



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 01:11 PM BST

PDB ID : 5X7R
Title : Crystal structure of Paenibacillus sp. 598K alpha-1,6-glucosyltransferase complexed with isomaltohexaose
Authors : Fujimoto, Z.; Kishine, N.; Suzuki, N.; Momma, M.; Ichinose, H.; Kimura, A.; Funane, K.
Deposited on : 2017-02-27
Resolution : 1.95 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

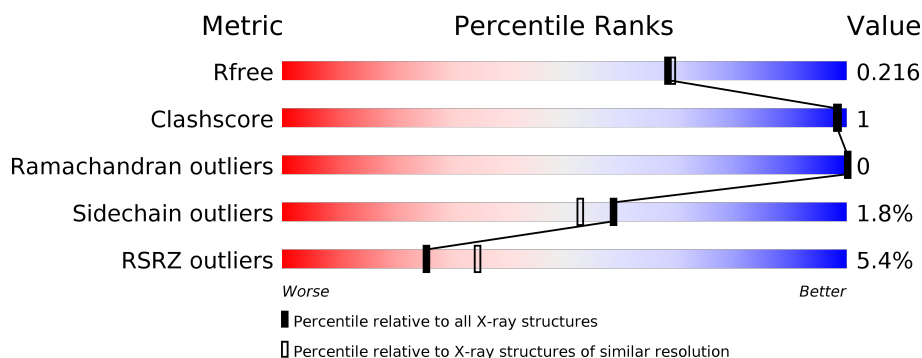
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	1263	<div> <div>6%</div> <div> <div></div> <div>96%</div> <div>..</div> </div> </div>
1	B	1263	<div> <div>5%</div> <div> <div></div> <div>96%</div> <div>..</div> </div> </div>
2	C	5	<div> <div>40%</div> <div>40%</div> <div>20%</div> </div>
3	D	3	<div> <div>67%</div> <div>33%</div> </div>
3	F	3	<div> <div>100%</div> </div>
4	E	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	2	
5	H	2	
5	I	2	

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
5	GLC	H	1	-	-	-	X
8	GLC	A	1461	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 21450 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 Glycoside hydrolase family 31 alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1247	Total	C	N	O	S	0	0	0
			9601	6023	1633	1923	22			
1	B	1247	Total	C	N	O	S	0	0	0
			9601	6023	1633	1923	22			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	HIS	-	expression tag	UNP A0A193PKW5
A	20	HIS	-	expression tag	UNP A0A193PKW5
A	21	HIS	-	expression tag	UNP A0A193PKW5
A	22	HIS	-	expression tag	UNP A0A193PKW5
A	23	HIS	-	expression tag	UNP A0A193PKW5
A	24	HIS	-	expression tag	UNP A0A193PKW5
A	25	SER	-	expression tag	UNP A0A193PKW5
A	26	SER	-	expression tag	UNP A0A193PKW5
A	27	GLY	-	expression tag	UNP A0A193PKW5
A	28	LEU	-	expression tag	UNP A0A193PKW5
A	29	VAL	-	expression tag	UNP A0A193PKW5
A	30	PRO	-	expression tag	UNP A0A193PKW5
A	31	ARG	-	expression tag	UNP A0A193PKW5
A	32	GLY	-	expression tag	UNP A0A193PKW5
A	33	SER	-	expression tag	UNP A0A193PKW5
A	34	HIS	-	expression tag	UNP A0A193PKW5
A	35	MET	-	expression tag	UNP A0A193PKW5
B	19	HIS	-	expression tag	UNP A0A193PKW5
B	20	HIS	-	expression tag	UNP A0A193PKW5
B	21	HIS	-	expression tag	UNP A0A193PKW5
B	22	HIS	-	expression tag	UNP A0A193PKW5
B	23	HIS	-	expression tag	UNP A0A193PKW5
B	24	HIS	-	expression tag	UNP A0A193PKW5
B	25	SER	-	expression tag	UNP A0A193PKW5
B	26	SER	-	expression tag	UNP A0A193PKW5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	GLY	-	expression tag	UNP A0A193PKW5
B	28	LEU	-	expression tag	UNP A0A193PKW5
B	29	VAL	-	expression tag	UNP A0A193PKW5
B	30	PRO	-	expression tag	UNP A0A193PKW5
B	31	ARG	-	expression tag	UNP A0A193PKW5
B	32	GLY	-	expression tag	UNP A0A193PKW5
B	33	SER	-	expression tag	UNP A0A193PKW5
B	34	HIS	-	expression tag	UNP A0A193PKW5
B	35	MET	-	expression tag	UNP A0A193PKW5

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	C	5	Total	C	O	0	0	0
			56	30	26			

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



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

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



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

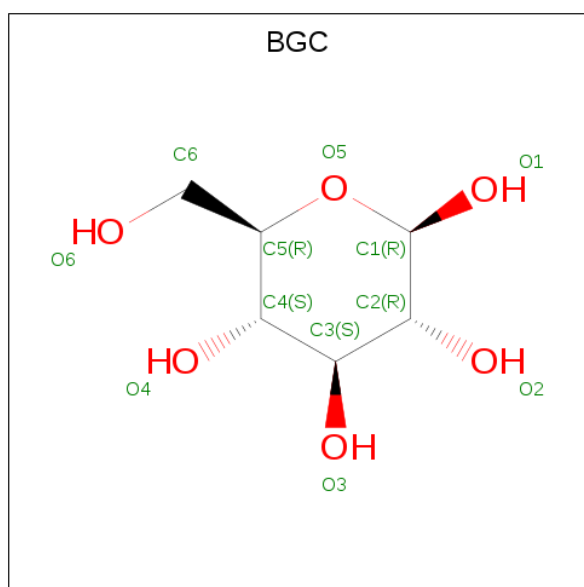
- Molecule 5 is an oligosaccharide called 4,6-dideoxy-4-{[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	2	Total	C	N	O	0	0	1
			22	13	1	8			
5	I	2	Total	C	N	O	0	0	1
			22	13	1	8			

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

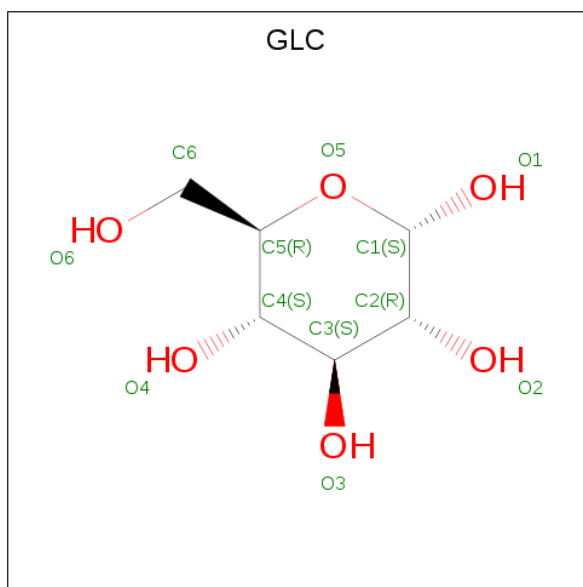
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Ca	0	0
			3	3		
6	A	3	Total	Ca	0	0
			3	3		

- Molecule 7 is beta-D-glucopyranose (three-letter code: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			12	6	6		
7	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 8 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			12	6	6		
8	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 9 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	2	Total	Ni	0	0
			2	2		
9	A	2	Total	Ni	0	0
			2	2		

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

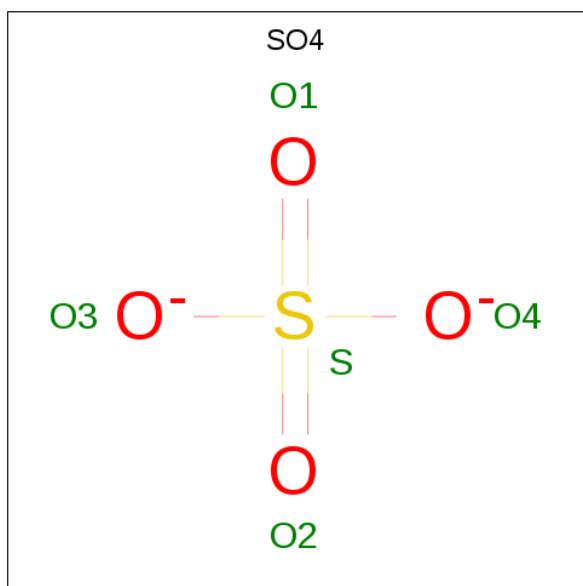
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	10	Total	Mg	0	0
			10	10		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	10	Total	Mg	0	0
			10	10		

- Molecule 11 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



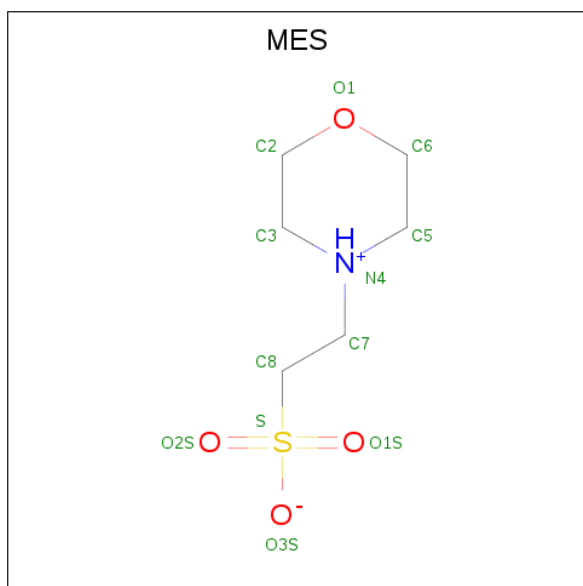
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	A	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		
11	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 12 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



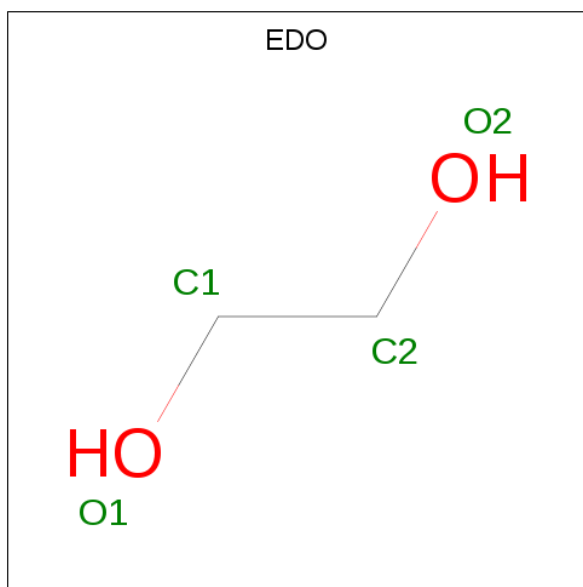
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
12	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
12	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
12	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
12	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
12	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
12	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
12	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
12	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
12	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
12	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
12	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
12	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 13 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

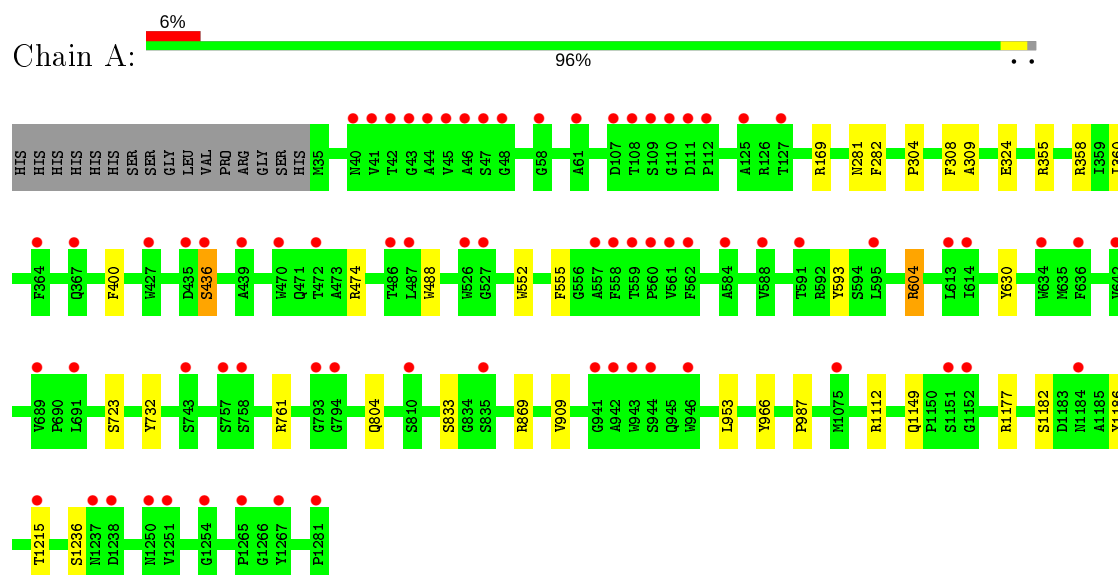
- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	828	Total O 828 828	0	0
14	B	824	Total O 824 824	0	0

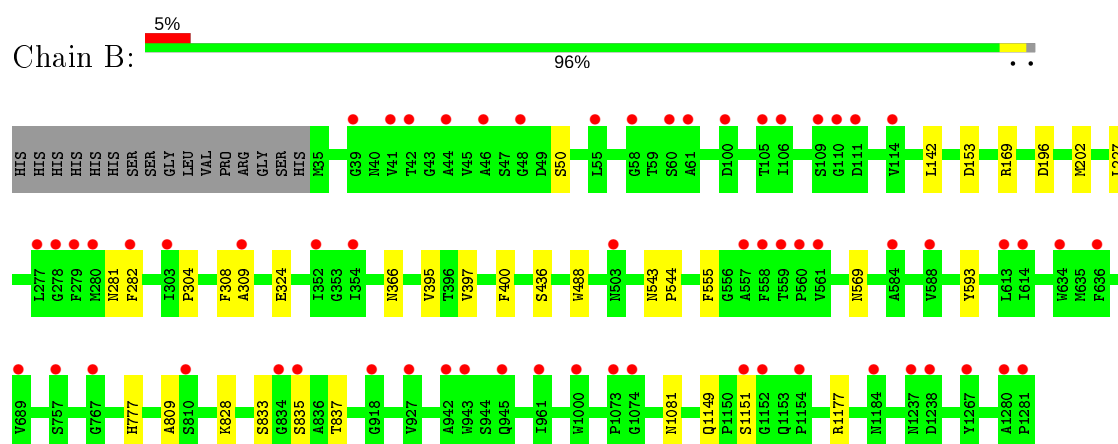
3 Residue-property plots [i](#)

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

- Molecule 1: Glycoside hydrolase family 31 alpha-glucosidase



- Molecule 1: Glycoside hydrolase family 31 alpha-glucosidase



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





- Molecule 3: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain D:



- Molecule 3: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain F:



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

Chain E:



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

Chain G:



- Molecule 5: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain H:



- Molecule 5: 4,6-dideoxy-4-[(1S,4R,5S,6S)-4,5,6-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	184.33Å 271.26Å 133.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.46 – 1.95 47.51 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.4 (152.46-1.95) 96.8 (47.51-1.94)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.82 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.178 , 0.208 0.188 , 0.216	Depositor DCC
R_{free} test set	12052 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.710	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21450	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, MG, BGC, CA, GLC, EDO, AC1, SO4, MES

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	0.45	0/9863	0.68	5/13473 (0.0%)
1	B	0.46	0/9863	0.68	2/13473 (0.0%)
All	All	0.46	0/19726	0.68	7/26946 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	355	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	474	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	869	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	1112	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	B	196	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	358	ARG	NE-CZ-NH1	5.02	122.81	120.30

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	9601	0	8954	14	1
1	B	9601	0	8954	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	56	0	48	1	0
3	D	34	0	30	0	0
3	F	34	0	30	0	0
4	E	23	0	21	0	0
4	G	23	0	21	0	0
5	H	22	0	10	0	0
5	I	22	0	10	0	1
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	12	0	12	0	0
7	B	12	0	12	0	0
8	A	12	0	12	0	0
8	B	12	0	12	0	0
9	A	2	0	0	0	0
9	B	2	0	0	0	0
10	A	10	0	0	0	0
10	B	10	0	0	0	0
11	A	30	0	0	0	0
11	B	50	0	0	0	0
12	A	96	0	104	1	0
12	B	96	0	104	1	0
13	A	16	0	24	0	0
13	B	16	0	24	0	0
14	A	828	0	0	2	0
14	B	824	0	0	2	0
All	All	21450	0	18382	21	1

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 1.

All (21) 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:360:ILE:HD13	1:B:397:VAL:HG12	1.67	0.76
1:B:777:HIS:CD2	14:B:2387:HOH:O	2.49	0.64
12:B:1711:MES:O1S	14:B:2001:HOH:O	2.12	0.63
1:A:761:ARG:NH1	14:A:2006:HOH:O	2.33	0.62
1:A:604:ARG:HD3	1:A:732:TYR:CD1	2.36	0.61
1:A:436:SER:HA	2:C:3:GLC:O2	2.05	0.57
1:B:366:ASN:HB2	1:B:569:ASN:ND2	2.24	0.52
1:A:360:ILE:HD12	1:B:395:VAL:CG1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:TYR:OH	14:A:2001:HOH:O	2.20	0.48
1:A:987:PRO:HG2	12:A:1711:MES:H51	1.96	0.47
1:A:909:VAL:HG21	1:A:953:LEU:HD12	1.95	0.47
1:A:282:PHE:CG	1:A:309:ALA:HB3	2.53	0.44
1:A:304:PRO:HB2	1:B:593:TYR:CE1	2.52	0.44
1:B:282:PHE:CG	1:B:309:ALA:HB3	2.52	0.44
1:A:360:ILE:HD12	1:B:395:VAL:HG11	1.98	0.44
1:B:543:ASN:HB3	1:B:544:PRO:HD2	2.01	0.43
1:A:593:TYR:CE1	1:B:304:PRO:HB2	2.55	0.41
1:B:809:ALA:O	1:B:828:LYS:NZ	2.40	0.41
1:A:604:ARG:HD3	1:A:732:TYR:CE1	2.54	0.41
1:A:1182:SER:HB3	1:A:1186:TYR:CD1	2.56	0.41
1:B:142:LEU:N	1:B:142:LEU:HD23	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:THR:OG1	5:I:2:AC1:O6B[6_555]	1.99	0.21

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	1245/1263 (99%)	1215 (98%)	30 (2%)	0	100	100
1	B	1245/1263 (99%)	1215 (98%)	30 (2%)	0	100	100
All	All	2490/2526 (99%)	2430 (98%)	60 (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	997/1011 (99%)	980 (98%)	17 (2%)	60	55
1	B	997/1011 (99%)	978 (98%)	19 (2%)	57	50
All	All	1994/2022 (99%)	1958 (98%)	36 (2%)	59	53

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ARG
1	A	281	ASN
1	A	308	PHE
1	A	324	GLU
1	A	400	PHE
1	A	436	SER
1	A	488	TRP
1	A	552	TRP
1	A	555	PHE
1	A	604	ARG
1	A	723	SER
1	A	804	GLN
1	A	833	SER
1	A	966	TYR
1	A	1149	GLN
1	A	1177	ARG
1	A	1236	SER
1	B	50	SER
1	B	153	ASP
1	B	169	ARG
1	B	202	MET
1	B	227	LEU
1	B	281	ASN
1	B	308	PHE
1	B	324	GLU
1	B	400	PHE
1	B	436	SER

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Mol	Chain	Res	Type
1	B	488	TRP
1	B	555	PHE
1	B	833	SER
1	B	835	SER
1	B	837	THR
1	B	1081	ASN
1	B	1149	GLN
1	B	1151	SER
1	B	1177	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	949	GLN
1	A	1226	HIS
1	B	440	GLN
1	B	777	HIS
1	B	1213	ASN
1	B	1226	HIS
1	B	1250	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 ⓘ

Of 19 monosaccharides modelled in this entry, 17 were used 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
2	BGC	C	1	2	12,12,12	0.47	0	17,17,17	1.06	1 (5%)
2	GLC	C	2	2	11,11,12	0.37	0	15,15,17	0.57	0
2	GLC	C	3	2	11,11,12	0.47	0	15,15,17	0.94	1 (6%)
2	GLC	C	4	2	11,11,12	0.51	0	15,15,17	1.03	0
2	GLC	C	5	2	11,11,12	0.70	0	15,15,17	0.85	1 (6%)
3	GLC	D	1	3	12,12,12	0.67	0	17,17,17	0.62	0
3	GLC	D	2	3	11,11,12	0.39	0	15,15,17	1.11	2 (13%)
3	GLC	D	3	3	11,11,12	0.49	0	15,15,17	0.88	0
4	GLC	E	1	4	12,12,12	0.60	0	17,17,17	1.15	1 (5%)
4	GLC	E	2	4	11,11,12	0.45	0	15,15,17	1.06	1 (6%)
3	GLC	F	1	3	12,12,12	0.57	0	17,17,17	0.91	1 (5%)
3	GLC	F	2	3	11,11,12	0.41	0	15,15,17	1.08	1 (6%)
3	GLC	F	3	3	11,11,12	0.37	0	15,15,17	1.01	1 (6%)
4	GLC	G	1	4	12,12,12	0.53	0	17,17,17	0.70	0
4	GLC	G	2	4	11,11,12	0.39	0	15,15,17	0.88	1 (6%)
5	AC1	H	2	5	21,22,23	0.63	0	22,32,34	1.04	2 (9%)
5	AC1	I	2	5	21,22,23	0.74	0	22,32,34	1.06	1 (4%)

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	BGC	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	-	0/2/19/22	0/1/1/1
2	GLC	C	4	2	-	1/2/19/22	0/1/1/1
2	GLC	C	5	2	-	0/2/19/22	0/1/1/1
3	GLC	D	1	3	-	0/2/22/22	0/1/1/1
3	GLC	D	2	3	-	0/2/19/22	0/1/1/1
3	GLC	D	3	3	-	1/2/19/22	0/1/1/1
4	GLC	E	1	4	-	2/2/22/22	0/1/1/1
4	GLC	E	2	4	-	2/2/19/22	0/1/1/1
3	GLC	F	1	3	-	0/2/22/22	0/1/1/1
3	GLC	F	2	3	-	0/2/19/22	0/1/1/1
3	GLC	F	3	3	-	0/2/19/22	0/1/1/1
4	GLC	G	1	4	-	2/2/22/22	0/1/1/1
4	GLC	G	2	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AC1	H	2	5	-	2/6/43/46	0/2/2/2
5	AC1	I	2	5	-	3/6/43/46	0/2/2/2

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	1	GLC	C1-O5-C5	3.62	120.50	113.66
5	H	2	AC1	C2-C3-C4	-3.07	107.92	110.63
5	I	2	AC1	C7B-C1B-N4A	-3.04	106.13	110.68
4	E	2	GLC	C1-O5-C5	2.90	116.12	112.19
3	F	2	GLC	C1-O5-C5	2.45	115.51	112.19
3	D	2	GLC	C1-O5-C5	2.44	115.50	112.19
3	F	3	GLC	C1-O5-C5	2.36	115.39	112.19
2	C	3	GLC	C1-O5-C5	2.29	115.29	112.19
3	D	2	GLC	C1-C2-C3	2.23	112.41	109.67
4	G	2	GLC	C1-O5-C5	2.16	115.11	112.19
5	H	2	AC1	C7B-C1B-N4A	-2.13	107.48	110.68
2	C	1	BGC	O2-C2-C3	-2.12	105.44	110.35
2	C	5	GLC	C1-O5-C5	2.07	115.00	112.19
3	F	1	GLC	C3-C4-C5	2.05	113.89	110.24

There are no chirality outliers.

All (13) torsion outliers are listed below:

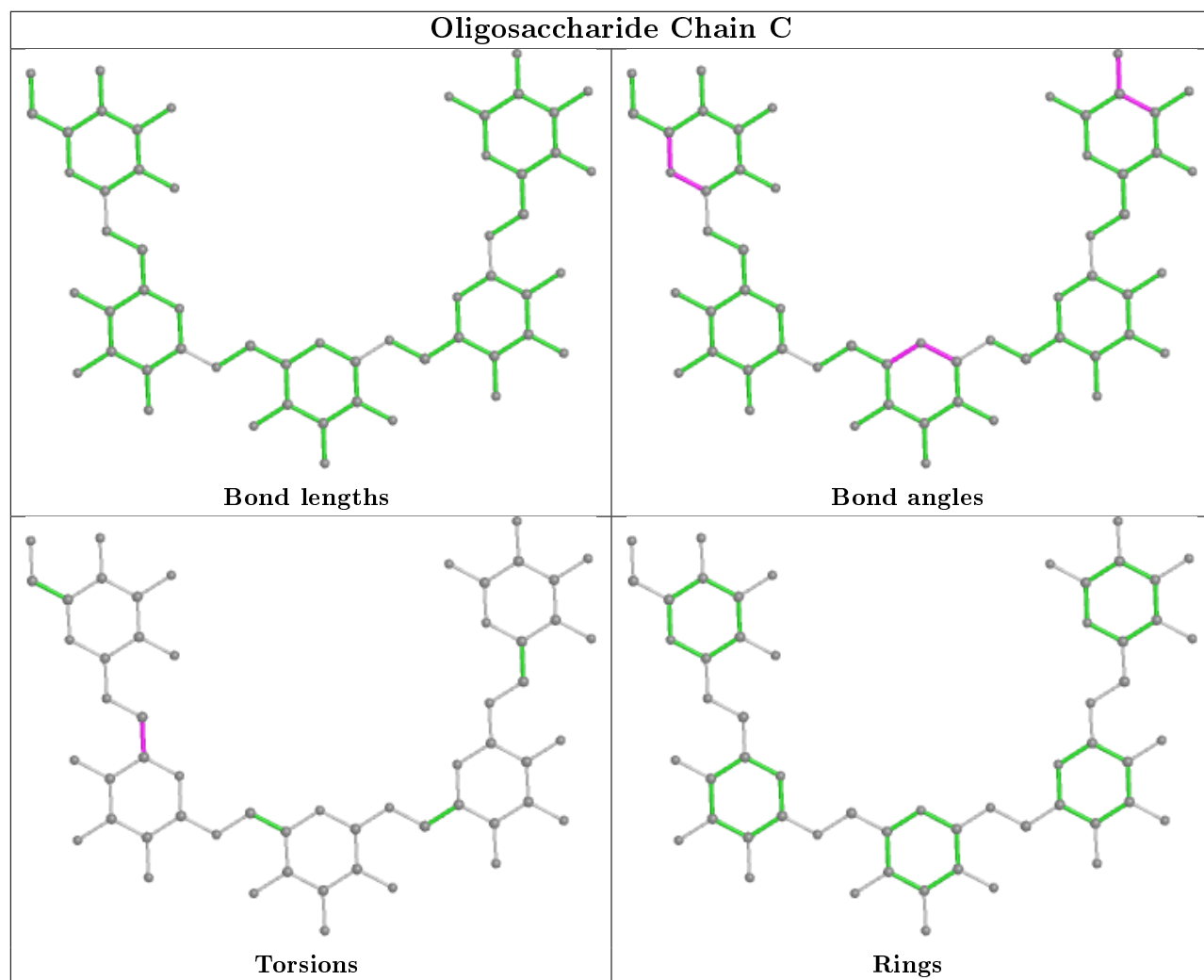
Mol	Chain	Res	Type	Atoms
5	I	2	AC1	C4A-C5B-C6B-O6B
5	I	2	AC1	C7B-C5B-C6B-O6B
4	G	1	GLC	O5-C5-C6-O6
4	E	1	GLC	C4-C5-C6-O6
4	E	1	GLC	O5-C5-C6-O6
4	G	1	GLC	C4-C5-C6-O6
4	E	2	GLC	C4-C5-C6-O6
2	C	4	GLC	C4-C5-C6-O6
4	E	2	GLC	O5-C5-C6-O6
5	H	2	AC1	C5-C4-N4A-C1B
5	H	2	AC1	C3-C4-N4A-C1B
5	I	2	AC1	C5-C4-N4A-C1B
3	D	3	GLC	C4-C5-C6-O6

There are no ring outliers.

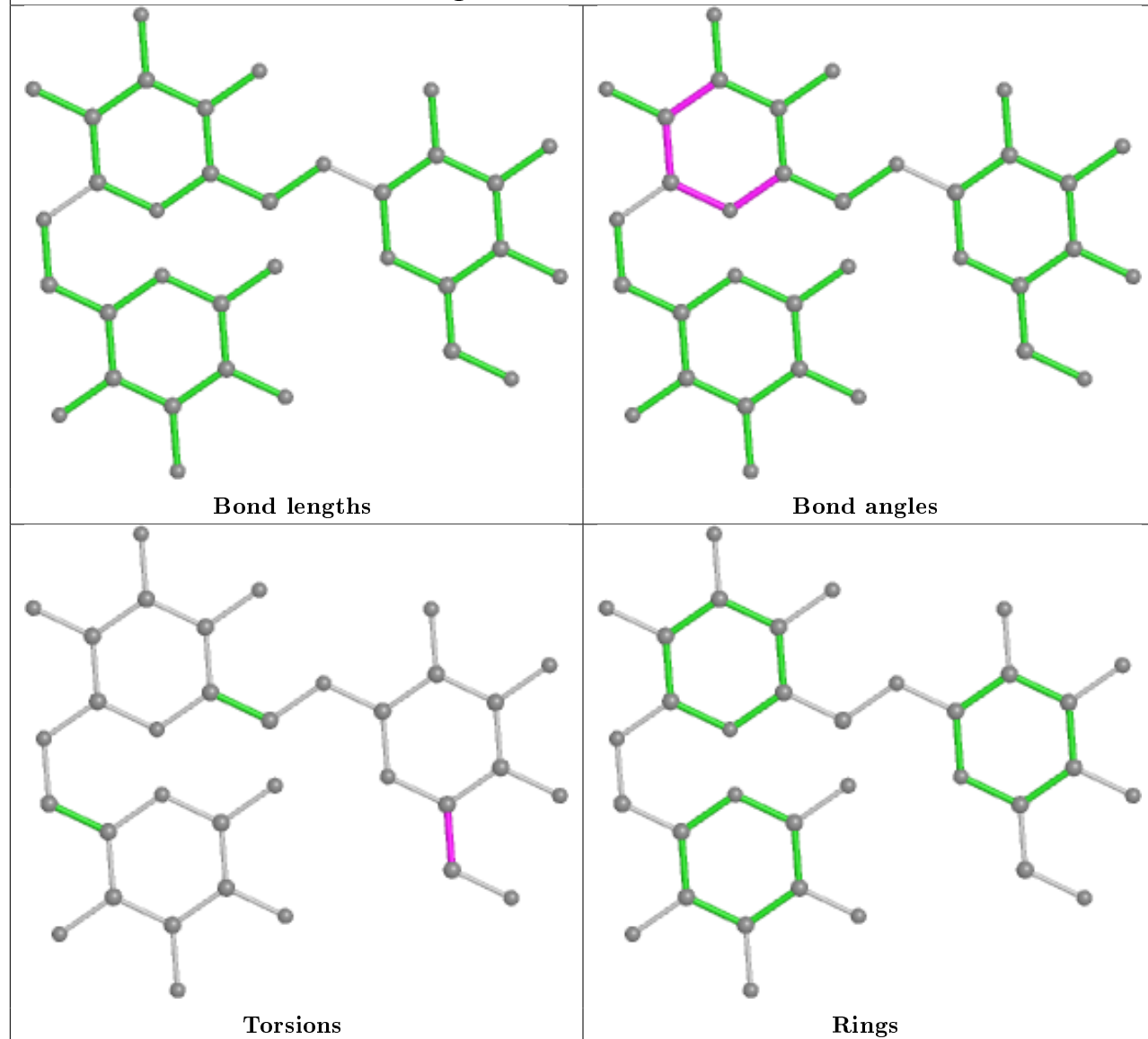
2 monomers are involved in 2 short contacts:

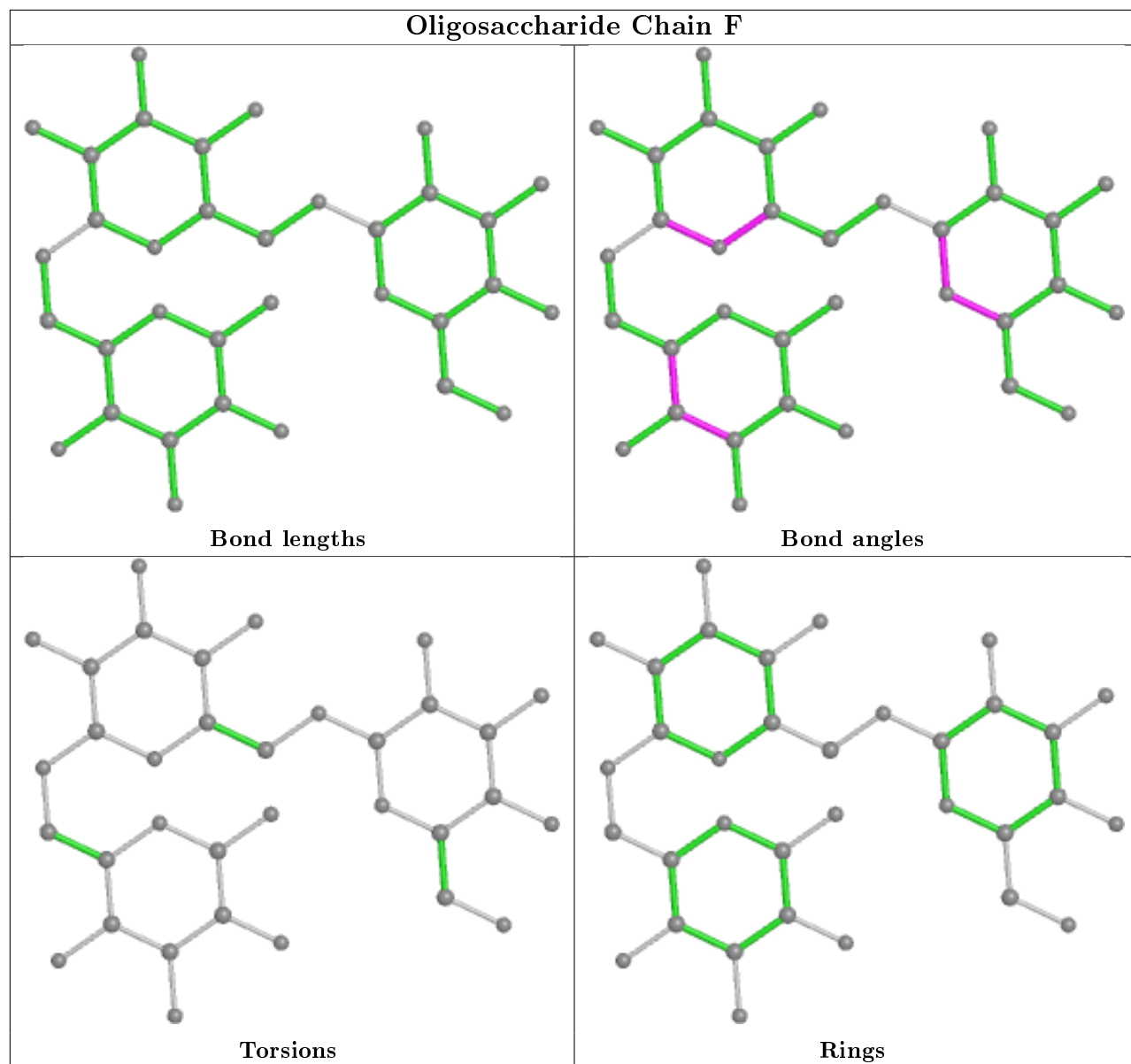
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	GLC	1	0
5	I	2	AC1	0	1

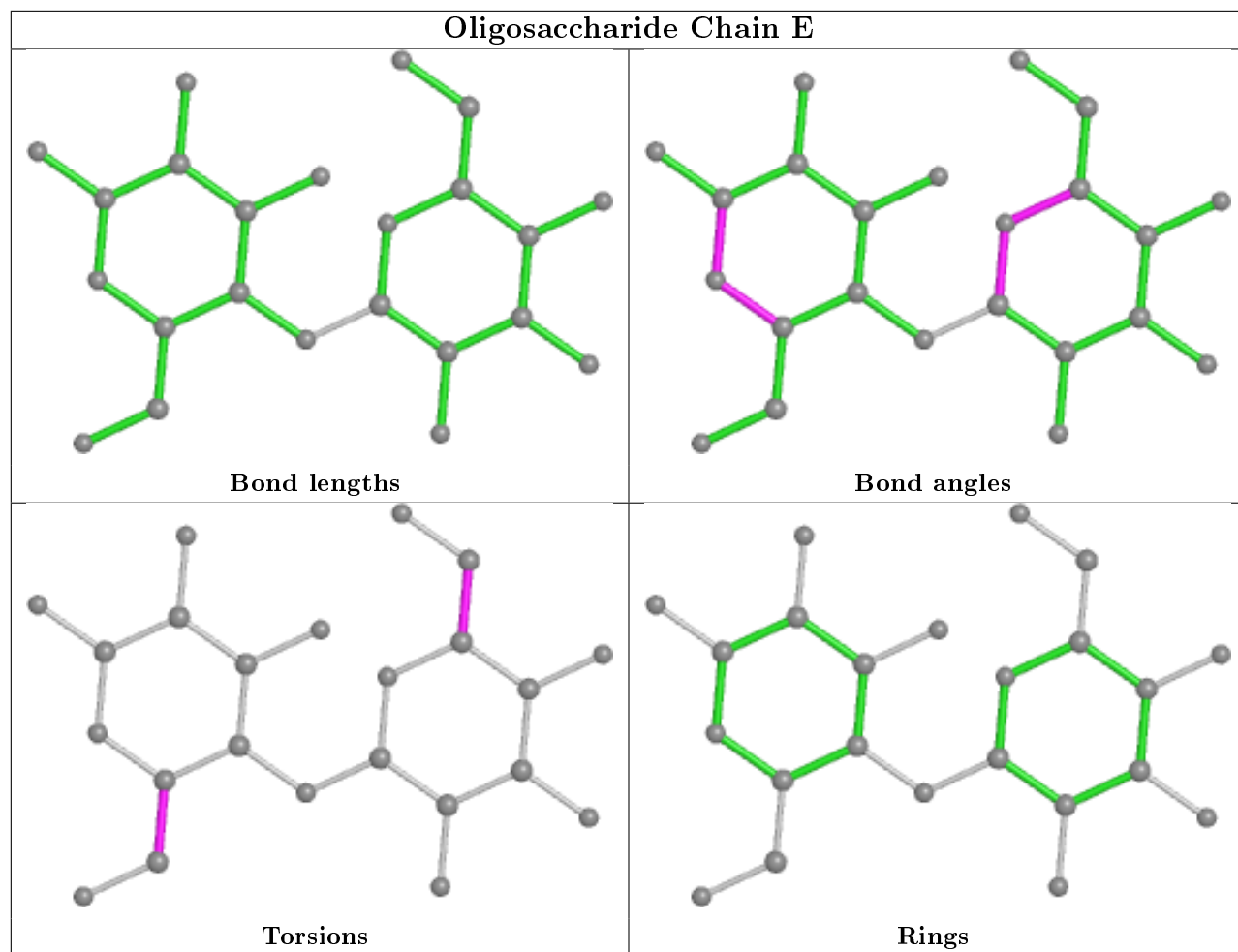
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

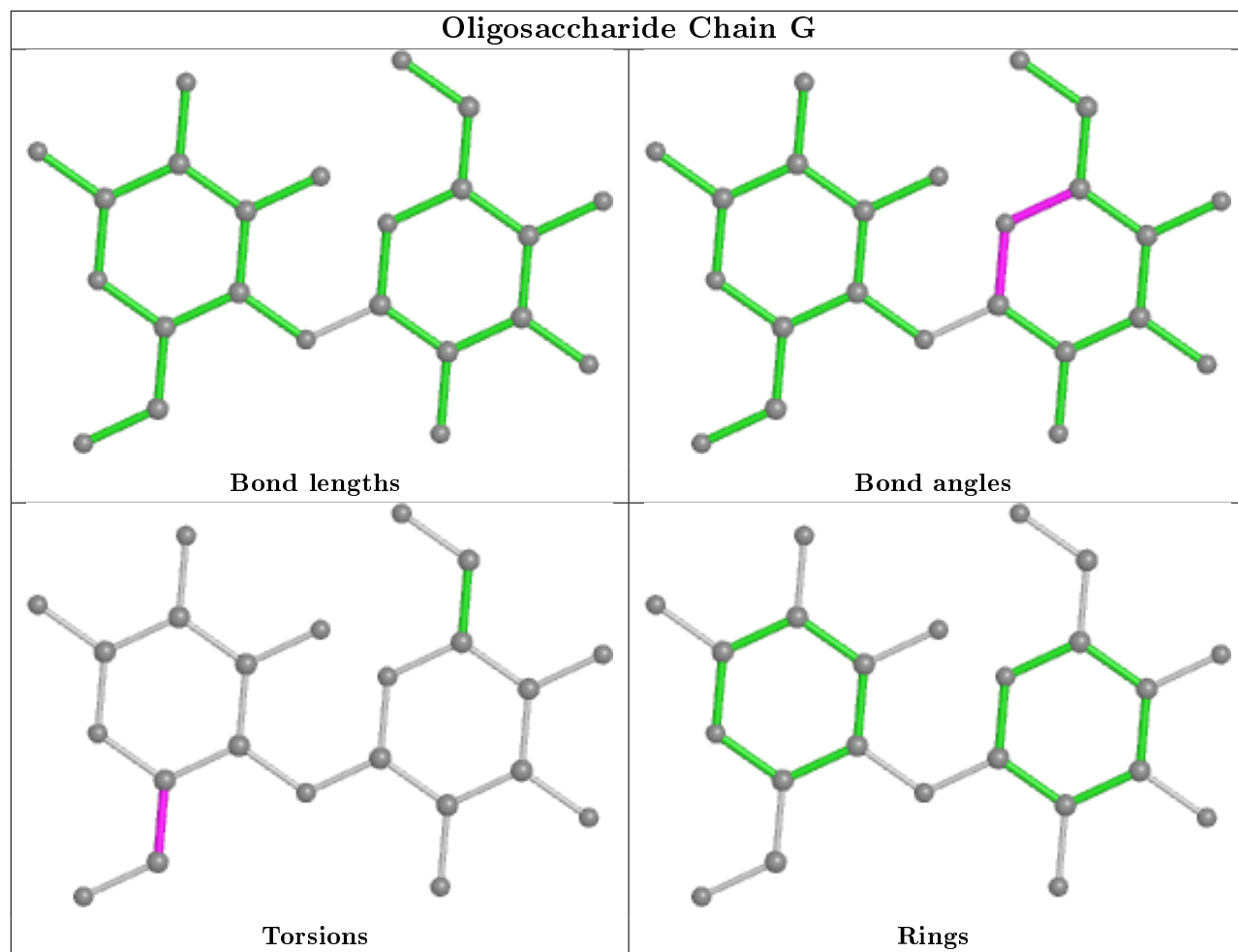


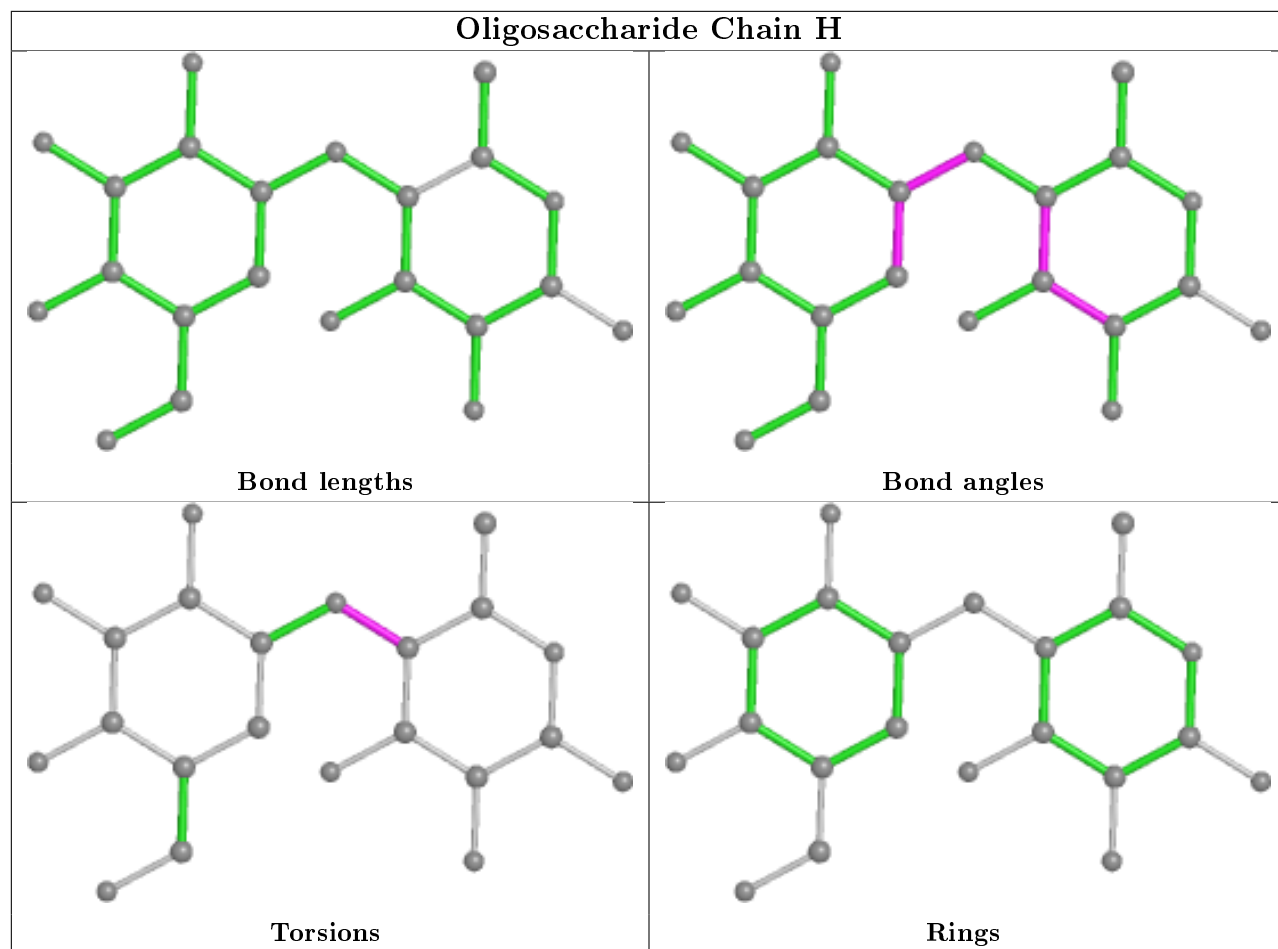
Oligosaccharide Chain D

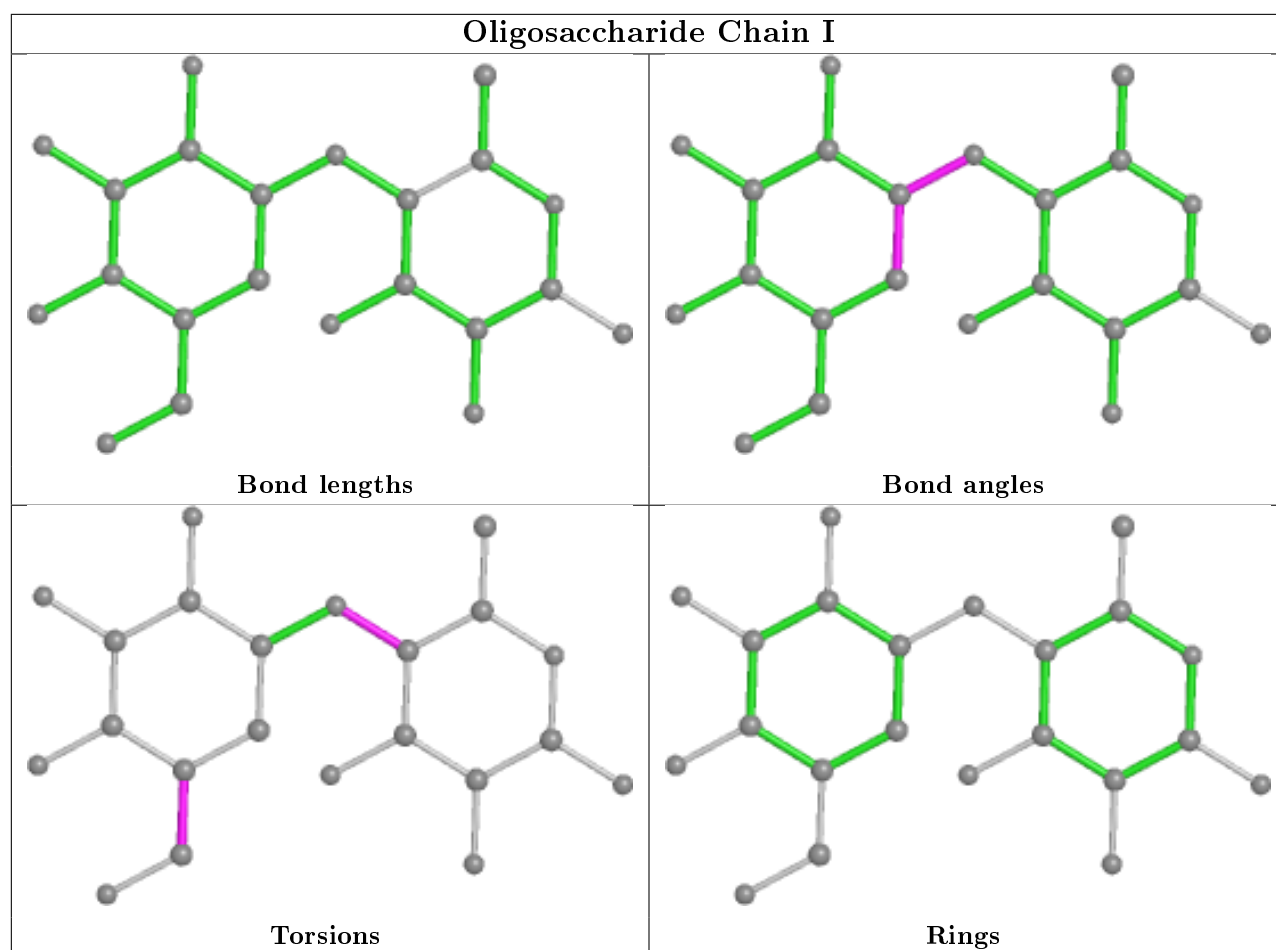












5.6 Ligand geometry [i](#)

Of 74 ligands modelled in this entry, 30 are monoatomic - leaving 44 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	$\# Z > 2$
12	MES	A	1708	-	12,12,12	2.31	1 (8%)	14,16,16	1.39	3 (21%)
12	MES	B	1708	-	12,12,12	1.93	1 (8%)	14,16,16	1.95	3 (21%)
12	MES	A	1706	-	12,12,12	2.14	1 (8%)	14,16,16	1.46	2 (14%)
12	MES	A	1704	-	12,12,12	1.98	1 (8%)	14,16,16	1.39	2 (14%)
12	MES	A	1713	-	12,12,12	2.26	1 (8%)	14,16,16	1.69	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	MES	B	1701	-	12,12,12	2.33	1 (8%)	14,16,16	1.27	2 (14%)
13	EDO	B	1803	-	3,3,3	0.27	0	2,2,2	0.67	0
13	EDO	A	1804	-	3,3,3	0.63	0	2,2,2	0.78	0
11	SO4	A	1701	-	4,4,4	0.31	0	6,6,6	0.12	0
13	EDO	B	1802	-	3,3,3	0.38	0	2,2,2	0.24	0
11	SO4	B	1703	-	4,4,4	0.29	0	6,6,6	0.17	0
11	SO4	B	1704	-	4,4,4	0.35	0	6,6,6	0.15	0
11	SO4	B	1713	-	4,4,4	0.45	0	6,6,6	0.24	0
12	MES	B	1707	-	12,12,12	2.07	1 (8%)	14,16,16	1.57	2 (14%)
11	SO4	A	1707	-	4,4,4	0.31	0	6,6,6	0.22	0
12	MES	B	1706	-	12,12,12	2.16	1 (8%)	14,16,16	1.62	2 (14%)
11	SO4	A	1703	-	4,4,4	0.27	0	6,6,6	0.17	0
12	MES	B	1711	-	12,12,12	2.08	1 (8%)	14,16,16	1.34	2 (14%)
11	SO4	B	1709	-	4,4,4	0.35	0	6,6,6	0.14	0
11	SO4	B	1702	-	4,4,4	0.34	0	6,6,6	0.34	0
8	GLC	A	1461	-	12,12,12	0.71	0	17,17,17	0.71	0
12	MES	A	1712	-	12,12,12	2.30	1 (8%)	14,16,16	1.20	1 (7%)
12	MES	B	1716	-	12,12,12	2.14	1 (8%)	14,16,16	1.50	2 (14%)
12	MES	B	1714	-	12,12,12	2.15	1 (8%)	14,16,16	1.11	1 (7%)
11	SO4	B	1718	-	4,4,4	0.39	0	6,6,6	0.24	0
13	EDO	B	1801	-	3,3,3	0.46	0	2,2,2	0.02	0
7	BGC	B	1401	-	12,12,12	0.46	0	17,17,17	0.62	0
12	MES	A	1709	-	12,12,12	2.08	1 (8%)	14,16,16	1.77	1 (7%)
11	SO4	B	1715	-	4,4,4	0.40	0	6,6,6	0.23	0
11	SO4	A	1702	-	4,4,4	0.36	0	6,6,6	0.27	0
12	MES	B	1712	-	12,12,12	2.21	1 (8%)	14,16,16	1.06	0
12	MES	A	1705	-	12,12,12	1.96	1 (8%)	14,16,16	1.99	2 (14%)
12	MES	A	1711	-	12,12,12	2.13	1 (8%)	14,16,16	1.71	5 (35%)
11	SO4	B	1710	-	4,4,4	0.33	0	6,6,6	0.29	0
11	SO4	B	1717	-	4,4,4	0.36	0	6,6,6	0.13	0
13	EDO	A	1801	-	3,3,3	0.45	0	2,2,2	0.28	0
11	SO4	A	1714	-	4,4,4	0.32	0	6,6,6	0.13	0
13	EDO	A	1803	-	3,3,3	0.33	0	2,2,2	0.46	0
11	SO4	A	1710	-	4,4,4	0.35	0	6,6,6	0.42	0
8	GLC	B	1461	-	12,12,12	0.61	0	17,17,17	0.73	0
11	SO4	B	1705	-	4,4,4	0.33	0	6,6,6	0.18	0
13	EDO	B	1804	-	3,3,3	0.39	0	2,2,2	0.65	0
7	BGC	A	1401	-	12,12,12	0.50	0	17,17,17	0.65	0
13	EDO	A	1802	-	3,3,3	0.40	0	2,2,2	0.42	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
12	MES	A	1708	-	-	0/6/14/14	0/1/1/1
12	MES	B	1708	-	-	0/6/14/14	0/1/1/1
12	MES	A	1706	-	-	3/6/14/14	0/1/1/1
12	MES	A	1704	-	-	3/6/14/14	0/1/1/1
12	MES	A	1713	-	-	5/6/14/14	0/1/1/1
12	MES	B	1701	-	-	2/6/14/14	0/1/1/1
13	EDO	B	1803	-	-	1/1/1/1	-
13	EDO	A	1804	-	-	0/1/1/1	-
13	EDO	B	1802	-	-	0/1/1/1	-
12	MES	B	1707	-	-	0/6/14/14	0/1/1/1
12	MES	B	1706	-	-	4/6/14/14	0/1/1/1
12	MES	B	1711	-	-	5/6/14/14	0/1/1/1
8	GLC	A	1461	-	-	0/2/22/22	0/1/1/1
12	MES	A	1712	-	-	0/6/14/14	0/1/1/1
12	MES	B	1716	-	-	2/6/14/14	0/1/1/1
12	MES	B	1714	-	-	0/6/14/14	0/1/1/1
13	EDO	B	1801	-	-	0/1/1/1	-
7	BGC	B	1401	-	-	0/2/22/22	0/1/1/1
12	MES	A	1709	-	-	0/6/14/14	0/1/1/1
12	MES	B	1712	-	-	3/6/14/14	0/1/1/1
12	MES	A	1705	-	-	5/6/14/14	0/1/1/1
12	MES	A	1711	-	-	5/6/14/14	0/1/1/1
7	BGC	A	1401	-	-	0/2/22/22	0/1/1/1
13	EDO	A	1803	-	-	1/1/1/1	-
8	GLC	B	1461	-	-	0/2/22/22	0/1/1/1
13	EDO	A	1801	-	-	0/1/1/1	-
13	EDO	B	1804	-	-	1/1/1/1	-
13	EDO	A	1802	-	-	0/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1708	MES	C8-S	-7.71	1.66	1.77
12	B	1701	MES	C8-S	-7.68	1.66	1.77
12	A	1712	MES	C8-S	-7.61	1.66	1.77
12	A	1713	MES	C8-S	-7.52	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	1712	MES	C8-S	-7.36	1.67	1.77
12	B	1706	MES	C8-S	-7.15	1.67	1.77
12	A	1706	MES	C8-S	-7.10	1.67	1.77
12	B	1714	MES	C8-S	-7.08	1.67	1.77
12	A	1711	MES	C8-S	-7.01	1.67	1.77
12	B	1716	MES	C8-S	-6.96	1.67	1.77
12	B	1711	MES	C8-S	-6.90	1.67	1.77
12	A	1709	MES	C8-S	-6.80	1.67	1.77
12	B	1707	MES	C8-S	-6.76	1.67	1.77
12	A	1704	MES	C8-S	-6.44	1.68	1.77
12	A	1705	MES	C8-S	-6.30	1.68	1.77
12	B	1708	MES	C8-S	-6.08	1.68	1.77

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	1705	MES	O2S-S-C8	6.15	114.33	106.92
12	A	1709	MES	O2S-S-C8	5.47	113.50	106.92
12	A	1713	MES	O2S-S-C8	4.93	112.85	106.92
12	B	1708	MES	O1S-S-C8	4.38	112.19	106.92
12	A	1706	MES	O3S-S-C8	4.09	112.39	105.77
12	B	1716	MES	O2S-S-C8	3.98	111.71	106.92
12	B	1707	MES	O2S-S-C8	3.55	111.19	106.92
12	B	1706	MES	O3S-S-C8	3.43	111.31	105.77
12	A	1711	MES	C6-C5-N4	3.35	115.19	110.10
12	A	1712	MES	O3S-S-C8	3.22	110.97	105.77
12	A	1704	MES	O2S-S-C8	3.18	110.74	106.92
12	B	1708	MES	O3S-S-C8	3.11	110.80	105.77
12	B	1711	MES	O3S-S-C8	2.92	110.49	105.77
12	B	1706	MES	O2S-S-C8	2.88	110.39	106.92
12	B	1716	MES	O3S-S-C8	2.83	110.34	105.77
12	B	1707	MES	O3S-S-C8	2.82	110.32	105.77
12	A	1705	MES	O3S-S-C8	2.82	110.32	105.77
12	A	1704	MES	O3S-S-C8	2.76	110.23	105.77
12	B	1701	MES	O1S-S-C8	2.75	110.23	106.92
12	A	1711	MES	O1S-S-C8	2.69	110.16	106.92
12	B	1714	MES	O1S-S-C8	2.45	109.87	106.92
12	A	1706	MES	O1S-S-C8	2.38	109.78	106.92
12	A	1711	MES	O3S-S-C8	2.34	109.55	105.77
12	B	1708	MES	O2S-S-C8	2.31	109.70	106.92
12	A	1708	MES	O2S-S-C8	2.25	109.62	106.92
12	A	1711	MES	O1-C2-C3	-2.24	106.87	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	1711	MES	O1S-S-C8	2.23	109.60	106.92
12	A	1708	MES	O1S-S-C8	2.20	109.57	106.92
12	A	1708	MES	O3S-S-C8	2.13	109.22	105.77
12	B	1701	MES	O3S-S-C8	2.04	109.08	105.77
12	A	1711	MES	O2S-S-C8	2.04	109.37	106.92

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	1713	MES	C8-C7-N4-C3
12	A	1713	MES	C8-C7-N4-C5
12	A	1713	MES	C7-C8-S-O1S
12	A	1713	MES	C7-C8-S-O3S
12	A	1711	MES	C8-C7-N4-C3
12	A	1711	MES	C8-C7-N4-C5
12	A	1711	MES	C7-C8-S-O2S
12	A	1706	MES	C7-C8-S-O2S
12	B	1706	MES	C7-C8-S-O1S
12	B	1716	MES	C8-C7-N4-C3
12	B	1716	MES	C8-C7-N4-C5
12	A	1705	MES	C7-C8-S-O1S
12	A	1705	MES	C7-C8-S-O3S
12	A	1711	MES	C7-C8-S-O3S
12	A	1706	MES	C7-C8-S-O3S
12	B	1706	MES	C7-C8-S-O3S
12	B	1706	MES	C8-C7-N4-C5
12	B	1711	MES	C8-C7-N4-C3
12	A	1705	MES	C8-C7-N4-C3
12	A	1705	MES	C8-C7-N4-C5
12	A	1704	MES	C7-C8-S-O3S
12	B	1711	MES	C7-C8-S-O3S
13	A	1803	EDO	O1-C1-C2-O2
12	A	1704	MES	C7-C8-S-O1S
12	A	1704	MES	C7-C8-S-O2S
12	A	1713	MES	C7-C8-S-O2S
12	A	1711	MES	C7-C8-S-O1S
12	A	1706	MES	C7-C8-S-O1S
12	B	1706	MES	C7-C8-S-O2S
12	B	1711	MES	C7-C8-S-O1S
12	B	1711	MES	C7-C8-S-O2S
12	A	1705	MES	C7-C8-S-O2S

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Mol	Chain	Res	Type	Atoms
12	B	1711	MES	C8-C7-N4-C5
12	B	1712	MES	C8-C7-N4-C3
12	B	1712	MES	C8-C7-N4-C5
12	B	1701	MES	C8-C7-N4-C3
12	B	1701	MES	C8-C7-N4-C5
13	B	1803	EDO	O1-C1-C2-O2
13	B	1804	EDO	O1-C1-C2-O2
12	B	1712	MES	C7-C8-S-O3S

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	1711	MES	1	0
12	A	1711	MES	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	1247/1263 (98%)	0.35	73 (5%) 22 30	22, 32, 48, 79	0
1	B	1247/1263 (98%)	0.30	62 (4%) 28 39	21, 31, 48, 80	0
All	All	2494/2526 (98%)	0.33	135 (5%) 25 34	21, 32, 48, 80	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1237	ASN	5.3
1	B	1281	PRO	5.1
1	A	1237	ASN	4.8
1	A	58	GLY	4.7
1	B	61	ALA	4.7
1	B	60	SER	3.9
1	A	42	THR	3.9
1	A	1152	GLY	3.9
1	A	439	ALA	3.9
1	A	108	THR	3.9
1	A	588	VAL	3.8
1	A	109	SER	3.7
1	A	561	VAL	3.6
1	B	58	GLY	3.5
1	A	943	TRP	3.5
1	A	364	PHE	3.5
1	B	110	GLY	3.5
1	A	743	SER	3.4
1	B	1151	SER	3.4
1	A	46	ALA	3.3
1	A	1267	TYR	3.3
1	A	557	ALA	3.2
1	A	1281	PRO	3.2
1	A	793	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	43	GLY	3.1
1	B	1152	GLY	3.1
1	A	562	PHE	3.0
1	B	106	ILE	3.0
1	B	109	SER	3.0
1	B	114	VAL	3.0
1	A	613	LEU	3.0
1	A	794	GLY	3.0
1	A	560	PRO	3.0
1	B	834	GLY	3.0
1	A	486	THR	2.9
1	B	41	VAL	2.9
1	B	767	GLY	2.9
1	A	1151	SER	2.8
1	A	946	TRP	2.8
1	B	282	PHE	2.8
1	A	584	ALA	2.8
1	B	613	LEU	2.8
1	B	1074	GLY	2.8
1	B	835	SER	2.8
1	A	48	GLY	2.7
1	B	354	ILE	2.7
1	B	48	GLY	2.7
1	A	41	VAL	2.6
1	A	559	THR	2.6
1	B	503	ASN	2.6
1	B	1073	PRO	2.6
1	A	944	SER	2.6
1	B	557	ALA	2.6
1	B	614	ILE	2.6
1	B	689	VAL	2.6
1	B	942	ALA	2.6
1	B	943	TRP	2.6
1	A	436	SER	2.6
1	B	927	VAL	2.6
1	A	595	LEU	2.5
1	A	758	SER	2.5
1	B	1238	ASP	2.5
1	A	614	ILE	2.5
1	B	279	PHE	2.5
1	B	44	ALA	2.5
1	A	107	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	918	GLY	2.5
1	A	1250	ASN	2.5
1	B	1267	TYR	2.5
1	A	941	GLY	2.5
1	B	39	GLY	2.5
1	A	427	TRP	2.5
1	B	757	SER	2.5
1	B	561	VAL	2.5
1	A	691	LEU	2.5
1	B	46	ALA	2.5
1	A	1238	ASP	2.5
1	A	127	THR	2.5
1	A	835	SER	2.5
1	A	636	PHE	2.4
1	B	584	ALA	2.4
1	B	588	VAL	2.4
1	B	111	ASP	2.4
1	B	558	PHE	2.4
1	B	280	MET	2.4
1	B	810	SER	2.4
1	A	1215	THR	2.4
1	A	689	VAL	2.4
1	A	487	LEU	2.4
1	A	558	PHE	2.4
1	A	111	ASP	2.4
1	A	45	VAL	2.4
1	B	277	LEU	2.3
1	B	1184	ASN	2.3
1	B	42	THR	2.3
1	A	435	ASP	2.3
1	B	105	THR	2.3
1	A	40	ASN	2.3
1	A	1184	ASN	2.3
1	B	1000	TRP	2.3
1	A	757	SER	2.3
1	A	942	ALA	2.3
1	B	303	ILE	2.3
1	A	125	ALA	2.2
1	A	470	TRP	2.2
1	B	352	ILE	2.2
1	B	278	GLY	2.2
1	B	636	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	634	TRP	2.2
1	A	47	SER	2.2
1	B	1280	ALA	2.2
1	A	367	GLN	2.2
1	A	110	GLY	2.2
1	A	1254	GLY	2.2
1	A	1265	PRO	2.2
1	B	309	ALA	2.2
1	B	1154	PRO	2.1
1	B	945	GLN	2.1
1	A	642	VAL	2.1
1	A	526	TRP	2.1
1	A	527	GLY	2.1
1	A	1075	MET	2.1
1	A	44	ALA	2.1
1	A	591	THR	2.1
1	B	100	ASP	2.1
1	B	961	ILE	2.1
1	A	472	THR	2.0
1	A	810	SER	2.0
1	A	634	TRP	2.0
1	A	112	PRO	2.0
1	B	560	PRO	2.0
1	B	559	THR	2.0
1	A	1251	VAL	2.0
1	A	61	ALA	2.0
1	B	55	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

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

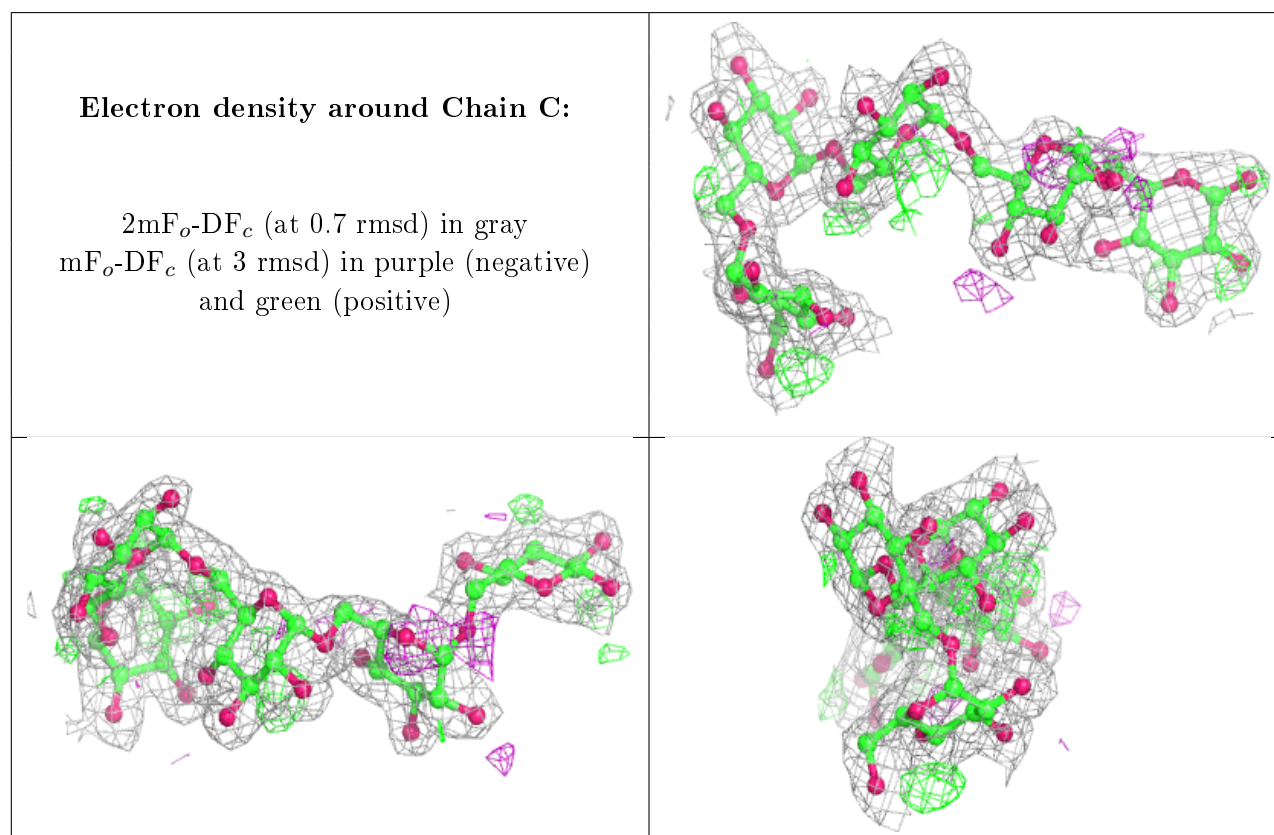
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GLC	H	1	1/12	0.63	0.40	72,72,72,72	0

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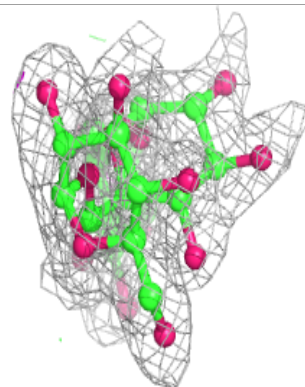
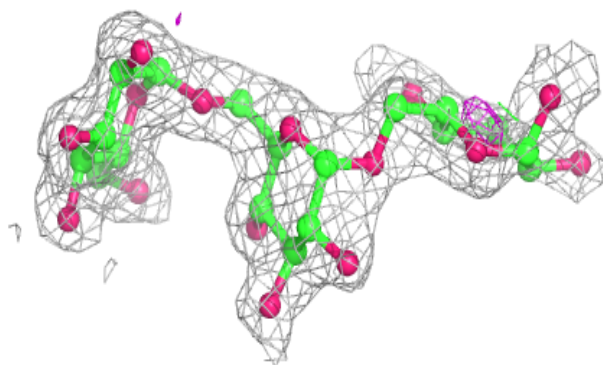
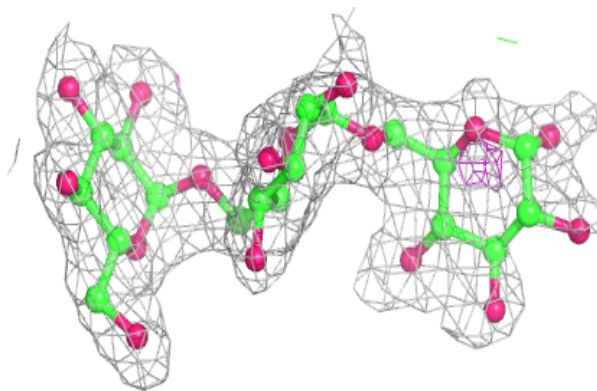
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLC	D	1	12/12	0.71	0.40	53,70,73,74	0
3	GLC	F	1	12/12	0.82	0.41	51,76,79,84	0
5	AC1	I	2	21/22	0.82	0.26	40,52,68,70	0
2	GLC	C	2	11/12	0.85	0.17	40,43,45,47	0
4	GLC	E	1	12/12	0.85	0.18	48,58,64,66	0
4	GLC	G	1	12/12	0.86	0.19	53,66,68,70	0
2	GLC	C	3	11/12	0.86	0.13	37,42,44,46	0
5	GLC	I	1	1/12	0.86	0.17	66,66,66,66	0
5	AC1	H	2	21/22	0.86	0.23	35,44,67,72	0
2	BGC	C	1	12/12	0.88	0.12	36,38,39,40	0
2	GLC	C	4	11/12	0.89	0.11	37,40,41,41	0
2	GLC	C	5	11/12	0.90	0.13	38,40,41,42	0
4	GLC	E	2	11/12	0.90	0.14	39,46,50,51	0
3	GLC	D	2	11/12	0.93	0.26	40,44,49,52	0
3	GLC	F	2	11/12	0.94	0.20	36,40,46,46	0
4	GLC	G	2	11/12	0.94	0.11	45,52,56,61	0
3	GLC	D	3	11/12	0.94	0.20	33,38,40,40	0
3	GLC	F	3	11/12	0.96	0.17	31,33,35,36	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.

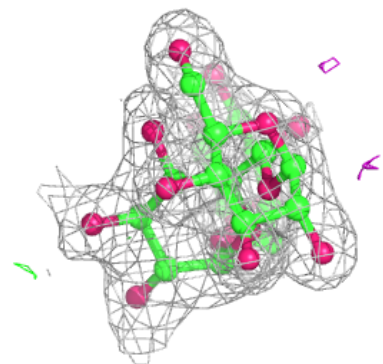
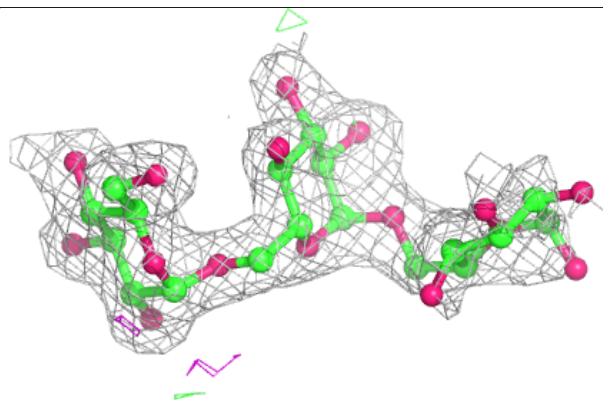
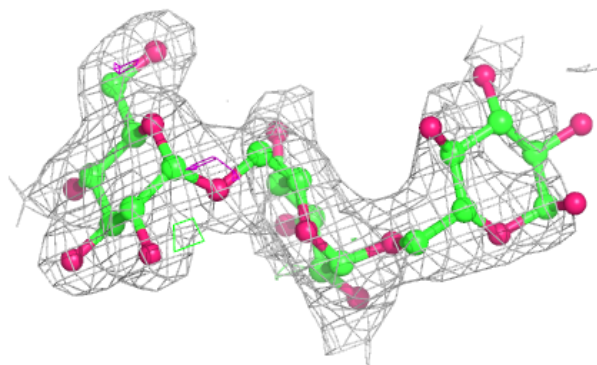


Electron density around Chain D:

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

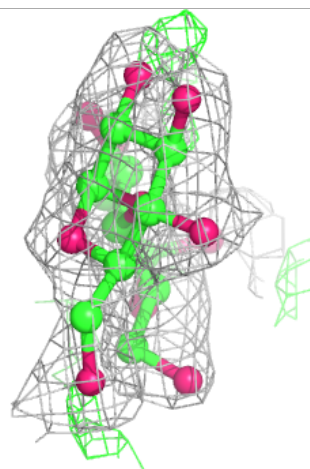
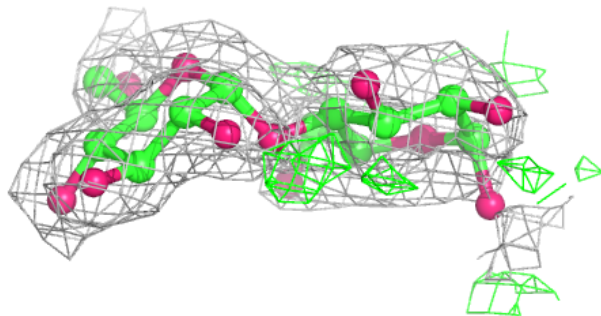
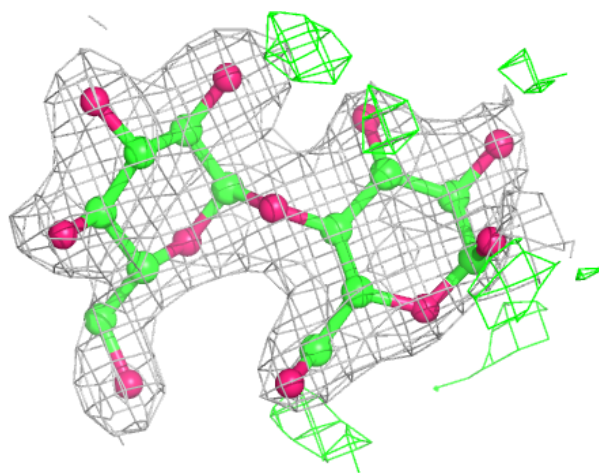
**Electron density around Chain F:**

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



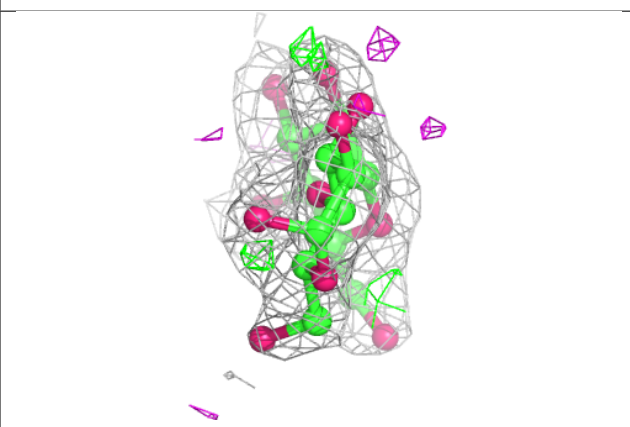
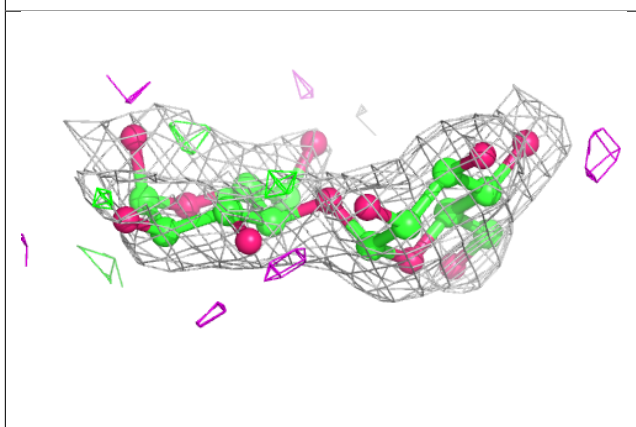
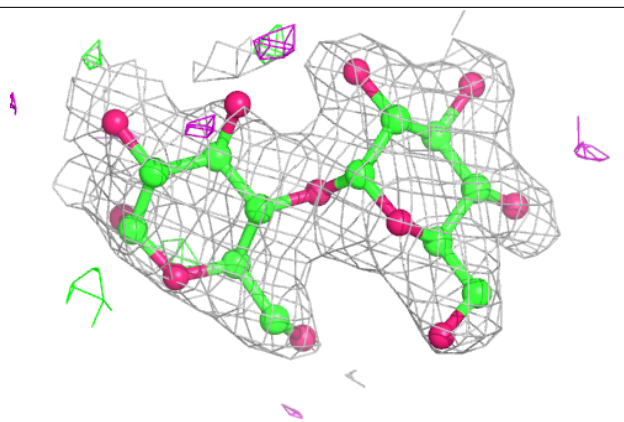
Electron density around Chain E:

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



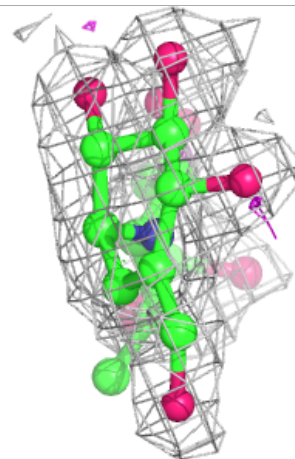
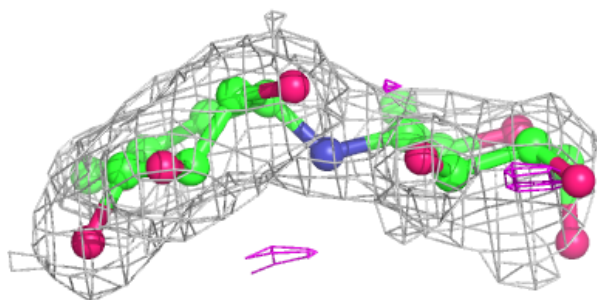
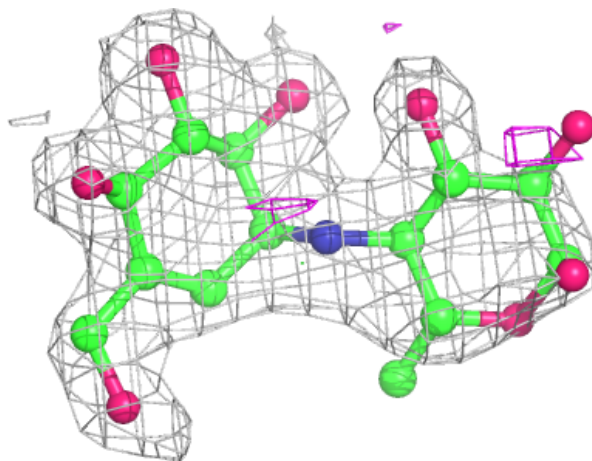
Electron density around Chain G:

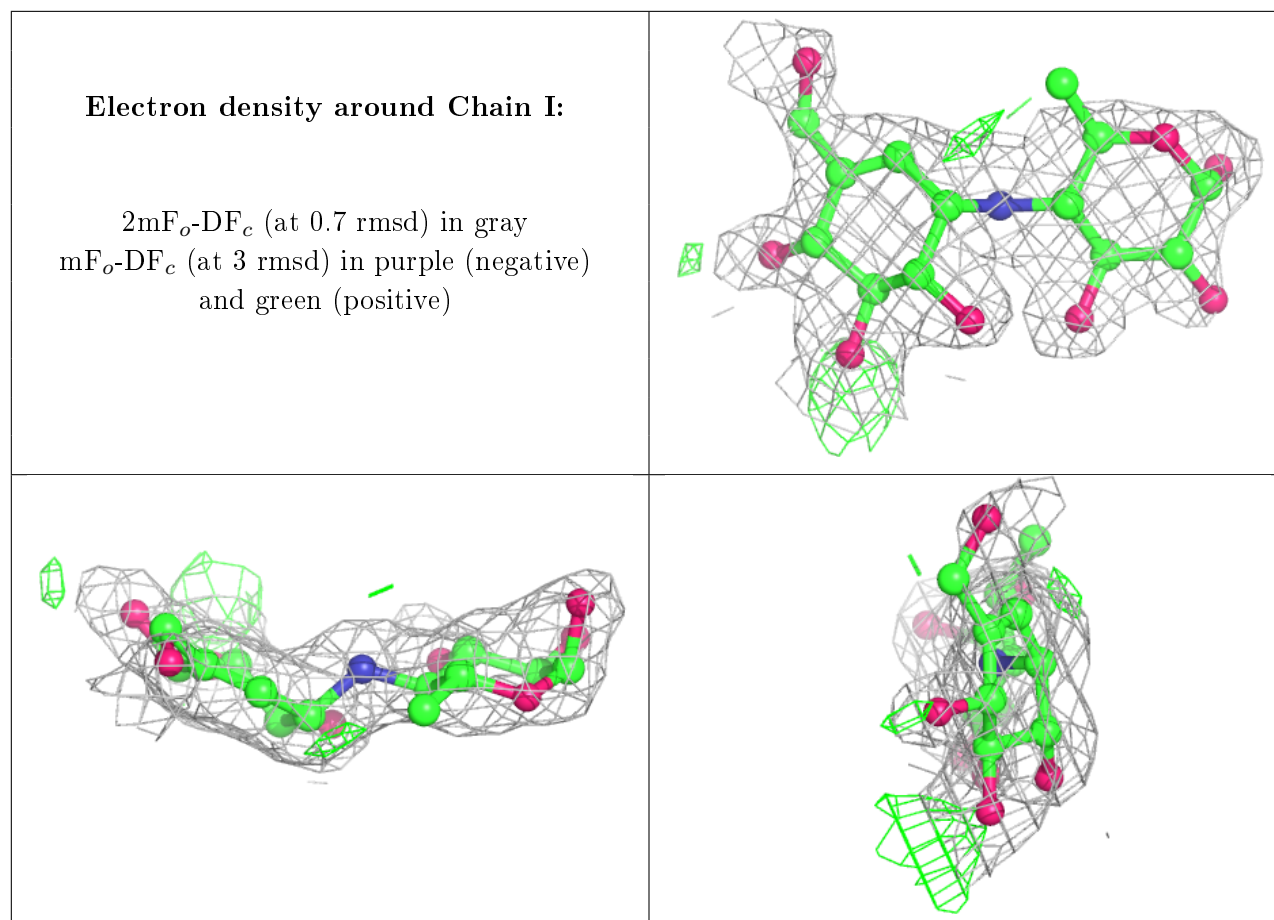
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

$2mF_o-DF_c$ (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
12	MES	B	1701	12/12	0.67	0.26	74,78,86,89	0
8	GLC	B	1461	12/12	0.68	0.39	52,71,77,77	0
8	GLC	A	1461	12/12	0.71	0.41	52,63,64,65	0
10	MG	B	1610	1/1	0.74	0.27	48,48,48,48	0
12	MES	A	1708	12/12	0.76	0.25	78,84,108,113	0
10	MG	B	1608	1/1	0.77	0.08	50,50,50,50	0
12	MES	A	1704	12/12	0.79	0.24	78,82,84,87	0
13	EDO	A	1804	4/4	0.81	0.19	30,36,36,43	0
11	SO4	A	1701	5/5	0.81	0.26	78,81,84,88	0
12	MES	A	1705	12/12	0.82	0.27	54,66,77,79	0
10	MG	B	1606	1/1	0.84	0.21	67,67,67,67	0
12	MES	B	1716	12/12	0.85	0.24	70,74,77,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
12	MES	B	1707	12/12	0.86	0.17	75,77,79,81	0
12	MES	B	1711	12/12	0.86	0.24	58,66,68,69	0
11	SO4	B	1703	5/5	0.86	0.32	84,87,90,91	0
12	MES	A	1706	12/12	0.86	0.23	81,86,89,90	0
10	MG	A	1610	1/1	0.87	0.24	58,58,58,58	0
12	MES	A	1711	12/12	0.87	0.22	59,64,68,71	0
11	SO4	B	1709	5/5	0.88	0.30	78,80,87,87	0
11	SO4	B	1713	5/5	0.88	0.19	57,61,67,67	0
10	MG	A	1604	1/1	0.88	0.07	57,57,57,57	0
10	MG	A	1606	1/1	0.88	0.15	67,67,67,67	0
10	MG	B	1604	1/1	0.89	0.08	64,64,64,64	0
12	MES	B	1706	12/12	0.89	0.27	72,74,77,80	0
11	SO4	B	1717	5/5	0.90	0.30	88,89,92,92	0
12	MES	A	1709	12/12	0.90	0.24	48,56,70,70	0
13	EDO	B	1803	4/4	0.90	0.19	49,52,52,54	0
12	MES	A	1713	12/12	0.90	0.23	68,70,74,75	0
11	SO4	A	1714	5/5	0.91	0.40	91,92,95,95	0
10	MG	B	1603	1/1	0.91	0.11	47,47,47,47	0
11	SO4	B	1702	5/5	0.91	0.17	58,60,64,66	0
11	SO4	B	1718	5/5	0.91	0.30	75,78,81,82	0
11	SO4	B	1715	5/5	0.92	0.28	64,66,67,71	0
13	EDO	A	1803	4/4	0.92	0.15	46,47,49,50	0
11	SO4	A	1702	5/5	0.92	0.18	54,57,59,68	0
12	MES	B	1712	12/12	0.92	0.16	52,57,58,58	0
11	SO4	A	1707	5/5	0.93	0.30	66,67,75,77	0
13	EDO	B	1804	4/4	0.93	0.14	31,35,35,43	0
13	EDO	A	1802	4/4	0.93	0.16	45,46,46,47	0
12	MES	B	1708	12/12	0.93	0.15	44,56,60,63	0
11	SO4	B	1704	5/5	0.94	0.17	58,58,64,69	0
10	MG	A	1605	1/1	0.94	0.14	53,53,53,53	0
13	EDO	B	1801	4/4	0.95	0.12	35,38,38,38	0
13	EDO	A	1801	4/4	0.95	0.10	33,36,36,38	0
9	NI	A	1502	1/1	0.95	0.07	43,43,43,43	0
10	MG	B	1605	1/1	0.95	0.17	48,48,48,48	0
6	CA	A	1303	1/1	0.96	0.10	33,33,33,33	0
11	SO4	A	1710	5/5	0.96	0.12	50,51,54,54	0
10	MG	A	1603	1/1	0.96	0.07	43,43,43,43	0
10	MG	B	1609	1/1	0.96	0.05	34,34,34,34	0
13	EDO	B	1802	4/4	0.96	0.14	41,42,42,42	0
10	MG	B	1607	1/1	0.96	0.04	36,36,36,36	0
10	MG	B	1602	1/1	0.97	0.05	34,34,34,34	0
10	MG	A	1607	1/1	0.97	0.09	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	SO4	A	1703	5/5	0.97	0.27	60,64,65,68	0
10	MG	A	1608	1/1	0.97	0.07	39,39,39,39	0
11	SO4	B	1705	5/5	0.97	0.26	58,58,60,61	0
11	SO4	B	1710	5/5	0.97	0.15	51,51,53,54	0
12	MES	B	1714	12/12	0.97	0.10	30,32,35,37	0
7	BGC	B	1401	12/12	0.97	0.11	23,25,26,27	0
10	MG	A	1601	1/1	0.98	0.08	31,31,31,31	0
9	NI	B	1502	1/1	0.98	0.05	54,54,54,54	0
6	CA	A	1302	1/1	0.98	0.08	28,28,28,28	0
7	BGC	A	1401	12/12	0.98	0.12	24,26,26,27	0
10	MG	A	1609	1/1	0.98	0.04	33,33,33,33	0
6	CA	A	1301	1/1	0.98	0.05	33,33,33,33	0
10	MG	B	1601	1/1	0.99	0.10	25,25,25,25	0
6	CA	B	1302	1/1	0.99	0.07	30,30,30,30	0
12	MES	A	1712	12/12	0.99	0.08	31,36,38,38	0
6	CA	B	1303	1/1	0.99	0.09	33,33,33,33	0
10	MG	A	1602	1/1	0.99	0.07	28,28,28,28	0
6	CA	B	1301	1/1	1.00	0.08	30,30,30,30	0
9	NI	A	1501	1/1	1.00	0.06	30,30,30,30	0
9	NI	B	1501	1/1	1.00	0.05	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.