



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 3, 2024 – 12:33 PM EDT

PDB ID : 8DL2
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 wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

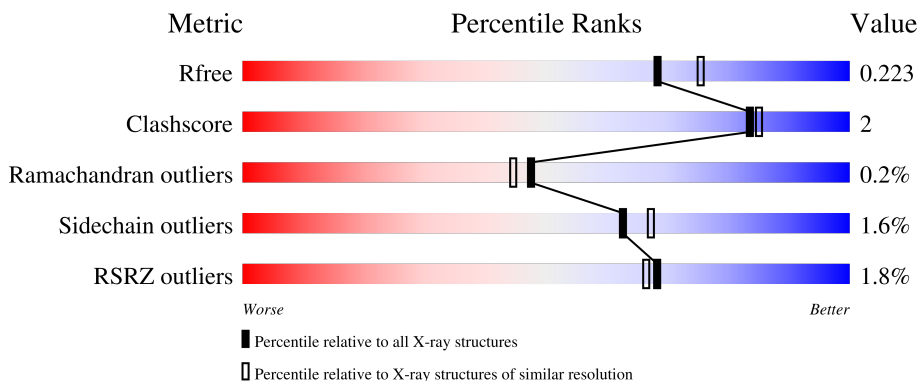
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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.





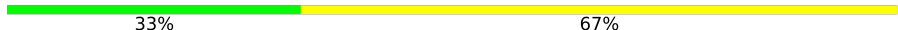

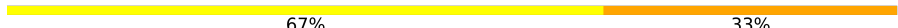
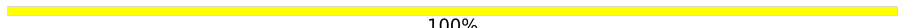

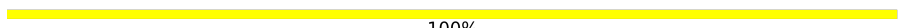
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	 91% 6%
1	B	738	 90% 6%
1	C	738	 90% 6%
1	D	738	 91% 5%
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	 100%
7	M	4	 50% 50%
7	S	4	 100%

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	712	Total 5718	C 3652	N 941	O 1103	S 22	0	5	0
1	B	712	Total 5713	C 3647	N 937	O 1107	S 22	0	4	0
1	C	709	Total 5680	C 3628	N 938	O 1092	S 22	0	2	0
1	D	712	Total 5681	C 3626	N 936	O 1097	S 22	0	1	0

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-glucopyranoside-(1-4)-beta-D-glucopyranose.

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

- 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-glucopyranoside-(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.

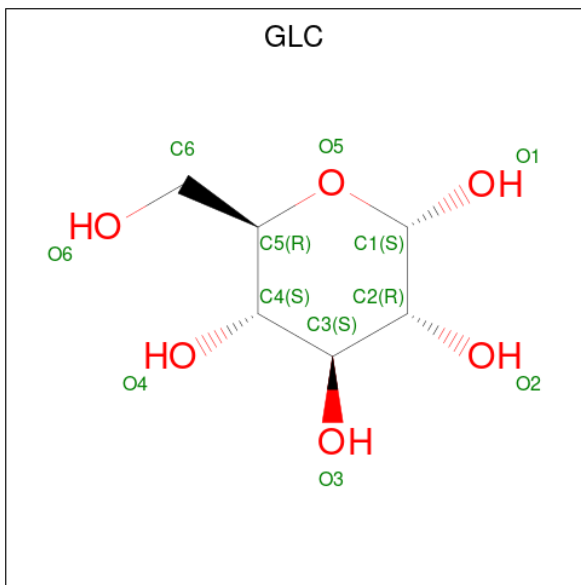
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	M	4	Total	C	N	O	0	0	0
			55	31	1	23			

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

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



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

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

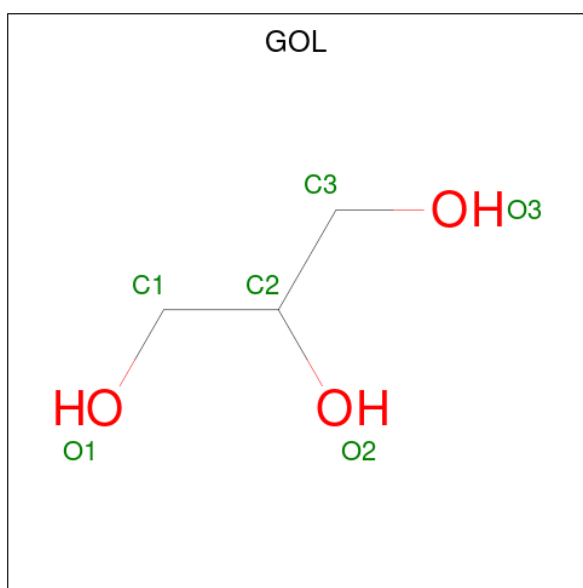
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
9	A	1	1	1	0	0
9	B	1	1	1	0	0
9	C	1	1	1	0	0
9	D	1	1	1	0	0

- Molecule 10 is TRIETHYLENE GLYCOL (three-letter code: 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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



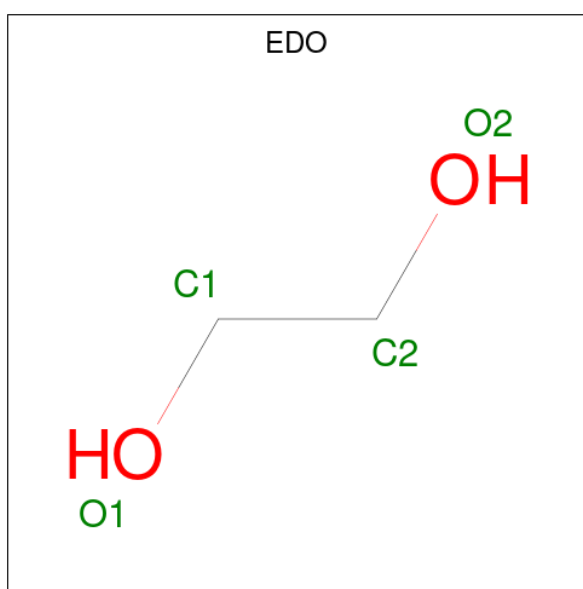
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		

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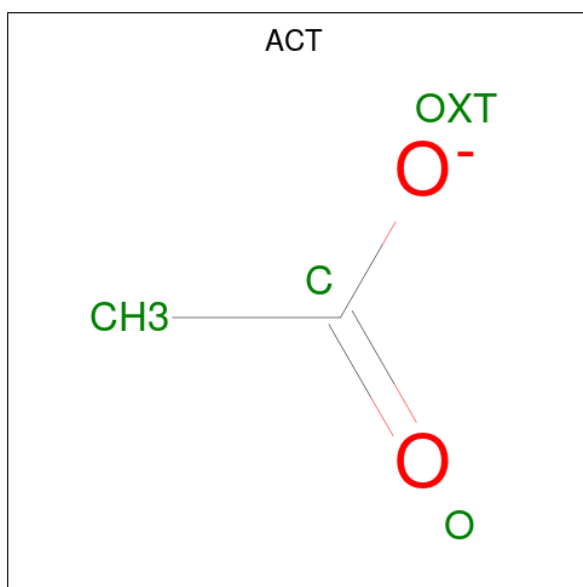
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			6	3	3		
11	B	1	Total	C	O	0	0
			6	3	3		
11	C	1	Total	C	O	0	0
			6	3	3		
11	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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 (three-letter code: ACT) (formula: C₂H₃O₂).

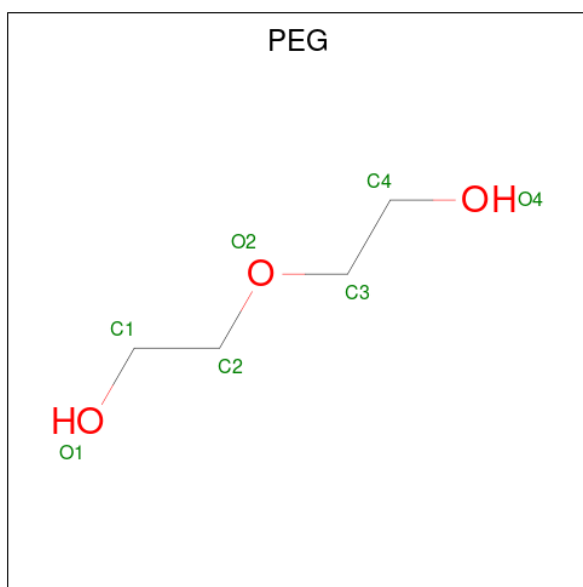


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O 4 2 2	0	0
13	B	1	Total C O 4 2 2	0	0
13	C	1	Total C O 4 2 2	0	0

- Molecule 14 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 15 is DI(HYDROXYETHYL)ETHER (three-letter code: 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 (three-letter code: CL) (formula: Cl).

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

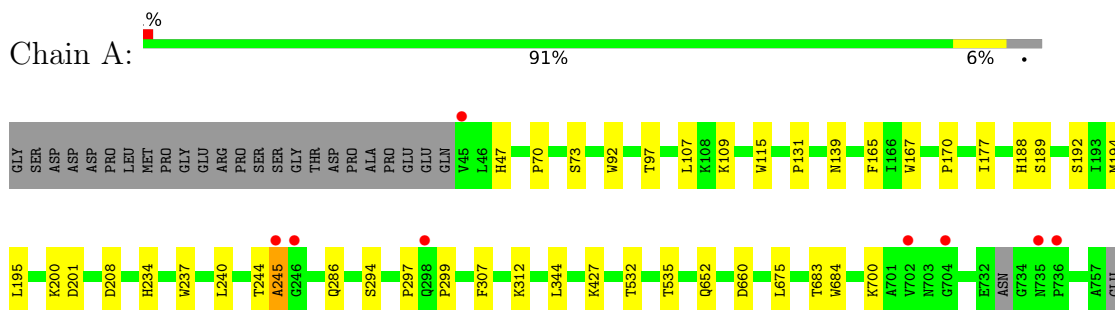
- Molecule 17 is water.

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		

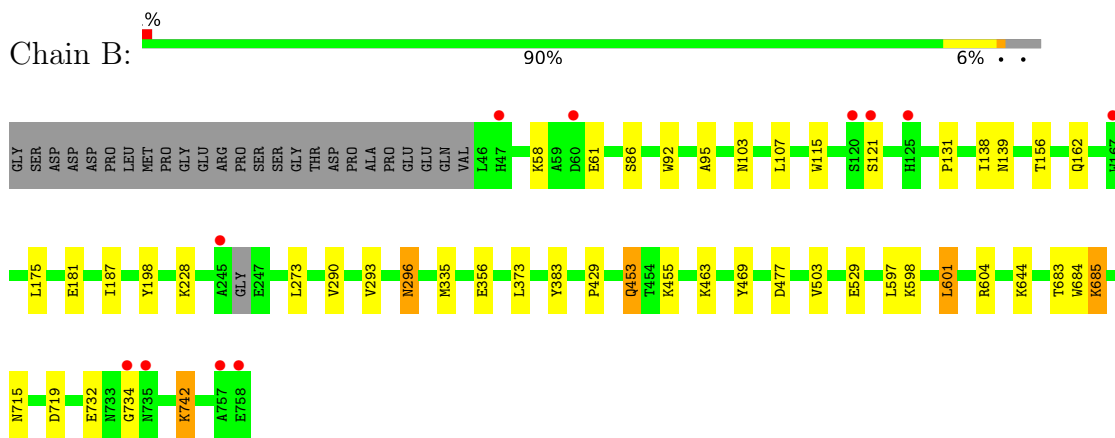
3 Residue-property plots [i](#)

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.

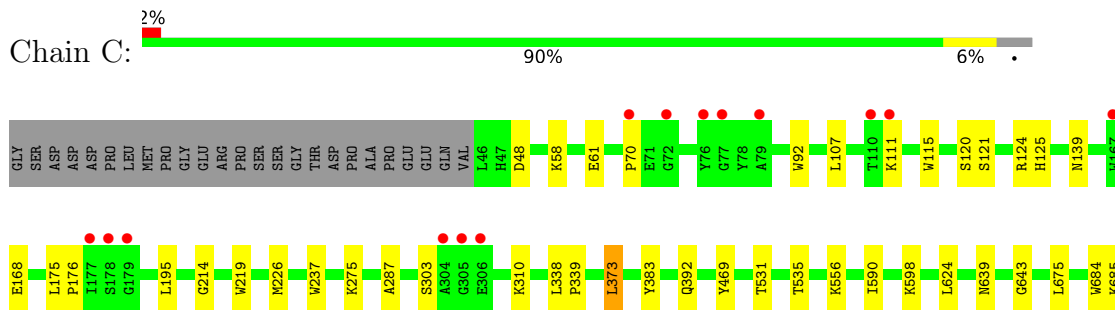
- Molecule 1: Alpha amylase, catalytic domain protein

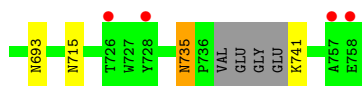


- Molecule 1: Alpha amylase, catalytic domain protein

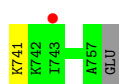
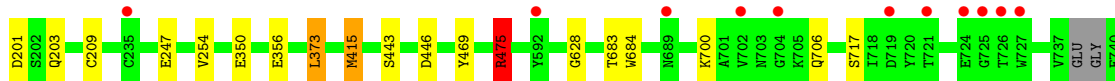
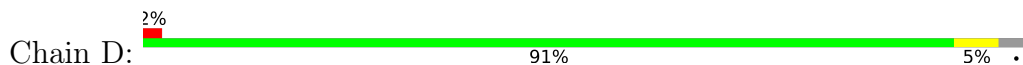


- Molecule 1: Alpha amylase, catalytic domain protein





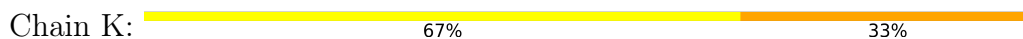
- Molecule 1: Alpha amylase, catalytic domain protein



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



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




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



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



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

Chain O:  33% 67%

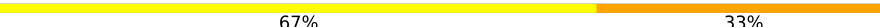
GLC1
GLC2
AC13

- Molecule 3: 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 N:  33% 67%


GLC1
GLC2
AC13

- Molecule 3: 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 V:  67% 33%

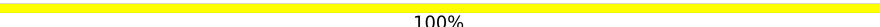
GLC1
GLC2
AC13

- Molecule 3: 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 Q:  67% 33%

GLC1
GLC2
AC13

- Molecule 4: α -D-glucopyranose-(1-4)- 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 J:  100%


GLC1
GLC2
AC13
GLC4
GLC5

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

Chain P:  50% 50%

GLC1
GLC2

- 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:  100%


GLC1
AC12

- Molecule 7: 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

Chain M:  50%

GLC1
GLC2
AC13
GLC4

- Molecule 7: 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

Chain S:  100%

GLC1
GLC2
AC13
GLC4

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 47.74 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.60-1.99) 98.5 (47.74-1.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.98Å)	Xtrriage
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 (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtrriage
Anisotropy	0.036	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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: PGE, MN, PEG, CA, AC1, ACT, BGC, GLC, CL, GOL, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.72	0/5900	0.86	0/8032
1	B	0.73	1/5891 (0.0%)	0.85	0/8021
1	C	0.68	0/5853	0.82	1/7969 (0.0%)
1	D	0.70	0/5851	0.83	1/7973 (0.0%)
All	All	0.71	1/23495 (0.0%)	0.84	2/31995 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	529	GLU	CD-OE1	5.97	1.32	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	475	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	C	124	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5718	0	5343	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5713	0	5330	28	0
1	C	5680	0	5304	22	0
1	D	5681	0	5271	23	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
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	8	0
17	B	675	0	0	8	0
17	C	497	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	D	449	0	0	7	0
All	All	25774	0	21775	108	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

The worst 5 of 108 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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	713/738 (97%)	679 (95%)	32 (4%)	2 (0%)	41 37
1	B	712/738 (96%)	685 (96%)	25 (4%)	2 (0%)	41 37
1	C	707/738 (96%)	669 (95%)	37 (5%)	1 (0%)	51 49
1	D	709/738 (96%)	681 (96%)	27 (4%)	1 (0%)	51 49
All	All	2841/2952 (96%)	2714 (96%)	121 (4%)	6 (0%)	47 44

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	ALA

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Mol	Chain	Res	Type
1	A	307	PHE
1	B	734	GLY
1	D	102	GLN
1	B	121	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	608/639 (95%)	601 (99%)	7 (1%)	71	76
1	B	608/639 (95%)	596 (98%)	12 (2%)	55	58
1	C	602/639 (94%)	591 (98%)	11 (2%)	59	63
1	D	600/639 (94%)	590 (98%)	10 (2%)	60	65
All	All	2418/2556 (95%)	2378 (98%)	40 (2%)	62	65

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	735	ASN
1	D	475	ARG
1	C	741	LYS
1	D	373	LEU
1	D	684	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	550	GLN
1	D	91	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	1.21	2 (11%)
2	GLC	H	2	2,8	11,11,12	0.92	1 (9%)	15,15,17	1.32	1 (6%)
2	AC1	H	3	2	21,22,23	0.57	0	22,32,34	0.98	2 (9%)
3	GLC	I	1	3	12,12,12	0.67	0	17,17,17	0.97	2 (11%)
3	GLC	I	2	3	11,11,12	0.35	0	15,15,17	0.93	0
3	AC1	I	3	3	21,22,23	0.47	0	22,32,34	0.67	0
4	GLC	J	1	4	12,12,12	0.49	0	17,17,17	1.39	1 (5%)
4	GLC	J	2	4	11,11,12	0.72	0	15,15,17	1.21	2 (13%)
4	AC1	J	3	4	21,22,23	1.60	5 (23%)	22,32,34	1.58	3 (13%)
4	GLC	J	4	4	11,11,12	0.62	0	15,15,17	1.60	4 (26%)
4	GLC	J	5	4	11,11,12	0.81	0	15,15,17	1.22	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	0.84	0	15,15,17	1.77	5 (33%)
2	AC1	K	3	2	21,22,23	0.47	0	22,32,34	0.85	1 (4%)
3	GLC	L	1	3	12,12,12	0.62	0	17,17,17	1.47	3 (17%)
3	GLC	L	2	3	11,11,12	0.74	0	15,15,17	1.62	3 (20%)
3	AC1	L	3	3	21,22,23	0.66	0	22,32,34	0.67	0
7	GLC	M	1	7	12,12,12	0.56	0	17,17,17	1.71	5 (29%)
7	GLC	M	2	7	11,11,12	0.91	0	15,15,17	1.14	1 (6%)
7	AC1	M	3	7	21,22,23	1.31	2 (9%)	22,32,34	1.56	5 (22%)
7	GLC	M	4	7	11,11,12	1.28	1 (9%)	15,15,17	1.59	4 (26%)
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	0.55	0	15,15,17	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AC1	N	3	3	21,22,23	0.98	1 (4%)	22,32,34	1.68	5 (22%)
3	GLC	O	1	3	12,12,12	0.46	0	17,17,17	0.88	1 (5%)
3	GLC	O	2	3	11,11,12	0.43	0	15,15,17	1.69	4 (26%)
3	AC1	O	3	3	21,22,23	0.44	0	22,32,34	0.63	0
5	GLC	P	1	5	11,11,12	0.53	0	15,15,17	1.53	3 (20%)
5	GLC	P	2	5	11,11,12	0.99	0	15,15,17	1.94	4 (26%)
3	GLC	Q	1	3	12,12,12	0.68	0	17,17,17	1.91	3 (17%)
3	GLC	Q	2	3	11,11,12	0.98	1 (9%)	15,15,17	1.23	2 (13%)
3	AC1	Q	3	3	21,22,23	1.02	2 (9%)	22,32,34	1.71	6 (27%)
6	GLC	R	1	6	12,12,12	0.65	0	17,17,17	1.18	2 (11%)
6	AC1	R	2	6	21,22,23	0.38	0	22,32,34	0.80	1 (4%)
7	GLC	S	1	7	12,12,12	0.63	0	17,17,17	1.49	4 (23%)
7	GLC	S	2	7	11,11,12	0.65	0	15,15,17	1.21	2 (13%)
7	AC1	S	3	7	21,22,23	1.07	1 (4%)	22,32,34	1.63	6 (27%)
7	GLC	S	4	7	11,11,12	0.60	0	15,15,17	1.68	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	0.86	0	15,15,17	1.57	3 (20%)
3	AC1	V	3	3	21,22,23	1.21	1 (4%)	22,32,34	1.56	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	-	4/6/43/46	0/2/2/2
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AC1	K	3	2	-	4/6/43/46	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

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3	AC1	C1B-N4A	4.50	1.55	1.47
7	M	3	AC1	C1B-N4A	3.83	1.54	1.47
3	V	3	AC1	C1B-N4A	3.70	1.54	1.47
7	S	3	AC1	C1B-N4A	3.31	1.53	1.47
4	J	3	AC1	C1B-C7B	3.03	1.54	1.50

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	1	GLC	C4-C3-C2	5.52	120.46	110.82
3	L	2	GLC	C1-O5-C5	4.48	118.26	112.19
7	M	3	AC1	C7B-C1B-N4A	4.26	117.08	110.68
4	J	3	AC1	O6B-C6B-C5B	-4.12	102.63	112.50
5	P	2	GLC	O3-C3-C2	4.03	117.71	109.99

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

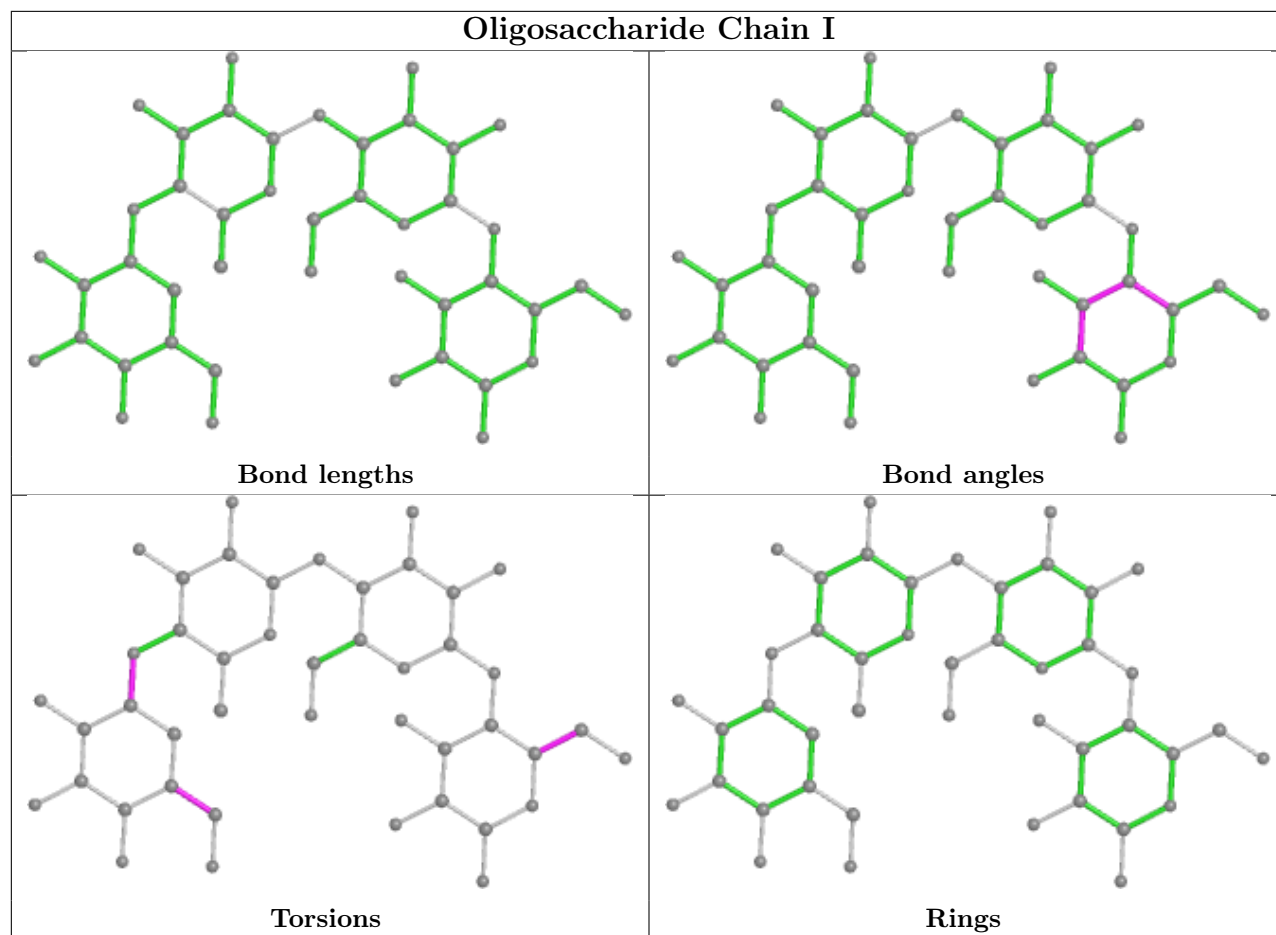
Mol	Chain	Res	Type	Atoms
2	H	3	AC1	C2B-C1B-N4A-C4
2	K	3	AC1	C2B-C1B-N4A-C4
3	I	3	AC1	C2B-C1B-N4A-C4
3	I	3	AC1	C4A-C5B-C6B-O6B
3	I	3	AC1	C7B-C5B-C6B-O6B

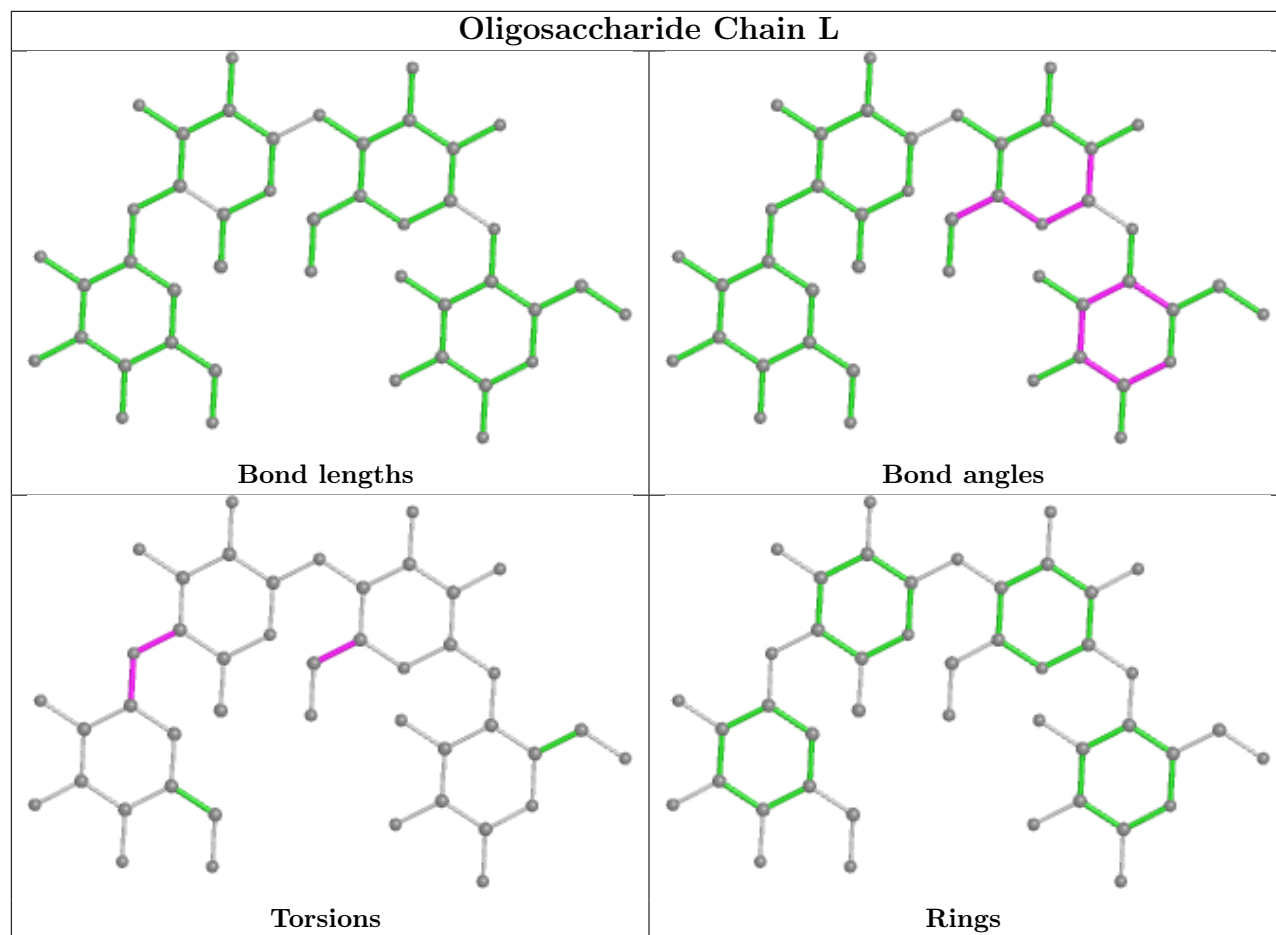
There are no ring outliers.

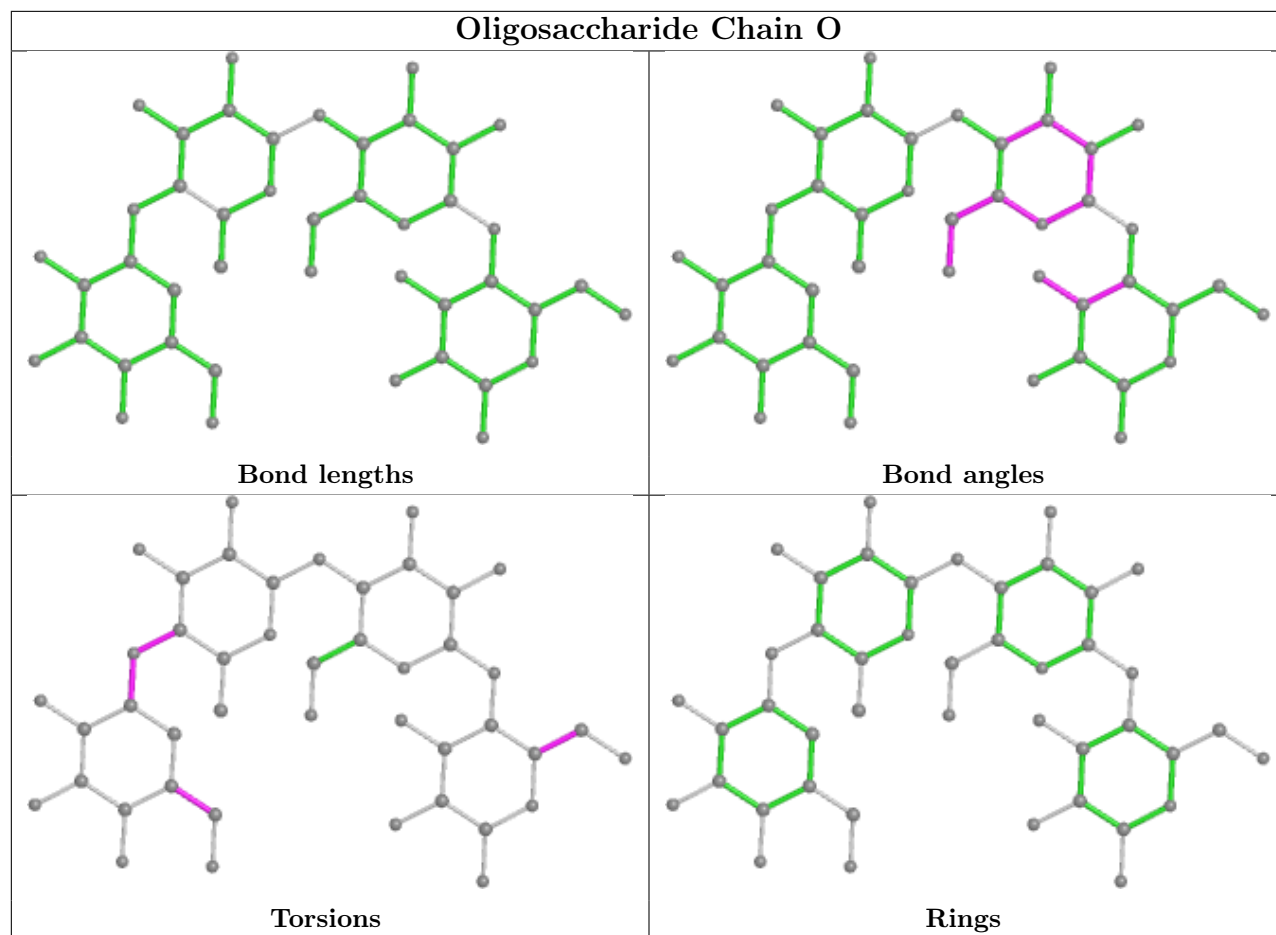
9 monomers are involved in 9 short contacts:

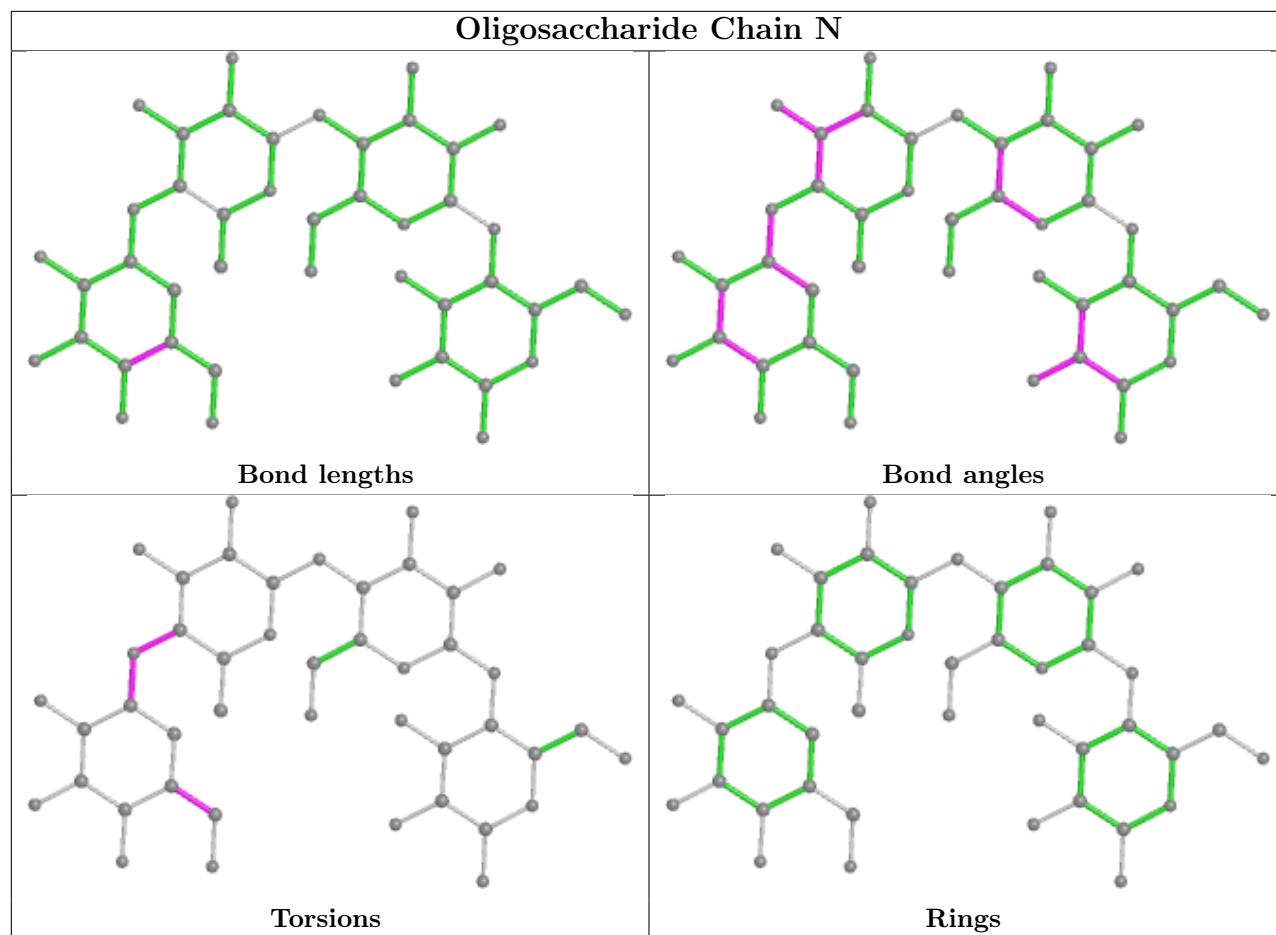
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1	GLC	1	0
3	Q	3	AC1	1	0
2	K	3	AC1	1	0
7	M	4	GLC	1	0
3	V	3	AC1	3	0
3	N	2	GLC	1	0
2	H	3	AC1	1	0
7	M	3	AC1	1	0
5	P	1	GLC	3	0

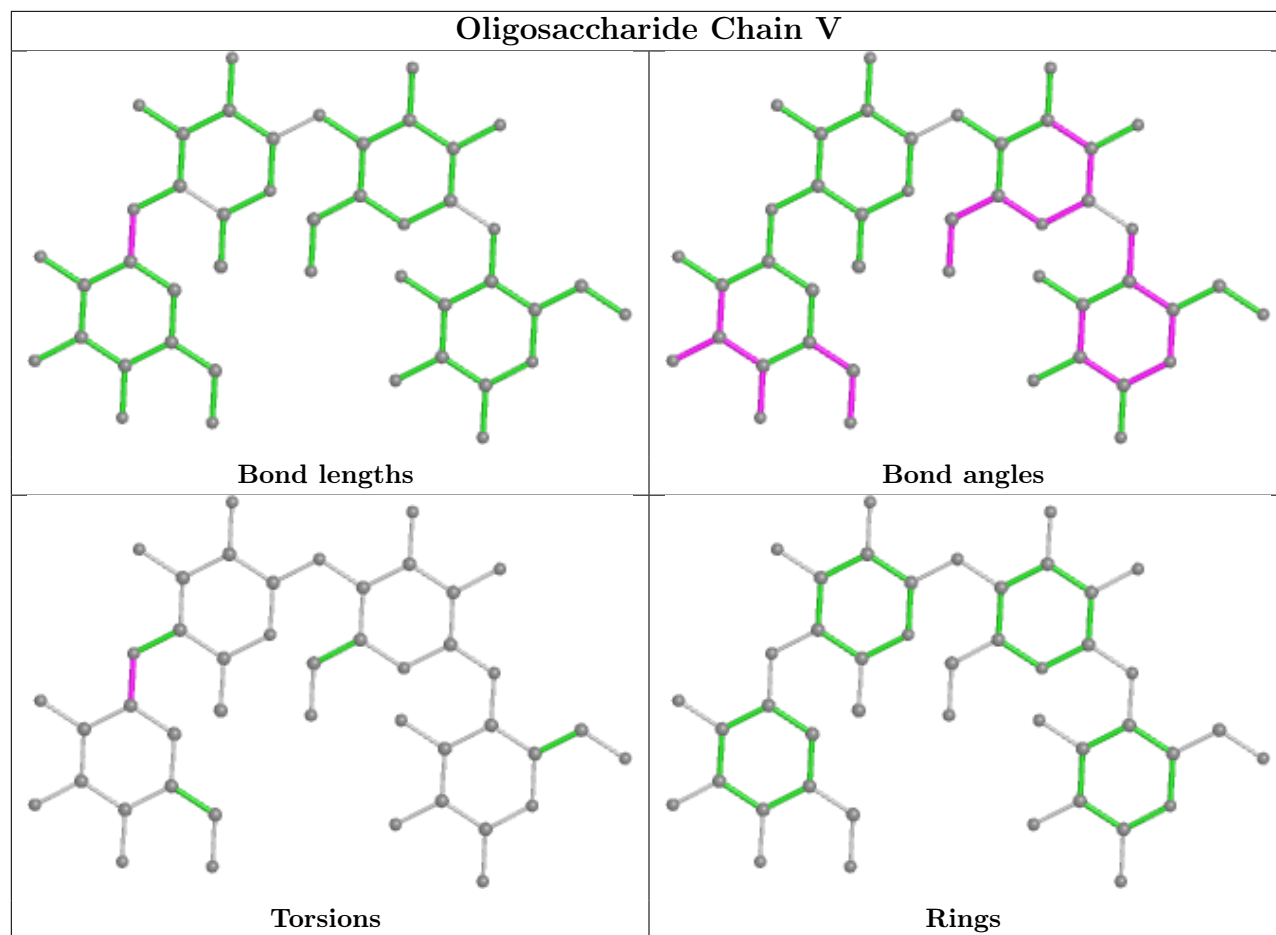
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

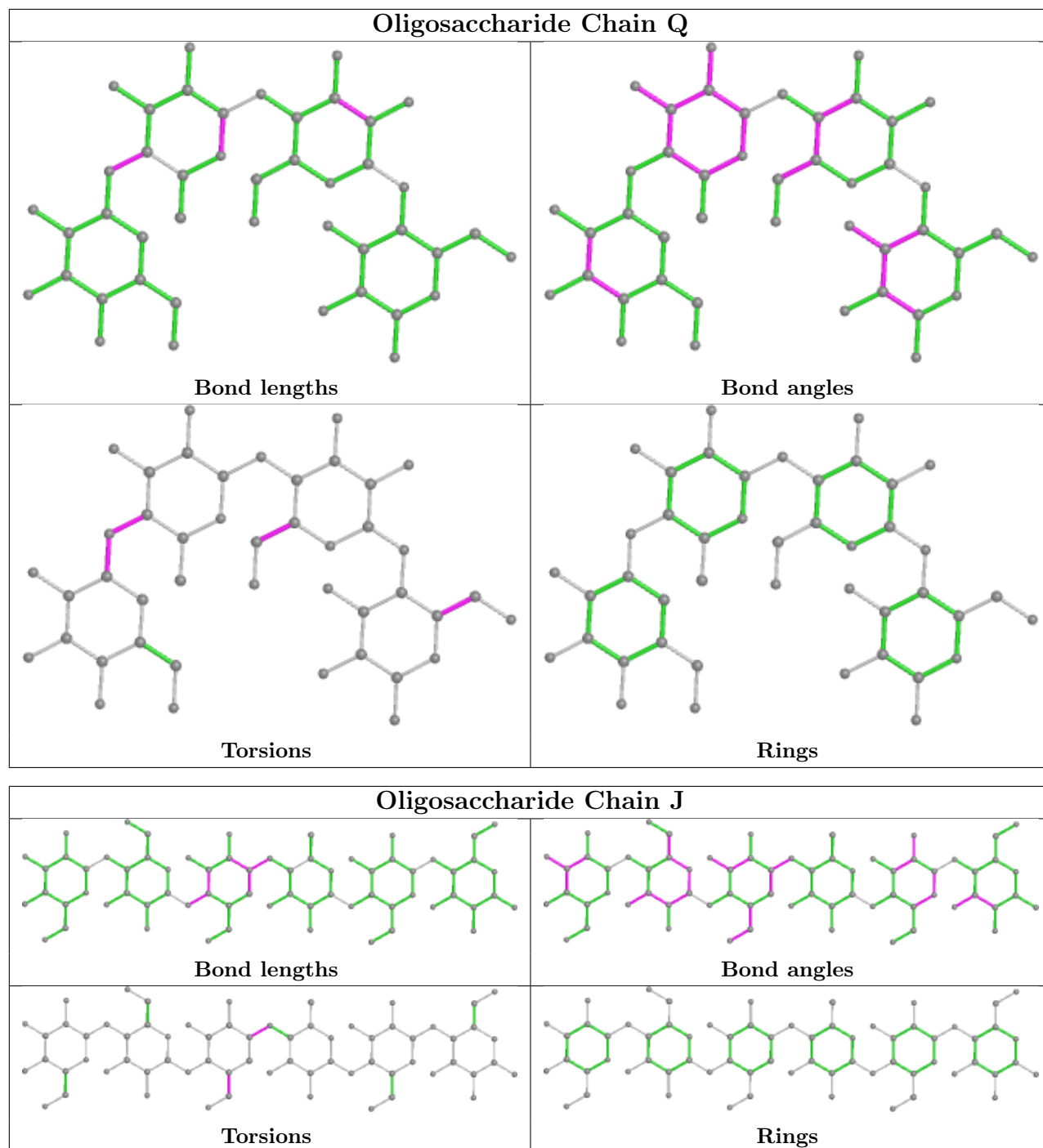


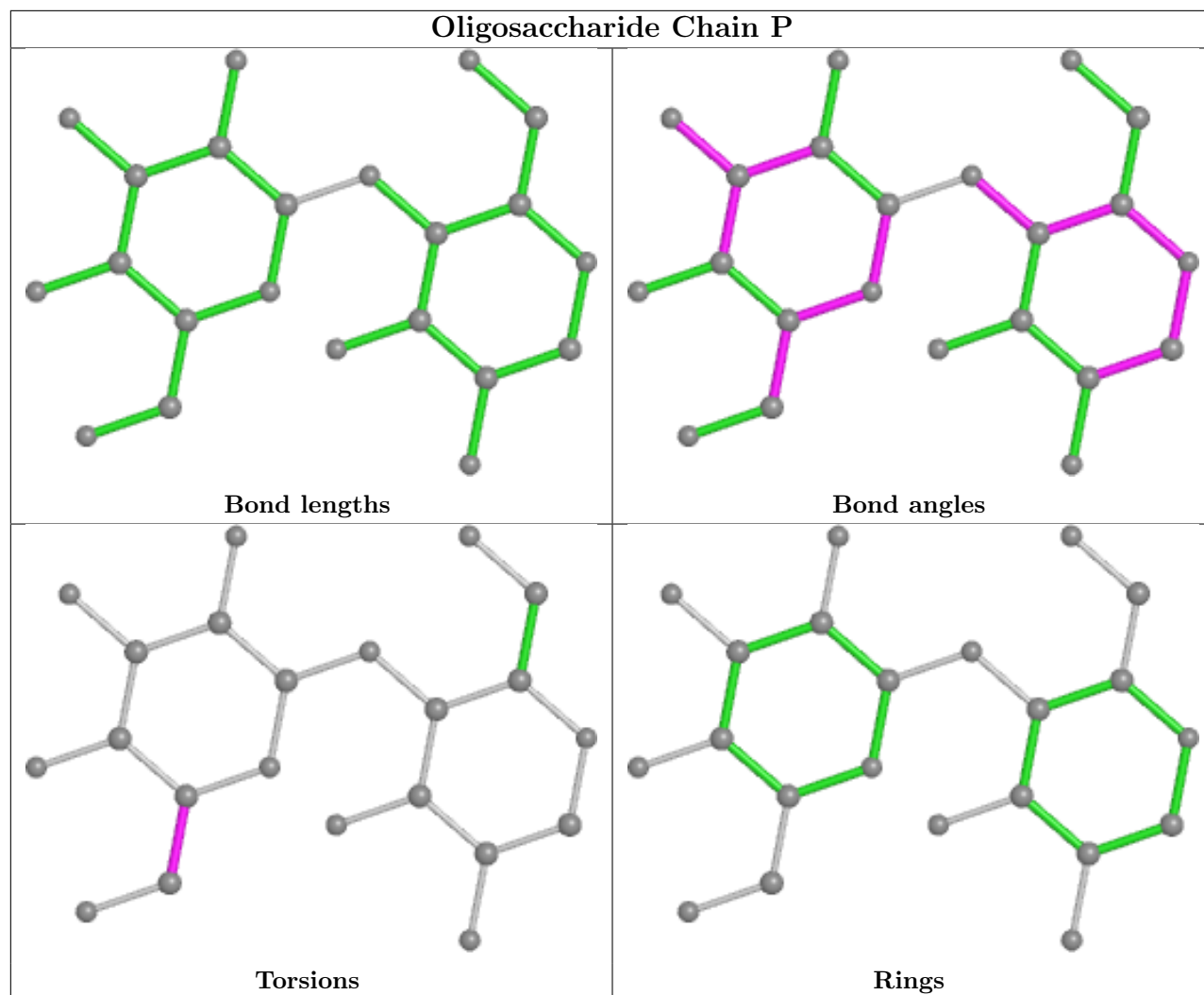


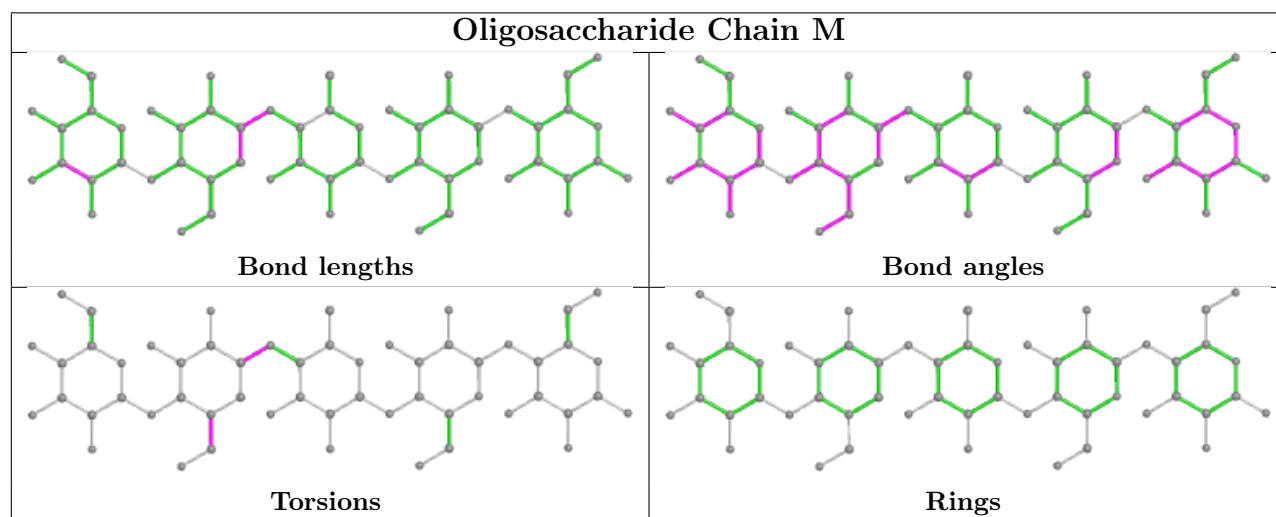
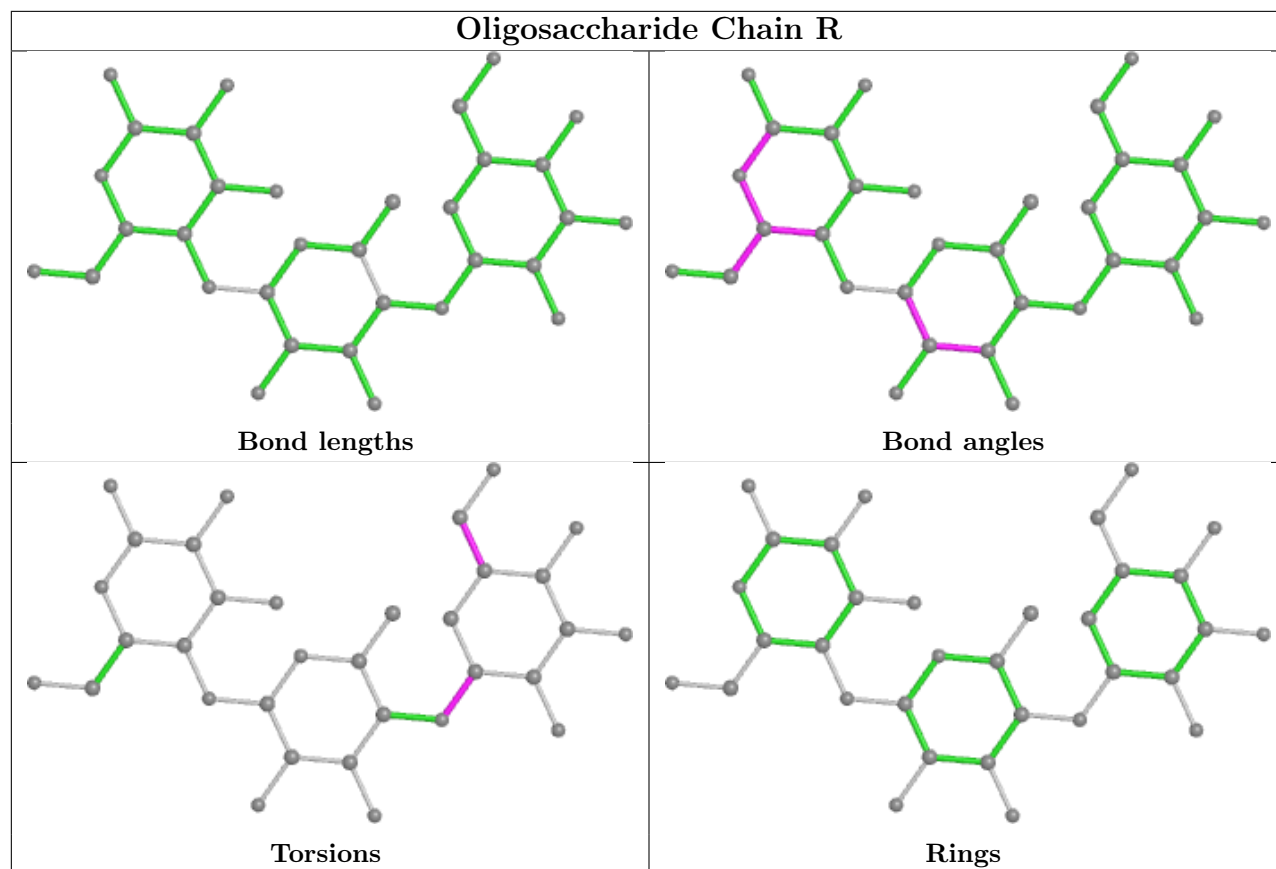


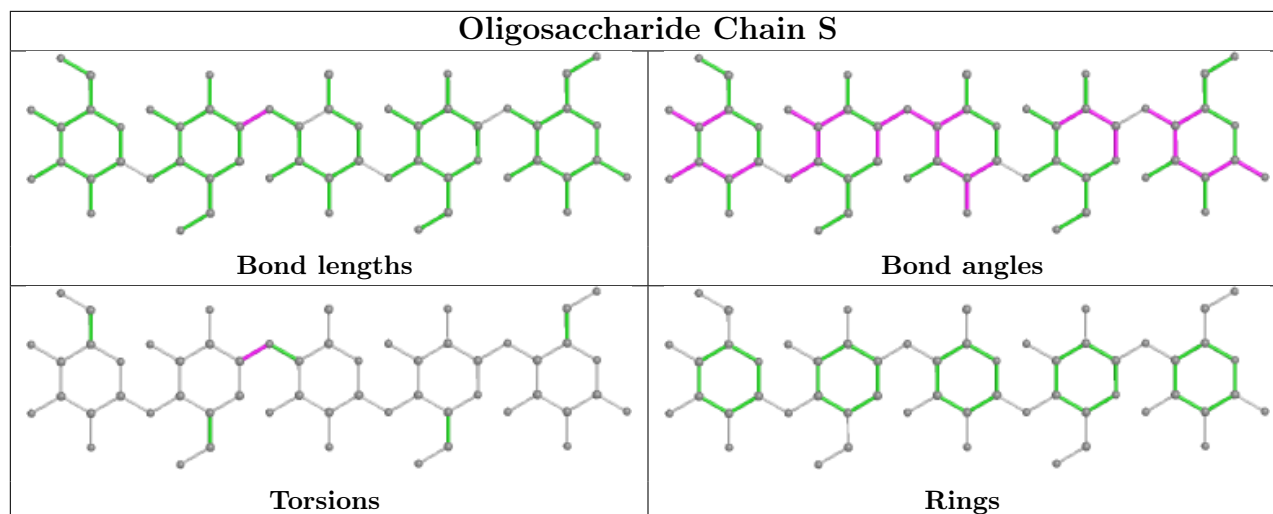












5.6 Ligand geometry [i](#)

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
11	GOL	A	804	-	5,5,5	0.10	0	5,5,5	0.35	0
10	PGE	B	807	-	9,9,9	0.29	0	8,8,8	0.20	0
11	GOL	B	805	-	5,5,5	0.11	0	5,5,5	0.27	0
11	GOL	B	806	-	5,5,5	0.19	0	5,5,5	0.63	0
11	GOL	C	803	-	5,5,5	0.08	0	5,5,5	0.28	0
8	GLC	A	801[B]	2	12,12,12	0.64	0	17,17,17	1.03	0
12	EDO	A	805	-	3,3,3	0.34	0	2,2,2	0.22	0
15	PEG	D	803	-	6,6,6	0.44	0	5,5,5	0.23	0
13	ACT	A	806	-	3,3,3	1.22	1 (33%)	3,3,3	0.58	0
8	GLC	B	801	2	12,12,12	0.75	0	17,17,17	1.21	1 (5%)
11	GOL	B	803	-	5,5,5	0.13	0	5,5,5	0.37	0
13	ACT	C	804	-	3,3,3	0.65	0	3,3,3	1.05	0
10	PGE	A	803	-	9,9,9	0.38	0	8,8,8	0.39	0
15	PEG	B	804	-	6,6,6	0.58	0	5,5,5	0.41	0
11	GOL	C	802	-	5,5,5	0.17	0	5,5,5	0.36	0
12	EDO	D	804	-	3,3,3	0.31	0	2,2,2	0.75	0
13	ACT	B	808	-	3,3,3	1.44	1 (33%)	3,3,3	0.76	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
11	GOL	A	804	-	-	0/4/4/4	-
10	PGE	B	807	-	-	5/7/7/7	-
11	GOL	B	805	-	-	4/4/4/4	-
11	GOL	B	806	-	-	0/4/4/4	-
11	GOL	C	803	-	-	1/4/4/4	-
8	GLC	A	801[B]	2	-	1/2/22/22	0/1/1/1
12	EDO	A	805	-	-	0/1/1/1	-
15	PEG	D	803	-	-	1/4/4/4	-
8	GLC	B	801	2	-	0/2/22/22	0/1/1/1
11	GOL	B	803	-	-	2/4/4/4	-
10	PGE	A	803	-	-	3/7/7/7	-
15	PEG	B	804	-	-	0/4/4/4	-
11	GOL	C	802	-	-	2/4/4/4	-
12	EDO	D	804	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	808	ACT	OXT-C	-2.48	1.18	1.30
13	A	806	ACT	OXT-C	-2.08	1.20	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	801	GLC	O3-C3-C2	-2.19	105.29	110.35

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

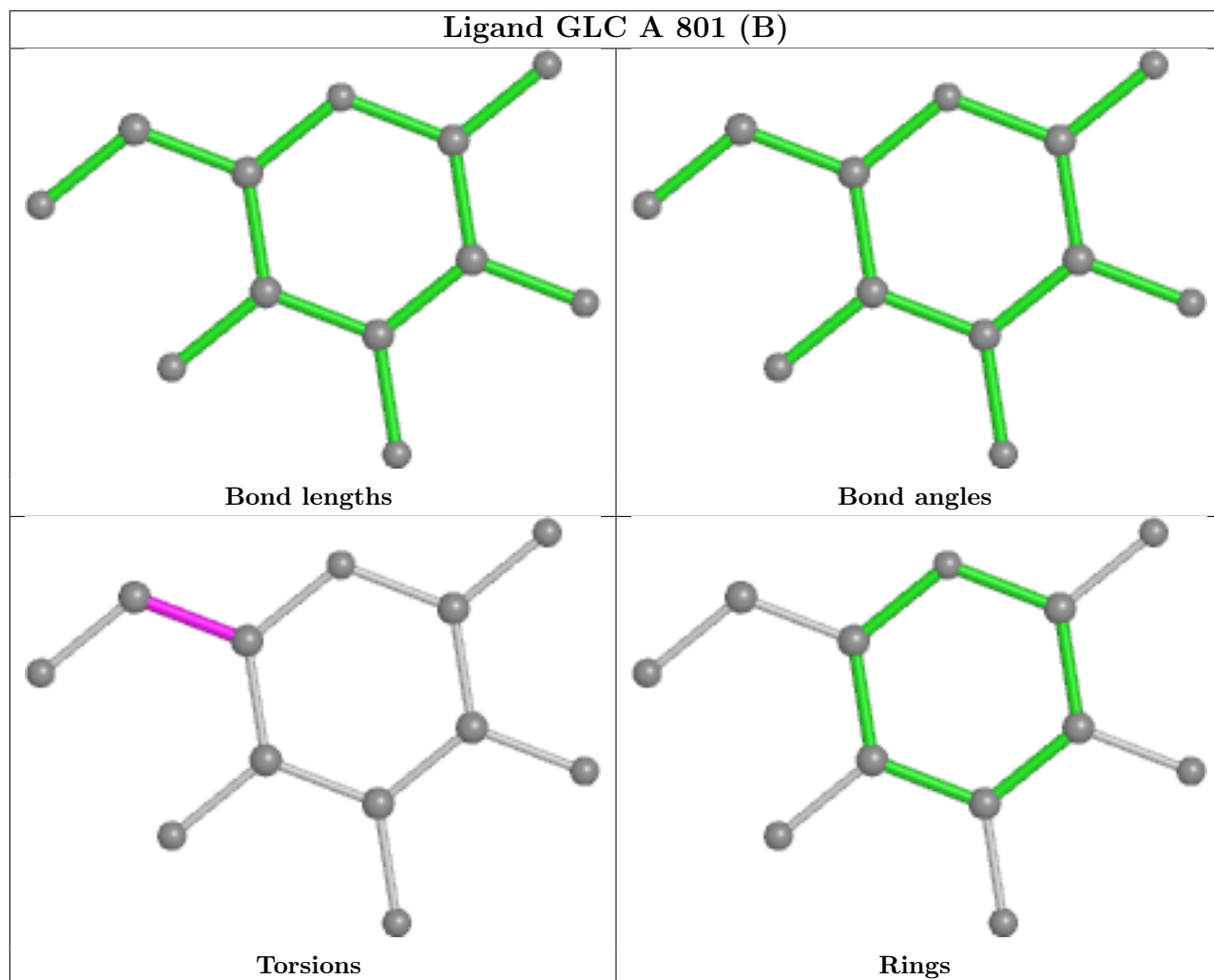
Mol	Chain	Res	Type	Atoms
11	B	803	GOL	C1-C2-C3-O3
11	B	805	GOL	O1-C1-C2-O2
11	B	805	GOL	O1-C1-C2-C3
11	B	805	GOL	C1-C2-C3-O3
11	C	802	GOL	O1-C1-C2-C3

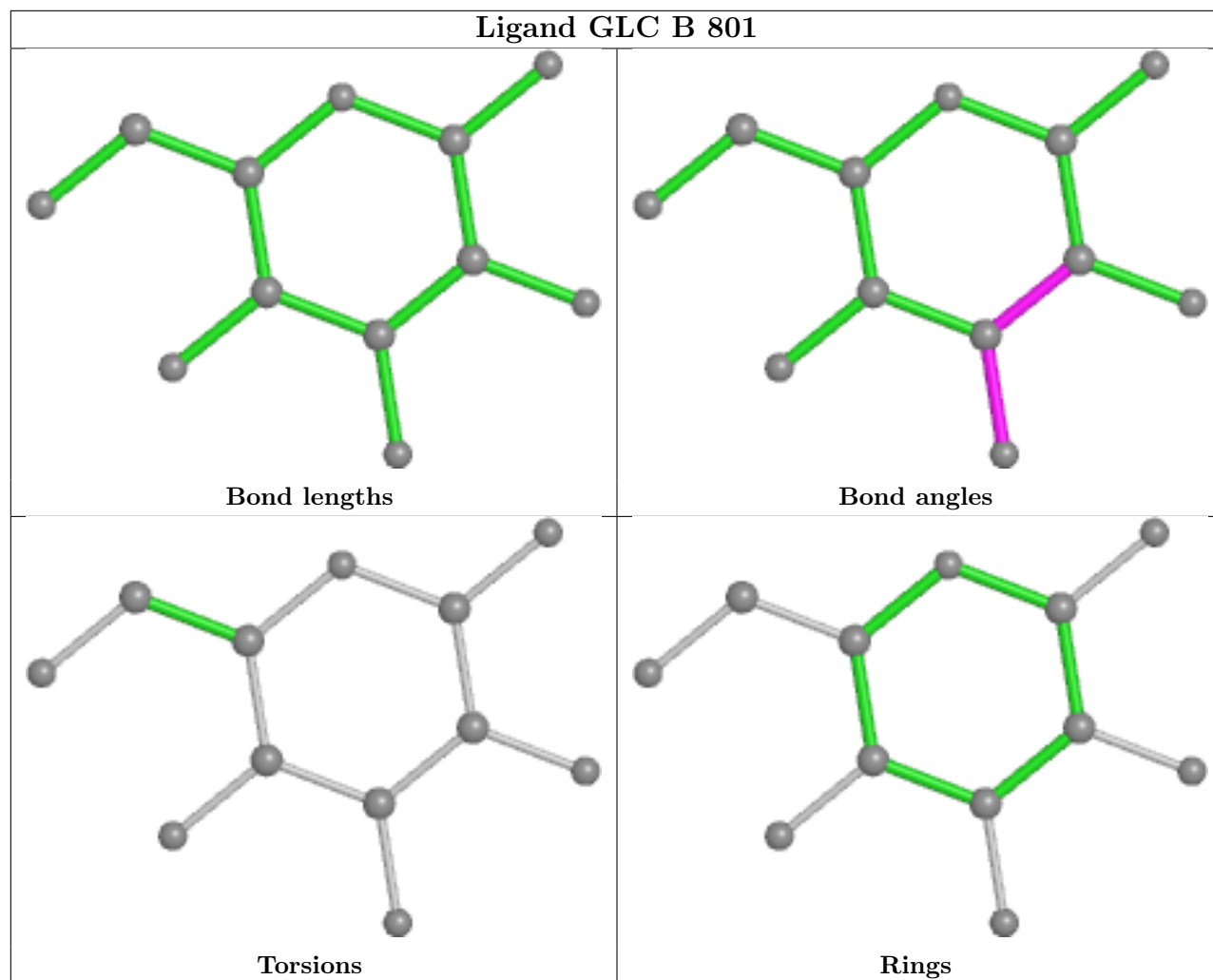
There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	804	GOL	1	0
11	B	805	GOL	1	0
11	B	806	GOL	1	0
11	C	803	GOL	1	0
12	A	805	EDO	1	0
15	D	803	PEG	1	0
13	A	806	ACT	1	0
10	A	803	PGE	2	0
15	B	804	PEG	2	0
12	D	804	EDO	2	0
13	B	808	ACT	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.27	8 (1%) 80 79	8, 21, 46, 69	0
1	B	712/738 (96%)	-0.22	11 (1%) 73 72	7, 18, 45, 75	0
1	C	709/738 (96%)	-0.04	18 (2%) 57 56	14, 26, 52, 81	0
1	D	712/738 (96%)	0.02	15 (2%) 63 62	13, 28, 50, 75	0
All	All	2845/2952 (96%)	-0.13	52 (1%) 68 66	7, 24, 48, 81	0

The worst 5 of 52 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	ALA	5.9
1	A	246	GLY	5.5
1	D	167	TRP	4.4
1	A	45	VAL	4.3
1	C	76	TYR	4.1

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
3	GLC	I	1	12/12	0.79	0.27	44,68,76,79	0
3	GLC	O	1	12/12	0.80	0.27	51,80,84,90	0

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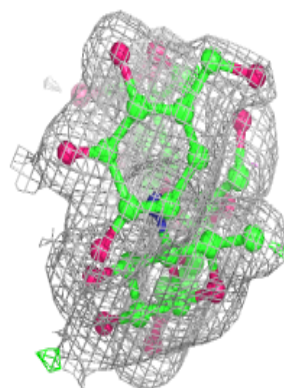
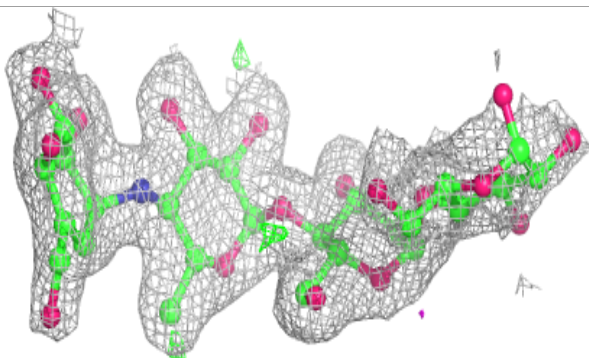
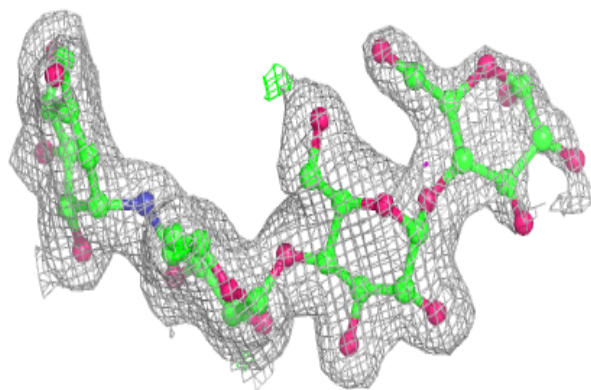
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLC	Q	1	12/12	0.87	0.16	32,53,59,59	0
3	GLC	L	1	12/12	0.89	0.22	27,52,55,59	0
5	GLC	P	2	11/12	0.89	0.18	38,42,56,71	0
7	GLC	S	1	12/12	0.89	0.14	34,40,44,45	0
4	GLC	J	5	11/12	0.90	0.18	27,31,46,63	0
6	AC1	R	2	21/22	0.91	0.19	32,43,54,57	0
3	GLC	N	1	12/12	0.91	0.14	30,56,59,62	0
2	BGC	K	1	12/12	0.92	0.14	24,34,37,40	12
2	BGC	H	1[A]	12/12	0.92	0.10	21,31,34,35	12
3	GLC	V	1	12/12	0.93	0.10	25,33,34,34	0
3	AC1	O	3	21/22	0.93	0.11	25,32,42,50	0
7	AC1	S	3	21/22	0.93	0.12	21,29,31,32	0
3	AC1	Q	3	21/22	0.94	0.11	17,27,53,62	0
3	AC1	V	3	21/22	0.94	0.10	19,23,26,33	0
7	GLC	S	4	11/12	0.94	0.10	23,25,28,32	0
4	AC1	J	3	21/22	0.95	0.10	12,16,19,25	0
3	AC1	N	3	21/22	0.95	0.13	18,23,43,48	0
2	AC1	H	3	21/22	0.95	0.11	14,22,34,48	0
6	GLC	R	1	12/12	0.95	0.18	37,43,44,46	0
3	GLC	V	2	11/12	0.95	0.08	20,24,27,28	0
7	GLC	M	1	12/12	0.95	0.09	16,20,24,27	0
3	GLC	O	2	11/12	0.95	0.08	25,32,35,38	0
3	AC1	I	3	21/22	0.95	0.09	18,25,37,47	0
2	AC1	K	3	21/22	0.95	0.12	16,21,33,44	0
3	GLC	Q	2	11/12	0.96	0.07	17,22,26,33	0
7	AC1	M	3	21/22	0.96	0.08	11,14,16,23	0
3	AC1	L	3	21/22	0.96	0.09	11,15,24,31	0
4	GLC	J	1	12/12	0.96	0.10	17,22,28,28	0
2	GLC	K	2	11/12	0.96	0.10	15,17,21,27	0
3	GLC	N	2	11/12	0.97	0.10	21,22,25,26	0
4	GLC	J	4	11/12	0.97	0.08	13,15,19,21	0
3	GLC	I	2	11/12	0.97	0.07	20,26,36,41	0
7	GLC	M	4	11/12	0.97	0.07	12,14,16,17	0
5	GLC	P	1	11/12	0.97	0.07	23,27,31,35	0
7	GLC	S	2	11/12	0.97	0.10	29,32,36,38	0
2	GLC	H	2	11/12	0.97	0.13	12,15,17,20	0
4	GLC	J	2	11/12	0.97	0.08	13,15,16,17	0
3	GLC	L	2	11/12	0.98	0.08	16,20,23,27	0
7	GLC	M	2	11/12	0.98	0.07	12,13,14,15	0

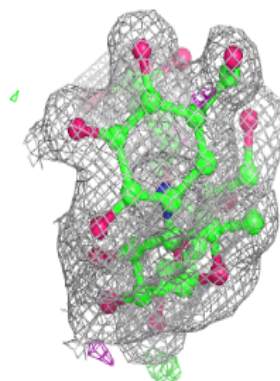
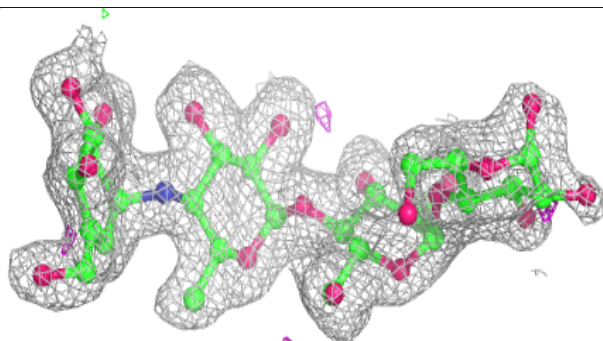
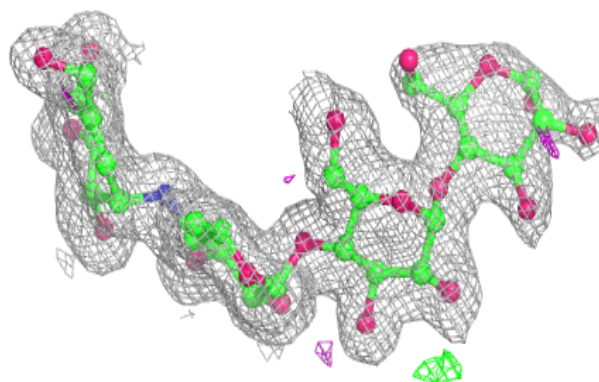
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

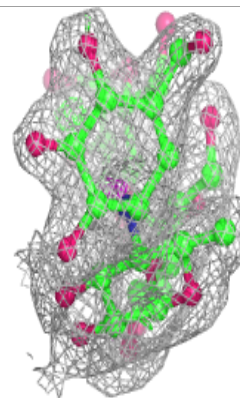
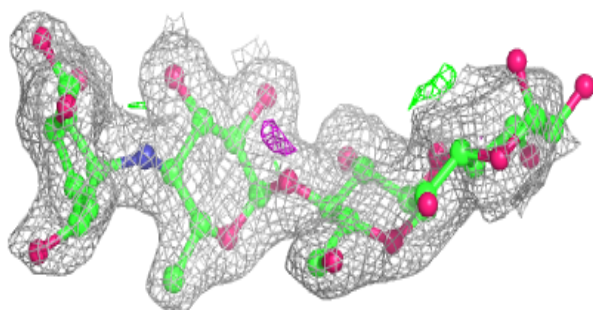
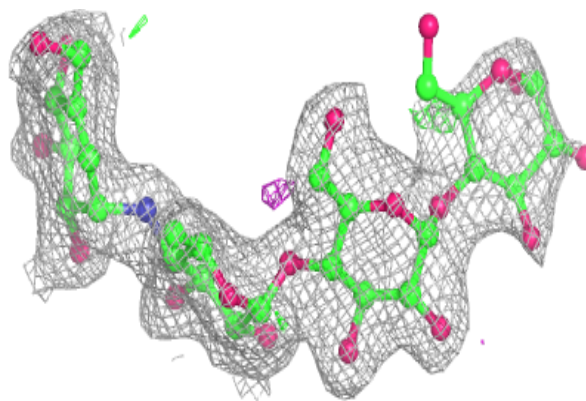
**Electron density around Chain L:**

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

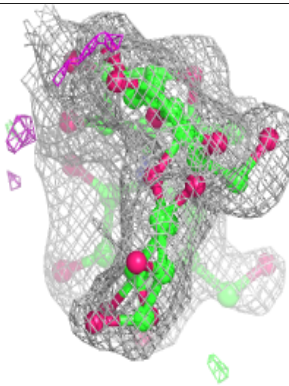
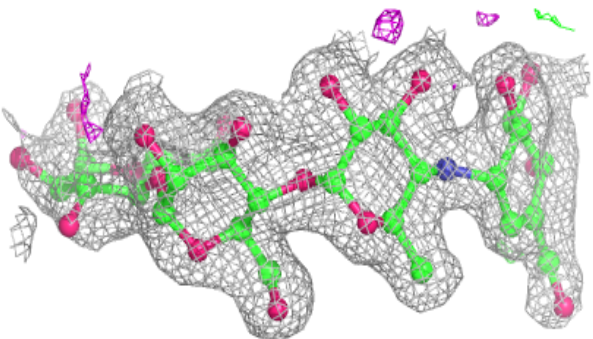
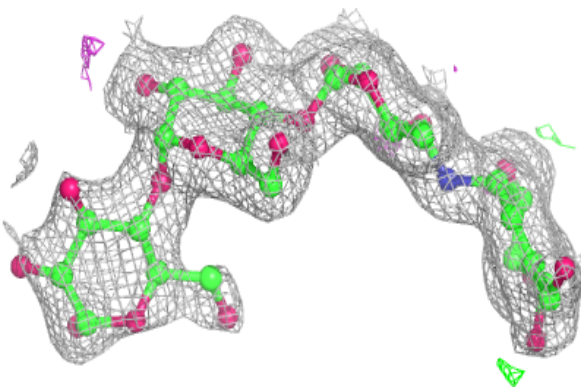


Electron density around Chain O:

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

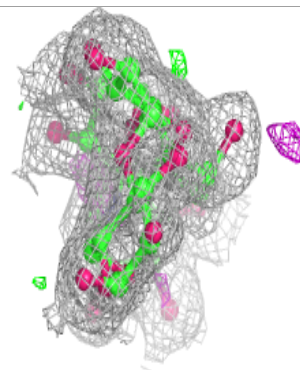
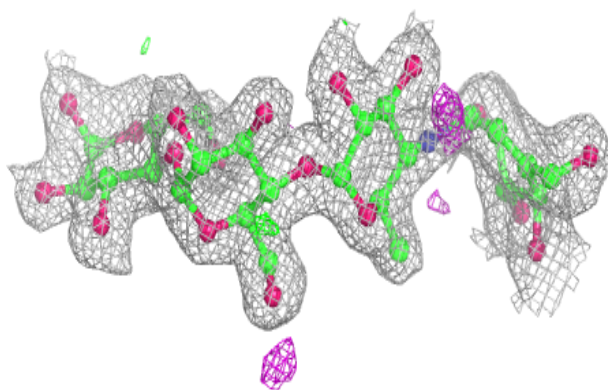
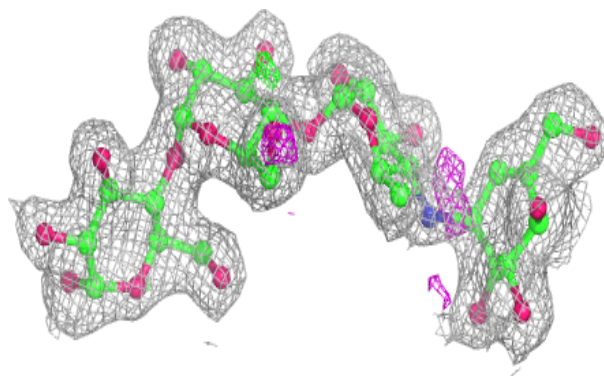
**Electron density around Chain N:**

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

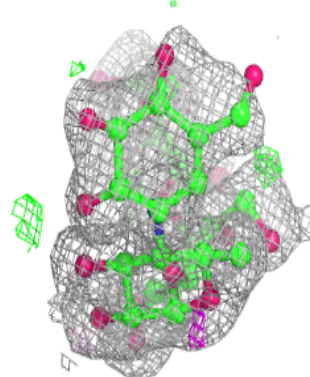
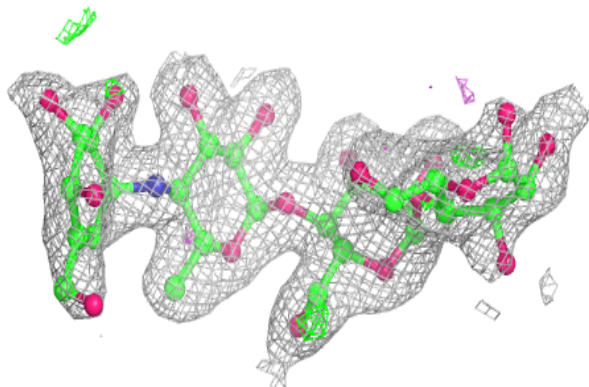
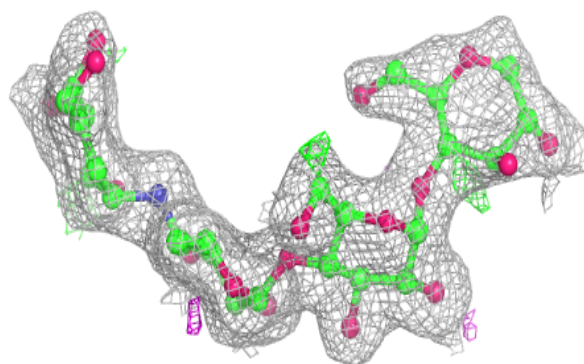


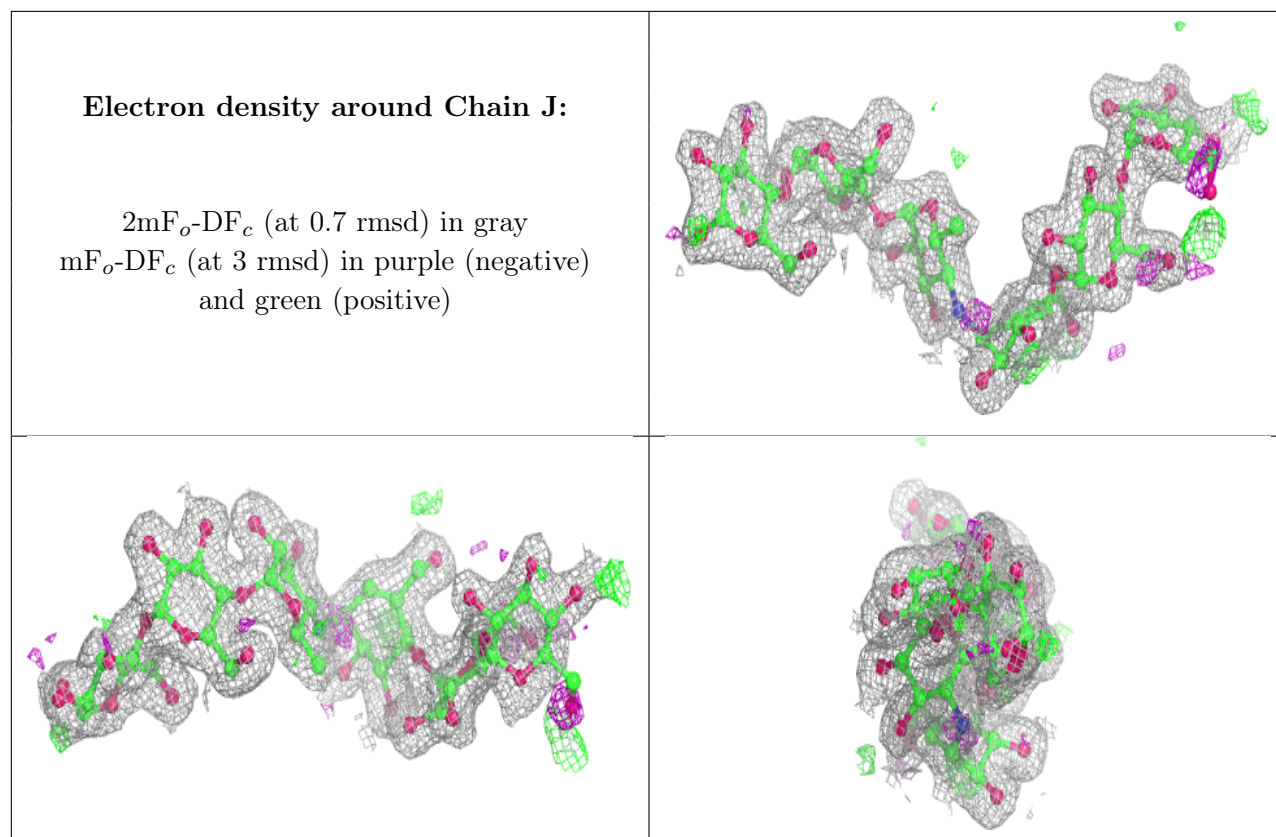
Electron density around Chain V:

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

**Electron density around Chain Q:**

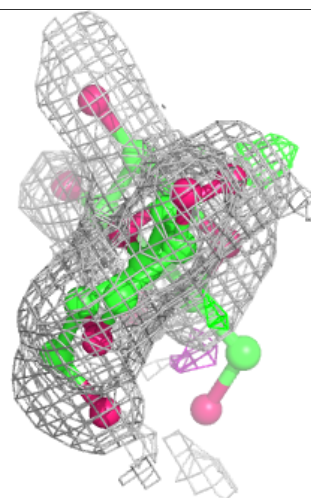
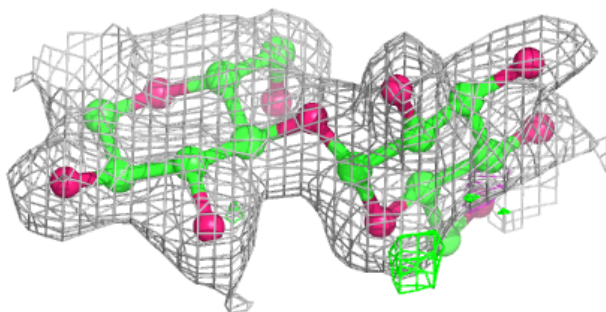
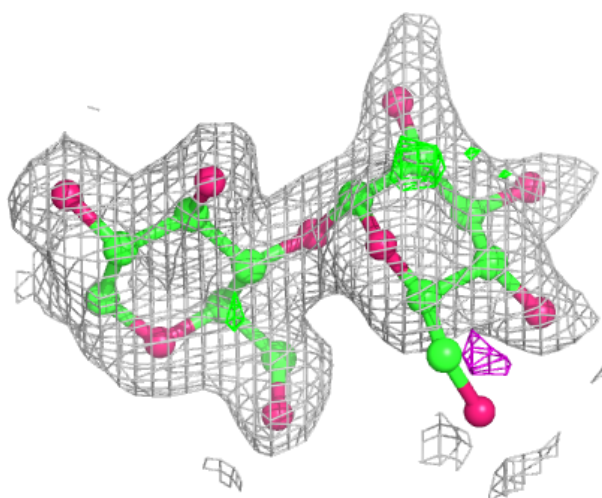
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





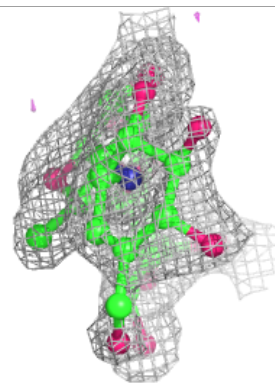
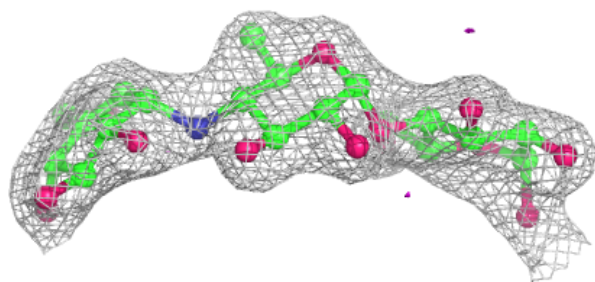
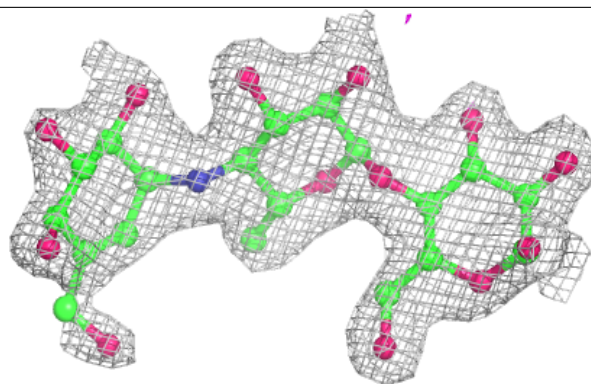
Electron density around Chain P:

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

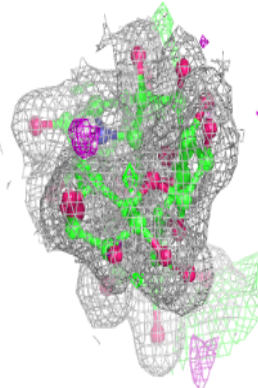
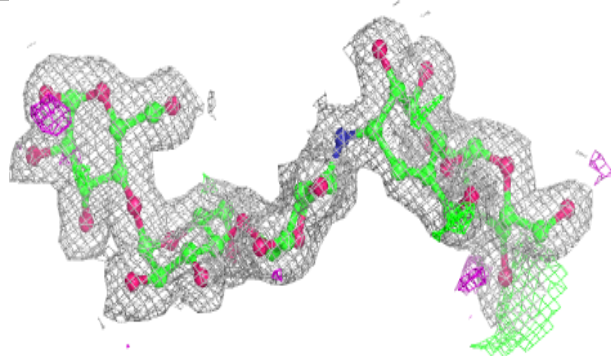
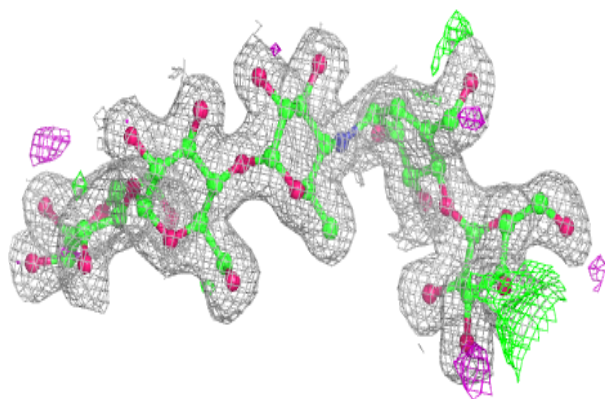


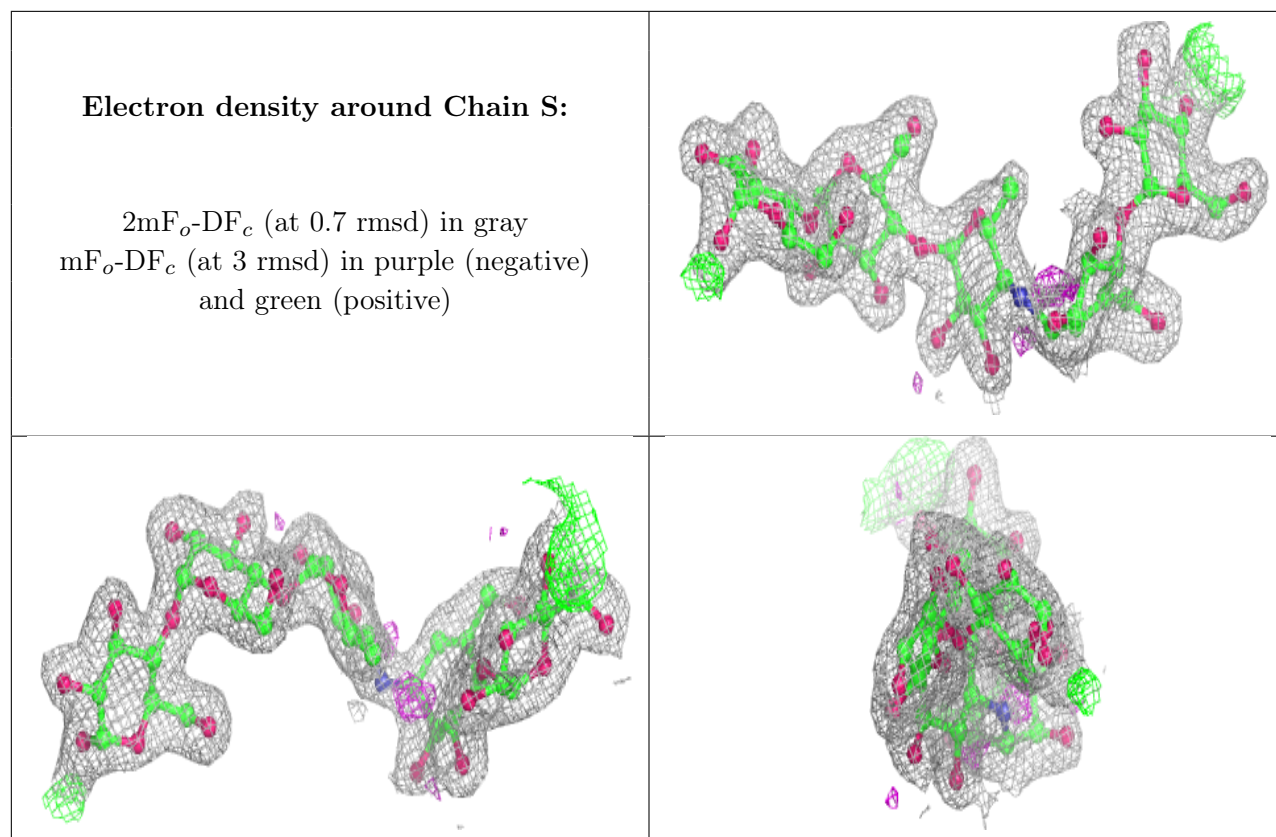
Electron density around Chain R:

$2mF_o-DF_c$ (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
12	EDO	D	804	4/4	0.72	0.15	42,45,46,46	0
15	PEG	B	804	7/7	0.75	0.28	38,47,58,58	0
11	GOL	C	803	6/6	0.76	0.22	61,64,66,66	0
15	PEG	D	803	7/7	0.77	0.24	37,45,48,49	0
11	GOL	A	804	6/6	0.83	0.23	58,61,62,67	0
11	GOL	B	803	6/6	0.83	0.18	39,43,46,48	0
10	PGE	B	807	10/10	0.86	0.13	36,47,54,59	0
11	GOL	B	805	6/6	0.88	0.21	51,61,63,64	0
11	GOL	C	802	6/6	0.89	0.23	33,44,48,49	0
16	CL	D	802	1/1	0.89	0.07	51,51,51,51	0
10	PGE	A	803	10/10	0.90	0.12	34,39,46,47	0
11	GOL	B	806	6/6	0.91	0.16	21,32,33,39	0
8	GLC	B	801	12/12	0.92	0.13	21,25,26,27	12
8	GLC	A	801[B]	12/12	0.94	0.10	21,30,33,34	12

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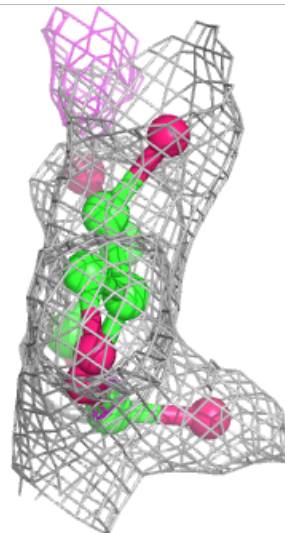
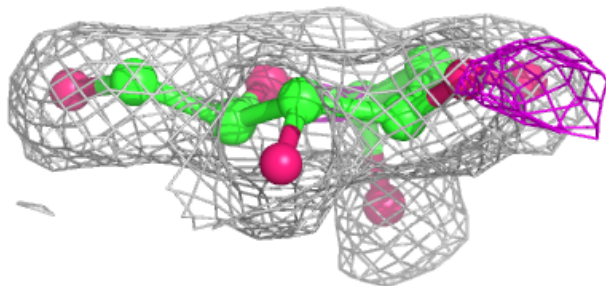
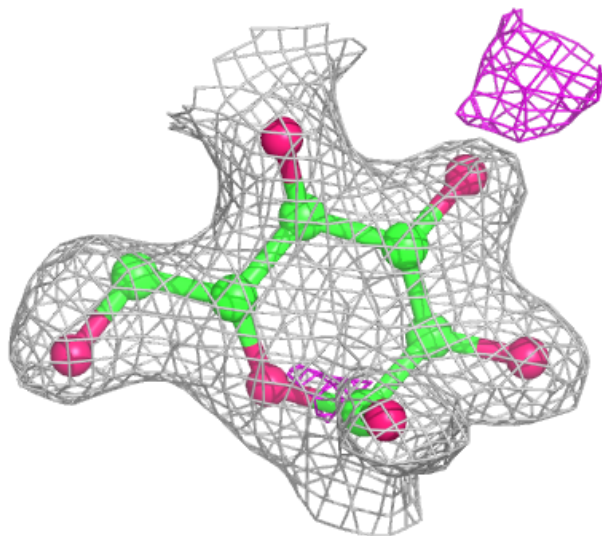
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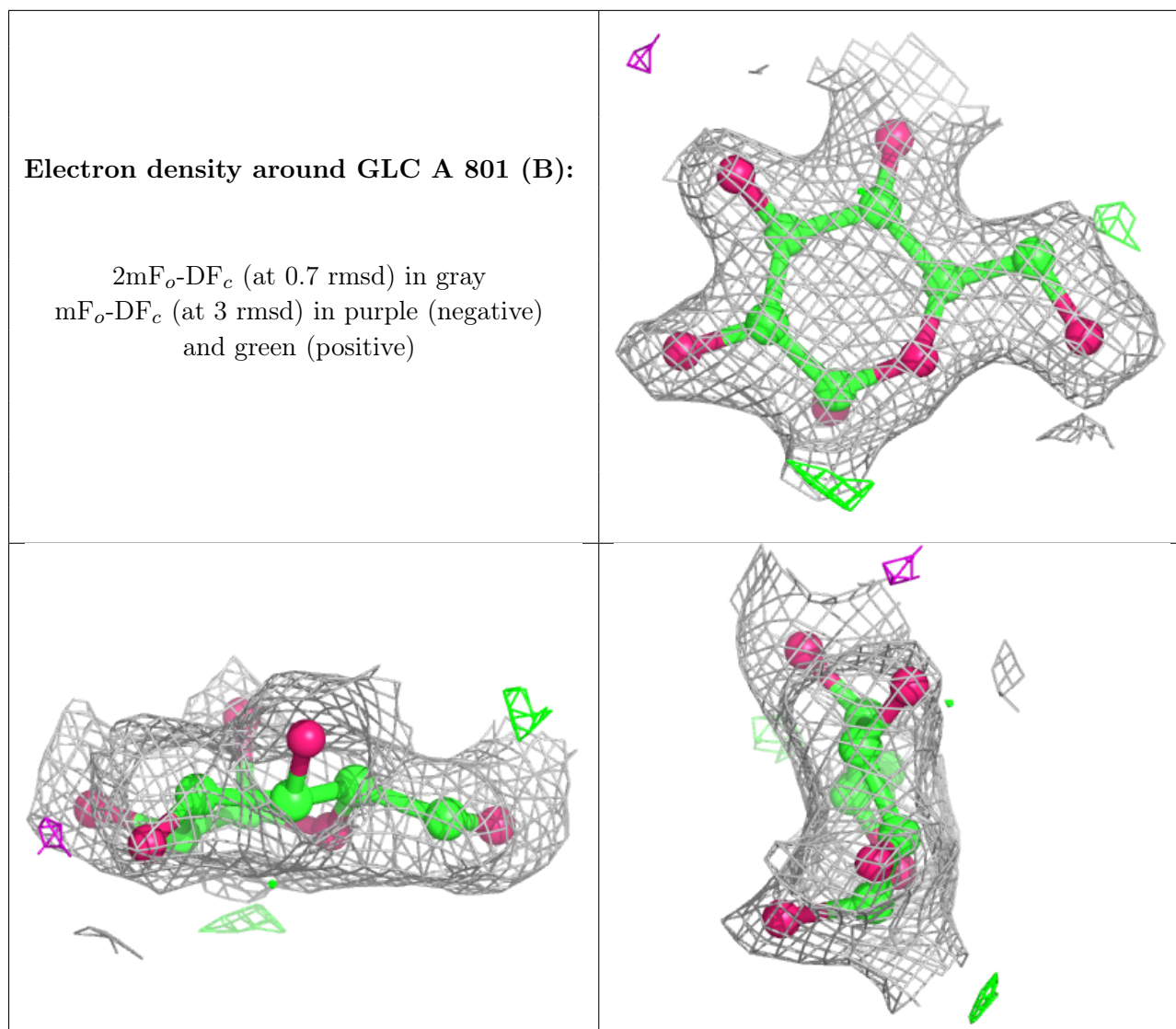
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	ACT	B	808	4/4	0.95	0.21	24,25,31,32	0
12	EDO	A	805	4/4	0.95	0.08	18,23,26,26	0
13	ACT	C	804	4/4	0.96	0.17	29,31,33,35	0
13	ACT	A	806	4/4	0.96	0.13	28,30,32,35	0
14	MN	D	805	1/1	0.98	0.04	36,36,36,36	0
14	MN	C	805	1/1	0.98	0.03	31,31,31,31	0
14	MN	A	807	1/1	0.99	0.03	21,21,21,21	0
9	CA	D	801	1/1	0.99	0.07	18,18,18,18	0
9	CA	C	801	1/1	0.99	0.06	21,21,21,21	0
14	MN	B	809	1/1	1.00	0.03	20,20,20,20	0
9	CA	A	802	1/1	1.00	0.06	13,13,13,13	0
9	CA	B	802	1/1	1.00	0.09	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)





6.5 Other polymers [i](#)

There are no such residues in this entry.