



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:11 PM UTC

PDB ID : 6GN6 / pdb_00006gn6
Title : Alpha-L-fucosidase isoenzyme 1 from Paenibacillus thiaminolyticus
Authors : Kovalova, T.; Koval, T.; Lipovova, P.; Dohnalek, J.
Deposited on : 2018-05-30
Resolution : 2.20 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

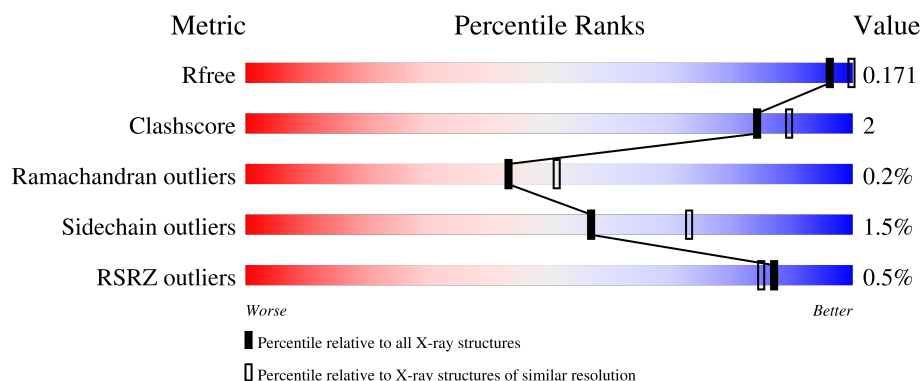
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



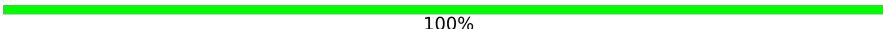
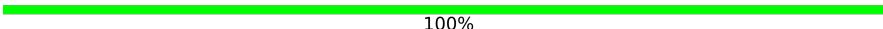
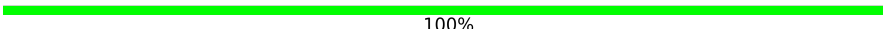
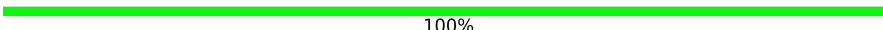
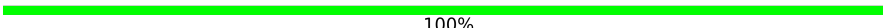
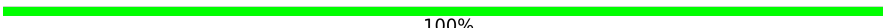
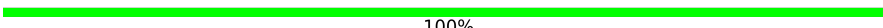
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	447	
1	B	447	
1	C	447	
1	D	447	
1	E	447	

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Mol	Chain	Length	Quality of chain
1	F	447	 89% 6%
2	G	2	 100%
2	H	2	 100%
2	I	2	 100%
2	J	2	 100%
2	K	2	 100%
2	L	2	 50% 50%
2	M	2	 100%
2	N	2	 100%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 22428 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-L-fucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	2	0
			3416	2184	593	626	13			
1	B	421	Total	C	N	O	S	0	3	0
			3424	2190	595	626	13			
1	C	421	Total	C	N	O	S	0	1	0
			3408	2179	590	626	13			
1	D	425	Total	C	N	O	S	0	1	0
			3444	2202	599	629	14			
1	E	421	Total	C	N	O	S	0	2	0
			3416	2184	593	626	13			
1	F	428	Total	C	N	O	S	0	2	0
			3473	2218	605	636	14			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP E3PQQ9
A	-19	GLY	-	expression tag	UNP E3PQQ9
A	-18	HIS	-	expression tag	UNP E3PQQ9
A	-17	HIS	-	expression tag	UNP E3PQQ9
A	-16	HIS	-	expression tag	UNP E3PQQ9
A	-15	HIS	-	expression tag	UNP E3PQQ9
A	-14	HIS	-	expression tag	UNP E3PQQ9
A	-13	HIS	-	expression tag	UNP E3PQQ9
A	-12	HIS	-	expression tag	UNP E3PQQ9
A	-11	HIS	-	expression tag	UNP E3PQQ9
A	-10	HIS	-	expression tag	UNP E3PQQ9
A	-9	HIS	-	expression tag	UNP E3PQQ9
A	-8	SER	-	expression tag	UNP E3PQQ9
A	-7	SER	-	expression tag	UNP E3PQQ9
A	-6	GLY	-	expression tag	UNP E3PQQ9
A	-5	HIS	-	expression tag	UNP E3PQQ9
A	-4	ILE	-	expression tag	UNP E3PQQ9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLU	-	expression tag	UNP E3PQQ9
A	-2	GLY	-	expression tag	UNP E3PQQ9
A	-1	ARG	-	expression tag	UNP E3PQQ9
A	0	HIS	-	expression tag	UNP E3PQQ9
B	-20	MET	-	initiating methionine	UNP E3PQQ9
B	-19	GLY	-	expression tag	UNP E3PQQ9
B	-18	HIS	-	expression tag	UNP E3PQQ9
B	-17	HIS	-	expression tag	UNP E3PQQ9
B	-16	HIS	-	expression tag	UNP E3PQQ9
B	-15	HIS	-	expression tag	UNP E3PQQ9
B	-14	HIS	-	expression tag	UNP E3PQQ9
B	-13	HIS	-	expression tag	UNP E3PQQ9
B	-12	HIS	-	expression tag	UNP E3PQQ9
B	-11	HIS	-	expression tag	UNP E3PQQ9
B	-10	HIS	-	expression tag	UNP E3PQQ9
B	-9	HIS	-	expression tag	UNP E3PQQ9
B	-8	SER	-	expression tag	UNP E3PQQ9
B	-7	SER	-	expression tag	UNP E3PQQ9
B	-6	GLY	-	expression tag	UNP E3PQQ9
B	-5	HIS	-	expression tag	UNP E3PQQ9
B	-4	ILE	-	expression tag	UNP E3PQQ9
B	-3	GLU	-	expression tag	UNP E3PQQ9
B	-2	GLY	-	expression tag	UNP E3PQQ9
B	-1	ARG	-	expression tag	UNP E3PQQ9
B	0	HIS	-	expression tag	UNP E3PQQ9
C	-20	MET	-	initiating methionine	UNP E3PQQ9
C	-19	GLY	-	expression tag	UNP E3PQQ9
C	-18	HIS	-	expression tag	UNP E3PQQ9
C	-17	HIS	-	expression tag	UNP E3PQQ9
C	-16	HIS	-	expression tag	UNP E3PQQ9
C	-15	HIS	-	expression tag	UNP E3PQQ9
C	-14	HIS	-	expression tag	UNP E3PQQ9
C	-13	HIS	-	expression tag	UNP E3PQQ9
C	-12	HIS	-	expression tag	UNP E3PQQ9
C	-11	HIS	-	expression tag	UNP E3PQQ9
C	-10	HIS	-	expression tag	UNP E3PQQ9
C	-9	HIS	-	expression tag	UNP E3PQQ9
C	-8	SER	-	expression tag	UNP E3PQQ9
C	-7	SER	-	expression tag	UNP E3PQQ9
C	-6	GLY	-	expression tag	UNP E3PQQ9
C	-5	HIS	-	expression tag	UNP E3PQQ9
C	-4	ILE	-	expression tag	UNP E3PQQ9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLU	-	expression tag	UNP E3PQQ9
C	-2	GLY	-	expression tag	UNP E3PQQ9
C	-1	ARG	-	expression tag	UNP E3PQQ9
C	0	HIS	-	expression tag	UNP E3PQQ9
D	-20	MET	-	initiating methionine	UNP E3PQQ9
D	-19	GLY	-	expression tag	UNP E3PQQ9
D	-18	HIS	-	expression tag	UNP E3PQQ9
D	-17	HIS	-	expression tag	UNP E3PQQ9
D	-16	HIS	-	expression tag	UNP E3PQQ9
D	-15	HIS	-	expression tag	UNP E3PQQ9
D	-14	HIS	-	expression tag	UNP E3PQQ9
D	-13	HIS	-	expression tag	UNP E3PQQ9
D	-12	HIS	-	expression tag	UNP E3PQQ9
D	-11	HIS	-	expression tag	UNP E3PQQ9
D	-10	HIS	-	expression tag	UNP E3PQQ9
D	-9	HIS	-	expression tag	UNP E3PQQ9
D	-8	SER	-	expression tag	UNP E3PQQ9
D	-7	SER	-	expression tag	UNP E3PQQ9
D	-6	GLY	-	expression tag	UNP E3PQQ9
D	-5	HIS	-	expression tag	UNP E3PQQ9
D	-4	ILE	-	expression tag	UNP E3PQQ9
D	-3	GLU	-	expression tag	UNP E3PQQ9
D	-2	GLY	-	expression tag	UNP E3PQQ9
D	-1	ARG	-	expression tag	UNP E3PQQ9
D	0	HIS	-	expression tag	UNP E3PQQ9
E	-20	MET	-	initiating methionine	UNP E3PQQ9
E	-19	GLY	-	expression tag	UNP E3PQQ9
E	-18	HIS	-	expression tag	UNP E3PQQ9
E	-17	HIS	-	expression tag	UNP E3PQQ9
E	-16	HIS	-	expression tag	UNP E3PQQ9
E	-15	HIS	-	expression tag	UNP E3PQQ9
E	-14	HIS	-	expression tag	UNP E3PQQ9
E	-13	HIS	-	expression tag	UNP E3PQQ9
E	-12	HIS	-	expression tag	UNP E3PQQ9
E	-11	HIS	-	expression tag	UNP E3PQQ9
E	-10	HIS	-	expression tag	UNP E3PQQ9
E	-9	HIS	-	expression tag	UNP E3PQQ9
E	-8	SER	-	expression tag	UNP E3PQQ9
E	-7	SER	-	expression tag	UNP E3PQQ9
E	-6	GLY	-	expression tag	UNP E3PQQ9
E	-5	HIS	-	expression tag	UNP E3PQQ9
E	-4	ILE	-	expression tag	UNP E3PQQ9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLU	-	expression tag	UNP E3PQQ9
E	-2	GLY	-	expression tag	UNP E3PQQ9
E	-1	ARG	-	expression tag	UNP E3PQQ9
E	0	HIS	-	expression tag	UNP E3PQQ9
F	-20	MET	-	initiating methionine	UNP E3PQQ9
F	-19	GLY	-	expression tag	UNP E3PQQ9
F	-18	HIS	-	expression tag	UNP E3PQQ9
F	-17	HIS	-	expression tag	UNP E3PQQ9
F	-16	HIS	-	expression tag	UNP E3PQQ9
F	-15	HIS	-	expression tag	UNP E3PQQ9
F	-14	HIS	-	expression tag	UNP E3PQQ9
F	-13	HIS	-	expression tag	UNP E3PQQ9
F	-12	HIS	-	expression tag	UNP E3PQQ9
F	-11	HIS	-	expression tag	UNP E3PQQ9
F	-10	HIS	-	expression tag	UNP E3PQQ9
F	-9	HIS	-	expression tag	UNP E3PQQ9
F	-8	SER	-	expression tag	UNP E3PQQ9
F	-7	SER	-	expression tag	UNP E3PQQ9
F	-6	GLY	-	expression tag	UNP E3PQQ9
F	-5	HIS	-	expression tag	UNP E3PQQ9
F	-4	ILE	-	expression tag	UNP E3PQQ9
F	-3	GLU	-	expression tag	UNP E3PQQ9
F	-2	GLY	-	expression tag	UNP E3PQQ9
F	-1	ARG	-	expression tag	UNP E3PQQ9
F	0	HIS	-	expression tag	UNP E3PQQ9

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



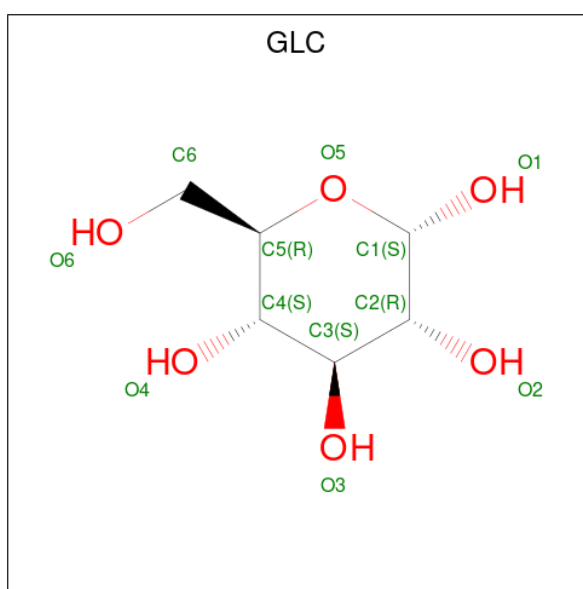
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	G	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			
2	I	2	Total	C	O	0	0	0
			23	12	11			
2	J	2	Total	C	O	0	0	0
			23	12	11			

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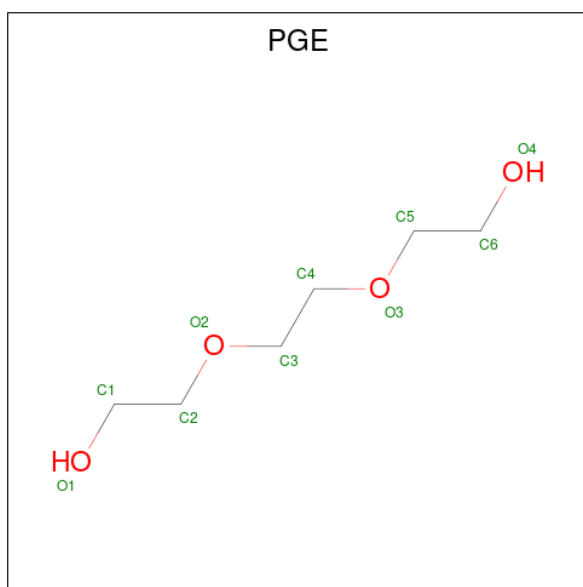
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	K	2	Total	C	O	0	0	0
			23	12	11			
2	L	2	Total	C	O	0	0	0
			23	12	11			
2	M	2	Total	C	O	0	0	0
			23	12	11			
2	N	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



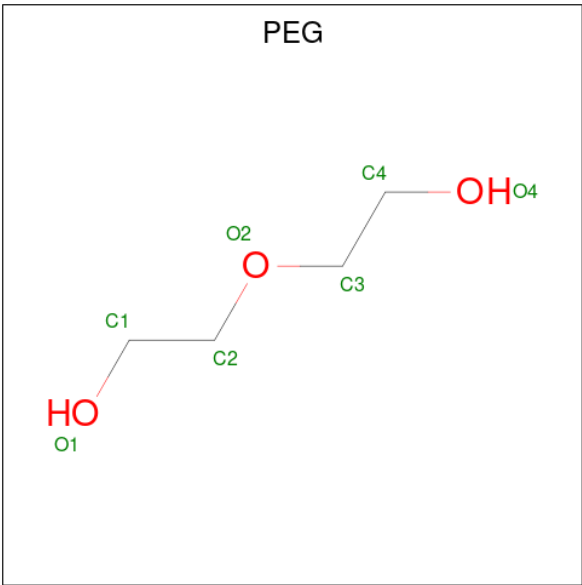
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		
3	E	1	Total	C	O	0	0
			12	6	6		
3	F	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



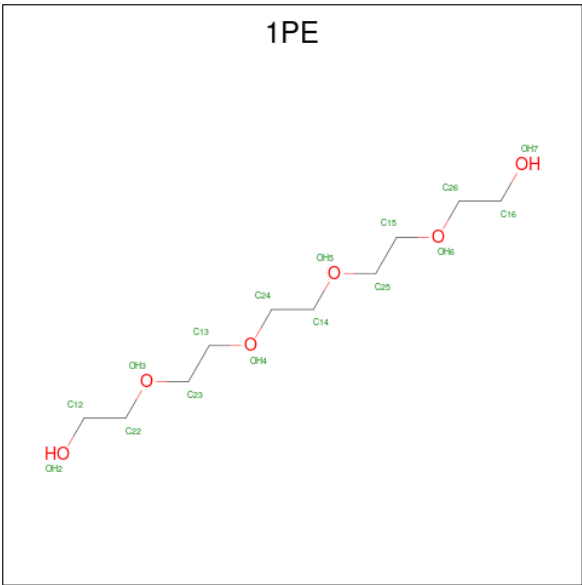
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	D	1	Total	C	O	0	0
			10	6	4		
4	E	1	Total	C	O	0	0
			10	6	4		
4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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



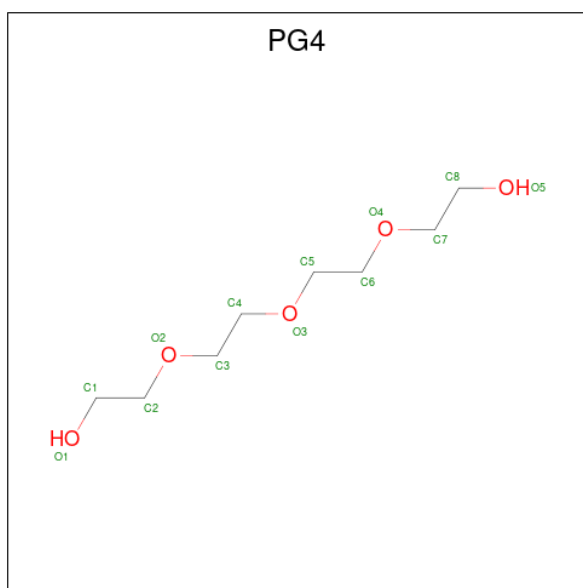
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



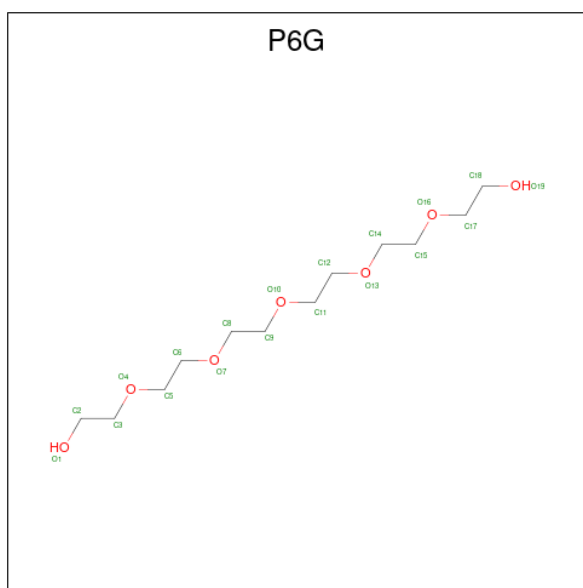
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			16	10	6		
6	F	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			19	12	7		
8	E	1	Total	C	O	0	0
			19	12	7		

- Molecule 9 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total 1	Na 1	0	0
9	F	1	Total 1	Na 1	0	0

- Molecule 10 is water.

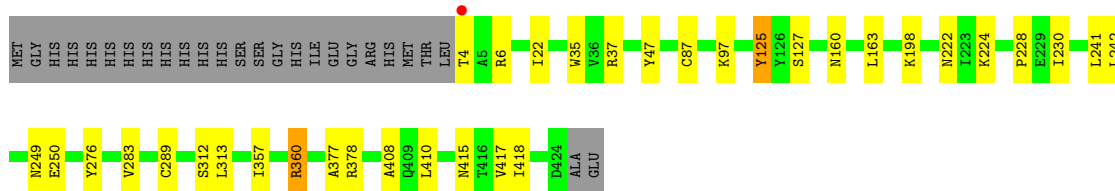
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	255	Total 255	O 255	0	0
10	B	247	Total 247	O 247	0	0
10	C	218	Total 218	O 218	0	0
10	D	226	Total 226	O 226	0	0
10	E	226	Total 226	O 226	0	0
10	F	220	Total 220	O 220	0	0

3 Residue-property plots

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.

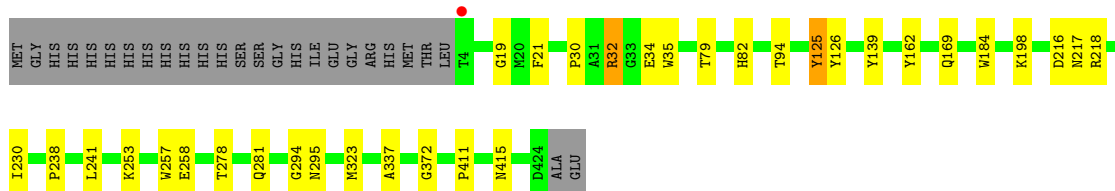
- Molecule 1: Alpha-L-fucosidase

Chain A: 



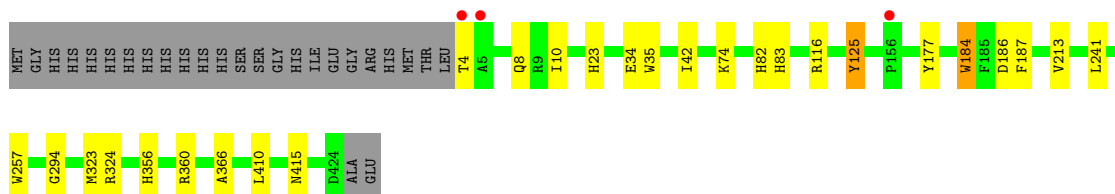
- Molecule 1: Alpha-L-fucosidase

Chain B: 



- Molecule 1: Alpha-L-fucosidase

Chain C: 



- Molecule 1: Alpha-L-fucosidase

Chain D: 





- Molecule 1: Alpha-L-fucosidase

Chain E: 87% 7% 6%



- Molecule 1: Alpha-L-fucosidase

Chain F: 89% 6% .



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

Chain G: 100%



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

Chain H: 100%



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

Chain I: 100%



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

Chain J: 100%



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

Chain K:  100%



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

Chain L:  50% 50%

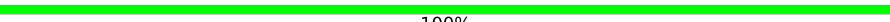


- Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain M:  100%



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

Chain N:  100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.77Å 148.76Å 194.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 2.20 48.93 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.93-2.20) 99.2 (48.93-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.167 , 0.217 (Not available) , 0.171	Depositor DCC
R_{free} test set	7763 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22428	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 1PE, PG4, PEG, PGE, P6G, GLC

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	1.13	6/3524 (0.2%)	1.10	0/4790
1	B	1.19	9/3536 (0.3%)	1.11	1/4806 (0.0%)
1	C	1.15	7/3513 (0.2%)	1.06	0/4776
1	D	1.19	9/3550 (0.3%)	1.09	1/4825 (0.0%)
1	E	1.19	10/3524 (0.3%)	1.12	2/4790 (0.0%)
1	F	1.13	3/3582 (0.1%)	1.11	4/4867 (0.1%)
All	All	1.16	44/21229 (0.2%)	1.10	8/28854 (0.0%)

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	92	ALA	C-O	-8.38	1.13	1.24
1	E	177	TYR	N-CA	7.73	1.53	1.46
1	D	37	ARG	N-CA	7.33	1.55	1.46
1	A	313	LEU	N-CA	7.16	1.55	1.46
1	E	126	TYR	C-O	6.41	1.31	1.23
1	D	261	ILE	C-O	-6.41	1.17	1.24
1	C	366	ALA	C-O	-6.20	1.16	1.24
1	B	372	GLY	C-O	-6.14	1.17	1.24
1	D	19	GLY	N-CA	6.04	1.50	1.45
1	F	265	HIS	N-CA	5.99	1.53	1.46
1	E	63	ALA	C-O	-5.94	1.17	1.24
1	C	356	HIS	N-CA	-5.91	1.39	1.46
1	D	23	HIS	C-O	-5.82	1.17	1.24
1	F	307	GLU	N-CA	-5.79	1.39	1.46
1	E	194	GLY	C-O	5.74	1.31	1.24
1	E	125	TYR	N-CA	-5.71	1.39	1.46
1	B	19	GLY	N-CA	5.64	1.50	1.44
1	D	365	ILE	N-CA	-5.64	1.39	1.46
1	A	127	SER	C-O	5.62	1.30	1.24
1	B	139	TYR	C-O	-5.62	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	408	ALA	C-O	-5.60	1.17	1.24
1	A	22	ILE	C-O	-5.60	1.17	1.24
1	E	381	ALA	C-O	-5.56	1.17	1.24
1	A	417	VAL	C-O	-5.51	1.17	1.24
1	C	213	VAL	C-O	-5.51	1.17	1.24
1	B	337	ALA	C-O	-5.47	1.17	1.24
1	C	184	TRP	C-O	-5.42	1.17	1.24
1	E	57	VAL	C-O	-5.35	1.17	1.24
1	E	101	THR	N-CA	5.35	1.52	1.45
1	C	42	ILE	N-CA	-5.32	1.40	1.46
1	B	94	THR	C-O	5.31	1.30	1.23
1	D	166	MET	N-CA	-5.28	1.40	1.46
1	E	283	VAL	N-CA	-5.26	1.40	1.46
1	C	323	MET	C-O	-5.25	1.17	1.24
1	B	253	LYS	N-CA	5.19	1.54	1.46
1	B	323	MET	C-O	-5.19	1.18	1.24
1	B	82	HIS	CE1-NE2	5.18	1.37	1.32
1	B	238	PRO	C-O	5.15	1.29	1.23
1	D	212	ASN	C-O	-5.11	1.17	1.24
1	C	324	ARG	C-O	-5.09	1.18	1.24
1	F	305	LYS	C-O	-5.05	1.17	1.24
1	D	249	ASN	N-CA	5.04	1.52	1.45
1	A	283	VAL	C-O	-5.01	1.18	1.24
1	E	127	SER	N-CA	-5.00	1.40	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	308	ILE	N-CA-C	-6.00	103.07	108.95
1	E	164	ASP	N-CA-C	-5.86	104.90	111.28
1	B	162	TYR	N-CA-CB	5.52	118.01	110.01
1	F	122	VAL	CA-C-N	5.26	125.23	121.65
1	F	122	VAL	C-N-CA	5.26	125.23	121.65
1	E	161	ARG	N-CA-C	-5.12	105.78	111.36
1	F	249	ASN	CA-C-N	5.07	127.32	120.38
1	F	249	ASN	C-N-CA	5.07	127.32	120.38

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	3416	0	3270	22	0
1	B	3424	0	3279	13	0
1	C	3408	0	3257	12	0
1	D	3444	0	3303	16	0
1	E	3416	0	3270	14	0
1	F	3473	0	3329	18	0
2	G	23	0	21	0	0
2	H	23	0	21	0	0
2	I	23	0	21	0	0
2	J	23	0	21	0	0
2	K	23	0	21	0	0
2	L	23	0	21	1	0
2	M	23	0	21	0	0
2	N	23	0	21	0	0
3	A	12	0	12	1	0
3	B	12	0	12	2	0
3	C	12	0	12	3	0
3	D	12	0	12	2	0
3	E	12	0	12	2	0
3	F	12	0	12	2	0
4	A	20	0	28	1	0
4	B	10	0	14	0	0
4	C	20	0	28	1	0
4	D	20	0	28	2	0
4	E	20	0	28	0	0
4	F	10	0	14	0	0
5	B	14	0	20	1	0
6	B	16	0	22	0	0
6	F	16	0	22	0	0
7	B	13	0	18	1	0
8	C	19	0	26	0	0
8	E	19	0	26	0	0
9	C	1	0	0	0	0
9	F	1	0	0	0	0
10	A	255	0	0	1	0
10	B	247	0	0	0	0
10	C	218	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	226	0	0	0	0
10	E	226	0	0	1	0
10	F	220	0	0	0	0
All	All	22428	0	20222	94	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.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:ASN:OD1	1:D:151:GLU:HG2	1.78	0.83
1:E:360:ARG:HH21	1:E:360:ARG:HG3	1.57	0.69
1:B:30:PRO:O	1:B:32:ARG:HG2	1.95	0.66
1:A:360:ARG:HH11	1:A:360:ARG:HG3	1.60	0.66
1:A:360:ARG:HB2	1:A:410:LEU:HG	1.76	0.65
1:C:257:TRP:CE2	1:C:294:GLY:HA3	2.32	0.64
1:E:280:LYS:O	1:E:284:ARG:HG3	1.98	0.64
1:F:35:TRP:HE1	3:F:501:GLC:H2	1.63	0.64
1:E:176:ASN:HA	2:L:1:GLC:H1	1.81	0.63
1:D:258:GLU:HB2	1:D:295:ASN:HB2	1.82	0.62
1:D:360:ARG:HB2	1:D:410:LEU:HG	1.83	0.61
1:D:146:MET:HA	1:D:146:MET:HE2	1.83	0.60
1:A:357:ILE:HD11	1:A:418:ILE:HD12	1.86	0.56
1:B:216:ASP:OD2	1:B:218:ARG:HG3	2.06	0.56
1:A:224:LYS:O	1:A:250:GLU:HG3	2.06	0.55
1:E:195:GLU:OE2	1:E:195:GLU:HA	2.06	0.55
1:A:163:LEU:HD13	1:A:198:LYS:HG3	1.89	0.55
1:B:258:GLU:HB2	1:B:295:ASN:HB2	1.90	0.54
1:F:360:ARG:HB2	1:F:410:LEU:HG	1.91	0.53
1:E:360:ARG:HB2	1:E:410:LEU:HG	1.90	0.53
1:C:74:LYS:HD3	4:C:503:PGE:H52	1.90	0.53
1:C:82:HIS:HD1	1:C:83:HIS:H	1.56	0.52
1:E:35:TRP:HE1	3:E:501:GLC:H2	1.73	0.52
1:A:360:ARG:HG3	1:A:360:ARG:NH1	2.24	0.52
1:D:198:LYS:HE3	4:D:503:PGE:H4	1.92	0.52
1:E:360:ARG:HG3	1:E:360:ARG:NH2	2.24	0.51
1:A:377:ALA:C	1:A:378[B]:ARG:HG2	2.35	0.51
1:B:198:LYS:HE2	7:B:506:PG4:O4	2.10	0.51
1:A:249:ASN:OD1	1:A:249:ASN:C	2.53	0.51
1:A:125:TYR:C	1:A:125:TYR:CD1	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:PRO:HB3	1:F:274:ARG:NH2	2.27	0.50
1:F:360:ARG:HG3	1:F:360:ARG:HH11	1.76	0.50
1:A:6:ARG:HG2	10:A:607:HOH:O	2.12	0.50
1:C:360:ARG:HB2	1:C:410:LEU:HG	1.94	0.49
1:D:222:ASN:C	1:D:222:ASN:OD1	2.56	0.49
1:E:360:ARG:HG3	1:E:360:ARG:O	2.12	0.49
1:A:37:ARG:HG3	1:A:47:TYR:CE1	2.48	0.49
1:B:35:TRP:HE1	3:B:501:GLC:H2	1.78	0.49
1:B:126:TYR:OH	1:B:169:GLN:NE2	2.43	0.48
1:A:377:ALA:C	1:A:378[A]:ARG:HG2	2.37	0.48
1:F:34:GLU:OE2	3:F:501:GLC:O3	2.32	0.48
1:C:186:ASP:OD1	1:C:187:PHE:HB3	2.12	0.48
1:E:34:GLU:OE2	3:E:501:GLC:O3	2.31	0.48
1:A:242:LEU:HD22	1:A:289:CYS:SG	2.54	0.47
1:C:35:TRP:HE1	3:C:501:GLC:H2	1.79	0.47
1:F:128:ILE:HD12	1:F:197:TRP:CE2	2.50	0.47
1:A:360:ARG:HG3	1:A:360:ARG:O	2.14	0.47
1:B:34:GLU:OE2	3:B:501:GLC:O3	2.33	0.46
1:A:276:TYR:HE2	1:A:312:SER:HG	1.62	0.46
1:D:149:ASN:CG	1:D:151:GLU:HG2	2.40	0.45
1:B:278:THR:OG1	1:B:281:GLN:HG3	2.17	0.45
1:D:242:LEU:HD22	1:D:289:CYS:SG	2.55	0.45
1:E:186:ASP:OD1	1:E:187:PHE:HB3	2.16	0.45
1:F:34:GLU:CD	1:F:34:GLU:H	2.24	0.45
1:A:160:ASN:OD1	4:A:504:PGE:H62	2.16	0.45
1:A:35:TRP:HE1	3:A:501:GLC:H2	1.81	0.45
1:F:241:LEU:HD12	1:F:241:LEU:O	2.17	0.44
1:D:35:TRP:HE1	3:D:501:GLC:H2	1.83	0.44
1:B:79:THR:HA	1:B:125:TYR:HB3	1.99	0.44
1:C:125:TYR:CD1	1:C:125:TYR:C	2.95	0.44
1:D:79:THR:HA	1:D:125:TYR:HB3	1.99	0.44
1:F:241:LEU:C	1:F:241:LEU:CD1	2.91	0.44
1:A:357:ILE:HD11	1:A:418:ILE:CD1	2.48	0.43
1:C:34:GLU:OE2	3:C:501:GLC:O3	2.36	0.43
1:F:89:PHE:HA	1:F:106:ASP:OD1	2.18	0.43
1:C:23:HIS:NE2	3:C:501:GLC:O4	2.42	0.43
1:B:257:TRP:CE2	1:B:294:GLY:HA3	2.53	0.43
1:C:4:THR:O	1:C:8:GLN:HB2	2.19	0.43
1:C:116:ARG:NH1	1:C:177:TYR:O	2.44	0.43
1:E:303:ASN:OD1	1:E:303:ASN:C	2.62	0.43
1:D:37:ARG:HG3	1:D:47:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:TYR:CD1	1:F:125:TYR:C	2.97	0.42
1:A:377:ALA:O	1:A:378[B]:ARG:HG2	2.19	0.42
1:D:34:GLU:OE2	3:D:501:GLC:O3	2.38	0.42
1:A:87:CYS:O	1:A:97:LYS:HA	2.19	0.42
1:E:206:ILE:HG21	1:E:215:ILE:HD11	2.00	0.42
1:E:128:ILE:HD12	1:E:197:TRP:CE2	2.55	0.42
1:F:5:ALA:O	1:F:9:ARG:HG2	2.20	0.42
1:F:360:ARG:HG3	1:F:360:ARG:O	2.20	0.42
1:D:360:ARG:HH11	1:D:360:ARG:HG3	1.84	0.41
1:F:196:LYS:HA	1:F:196:LYS:HD3	1.77	0.41
1:F:195:GLU:OE1	1:F:195:GLU:HA	2.20	0.41
1:A:224:LYS:O	1:A:249:ASN:HB2	2.21	0.41
1:F:242:LEU:HD22	1:F:289:CYS:SG	2.61	0.41
1:F:282:VAL:HG13	1:F:296:MET:HE1	2.02	0.41
1:D:205:MET:HG3	4:D:502:PGE:H22	2.03	0.41
1:B:125:TYR:C	1:B:125:TYR:CD1	2.99	0.41
1:B:217:ASN:HD21	5:B:502:PEG:H41	1.85	0.40
1:D:16:ASP:HB3	1:D:74:LYS:HB2	2.03	0.40
1:E:378[A]:ARG:HD2	10:E:607:HOH:O	2.21	0.40
1:F:290:VAL:HG21	1:F:330:ILE:HG23	2.03	0.40
1:A:222:ASN:O	1:A:228:PRO:HB3	2.22	0.40
1:C:241:LEU:HD12	1:C:241:LEU:C	2.47	0.40
1:D:43:PRO:O	1:D:44:VAL:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	421/447 (94%)	410 (97%)	10 (2%)	1 (0%)	43 51
1	B	422/447 (94%)	403 (96%)	18 (4%)	1 (0%)	43 51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	420/447 (94%)	404 (96%)	15 (4%)	1 (0%)	43	51
1	D	424/447 (95%)	410 (97%)	13 (3%)	1 (0%)	43	51
1	E	421/447 (94%)	408 (97%)	13 (3%)	0	100	100
1	F	428/447 (96%)	413 (96%)	14 (3%)	1 (0%)	43	51
All	All	2536/2682 (95%)	2448 (96%)	83 (3%)	5 (0%)	43	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	ASN
1	D	415	ASN
1	B	415	ASN
1	C	415	ASN
1	F	415	ASN

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	352/372 (95%)	347 (99%)	5 (1%)	59	75
1	B	353/372 (95%)	347 (98%)	6 (2%)	53	69
1	C	351/372 (94%)	348 (99%)	3 (1%)	70	84
1	D	355/372 (95%)	349 (98%)	6 (2%)	53	69
1	E	352/372 (95%)	346 (98%)	6 (2%)	53	69
1	F	358/372 (96%)	352 (98%)	6 (2%)	53	69
All	All	2121/2232 (95%)	2089 (98%)	32 (2%)	57	73

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	125	TYR

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Mol	Chain	Res	Type
1	A	230	ILE
1	A	241	LEU
1	A	360	ARG
1	B	21	PHE
1	B	32	ARG
1	B	125	TYR
1	B	184	TRP
1	B	230	ILE
1	B	241	LEU
1	C	10	ILE
1	C	125	TYR
1	C	184	TRP
1	D	21	PHE
1	D	66	LYS
1	D	226	ARG
1	D	241	LEU
1	D	258	GLU
1	D	284	ARG
1	E	21	PHE
1	E	166	MET
1	E	184	TRP
1	E	241	LEU
1	E	307	GLU
1	E	360	ARG
1	F	21	PHE
1	F	151	GLU
1	F	184	TRP
1	F	196	LYS
1	F	241	LEU
1	F	424	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	212	ASN
1	A	389	GLN
1	C	55	ASN
1	C	169	GLN
1	D	389	GLN
1	E	272	HIS
1	F	0	HIS

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Mol	Chain	Res	Type
1	F	132	HIS
1	F	160	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

16 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GLC	G	1	2	12,12,12	0.72	0	17,17,17	0.59	0
2	GLC	G	2	2	11,11,12	0.92	0	15,15,17	0.59	0
2	GLC	H	1	2	12,12,12	0.67	0	17,17,17	0.59	0
2	GLC	H	2	2	11,11,12	0.66	0	15,15,17	0.87	0
2	GLC	I	1	2	12,12,12	0.70	0	17,17,17	0.64	0
2	GLC	I	2	2	11,11,12	0.89	0	15,15,17	1.03	0
2	GLC	J	1	2	12,12,12	0.52	0	17,17,17	0.74	0
2	GLC	J	2	2	11,11,12	0.51	0	15,15,17	0.74	0
2	GLC	K	1	2	12,12,12	0.74	0	17,17,17	0.86	0
2	GLC	K	2	2	11,11,12	0.71	0	15,15,17	1.07	0
2	GLC	L	1	2	12,12,12	0.71	0	17,17,17	1.17	1 (5%)
2	GLC	L	2	2	11,11,12	0.71	0	15,15,17	1.02	2 (13%)
2	GLC	M	1	2	12,12,12	0.79	0	17,17,17	0.70	0
2	GLC	M	2	2	11,11,12	1.15	0	15,15,17	0.91	0
2	GLC	N	1	2	12,12,12	0.60	0	17,17,17	0.60	0
2	GLC	N	2	2	11,11,12	0.65	0	15,15,17	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	G	1	2	-	0/2/22/22	0/1/1/1
2	GLC	G	2	2	-	0/2/19/22	0/1/1/1
2	GLC	H	1	2	-	0/2/22/22	0/1/1/1
2	GLC	H	2	2	-	2/2/19/22	0/1/1/1
2	GLC	I	1	2	-	0/2/22/22	0/1/1/1
2	GLC	I	2	2	-	2/2/19/22	0/1/1/1
2	GLC	J	1	2	-	0/2/22/22	0/1/1/1
2	GLC	J	2	2	-	0/2/19/22	0/1/1/1
2	GLC	K	1	2	-	0/2/22/22	0/1/1/1
2	GLC	K	2	2	-	2/2/19/22	0/1/1/1
2	GLC	L	1	2	-	2/2/22/22	0/1/1/1
2	GLC	L	2	2	-	0/2/19/22	0/1/1/1
2	GLC	M	1	2	-	0/2/22/22	0/1/1/1
2	GLC	M	2	2	-	0/2/19/22	0/1/1/1
2	GLC	N	1	2	-	2/2/22/22	0/1/1/1
2	GLC	N	2	2	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	2	GLC	C3-C4-C5	2.29	114.39	110.23
2	L	2	GLC	O4-C4-C3	-2.19	105.22	110.38
2	L	1	GLC	O2-C2-C3	-2.02	105.61	110.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	2	GLC	C4-C5-C6-O6
2	L	1	GLC	O5-C5-C6-O6
2	L	1	GLC	C4-C5-C6-O6
2	I	2	GLC	C4-C5-C6-O6
2	H	2	GLC	O5-C5-C6-O6
2	N	1	GLC	C4-C5-C6-O6
2	K	2	GLC	C4-C5-C6-O6

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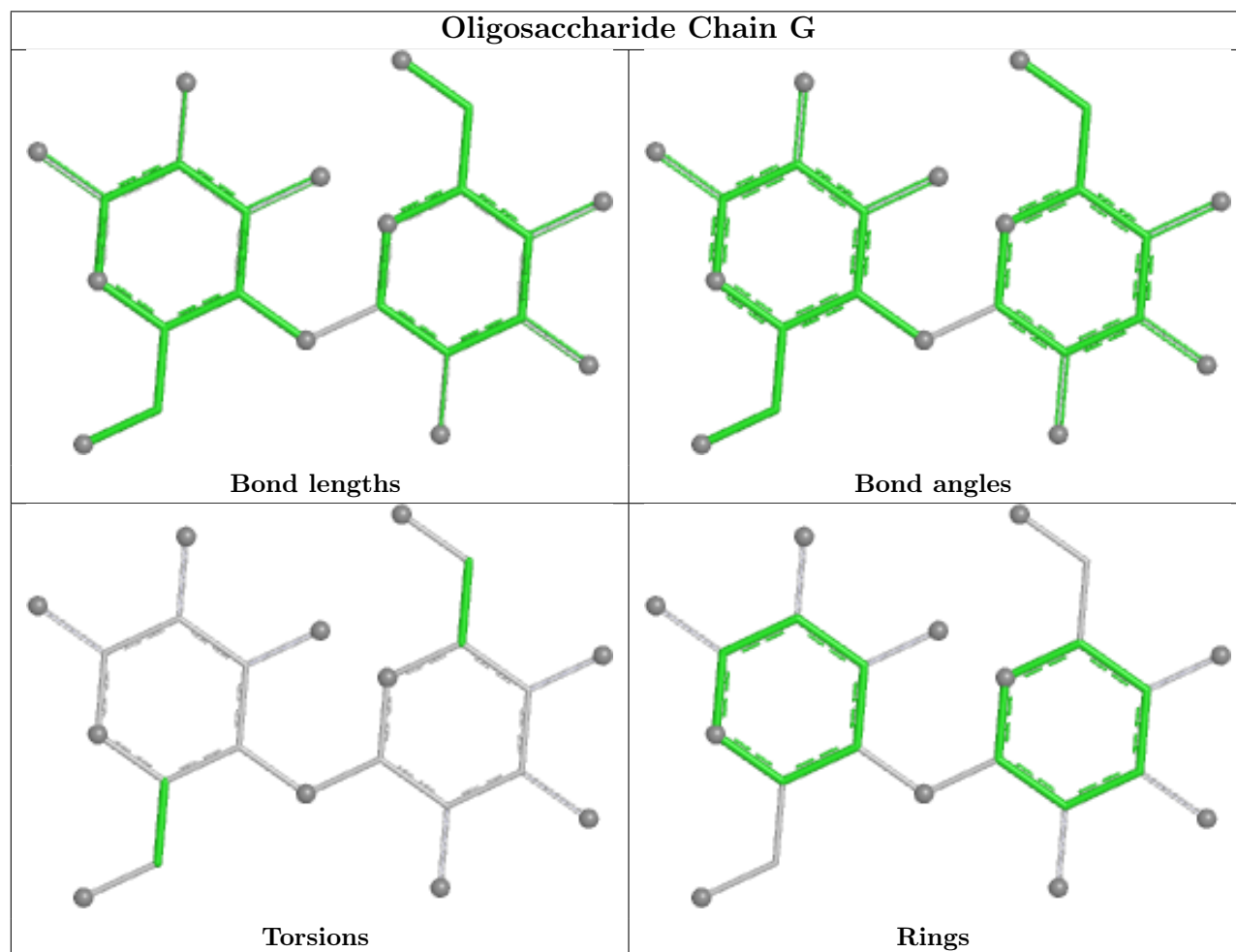
Mol	Chain	Res	Type	Atoms
2	N	1	GLC	O5-C5-C6-O6
2	N	2	GLC	C4-C5-C6-O6
2	K	2	GLC	O5-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6

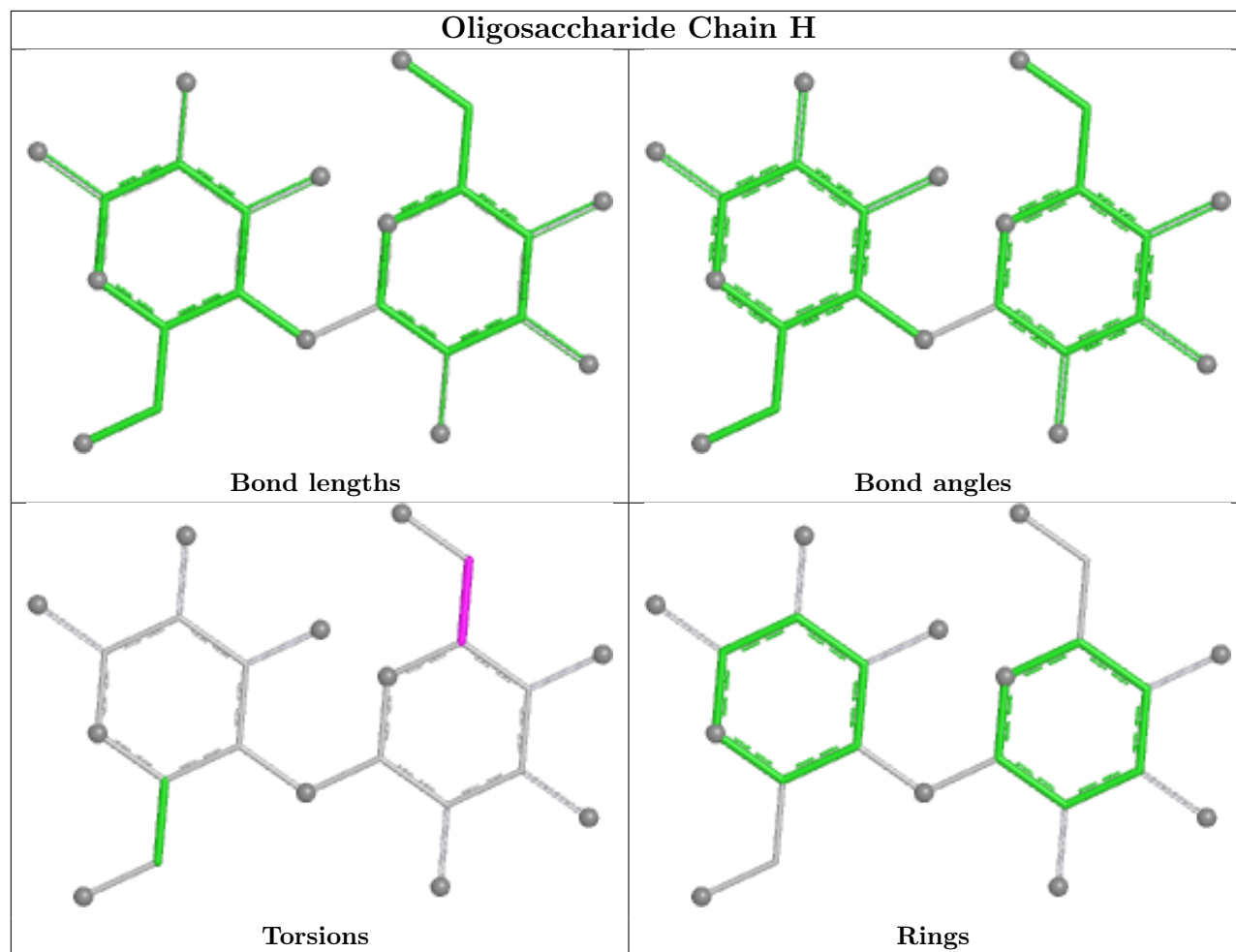
There are no ring outliers.

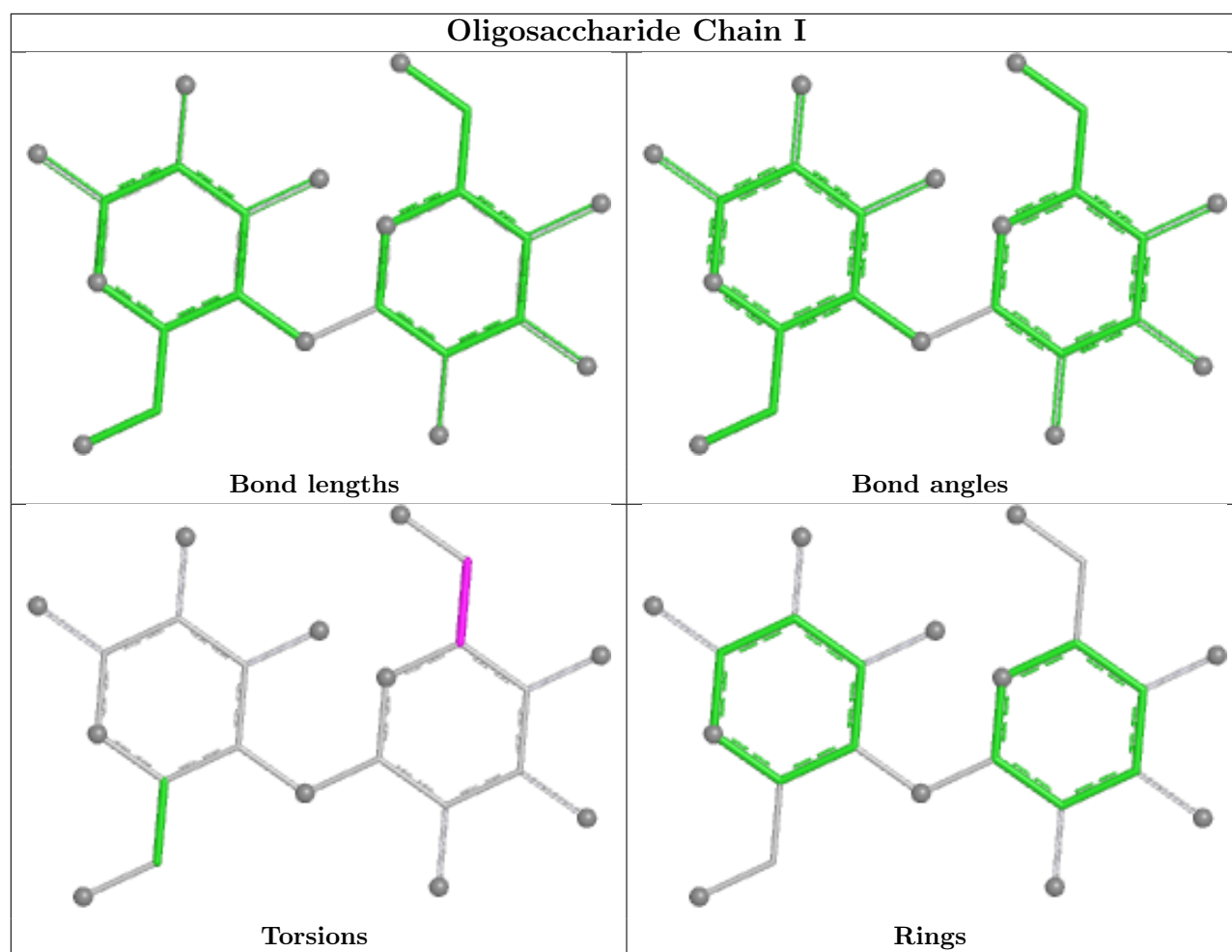
1 monomer is involved in 1 short contact:

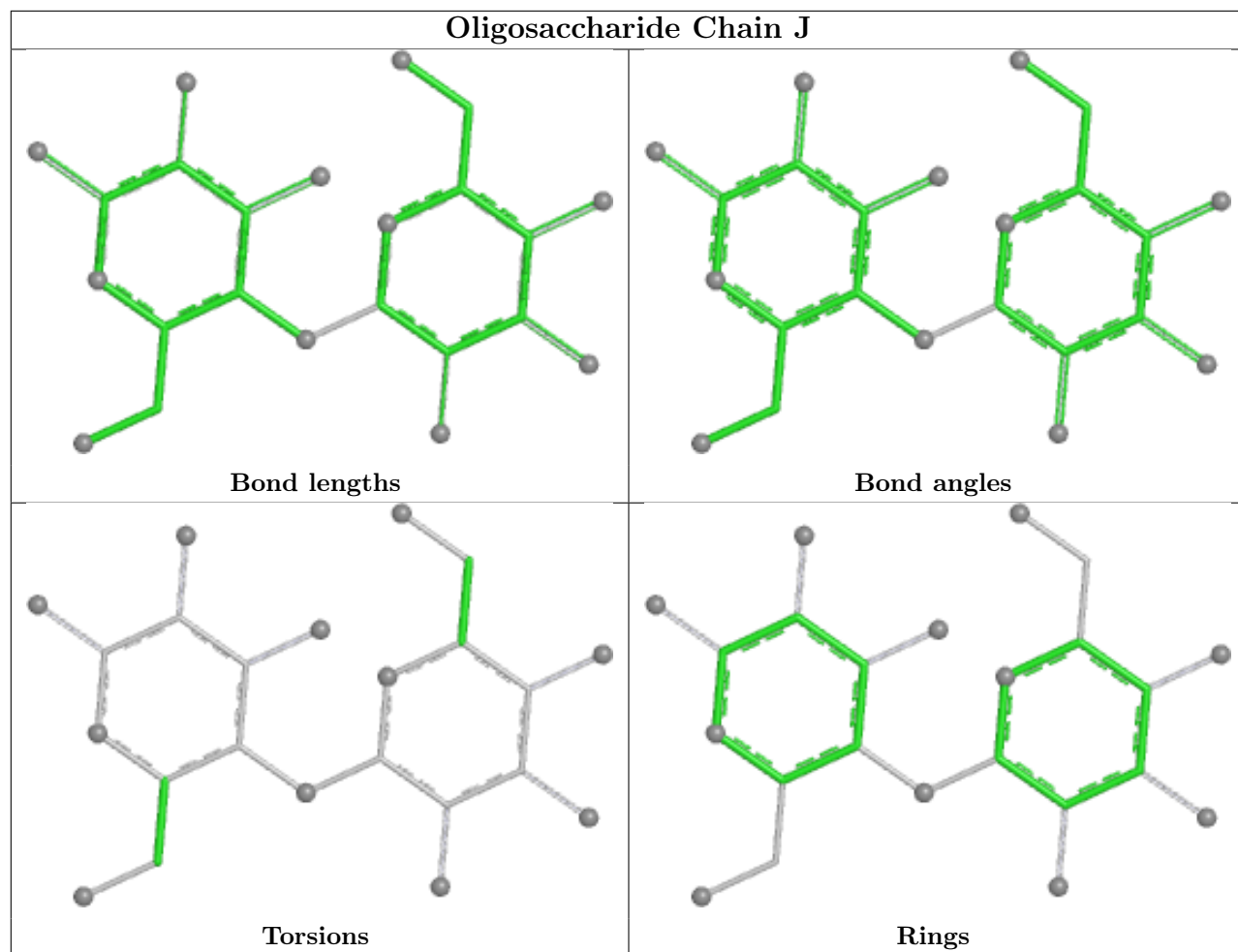
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	GLC	1	0

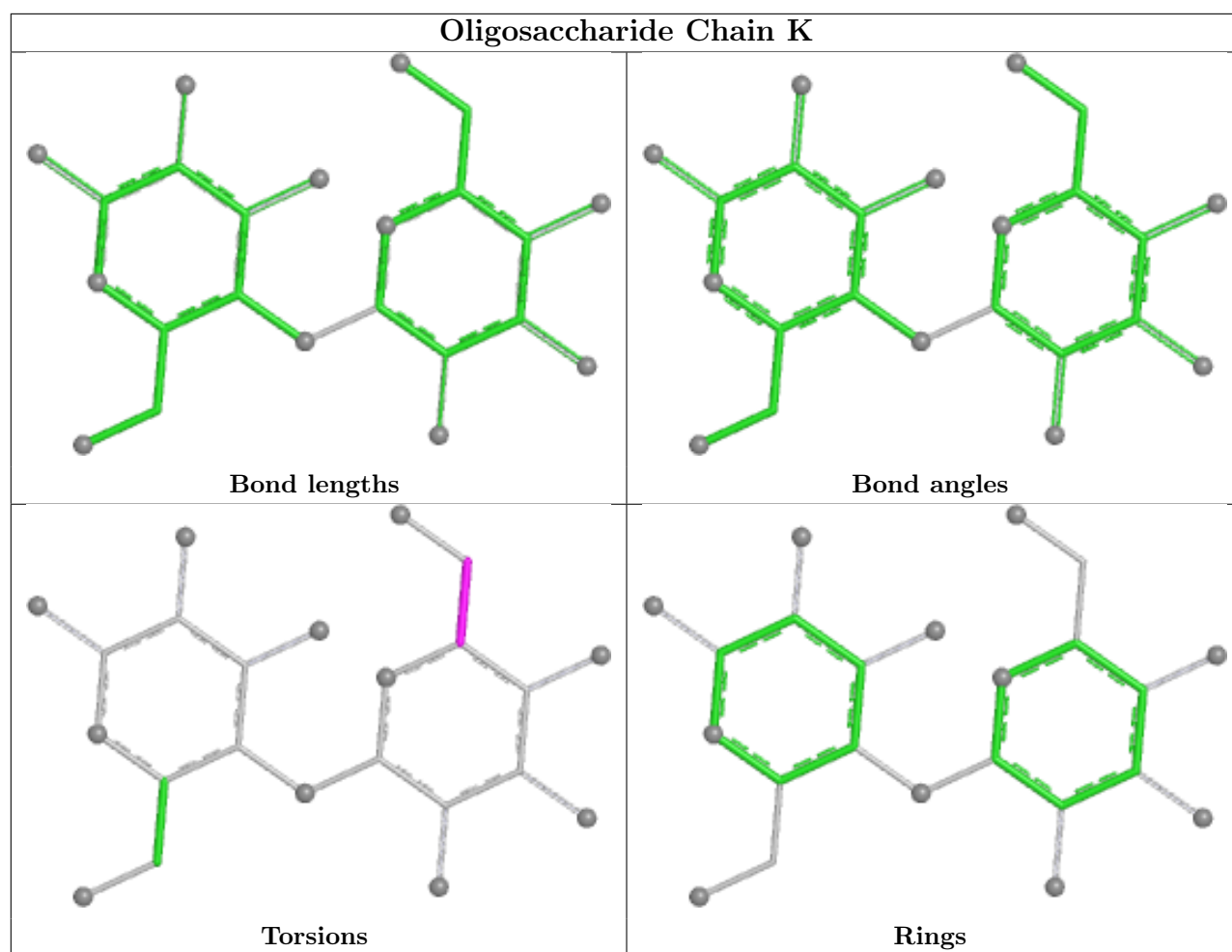
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

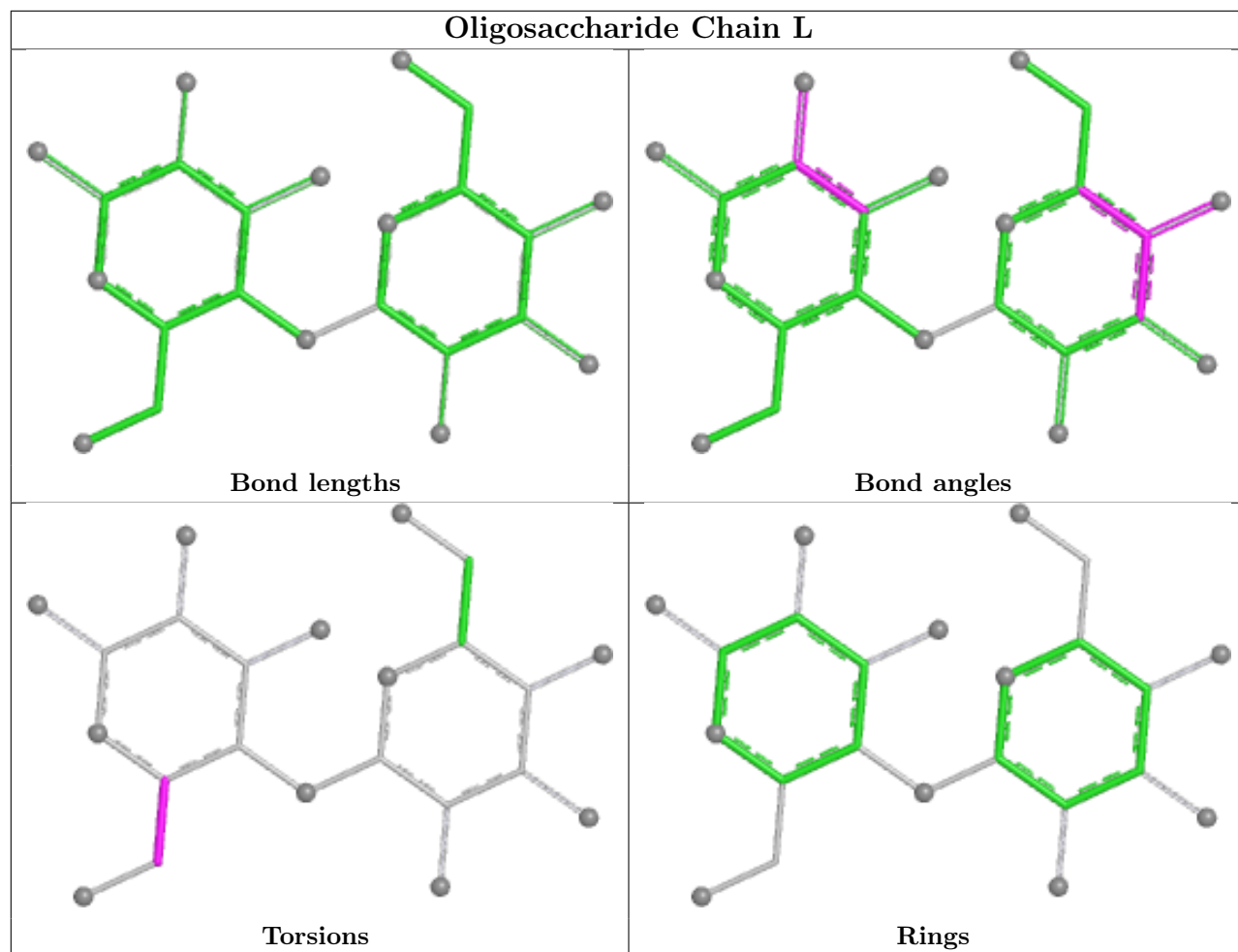


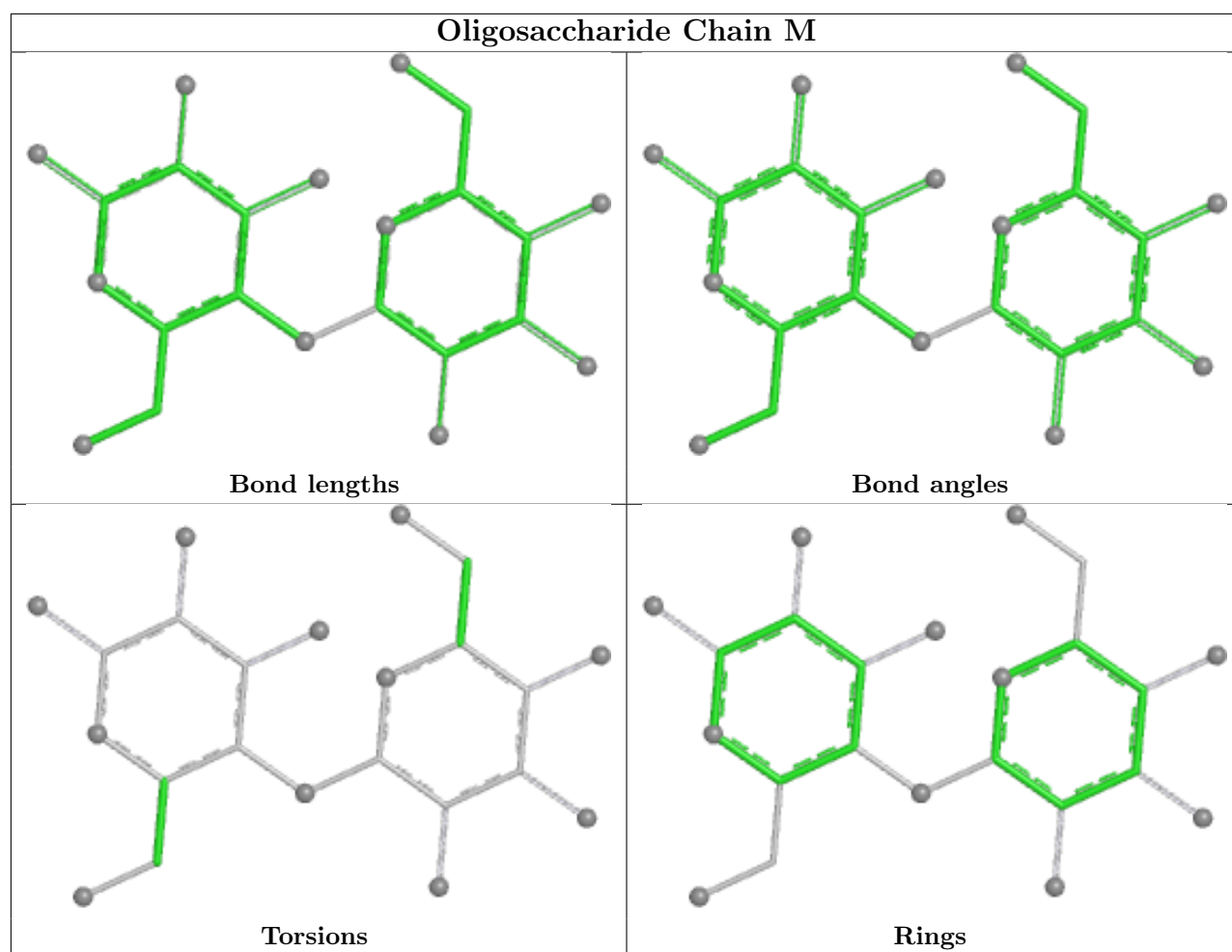


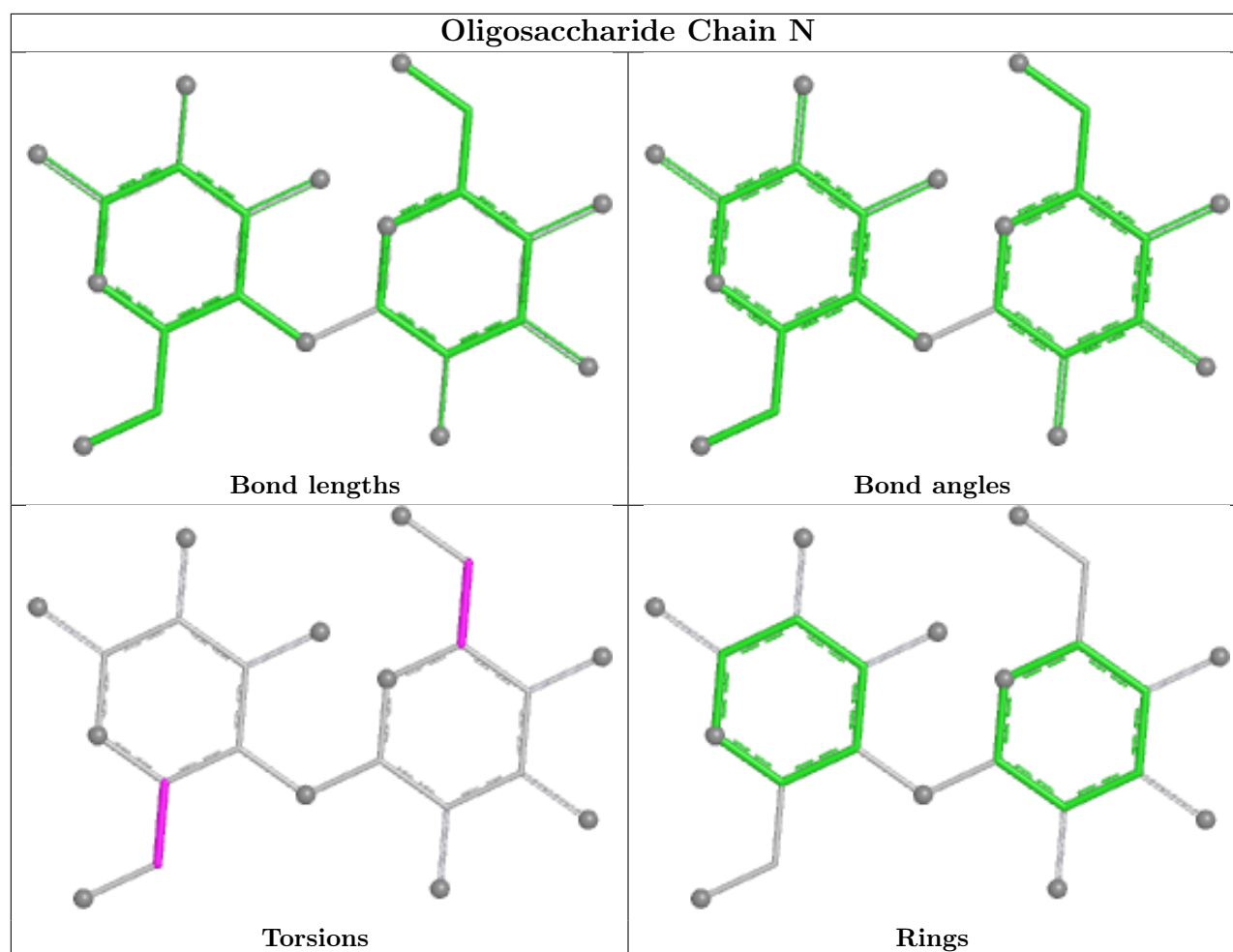












5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	$\# Z > 2$
3	GLC	E	501	-	12,12,12	0.74	0	17,17,17	2.12	6 (35%)
4	PGE	B	504	-	9,9,9	0.85	0	8,8,8	0.88	0
4	PGE	C	504	-	9,9,9	0.56	0	8,8,8	0.46	0
4	PGE	D	502	-	9,9,9	0.77	0	8,8,8	0.78	0
3	GLC	B	501	-	12,12,12	0.78	0	17,17,17	2.33	10 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	1PE	F	505	9	15,15,15	0.77	0	14,14,14	0.53	0
3	GLC	F	501	-	12,12,12	0.72	0	17,17,17	2.22	6 (35%)
4	PGE	D	503	-	9,9,9	0.58	0	8,8,8	0.56	0
4	PGE	A	504	-	9,9,9	0.71	0	8,8,8	0.82	0
3	GLC	D	501	-	12,12,12	0.93	1 (8%)	17,17,17	2.17	7 (41%)
3	GLC	C	501	-	12,12,12	0.75	0	17,17,17	2.01	4 (23%)
4	PGE	E	507	-	9,9,9	0.91	0	8,8,8	0.77	0
8	P6G	C	502	9	18,18,18	0.78	0	17,17,17	0.92	0
4	PGE	A	505	-	9,9,9	0.78	0	8,8,8	0.88	0
3	GLC	A	501	-	12,12,12	0.75	0	17,17,17	2.39	10 (58%)
4	PGE	F	504	-	9,9,9	0.74	0	8,8,8	0.77	0
5	PEG	B	503	-	6,6,6	0.67	0	5,5,5	0.24	0
6	1PE	B	505	-	15,15,15	0.61	0	14,14,14	0.32	0
5	PEG	B	502	-	6,6,6	0.54	0	5,5,5	0.31	0
7	PG4	B	506	-	12,12,12	0.69	0	11,11,11	0.37	0
4	PGE	C	503	-	9,9,9	1.08	0	8,8,8	1.46	2 (25%)
4	PGE	E	506	-	9,9,9	0.87	0	8,8,8	0.77	0
8	P6G	E	508	-	18,18,18	0.82	0	17,17,17	0.97	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
3	GLC	E	501	-	-	0/2/22/22	0/1/1/1
4	PGE	B	504	-	-	2/7/7/7	-
4	PGE	C	504	-	-	2/7/7/7	-
4	PGE	D	502	-	-	5/7/7/7	-
3	GLC	B	501	-	-	0/2/22/22	0/1/1/1
6	1PE	F	505	9	-	7/13/13/13	-
3	GLC	F	501	-	-	0/2/22/22	0/1/1/1
4	PGE	D	503	-	-	5/7/7/7	-
4	PGE	A	504	-	-	4/7/7/7	-
3	GLC	D	501	-	-	1/2/22/22	0/1/1/1
3	GLC	C	501	-	-	2/2/22/22	0/1/1/1
4	PGE	E	507	-	-	4/7/7/7	-
8	P6G	C	502	9	-	7/16/16/16	-
4	PGE	A	505	-	-	1/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLC	A	501	-	-	2/2/22/22	0/1/1/1
4	PGE	F	504	-	-	7/7/7/7	-
5	PEG	B	503	-	-	2/4/4/4	-
6	1PE	B	505	-	-	7/13/13/13	-
5	PEG	B	502	-	-	2/4/4/4	-
7	PG4	B	506	-	-	2/10/10/10	-
4	PGE	C	503	-	-	5/7/7/7	-
4	PGE	E	506	-	-	2/7/7/7	-
8	P6G	E	508	-	-	8/16/16/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	GLC	O5-C5	-2.18	1.39	1.44

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	501	GLC	O5-C1-C2	-5.33	100.93	110.30
3	E	501	GLC	O5-C1-C2	-4.90	101.69	110.30
3	A	501	GLC	C4-C3-C2	4.34	118.44	110.83
3	D	501	GLC	O2-C2-C1	4.31	119.19	109.25
3	C	501	GLC	O5-C1-C2	-4.02	103.22	110.30
3	B	501	GLC	C4-C3-C2	3.76	117.44	110.83
3	D	501	GLC	C4-C3-C2	3.67	117.28	110.83
3	E	501	GLC	C3-C4-C5	3.56	116.69	110.23
3	F	501	GLC	C4-C3-C2	3.51	117.00	110.83
3	A	501	GLC	O5-C1-C2	-3.50	104.14	110.30
3	A	501	GLC	C1-C2-C3	-3.44	103.33	110.36
3	D	501	GLC	O3-C3-C2	-3.41	102.34	110.38
3	B	501	GLC	C3-C4-C5	3.33	116.28	110.23
3	E	501	GLC	O6-C6-C5	-3.30	100.10	111.33
3	B	501	GLC	O2-C2-C1	3.22	116.67	109.25
3	C	501	GLC	C4-C3-C2	3.15	116.36	110.83
3	F	501	GLC	C3-C4-C5	3.11	115.88	110.23
3	A	501	GLC	O2-C2-C1	3.06	116.31	109.25
3	F	501	GLC	O6-C6-C5	-3.06	100.91	111.33
3	B	501	GLC	O1-C1-O5	-3.01	101.46	110.41
3	B	501	GLC	O1-C1-C2	2.99	117.65	108.98
3	D	501	GLC	C3-C4-C5	2.97	115.62	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	GLC	C3-C4-C5	2.97	115.62	110.23
3	B	501	GLC	C1-C2-C3	-2.82	104.60	110.36
3	C	501	GLC	C3-C4-C5	2.82	115.34	110.23
3	A	501	GLC	O3-C3-C4	-2.77	103.85	110.38
3	B	501	GLC	O6-C6-C5	-2.62	102.41	111.33
3	E	501	GLC	O3-C3-C2	-2.62	104.20	110.38
4	C	503	PGE	O2-C3-C4	2.54	121.93	110.35
3	C	501	GLC	O1-C1-C2	2.52	116.29	108.98
3	B	501	GLC	O3-C3-C2	-2.48	104.54	110.38
3	F	501	GLC	C1-C2-C3	-2.47	105.31	110.36
3	A	501	GLC	O3-C3-C2	-2.41	104.69	110.38
3	A	501	GLC	O6-C6-C5	-2.38	103.21	111.33
3	E	501	GLC	C4-C3-C2	2.37	114.98	110.83
3	A	501	GLC	O5-C5-C4	2.34	113.91	109.70
3	E	501	GLC	O4-C4-C5	-2.31	103.63	109.32
3	D	501	GLC	O1-C1-O5	-2.29	103.62	110.41
4	C	503	PGE	C5-O3-C4	2.27	123.18	113.26
3	B	501	GLC	O5-C5-C4	2.20	113.66	109.70
3	D	501	GLC	O5-C5-C4	2.20	113.66	109.70
3	B	501	GLC	C1-O5-C5	-2.17	109.46	113.65
3	F	501	GLC	O3-C3-C2	-2.14	105.33	110.38
3	D	501	GLC	O6-C6-C5	-2.09	104.22	111.33
3	A	501	GLC	O1-C1-O5	-2.01	104.45	110.41

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	503	PGE	C3-C4-O3-C5
6	F	505	1PE	OH5-C14-C24-OH4
6	B	505	1PE	OH6-C15-C25-OH5
6	B	505	1PE	OH4-C13-C23-OH3
4	E	507	PGE	O2-C3-C4-O3
6	F	505	1PE	OH4-C13-C23-OH3
4	D	503	PGE	O2-C3-C4-O3
8	E	508	P6G	O13-C14-C15-O16
8	E	508	P6G	O10-C11-C12-O13
8	C	502	P6G	O13-C14-C15-O16
4	F	504	PGE	O2-C3-C4-O3
4	B	504	PGE	O3-C5-C6-O4
4	C	503	PGE	O3-C5-C6-O4
4	F	504	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
3	C	501	GLC	C4-C5-C6-O6
4	D	502	PGE	O2-C3-C4-O3
8	C	502	P6G	O10-C11-C12-O13
8	E	508	P6G	C15-C14-O13-C12
4	C	503	PGE	O1-C1-C2-O2
4	E	507	PGE	O3-C5-C6-O4
6	B	505	1PE	OH2-C12-C22-OH3
4	D	503	PGE	O3-C5-C6-O4
8	C	502	P6G	O16-C17-C18-O19
4	A	504	PGE	O1-C1-C2-O2
4	D	502	PGE	O3-C5-C6-O4
4	E	507	PGE	O1-C1-C2-O2
7	B	506	PG4	O2-C3-C4-O3
3	A	501	GLC	C4-C5-C6-O6
4	E	506	PGE	O3-C5-C6-O4
5	B	503	PEG	O1-C1-C2-O2
6	B	505	1PE	OH5-C14-C24-OH4
4	A	505	PGE	O3-C5-C6-O4
8	C	502	P6G	O7-C8-C9-O10
3	C	501	GLC	O5-C5-C6-O6
6	F	505	1PE	C13-C23-OH3-C22
4	F	504	PGE	C1-C2-O2-C3
7	B	506	PG4	C1-C2-O2-C3
4	D	502	PGE	C3-C4-O3-C5
8	E	508	P6G	C12-C11-O10-C9
4	A	504	PGE	C1-C2-O2-C3
4	E	507	PGE	C1-C2-O2-C3
4	D	503	PGE	C1-C2-O2-C3
4	F	504	PGE	C4-C3-O2-C2
6	B	505	1PE	C23-C13-OH4-C24
8	C	502	P6G	O1-C2-C3-O4
6	B	505	1PE	C12-C22-OH3-C23
4	A	504	PGE	C4-C3-O2-C2
4	D	503	PGE	C3-C4-O3-C5
4	B	504	PGE	C1-C2-O2-C3
4	D	502	PGE	C1-C2-O2-C3
4	C	503	PGE	C1-C2-O2-C3
8	E	508	P6G	C2-C3-O4-C5
4	D	502	PGE	C6-C5-O3-C4
6	F	505	1PE	C14-C24-OH4-C13
4	F	504	PGE	C3-C4-O3-C5
4	D	503	PGE	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
4	F	504	PGE	O1-C1-C2-O2
6	F	505	1PE	C23-C13-OH4-C24
5	B	502	PEG	C4-C3-O2-C2
4	C	504	PGE	C1-C2-O2-C3
3	D	501	GLC	C4-C5-C6-O6
4	E	506	PGE	C3-C4-O3-C5
4	F	504	PGE	C6-C5-O3-C4
8	C	502	P6G	C18-C17-O16-C15
4	C	504	PGE	O1-C1-C2-O2
8	E	508	P6G	C18-C17-O16-C15
8	C	502	P6G	C11-C12-O13-C14
4	A	504	PGE	C6-C5-O3-C4
6	F	505	1PE	C12-C22-OH3-C23
5	B	502	PEG	C1-C2-O2-C3
4	C	503	PGE	O2-C3-C4-O3
8	E	508	P6G	C6-C5-O4-C3
6	F	505	1PE	C15-C25-OH5-C14
3	A	501	GLC	O5-C5-C6-O6
8	E	508	P6G	O16-C17-C18-O19
5	B	503	PEG	C1-C2-O2-C3
6	B	505	1PE	C13-C23-OH3-C22

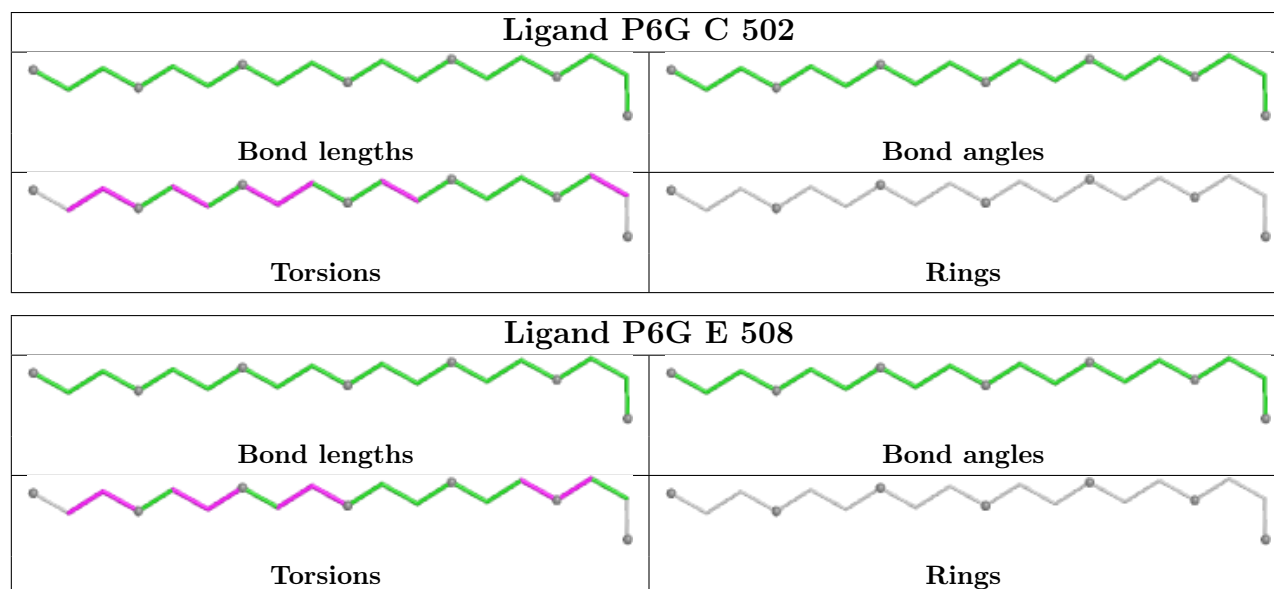
There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	GLC	2	0
4	D	502	PGE	1	0
3	B	501	GLC	2	0
3	F	501	GLC	2	0
4	D	503	PGE	1	0
4	A	504	PGE	1	0
3	D	501	GLC	2	0
3	C	501	GLC	3	0
3	A	501	GLC	1	0
5	B	502	PEG	1	0
7	B	506	PG4	1	0
4	C	503	PGE	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	421/447 (94%)	-0.37	1 (0%) 91 90	16, 31, 57, 86	2 (0%)
1	B	421/447 (94%)	-0.42	1 (0%) 91 90	16, 28, 55, 90	3 (0%)
1	C	421/447 (94%)	-0.31	3 (0%) 84 82	20, 32, 59, 94	2 (0%)
1	D	425/447 (95%)	-0.32	5 (1%) 76 74	15, 31, 63, 110	1 (0%)
1	E	421/447 (94%)	-0.38	2 (0%) 87 85	17, 30, 57, 79	2 (0%)
1	F	428/447 (95%)	-0.32	0 100 100	19, 32, 60, 87	2 (0%)
All	All	2537/2682 (94%)	-0.35	12 (0%) 87 85	15, 31, 59, 110	12 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	3.7
1	D	3	LEU	3.5
1	C	4	THR	3.3
1	D	2	THR	2.9
1	C	156	PRO	2.5
1	A	4	THR	2.4
1	E	4	THR	2.4
1	E	424	ASP	2.3
1	D	0	HIS	2.3
1	B	4	THR	2.2
1	C	5	ALA	2.1
1	D	230	ILE	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

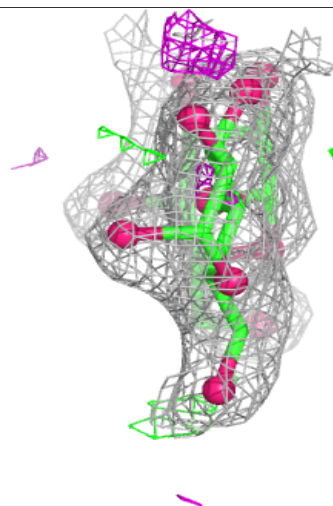
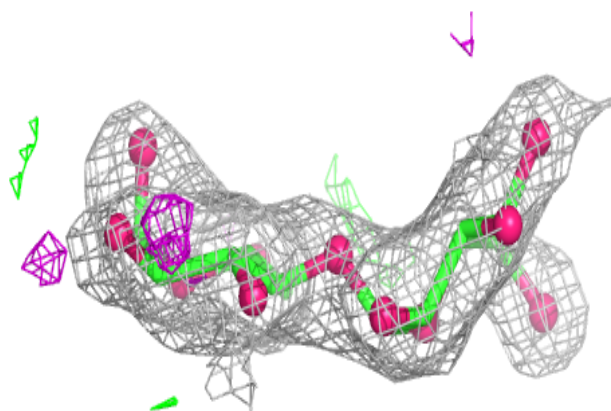
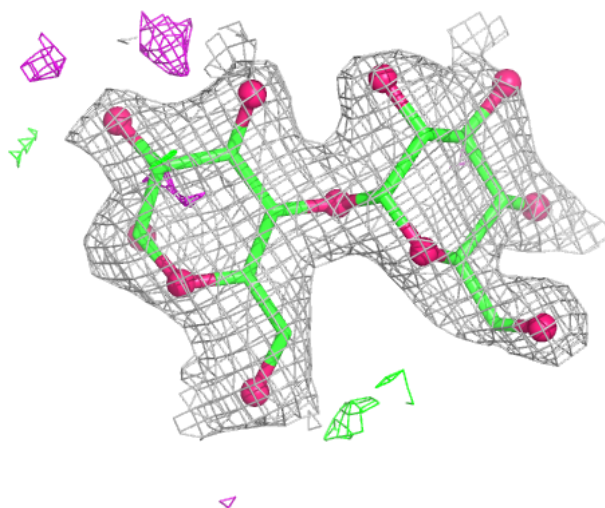
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	J	1	12/12	0.76	0.15	75,91,99,110	0
2	GLC	J	2	11/12	0.77	0.14	89,97,104,106	0
2	GLC	H	2	11/12	0.79	0.13	64,76,82,85	0
2	GLC	K	2	11/12	0.82	0.14	59,67,76,84	0
2	GLC	L	2	11/12	0.83	0.14	33,39,42,44	11
2	GLC	H	1	12/12	0.84	0.13	52,72,84,103	0
2	GLC	N	2	11/12	0.84	0.12	61,68,72,73	0
2	GLC	I	1	12/12	0.85	0.13	58,67,73,73	0
2	GLC	N	1	12/12	0.87	0.11	58,66,73,78	0
2	GLC	I	2	11/12	0.88	0.12	63,73,80,81	0
2	GLC	L	1	12/12	0.89	0.14	28,41,44,46	12
2	GLC	G	1	12/12	0.89	0.10	55,58,64,66	0
2	GLC	G	2	11/12	0.90	0.10	49,57,63,66	0
2	GLC	M	1	12/12	0.90	0.10	47,53,58,59	0
2	GLC	M	2	11/12	0.91	0.10	49,56,58,59	0
2	GLC	K	1	12/12	0.92	0.09	44,54,59,66	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.

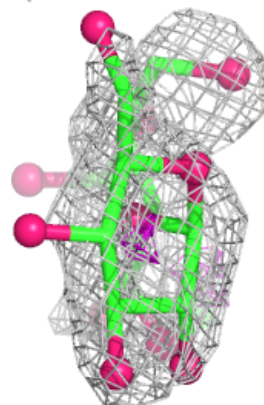
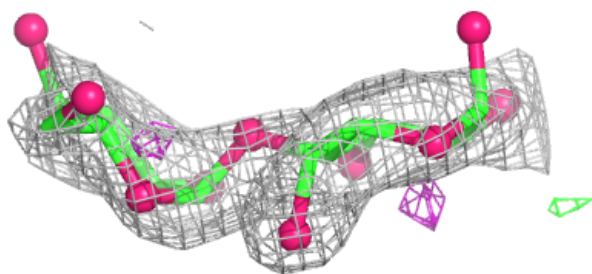
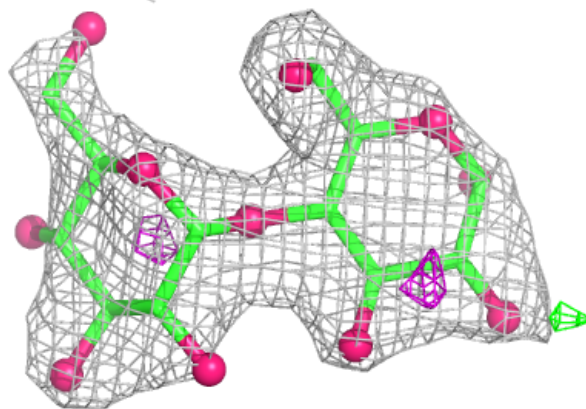
Electron density around Chain G:

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



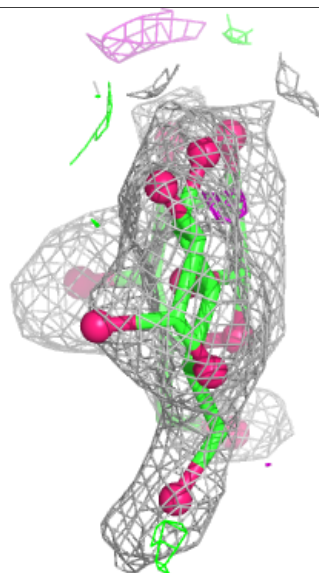
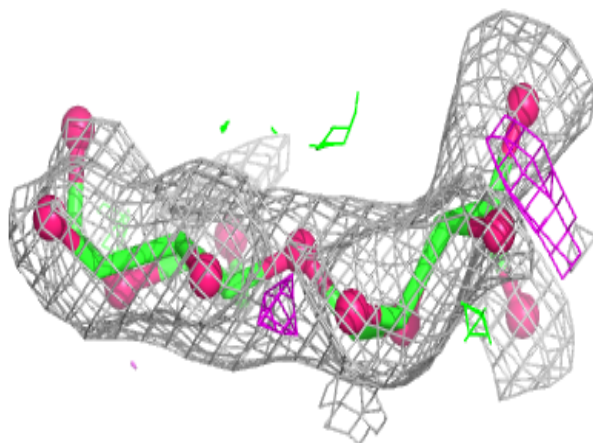
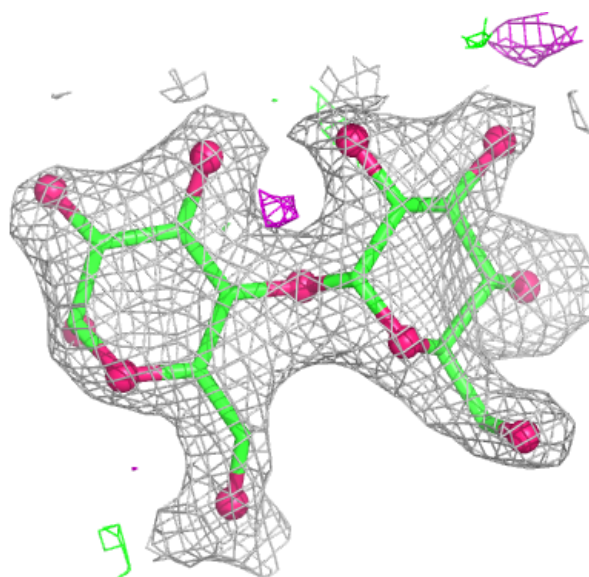
Electron density around Chain H:

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



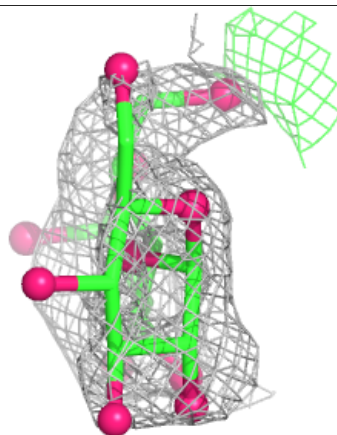
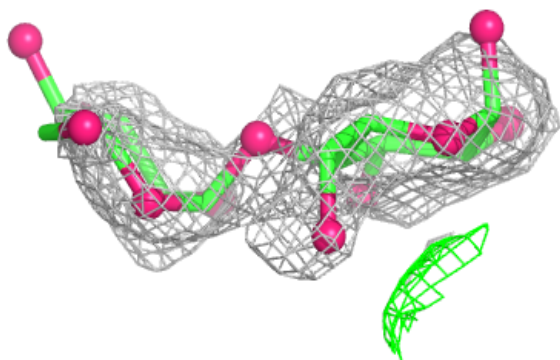
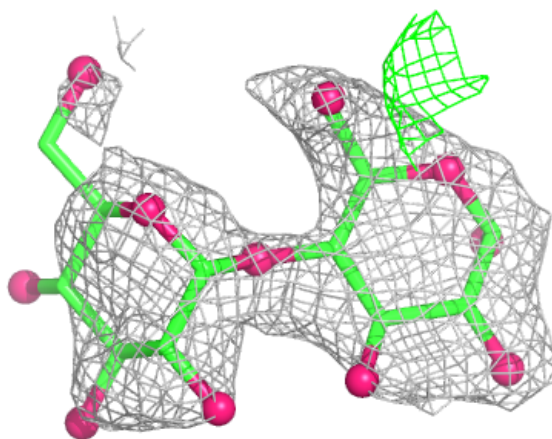
Electron density around Chain I:

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



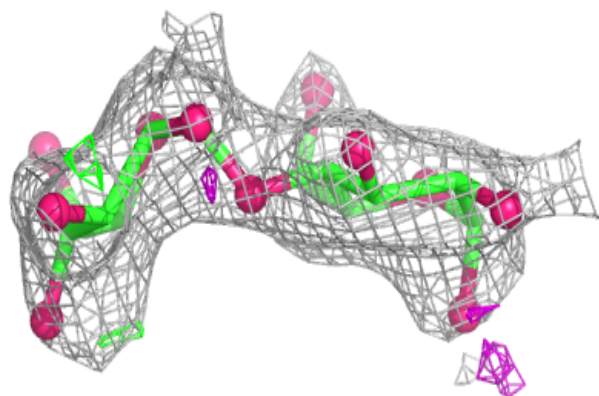
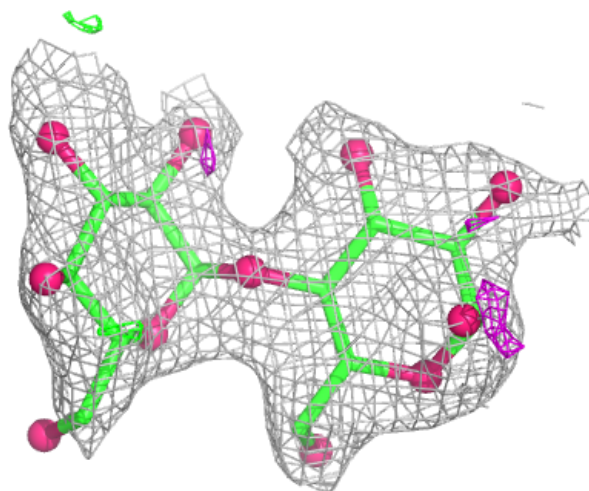
Electron density around Chain J:

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



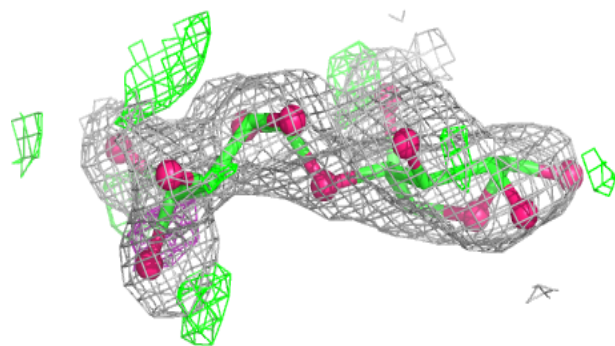
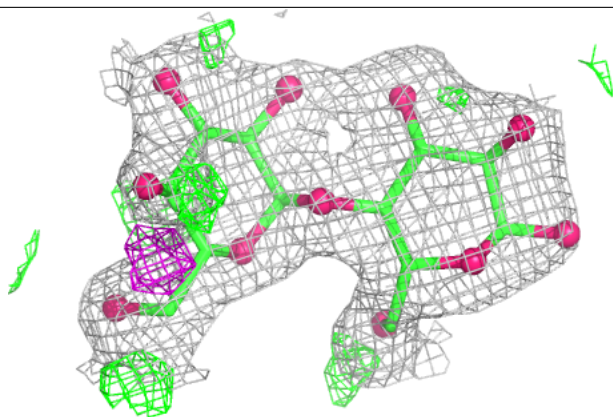
Electron density around Chain K:

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



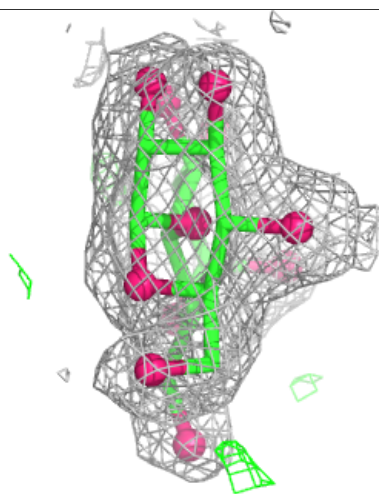
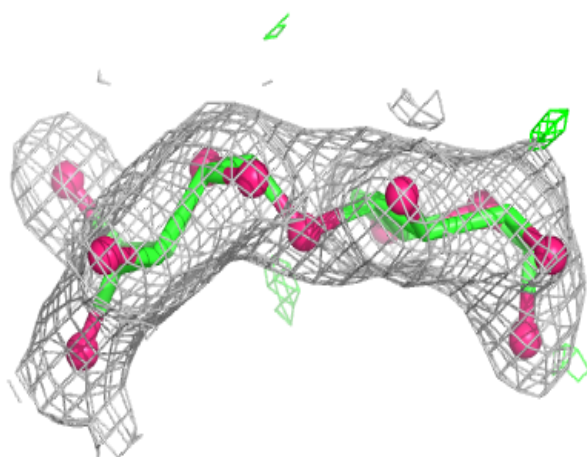
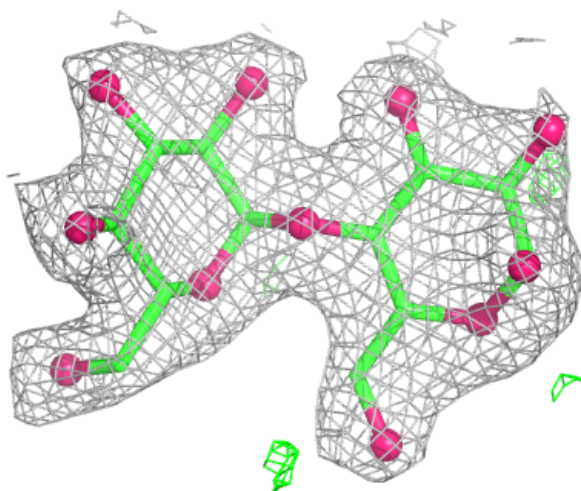
Electron density around Chain L:

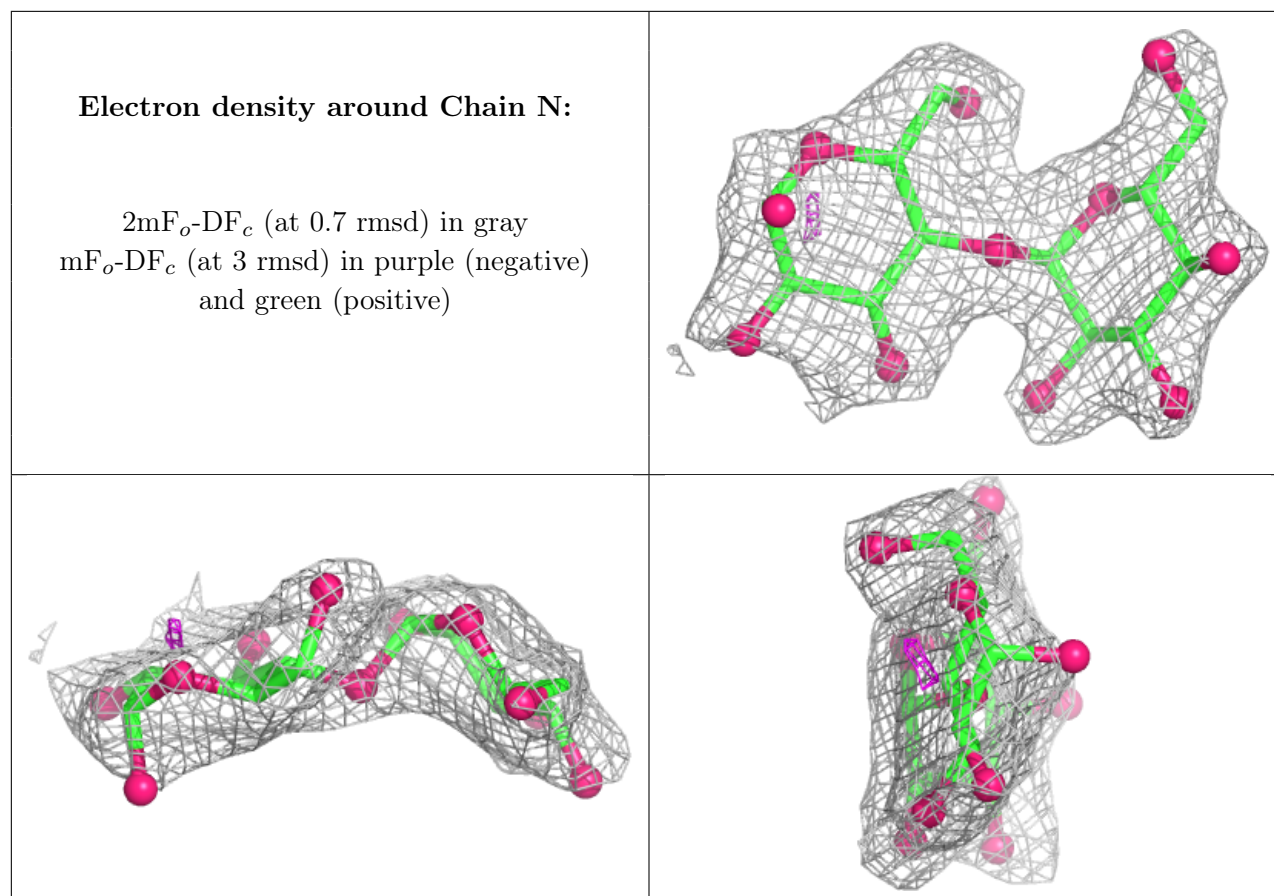
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain M:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PGE	D	502	10/10	0.81	0.17	65,72,75,81	0
4	PGE	B	504	10/10	0.82	0.18	65,69,81,83	0
4	PGE	C	503	10/10	0.86	0.16	55,69,78,80	0
8	P6G	E	508	19/19	0.86	0.17	52,70,77,80	0
3	GLC	A	501	12/12	0.87	0.15	36,52,64,73	0
3	GLC	B	501	12/12	0.87	0.14	40,53,57,65	0
3	GLC	C	501	12/12	0.87	0.14	37,57,66,74	0
6	1PE	B	505	16/16	0.87	0.16	60,70,76,77	0
6	1PE	F	505	16/16	0.87	0.17	56,73,82,83	0
4	PGE	A	504	10/10	0.87	0.15	63,80,84,85	0
4	PGE	E	506	10/10	0.88	0.16	62,67,77,78	0
4	PGE	A	505	10/10	0.88	0.14	60,74,83,84	0
3	GLC	F	501	12/12	0.88	0.14	37,55,61,69	0

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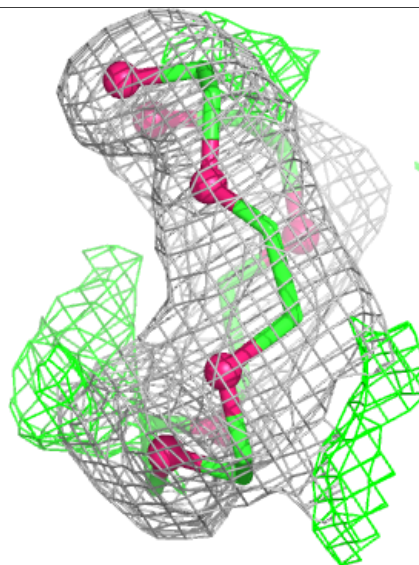
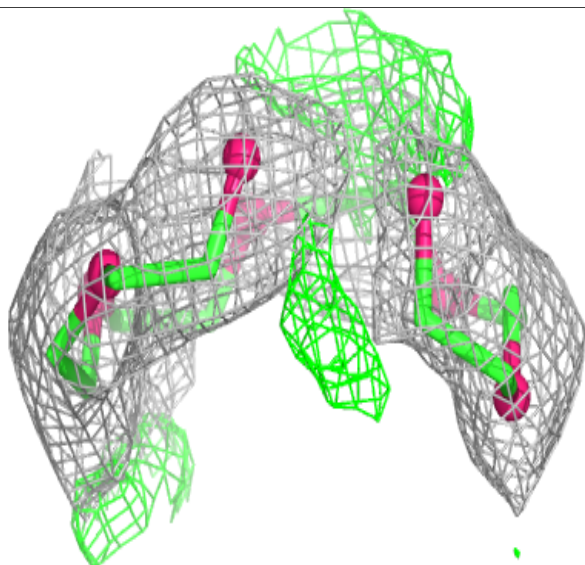
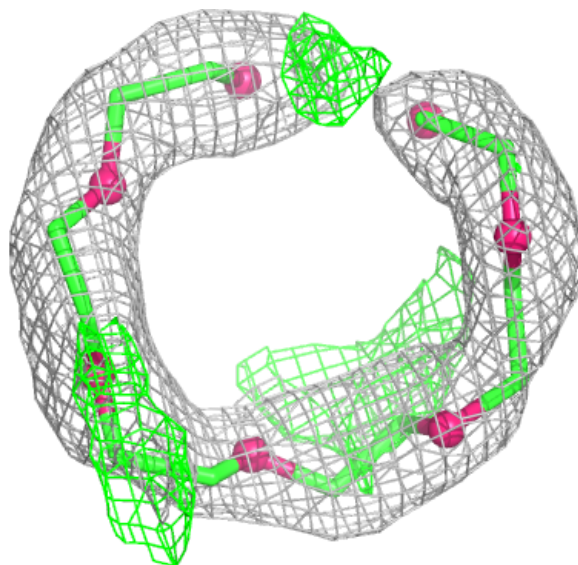
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	PG4	B	506	13/13	0.88	0.15	56,64,81,94	0
4	PGE	D	503	10/10	0.88	0.15	61,67,71,72	0
4	PGE	E	507	10/10	0.90	0.14	62,64,69,72	0
4	PGE	F	504	10/10	0.90	0.15	49,74,86,90	0
3	GLC	E	501	12/12	0.90	0.12	34,52,57,68	0
9	NA	C	505	1/1	0.90	0.12	69,69,69,69	0
9	NA	F	506	1/1	0.90	0.12	63,63,63,63	0
8	P6G	C	502	19/19	0.91	0.14	52,65,81,81	0
3	GLC	D	501	12/12	0.91	0.12	33,51,59,59	0
5	PEG	B	503	7/7	0.92	0.13	60,63,67,68	0
4	PGE	C	504	10/10	0.92	0.12	58,65,74,77	0
5	PEG	B	502	7/7	0.94	0.12	54,60,62,63	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.

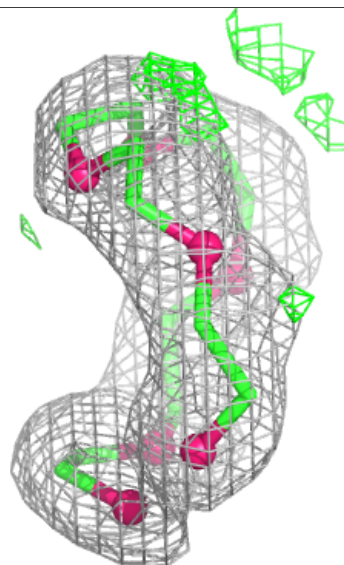
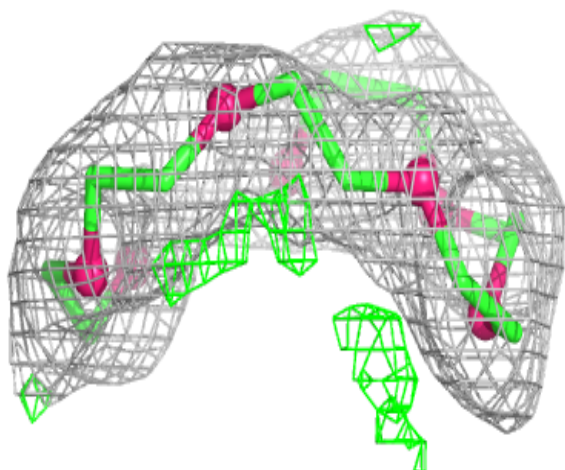
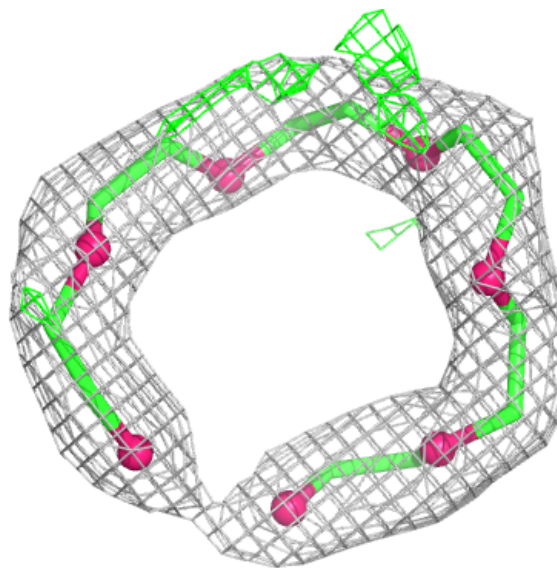
Electron density around P6G E 508:

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



Electron density around P6G C 502:

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.