



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:59 AM UTC

PDB ID : 8DL1 / pdb_00008dl1
Title : BoGH13ASus-E523Q from Bacteroides ovatus bound to maltoheptaose
Authors : Brown, H.A.; DeVeaux, A.L.; Koropatkin, N.M.
Deposited on : 2022-07-06
Resolution : 2.09 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

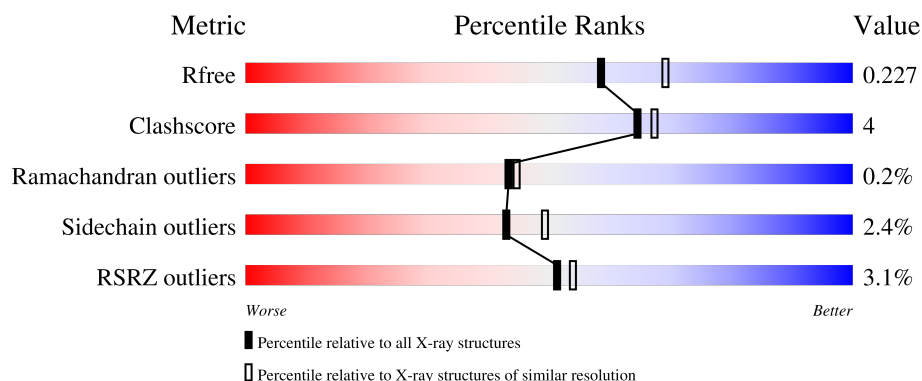
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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.



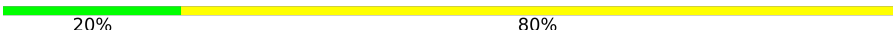
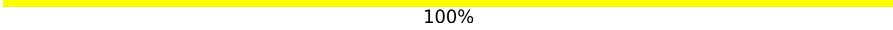
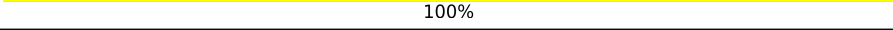
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	738	 2% 87% 9% ..
1	B	738	 2% 88% 7% .
1	C	738	 4% 86% 10% ..
1	D	738	 5% 86% 9% .
2	G	5	 100%

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Mol	Chain	Length	Quality of chain
2	H	5	 20%80%
2	I	5	 20%80%
2	J	5	 40%60%
2	K	5	 80%20%
3	L	3	 67%33%
3	M	3	 100%
4	N	4	 75%25%
5	O	7	 86%14%
6	P	7	 100%
7	Q	6	 17%83%
8	R	5	 40%60%

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
10	ACT	D	805	-	-	X	-
13	1PE	C	2301	-	-	X	-
9	EDO	A	2316	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 25543 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, catalytic domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	1	0
			5726	3652	943	1108	23			
1	B	708	Total	C	N	O	S	0	2	0
			5664	3613	932	1096	23			
1	C	712	Total	C	N	O	S	0	0	0
			5698	3635	940	1101	22			
1	D	706	Total	C	N	O	S	0	1	0
			5613	3586	925	1080	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	expression tag	UNP A7M087
A	523	GLN	GLU	engineered mutation	UNP A7M087
B	21	GLY	-	expression tag	UNP A7M087
B	523	GLN	GLU	engineered mutation	UNP A7M087
C	21	GLY	-	expression tag	UNP A7M087
C	523	GLN	GLU	engineered mutation	UNP A7M087
D	21	GLY	-	expression tag	UNP A7M087
D	523	GLN	GLU	engineered mutation	UNP A7M087

- 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	G	5	Total	C O	0	0	0
			56	30 26			

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

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



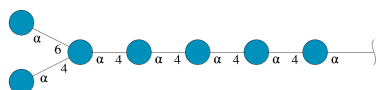
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	L	3	Total	C	O	0	0	0
			34	18	16			
3	M	3	Total	C	O	0	0	0
			34	18	16			

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



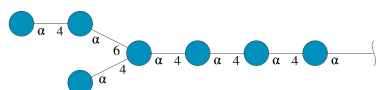
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
4	N	4	Total	C	O	0	0	0
			45	24	21			

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



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

- 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-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



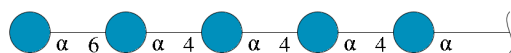
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
6	P	7	Total	C	O	0	0	0
			78	42	36			

- Molecule 7 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-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
7	Q	6	Total	C	O	0	0	0
			67	36	31			

- Molecule 8 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-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
8	R	5	Total	C	O	0	0	0
			56	30	26			

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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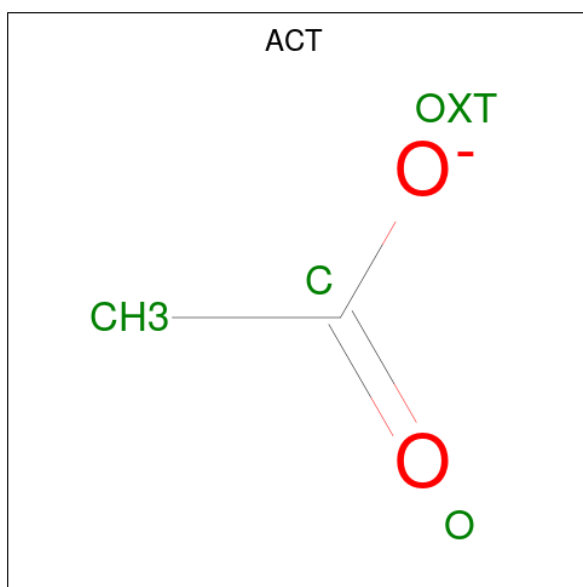
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 4	C 2	O 2	0	0
9	A	1	Total 4	C 2	O 2	0	0
9	A	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0	0
9	B	1	Total 4	C 2	O 2	0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

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

- Molecule 10 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

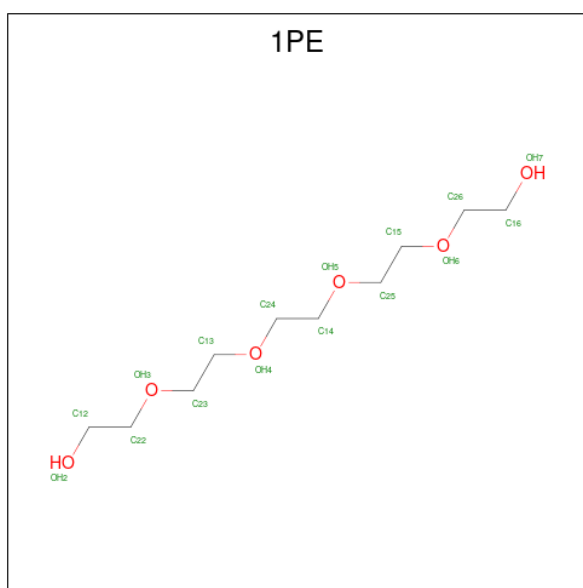
- Molecule 11 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	Ca	0	0
			1	1		
11	B	1	Total	Ca	0	0
			1	1		
11	C	1	Total	Ca	0	0
			1	1		
11	D	1	Total	Ca	0	0
			1	1		

- Molecule 12 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

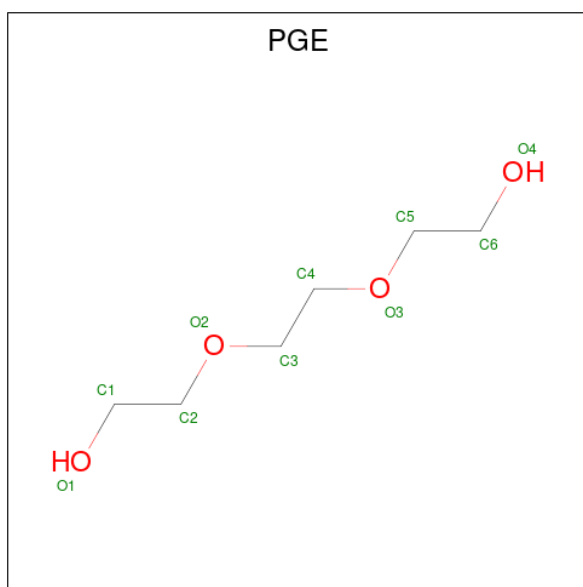
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	1	Total	Mn	0	0
			1	1		
12	B	1	Total	Mn	0	0
			1	1		
12	C	1	Total	Mn	0	0
			1	1		
12	D	1	Total	Mn	0	0
			1	1		

- Molecule 13 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			16	10	6		

- Molecule 14 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).

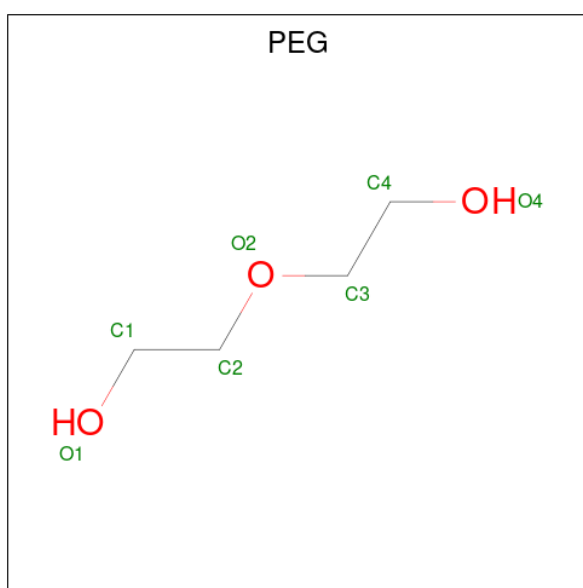


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 15 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	1	Total	Na	0	0
			1	1		

- Molecule 16 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 17 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

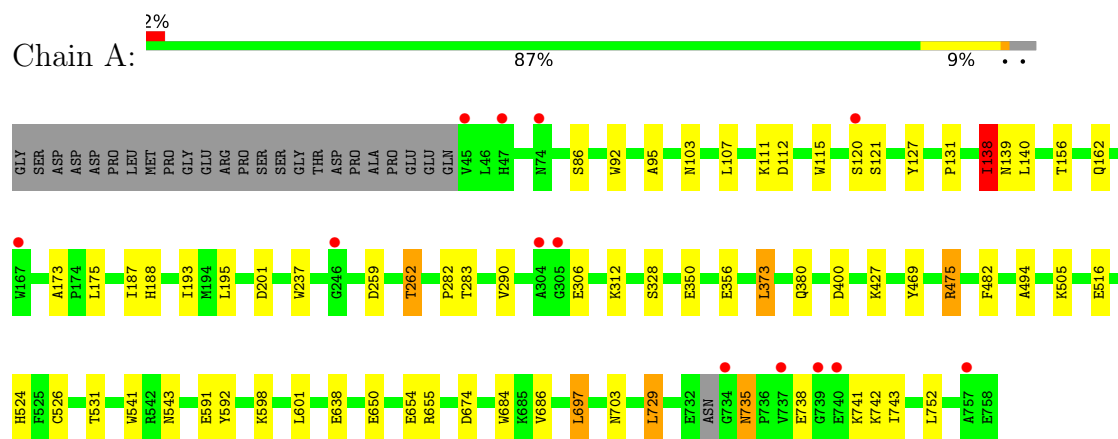
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	587	Total	O	0	0
			587	587		
18	B	488	Total	O	0	0
			488	488		
18	C	462	Total	O	0	0
			462	462		
18	D	350	Total	O	0	0
			350	350		

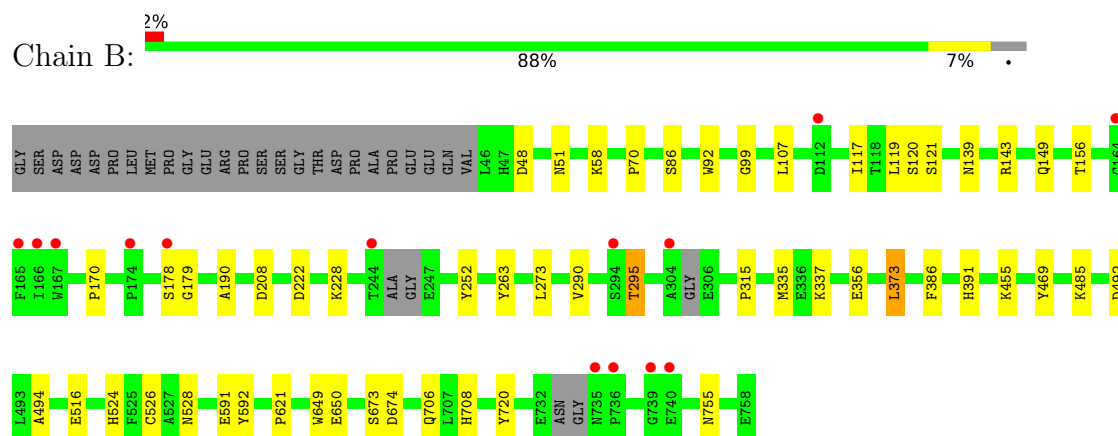
3 Residue-property plots [i](#)

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.

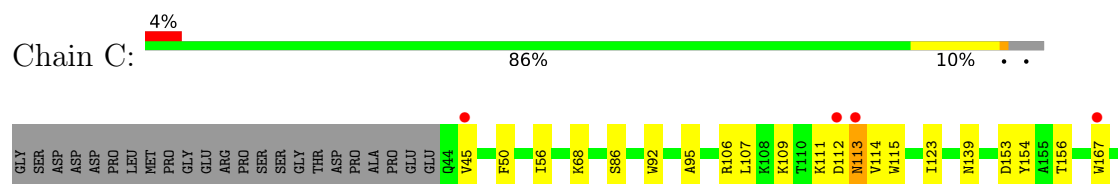
- Molecule 1: Alpha amylase, catalytic domain protein

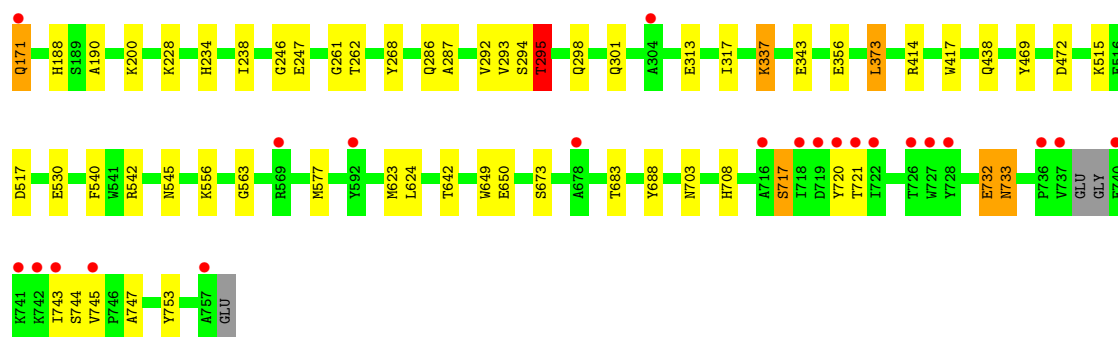


- Molecule 1: Alpha amylase, catalytic domain protein

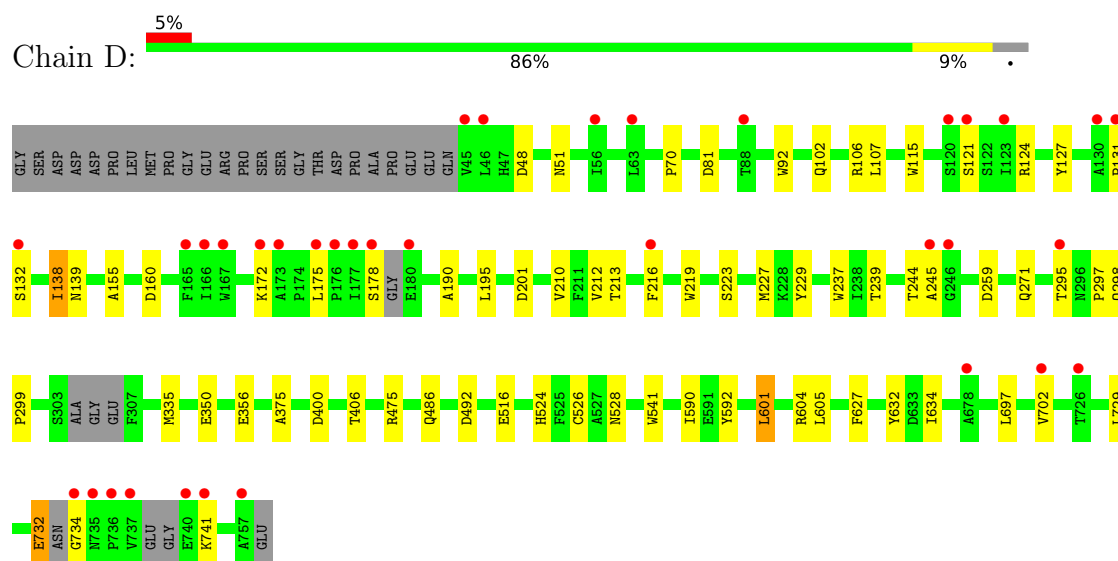


- Molecule 1: Alpha amylase, catalytic domain protein

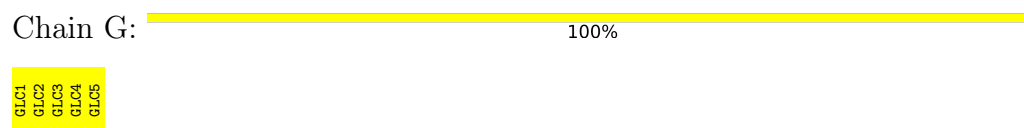




- Molecule 1: Alpha amylase, catalytic domain protein



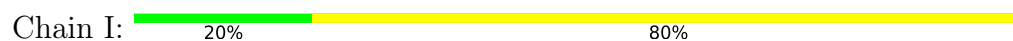
- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose





- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain J:



- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain K:



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain L:



- Molecule 3: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:



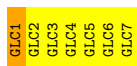
- Molecule 4: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain N:

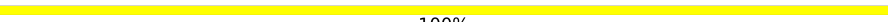


- Molecule 5: alpha-D-glucopyranose-(1-4)-[alpha-D-glucopyranose-(1-6)]alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain O:

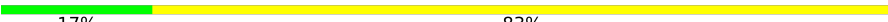


- Molecule 6: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-6)-[alpha-D-glucopyranose-(1-4)]alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain P:  100%

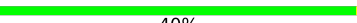
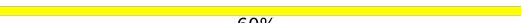
GLC1
GLC2
GLC3
GLC4
GLC5
GLC6
GLC7

- Molecule 7: 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 Q:  17%  83%

GLC1
GLC2
GLC3
GLC4
GLC5
GLC6

- Molecule 8: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain R:  40%  60%

GLC1
GLC2
GLC3
GLC4
GLC5

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.68Å 128.64Å 149.76Å 90.00° 105.37° 90.00°	Depositor
Resolution (Å)	47.93 – 2.09 47.93 – 2.09	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.93-2.09) 98.7 (47.93-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.177 , 0.223 0.185 , 0.227	Depositor DCC
R_{free} test set	10581 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25543	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: EDO, CA, CL, PGE, 1PE, GLC, PEG, NA, MN, 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	1.02	0/5895	1.27	9/8021 (0.1%)
1	B	1.01	0/5832	1.29	4/7939 (0.1%)
1	C	1.01	2/5864 (0.0%)	1.33	12/7986 (0.2%)
1	D	1.02	0/5779	1.31	6/7875 (0.1%)
All	All	1.01	2/23370 (0.0%)	1.30	31/31821 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	745	VAL	N-CA	5.51	1.50	1.46
1	C	188	HIS	CE1-NE2	5.43	1.38	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	642	THR	CA-C-N	6.62	126.39	120.10
1	C	642	THR	C-N-CA	6.62	126.39	120.10
1	C	744	SER	CA-C-N	6.55	127.06	122.60
1	C	744	SER	C-N-CA	6.55	127.06	122.60
1	A	138	ILE	CB-CA-C	6.13	118.70	110.42
1	C	721	THR	CB-CA-C	6.13	121.76	111.22
1	D	492	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	282	PRO	CA-C-N	5.70	127.92	120.28
1	A	282	PRO	C-N-CA	5.70	127.92	120.28
1	C	295	THR	N-CA-CB	-5.69	100.65	110.32
1	B	492	ASP	CA-CB-CG	5.62	118.22	112.60
1	D	201	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	400	ASP	CB-CA-C	5.51	118.53	110.26
1	C	238	ILE	CA-C-O	-5.46	116.38	120.96
1	D	406	THR	CB-CA-C	5.42	121.21	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	472	ASP	CA-CB-CG	-5.40	107.20	112.60
1	A	729	LEU	CA-C-N	5.39	127.50	120.28
1	A	729	LEU	C-N-CA	5.39	127.50	120.28
1	A	531	THR	CA-CB-OG1	-5.34	101.58	109.60
1	B	674	ASP	CA-CB-CG	5.27	117.87	112.60
1	C	294	SER	CA-C-N	5.24	128.99	120.60
1	C	294	SER	C-N-CA	5.24	128.99	120.60
1	D	102	GLN	CA-C-N	5.17	127.47	120.38
1	D	102	GLN	C-N-CA	5.17	127.47	120.38
1	B	179	GLY	CA-C-O	-5.17	116.99	122.01
1	A	187	ILE	CA-C-N	5.15	129.38	120.58
1	A	187	ILE	C-N-CA	5.15	129.38	120.58
1	C	123	ILE	N-CA-C	-5.13	105.49	110.42
1	B	228	LYS	CB-CA-C	5.13	118.10	109.48
1	D	400	ASP	CB-CA-C	5.08	118.62	110.29
1	C	156	THR	CA-CB-OG1	-5.06	102.01	109.60

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	5726	0	5357	39	0
1	B	5664	0	5266	40	0
1	C	5698	0	5310	55	0
1	D	5613	0	5186	37	0
2	G	56	0	48	0	0
2	H	56	0	48	0	0
2	I	56	0	48	0	0
2	J	56	0	48	0	0
2	K	56	0	48	1	0
3	L	34	0	30	0	0
3	M	34	0	30	0	0
4	N	45	0	39	1	0
5	O	78	0	66	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	78	0	66	0	0
7	Q	67	0	57	0	0
8	R	56	0	48	0	0
9	A	68	0	102	7	0
9	B	80	0	120	10	0
9	C	52	0	78	6	0
9	D	20	0	30	2	0
10	A	16	0	12	0	0
10	D	4	0	3	2	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	C	1	0	0	0	0
12	D	1	0	0	0	0
13	C	16	0	22	19	0
14	C	10	0	14	1	0
15	C	1	0	0	0	0
16	C	7	0	10	2	0
17	D	1	0	0	0	0
18	A	587	0	0	5	0
18	B	488	0	0	8	0
18	C	462	0	0	8	0
18	D	350	0	0	2	0
All	All	25543	0	22086	179	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 4.

All (179) 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:C:92:TRP:HE1	13:C:2301:1PE:H162	1.27	0.97
1:B:190:ALA:O	1:B:295:THR:HG21	1.72	0.90
1:C:50:PHE:H	16:C:2312:PEG:H21	1.46	0.79
1:D:271:GLN:HG3	10:D:805:ACT:H1	1.66	0.77
1:C:92:TRP:NE1	13:C:2301:1PE:H162	2.00	0.76
1:A:259:ASP:OD2	18:A:2401:HOH:O	2.05	0.74
1:D:590:ILE:HD11	1:D:604:ARG:NH1	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:650:GLU:OE1	18:C:2401:HOH:O	2.08	0.71
1:D:212:VAL:HG23	1:D:227:MET:HE2	1.71	0.70
1:C:92:TRP:HE1	13:C:2301:1PE:C16	2.02	0.70
9:B:3304:EDO:H11	18:B:3718:HOH:O	1.92	0.70
1:D:210:VAL:HG12	1:D:227:MET:HE1	1.76	0.67
1:C:154:TYR:CE2	16:C:2312:PEG:H22	2.30	0.67
1:A:735:ASN:OD1	1:A:735:ASN:N	2.28	0.66
1:C:261:GLY:O	13:C:2301:1PE:H121	1.95	0.65
1:A:598:LYS:NZ	18:A:2404:HOH:O	2.30	0.64
1:B:335:MET:HE1	18:B:3777:HOH:O	1.97	0.64
1:B:335:MET:HE2	1:B:386:PHE:HA	1.79	0.64
1:B:391:HIS:ND1	9:B:3316:EDO:C2	2.63	0.62
1:A:655:ARG:HE	9:A:2316:EDO:H22	1.63	0.62
1:C:414:ARG:HH12	9:C:2314:EDO:H12	1.64	0.62
1:D:297:PRO:O	1:D:299:PRO:HD3	2.01	0.60
1:C:190:ALA:O	1:C:295:THR:HG21	2.02	0.59
1:A:373:LEU:HD22	1:A:469:TYR:CZ	2.38	0.59
1:D:212:VAL:CG2	1:D:227:MET:HE2	2.32	0.59
1:A:697:LEU:HD12	1:A:697:LEU:C	2.27	0.59
13:C:2301:1PE:H252	13:C:2301:1PE:H231	1.83	0.59
1:C:261:GLY:O	13:C:2301:1PE:C12	2.50	0.58
1:C:373:LEU:HD22	1:C:469:TYR:CZ	2.38	0.58
1:A:654:GLU:HB3	9:A:2316:EDO:H21	1.85	0.57
1:C:747:ALA:O	18:C:2402:HOH:O	2.17	0.57
1:C:190:ALA:O	1:C:295:THR:CG2	2.53	0.57
1:D:212:VAL:HG12	1:D:216:PHE:HZ	1.69	0.57
1:B:58:LYS:NZ	18:B:3415:HOH:O	2.38	0.56
9:B:3304:EDO:C1	18:B:3718:HOH:O	2.50	0.56
13:C:2301:1PE:H231	13:C:2301:1PE:C14	2.35	0.56
1:B:391:HIS:ND1	9:B:3316:EDO:H22	2.21	0.56
1:A:494:ALA:O	1:A:526[A]:CYS:SG	2.65	0.56
1:B:373:LEU:HD22	1:B:469:TYR:CZ	2.42	0.55
1:C:708:HIS:HE2	1:C:720:TYR:HH	1.53	0.55
1:B:208:ASP:OD1	18:B:3401:HOH:O	2.18	0.55
1:B:591:GLU:HG2	1:B:592:TYR:CE2	2.42	0.55
1:C:247:GLU:HG3	1:C:292:VAL:HG13	1.90	0.54
1:C:107:LEU:HB3	1:C:115:TRP:HB3	1.90	0.54
1:C:515:LYS:NZ	1:C:517:ASP:OD1	2.40	0.54
1:A:107:LEU:HB3	1:A:115:TRP:HB3	1.88	0.54
1:D:210:VAL:HG12	1:D:227:MET:CE	2.38	0.53
1:D:486:GLN:OE1	18:D:901:HOH:O	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LYS:HB2	1:C:114:VAL:HB	1.90	0.53
1:B:170:PRO:HG3	1:B:208:ASP:O	2.08	0.53
1:D:524:HIS:CD2	1:D:526:CYS:HB3	2.44	0.53
1:C:732:GLU:O	1:C:733:ASN:CB	2.57	0.52
1:B:48:ASP:CG	1:B:70:PRO:HB3	2.35	0.52
1:B:524:HIS:CD2	1:B:526[A]:CYS:HB2	2.43	0.52
1:C:743:ILE:HD13	1:C:753:TYR:OH	2.09	0.52
1:B:706:GLN:HB2	1:B:755:ASN:ND2	2.25	0.52
1:D:124:ARG:HH22	1:D:160:ASP:CG	2.17	0.52
1:D:601:LEU:HD22	1:D:605:LEU:HG	1.92	0.51
1:B:650:GLU:HG3	18:B:3689:HOH:O	2.10	0.51
1:D:51:ASN:HA	18:D:1175:HOH:O	2.11	0.51
1:A:543:ASN:HD22	5:O:1:GLC:H62	1.76	0.50
13:C:2301:1PE:H141	9:C:2314:EDO:H11	1.93	0.50
1:B:92:TRP:CZ2	1:B:139:ASN:HB3	2.46	0.50
1:A:188:HIS:CD2	1:C:246:GLY:HA2	2.46	0.50
1:A:524:HIS:CD2	1:A:526[B]:CYS:HB2	2.46	0.50
1:D:107:LEU:HB3	1:D:115:TRP:HB3	1.94	0.50
1:C:317:ILE:O	1:C:623:MET:HA	2.13	0.49
1:A:591:GLU:OE1	1:A:592:TYR:CE2	2.66	0.49
1:B:494:ALA:O	1:B:526[B]:CYS:SG	2.71	0.48
1:C:683:THR:HA	18:C:2713:HOH:O	2.14	0.48
1:D:350:GLU:OE1	1:D:475:ARG:HD3	2.14	0.48
1:C:109:LYS:HE2	1:C:112:ASP:O	2.14	0.48
1:A:350:GLU:OE2	1:A:475:ARG:HD3	2.13	0.48
1:A:86:SER:O	1:A:95:ALA:HA	2.14	0.47
1:B:708:HIS:NE2	1:B:720:TYR:OH	2.45	0.47
1:C:92:TRP:CZ2	1:C:139:ASN:HB3	2.49	0.47
1:C:708:HIS:NE2	1:C:720:TYR:OH	2.35	0.47
1:A:654:GLU:CB	9:A:2316:EDO:H21	2.44	0.47
1:B:494:ALA:O	9:B:3307:EDO:H22	2.14	0.47
1:A:92:TRP:CZ2	1:A:139:ASN:HB3	2.50	0.47
1:B:528:ASN:H	9:B:3307:EDO:H21	1.80	0.47
13:C:2301:1PE:H231	13:C:2301:1PE:C25	2.45	0.47
1:C:113:ASN:H	1:C:113:ASN:HD22	1.62	0.46
1:C:153:ASP:HB3	13:C:2301:1PE:H251	1.95	0.46
1:B:190:ALA:HA	1:B:295:THR:HG23	1.96	0.46
1:A:592:TYR:CE1	2:K:2:GLC:H61	2.50	0.46
1:C:262:THR:HG23	13:C:2301:1PE:H232	1.96	0.46
1:C:313:GLU:OE2	9:C:2318:EDO:O1	2.27	0.46
1:C:286:GLN:HG2	1:C:287:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:LEU:HD11	9:A:2315:EDO:H22	1.97	0.46
1:B:335:MET:HB2	1:B:335:MET:HE3	1.66	0.46
1:A:120:SER:HB3	18:A:2888:HOH:O	2.16	0.46
1:B:107:LEU:HG	1:B:117:ILE:HB	1.97	0.46
1:C:624:LEU:HD23	1:C:624:LEU:H	1.81	0.46
1:A:655:ARG:HE	9:A:2316:EDO:C2	2.27	0.46
1:A:262:THR:HG21	18:A:2641:HOH:O	2.16	0.45
13:C:2301:1PE:H221	18:C:2431:HOH:O	2.15	0.45
1:A:195:LEU:O	1:A:237:TRP:HA	2.16	0.45
1:B:391:HIS:ND1	9:B:3316:EDO:H21	2.30	0.45
1:B:516:GLU:HG2	18:B:3546:HOH:O	2.16	0.45
1:D:127:TYR:OH	1:D:138:ILE:HD11	2.16	0.45
1:C:703:ASN:OD1	1:C:703:ASN:C	2.59	0.45
1:A:138:ILE:HD12	1:A:140:LEU:HD21	1.98	0.45
1:A:742:LYS:NZ	18:A:2441:HOH:O	2.50	0.45
1:C:438:GLN:HG3	18:C:2857:HOH:O	2.16	0.45
1:B:120:SER:HB2	1:B:121:SER:HA	1.99	0.45
1:D:697:LEU:HD12	1:D:697:LEU:C	2.41	0.45
9:C:2318:EDO:H22	18:C:2781:HOH:O	2.17	0.45
1:D:124:ARG:HD3	1:D:131:PRO:HA	1.99	0.45
1:D:92:TRP:CZ2	1:D:139:ASN:HB3	2.52	0.45
1:D:190:ALA:HA	1:D:295:THR:HB	1.98	0.45
1:D:195:LEU:O	1:D:237:TRP:HA	2.17	0.45
1:C:68:LYS:HA	1:C:113:ASN:O	2.17	0.45
1:A:752:LEU:C	1:A:752:LEU:HD23	2.43	0.44
1:B:273:LEU:HB2	1:B:290:VAL:HG22	1.99	0.44
1:C:262:THR:OG1	13:C:2301:1PE:H232	2.16	0.44
1:D:139:ASN:OD1	1:D:155:ALA:HB2	2.17	0.44
1:B:48:ASP:OD2	1:B:70:PRO:HB3	2.17	0.44
1:D:590:ILE:HD11	1:D:604:ARG:CZ	2.48	0.44
1:B:252:TYR:O	1:B:263:TYR:HA	2.17	0.44
1:A:131:PRO:O	1:A:162:GLN:NE2	2.48	0.44
1:A:138:ILE:CG2	1:A:156:THR:HG22	2.47	0.44
1:C:171:GLN:HB3	1:C:228:LYS:HG2	2.00	0.44
1:C:200:LYS:HB2	1:C:234:HIS:HB3	2.00	0.44
1:C:556:LYS:HG2	1:C:688:TYR:CE1	2.52	0.44
1:D:729:LEU:HB3	1:D:732:GLU:HG3	1.98	0.44
1:D:634:ILE:HA	9:D:804:EDO:H12	1.98	0.44
1:C:417:TRP:HB3	13:C:2301:1PE:H132	2.00	0.43
1:D:375:ALA:HB2	10:D:805:ACT:H3	1.99	0.43
1:B:315:PRO:HD2	1:B:621:PRO:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:GLU:HG3	9:C:2315:EDO:C2	2.48	0.43
1:D:475:ARG:HD2	1:D:541:TRP:CZ2	2.52	0.43
1:A:654:GLU:HB3	9:A:2316:EDO:C2	2.49	0.43
1:A:743:ILE:HG21	9:A:2315:EDO:H11	2.01	0.43
1:B:178:SER:HB3	9:B:3320:EDO:H12	2.01	0.43
1:D:627:PHE:HB3	1:D:632:TYR:HB2	2.01	0.43
1:C:286:GLN:HE22	13:C:2301:1PE:H261	1.83	0.43
1:C:717:SER:N	18:C:2450:HOH:O	2.52	0.43
1:C:530:GLU:HG2	1:C:540:PHE:CD2	2.54	0.43
13:C:2301:1PE:C22	18:C:2431:HOH:O	2.66	0.43
1:B:337:LYS:HE3	1:B:649:TRP:CE2	2.54	0.42
1:C:56:ILE:HG23	1:C:167:TRP:CH2	2.54	0.42
1:C:153:ASP:HB2	13:C:2301:1PE:C14	2.49	0.42
1:A:684:TRP:CE3	1:A:686:VAL:HG11	2.54	0.42
1:C:337:LYS:HG3	1:C:649:TRP:CZ2	2.54	0.42
1:B:222:ASP:C	1:B:222:ASP:OD1	2.63	0.42
1:B:455:LYS:HE2	18:B:3520:HOH:O	2.19	0.42
1:A:127:TYR:OH	1:A:138:ILE:HD11	2.20	0.42
1:D:213[B]:THR:OG1	1:D:219:TRP:HA	2.19	0.42
1:C:268:TYR:HB3	14:C:2302:PGE:H4	2.00	0.42
1:C:86:SER:O	1:C:95:ALA:HA	2.19	0.42
13:C:2301:1PE:H121	13:C:2301:1PE:H252	2.02	0.42
1:C:343:GLU:HG3	9:C:2315:EDO:H22	2.01	0.42
1:B:591:GLU:CG	1:B:592:TYR:CE2	3.03	0.41
1:A:674:ASP:OD2	1:A:703:ASN:ND2	2.51	0.41
1:B:335:MET:CE	1:B:386:PHE:HA	2.45	0.41
1:C:337:LYS:HA	1:C:337:LYS:HD2	1.79	0.41
1:D:475:ARG:HD2	1:D:541:TRP:CE2	2.55	0.41
1:A:201:ASP:HB2	1:A:427:LYS:HB3	2.03	0.41
1:D:81:ASP:OD2	1:D:106:ARG:HD3	2.20	0.41
1:D:634:ILE:HA	9:D:804:EDO:C1	2.49	0.41
1:A:380:GLN:HG3	1:A:469:TYR:OH	2.21	0.41
1:A:738:GLU:O	1:A:741:LYS:HB3	2.21	0.41
1:B:524:HIS:CD2	1:B:526[B]:CYS:HB3	2.55	0.41
1:D:175:LEU:HD23	1:D:175:LEU:HA	1.93	0.41
1:B:99:GLY:HA2	1:B:143:ARG:CZ	2.51	0.41
1:A:475:ARG:HD2	1:A:541:TRP:CE2	2.55	0.41
1:D:48:ASP:CG	1:D:70:PRO:HB3	2.46	0.41
1:B:149:GLN:HB3	9:B:3313:EDO:H11	2.02	0.41
1:B:526[B]:CYS:SG	9:B:3307:EDO:H22	2.61	0.41
1:D:172:LYS:HA	1:D:229:TYR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ALA:HB2	1:C:301:GLN:HG3	2.02	0.40
1:A:138:ILE:HD12	1:A:140:LEU:CD2	2.50	0.40
1:C:542:ARG:NH1	1:C:563:GLY:O	2.45	0.40
1:C:262:THR:CG2	13:C:2301:1PE:H232	2.51	0.40
1:B:86:SER:HA	1:B:139:ASN:O	2.22	0.40
1:C:545:ASN:HA	1:C:577:MET:O	2.22	0.40
1:D:592:TYR:CE1	4:N:1:GLC:H2	2.56	0.40
1:D:732:GLU:O	1:D:734:GLY:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	710/738 (96%)	681 (96%)	27 (4%)	2 (0%)	36	36
1	B	702/738 (95%)	664 (95%)	38 (5%)	0	100	100
1	C	708/738 (96%)	678 (96%)	29 (4%)	1 (0%)	48	50
1	D	697/738 (94%)	658 (94%)	36 (5%)	3 (0%)	30	28
All	All	2817/2952 (95%)	2681 (95%)	130 (5%)	6 (0%)	43	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	733	ASN
1	A	306	GLU
1	A	121	SER
1	D	298	GLN
1	D	245	ALA
1	D	121	SER

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	611/639 (96%)	589 (96%)	22 (4%)	31	34
1	B	601/639 (94%)	593 (99%)	8 (1%)	61	69
1	C	605/639 (95%)	592 (98%)	13 (2%)	47	54
1	D	589/639 (92%)	574 (98%)	15 (2%)	42	48
All	All	2406/2556 (94%)	2348 (98%)	58 (2%)	43	49

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	111	LYS
1	A	112	ASP
1	A	138	ILE
1	A	175	LEU
1	A	193	ILE
1	A	262	THR
1	A	283	THR
1	A	290	VAL
1	A	312	LYS
1	A	328	SER
1	A	356	GLU
1	A	373	LEU
1	A	475	ARG
1	A	482	PHE
1	A	505	LYS
1	A	516	GLU
1	A	601	LEU
1	A	638	GLU
1	A	650	GLU
1	A	697	LEU
1	A	735	ASN
1	B	51	ASN
1	B	119	LEU

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Mol	Chain	Res	Type
1	B	156	THR
1	B	295	THR
1	B	356	GLU
1	B	373	LEU
1	B	485	LYS
1	B	673	SER
1	C	45	VAL
1	C	106	ARG
1	C	113	ASN
1	C	171	GLN
1	C	293	VAL
1	C	295	THR
1	C	298	GLN
1	C	337	LYS
1	C	356	GLU
1	C	373	LEU
1	C	673	SER
1	C	717	SER
1	C	732	GLU
1	D	132	SER
1	D	138	ILE
1	D	178	SER
1	D	223	SER
1	D	239	THR
1	D	244	THR
1	D	259	ASP
1	D	335	MET
1	D	356	GLU
1	D	516	GLU
1	D	528	ASN
1	D	601	LEU
1	D	702	VAL
1	D	732	GLU
1	D	741	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	91	ASN
1	A	125	HIS
1	A	150	GLN

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Mol	Chain	Res	Type
1	A	233	ASN
1	A	286	GLN
1	A	421	ASN
1	A	539	HIS
1	A	546	HIS
1	A	693	ASN
1	B	218	ASN
1	B	286	GLN
1	B	550	GLN
1	B	681	GLN
1	B	689	ASN
1	C	113	ASN
1	C	149	GLN
1	C	286	GLN
1	C	296	ASN
1	C	380	GLN
1	D	218	ASN
1	D	311	ASN
1	D	408	ASN
1	D	706	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

60 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	G	1	2	12,12,12	0.71	0	17,17,17	1.82	4 (23%)
2	GLC	G	2	2	11,11,12	0.79	0	15,15,17	1.21	2 (13%)
2	GLC	G	3	2	11,11,12	0.78	0	15,15,17	0.92	1 (6%)
2	GLC	G	4	2	11,11,12	0.60	0	15,15,17	1.17	1 (6%)
2	GLC	G	5	2	11,11,12	0.53	0	15,15,17	1.29	1 (6%)
2	GLC	H	1	2	12,12,12	0.73	0	17,17,17	1.45	4 (23%)
2	GLC	H	2	2	11,11,12	0.63	0	15,15,17	1.36	4 (26%)
2	GLC	H	3	2	11,11,12	0.72	0	15,15,17	0.84	0
2	GLC	H	4	2	11,11,12	0.70	0	15,15,17	1.16	2 (13%)
2	GLC	H	5	2	11,11,12	0.88	1 (9%)	15,15,17	2.22	8 (53%)
2	GLC	I	1	2	12,12,12	0.64	0	17,17,17	1.80	5 (29%)
2	GLC	I	2	2	11,11,12	0.65	0	15,15,17	1.07	1 (6%)
2	GLC	I	3	2	11,11,12	0.71	0	15,15,17	0.70	0
2	GLC	I	4	2	11,11,12	0.62	0	15,15,17	1.03	1 (6%)
2	GLC	I	5	2	11,11,12	0.49	0	15,15,17	1.07	1 (6%)
2	GLC	J	1	2	12,12,12	0.63	0	17,17,17	1.36	3 (17%)
2	GLC	J	2	2	11,11,12	1.01	0	15,15,17	1.48	3 (20%)
2	GLC	J	3	2	11,11,12	0.85	0	15,15,17	1.15	0
2	GLC	J	4	2	11,11,12	0.50	0	15,15,17	0.69	0
2	GLC	J	5	2	11,11,12	0.73	0	15,15,17	1.22	2 (13%)
2	GLC	K	1	2	12,12,12	0.73	0	17,17,17	1.27	2 (11%)
2	GLC	K	2	2	11,11,12	0.87	0	15,15,17	1.37	3 (20%)
2	GLC	K	3	2	11,11,12	0.55	0	15,15,17	1.49	3 (20%)
2	GLC	K	4	2	11,11,12	0.55	0	15,15,17	1.51	2 (13%)
2	GLC	K	5	2	11,11,12	0.67	0	15,15,17	1.20	1 (6%)
3	GLC	L	1	3	12,12,12	0.37	0	17,17,17	1.12	0
3	GLC	L	2	3	11,11,12	0.91	1 (9%)	15,15,17	1.50	2 (13%)
3	GLC	L	3	3	11,11,12	0.66	0	15,15,17	0.78	0
3	GLC	M	1	3	12,12,12	0.66	0	17,17,17	1.21	2 (11%)
3	GLC	M	2	3	11,11,12	0.28	0	15,15,17	1.11	1 (6%)
3	GLC	M	3	3	11,11,12	0.48	0	15,15,17	0.99	1 (6%)
4	GLC	N	1	4	12,12,12	0.77	0	17,17,17	1.14	2 (11%)
4	GLC	N	2	4	11,11,12	0.61	0	15,15,17	1.44	3 (20%)
4	GLC	N	3	4	11,11,12	0.69	0	15,15,17	0.93	1 (6%)
4	GLC	N	4	4	11,11,12	0.50	0	15,15,17	1.31	2 (13%)
5	GLC	O	1	5	12,12,12	0.94	0	17,17,17	1.17	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GLC	O	2	5	11,11,12	0.83	1 (9%)	15,15,17	1.54	3 (20%)
5	GLC	O	3	5	11,11,12	0.97	1 (9%)	15,15,17	1.20	0
5	GLC	O	4	5	11,11,12	0.84	0	15,15,17	1.76	2 (13%)
5	GLC	O	5	5	11,11,12	0.91	0	15,15,17	1.56	3 (20%)
5	GLC	O	6	5	11,11,12	0.47	0	15,15,17	1.88	5 (33%)
5	GLC	O	7	5	11,11,12	1.32	2 (18%)	15,15,17	1.75	3 (20%)
6	GLC	P	1	6	12,12,12	0.70	0	17,17,17	2.20	5 (29%)
6	GLC	P	2	6	11,11,12	0.89	1 (9%)	15,15,17	1.24	2 (13%)
6	GLC	P	3	6	11,11,12	0.92	0	15,15,17	1.90	7 (46%)
6	GLC	P	4	6	11,11,12	0.63	0	15,15,17	1.52	2 (13%)
6	GLC	P	5	6	11,11,12	1.02	0	15,15,17	1.57	3 (20%)
6	GLC	P	6	6	11,11,12	0.59	0	15,15,17	1.34	2 (13%)
6	GLC	P	7	6	11,11,12	0.85	0	15,15,17	1.93	4 (26%)
7	GLC	Q	1	7	12,12,12	0.77	0	17,17,17	1.78	3 (17%)
7	GLC	Q	2	7	11,11,12	0.45	0	15,15,17	0.71	0
7	GLC	Q	3	7	11,11,12	0.92	0	15,15,17	1.84	4 (26%)
7	GLC	Q	4	7	11,11,12	0.83	0	15,15,17	1.51	3 (20%)
7	GLC	Q	5	7	11,11,12	1.30	1 (9%)	15,15,17	1.19	1 (6%)
7	GLC	Q	6	7	11,11,12	0.92	1 (9%)	15,15,17	1.95	2 (13%)
8	GLC	R	1	8	12,12,12	0.73	0	17,17,17	0.72	0
8	GLC	R	2	8	11,11,12	0.81	0	15,15,17	1.15	0
8	GLC	R	3	8	11,11,12	0.55	0	15,15,17	1.76	3 (20%)
8	GLC	R	4	8	11,11,12	0.97	0	15,15,17	1.17	1 (6%)
8	GLC	R	5	8	11,11,12	1.39	2 (18%)	15,15,17	1.63	4 (26%)

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	G	1	2	-	2/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	G	3	2	-	0/2/19/22	0/1/1/1
2	GLC	G	4	2	-	0/2/19/22	0/1/1/1
2	GLC	G	5	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	H	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	3	2	-	0/2/19/22	0/1/1/1
2	GLC	H	4	2	-	0/2/19/22	0/1/1/1
2	GLC	H	5	2	-	0/2/19/22	0/1/1/1
2	GLC	I	1	2	-	0/2/22/22	0/1/1/1
2	GLC	I	2	2	-	0/2/19/22	0/1/1/1
2	GLC	I	3	2	-	0/2/19/22	0/1/1/1
2	GLC	I	4	2	-	0/2/19/22	0/1/1/1
2	GLC	I	5	2	-	0/2/19/22	0/1/1/1
2	GLC	J	1	2	-	2/2/22/22	0/1/1/1
2	GLC	J	2	2	-	0/2/19/22	0/1/1/1
2	GLC	J	3	2	-	0/2/19/22	0/1/1/1
2	GLC	J	4	2	-	0/2/19/22	0/1/1/1
2	GLC	J	5	2	-	2/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	2/2/19/22	0/1/1/1
2	GLC	K	3	2	-	0/2/19/22	0/1/1/1
2	GLC	K	4	2	-	0/2/19/22	0/1/1/1
2	GLC	K	5	2	-	2/2/19/22	0/1/1/1
3	GLC	L	1	3	-	2/2/22/22	0/1/1/1
3	GLC	L	2	3	-	0/2/19/22	0/1/1/1
3	GLC	L	3	3	-	0/2/19/22	0/1/1/1
3	GLC	M	1	3	-	2/2/22/22	0/1/1/1
3	GLC	M	2	3	-	0/2/19/22	0/1/1/1
3	GLC	M	3	3	-	0/2/19/22	0/1/1/1
4	GLC	N	1	4	-	0/2/22/22	0/1/1/1
4	GLC	N	2	4	-	0/2/19/22	0/1/1/1
4	GLC	N	3	4	-	2/2/19/22	0/1/1/1
4	GLC	N	4	4	-	0/2/19/22	0/1/1/1
5	GLC	O	1	5	-	0/2/22/22	0/1/1/1
5	GLC	O	2	5	-	0/2/19/22	0/1/1/1
5	GLC	O	3	5	-	0/2/19/22	0/1/1/1
5	GLC	O	4	5	-	2/2/19/22	0/1/1/1
5	GLC	O	5	5	-	0/2/19/22	0/1/1/1
5	GLC	O	6	5	-	2/2/19/22	0/1/1/1
5	GLC	O	7	5	-	0/2/19/22	0/1/1/1
6	GLC	P	1	6	-	2/2/22/22	0/1/1/1
6	GLC	P	2	6	-	0/2/19/22	0/1/1/1
6	GLC	P	3	6	-	2/2/19/22	0/1/1/1
6	GLC	P	4	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GLC	P	5	6	-	0/2/19/22	0/1/1/1
6	GLC	P	6	6	-	2/2/19/22	0/1/1/1
6	GLC	P	7	6	-	2/2/19/22	0/1/1/1
7	GLC	Q	1	7	-	2/2/22/22	0/1/1/1
7	GLC	Q	2	7	-	0/2/19/22	0/1/1/1
7	GLC	Q	3	7	-	1/2/19/22	0/1/1/1
7	GLC	Q	4	7	-	0/2/19/22	0/1/1/1
7	GLC	Q	5	7	-	0/2/19/22	0/1/1/1
7	GLC	Q	6	7	-	0/2/19/22	0/1/1/1
8	GLC	R	1	8	-	0/2/22/22	0/1/1/1
8	GLC	R	2	8	-	1/2/19/22	0/1/1/1
8	GLC	R	3	8	-	1/2/19/22	0/1/1/1
8	GLC	R	4	8	-	0/2/19/22	0/1/1/1
8	GLC	R	5	8	-	0/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	2	GLC	O5-C1	-2.41	1.39	1.43
5	O	7	GLC	O5-C5	2.32	1.48	1.43
7	Q	5	GLC	C2-C3	2.31	1.56	1.52
2	H	5	GLC	O5-C5	2.14	1.47	1.43
8	R	5	GLC	C2-C3	2.08	1.55	1.52
5	O	7	GLC	C4-C5	2.07	1.57	1.53
8	R	5	GLC	O5-C1	2.07	1.47	1.43
5	O	2	GLC	C2-C3	2.07	1.55	1.52
7	Q	6	GLC	C2-C3	2.05	1.55	1.52
6	P	2	GLC	O5-C1	-2.03	1.40	1.43
5	O	3	GLC	O2-C2	2.02	1.47	1.43

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	6	GLC	C1-O5-C5	6.02	120.25	112.19
7	Q	3	GLC	C1-O5-C5	4.54	118.27	112.19
6	P	1	GLC	C1-O5-C5	4.53	122.42	113.65
6	P	1	GLC	O1-C1-C2	4.50	122.05	108.98
2	G	1	GLC	C1-O5-C5	4.42	122.20	113.65
8	R	3	GLC	C1-O5-C5	4.21	117.82	112.19
6	P	7	GLC	O5-C5-C6	4.17	115.78	107.66
2	K	4	GLC	C1-O5-C5	4.12	117.70	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	R	5	GLC	C1-O5-C5	4.09	117.67	112.19
6	P	5	GLC	C1-O5-C5	4.06	117.63	112.19
7	Q	1	GLC	O5-C5-C4	3.95	116.82	109.70
2	G	5	GLC	C1-O5-C5	3.94	117.47	112.19
5	O	4	GLC	C1-O5-C5	3.92	117.43	112.19
2	I	1	GLC	C1-O5-C5	3.84	121.08	113.65
6	P	3	GLC	C1-O5-C5	3.80	117.28	112.19
6	P	4	GLC	O3-C3-C2	-3.69	102.52	110.05
6	P	1	GLC	O5-C5-C4	3.64	116.25	109.70
3	L	2	GLC	C1-O5-C5	3.59	116.99	112.19
4	N	4	GLC	C1-O5-C5	3.53	116.91	112.19
7	Q	4	GLC	O5-C1-C2	-3.46	102.53	110.79
6	P	6	GLC	C1-O5-C5	3.40	116.74	112.19
2	H	5	GLC	C1-O5-C5	3.38	116.71	112.19
5	O	7	GLC	O2-C2-C3	3.37	117.13	110.15
5	O	7	GLC	O2-C2-C1	3.33	116.85	109.22
7	Q	1	GLC	C1-O5-C5	3.23	119.91	113.65
5	O	6	GLC	C2-C3-C4	-3.20	105.23	110.86
2	H	5	GLC	O5-C5-C4	3.20	118.61	110.83
2	H	5	GLC	O4-C4-C5	3.16	117.11	109.32
4	N	2	GLC	C1-O5-C5	-3.16	107.95	112.19
2	J	1	GLC	C1-O5-C5	3.15	119.75	113.65
5	O	2	GLC	O5-C5-C6	3.13	113.76	107.66
5	O	6	GLC	O2-C2-C1	3.12	116.37	109.22
7	Q	5	GLC	C1-O5-C5	3.12	116.36	112.19
5	O	6	GLC	C1-C2-C3	-3.11	105.12	109.64
2	G	1	GLC	O6-C6-C5	3.07	121.79	111.33
2	H	1	GLC	C1-O5-C5	3.06	119.57	113.65
2	H	5	GLC	O2-C2-C3	-3.02	103.89	110.15
5	O	4	GLC	C3-C4-C5	3.01	115.70	110.23
6	P	7	GLC	C1-C2-C3	3.01	114.03	109.64
2	K	2	GLC	C2-C3-C4	-2.99	105.61	110.86
2	I	4	GLC	C1-O5-C5	2.98	116.17	112.19
3	M	1	GLC	O5-C1-C2	-2.95	105.11	110.30
5	O	6	GLC	O5-C1-C2	-2.90	103.87	110.79
2	J	2	GLC	O2-C2-C3	-2.90	104.14	110.15
2	I	1	GLC	O2-C2-C1	-2.86	102.65	109.25
2	I	1	GLC	O4-C4-C3	-2.81	103.75	110.38
6	P	4	GLC	O2-C2-C3	-2.80	104.34	110.15
2	H	5	GLC	C1-C2-C3	2.78	113.70	109.64
5	O	5	GLC	C1-O5-C5	2.78	115.91	112.19
5	O	1	GLC	C1-C2-C3	2.78	116.02	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1	GLC	O4-C4-C3	-2.75	103.89	110.38
2	H	1	GLC	O6-C6-C5	2.75	120.68	111.33
3	M	1	GLC	O1-C1-C2	2.74	116.94	108.98
6	P	7	GLC	O5-C5-C4	-2.73	104.18	110.83
6	P	7	GLC	O3-C3-C2	-2.72	104.51	110.05
2	J	2	GLC	O5-C5-C6	2.70	112.92	107.66
6	P	3	GLC	C3-C4-C5	2.69	115.11	110.23
4	N	1	GLC	O1-C1-C2	2.66	116.71	108.98
4	N	2	GLC	C6-C5-C4	2.66	119.56	113.02
2	H	2	GLC	C2-C3-C4	-2.66	106.19	110.86
7	Q	1	GLC	C6-C5-C4	-2.66	106.50	113.02
5	O	2	GLC	O2-C2-C3	-2.65	104.66	110.15
8	R	4	GLC	C1-O5-C5	2.64	115.72	112.19
2	J	2	GLC	O6-C6-C5	-2.63	102.38	111.33
8	R	5	GLC	O3-C3-C2	2.61	115.39	110.05
8	R	5	GLC	O2-C2-C3	2.60	115.54	110.15
6	P	3	GLC	O2-C2-C3	2.60	115.53	110.15
2	K	2	GLC	O5-C5-C6	-2.58	102.64	107.66
7	Q	4	GLC	O3-C3-C2	-2.58	104.79	110.05
7	Q	3	GLC	O2-C2-C3	2.58	115.49	110.15
6	P	1	GLC	O5-C1-C2	-2.56	105.80	110.30
4	N	3	GLC	C1-O5-C5	2.54	115.59	112.19
2	K	1	GLC	O5-C5-C4	2.54	114.28	109.70
7	Q	3	GLC	C1-C2-C3	-2.53	105.97	109.64
6	P	6	GLC	C3-C4-C5	2.52	114.80	110.23
2	G	2	GLC	C1-O5-C5	2.52	115.56	112.19
6	P	1	GLC	O6-C6-C5	-2.47	102.92	111.33
6	P	3	GLC	C1-C2-C3	-2.46	106.06	109.64
5	O	5	GLC	O3-C3-C2	-2.45	105.05	110.05
2	K	3	GLC	C6-C5-C4	-2.42	107.08	113.02
7	Q	3	GLC	O2-C2-C1	2.41	114.73	109.22
8	R	3	GLC	O5-C1-C2	-2.39	105.09	110.79
2	K	3	GLC	O3-C3-C4	-2.39	104.75	110.38
4	N	2	GLC	O4-C4-C3	-2.38	104.77	110.38
2	G	1	GLC	O4-C4-C3	-2.37	104.78	110.38
2	J	5	GLC	C2-C3-C4	-2.36	106.70	110.86
2	K	3	GLC	O6-C6-C5	-2.36	103.28	111.33
6	P	5	GLC	O3-C3-C2	2.36	114.87	110.05
2	G	1	GLC	C4-C3-C2	-2.36	106.69	110.83
2	G	3	GLC	C1-O5-C5	2.33	115.30	112.19
2	H	1	GLC	O5-C5-C6	2.31	112.16	106.44
2	I	1	GLC	C3-C4-C5	2.30	114.41	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	5	GLC	C1-C2-C3	2.30	112.99	109.64
2	H	1	GLC	O4-C4-C3	-2.28	105.01	110.38
8	R	5	GLC	O4-C4-C5	2.25	114.87	109.32
6	P	5	GLC	C3-C4-C5	2.25	114.30	110.23
2	I	1	GLC	O5-C1-C2	2.24	114.24	110.30
6	P	2	GLC	C1-O5-C5	2.22	115.16	112.19
8	R	3	GLC	C1-C2-C3	-2.21	106.43	109.64
2	J	1	GLC	C4-C3-C2	-2.21	106.96	110.83
2	H	4	GLC	O5-C1-C2	-2.20	105.53	110.79
5	O	7	GLC	C1-C2-C3	-2.20	106.45	109.64
2	I	5	GLC	C1-C2-C3	2.19	112.84	109.64
7	Q	6	GLC	C1-C2-C3	2.19	112.84	109.64
2	G	2	GLC	C1-C2-C3	2.19	112.84	109.64
2	J	5	GLC	C1-O5-C5	2.19	115.12	112.19
3	M	2	GLC	C1-O5-C5	2.19	115.12	112.19
5	O	6	GLC	O5-C5-C6	2.19	111.92	107.66
2	H	5	GLC	O2-C2-C1	2.18	114.22	109.22
6	P	3	GLC	C2-C3-C4	-2.18	107.03	110.86
2	H	5	GLC	C6-C5-C4	-2.17	107.69	113.02
6	P	2	GLC	O4-C4-C3	2.17	115.49	110.38
2	K	1	GLC	O5-C1-C2	-2.16	106.50	110.30
2	G	4	GLC	O4-C4-C5	-2.14	104.05	109.32
2	H	4	GLC	O4-C4-C5	-2.13	104.07	109.32
6	P	3	GLC	O4-C4-C5	-2.11	104.12	109.32
7	Q	4	GLC	O4-C4-C3	2.10	115.33	110.38
6	P	3	GLC	O5-C1-C2	-2.10	105.79	110.79
5	O	5	GLC	O6-C6-C5	-2.09	104.22	111.33
2	K	4	GLC	O4-C4-C5	-2.07	104.24	109.32
2	H	2	GLC	C3-C4-C5	2.06	113.97	110.23
3	L	2	GLC	O2-C2-C1	-2.05	104.54	109.22
4	N	1	GLC	C4-C3-C2	-2.04	107.24	110.83
2	H	2	GLC	O4-C4-C5	-2.04	104.30	109.32
2	K	2	GLC	O5-C1-C2	-2.03	105.94	110.79
2	H	5	GLC	O6-C6-C5	-2.03	104.42	111.33
3	M	3	GLC	C1-C2-C3	-2.03	106.69	109.64
2	H	2	GLC	O5-C5-C6	2.03	111.61	107.66
4	N	4	GLC	O5-C1-C2	-2.02	105.98	110.79
2	I	2	GLC	C3-C4-C5	2.01	113.88	110.23
5	O	2	GLC	C3-C4-C5	-2.01	106.59	110.23

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	3	GLC	O5-C5-C6-O6
2	K	5	GLC	O5-C5-C6-O6
6	P	6	GLC	C4-C5-C6-O6
6	P	7	GLC	O5-C5-C6-O6
6	P	7	GLC	C4-C5-C6-O6
4	N	3	GLC	C4-C5-C6-O6
6	P	1	GLC	O5-C5-C6-O6
6	P	6	GLC	O5-C5-C6-O6
7	Q	1	GLC	C4-C5-C6-O6
2	K	5	GLC	C4-C5-C6-O6
3	M	1	GLC	O5-C5-C6-O6
6	P	1	GLC	C4-C5-C6-O6
5	O	6	GLC	O5-C5-C6-O6
3	M	1	GLC	C4-C5-C6-O6
7	Q	1	GLC	O5-C5-C6-O6
2	J	5	GLC	C4-C5-C6-O6
2	K	2	GLC	C4-C5-C6-O6
5	O	4	GLC	C4-C5-C6-O6
2	J	1	GLC	C4-C5-C6-O6
6	P	3	GLC	C4-C5-C6-O6
2	J	1	GLC	O5-C5-C6-O6
3	L	1	GLC	C4-C5-C6-O6
5	O	6	GLC	C4-C5-C6-O6
8	R	2	GLC	C4-C5-C6-O6
2	K	2	GLC	O5-C5-C6-O6
2	G	1	GLC	O5-C5-C6-O6
8	R	3	GLC	C4-C5-C6-O6
7	Q	3	GLC	C4-C5-C6-O6
5	O	4	GLC	O5-C5-C6-O6
6	P	3	GLC	O5-C5-C6-O6
2	J	5	GLC	O5-C5-C6-O6
3	L	1	GLC	O5-C5-C6-O6
2	G	1	GLC	C4-C5-C6-O6

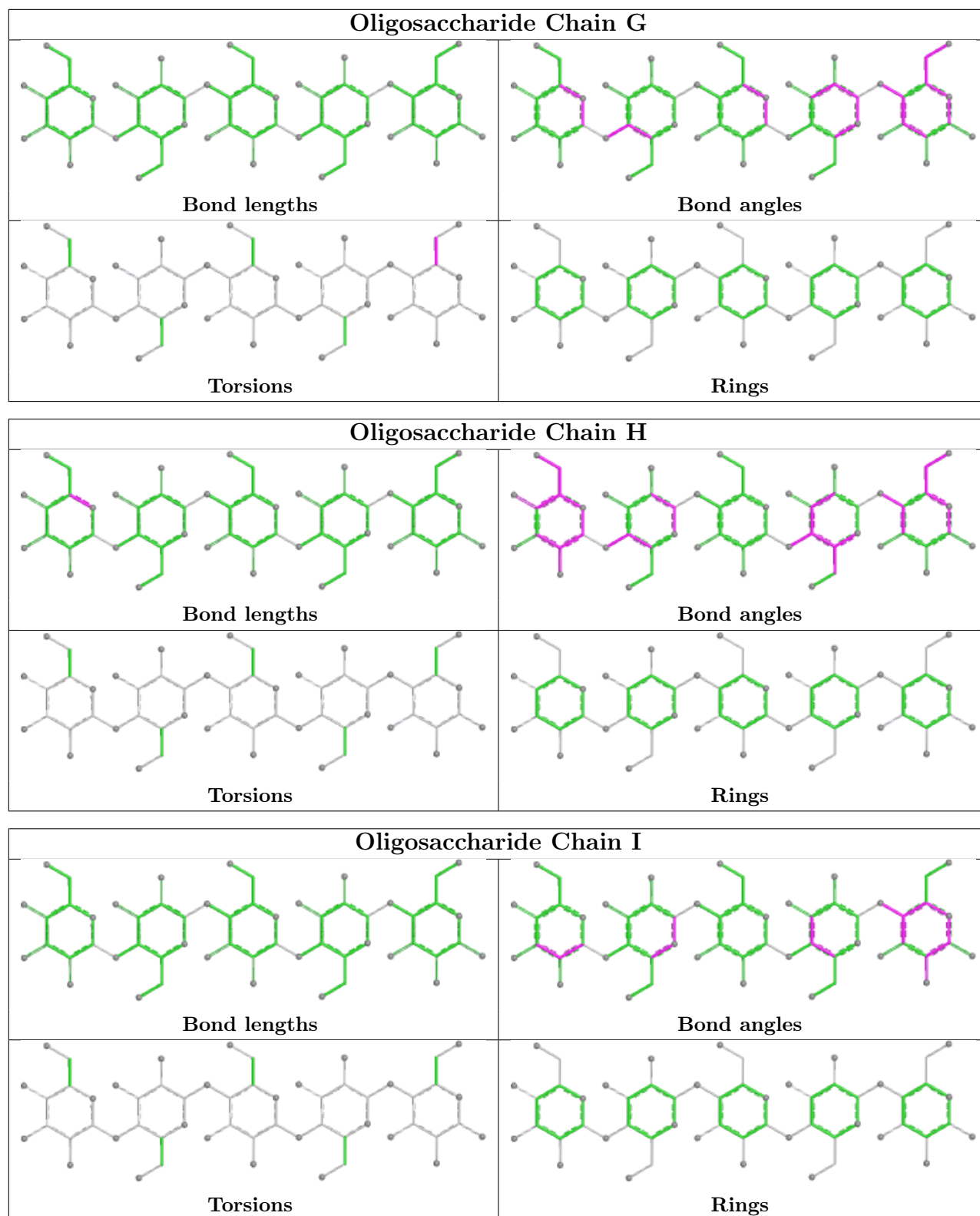
There are no ring outliers.

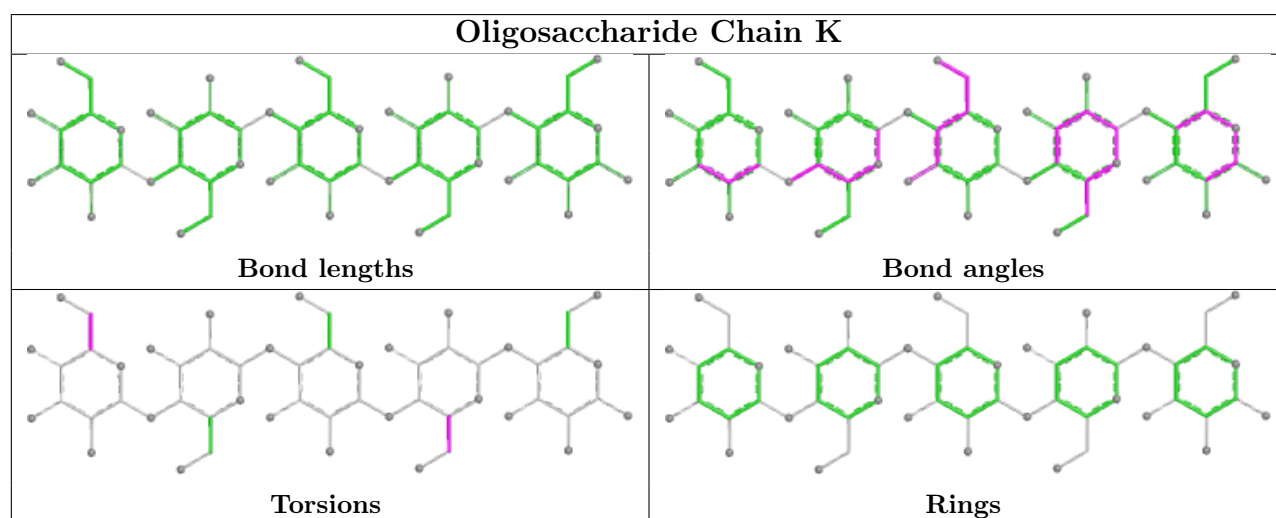
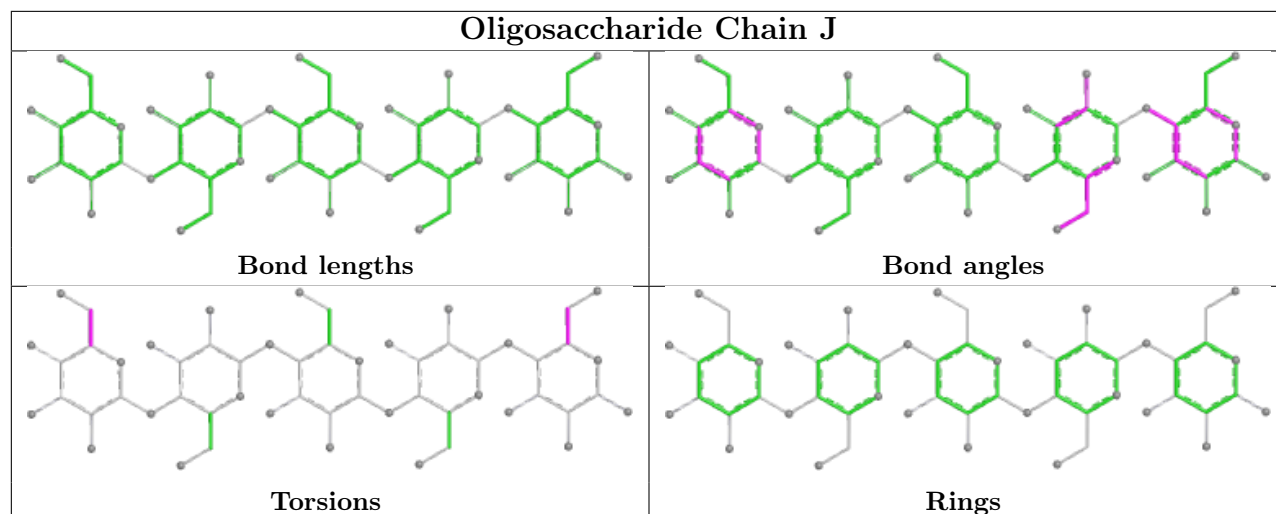
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	2	GLC	1	0
5	O	1	GLC	1	0
4	N	1	GLC	1	0

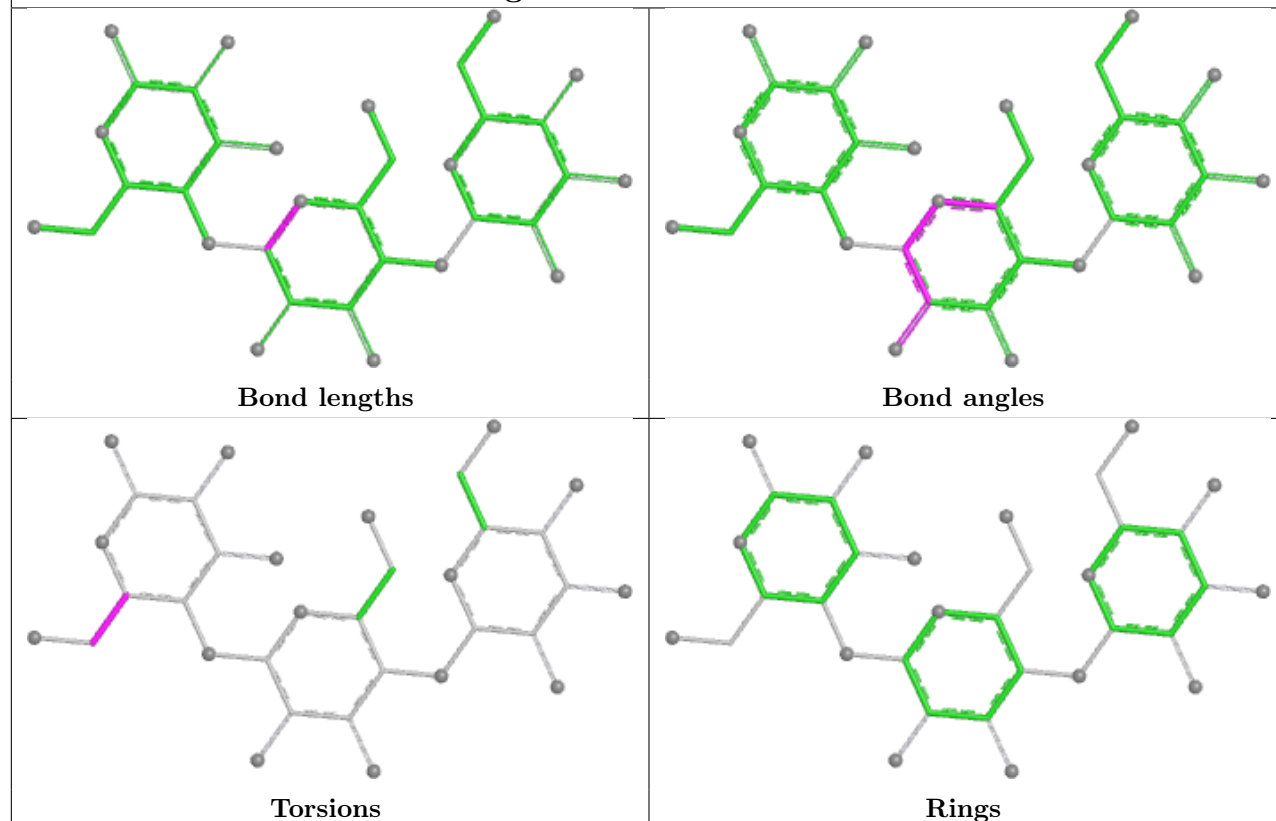
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

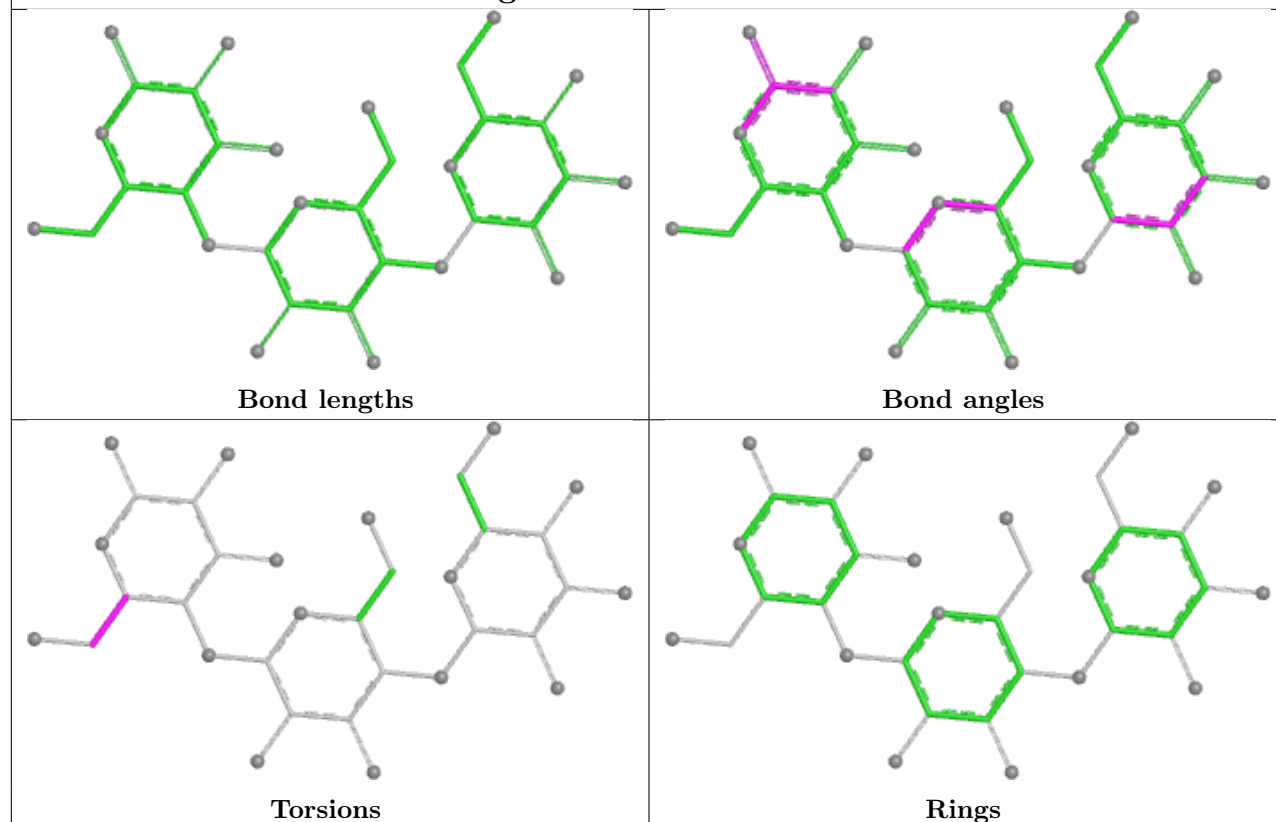


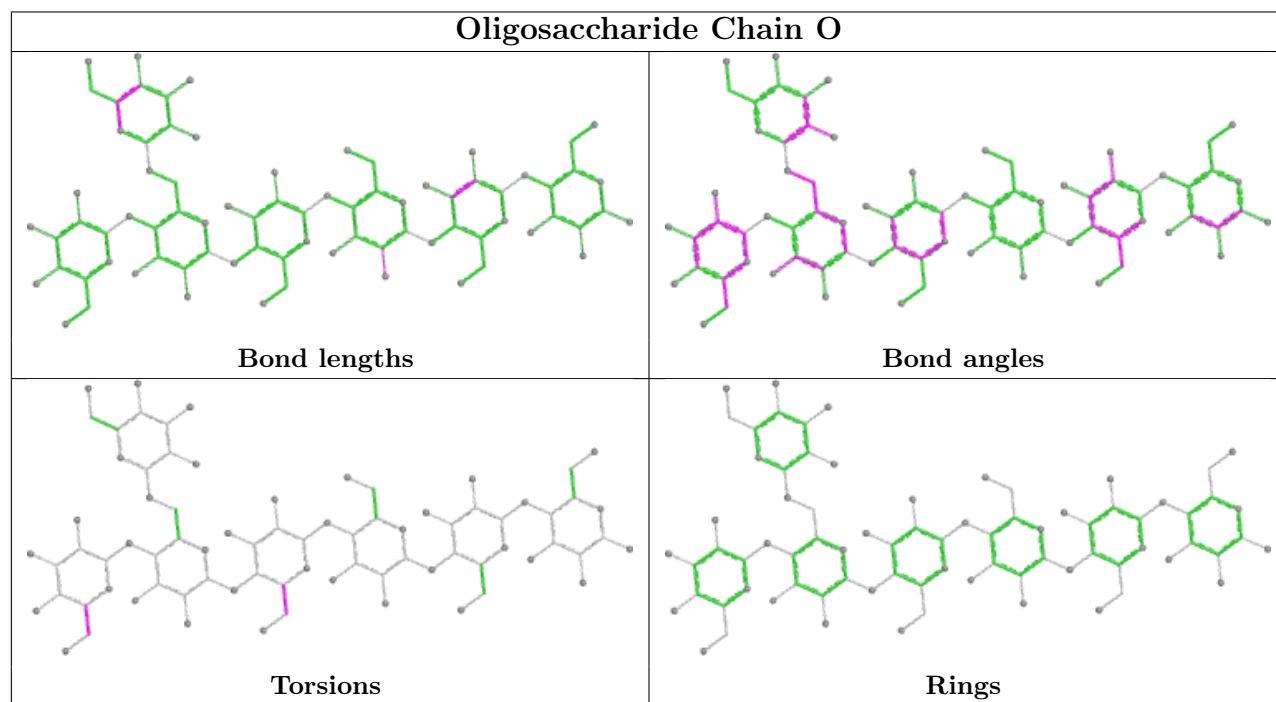
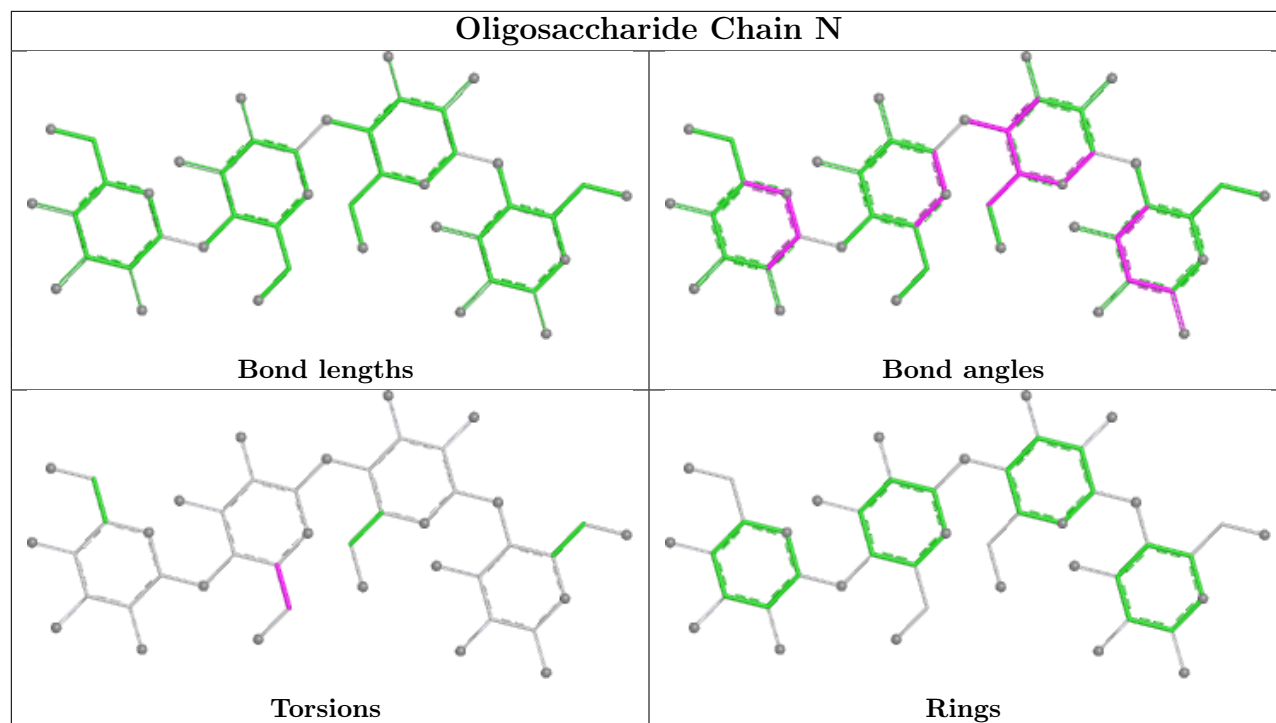


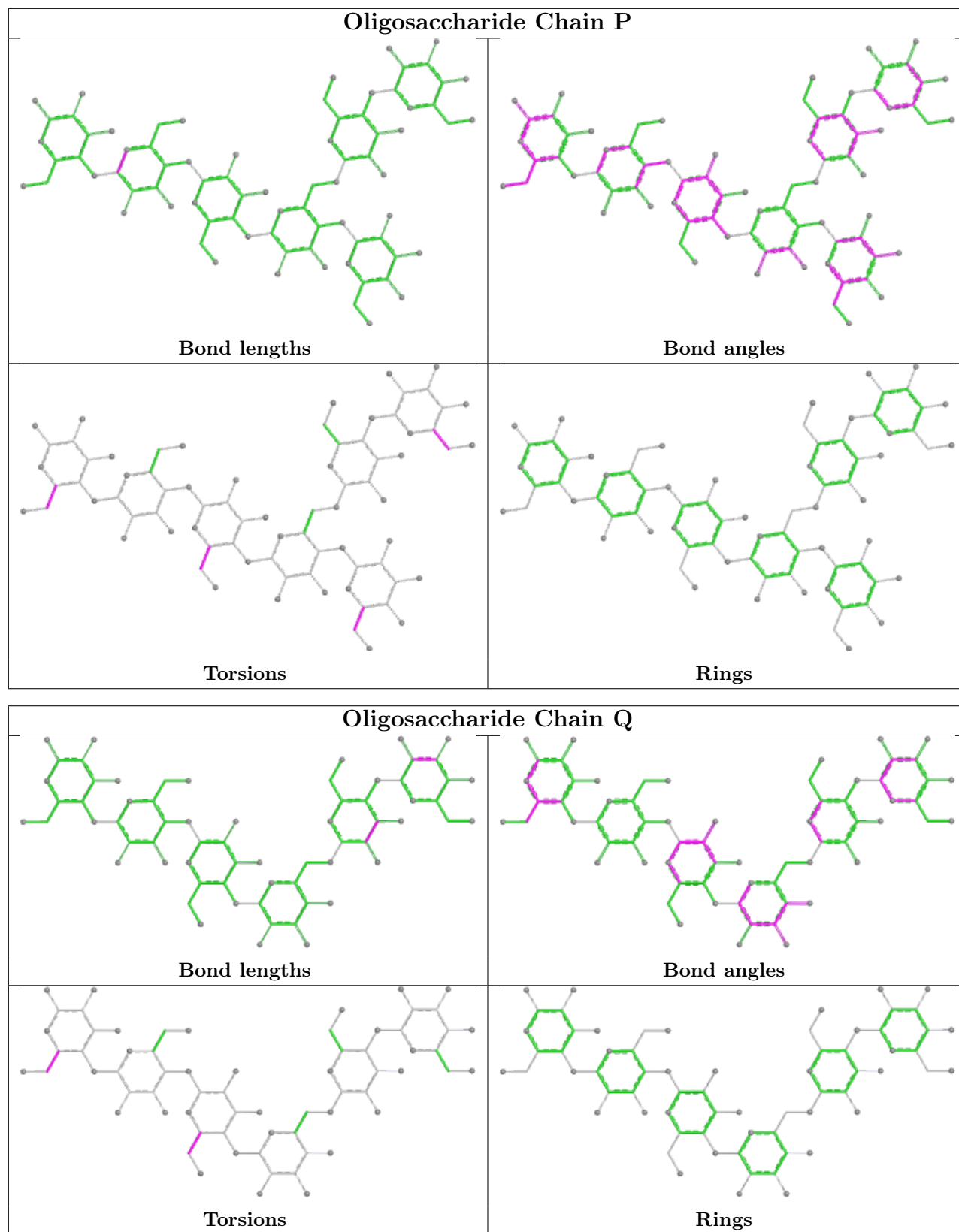
Oligosaccharide Chain L

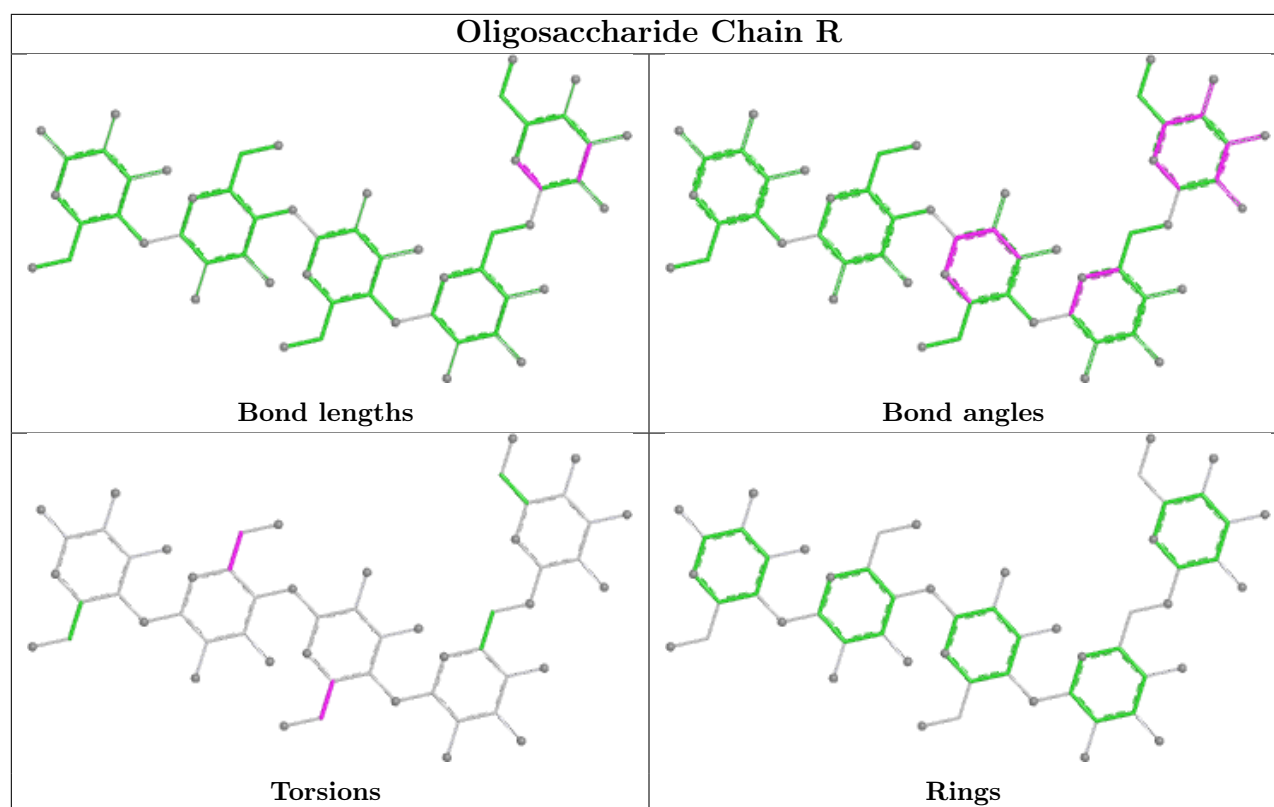


Oligosaccharide Chain M









5.6 Ligand geometry [i](#)

Of 73 ligands modelled in this entry, 10 are monoatomic - leaving 63 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	$\# Z > 2$
9	EDO	B	3312	-	3,3,3	0.13	0	2,2,2	0.23	0
9	EDO	B	3315	-	3,3,3	0.11	0	2,2,2	0.27	0
9	EDO	C	2306	-	3,3,3	0.18	0	2,2,2	0.06	0
9	EDO	A	2311	-	3,3,3	0.16	0	2,2,2	0.62	0
9	EDO	C	2311	-	3,3,3	0.07	0	2,2,2	0.13	0
9	EDO	A	2301	-	3,3,3	0.16	0	2,2,2	0.12	0
9	EDO	A	2309	-	3,3,3	0.08	0	2,2,2	0.29	0
9	EDO	C	2315	-	3,3,3	0.39	0	2,2,2	0.26	0
9	EDO	A	2307	-	3,3,3	0.04	0	2,2,2	0.14	0
9	EDO	C	2304	-	3,3,3	0.24	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	D	808	-	3,3,3	0.18	0	2,2,2	0.16	0
9	EDO	B	3308	-	3,3,3	0.06	0	2,2,2	0.50	0
9	EDO	A	2305	-	3,3,3	0.29	0	2,2,2	0.44	0
9	EDO	C	2313	-	3,3,3	0.38	0	2,2,2	0.57	0
9	EDO	C	2303	-	3,3,3	0.23	0	2,2,2	0.43	0
9	EDO	C	2317	-	3,3,3	0.20	0	2,2,2	0.13	0
9	EDO	B	3316	-	3,3,3	0.14	0	2,2,2	0.47	0
9	EDO	B	3302	-	3,3,3	0.22	0	2,2,2	0.33	0
9	EDO	D	809	-	3,3,3	0.22	0	2,2,2	0.21	0
9	EDO	A	2308	-	3,3,3	0.18	0	2,2,2	0.25	0
9	EDO	A	2316	-	3,3,3	0.58	0	2,2,2	0.61	0
9	EDO	B	3304	-	3,3,3	0.28	0	2,2,2	0.16	0
9	EDO	B	3306	-	3,3,3	0.07	0	2,2,2	0.26	0
9	EDO	A	2314	-	3,3,3	0.28	0	2,2,2	0.25	0
9	EDO	D	806	-	3,3,3	0.05	0	2,2,2	0.06	0
13	1PE	C	2301	-	15,15,15	0.34	0	14,14,14	0.35	0
9	EDO	C	2305	-	3,3,3	0.18	0	2,2,2	0.22	0
10	ACT	A	2319	-	3,3,3	1.26	0	3,3,3	0.81	0
9	EDO	C	2318	-	3,3,3	0.15	0	2,2,2	0.21	0
9	EDO	A	2321	-	3,3,3	0.11	0	2,2,2	0.23	0
9	EDO	B	3319	-	3,3,3	0.12	0	2,2,2	0.39	0
10	ACT	A	2302	-	3,3,3	1.31	0	3,3,3	0.51	0
9	EDO	B	3321	-	3,3,3	0.10	0	2,2,2	0.09	0
9	EDO	D	804	-	3,3,3	0.10	0	2,2,2	0.27	0
10	ACT	A	2320	-	3,3,3	1.11	0	3,3,3	0.69	0
9	EDO	A	2315	-	3,3,3	0.60	0	2,2,2	0.72	0
9	EDO	C	2307	-	3,3,3	0.30	0	2,2,2	0.46	0
10	ACT	D	805	-	3,3,3	0.90	0	3,3,3	1.03	0
9	EDO	B	3313	-	3,3,3	0.20	0	2,2,2	0.08	0
9	EDO	B	3314	-	3,3,3	0.30	0	2,2,2	0.41	0
16	PEG	C	2312	-	6,6,6	0.63	0	5,5,5	0.47	0
9	EDO	A	2303	-	3,3,3	0.21	0	2,2,2	0.14	0
9	EDO	D	807	-	3,3,3	0.11	0	2,2,2	0.08	0
9	EDO	B	3307	-	3,3,3	0.31	0	2,2,2	0.50	0
9	EDO	C	2319	-	3,3,3	0.12	0	2,2,2	0.14	0
9	EDO	B	3320	-	3,3,3	0.14	0	2,2,2	0.51	0
9	EDO	B	3303	-	3,3,3	0.14	0	2,2,2	0.28	0
9	EDO	B	3301	-	3,3,3	0.09	0	2,2,2	0.17	0
9	EDO	A	2317	-	3,3,3	0.10	0	2,2,2	0.14	0
9	EDO	B	3311	-	3,3,3	0.16	0	2,2,2	0.25	0
9	EDO	B	3322	-	3,3,3	0.11	0	2,2,2	0.05	0
14	PGE	C	2302	-	9,9,9	0.24	0	8,8,8	0.16	0
9	EDO	A	2323	-	3,3,3	0.16	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	A	2306	-	3,3,3	0.10	0	2,2,2	0.18	0
9	EDO	A	2310	-	3,3,3	0.23	0	2,2,2	0.10	0
9	EDO	B	3318	-	3,3,3	0.12	0	2,2,2	0.22	0
9	EDO	C	2314	-	3,3,3	0.19	0	2,2,2	0.39	0
9	EDO	C	2316	-	3,3,3	0.08	0	2,2,2	0.15	0
9	EDO	A	2318	-	3,3,3	0.13	0	2,2,2	0.23	0
9	EDO	A	2304	-	3,3,3	0.15	0	2,2,2	0.24	0
9	EDO	B	3305	-	3,3,3	0.09	0	2,2,2	0.15	0
9	EDO	B	3317	-	3,3,3	0.20	0	2,2,2	0.13	0
10	ACT	A	2322	-	3,3,3	1.08	0	3,3,3	0.84	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
9	EDO	B	3312	-	-	1/1/1/1	-
9	EDO	B	3315	-	-	0/1/1/1	-
9	EDO	C	2306	-	-	0/1/1/1	-
9	EDO	A	2311	-	-	1/1/1/1	-
9	EDO	C	2311	-	-	1/1/1/1	-
9	EDO	A	2301	-	-	1/1/1/1	-
9	EDO	A	2309	-	-	1/1/1/1	-
9	EDO	C	2315	-	-	1/1/1/1	-
9	EDO	A	2307	-	-	1/1/1/1	-
9	EDO	C	2304	-	-	0/1/1/1	-
9	EDO	D	808	-	-	1/1/1/1	-
9	EDO	B	3308	-	-	1/1/1/1	-
9	EDO	A	2305	-	-	1/1/1/1	-
9	EDO	C	2313	-	-	1/1/1/1	-
9	EDO	C	2303	-	-	1/1/1/1	-
9	EDO	C	2317	-	-	1/1/1/1	-
9	EDO	B	3316	-	-	0/1/1/1	-
9	EDO	B	3302	-	-	0/1/1/1	-
9	EDO	D	809	-	-	0/1/1/1	-
9	EDO	A	2308	-	-	1/1/1/1	-
9	EDO	A	2316	-	-	0/1/1/1	-
9	EDO	B	3304	-	-	1/1/1/1	-
9	EDO	B	3306	-	-	0/1/1/1	-
9	EDO	A	2314	-	-	0/1/1/1	-
9	EDO	D	806	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	1PE	C	2301	-	-	7/13/13/13	-
9	EDO	C	2305	-	-	1/1/1/1	-
9	EDO	C	2318	-	-	1/1/1/1	-
9	EDO	A	2321	-	-	0/1/1/1	-
9	EDO	B	3319	-	-	1/1/1/1	-
9	EDO	B	3321	-	-	1/1/1/1	-
9	EDO	D	804	-	-	0/1/1/1	-
9	EDO	A	2315	-	-	1/1/1/1	-
9	EDO	C	2307	-	-	1/1/1/1	-
9	EDO	B	3313	-	-	1/1/1/1	-
9	EDO	B	3314	-	-	1/1/1/1	-
16	PEG	C	2312	-	-	2/4/4/4	-
9	EDO	A	2303	-	-	1/1/1/1	-
9	EDO	D	807	-	-	1/1/1/1	-
9	EDO	B	3307	-	-	1/1/1/1	-
9	EDO	C	2319	-	-	1/1/1/1	-
9	EDO	B	3320	-	-	1/1/1/1	-
9	EDO	B	3303	-	-	1/1/1/1	-
9	EDO	B	3301	-	-	1/1/1/1	-
9	EDO	A	2317	-	-	0/1/1/1	-
9	EDO	B	3311	-	-	1/1/1/1	-
9	EDO	B	3322	-	-	1/1/1/1	-
14	PGE	C	2302	-	-	5/7/7/7	-
9	EDO	A	2323	-	-	0/1/1/1	-
9	EDO	A	2306	-	-	1/1/1/1	-
9	EDO	A	2310	-	-	1/1/1/1	-
9	EDO	B	3318	-	-	0/1/1/1	-
9	EDO	C	2314	-	-	1/1/1/1	-
9	EDO	C	2316	-	-	1/1/1/1	-
9	EDO	A	2318	-	-	1/1/1/1	-
9	EDO	A	2304	-	-	1/1/1/1	-
9	EDO	B	3305	-	-	1/1/1/1	-
9	EDO	B	3317	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (53) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
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Mol	Chain	Res	Type	Atoms
14	C	2302	PGE	O2-C3-C4-O3
13	C	2301	1PE	OH4-C13-C23-OH3
13	C	2301	1PE	OH5-C14-C24-OH4
16	C	2312	PEG	O1-C1-C2-O2
13	C	2301	1PE	OH7-C16-C26-OH6
14	C	2302	PGE	O1-C1-C2-O2
9	A	2304	EDO	O1-C1-C2-O2
9	A	2311	EDO	O1-C1-C2-O2
9	A	2318	EDO	O1-C1-C2-O2
9	B	3305	EDO	O1-C1-C2-O2
9	C	2313	EDO	O1-C1-C2-O2
9	A	2315	EDO	O1-C1-C2-O2
9	B	3308	EDO	O1-C1-C2-O2
9	B	3312	EDO	O1-C1-C2-O2
9	B	3313	EDO	O1-C1-C2-O2
9	B	3319	EDO	O1-C1-C2-O2
9	B	3321	EDO	O1-C1-C2-O2
9	C	2303	EDO	O1-C1-C2-O2
9	C	2307	EDO	O1-C1-C2-O2
13	C	2301	1PE	OH6-C15-C25-OH5
14	C	2302	PGE	O3-C5-C6-O4
9	A	2308	EDO	O1-C1-C2-O2
9	C	2305	EDO	O1-C1-C2-O2
9	C	2311	EDO	O1-C1-C2-O2
9	C	2318	EDO	O1-C1-C2-O2
9	A	2301	EDO	O1-C1-C2-O2
9	C	2316	EDO	O1-C1-C2-O2
13	C	2301	1PE	C16-C26-OH6-C15
13	C	2301	1PE	C23-C13-OH4-C24
14	C	2302	PGE	C1-C2-O2-C3
9	A	2306	EDO	O1-C1-C2-O2
9	B	3311	EDO	O1-C1-C2-O2
9	C	2314	EDO	O1-C1-C2-O2
9	C	2315	EDO	O1-C1-C2-O2
13	C	2301	1PE	C24-C14-OH5-C25
14	C	2302	PGE	C3-C4-O3-C5
9	A	2305	EDO	O1-C1-C2-O2
9	B	3301	EDO	O1-C1-C2-O2
9	D	808	EDO	O1-C1-C2-O2
9	A	2303	EDO	O1-C1-C2-O2
9	B	3322	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
9	C	2319	EDO	O1-C1-C2-O2
9	D	807	EDO	O1-C1-C2-O2
9	A	2307	EDO	O1-C1-C2-O2
9	A	2309	EDO	O1-C1-C2-O2
9	B	3303	EDO	O1-C1-C2-O2
9	B	3314	EDO	O1-C1-C2-O2
9	C	2317	EDO	O1-C1-C2-O2
9	A	2310	EDO	O1-C1-C2-O2
9	B	3304	EDO	O1-C1-C2-O2
9	B	3320	EDO	O1-C1-C2-O2
9	B	3307	EDO	O1-C1-C2-O2
16	C	2312	PEG	O2-C3-C4-O4

There are no ring outliers.

15 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	2315	EDO	2	0
9	B	3316	EDO	3	0
9	A	2316	EDO	5	0
9	B	3304	EDO	2	0
13	C	2301	1PE	19	0
9	C	2318	EDO	2	0
9	D	804	EDO	2	0
9	A	2315	EDO	2	0
10	D	805	ACT	2	0
9	B	3313	EDO	1	0
16	C	2312	PEG	2	0
9	B	3307	EDO	3	0
9	B	3320	EDO	1	0
14	C	2302	PGE	1	0
9	C	2314	EDO	2	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	713/738 (96%)	-0.32	13 (1%) 67 70	10, 19, 43, 62	1 (0%)
1	B	708/738 (95%)	-0.07	14 (1%) 65 67	11, 22, 48, 64	2 (0%)
1	C	712/738 (96%)	0.05	26 (3%) 45 47	11, 26, 52, 84	0
1	D	706/738 (95%)	0.37	35 (4%) 34 36	18, 34, 59, 80	1 (0%)
All	All	2839/2952 (96%)	0.01	88 (3%) 51 54	10, 25, 51, 84	4 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	737	VAL	5.3
1	B	735	ASN	5.2
1	D	737	VAL	5.0
1	A	167	TRP	5.0
1	D	167	TRP	4.9
1	A	740	GLU	4.7
1	D	45	VAL	4.7
1	A	739	GLY	4.4
1	D	165	PHE	4.3
1	C	757	ALA	4.1
1	D	734	GLY	3.8
1	A	304	ALA	3.8
1	B	167	TRP	3.7
1	D	757	ALA	3.7
1	B	304	ALA	3.7
1	C	722	ILE	3.6
1	A	45	VAL	3.5
1	B	740	GLU	3.5
1	A	734	GLY	3.3
1	C	743	ILE	3.3
1	C	721	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	742	LYS	3.1
1	C	113	ASN	3.0
1	D	735	ASN	3.0
1	C	592	TYR	3.0
1	B	165	PHE	3.0
1	D	741	LYS	2.9
1	D	177	ILE	2.9
1	D	245	ALA	2.9
1	C	718	ILE	2.8
1	B	244	THR	2.7
1	D	175	LEU	2.7
1	B	164	GLY	2.7
1	C	726	THR	2.6
1	D	736	PRO	2.6
1	C	112	ASP	2.6
1	C	720	TYR	2.6
1	D	726	THR	2.6
1	C	745	VAL	2.5
1	C	736	PRO	2.5
1	A	74	ASN	2.5
1	D	216	PHE	2.5
1	D	46	LEU	2.4
1	C	167	TRP	2.4
1	B	736	PRO	2.4
1	D	63	LEU	2.4
1	D	180	GLU	2.4
1	D	130	ALA	2.3
1	D	678	ALA	2.3
1	B	739	GLY	2.3
1	B	166	ILE	2.3
1	D	121	SER	2.3
1	D	56	ILE	2.3
1	D	123	ILE	2.3
1	C	304	ALA	2.3
1	B	294	SER	2.3
1	A	737	VAL	2.3
1	D	176	PRO	2.3
1	B	174	PRO	2.2
1	D	740	GLU	2.2
1	A	120	SER	2.2
1	D	132	SER	2.2
1	D	295	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	702	VAL	2.2
1	C	719	ASP	2.2
1	A	47	HIS	2.2
1	B	178	SER	2.2
1	D	120	SER	2.2
1	C	716	ALA	2.2
1	C	569	ARG	2.2
1	D	166	ILE	2.1
1	A	305	GLY	2.1
1	D	246	GLY	2.1
1	A	757	ALA	2.1
1	C	728	TYR	2.1
1	C	171	GLN	2.1
1	C	45	VAL	2.1
1	D	178	SER	2.1
1	D	88	THR	2.1
1	A	246	GLY	2.1
1	D	131	PRO	2.0
1	C	740	GLU	2.0
1	C	678	ALA	2.0
1	C	727	TRP	2.0
1	D	173	ALA	2.0
1	B	112	ASP	2.0
1	C	741	LYS	2.0
1	D	172	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	I	1	12/12	0.81	0.13	29,43,53,54	0
2	GLC	H	1	12/12	0.82	0.13	21,37,41,43	0
2	GLC	K	1	12/12	0.83	0.12	35,58,63,65	0

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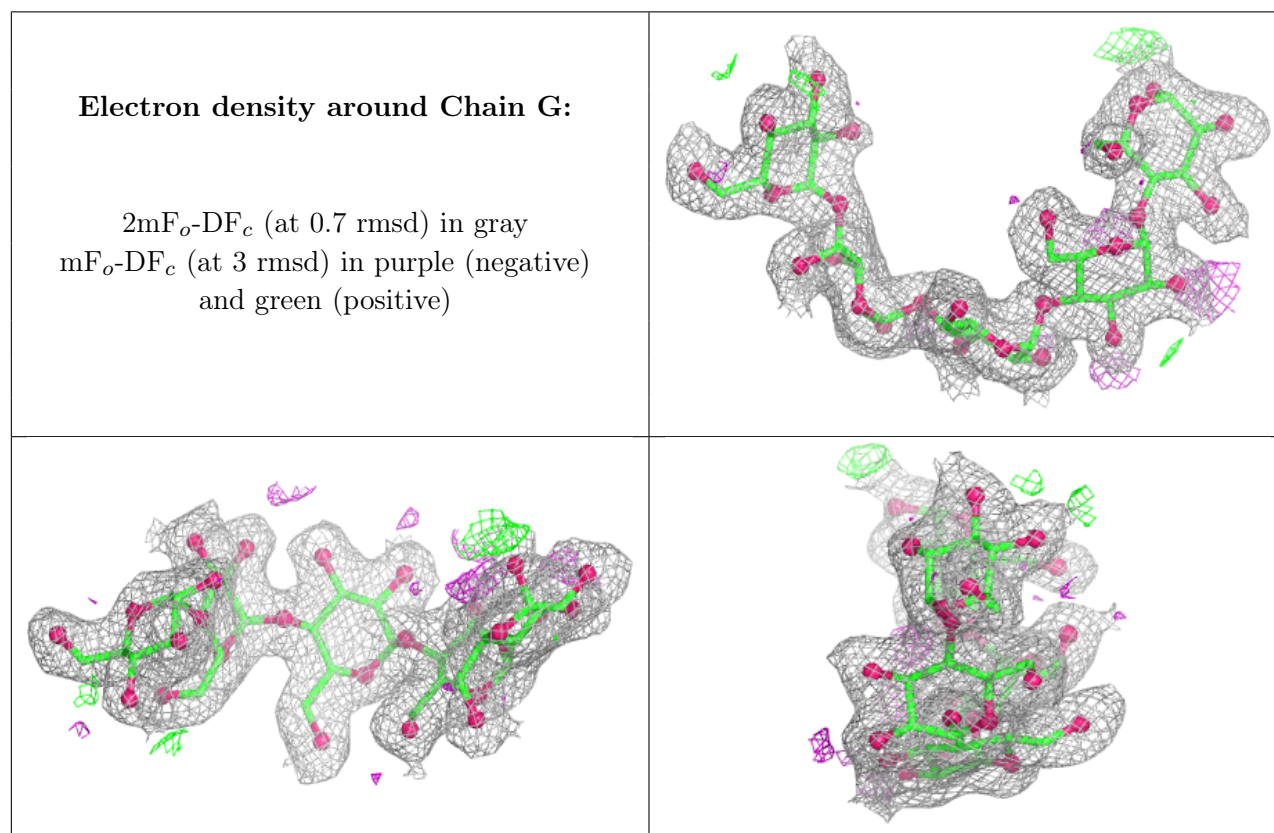
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	K	3	11/12	0.83	0.11	13,16,21,22	0
2	GLC	G	1	12/12	0.85	0.14	21,35,43,49	0
5	GLC	O	6	11/12	0.85	0.12	51,59,65,69	0
2	GLC	H	5	11/12	0.86	0.11	34,39,43,56	0
2	GLC	K	2	11/12	0.86	0.10	19,25,30,34	0
5	GLC	O	1	12/12	0.87	0.11	32,46,55,56	0
6	GLC	P	4	11/12	0.87	0.10	25,29,35,47	0
6	GLC	P	5	11/12	0.87	0.11	21,35,41,43	0
2	GLC	G	5	11/12	0.88	0.11	26,29,32,37	0
5	GLC	O	4	11/12	0.89	0.09	15,18,19,20	0
2	GLC	H	2	11/12	0.89	0.10	13,14,15,17	0
3	GLC	M	1	12/12	0.89	0.10	43,48,52,58	0
2	GLC	I	5	11/12	0.89	0.12	38,44,47,49	0
2	GLC	J	3	11/12	0.91	0.09	22,29,30,31	0
4	GLC	N	4	11/12	0.92	0.08	52,55,63,65	0
2	GLC	J	4	11/12	-	-	31,33,35,37	0
2	GLC	J	5	11/12	-	-	45,49,53,56	0
3	GLC	L	3	11/12	0.92	0.09	30,32,38,42	0
5	GLC	O	3	11/12	0.93	0.08	18,20,21,22	0
2	GLC	J	1	12/12	0.93	0.07	38,54,57,67	0
2	GLC	K	4	11/12	-	-	19,21,24,28	0
2	GLC	K	5	11/12	-	-	33,40,51,58	0
4	GLC	N	1	12/12	0.93	0.07	29,33,37,40	0
3	GLC	L	1	12/12	0.93	0.07	23,28,36,39	0
2	GLC	H	3	11/12	0.93	0.08	13,15,16,17	0
5	GLC	O	2	11/12	0.94	0.08	20,25,31,31	0
2	GLC	I	2	11/12	0.94	0.07	17,18,22,25	0
2	GLC	H	4	11/12	0.95	0.07	20,21,25,26	0
6	GLC	P	1	12/12	0.95	0.06	21,24,25,30	0
6	GLC	P	2	11/12	0.95	0.07	18,20,22,23	0
6	GLC	P	3	11/12	0.95	0.07	16,21,23,24	0
3	GLC	M	2	11/12	0.95	0.06	38,44,46,50	0
5	GLC	O	5	11/12	0.95	0.07	20,25,34,37	0
4	GLC	N	2	11/12	0.96	0.06	22,29,36,42	0
4	GLC	N	3	11/12	0.96	0.06	30,36,44,50	0
2	GLC	J	2	11/12	0.96	0.05	23,26,30,31	0
2	GLC	G	2	11/12	0.96	0.06	11,14,15,17	0
2	GLC	I	4	11/12	0.96	0.06	20,22,24,29	0
5	GLC	O	7	11/12	-	-	25,34,38,38	0
3	GLC	M	3	11/12	0.96	0.07	47,55,58,58	0
3	GLC	L	2	11/12	0.96	0.06	21,23,26,27	0
2	GLC	I	3	11/12	0.97	0.04	15,16,17,18	0

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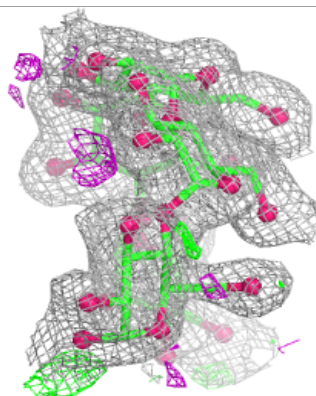
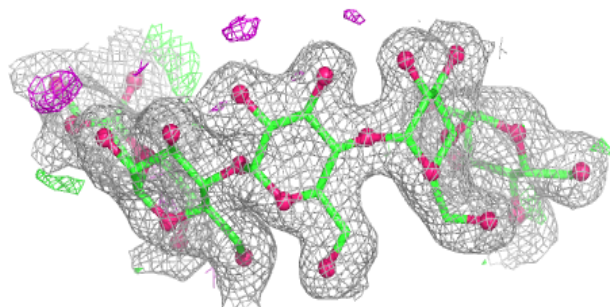
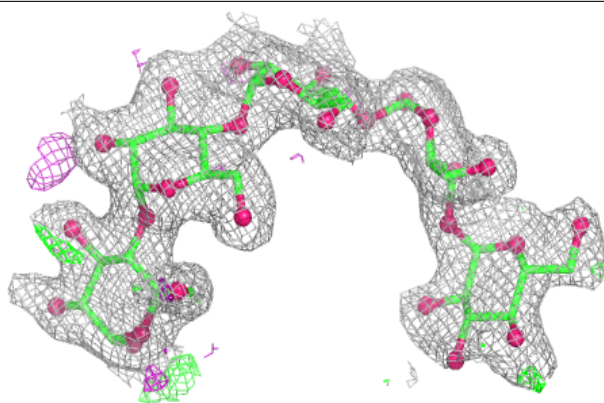
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	G	3	11/12	0.97	0.05	9,11,12,13	0
2	GLC	G	4	11/12	0.97	0.06	16,17,18,21	0
6	GLC	P	6	11/12	-	-	46,51,55,56	0
6	GLC	P	7	11/12	-	-	65,75,85,91	0
7	GLC	Q	1	12/12	-	-	33,36,43,45	0
7	GLC	Q	2	11/12	-	-	30,35,36,42	0
7	GLC	Q	3	11/12	-	-	24,29,29,32	0
7	GLC	Q	4	11/12	-	-	28,33,35,36	0
7	GLC	Q	5	11/12	-	-	25,33,38,45	0
7	GLC	Q	6	11/12	-	-	42,56,59,60	0
8	GLC	R	1	12/12	-	-	27,33,36,36	0
8	GLC	R	2	11/12	-	-	29,32,38,40	0
8	GLC	R	3	11/12	-	-	20,26,28,32	0
8	GLC	R	4	11/12	-	-	32,36,41,42	0
8	GLC	R	5	11/12	-	-	34,44,46,47	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.

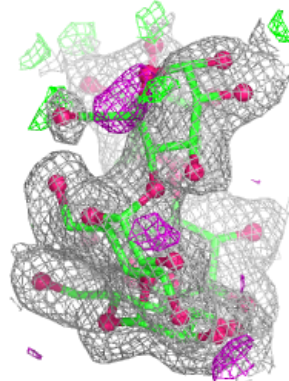
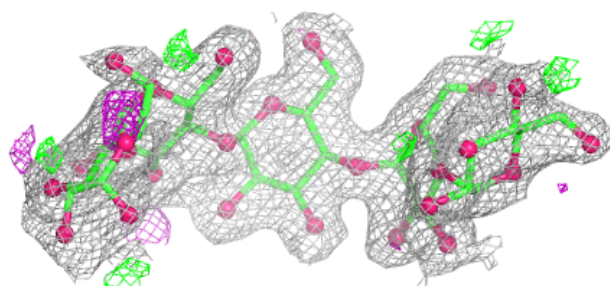
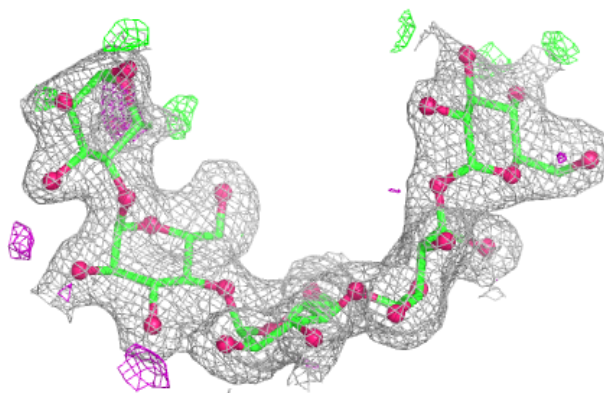


Electron density around Chain H:

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

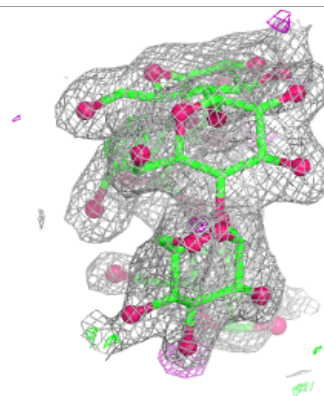
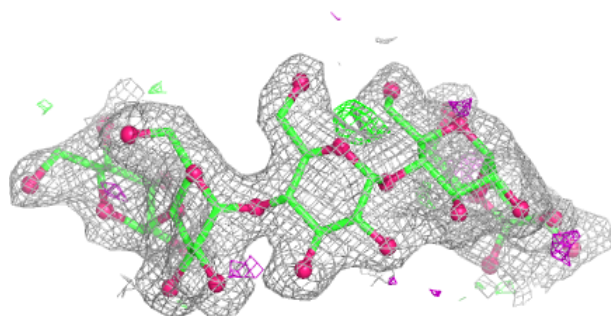
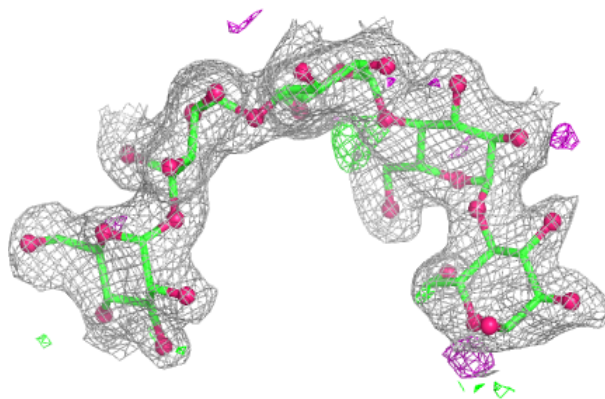
**Electron density around Chain I:**

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

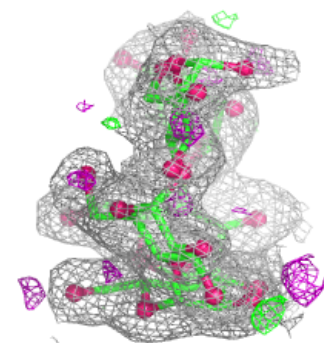
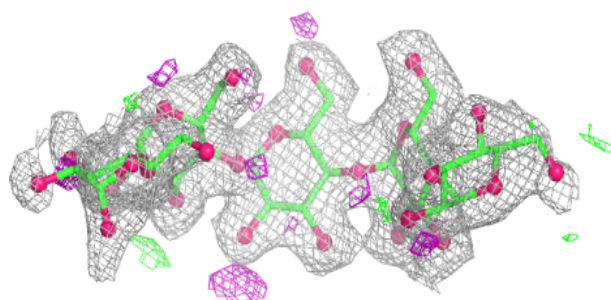
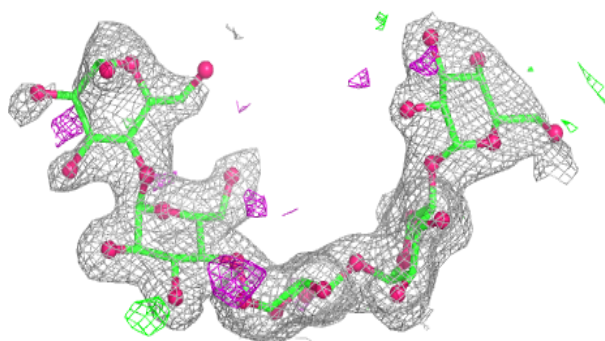


Electron density around Chain J:

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

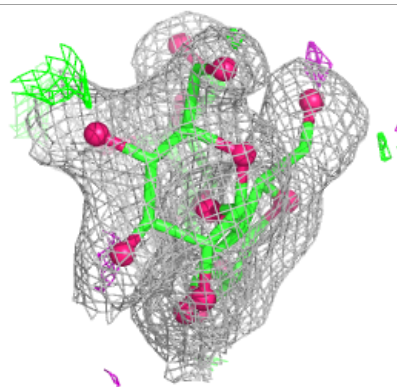
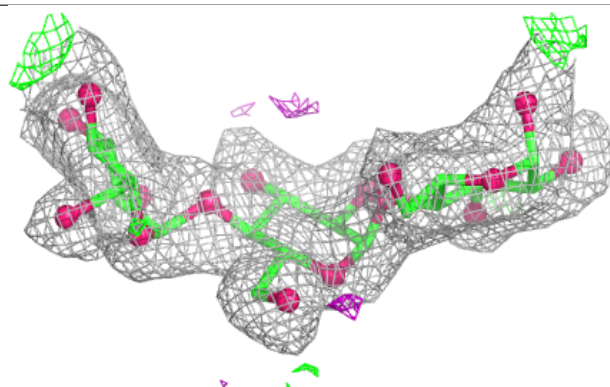
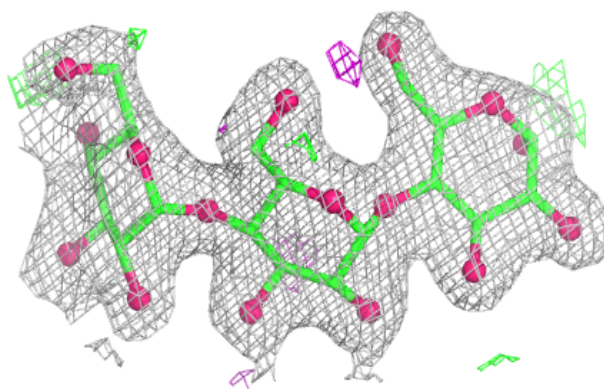
**Electron density around Chain K:**

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

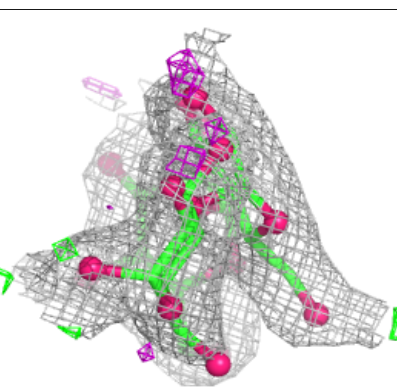
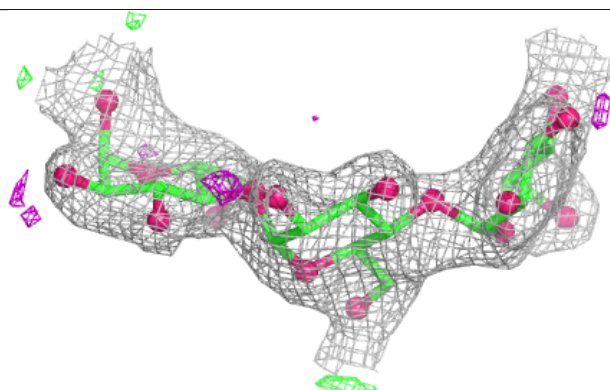
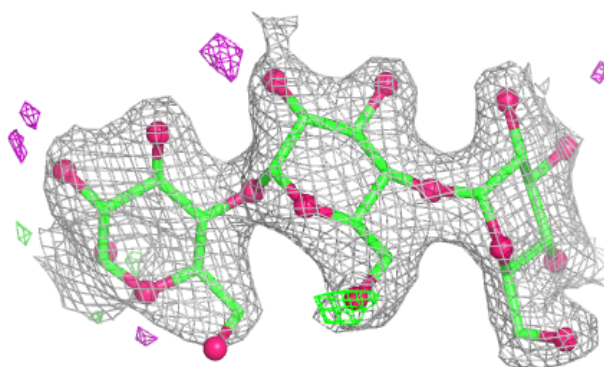


Electron density around Chain L:

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

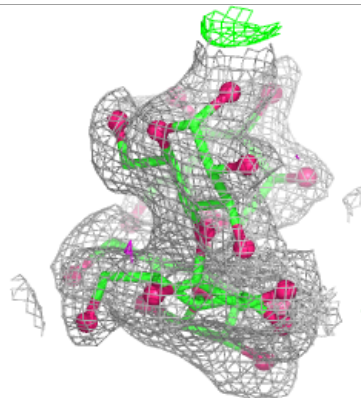
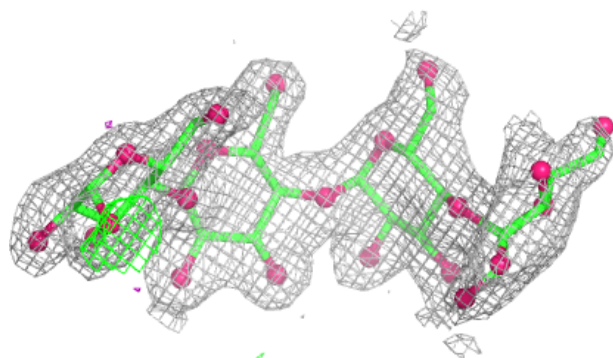
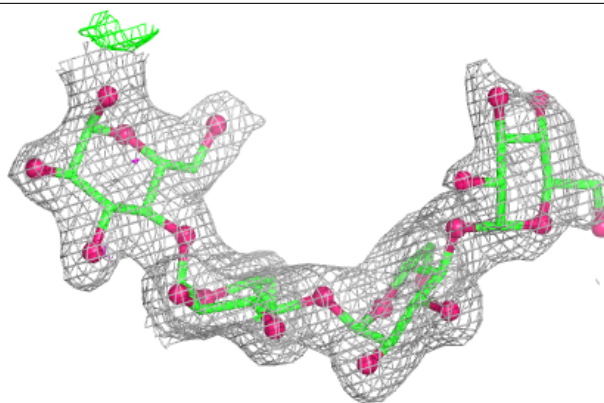
**Electron density around Chain M:**

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

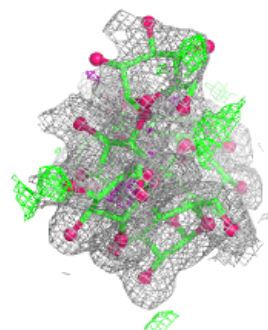
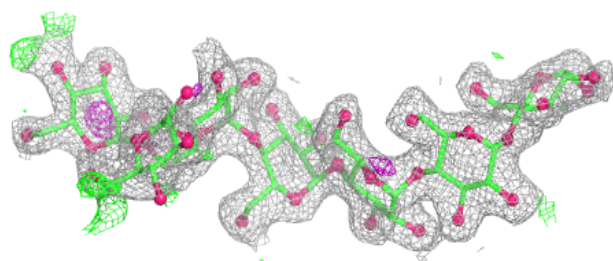
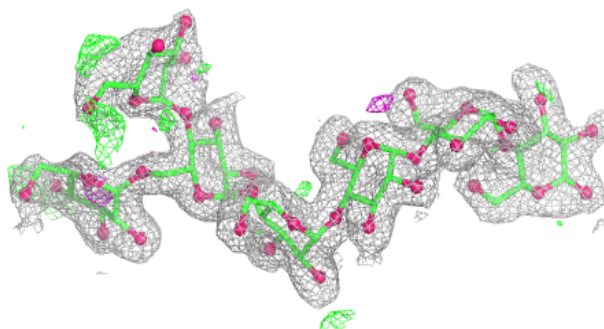


Electron density around Chain N:

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

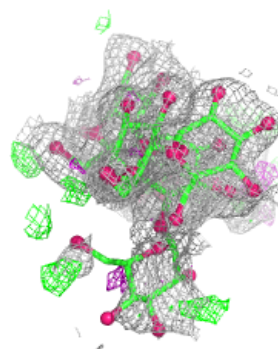
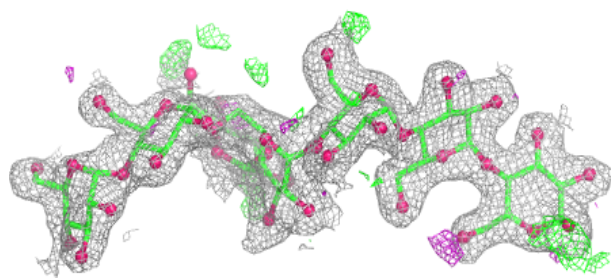
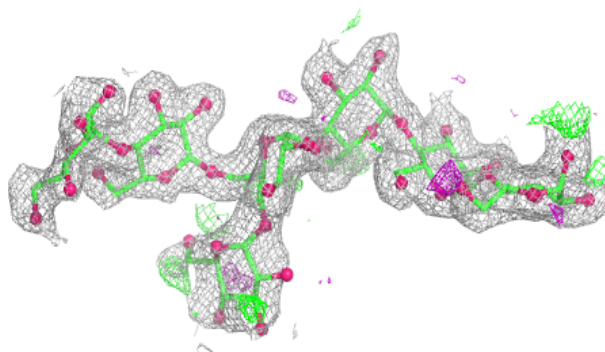
**Electron density around Chain O:**

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

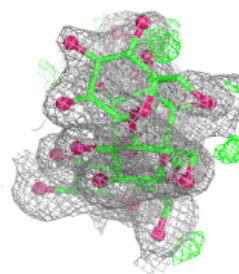
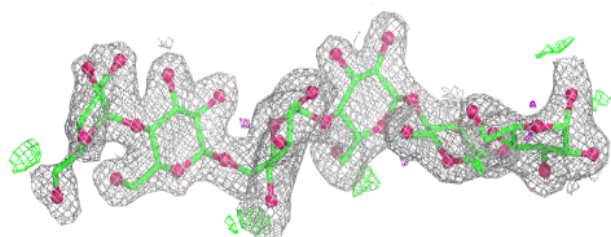
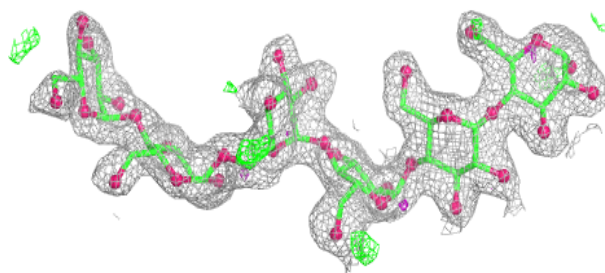


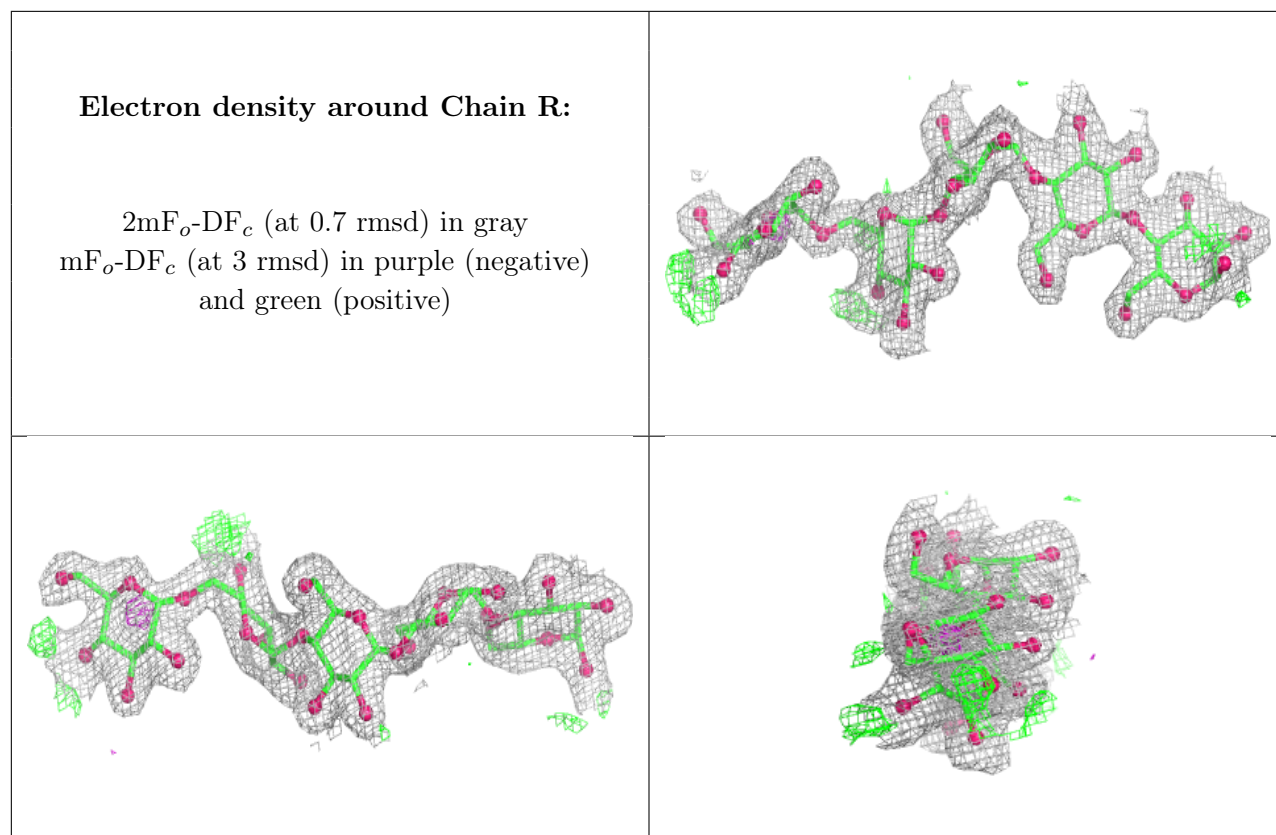
Electron density around Chain P:

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

**Electron density around Chain Q:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	ACT	A	2302	4/4	0.64	0.20	43,44,44,47	0
9	EDO	A	2303	4/4	0.68	0.31	52,54,57,65	0
9	EDO	A	2316	4/4	0.73	0.24	34,37,39,42	0
9	EDO	B	3321	4/4	0.74	0.23	65,67,68,69	0
9	EDO	B	3317	4/4	0.75	0.21	47,51,52,53	0
9	EDO	B	3301	4/4	0.76	0.21	60,63,67,68	0
9	EDO	B	3311	4/4	0.78	0.17	51,52,53,58	0
9	EDO	C	2307	4/4	0.79	0.23	50,50,51,53	0
9	EDO	C	2304	4/4	0.80	0.18	49,59,62,62	0
9	EDO	A	2314	4/4	0.80	0.25	56,57,60,61	0
9	EDO	D	808	4/4	0.80	0.22	62,62,64,65	0
9	EDO	A	2310	4/4	0.80	0.18	46,55,56,56	0
9	EDO	D	806	4/4	0.81	0.22	65,65,66,71	0
9	EDO	B	3307	4/4	0.81	0.20	45,52,53,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	EDO	B	3322	4/4	0.81	0.15	52,52,53,54	0
17	CL	D	803	1/1	0.81	0.22	68,68,68,68	0
9	EDO	C	2315	4/4	0.82	0.17	46,46,47,51	0
9	EDO	C	2318	4/4	0.82	0.16	47,48,48,50	0
9	EDO	A	2305	4/4	0.83	0.21	44,50,51,54	0
15	NA	C	2310	1/1	0.83	0.15	49,49,49,49	0
16	PEG	C	2312	7/7	0.83	0.20	43,51,54,58	0
9	EDO	B	3320	4/4	0.83	0.19	55,56,60,60	0
9	EDO	C	2316	4/4	0.84	0.19	50,53,53,58	0
9	EDO	A	2315	4/4	0.84	0.17	42,46,46,47	0
9	EDO	C	2311	4/4	0.84	0.16	51,52,54,55	0
9	EDO	A	2304	4/4	0.84	0.15	37,43,44,49	0
9	EDO	C	2305	4/4	0.85	0.15	40,45,49,49	0
9	EDO	B	3316	4/4	0.85	0.15	41,44,45,47	0
10	ACT	A	2319	4/4	0.85	0.15	40,41,47,49	0
10	ACT	D	805	4/4	0.85	0.18	58,59,61,63	0
9	EDO	A	2308	4/4	0.85	0.23	52,54,54,58	0
9	EDO	C	2319	4/4	0.85	0.14	52,58,59,60	0
9	EDO	C	2314	4/4	0.85	0.18	49,50,51,51	0
9	EDO	A	2323	4/4	0.86	0.14	48,50,53,54	0
10	ACT	A	2322	4/4	0.86	0.17	49,58,58,62	0
9	EDO	B	3308	4/4	0.86	0.15	39,46,46,47	0
9	EDO	B	3306	4/4	0.87	0.14	56,56,58,59	0
9	EDO	A	2301	4/4	0.87	0.15	51,53,54,54	0
9	EDO	B	3302	4/4	0.87	0.17	50,51,53,53	0
14	PGE	C	2302	10/10	0.87	0.19	50,66,68,72	0
9	EDO	B	3303	4/4	0.87	0.20	51,52,53,55	0
9	EDO	B	3315	4/4	0.87	0.20	54,57,57,63	0
9	EDO	C	2303	4/4	0.87	0.16	51,52,52,54	0
9	EDO	C	2306	4/4	0.88	0.14	50,51,54,56	0
9	EDO	B	3313	4/4	0.88	0.14	44,47,48,49	0
9	EDO	A	2317	4/4	0.88	0.17	46,53,55,58	0
9	EDO	A	2311	4/4	0.89	0.13	53,55,55,56	0
9	EDO	A	2321	4/4	0.89	0.14	46,49,50,53	0
9	EDO	D	807	4/4	0.89	0.19	54,65,66,68	0
9	EDO	A	2307	4/4	0.89	0.15	53,58,60,62	0
9	EDO	B	3319	4/4	0.90	0.15	41,47,48,49	0
13	1PE	C	2301	16/16	0.90	0.16	25,43,52,52	0
9	EDO	D	809	4/4	0.90	0.14	47,49,51,51	0
9	EDO	D	804	4/4	0.90	0.20	41,47,47,50	0
9	EDO	C	2317	4/4	0.90	0.14	39,39,40,42	0
9	EDO	B	3305	4/4	0.90	0.13	53,53,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	EDO	A	2309	4/4	0.91	0.12	42,43,46,46	0
9	EDO	A	2306	4/4	0.91	0.18	47,48,49,53	0
9	EDO	B	3304	4/4	0.91	0.12	41,44,44,49	0
9	EDO	B	3318	4/4	0.91	0.14	53,55,57,59	0
9	EDO	C	2313	4/4	0.91	0.12	35,38,40,40	0
9	EDO	B	3314	4/4	0.91	0.12	39,40,44,45	0
10	ACT	A	2320	4/4	0.91	0.14	35,36,38,43	0
9	EDO	A	2318	4/4	0.92	0.14	35,43,45,49	0
9	EDO	B	3312	4/4	0.92	0.12	33,42,43,45	0
11	CA	D	801	1/1	0.99	0.03	23,23,23,23	0
12	MN	A	2313	1/1	0.99	0.06	36,36,36,36	0
12	MN	B	3310	1/1	0.99	0.07	33,33,33,33	0
12	MN	C	2309	1/1	0.99	0.06	41,41,41,41	0
12	MN	D	802	1/1	0.99	0.07	47,47,47,47	0
11	CA	B	3309	1/1	1.00	0.01	14,14,14,14	0
11	CA	C	2308	1/1	1.00	0.01	15,15,15,15	0
11	CA	A	2312	1/1	1.00	0.01	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.