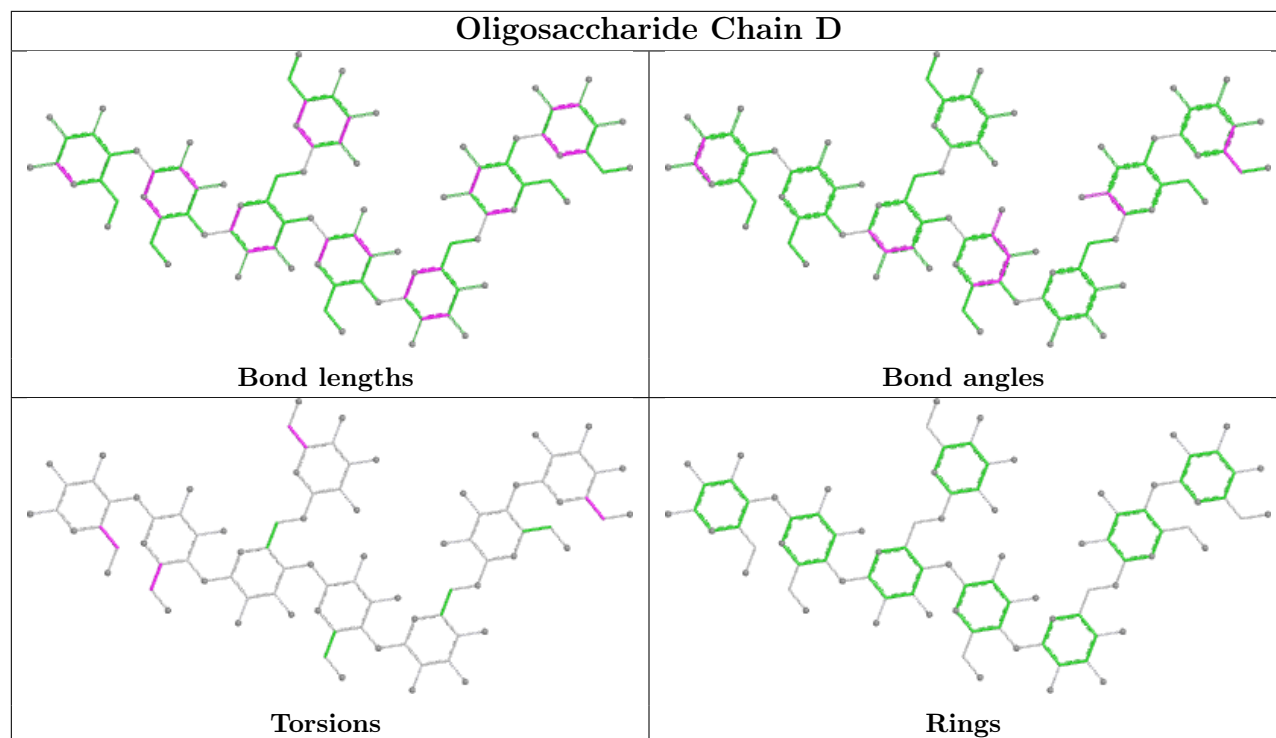
Oligosaccharide Chain C



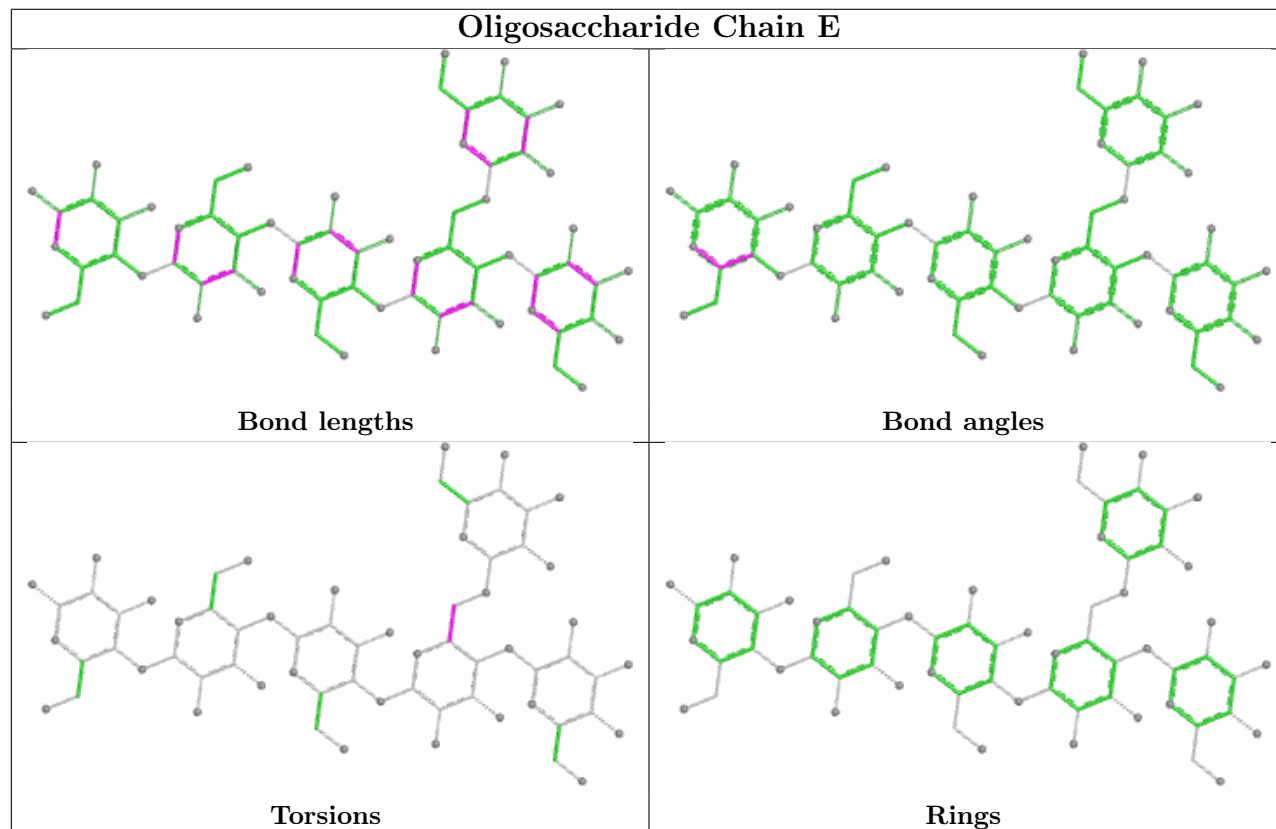
Oligosaccharide Chain H



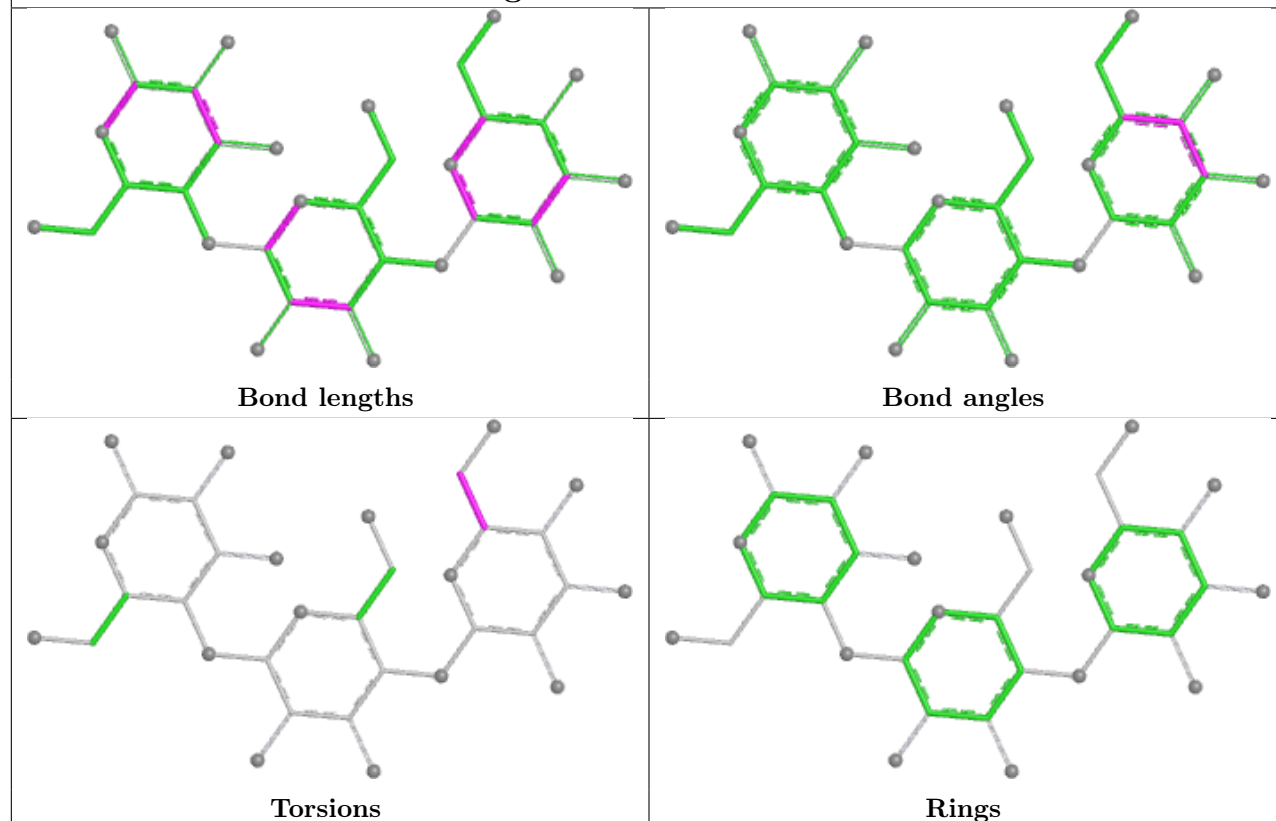
Oligosaccharide Chain D



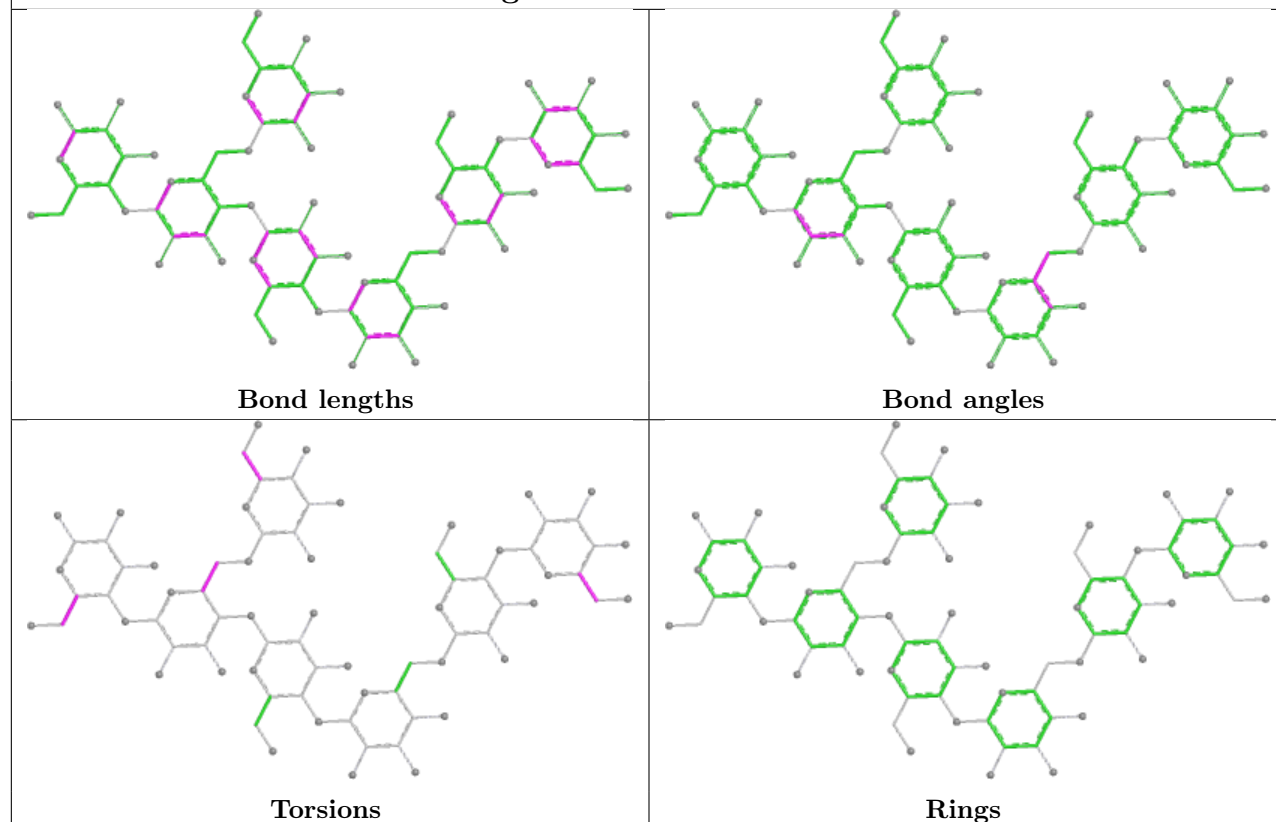
Oligosaccharide Chain E



Oligosaccharide Chain F



Oligosaccharide Chain G



5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z > 2$
8	GOL	A	721	-	5,5,5	0.33	0	5,5,5	0.64	0
9	ACT	A	722	-	3,3,3	0.85	0	3,3,3	0.91	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
8	GOL	A	721	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	721	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	721	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	648/670 (96%)	-0.21	10 (1%) 72 71	20, 33, 57, 80	0
1	B	649/670 (96%)	0.47	23 (3%) 47 46	29, 51, 75, 98	0
All	All	1297/1340 (96%)	0.13	33 (2%) 58 57	20, 42, 70, 98	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	231	ALA	4.3
1	A	242	THR	4.0
1	A	675	SER	3.5
1	B	105	ILE	3.4
1	B	647	THR	3.2
1	B	692	ASN	3.0
1	B	44	TRP	3.0
1	A	231	ALA	2.9
1	B	564	ASP	2.8
1	A	672	ASP	2.8
1	A	230	ASN	2.7
1	B	626	ILE	2.7
1	B	680	LEU	2.6
1	B	674	ASP	2.6
1	A	105	ILE	2.6
1	A	243	LYS	2.5
1	A	232	PRO	2.3
1	B	240	THR	2.3
1	B	654	THR	2.3
1	B	676	TYR	2.3
1	B	584	THR	2.2
1	B	682	GLY	2.2
1	B	134	ARG	2.2
1	A	43	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	686	VAL	2.1
1	B	575	LYS	2.1
1	B	510	ALA	2.1
1	B	627	ALA	2.1
1	B	675	SER	2.1
1	B	76	GLY	2.0
1	B	547	TYR	2.0
1	B	623	TYR	2.0
1	A	692	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

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

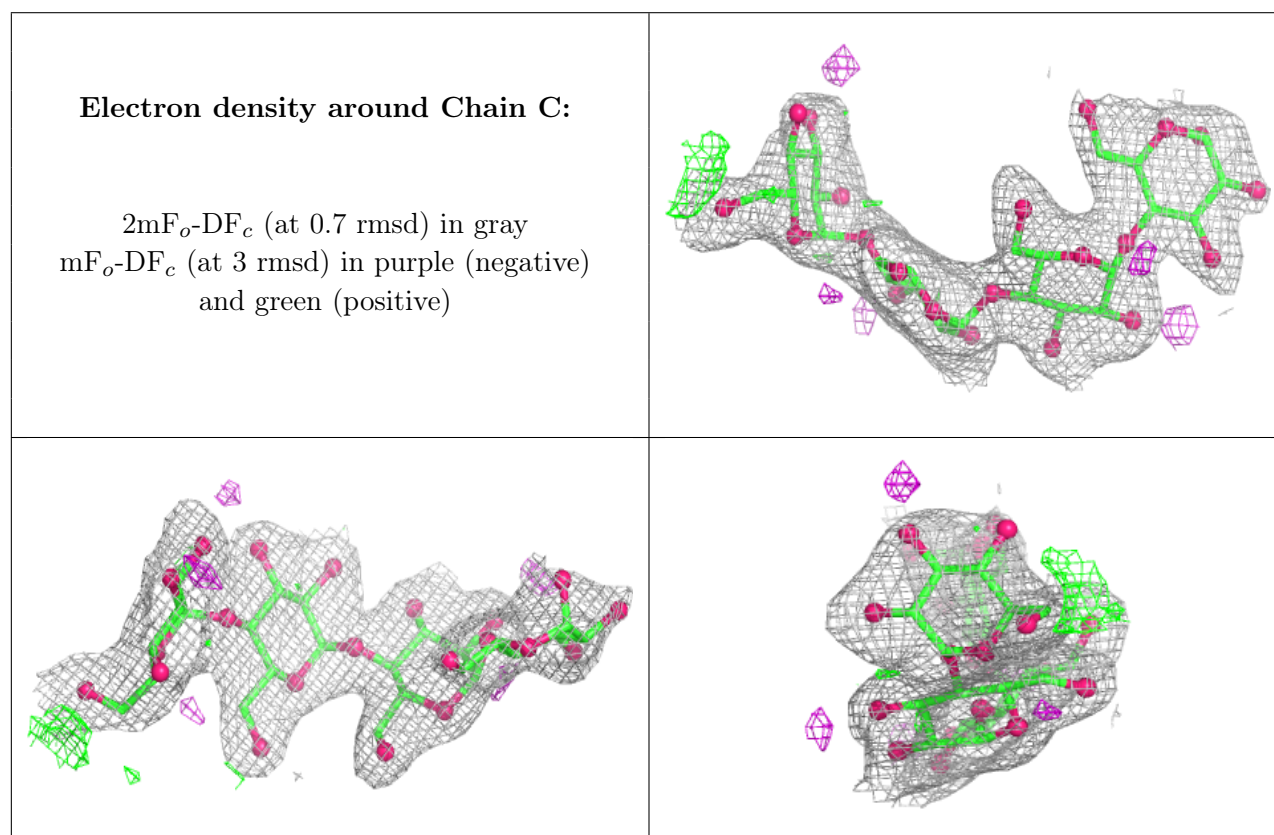
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	H	1	12/12	0.62	0.17	72,84,86,89	0
2	GLC	H	4	11/12	0.63	0.18	74,75,82,86	0
3	GLC	D	1	12/12	0.71	0.21	52,64,71,74	0
3	GLC	D	7	11/12	0.78	0.16	52,56,60,68	0
4	GLC	E	2	11/12	0.79	0.14	46,62,69,69	0
2	GLC	C	4	11/12	0.80	0.14	45,59,67,74	0
5	GLC	F	3	11/12	0.80	0.15	58,66,74,80	0
4	GLC	E	1	12/12	0.81	0.14	60,66,78,79	0
4	GLC	E	5	11/12	0.83	0.12	56,61,74,79	0
2	GLC	H	2	11/12	0.83	0.12	61,63,67,68	0
2	GLC	H	3	11/12	0.84	0.12	50,63,67,71	0
6	GLC	G	6	11/12	0.84	0.13	59,66,72,78	0
4	GLC	E	6	11/12	0.85	0.15	67,74,77,77	0
6	GLC	G	1	12/12	0.88	0.10	40,56,63,68	0
2	GLC	C	1	12/12	0.88	0.14	41,59,71,74	0
6	GLC	G	7	11/12	0.88	0.12	46,57,65,70	0
3	GLC	D	8	11/12	0.91	0.11	35,47,56,60	0
6	GLC	G	5	11/12	0.92	0.10	44,48,58,62	0
6	GLC	G	2	11/12	0.93	0.08	37,44,48,48	0

Continued on next page...

Continued from previous page...

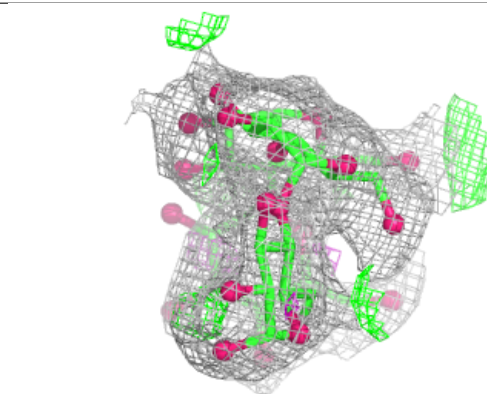
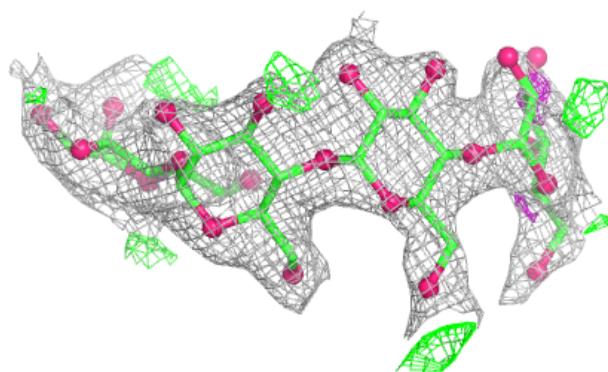
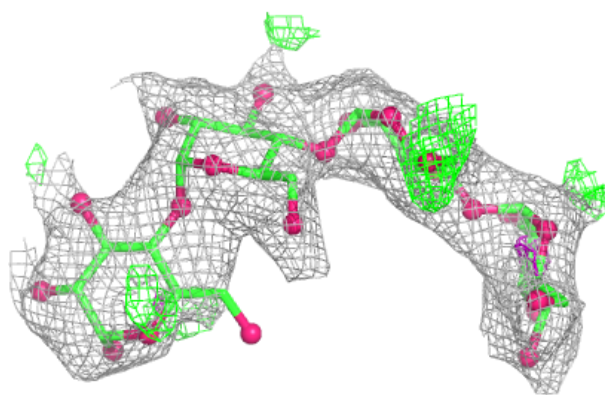
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GLC	F	2	11/12	0.93	0.08	36,39,42,44	0
5	GLC	F	1	12/12	0.94	0.09	37,38,49,50	0
4	GLC	E	4	11/12	0.94	0.08	31,34,43,52	0
2	GLC	C	2	11/12	0.94	0.07	35,40,47,53	0
3	GLC	D	2	11/12	0.94	0.08	29,36,55,57	0
6	GLC	G	4	11/12	0.95	0.08	34,43,48,50	0
2	GLC	C	3	11/12	0.95	0.08	31,35,42,45	0
3	GLC	D	5	11/12	0.95	0.07	23,26,31,35	0
6	GLC	G	3	11/12	0.95	0.07	33,38,43,46	0
3	GLC	D	6	11/12	0.96	0.07	24,29,36,37	0
4	GLC	E	3	11/12	0.96	0.08	24,34,40,47	0
3	GLC	D	3	11/12	0.96	0.06	21,26,30,33	0
3	GLC	D	4	11/12	0.97	0.05	17,24,27,28	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.

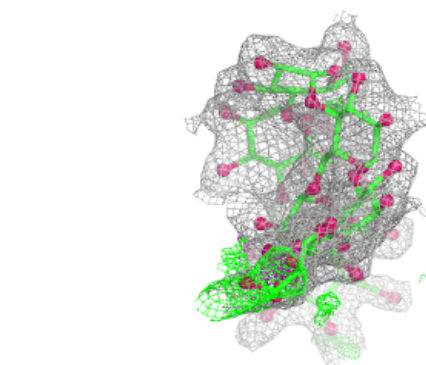
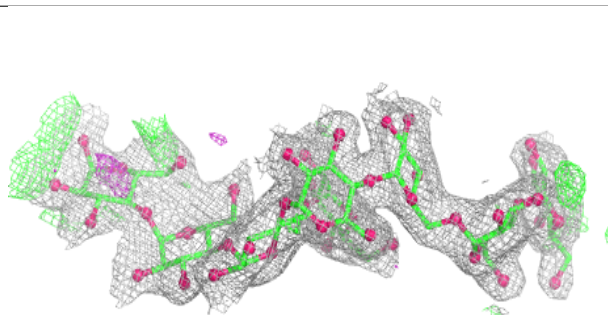
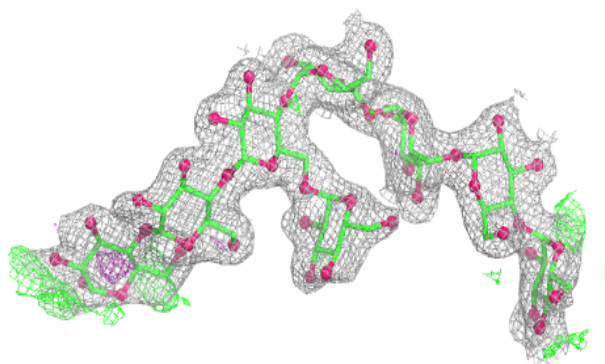


Electron density around Chain H:

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

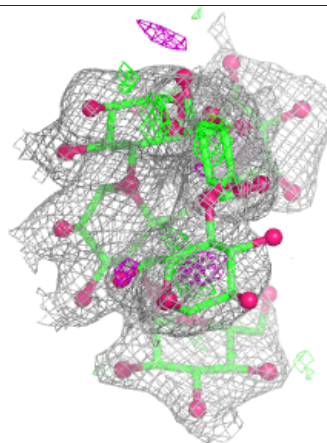
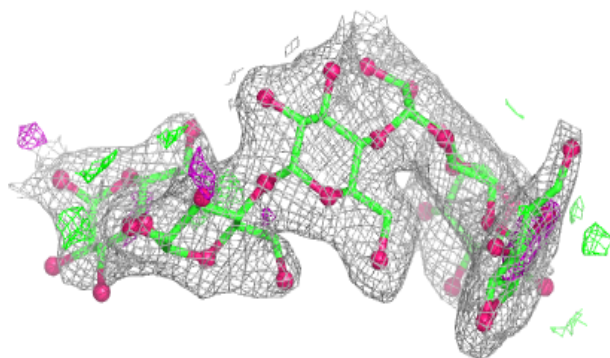
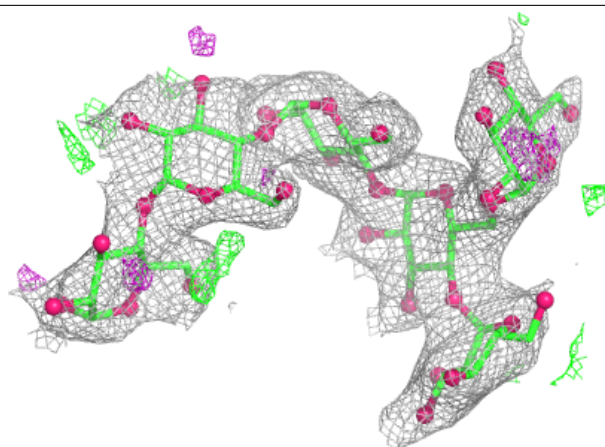
**Electron density around Chain D:**

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

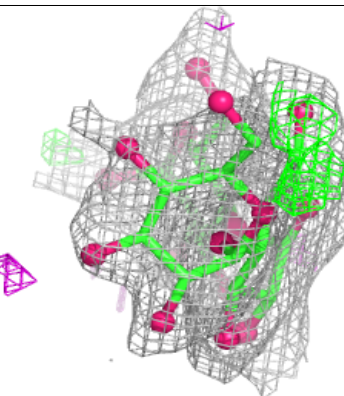
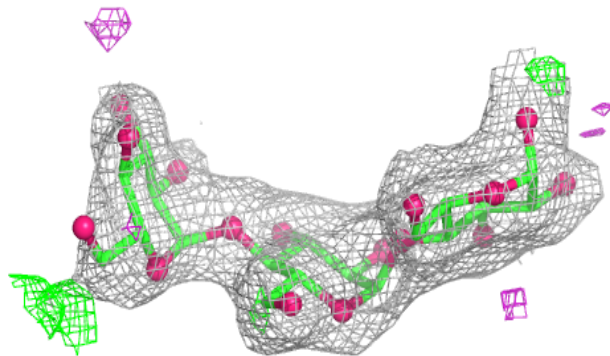
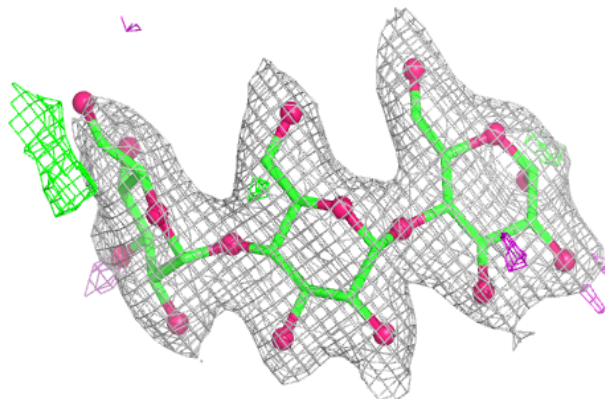


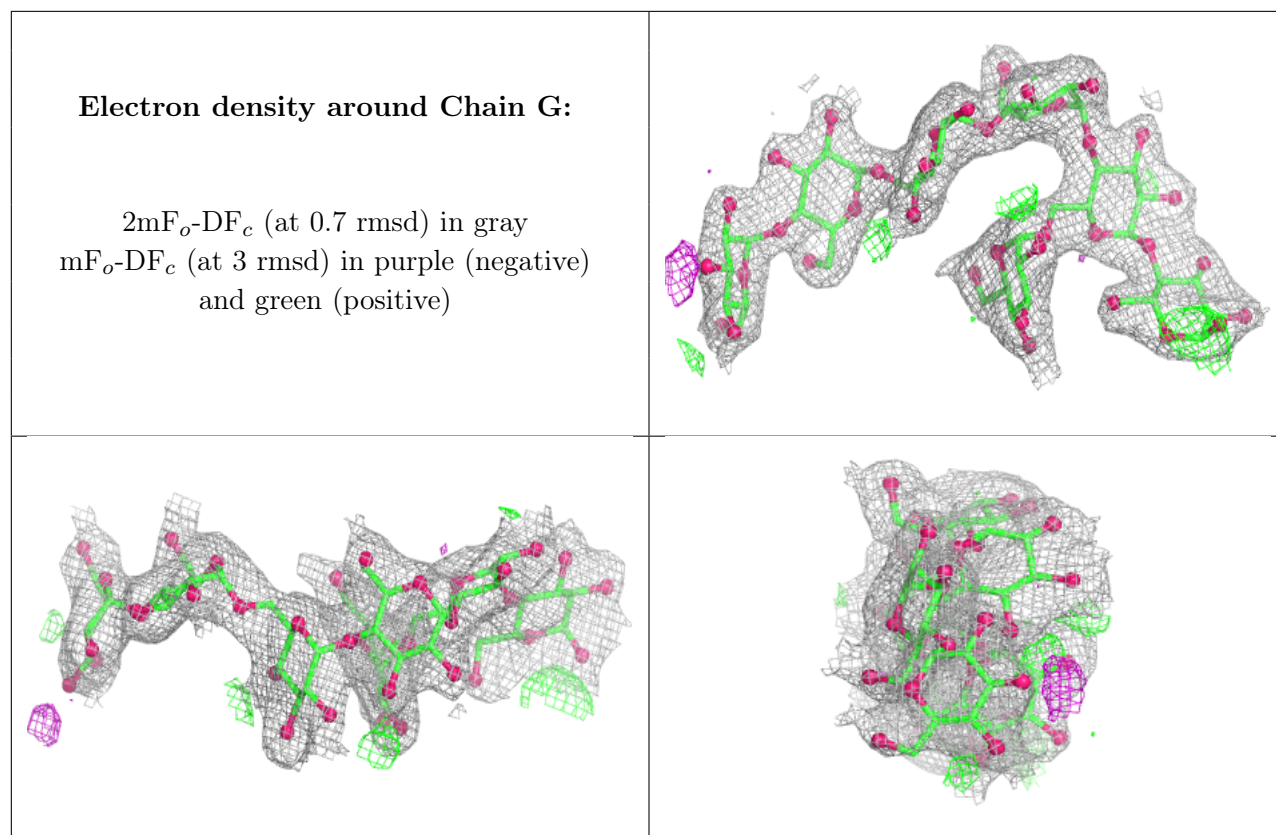
Electron density around Chain E:

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

**Electron density around Chain F:**

$2mF_o-DF_c$ (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($\text{\AA}^2$)	Q<0.9
8	GOL	A	721	6/6	0.78	0.16	49,53,63,63	0
9	ACT	A	722	4/4	0.89	0.15	50,56,59,64	0
7	CA	A	720	1/1	0.91	0.26	89,89,89,89	0
7	CA	B	716	1/1	0.93	0.10	77,77,77,77	0
7	CA	B	715	1/1	0.96	0.08	41,41,41,41	0
7	CA	A	719	1/1	0.99	0.02	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.