



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:43 PM UTC

PDB ID : 8DL2 / pdb_00008dl2
Title : BoGH13ASus from Bacteroides ovatus bound to acarbose
Authors : Brown, H.A.; DeVeaux, A.L.; Koropatkin, N.M.
Deposited on : 2022-07-06
Resolution : 1.99 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:

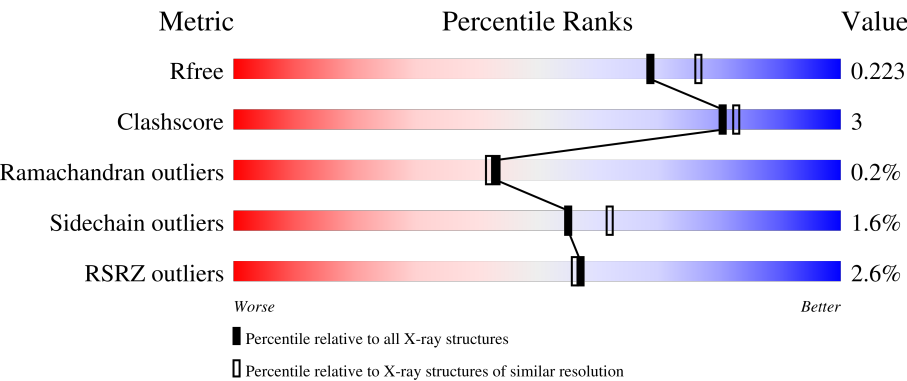
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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.



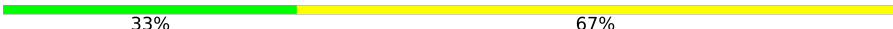
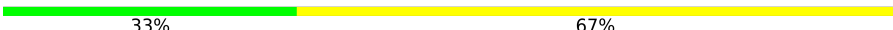
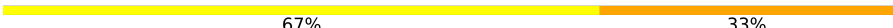
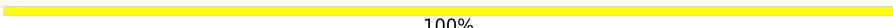
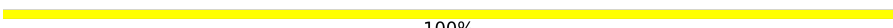
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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% 89% 7% .
1	B	738	2% 90% 6% ..
1	C	738	3% 89% 7% .
1	D	738	2% 91%
2	H	3	67% 33%

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Mol	Chain	Length	Quality of chain
2	K	3	 67% 33%
3	I	3	 67% 33%
3	L	3	 33% 67%
3	N	3	 33% 67%
3	O	3	 33% 67%
3	Q	3	 67% 33%
3	V	3	 67% 33%
4	J	5	 100%
5	P	2	 50% 50%
6	R	2	 50% 50%
7	M	4	 50% 50%
7	S	4	 100%

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 25774 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	712	Total	C	N	O	S	0	5	0
			5718	3652	941	1103	22			
1	B	712	Total	C	N	O	S	0	4	0
			5713	3647	937	1107	22			
1	C	709	Total	C	N	O	S	0	2	0
			5680	3628	938	1092	22			
1	D	712	Total	C	N	O	S	0	1	0
			5681	3626	936	1097	22			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	expression tag	UNP A7M087
B	21	GLY	-	expression tag	UNP A7M087
C	21	GLY	-	expression tag	UNP A7M087
D	21	GLY	-	expression tag	UNP A7M087

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	3	Total	C	N	O	0	1	0
			44	25	1	18			
2	K	3	Total	C	N	O	0	0	0
			44	25	1	18			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	3	Total	C	N	O	0	0	0
			44	25	1	18			
3	L	3	Total	C	N	O	0	0	0
			44	25	1	18			
3	O	3	Total	C	N	O	0	0	0
			44	25	1	18			
3	N	3	Total	C	N	O	0	0	0
			44	25	1	18			
3	V	3	Total	C	N	O	0	0	0
			44	25	1	18			
3	Q	3	Total	C	N	O	0	0	0
			44	25	1	18			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	5	Total	C	N	O	0	0	0
			66	37	1	28			

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
5	P	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 6 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
6	R	2	Total	C	N	O	0	0	0
			33	19	1	13			

- Molecule 7 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-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-(1-4)-alpha-D-glucopyranose.

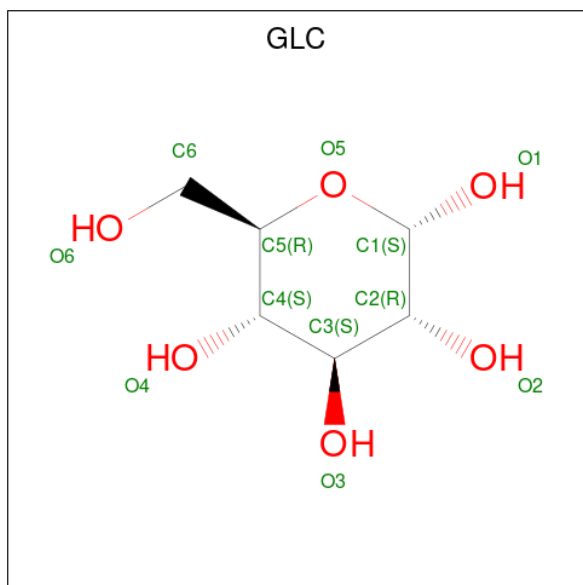
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	M	4	Total	C	N	O	0	0	0
			55	31	1	23			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	S	4	Total	C	N	O	0	0	0
			55	31	1	23			

- Molecule 8 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



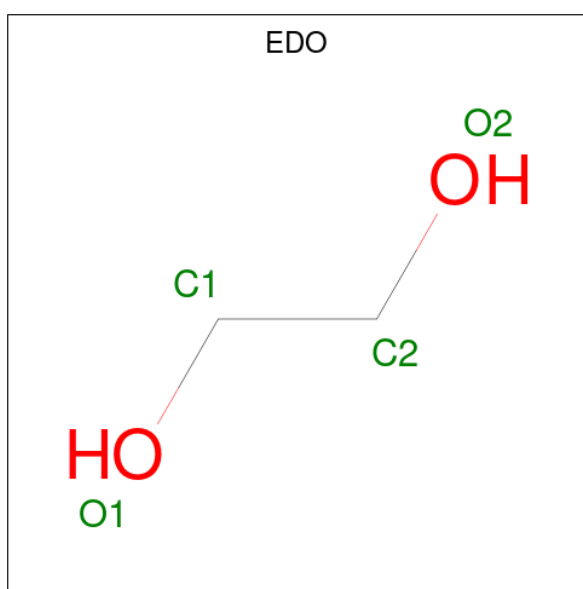
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		

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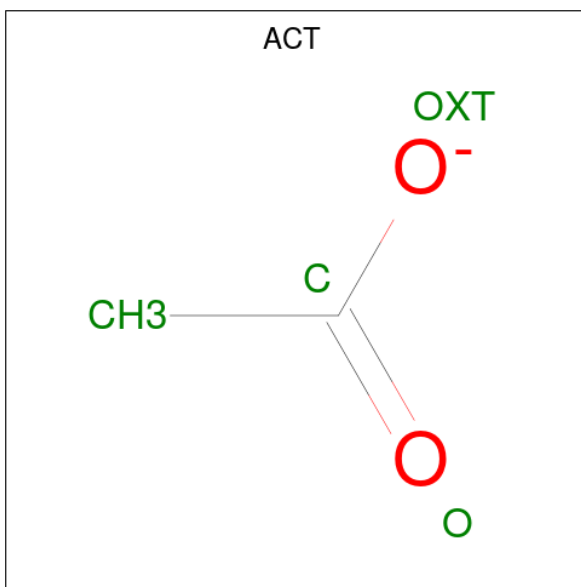
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		
11	C	1	Total	C	O	0	0
			6	3	3		
11	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 13 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 14 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 15 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

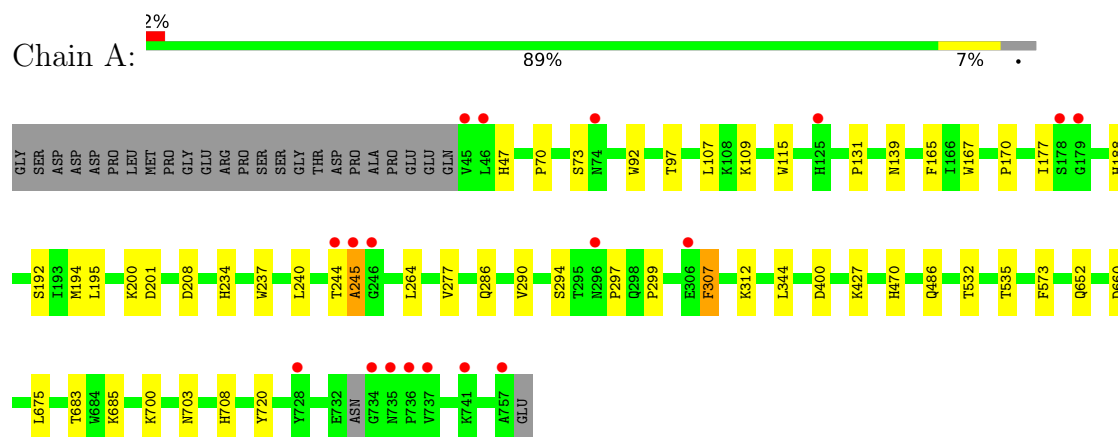
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	655	Total	O	0	0
			655	655		
17	B	675	Total	O	0	0
			675	675		
17	C	497	Total	O	0	0
			497	497		
17	D	449	Total	O	0	0
			449	449		

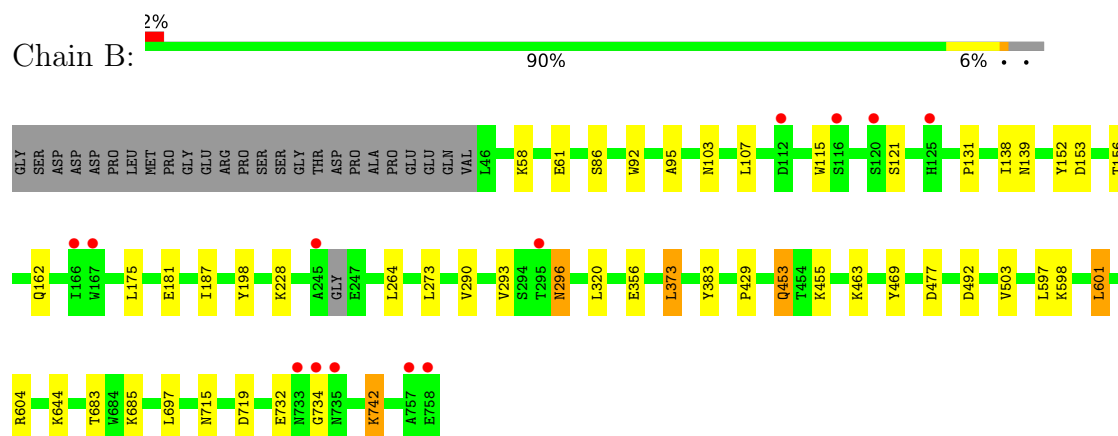
3 Residue-property plots [i](#)

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.

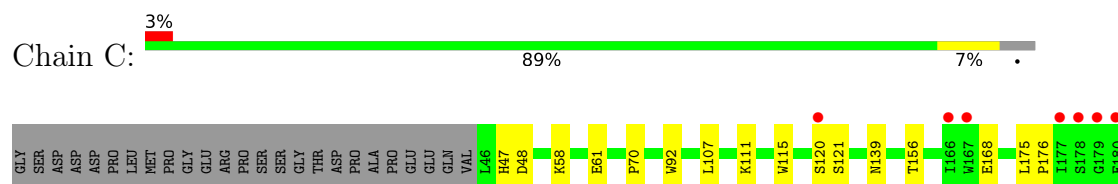
- Molecule 1: Alpha amylase, catalytic domain protein

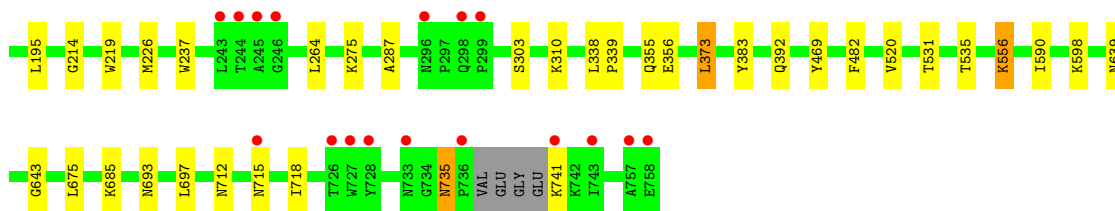


- Molecule 1: Alpha amylase, catalytic domain protein

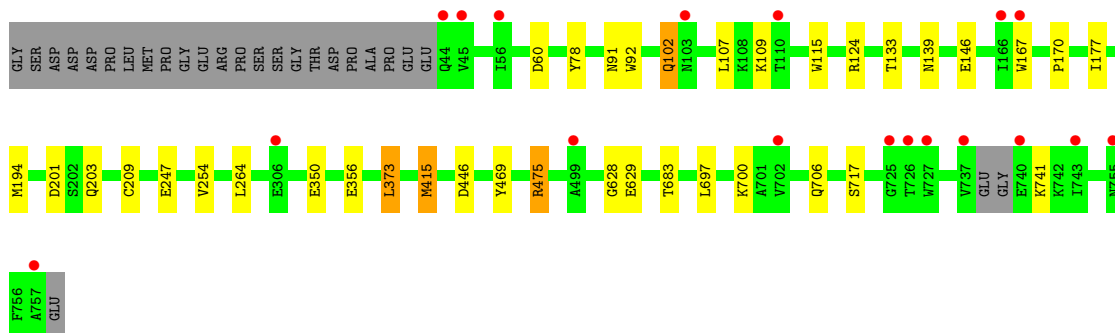


- Molecule 1: Alpha amylase, catalytic domain protein





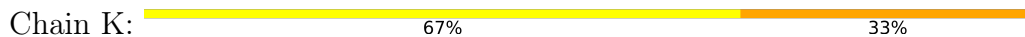
- Molecule 1: Alpha amylase, catalytic domain protein



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



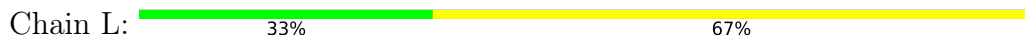
- Molecule 2: 4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino\}$ -alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-beta-D-glucopyranose



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



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





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

Chain O: 33% 67%



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

Chain N: 33% 67%



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

Chain V: 67% 33%



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

Chain Q: 67% 33%



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

Chain J: 100%



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

Chain P: 50% 50%



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

Chain R:  50% 50%

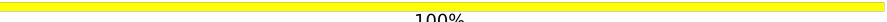


- Molecule 7: α -D-glucopyranose-(1-4)-4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain M:  50% 50%



- Molecule 7: α -D-glucopyranose-(1-4)-4,6-dideoxy-4- $\{[(1S,4R,5S,6S)-4,5,6\text{-trihydroxy-3-(hydroxymethyl)cyclohex-2-en-1-yl]amino}\}$ - α -D-glucopyranose-(1-4)- α -D-glucopyranose-(1-4)- α -D-glucopyranose

Chain S:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.08Å 125.31Å 150.78Å 90.00° 102.11° 90.00°	Depositor
Resolution (Å)	38.60 – 1.99 38.60 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.60-1.99) 98.5 (38.60-1.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.175 , 0.219 0.184 , 0.223	Depositor DCC
R_{free} test set	12246 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.8	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	25774	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: GLC, AC1, PGE, GOL, PEG, BGC, ACT, CA, CL, EDO, MN

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	1.03	0/5900	1.30	5/8032 (0.1%)
1	B	1.05	0/5891	1.29	2/8021 (0.0%)
1	C	1.01	1/5853 (0.0%)	1.28	2/7969 (0.0%)
1	D	1.02	0/5851	1.30	1/7973 (0.0%)
All	All	1.03	1/23495 (0.0%)	1.29	10/31995 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	520	VAL	C-O	5.03	1.29	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	LEU	N-CA-CB	-5.62	101.36	110.81
1	B	492	ASP	CA-CB-CG	5.41	118.01	112.60
1	A	277	VAL	N-CA-C	-5.16	107.54	111.62
1	C	556	LYS	CB-CA-C	5.16	119.62	110.85
1	D	629	GLU	CB-CG-CD	5.14	121.33	112.60
1	A	486	GLN	CA-C-O	-5.13	114.80	120.60
1	A	400	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	307	PHE	CA-CB-CG	-5.11	108.69	113.80
1	A	573	PHE	CA-CB-CG	-5.10	108.70	113.80
1	C	156	THR	CA-CB-OG1	-5.08	101.99	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	5718	0	5343	30	0
1	B	5713	0	5330	30	0
1	C	5680	0	5304	25	0
1	D	5681	0	5271	24	0
2	H	44	0	25	1	0
2	K	44	0	27	1	0
3	I	44	0	30	0	0
3	L	44	0	30	0	0
3	N	44	0	30	1	0
3	O	44	0	30	0	0
3	Q	44	0	30	1	0
3	V	44	0	29	3	0
4	J	66	0	48	0	0
5	P	22	0	19	3	0
6	R	33	0	21	0	0
7	M	55	0	39	2	0
7	S	55	0	39	0	0
8	A	12	0	5	0	0
8	B	12	0	8	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	10	0	14	2	0
10	B	10	0	14	0	0
11	A	6	0	8	1	0
11	B	18	0	24	2	0
11	C	12	0	16	1	0
12	A	4	0	6	1	0
12	D	4	0	6	2	0
13	A	4	0	3	1	0
13	B	4	0	3	1	0
13	C	4	0	3	0	0
14	A	1	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	B	7	0	10	2	0
15	D	7	0	10	1	0
16	D	1	0	0	0	0
17	A	655	0	0	10	0
17	B	675	0	0	7	0
17	C	497	0	0	5	0
17	D	449	0	0	7	0
All	All	25774	0	21775	117	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (117) 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)
5:P:1:GLC:C1	3:V:3:AC1:O4	1.66	1.41
1:A:188:HIS:HD2	17:A:1399:HOH:O	1.59	0.85
15:B:804:PEG:H12	17:B:1089:HOH:O	1.84	0.77
1:B:181:GLU:OE2	17:B:901:HOH:O	2.04	0.75
1:C:120:SER:O	17:C:901:HOH:O	2.03	0.75
5:P:1:GLC:C1	3:V:3:AC1:C4A	2.64	0.75
1:C:715:ASN:HB3	17:C:1097:HOH:O	1.90	0.70
1:D:91:ASN:OD1	17:D:901:HOH:O	2.09	0.70
1:D:254:VAL:HG11	1:D:415:MET:HE3	1.73	0.70
1:A:188:HIS:CD2	17:A:1399:HOH:O	2.40	0.69
1:A:652:GLN:OE1	17:A:901:HOH:O	2.13	0.66
1:A:286:GLN:OE1	17:A:902:HOH:O	2.13	0.66
1:D:146:GLU:HG3	17:D:1244:HOH:O	1.96	0.66
1:D:78:TYR:O	1:D:109:LYS:NZ	2.30	0.64
1:B:107:LEU:HB3	1:B:115:TRP:HB3	1.79	0.64
1:D:254:VAL:HG11	1:D:415:MET:CE	2.29	0.62
1:B:715[B]:ASN:CG	11:B:805:GOL:O3	2.44	0.60
15:B:804:PEG:C1	17:B:1089:HOH:O	2.48	0.60
1:D:373:LEU:HD22	1:D:469:TYR:CZ	2.37	0.59
1:C:373:LEU:HD22	1:C:469:TYR:CZ	2.38	0.59
1:D:92:TRP:CD1	3:Q:3:AC1:HCB1	2.38	0.59
1:A:107:LEU:HB3	1:A:115:TRP:HB3	1.85	0.58
1:B:198:TYR:CE1	1:B:453[B]:GLN:OE1	2.58	0.57
1:B:356:GLU:OE1	17:B:903:HOH:O	2.18	0.56
1:D:203:GLN:O	17:D:902:HOH:O	2.18	0.56
1:B:463:LYS:HE2	17:B:1464:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LYS:NZ	17:A:913:HOH:O	2.39	0.55
1:A:165:PHE:HB2	11:A:804:GOL:C3	2.36	0.54
1:A:700:LYS:HB3	17:A:970:HOH:O	2.06	0.54
1:A:244:THR:O	1:A:245:ALA:HB3	2.09	0.53
1:B:683:THR:OG1	13:B:808:ACT:H3	2.08	0.53
1:C:168:GLU:HB3	17:C:1151:HOH:O	2.10	0.52
1:A:177:ILE:HG21	1:A:194:MET:HE1	1.92	0.51
1:D:446:ASP:OD2	17:D:904:HOH:O	2.19	0.51
1:A:200:LYS:HD3	1:A:234:HIS:CE1	2.45	0.51
1:B:455:LYS:HD3	1:B:503:VAL:HG23	1.92	0.51
1:B:187:ILE:HD11	1:B:293:VAL:CG1	2.40	0.51
1:B:296:ASN:O	1:B:296:ASN:ND2	2.38	0.51
1:C:275:LYS:HD3	1:C:287:ALA:HB2	1.91	0.51
1:B:138:ILE:CG2	1:B:156:THR:HG22	2.40	0.50
1:C:107:LEU:HB3	1:C:115:TRP:HB3	1.93	0.50
1:B:429:PRO:HB2	1:B:453[A]:GLN:HE21	1.76	0.50
1:B:644:LYS:HE3	17:B:1181:HOH:O	2.11	0.50
1:A:170:PRO:HG2	1:A:208:ASP:O	2.12	0.49
1:C:58:LYS:HB2	1:C:61:GLU:HB2	1.94	0.49
1:C:92:TRP:CZ2	1:C:139:ASN:HB3	2.48	0.49
1:D:124:ARG:NH2	1:D:133:THR:O	2.46	0.49
1:C:48:ASP:HB3	1:C:70:PRO:HG3	1.96	0.48
1:A:167:TRP:CD1	10:A:803:PGE:H32	2.49	0.48
1:B:198:TYR:CE1	1:B:453[B]:GLN:CD	2.92	0.48
1:D:247:GLU:OE2	17:D:903:HOH:O	2.19	0.48
1:D:350:GLU:OE2	1:D:475:ARG:HD3	2.14	0.47
1:A:708:HIS:NE2	1:A:720:TYR:OH	2.45	0.47
1:A:92:TRP:CZ2	1:A:139:ASN:HB3	2.49	0.47
1:A:660:ASP:OD2	17:A:903:HOH:O	2.20	0.47
1:B:273:LEU:HB2	1:B:290:VAL:HG22	1.95	0.47
1:C:735:ASN:N	1:C:735:ASN:OD1	2.48	0.47
1:A:195:LEU:O	1:A:237:TRP:HA	2.15	0.47
1:C:693:ASN:HB2	11:C:803:GOL:H32	1.97	0.46
1:D:700:LYS:HG2	1:D:706:GLN:HG2	1.97	0.46
1:A:470:HIS:NE2	17:A:910:HOH:O	2.36	0.46
1:D:201:ASP:OD1	1:D:201:ASP:C	2.58	0.46
1:A:685:LYS:NZ	17:A:926:HOH:O	2.49	0.46
1:C:195:LEU:O	1:C:237:TRP:HA	2.14	0.46
1:A:70:PRO:HG2	1:A:73:SER:HB3	1.96	0.46
1:C:226:MET:HG2	17:C:1101:HOH:O	2.16	0.46
1:B:373:LEU:HD22	1:B:469:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:ILE:HD13	1:D:194:MET:HE1	1.97	0.46
1:D:167:TRP:HA	12:D:804:EDO:C1	2.45	0.45
15:D:803:PEG:H12	17:D:1161:HOH:O	2.16	0.45
1:C:531:THR:O	1:C:535:THR:HG23	2.16	0.45
1:C:373:LEU:HB3	1:C:383:TYR:CE2	2.51	0.45
1:A:683:THR:OG1	13:A:806:ACT:H3	2.16	0.45
1:D:60:ASP:OD1	1:D:124:ARG:HD2	2.17	0.45
1:B:92:TRP:CZ2	1:B:139:ASN:HB3	2.52	0.45
1:D:92:TRP:CZ2	1:D:139:ASN:HB3	2.52	0.44
3:N:1:GLC:H62	3:N:2:GLC:H5	1.98	0.44
11:B:806:GOL:H32	7:M:4:GLC:O6	2.17	0.44
1:A:201:ASP:HB2	1:A:427:LYS:HB3	2.00	0.44
5:P:1:GLC:C2	3:V:3:AC1:O4	2.57	0.44
1:D:170:PRO:HG3	1:D:209:CYS:HB3	2.00	0.44
1:A:97:THR:HG23	1:B:601:LEU:HD13	2.00	0.43
1:B:92:TRP:CD1	2:K:3:AC1:HCB1	2.53	0.43
1:B:719:ASP:HB3	1:B:742:LYS:HD3	2.01	0.43
1:A:192[B]:SER:HA	1:A:240:LEU:O	2.19	0.43
1:A:532:THR:O	1:A:535:THR:HB	2.18	0.43
1:A:192[A]:SER:HA	1:A:240:LEU:O	2.19	0.43
1:C:214:GLY:HA2	1:C:219:TRP:CZ3	2.53	0.43
1:B:373:LEU:HB3	1:B:383:TYR:CE2	2.54	0.42
1:D:628:GLY:HA3	17:D:938:HOH:O	2.17	0.42
1:B:131:PRO:O	1:B:162:GLN:NE2	2.52	0.42
1:B:597:LEU:O	1:B:604:ARG:HD2	2.19	0.42
1:C:310:LYS:HD2	17:C:1030:HOH:O	2.20	0.42
1:C:590:ILE:O	1:C:598:LYS:HG2	2.20	0.42
1:B:86:SER:O	1:B:95:ALA:HA	2.19	0.42
1:B:697:LEU:C	1:B:697:LEU:HD12	2.45	0.42
1:A:167:TRP:HD1	10:A:803:PGE:H32	1.84	0.41
1:A:297:PRO:O	1:A:299:PRO:HD3	2.20	0.41
1:B:58:LYS:HB2	1:B:61:GLU:HB2	2.02	0.41
1:C:303:SER:CB	1:C:392:GLN:HE21	2.33	0.41
1:C:697:LEU:C	1:C:697:LEU:HD12	2.45	0.41
1:A:92:TRP:CD1	2:H:3:AC1:HCB1	2.56	0.41
1:C:712:ASN:CG	1:C:718:ILE:HD12	2.45	0.41
1:D:167:TRP:HA	12:D:804:EDO:O1	2.20	0.41
1:B:152:TYR:O	1:B:153:ASP:C	2.62	0.41
1:B:598:LYS:HD2	17:B:1280:HOH:O	2.20	0.41
1:C:338:LEU:N	1:C:339:PRO:CD	2.84	0.41
1:C:639:ASN:O	1:C:643:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:GLN:O	1:C:356:GLU:C	2.64	0.41
1:D:107:LEU:HB3	1:D:115:TRP:HB3	2.02	0.41
1:C:175:LEU:HA	1:C:176:PRO:HD3	1.93	0.41
1:A:703:ASN:OD1	1:A:703:ASN:C	2.65	0.40
12:A:805:EDO:H11	17:A:1384:HOH:O	2.20	0.40
1:D:177:ILE:HD13	1:D:194:MET:CE	2.51	0.40
1:B:477:ASP:OD1	7:M:3:AC1:HCB2	2.22	0.40
1:D:697:LEU:HD12	1:D:697:LEU:C	2.46	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	713/738 (97%)	679 (95%)	32 (4%)	2 (0%)	36	35
1	B	712/738 (96%)	685 (96%)	25 (4%)	2 (0%)	36	35
1	C	707/738 (96%)	669 (95%)	37 (5%)	1 (0%)	48	46
1	D	709/738 (96%)	681 (96%)	27 (4%)	1 (0%)	48	46
All	All	2841/2952 (96%)	2714 (96%)	121 (4%)	6 (0%)	43	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	ALA
1	A	307	PHE
1	B	734	GLY
1	D	102	GLN
1	B	121	SER
1	C	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	608/639 (95%)	600 (99%)	8 (1%)	61	68
1	B	608/639 (95%)	596 (98%)	12 (2%)	48	54
1	C	602/639 (94%)	592 (98%)	10 (2%)	53	60
1	D	600/639 (94%)	591 (98%)	9 (2%)	57	64
All	All	2418/2556 (95%)	2379 (98%)	39 (2%)	55	62

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	131	PRO
1	A	264	LEU
1	A	290	VAL
1	A	294	SER
1	A	312	LYS
1	A	344	LEU
1	A	675	LEU
1	B	103	ASN
1	B	175	LEU
1	B	228	LYS
1	B	264	LEU
1	B	296	ASN
1	B	373	LEU
1	B	453[A]	GLN
1	B	453[B]	GLN
1	B	601	LEU
1	B	685	LYS
1	B	732	GLU
1	B	742	LYS
1	C	47	HIS
1	C	111	LYS
1	C	264	LEU
1	C	373	LEU

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Mol	Chain	Res	Type
1	C	482	PHE
1	C	556	LYS
1	C	675	LEU
1	C	685	LYS
1	C	735	ASN
1	C	741	LYS
1	D	102	GLN
1	D	264	LEU
1	D	356	GLU
1	D	373	LEU
1	D	415	MET
1	D	475	ARG
1	D	683	THR
1	D	717	SER
1	D	741	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	74	ASN
1	A	103	ASN
1	A	234	HIS
1	A	286	GLN
1	A	311	ASN
1	A	706	GLN
1	B	150	GLN
1	B	408	ASN
1	B	421	ASN
1	B	706	GLN
1	C	203	GLN
1	C	217	ASN
1	C	233	ASN
1	C	311	ASN
1	C	392	GLN
1	C	393	ASN
1	C	550	GLN
1	D	91	ASN
1	D	103	ASN
1	D	203	GLN
1	D	296	ASN
1	D	311	ASN

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Mol	Chain	Res	Type
1	D	392	GLN
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 ⓘ

41 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	BGC	H	1[A]	2	12,12,12	0.84	1 (8%)	17,17,17	1.20	1 (5%)
2	GLC	H	2	2,8	11,11,12	0.88	1 (9%)	15,15,17	1.22	1 (6%)
2	AC1	H	3	2	21,22,23	0.55	0	22,32,34	0.80	1 (4%)
3	GLC	I	1	3	12,12,12	0.66	0	17,17,17	0.96	2 (11%)
3	GLC	I	2	3	11,11,12	0.34	0	15,15,17	0.91	0
3	AC1	I	3	3	21,22,23	0.45	0	22,32,34	0.66	0
4	GLC	J	1	4	12,12,12	0.49	0	17,17,17	1.37	1 (5%)
4	GLC	J	2	4	11,11,12	0.71	0	15,15,17	1.19	2 (13%)
4	AC1	J	3	4	21,22,23	1.62	5 (23%)	22,32,34	1.42	3 (13%)
4	GLC	J	4	4	11,11,12	0.63	0	15,15,17	1.44	3 (20%)
4	GLC	J	5	4	11,11,12	0.78	0	15,15,17	1.17	2 (13%)
2	BGC	K	1	2,8	12,12,12	0.77	0	17,17,17	1.04	1 (5%)
2	GLC	K	2	2,8	11,11,12	0.81	0	15,15,17	1.67	5 (33%)
2	AC1	K	3	2	21,22,23	0.46	0	22,32,34	0.81	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GLC	L	1	3	12,12,12	0.62	0	17,17,17	1.47	4 (23%)
3	GLC	L	2	3	11,11,12	0.73	0	15,15,17	1.51	1 (6%)
3	AC1	L	3	3	21,22,23	0.65	0	22,32,34	0.63	0
7	GLC	M	1	7	12,12,12	0.55	0	17,17,17	1.71	5 (29%)
7	GLC	M	2	7	11,11,12	0.88	0	15,15,17	1.08	1 (6%)
7	AC1	M	3	7	21,22,23	1.34	2 (9%)	22,32,34	1.50	4 (18%)
7	GLC	M	4	7	11,11,12	1.25	1 (9%)	15,15,17	1.40	3 (20%)
3	GLC	N	1	3	12,12,12	0.62	0	17,17,17	1.28	2 (11%)
3	GLC	N	2	3	11,11,12	0.54	0	15,15,17	1.00	1 (6%)
3	AC1	N	3	3	21,22,23	0.89	1 (4%)	22,32,34	1.57	3 (13%)
3	GLC	O	1	3	12,12,12	0.46	0	17,17,17	0.87	1 (5%)
3	GLC	O	2	3	11,11,12	0.42	0	15,15,17	1.55	3 (20%)
3	AC1	O	3	3	21,22,23	0.43	0	22,32,34	0.59	0
5	GLC	P	1	5	11,11,12	0.51	0	15,15,17	1.40	2 (13%)
5	GLC	P	2	5	11,11,12	0.97	0	15,15,17	1.82	3 (20%)
3	GLC	Q	1	3	12,12,12	0.67	0	17,17,17	1.90	3 (17%)
3	GLC	Q	2	3	11,11,12	0.95	1 (9%)	15,15,17	1.15	2 (13%)
3	AC1	Q	3	3	21,22,23	0.90	1 (4%)	22,32,34	1.47	4 (18%)
6	GLC	R	1	6	12,12,12	0.66	0	17,17,17	1.16	1 (5%)
6	AC1	R	2	6	21,22,23	0.36	0	22,32,34	0.80	0
7	GLC	S	1	7	12,12,12	0.63	0	17,17,17	1.48	4 (23%)
7	GLC	S	2	7	11,11,12	0.65	0	15,15,17	1.07	1 (6%)
7	AC1	S	3	7	21,22,23	1.06	1 (4%)	22,32,34	1.52	5 (22%)
7	GLC	S	4	7	11,11,12	0.58	0	15,15,17	1.56	3 (20%)
3	GLC	V	1	3	12,12,12	0.64	0	17,17,17	1.48	4 (23%)
3	GLC	V	2	3	11,11,12	0.84	0	15,15,17	1.47	2 (13%)
3	AC1	V	3	3	21,22,23	1.22	2 (9%)	22,32,34	1.39	4 (18%)

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	H	1[A]	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2,8	-	0/2/19/22	0/1/1/1
2	AC1	H	3	2	-	3/6/43/46	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	I	1	3	-	2/2/22/22	0/1/1/1
3	GLC	I	2	3	-	0/2/19/22	0/1/1/1
3	AC1	I	3	3	-	3/6/43/46	0/2/2/2
4	GLC	J	1	4	-	0/2/22/22	0/1/1/1
4	GLC	J	2	4	-	0/2/19/22	0/1/1/1
4	AC1	J	3	4	-	3/6/43/46	0/2/2/2
4	GLC	J	4	4	-	0/2/19/22	0/1/1/1
4	GLC	J	5	4	-	0/2/19/22	0/1/1/1
2	BGC	K	1	2,8	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2,8	-	2/2/19/22	0/1/1/1
2	AC1	K	3	2	-	3/6/43/46	0/2/2/2
3	GLC	L	1	3	-	0/2/22/22	0/1/1/1
3	GLC	L	2	3	-	2/2/19/22	0/1/1/1
3	AC1	L	3	3	-	2/6/43/46	0/2/2/2
7	GLC	M	1	7	-	0/2/22/22	0/1/1/1
7	GLC	M	2	7	-	0/2/19/22	0/1/1/1
7	AC1	M	3	7	-	3/6/43/46	0/2/2/2
7	GLC	M	4	7	-	0/2/19/22	0/1/1/1
3	GLC	N	1	3	-	0/2/22/22	0/1/1/1
3	GLC	N	2	3	-	0/2/19/22	0/1/1/1
3	AC1	N	3	3	-	4/6/43/46	0/2/2/2
3	GLC	O	1	3	-	2/2/22/22	0/1/1/1
3	GLC	O	2	3	-	0/2/19/22	0/1/1/1
3	AC1	O	3	3	-	4/6/43/46	0/2/2/2
5	GLC	P	1	5	-	0/2/19/22	0/1/1/1
5	GLC	P	2	5	-	1/2/19/22	0/1/1/1
3	GLC	Q	1	3	-	2/2/22/22	0/1/1/1
3	GLC	Q	2	3	-	2/2/19/22	0/1/1/1
3	AC1	Q	3	3	-	2/6/43/46	0/2/2/2
6	GLC	R	1	6	-	0/2/22/22	0/1/1/1
6	AC1	R	2	6	-	3/6/43/46	0/2/2/2
7	GLC	S	1	7	-	0/2/22/22	0/1/1/1
7	GLC	S	2	7	-	0/2/19/22	0/1/1/1
7	AC1	S	3	7	-	1/6/43/46	0/2/2/2
7	GLC	S	4	7	-	0/2/19/22	0/1/1/1
3	GLC	V	1	3	-	0/2/22/22	0/1/1/1
3	GLC	V	2	3	-	0/2/19/22	0/1/1/1
3	AC1	V	3	3	-	1/6/43/46	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	AC1	C1B-N4A	4.61	1.55	1.47
7	M	3	AC1	C1B-N4A	3.92	1.54	1.47
3	V	3	AC1	C1B-N4A	3.79	1.54	1.47
7	S	3	AC1	C1B-N4A	3.39	1.53	1.47
4	J	3	AC1	C1B-C7B	3.03	1.54	1.50
4	J	3	AC1	C2B-C1B	2.94	1.56	1.53
7	M	3	AC1	C1B-C7B	2.76	1.54	1.50
3	Q	2	GLC	C2-C3	2.68	1.56	1.52
2	H	2	GLC	O5-C1	-2.65	1.39	1.43
4	J	3	AC1	O4-C4A	2.60	1.47	1.42
4	J	3	AC1	C3B-C4A	2.50	1.56	1.53
2	H	1[A]	BGC	O1-C1	2.27	1.46	1.39
3	Q	3	AC1	O5-C1	-2.20	1.40	1.43
3	N	3	AC1	C4A-C5B	-2.13	1.49	1.51
7	M	4	GLC	C2-C3	2.12	1.55	1.52
3	V	3	AC1	C4A-C5B	-2.01	1.49	1.51

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	1	GLC	C4-C3-C2	5.48	120.46	110.83
3	L	2	GLC	C1-O5-C5	4.54	118.26	112.19
7	M	3	AC1	C7B-C1B-N4A	4.35	117.08	110.68
4	J	3	AC1	C7B-C1B-N4A	3.83	116.31	110.68
5	P	2	GLC	O3-C3-C2	3.75	117.71	110.05
3	N	3	AC1	O3-C3-C4	-3.72	102.18	109.58
3	N	3	AC1	C7B-C1B-N4A	3.67	116.08	110.68
4	J	1	GLC	O3-C3-C2	-3.44	102.27	110.38
5	P	2	GLC	C2-C3-C4	-3.39	104.89	110.86
7	M	1	GLC	C1-C2-C3	3.29	117.07	110.36
5	P	2	GLC	C1-O5-C5	-3.25	107.83	112.19
3	Q	3	AC1	C2B-C3B-C4A	3.23	115.33	110.22
4	J	3	AC1	O6B-C6B-C5B	-3.21	102.63	112.74
7	M	1	GLC	O5-C5-C4	3.20	115.46	109.70
2	K	2	GLC	C1-C2-C3	3.18	114.28	109.64
3	V	1	GLC	C1-C2-C3	3.13	116.75	110.36
2	H	2	GLC	C1-C2-C3	3.06	114.10	109.64
7	S	3	AC1	C7B-C1B-N4A	3.06	115.18	110.68
3	Q	1	GLC	O3-C3-C2	-3.06	103.17	110.38
7	S	4	GLC	O3-C3-C2	-3.05	103.83	110.05
7	M	1	GLC	O3-C3-C2	-2.98	103.35	110.38
7	S	4	GLC	C1-C2-C3	2.94	113.93	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	S	3	AC1	O3B-C3B-C2B	2.94	117.31	110.38
3	O	2	GLC	C1-O5-C5	2.94	116.13	112.19
3	V	2	GLC	C1-O5-C5	2.94	116.12	112.19
2	K	3	AC1	C7B-C1B-N4A	-2.91	106.39	110.68
7	M	4	GLC	O4-C4-C5	2.91	116.49	109.32
3	V	3	AC1	O6B-C6B-C5B	-2.90	103.63	112.74
7	S	4	GLC	O4-C4-C5	2.82	116.28	109.32
3	Q	1	GLC	C1-C2-C3	2.79	116.04	110.36
3	V	3	AC1	C2B-C3B-C4A	-2.78	105.81	110.22
3	N	1	GLC	C1-C2-C3	2.76	115.98	110.36
3	L	1	GLC	O5-C1-C2	-2.73	105.49	110.30
7	M	1	GLC	O5-C1-C2	2.72	115.08	110.30
7	S	1	GLC	O4-C4-C3	2.70	116.75	110.38
4	J	2	GLC	O2-C2-C3	-2.70	104.55	110.15
7	M	2	GLC	C1-O5-C5	2.70	115.81	112.19
7	S	1	GLC	C3-C4-C5	-2.69	105.35	110.23
7	S	1	GLC	O1-C1-C2	2.67	116.74	108.98
3	V	1	GLC	O5-C5-C4	2.66	114.48	109.70
3	V	1	GLC	C1-O5-C5	2.65	118.77	113.65
3	Q	2	GLC	C6-C5-C4	2.58	119.36	113.02
2	K	2	GLC	C1-O5-C5	2.58	115.64	112.19
3	Q	3	AC1	O5-C1-C2	2.57	116.93	110.79
7	S	3	AC1	O4-C4A-C3B	-2.57	105.18	110.53
3	L	1	GLC	C4-C3-C2	-2.56	106.34	110.83
4	J	4	GLC	C1-O5-C5	2.54	115.59	112.19
5	P	1	GLC	O4-C4-C5	-2.52	103.12	109.32
5	P	1	GLC	C1-O5-C5	2.52	115.56	112.19
6	R	1	GLC	C1-O5-C5	2.50	118.48	113.65
3	N	1	GLC	O2-C2-C3	-2.45	104.60	110.38
4	J	5	GLC	O3-C3-C2	2.45	115.05	110.05
7	M	3	AC1	O6B-C6B-C5B	-2.45	105.04	112.74
7	M	3	AC1	O4-C4A-C5B	-2.44	106.09	110.75
4	J	2	GLC	C1-O5-C5	2.44	115.45	112.19
2	K	2	GLC	C2-C3-C4	-2.43	106.58	110.86
2	H	3	AC1	O2-C2-C3	2.41	115.15	110.15
2	K	2	GLC	O6-C6-C5	-2.41	103.11	111.33
3	V	3	AC1	O4-C4A-C3B	-2.41	105.51	110.53
3	V	1	GLC	O4-C4-C5	-2.36	103.52	109.32
3	Q	3	AC1	C3B-C4A-C5B	2.35	115.37	111.67
3	V	3	AC1	O3B-C3B-C2B	2.34	115.90	110.38
3	N	2	GLC	O5-C5-C4	-2.32	105.18	110.83
3	O	2	GLC	O6-C6-C5	-2.30	103.49	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	4	GLC	C1-C2-C3	2.28	112.96	109.64
7	S	3	AC1	C5-C4-N4A	2.27	117.99	111.74
4	J	3	AC1	O3B-C3B-C2B	2.27	115.73	110.38
2	H	1[A]	BGC	O2-C2-C3	-2.26	105.05	110.38
7	M	4	GLC	O3-C3-C2	-2.24	105.48	110.05
7	M	1	GLC	C1-O5-C5	2.24	117.98	113.65
3	O	1	GLC	O3-C3-C4	-2.23	105.11	110.38
4	J	4	GLC	O5-C5-C6	2.21	111.97	107.66
3	Q	3	AC1	O3-C3-C4	2.18	113.92	109.58
2	K	1	BGC	O4-C4-C5	2.17	114.68	109.32
7	S	2	GLC	C1-C2-C3	2.17	112.81	109.64
7	S	3	AC1	O2-C2-C1	2.17	114.20	109.22
3	V	2	GLC	O6-C6-C5	-2.17	103.95	111.33
3	N	3	AC1	C2B-C3B-C4A	-2.16	106.80	110.22
7	M	4	GLC	O5-C1-C2	2.15	115.92	110.79
3	O	2	GLC	C2-C3-C4	-2.15	107.08	110.86
2	K	2	GLC	C6-C5-C4	-2.14	107.77	113.02
3	Q	2	GLC	C3-C4-C5	-2.13	106.37	110.23
7	M	3	AC1	C2B-C3B-C4A	-2.13	106.85	110.22
4	J	5	GLC	O3-C3-C4	-2.10	105.42	110.38
3	I	1	GLC	C3-C4-C5	2.09	114.02	110.23
3	L	1	GLC	C1-C2-C3	-2.03	106.22	110.36
7	S	1	GLC	C1-C2-C3	2.02	114.47	110.36
3	I	1	GLC	C4-C3-C2	2.02	114.37	110.83
3	L	1	GLC	C3-C4-C5	-2.00	106.61	110.23

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	3	AC1	C2B-C1B-N4A-C4
2	K	3	AC1	C2B-C1B-N4A-C4
3	I	3	AC1	C2B-C1B-N4A-C4
3	I	3	AC1	C4A-C5B-C6B-O6B
3	I	3	AC1	C7B-C5B-C6B-O6B
3	L	3	AC1	C2B-C1B-N4A-C4
3	O	3	AC1	C2B-C1B-N4A-C4
3	N	3	AC1	C2B-C1B-N4A-C4
3	N	3	AC1	C4A-C5B-C6B-O6B
3	N	3	AC1	C7B-C5B-C6B-O6B
3	V	3	AC1	C7B-C1B-N4A-C4
3	Q	3	AC1	C2B-C1B-N4A-C4

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Mol	Chain	Res	Type	Atoms
4	J	3	AC1	C7B-C1B-N4A-C4
6	R	2	AC1	C2B-C1B-N4A-C4
6	R	2	AC1	C4A-C5B-C6B-O6B
6	R	2	AC1	C7B-C5B-C6B-O6B
7	M	3	AC1	C7B-C1B-N4A-C4
7	M	3	AC1	C4A-C5B-C6B-O6B
7	M	3	AC1	C7B-C5B-C6B-O6B
7	S	3	AC1	C7B-C1B-N4A-C4
3	Q	1	GLC	O5-C5-C6-O6
3	I	1	GLC	C4-C5-C6-O6
3	I	1	GLC	O5-C5-C6-O6
3	O	1	GLC	O5-C5-C6-O6
3	Q	1	GLC	C4-C5-C6-O6
5	P	2	GLC	O5-C5-C6-O6
2	K	2	GLC	C4-C5-C6-O6
3	Q	2	GLC	O5-C5-C6-O6
2	K	3	AC1	C5-C4-N4A-C1B
3	Q	3	AC1	C5-C4-N4A-C1B
3	O	1	GLC	C4-C5-C6-O6
3	Q	2	GLC	C4-C5-C6-O6
3	L	2	GLC	C4-C5-C6-O6
3	O	3	AC1	C4A-C5B-C6B-O6B
3	O	3	AC1	C7B-C5B-C6B-O6B
4	J	3	AC1	C4A-C5B-C6B-O6B
4	J	3	AC1	C7B-C5B-C6B-O6B
3	L	2	GLC	O5-C5-C6-O6
2	K	2	GLC	O5-C5-C6-O6
2	H	3	AC1	C5-C4-N4A-C1B
2	K	3	AC1	C3-C4-N4A-C1B
3	L	3	AC1	C5-C4-N4A-C1B
2	H	3	AC1	C7B-C5B-C6B-O6B
3	O	3	AC1	C5-C4-N4A-C1B
3	N	3	AC1	C5-C4-N4A-C1B

There are no ring outliers.

9 monomers are involved in 9 short contacts:

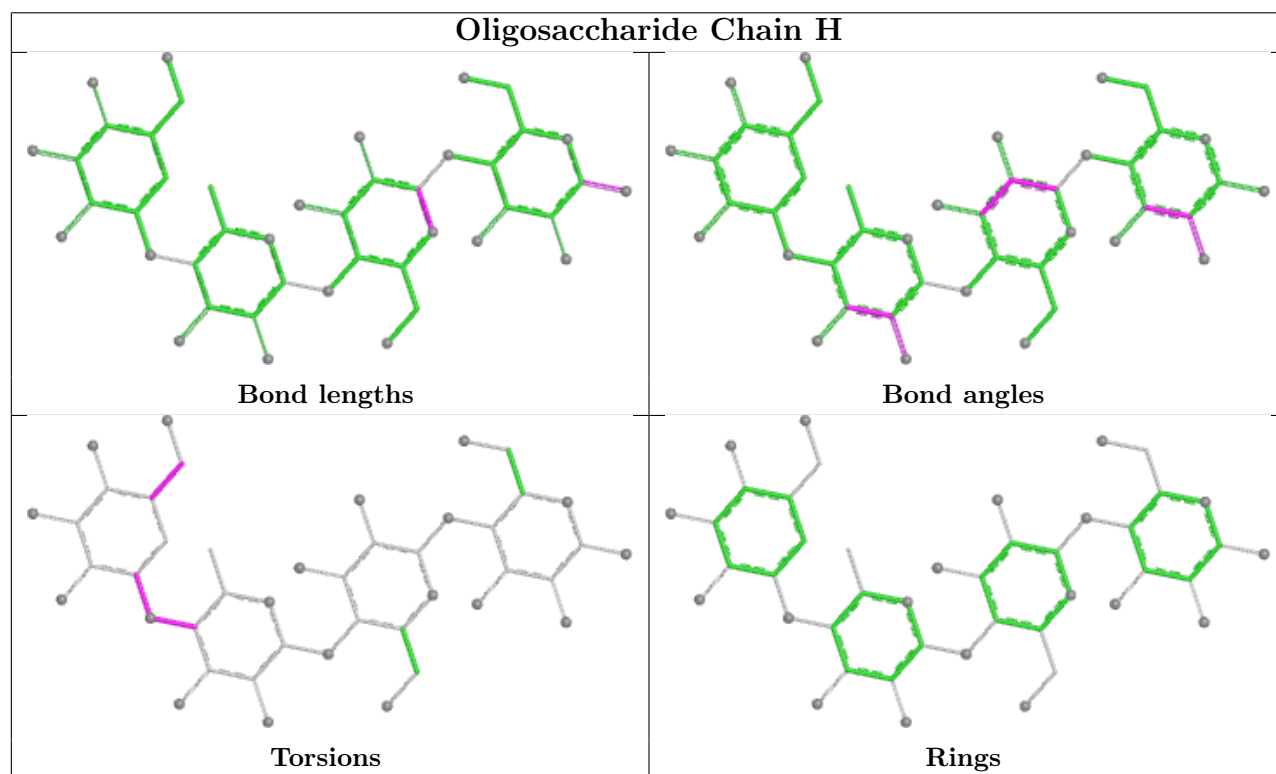
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	3	AC1	1	0
7	M	4	GLC	1	0
5	P	1	GLC	3	0
7	M	3	AC1	1	0

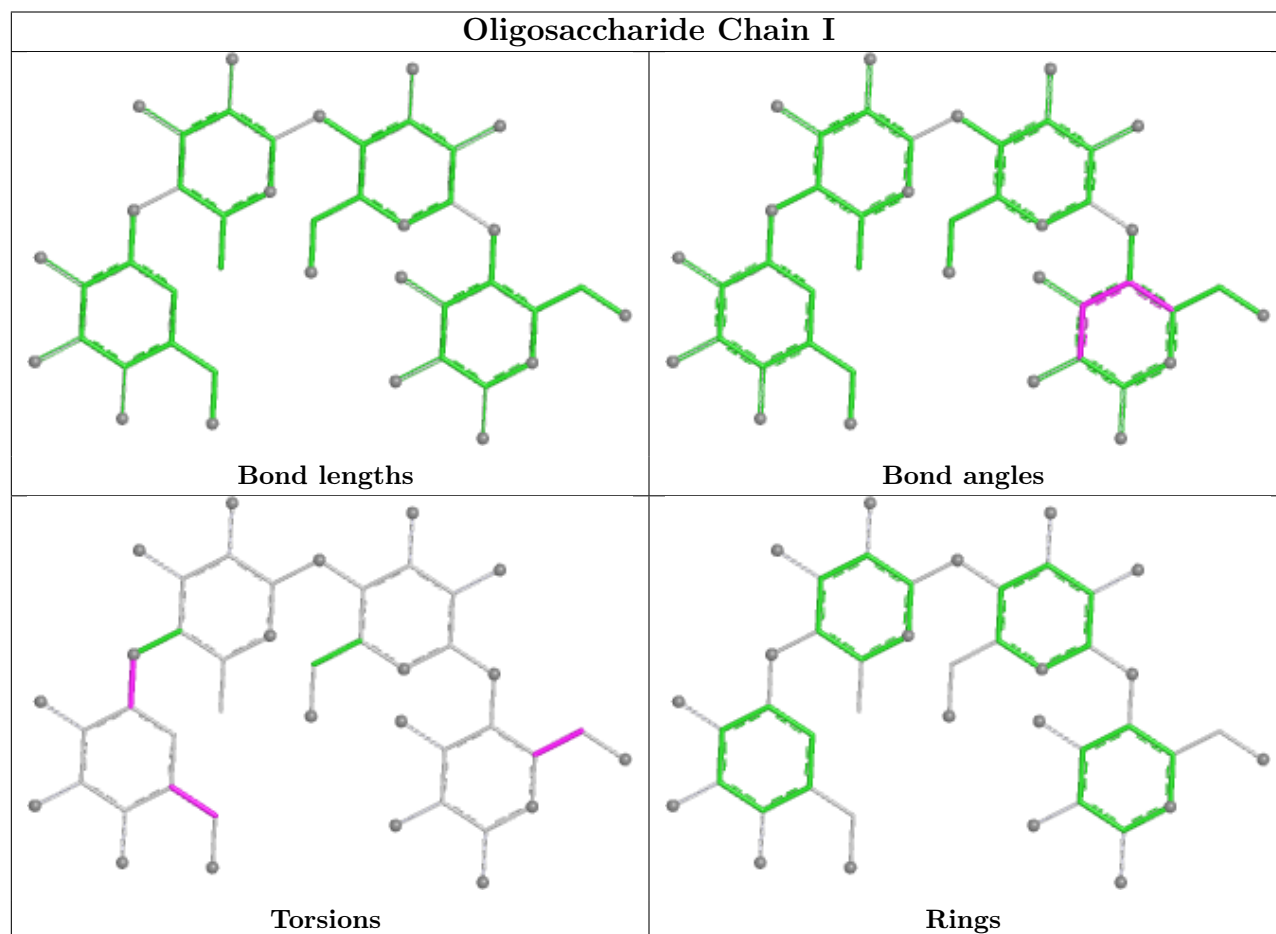
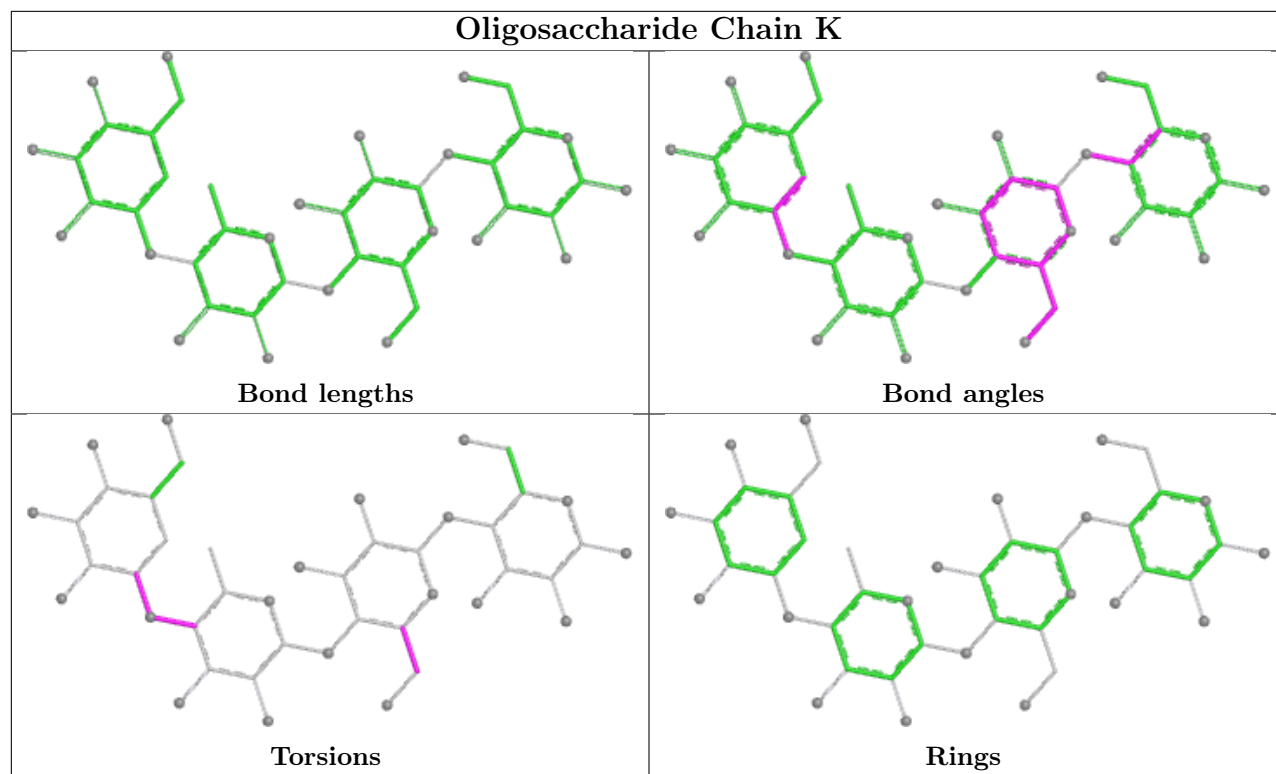
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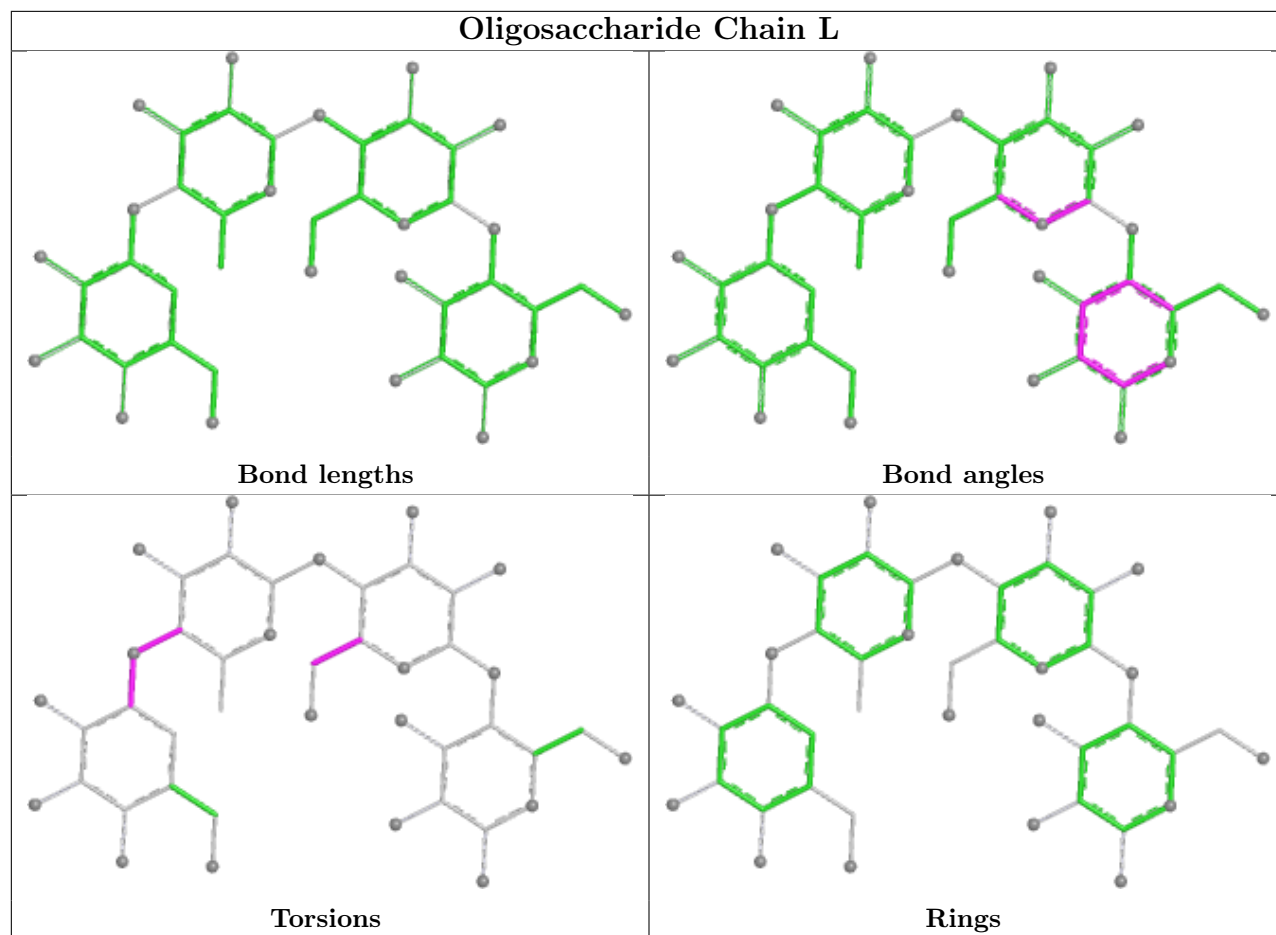
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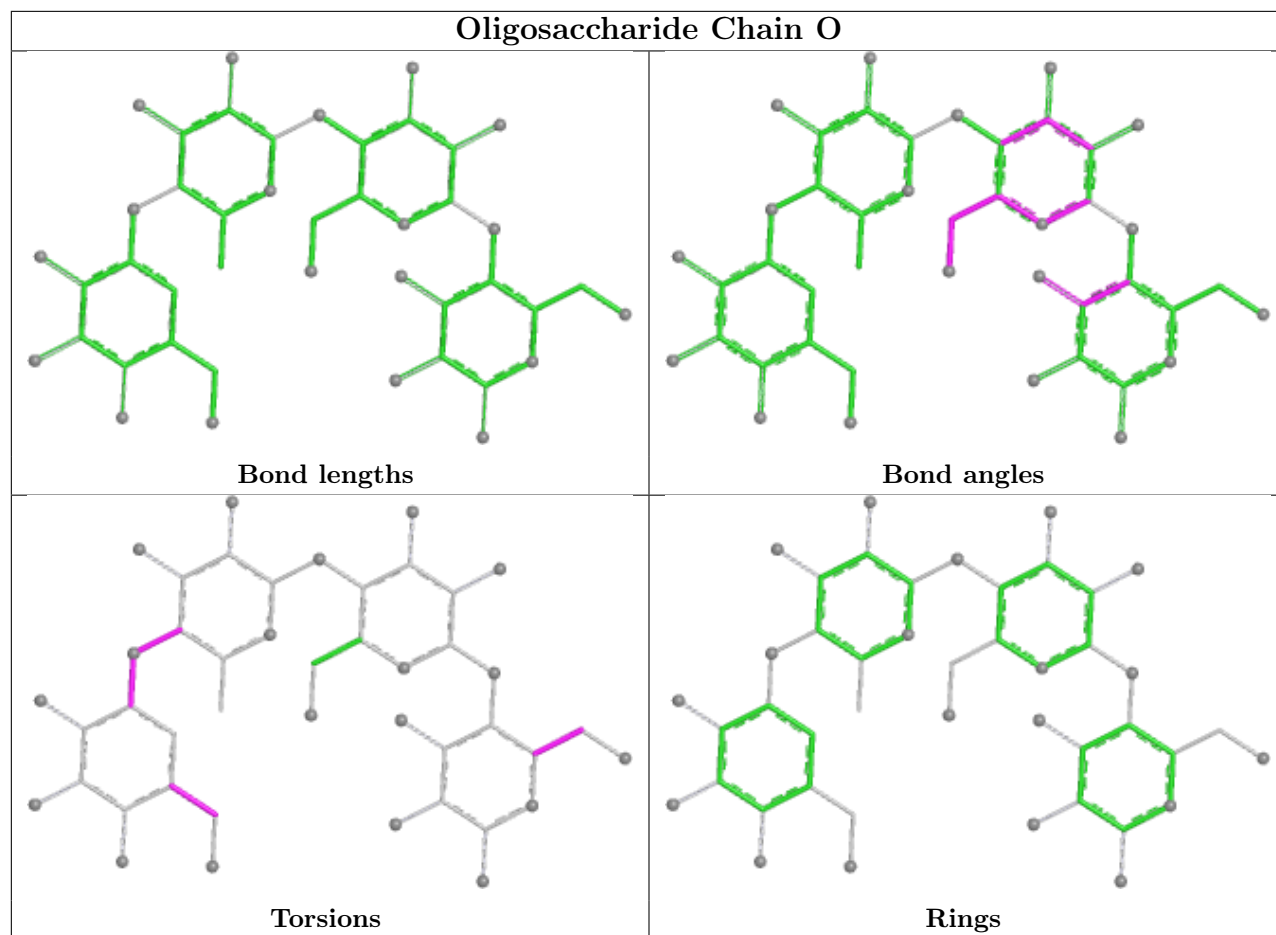
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	2	GLC	1	0
3	Q	3	AC1	1	0
2	K	3	AC1	1	0
3	N	1	GLC	1	0
3	V	3	AC1	3	0

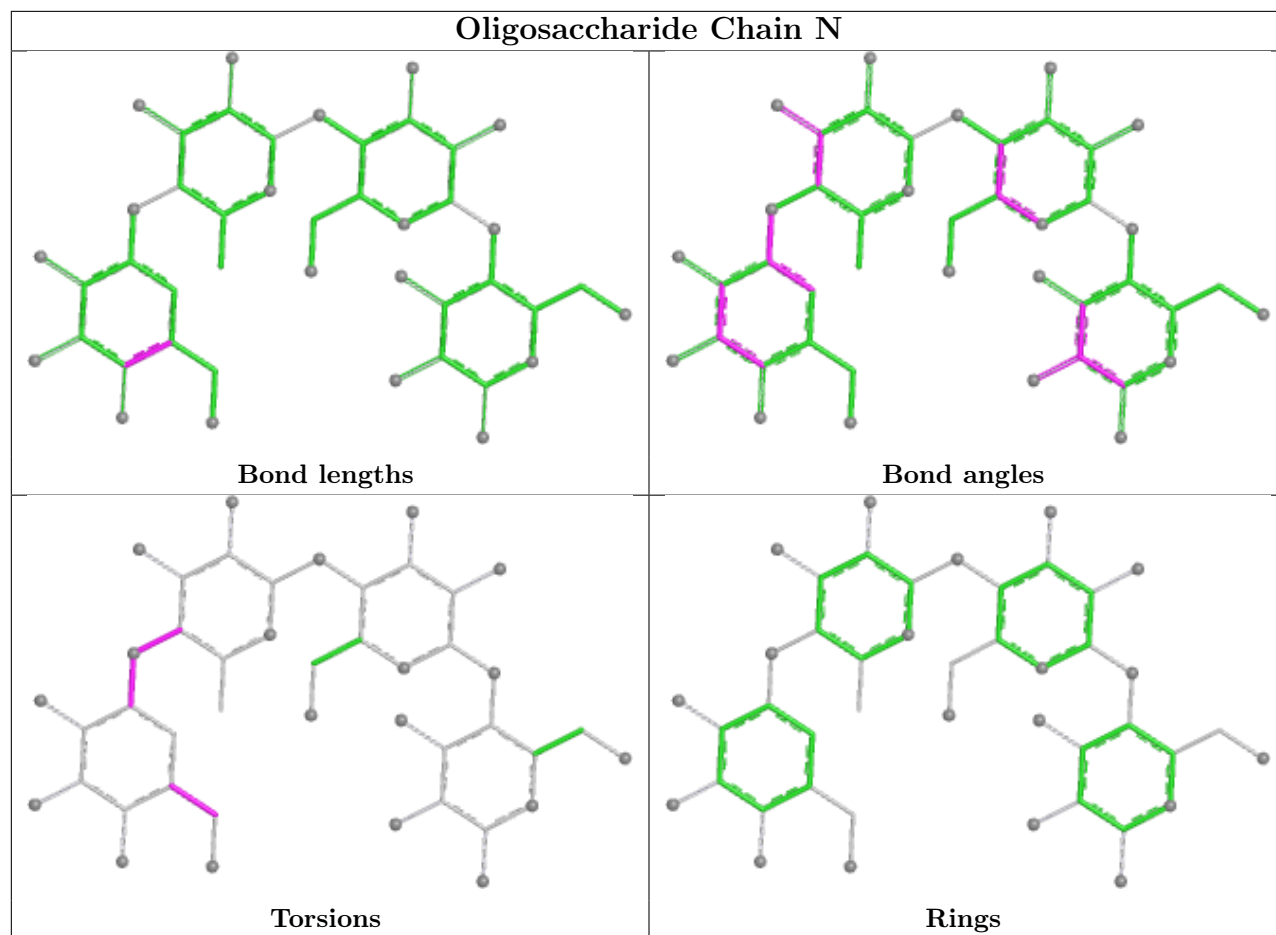
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

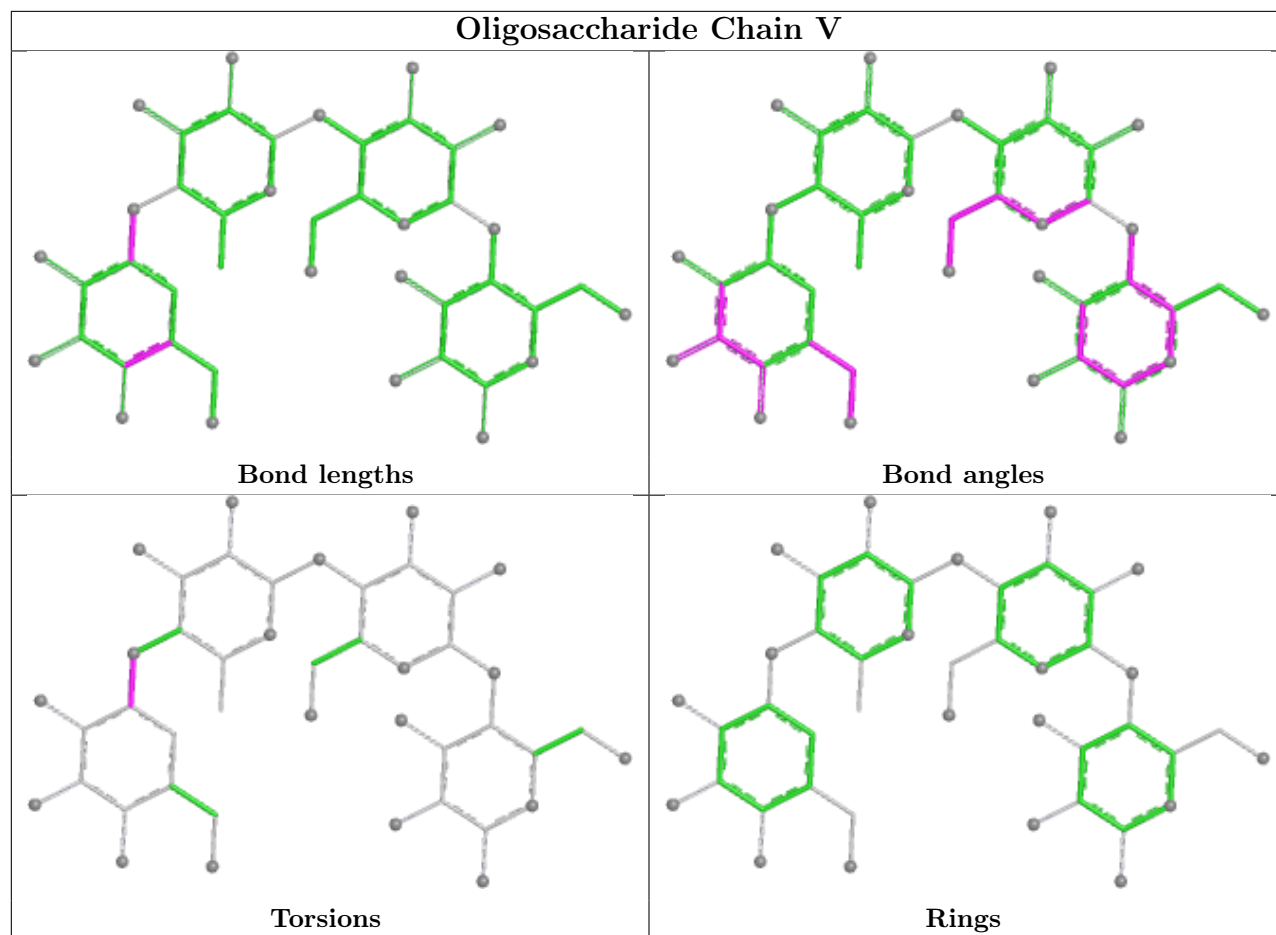




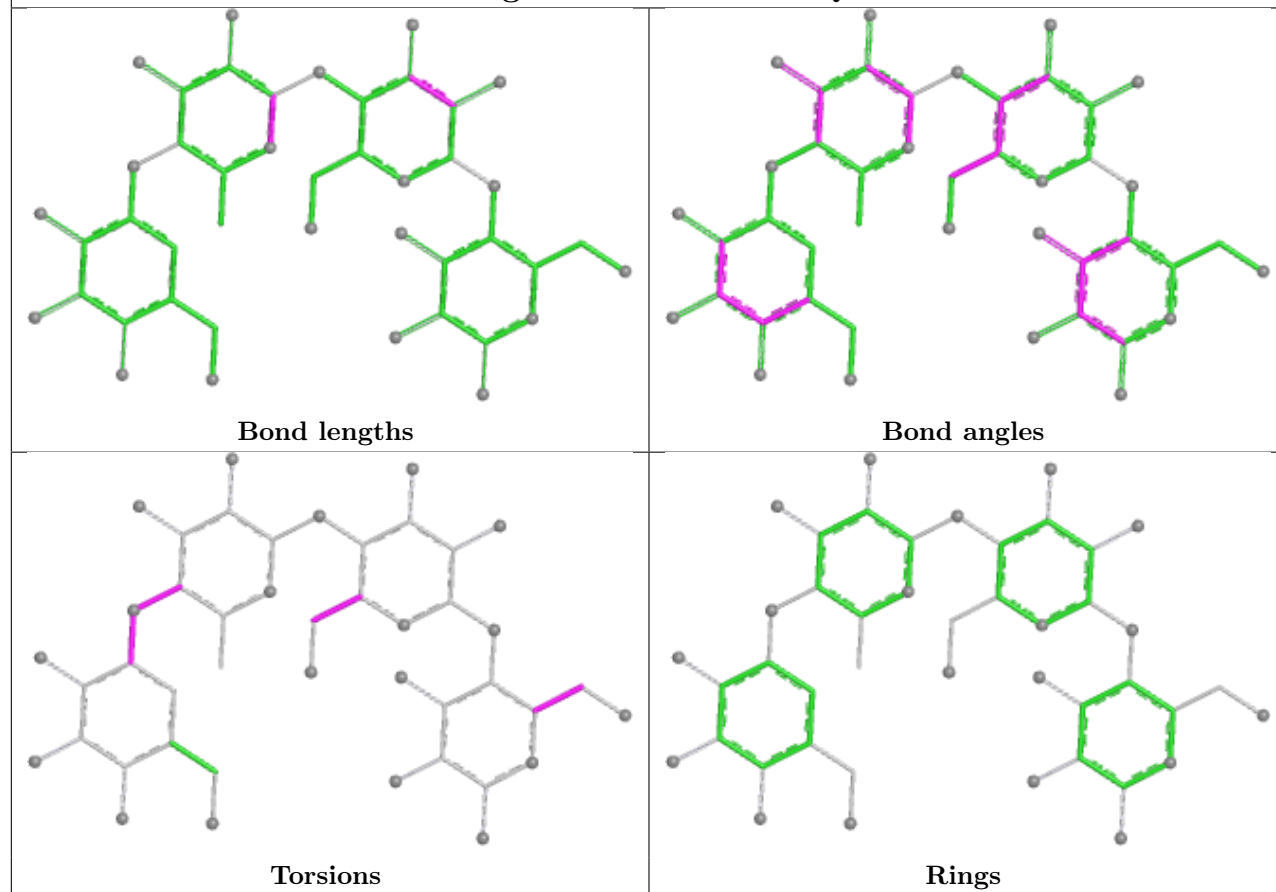




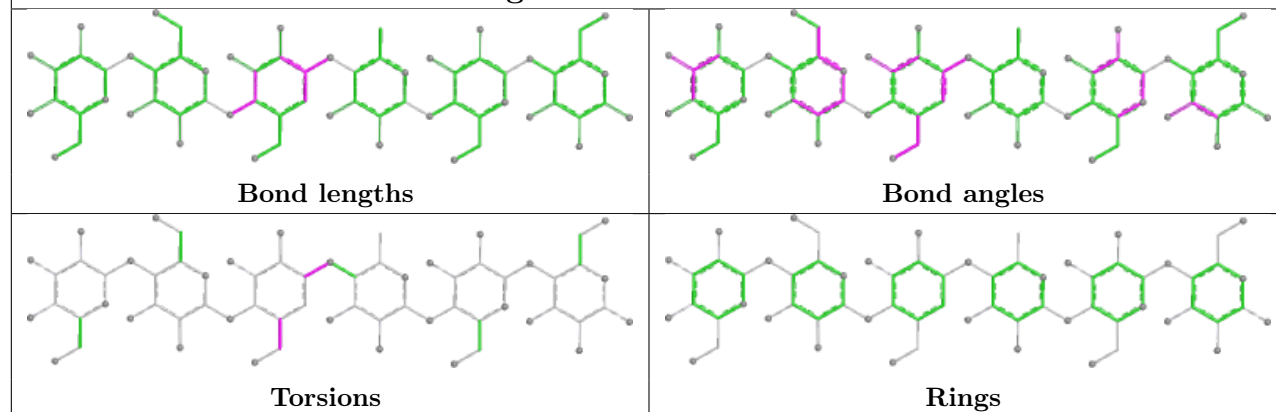


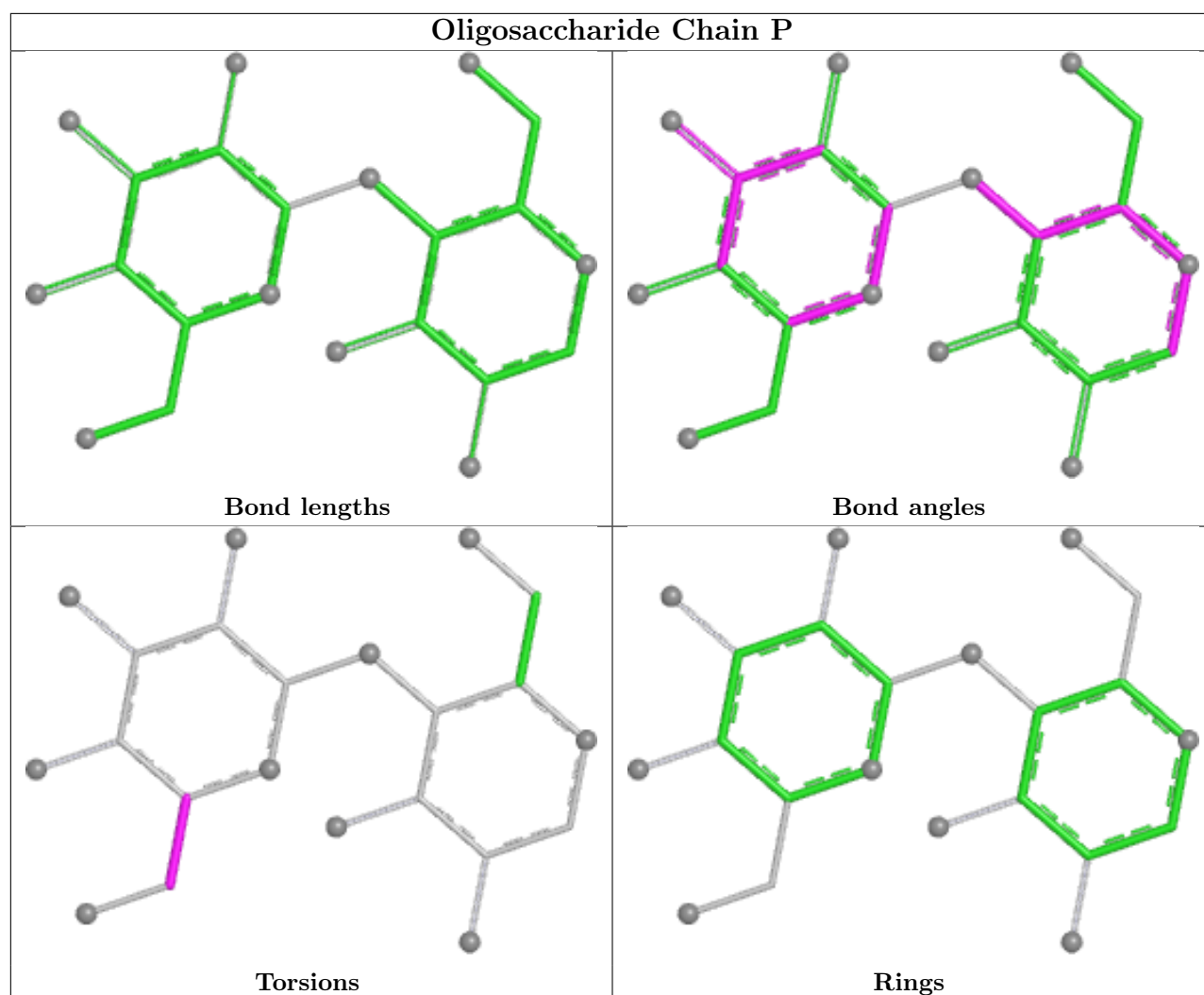


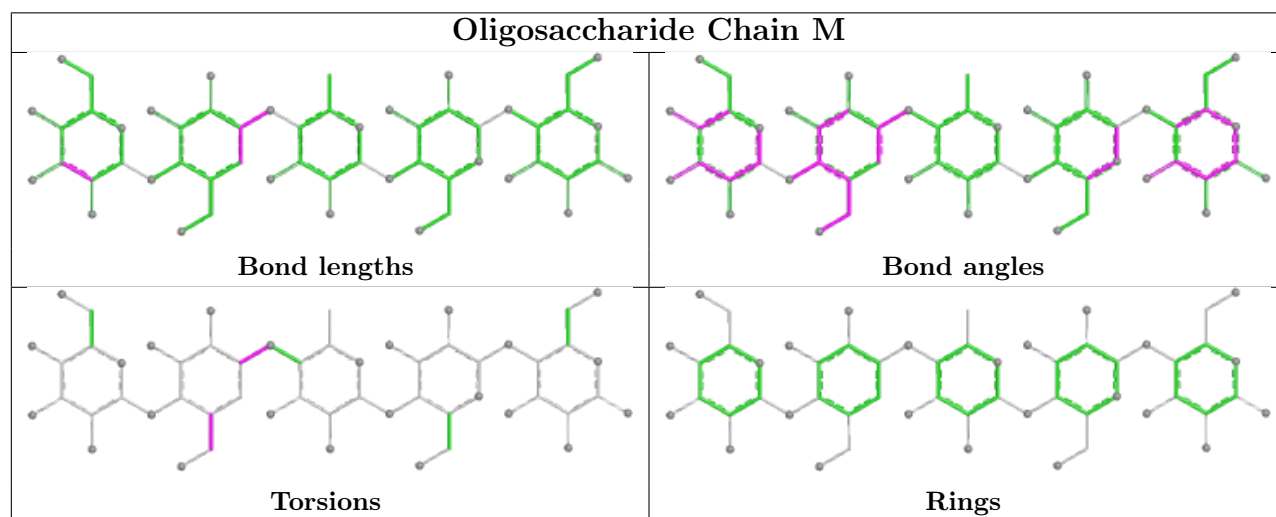
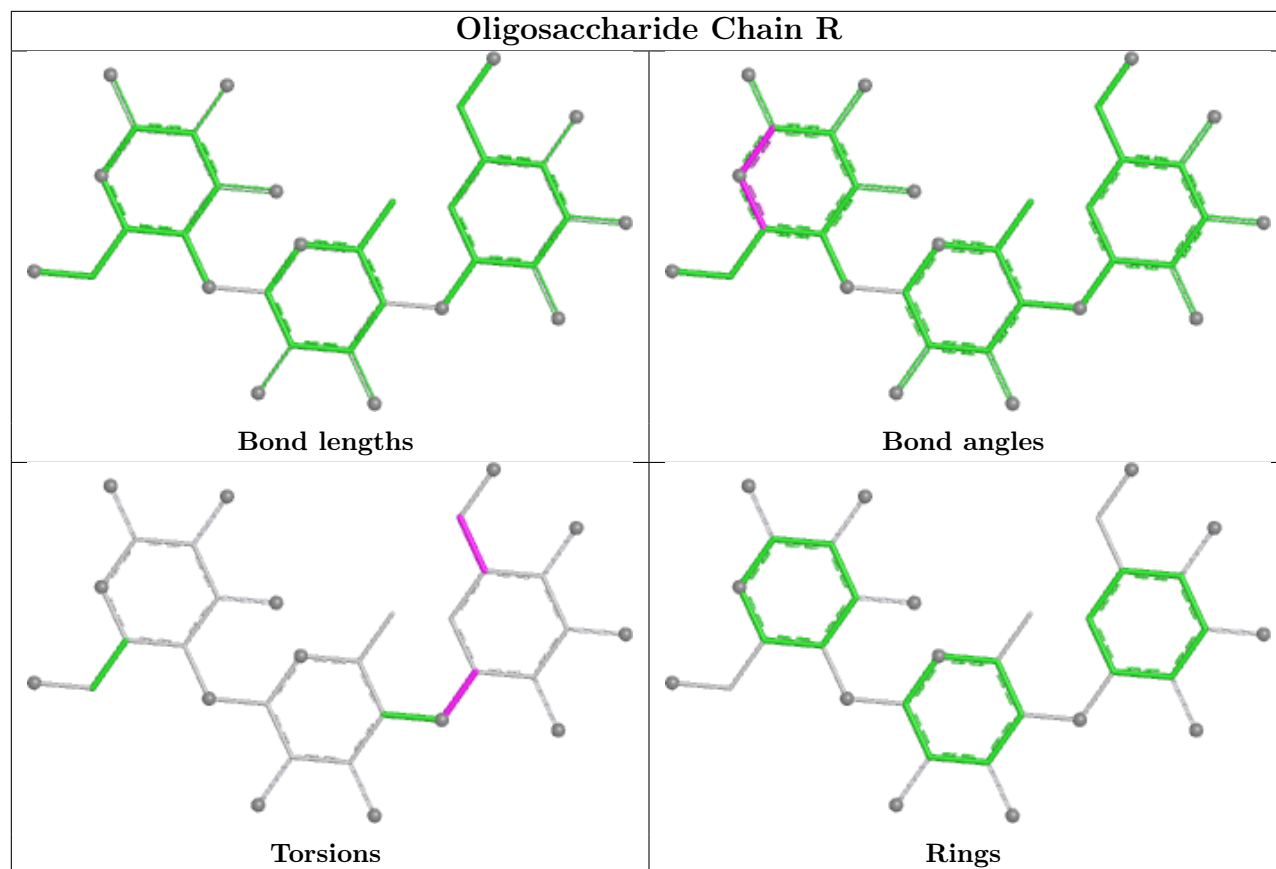
Oligosaccharide Chain Q

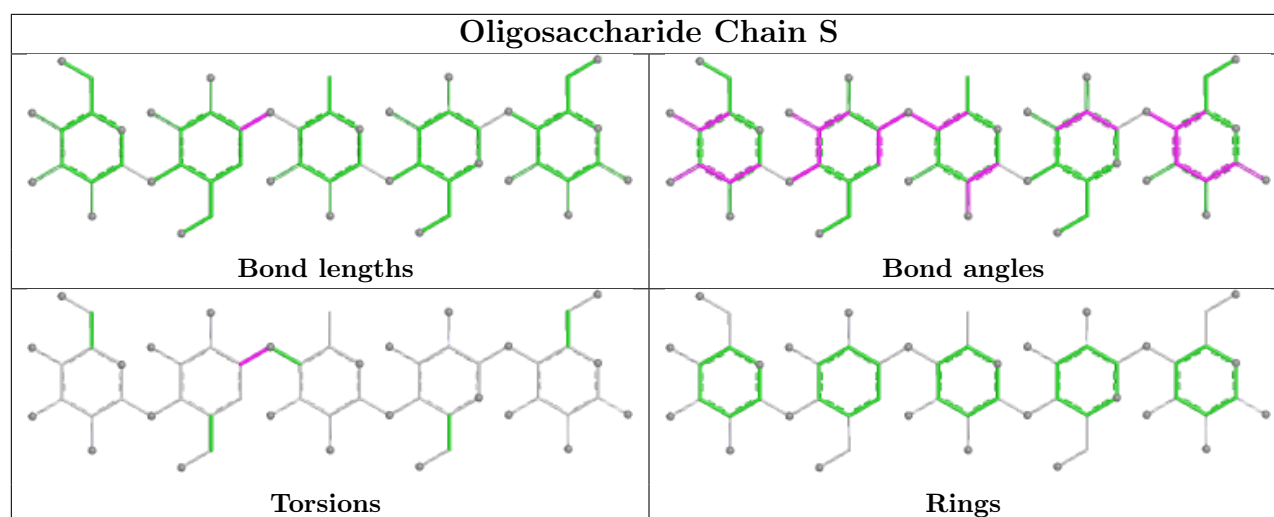


Oligosaccharide Chain J









5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 9 are monoatomic - leaving 17 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	$\# Z > 2$
13	ACT	C	804	-	3,3,3	0.69	0	3,3,3	1.04	0
12	EDO	A	805	-	3,3,3	0.32	0	2,2,2	0.16	0
11	GOL	B	806	-	5,5,5	0.19	0	5,5,5	0.66	0
15	PEG	D	803	-	6,6,6	0.44	0	5,5,5	0.23	0
15	PEG	B	804	-	6,6,6	0.59	0	5,5,5	0.40	0
11	GOL	B	805	-	5,5,5	0.11	0	5,5,5	0.26	0
11	GOL	C	802	-	5,5,5	0.17	0	5,5,5	0.36	0
8	GLC	B	801	2	12,12,12	0.76	0	17,17,17	1.20	2 (11%)
11	GOL	B	803	-	5,5,5	0.13	0	5,5,5	0.39	0
10	PGE	B	807	-	9,9,9	0.29	0	8,8,8	0.19	0
10	PGE	A	803	-	9,9,9	0.38	0	8,8,8	0.39	0
12	EDO	D	804	-	3,3,3	0.29	0	2,2,2	0.65	0
13	ACT	A	806	-	3,3,3	1.27	1 (33%)	3,3,3	0.59	0
13	ACT	B	808	-	3,3,3	1.50	1 (33%)	3,3,3	0.76	0
11	GOL	C	803	-	5,5,5	0.08	0	5,5,5	0.27	0
8	GLC	A	801[B]	2	12,12,12	0.64	0	17,17,17	1.02	0
11	GOL	A	804	-	5,5,5	0.11	0	5,5,5	0.35	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	EDO	A	805	-	-	0/1/1/1	-
11	GOL	B	806	-	-	0/4/4/4	-
15	PEG	D	803	-	-	1/4/4/4	-
15	PEG	B	804	-	-	0/4/4/4	-
11	GOL	B	805	-	-	4/4/4/4	-
11	GOL	C	802	-	-	2/4/4/4	-
8	GLC	B	801	2	-	0/2/22/22	0/1/1/1
11	GOL	B	803	-	-	2/4/4/4	-
10	PGE	B	807	-	-	5/7/7/7	-
10	PGE	A	803	-	-	3/7/7/7	-
12	EDO	D	804	-	-	1/1/1/1	-
11	GOL	C	803	-	-	1/4/4/4	-
8	GLC	A	801[B]	2	-	1/2/22/22	0/1/1/1
11	GOL	A	804	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	808	ACT	OXT-C	-2.58	1.18	1.30
13	A	806	ACT	OXT-C	-2.18	1.20	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	801	GLC	O3-C3-C2	-2.16	105.29	110.38
8	B	801	GLC	C1-C2-C3	-2.02	106.24	110.36

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	B	803	GOL	C1-C2-C3-O3
11	B	805	GOL	O1-C1-C2-O2
11	B	805	GOL	O1-C1-C2-C3
11	B	805	GOL	C1-C2-C3-O3
11	C	802	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	B	807	PGE	O3-C5-C6-O4
11	B	803	GOL	O2-C2-C3-O3
10	B	807	PGE	O1-C1-C2-O2
15	D	803	PEG	O1-C1-C2-O2
11	B	805	GOL	O2-C2-C3-O3
11	C	802	GOL	O1-C1-C2-O2
10	A	803	PGE	O2-C3-C4-O3
10	A	803	PGE	C4-C3-O2-C2
10	B	807	PGE	C4-C3-O2-C2
11	C	803	GOL	C1-C2-C3-O3
10	A	803	PGE	O3-C5-C6-O4
10	B	807	PGE	C3-C4-O3-C5
8	A	801[B]	GLC	O5-C5-C6-O6
12	D	804	EDO	O1-C1-C2-O2
10	B	807	PGE	C1-C2-O2-C3

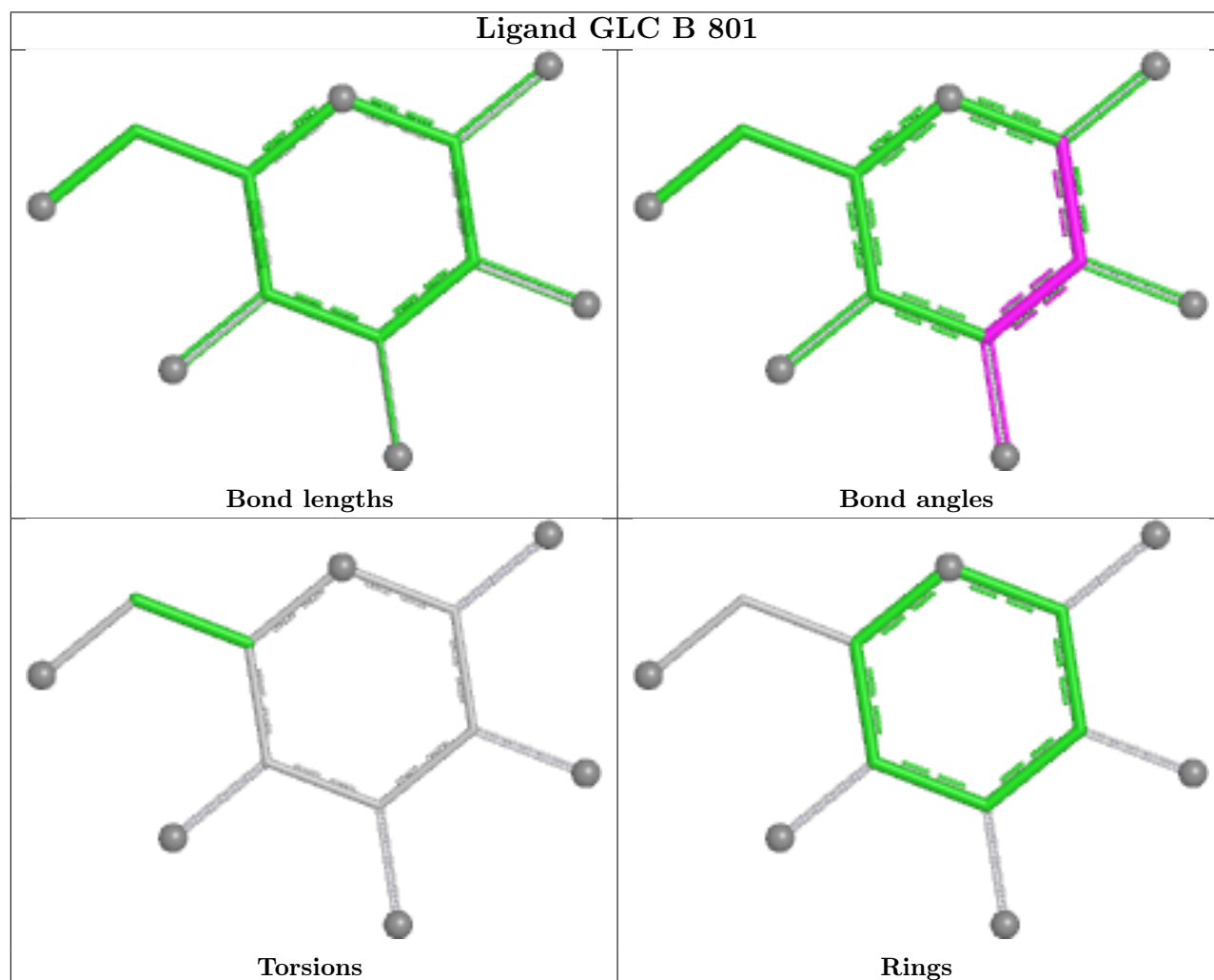
There are no ring outliers.

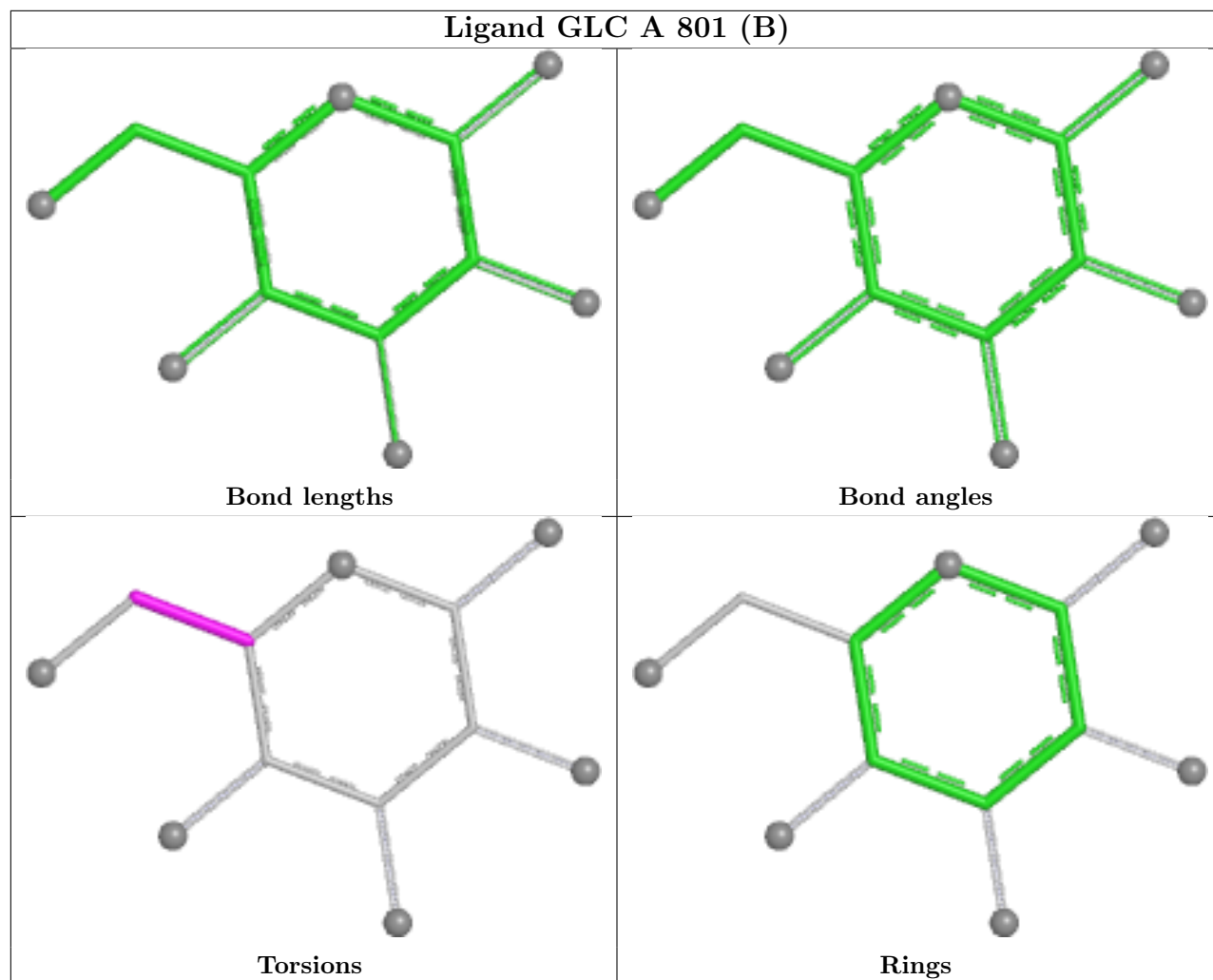
11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	805	EDO	1	0
11	B	806	GOL	1	0
15	D	803	PEG	1	0
15	B	804	PEG	2	0
11	B	805	GOL	1	0
10	A	803	PGE	2	0
12	D	804	EDO	2	0
13	A	806	ACT	1	0
13	B	808	ACT	1	0
11	C	803	GOL	1	0
11	A	804	GOL	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	712/738 (96%)	-0.02	18 (2%) 58 58	8, 21, 46, 69	5 (0%)
1	B	712/738 (96%)	-0.15	13 (1%) 67 67	7, 18, 45, 75	4 (0%)
1	C	709/738 (96%)	0.22	24 (3%) 48 47	13, 26, 52, 81	2 (0%)
1	D	712/738 (96%)	0.24	18 (2%) 58 58	13, 28, 50, 75	1 (0%)
All	All	2845/2952 (96%)	0.07	73 (2%) 57 56	7, 24, 48, 81	12 (0%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	45	VAL	5.3
1	B	167	TRP	4.9
1	C	167	TRP	4.8
1	A	245	ALA	4.6
1	D	167	TRP	4.6
1	B	245	ALA	4.3
1	A	735	ASN	4.2
1	A	736	PRO	3.8
1	D	45	VAL	3.8
1	A	246	GLY	3.7
1	A	757	ALA	3.6
1	A	244	THR	3.4
1	C	736	PRO	3.3
1	D	757	ALA	3.3
1	A	178	SER	3.3
1	B	734	GLY	3.1
1	C	733	ASN	3.1
1	C	245	ALA	3.1
1	A	179	GLY	3.1
1	A	734	GLY	3.0
1	C	166	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	44	GLN	2.9
1	B	757	ALA	2.9
1	C	758	GLU	2.8
1	A	74	ASN	2.8
1	D	743	ILE	2.8
1	B	758	GLU	2.8
1	C	244	THR	2.7
1	B	120	SER	2.7
1	D	740	GLU	2.6
1	A	728	TYR	2.6
1	C	299	PRO	2.6
1	B	735	ASN	2.6
1	C	726	THR	2.6
1	C	180	GLU	2.5
1	A	737	VAL	2.5
1	D	166	ILE	2.5
1	C	179	GLY	2.4
1	D	725	GLY	2.4
1	B	295	THR	2.4
1	C	727	TRP	2.4
1	B	166	ILE	2.4
1	D	702	VAL	2.4
1	B	116	SER	2.4
1	C	178	SER	2.4
1	D	110	THR	2.4
1	B	733	ASN	2.4
1	C	715	ASN	2.4
1	C	246	GLY	2.4
1	D	737	VAL	2.4
1	D	306	GLU	2.3
1	B	125	HIS	2.3
1	D	755	ASN	2.3
1	C	243	LEU	2.3
1	A	125[A]	HIS	2.3
1	D	727	TRP	2.2
1	C	296	ASN	2.2
1	C	728	TYR	2.2
1	C	177	ILE	2.2
1	C	120	SER	2.2
1	A	741	LYS	2.2
1	D	103	ASN	2.1
1	A	306	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	743	ILE	2.1
1	C	741	LYS	2.1
1	C	298	GLN	2.1
1	B	112	ASP	2.1
1	A	46	LEU	2.1
1	D	499	ALA	2.1
1	D	56	ILE	2.0
1	D	726	THR	2.0
1	A	296	ASN	2.0
1	C	757	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GLC	J	1	12/12	0.68	0.15	17,22,28,28	0
2	BGC	H	1[A]	12/12	0.84	0.15	21,31,34,35	12
5	GLC	P	1	11/12	0.84	0.13	23,27,31,35	0
2	BGC	K	1	12/12	-	-	24,34,37,40	12
3	GLC	I	1	12/12	0.85	0.14	44,68,76,79	0
2	AC1	K	3	21/22	-	-	16,21,33,44	0
2	GLC	K	2	11/12	0.86	0.13	15,17,21,27	0
3	GLC	N	1	12/12	0.87	0.12	30,56,59,62	0
3	GLC	Q	1	12/12	0.89	0.10	32,53,59,59	0
3	AC1	Q	3	21/22	0.91	0.10	17,27,53,62	0
3	GLC	L	2	11/12	-	-	16,20,23,27	0
3	AC1	L	3	21/22	-	-	11,15,24,31	0
3	GLC	O	2	11/12	0.92	0.07	25,32,35,38	0
3	GLC	O	1	12/12	0.92	0.08	51,80,84,90	0
4	GLC	J	2	11/12	0.93	0.08	13,15,16,17	0
4	AC1	J	3	21/22	0.93	0.09	12,16,19,25	0
3	AC1	O	3	21/22	0.93	0.08	25,32,42,50	0
2	AC1	H	3	21/22	0.94	0.08	14,22,34,48	0

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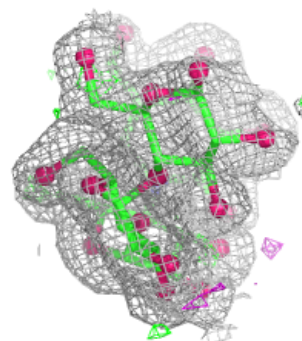
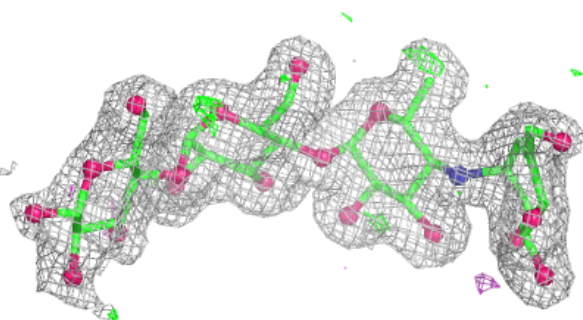
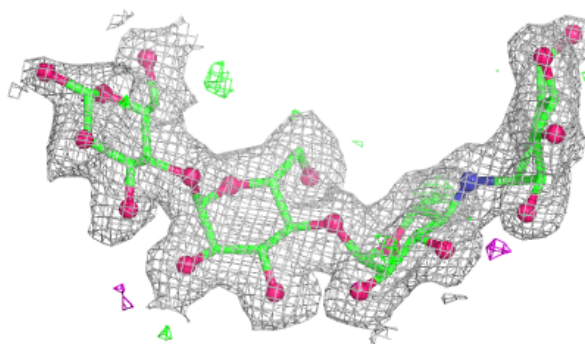
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GLC	V	1	12/12	-	-	25,33,34,34	0
3	GLC	V	2	11/12	-	-	20,24,27,28	0
3	AC1	V	3	21/22	-	-	19,23,26,33	0
3	GLC	L	1	12/12	0.94	0.07	27,52,55,59	0
3	GLC	Q	2	11/12	0.95	0.07	17,22,26,33	0
3	AC1	N	3	21/22	0.95	0.08	18,23,43,48	0
2	GLC	H	2	11/12	0.95	0.07	12,15,17,20	0
5	GLC	P	2	11/12	0.95	0.07	38,42,56,71	0
7	GLC	M	1	12/12	0.95	0.06	16,20,24,27	0
4	GLC	J	4	11/12	-	-	13,15,19,21	0
4	GLC	J	5	11/12	-	-	27,31,46,63	0
7	AC1	M	3	21/22	0.95	0.07	11,14,16,23	0
3	GLC	N	2	11/12	0.96	0.06	21,22,25,26	0
6	GLC	R	1	12/12	-	-	37,43,44,46	0
6	AC1	R	2	21/22	-	-	32,43,54,57	0
3	AC1	I	3	21/22	0.96	0.06	18,25,37,47	0
7	GLC	M	4	11/12	0.96	0.06	12,14,16,17	0
3	GLC	I	2	11/12	0.97	0.05	20,26,36,41	0
7	GLC	M	2	11/12	0.97	0.04	12,13,14,15	0
7	GLC	S	1	12/12	-	-	34,40,44,45	0
7	GLC	S	2	11/12	-	-	29,32,36,38	0
7	AC1	S	3	21/22	-	-	21,29,31,32	0
7	GLC	S	4	11/12	-	-	23,25,28,32	0

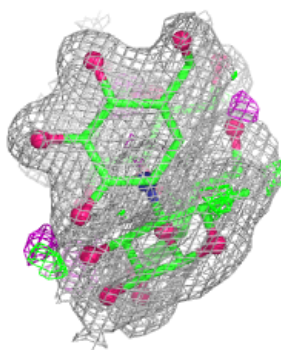
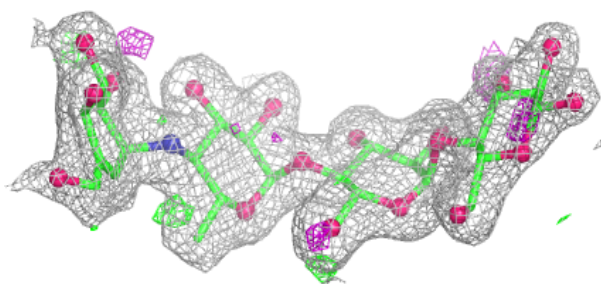
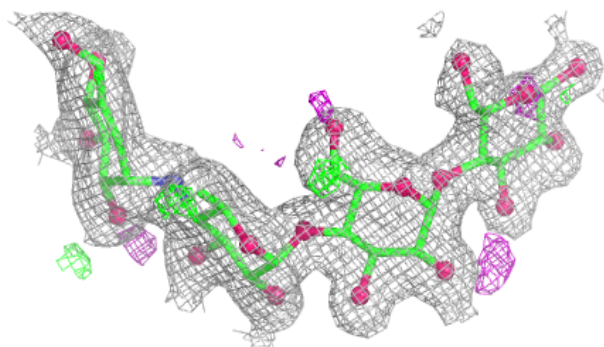
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

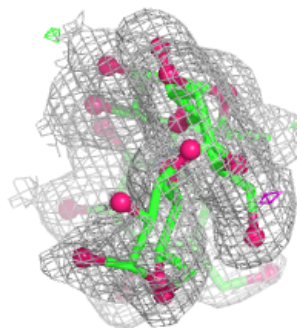
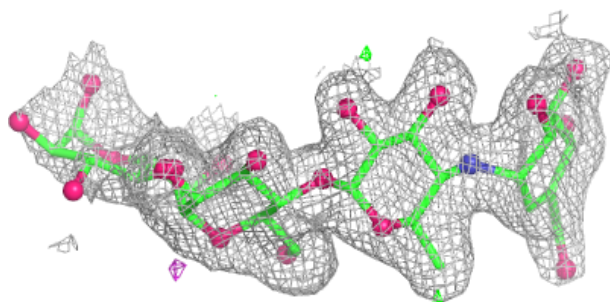
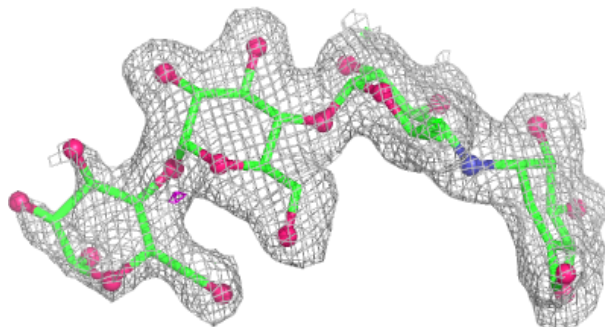
**Electron density around Chain K:**

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and green (positive)

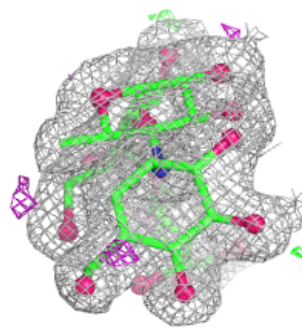
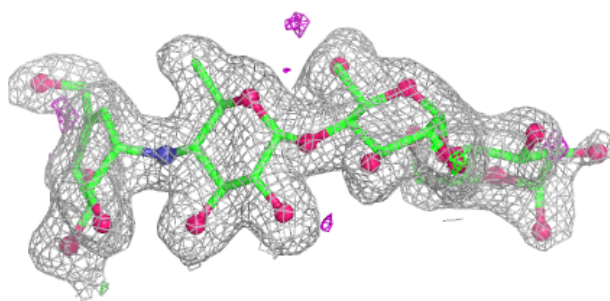
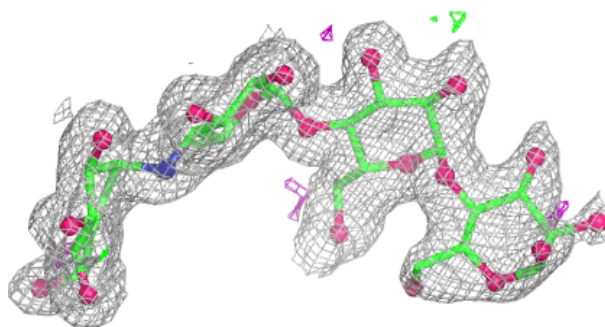


Electron density around Chain I:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

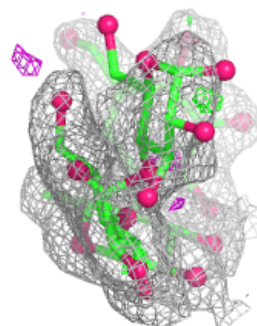
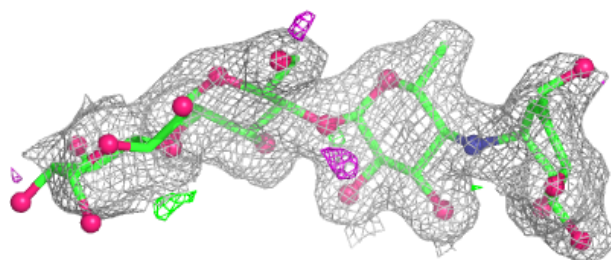
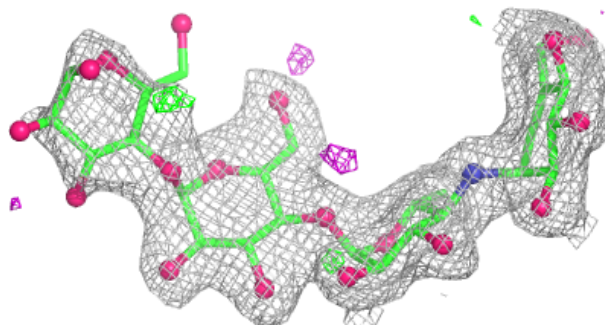
**Electron density around Chain L:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

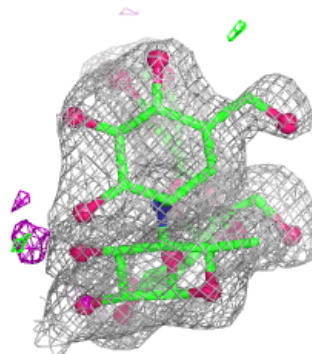
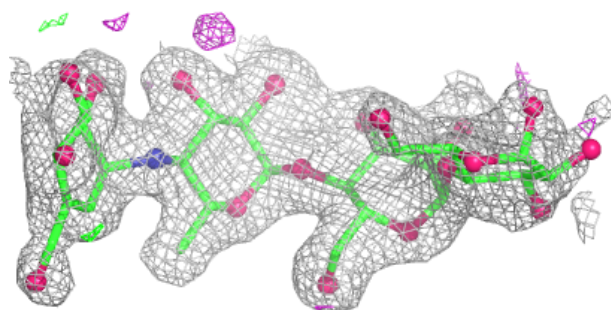
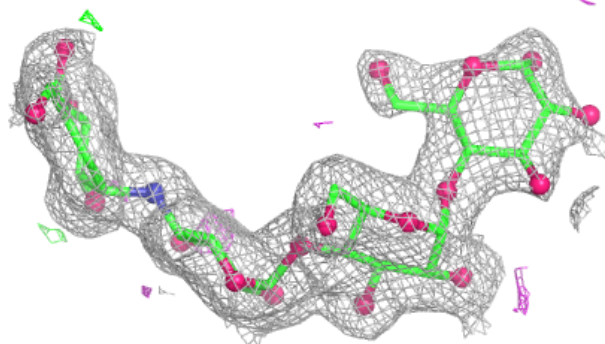


Electron density around Chain O:

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

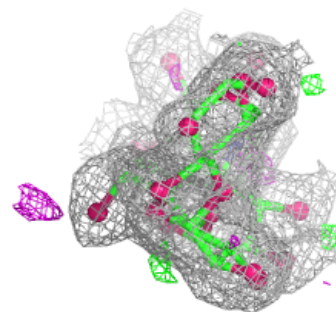
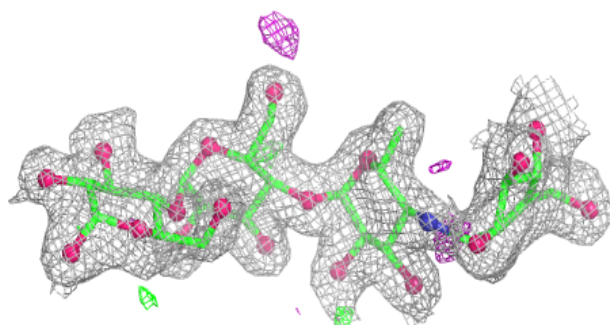
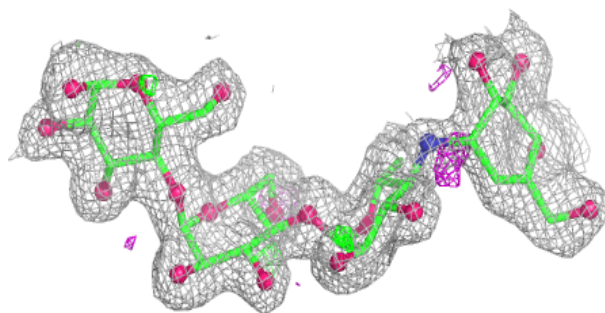
**Electron density around Chain N:**

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and green (positive)

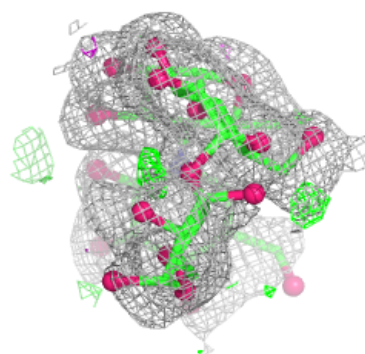
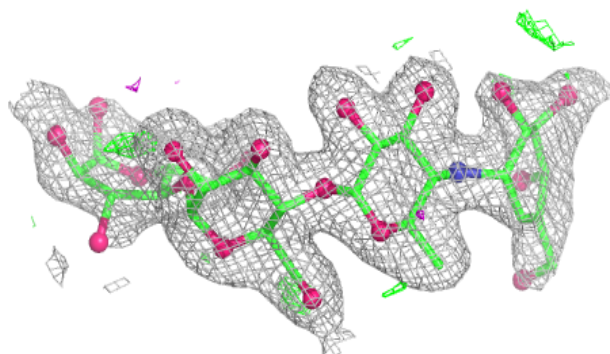
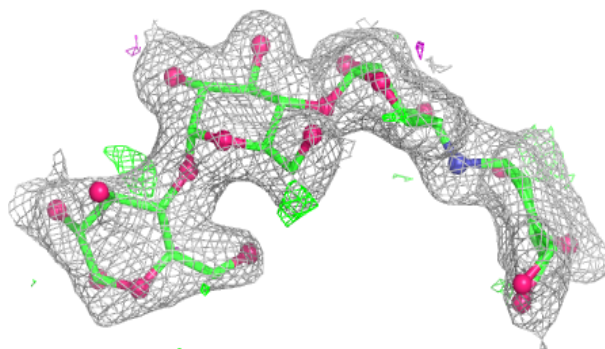


Electron density around Chain V:

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and green (positive)

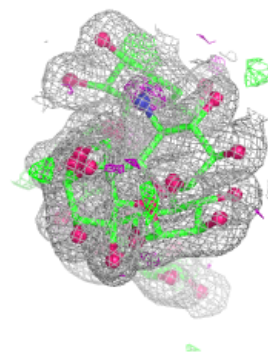
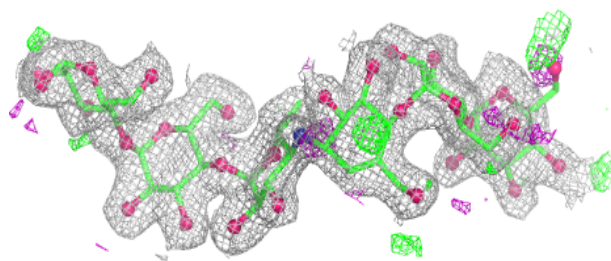
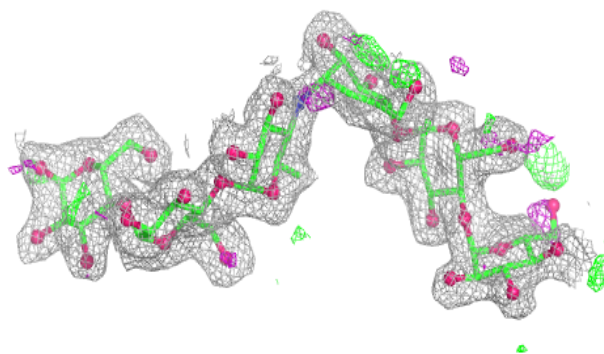
**Electron density around Chain Q:**

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and green (positive)



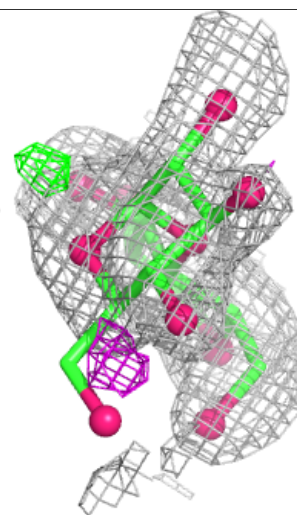
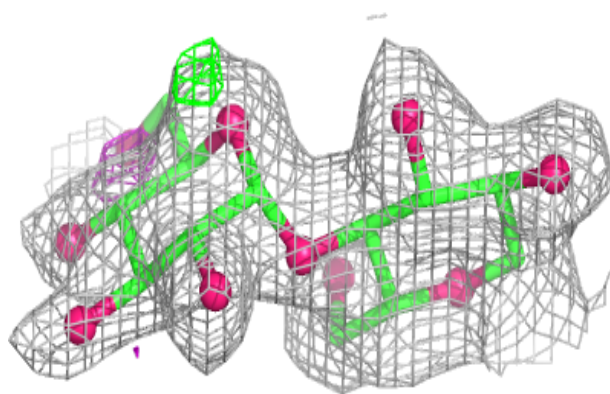
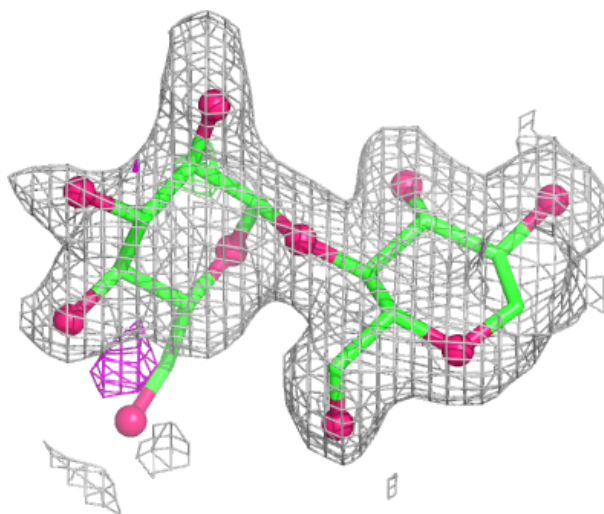
Electron density around Chain J:

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and green (positive)



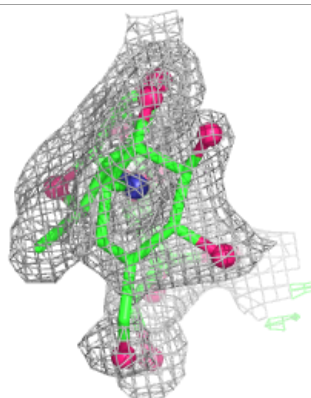
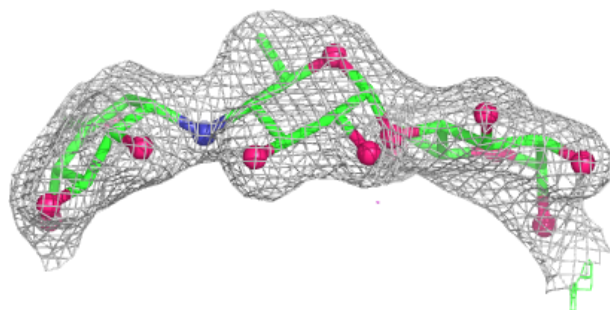
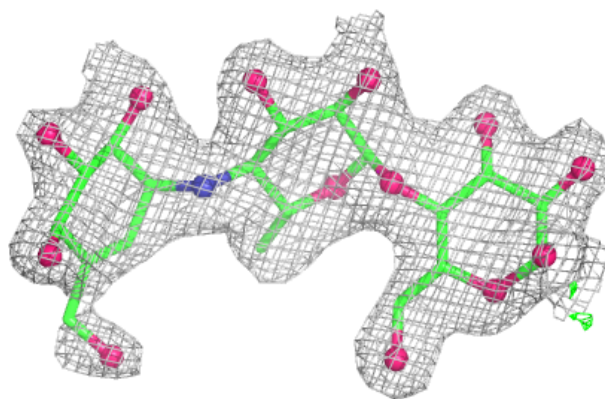
Electron density around Chain P:

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

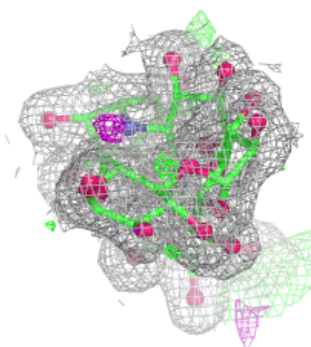
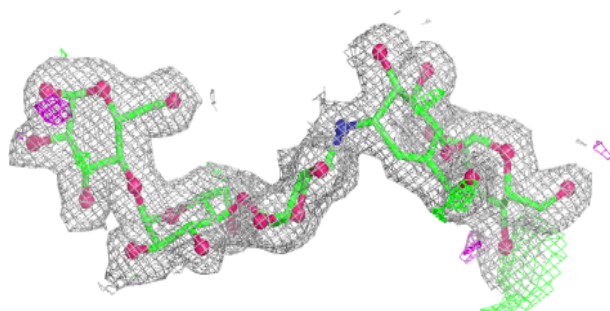
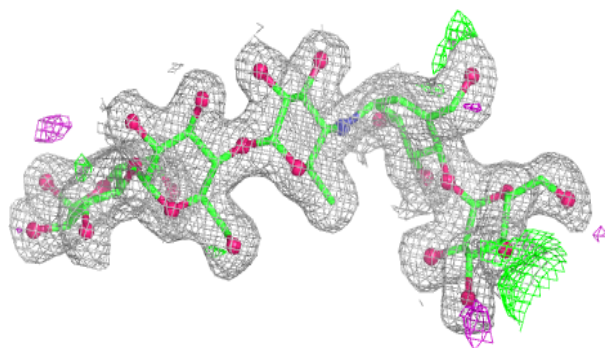


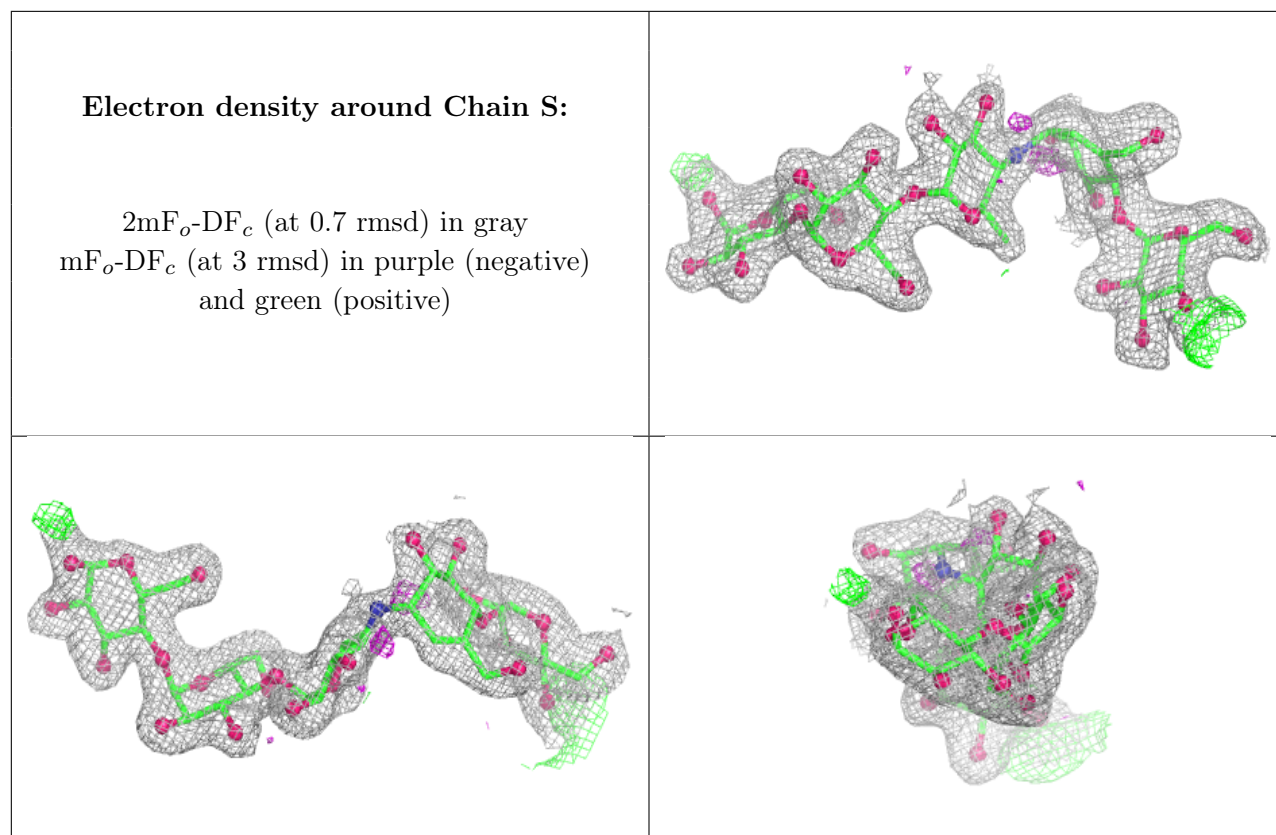
Electron density around Chain R:

$2mF_o-DF_c$ (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)





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
11	GOL	B	803	6/6	0.74	0.18	39,43,46,48	0
15	PEG	B	804	7/7	0.74	0.24	38,47,58,58	0
12	EDO	D	804	4/4	0.81	0.18	42,45,46,46	0
11	GOL	C	803	6/6	0.81	0.18	61,64,66,66	0
11	GOL	B	805	6/6	0.84	0.19	51,61,63,64	0
15	PEG	D	803	7/7	0.84	0.15	37,45,48,49	0
11	GOL	A	804	6/6	0.85	0.17	58,61,62,67	0
8	GLC	B	801	12/12	0.86	0.10	21,25,26,27	12
11	GOL	C	802	6/6	0.86	0.15	33,44,48,49	0
10	PGE	A	803	10/10	0.87	0.13	34,39,46,47	0
10	PGE	B	807	10/10	0.88	0.14	36,47,54,59	0
8	GLC	A	801[B]	12/12	0.90	0.09	21,30,33,34	12
16	CL	D	802	1/1	0.90	0.11	51,51,51,51	0
13	ACT	A	806	4/4	0.91	0.10	28,30,32,35	0

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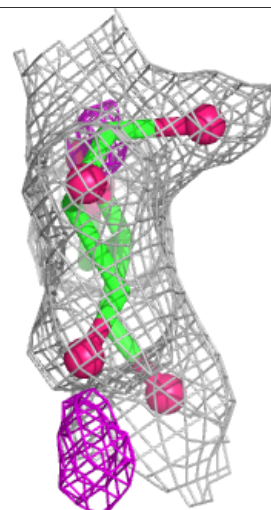
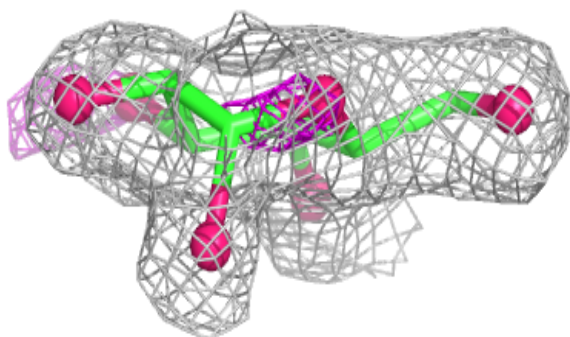
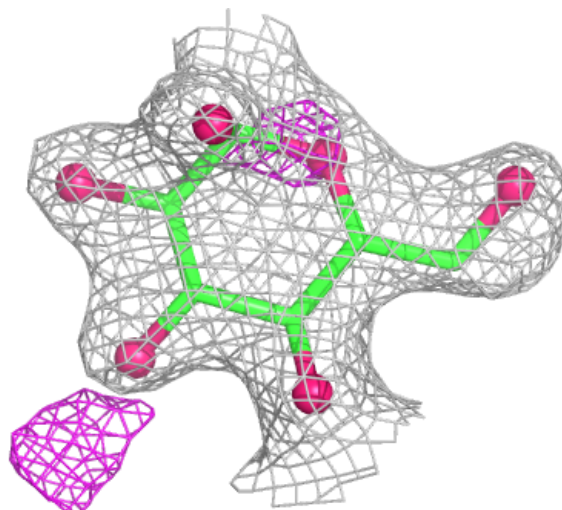
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
11	GOL	B	806	6/6	0.94	0.12	21,32,33,39	0
13	ACT	B	808	4/4	0.94	0.13	24,25,31,32	0
13	ACT	C	804	4/4	0.94	0.10	29,31,33,35	0
12	EDO	A	805	4/4	0.95	0.08	18,23,26,26	0
9	CA	C	801	1/1	0.98	0.03	21,21,21,21	0
14	MN	D	805	1/1	0.99	0.04	36,36,36,36	0
9	CA	D	801	1/1	0.99	0.02	18,18,18,18	0
14	MN	A	807	1/1	0.99	0.06	21,21,21,21	0
14	MN	C	805	1/1	0.99	0.05	31,31,31,31	0
14	MN	B	809	1/1	1.00	0.04	20,20,20,20	0
9	CA	A	802	1/1	1.00	0.02	13,13,13,13	0
9	CA	B	802	1/1	1.00	0.01	13,13,13,13	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

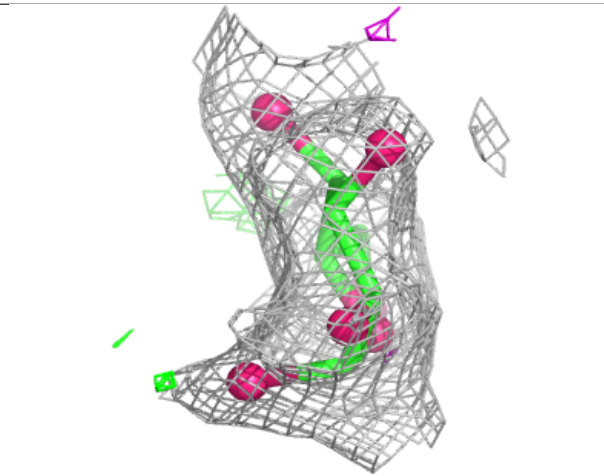
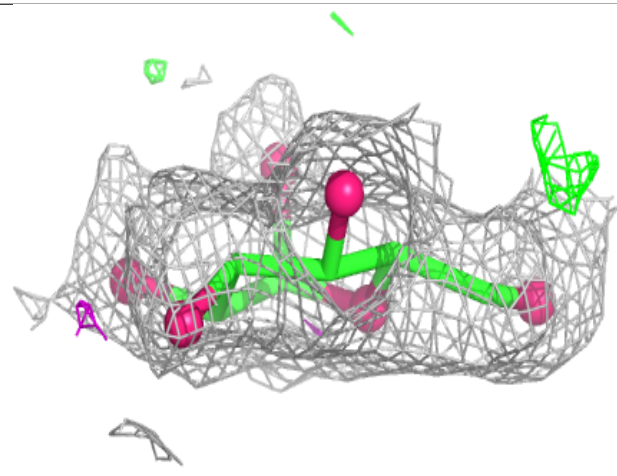
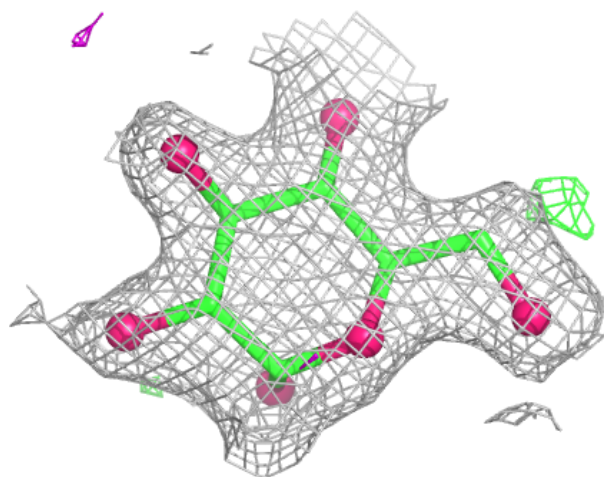
Electron density around GLC B 801:

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



Electron density around GLC A 801 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.