Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 01:36 pm GMT

PDB ID	:	6GN6
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)

The following versions of software and data (see references (i)) were used in the production of this report:

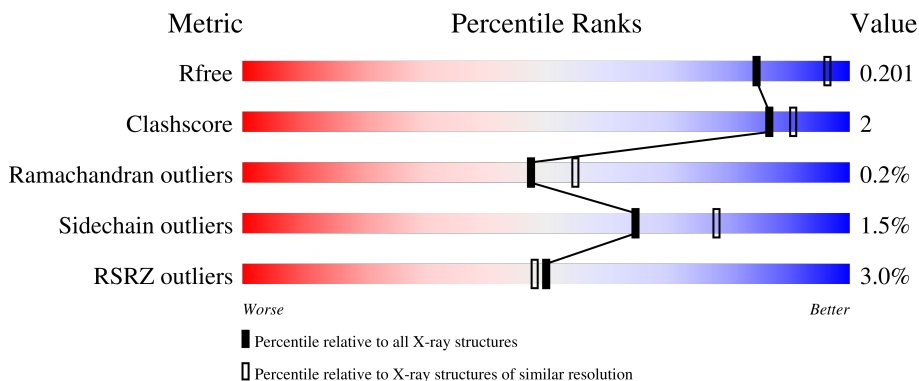|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1   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	Percentile Ranks	Value
Rfree		0.201
Clashscore		2
Ramachandran outliers		0.2%
Sidechain outliers		1.5%
RSRZ outliers		3.0%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 <=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	3% / 88% / 6% / 6%
1	B	447	3% / 89% / · · / 6%
1	C	447	4% / 89% / 5% / 6%
1	D	447	4% / 89% / 6% / 5%
1	E	447	% / 90% / · · / 6%

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Mol	Chain	Length	Quality of chain
1	F	447	3% ▮ 90% ▮ 5% ·
2	G	2	100%
2	H	2	50% 50%
2	I	2	50% 50%
2	J	2	100%
2	K	2	100%
2	L	2	50% 50%
2	M	2	100%
2	N	2	100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	J	2	-	-	-	X

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

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

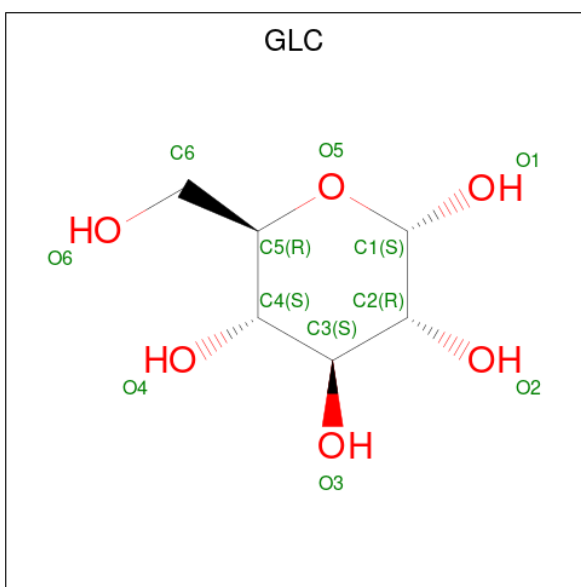- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.

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

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

- Molecule 3 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).

GLC

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

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

PGE

O4
OH

C5
C6

C4

O2
O

O3

C3

C1

C2

HO
O1
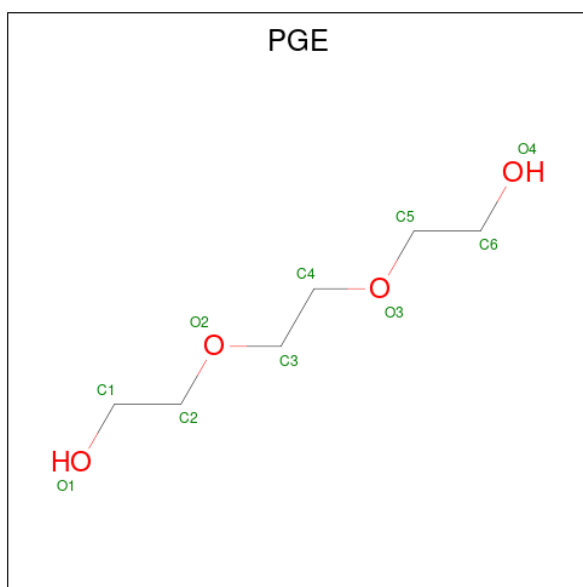
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 10	C 6	O 4	0	0
4	A	1	Total 10	C 6	O 4	0	0
4	B	1	Total 10	C 6	O 4	0	0
4	C	1	Total 10	C 6	O 4	0	0
4	C	1	Total 10	C 6	O 4	0	0
4	D	1	Total 10	C 6	O 4	0	0
4	D	1	Total 10	C 6	O 4	0	0
4	E	1	Total 10	C 6	O 4	0	0
4	E	1	Total 10	C 6	O 4	0	0
4	F	1	Total 10	C 6	O 4	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

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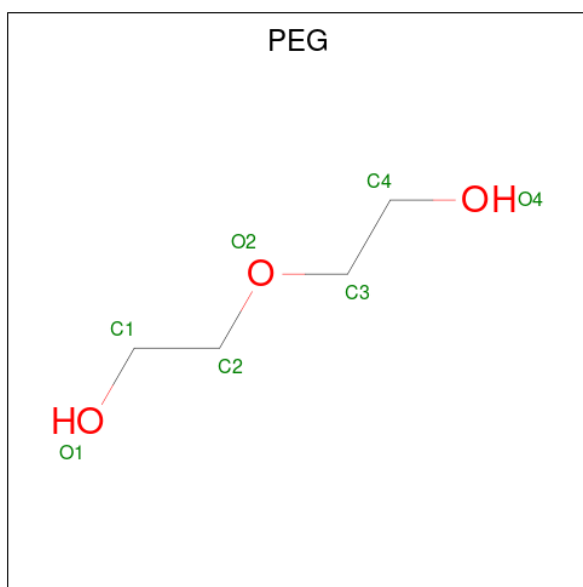
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 7	C 4	O 3	0	0
5	B	1	Total 7	C 4	O 3	0	0

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

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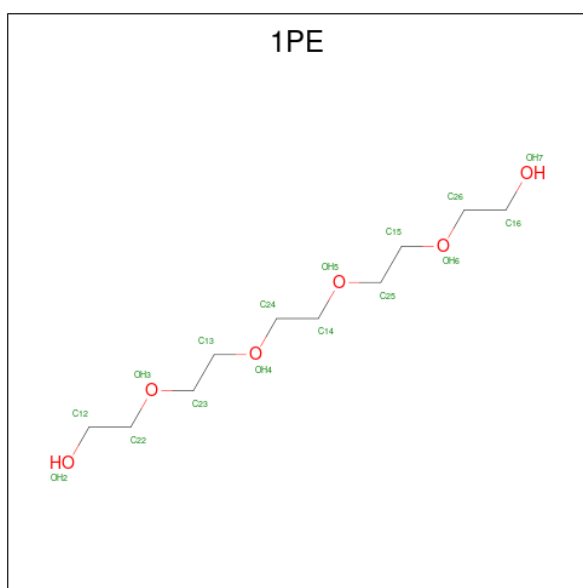
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 16	C 10	O 6	0	0
6	F	1	Total 16	C 10	O 6	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).
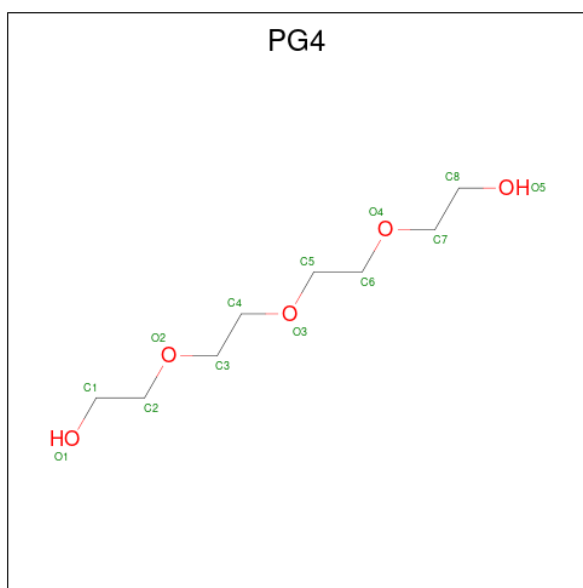
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 13	C 8	O 5	0	0

- Molecule 8 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).
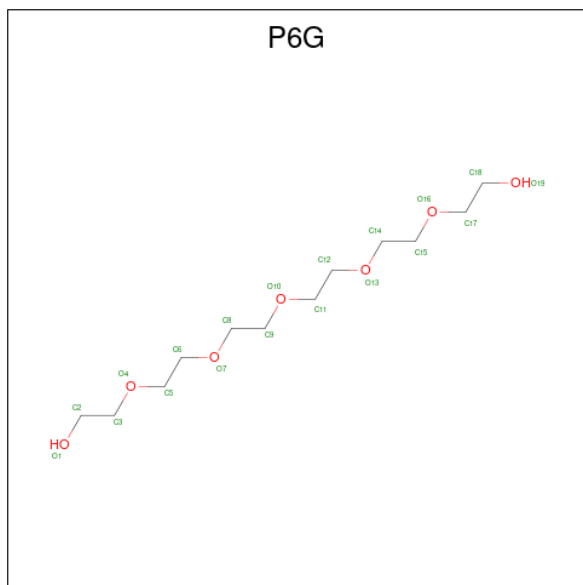
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total 19	C 12	O 7	0	0
8	E	1	Total 19	C 12	O 7	0	0

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	255	Total O 255 255		0	0
10	B	247	Total O 247 247		0	0
10	C	218	Total O 218 218		0	0
10	D	226	Total O 226 226		0	0
10	E	226	Total O 226 226		0	0
10	F	220	Total O 220 220		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.
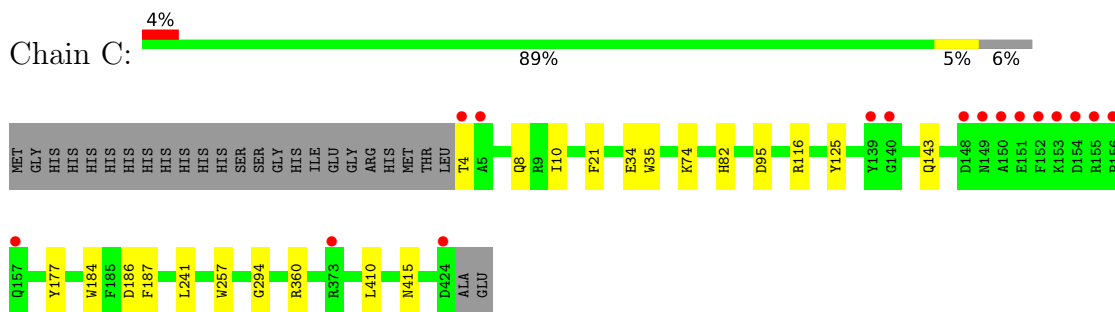
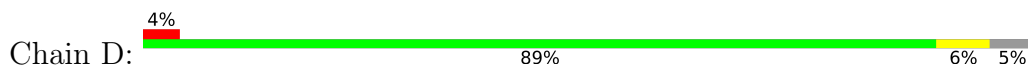- Molecule 1: Alpha-L-fucosidase

Chain A:

- Molecule 1: Alpha-L-fucosidase

Chain B:

- Molecule 1: Alpha-L-fucosidase

Chain C:

- Molecule 1: Alpha-L-fucosidase
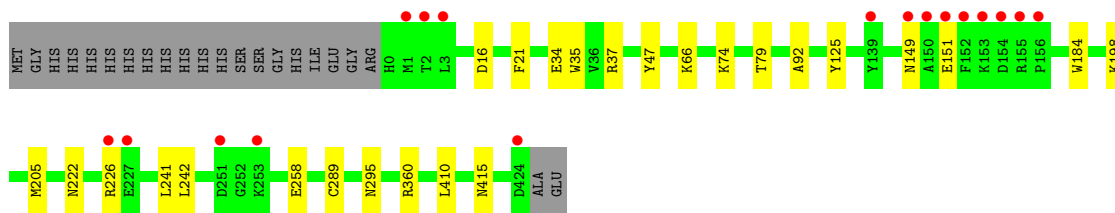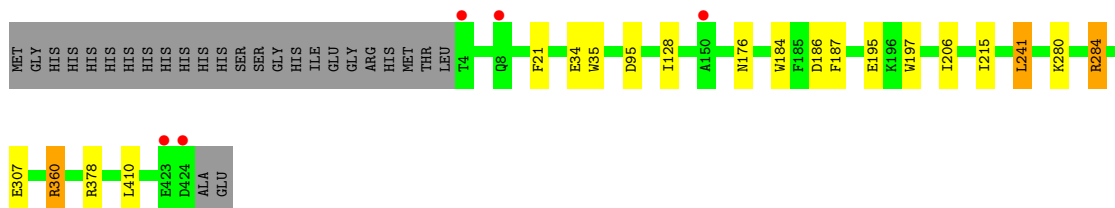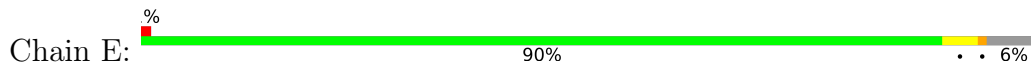
Chain D:

• Molecule 1: Alpha-L-fucosidase

Chain E:
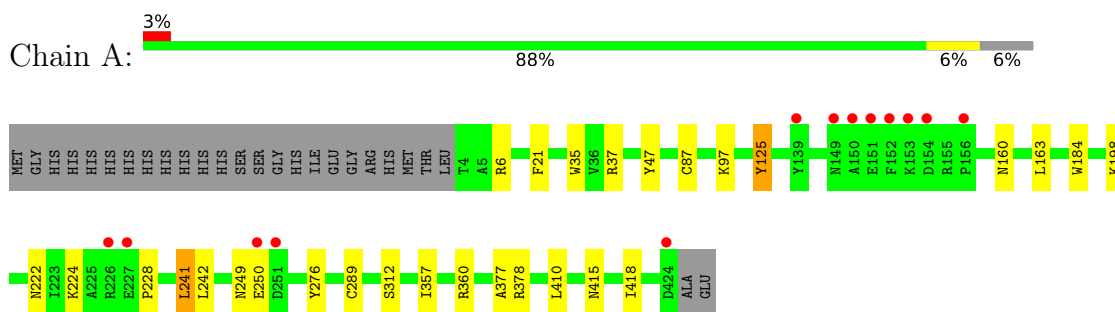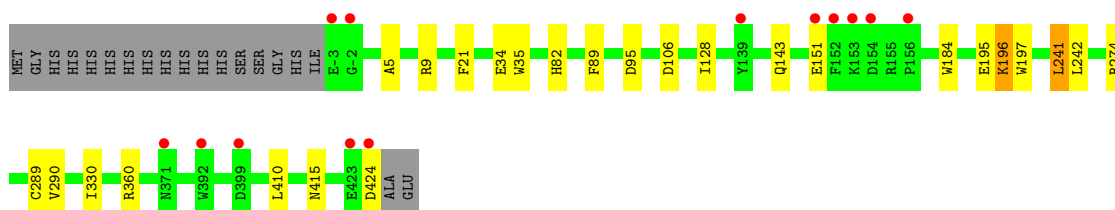

• Molecule 1: Alpha-L-fucosidase

• Molecule 1: Alpha-L-fucosidase
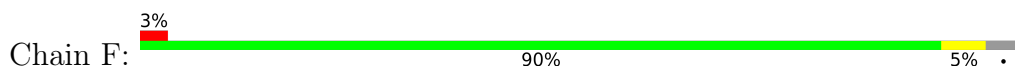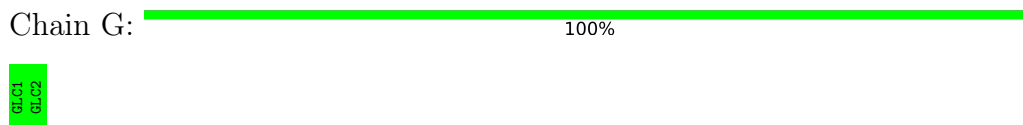
Chain F:

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

Chain G:

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

Chain H:

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

Chain I:

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

Chain J:

100%

GLC1 GLC2

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

Chain K:

100%

GLC1 GLC2

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

Chain L:

50% 50%

GLC1 GLC2

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

Chain M:

100%

GLC1 GLC2

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

Chain N:

100%

GLC1 GLC2

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.23 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.167 , 0.217 0.176 , 0.201	Depositor DCC
R_{free} test set	7763 reflections (4.92%)	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)	0.38 , 52.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PEG, 1PE, NA, P6G, GLC, PG4, PGE

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	0.80	0/3524	0.87	1/4790 (0.0%)
1	B	0.85	1/3536 (0.0%)	0.89	0/4806
1	C	0.82	0/3513	0.83	0/4776
1	D	0.83	1/3550 (0.0%)	0.84	0/4825
1	E	0.84	0/3524	0.89	2/4790 (0.0%)
1	F	0.80	0/3582	0.86	0/4867
All	All	0.82	2/21229 (0.0%)	0.86	3/28854 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	258	GLU	CD-OE2	5.64	1.31	1.25
1	D	92	ALA	C-O	-5.42	1.13	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	241	LEU	CA-CB-CG	6.28	129.75	115.30
1	E	284	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	E	241	LEU	CA-CB-CG	5.18	127.22	115.30

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	12	0
1	C	3408	0	3257	10	0
1	D	3444	0	3303	14	0
1	E	3416	0	3270	14	0
1	F	3473	0	3329	17	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	3	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	1	0
10	D	226	0	0	0	0
10	E	226	0	0	2	0
10	F	220	0	0	1	0
All	All	22428	0	20222	88	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 (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95[A]:ASP:OD1	10:C:601:HOH:O	1.69	1.10
1:E:95[B]:ASP:OD1	10:E:601:HOH:O	1.85	0.93
1:F:95[B]:ASP:OD1	10:F:601:HOH:O	1.89	0.91
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:A:357:ILE:HD11	1:A:418:ILE:HD12	1.86	0.56
1:E:195:GLU:OE2	1:E:195:GLU:HA	2.06	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: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: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:B:198:LYS:HE2	7:B:506:PG4:O4	2.10	0.51
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: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:F:34:GLU:OE2	3:F:501:GLC:O3	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:82:HIS:HE2	3:F:501:GLC:H3	1.79	0.47
1:A:242:LEU:HD22	1:A:289:CYS:SG	2.54	0.47
1:A:377:ALA:C	1:A:378[B]:ARG:HG2	2.35	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:A:249:ASN:OD1	1:A:249:ASN:C	2.53	0.46
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:A:125:TYR:C	1:A:125:TYR:CD1	2.89	0.46
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: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:D:222:ASN:C	1:D:222:ASN:OD1	2.56	0.44
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:A:377:ALA:C	1:A:378[A]:ARG:HG2	2.37	0.44
1:C:82:HIS:HE2	3:C:501:GLC:H3	1.81	0.44
1:D:79:THR:HA	1:D:125:TYR:HB3	1.99	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: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:D:37:ARG:HG3	1:D:47:TYR:CE1	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:205:MET:HG3	4:D:502:PGE:H22	2.03	0.41
1:D:149:ASN:CG	1:D:151:GLU:HG2	2.40	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:34:GLU:H	1:F:34:GLU:CD	2.24	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

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%)	47	55
1	B	422/447 (94%)	403 (96%)	18 (4%)	1 (0%)	47	55
1	C	420/447 (94%)	404 (96%)	15 (4%)	1 (0%)	47	55
1	D	424/447 (95%)	410 (97%)	13 (3%)	1 (0%)	47	55
1	E	421/447 (94%)	408 (97%)	13 (3%)	0	100	100
1	F	428/447 (96%)	413 (96%)	14 (3%)	1 (0%)	47	55
All	All	2536/2682 (95%)	2448 (96%)	83 (3%)	5 (0%)	47	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	415	ASN
1	D	415	ASN

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Mol	Chain	Res	Type
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%)	348 (99%)	4 (1%)	73	85
1	B	353/372 (95%)	348 (99%)	5 (1%)	67	80
1	C	351/372 (94%)	345 (98%)	6 (2%)	60	74
1	D	355/372 (95%)	350 (99%)	5 (1%)	67	80
1	E	352/372 (95%)	347 (99%)	5 (1%)	67	80
1	F	358/372 (96%)	351 (98%)	7 (2%)	55	69
All	All	2121/2232 (95%)	2089 (98%)	32 (2%)	65	78

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

Mol	Chain	Res	Type
1	A	21	PHE
1	A	125	TYR
1	A	184	TRP
1	A	241	LEU
1	B	21	PHE
1	B	32	ARG
1	B	125	TYR
1	B	184	TRP
1	B	241	LEU
1	C	10	ILE
1	C	21	PHE
1	C	125	TYR
1	C	143	GLN
1	C	184	TRP
1	C	241	LEU

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Mol	Chain	Res	Type
1	D	21	PHE
1	D	66	LYS
1	D	184	TRP
1	D	226	ARG
1	D	241	LEU
1	E	21	PHE
1	E	184	TRP
1	E	241	LEU
1	E	307	GLU
1	E	360	ARG
1	F	21	PHE
1	F	143	GLN
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. There are no such sidechains identified.

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	0.58	0
2	GLC	G	2	2	11,11,12	0.93	0	15,15,17	0.68	0
2	GLC	H	1	2	12,12,12	0.67	0	17,17,17	0.60	0
2	GLC	H	2	2	11,11,12	0.67	0	15,15,17	1.01	1 (6%)
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	0.90	0	15,15,17	1.14	1 (6%)
2	GLC	J	1	2	12,12,12	0.52	0	17,17,17	0.75	0
2	GLC	J	2	2	11,11,12	0.52	0	15,15,17	0.86	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	1.15	0
2	GLC	L	1	2	12,12,12	0.71	0	17,17,17	1.18	1 (5%)
2	GLC	L	2	2	11,11,12	0.72	0	15,15,17	1.05	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	1.17	0	15,15,17	1.07	0
2	GLC	N	1	2	12,12,12	0.59	0	17,17,17	0.60	0
2	GLC	N	2	2	11,11,12	0.66	0	15,15,17	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	2	GLC	C3-C4-C5	2.32	114.39	110.24
2	L	2	GLC	O4-C4-C3	-2.22	105.22	110.35
2	H	2	GLC	O5-C5-C6	2.12	110.52	107.20
2	I	2	GLC	C1-C2-C3	2.05	112.19	109.67
2	L	1	GLC	O2-C2-C3	-2.05	105.61	110.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

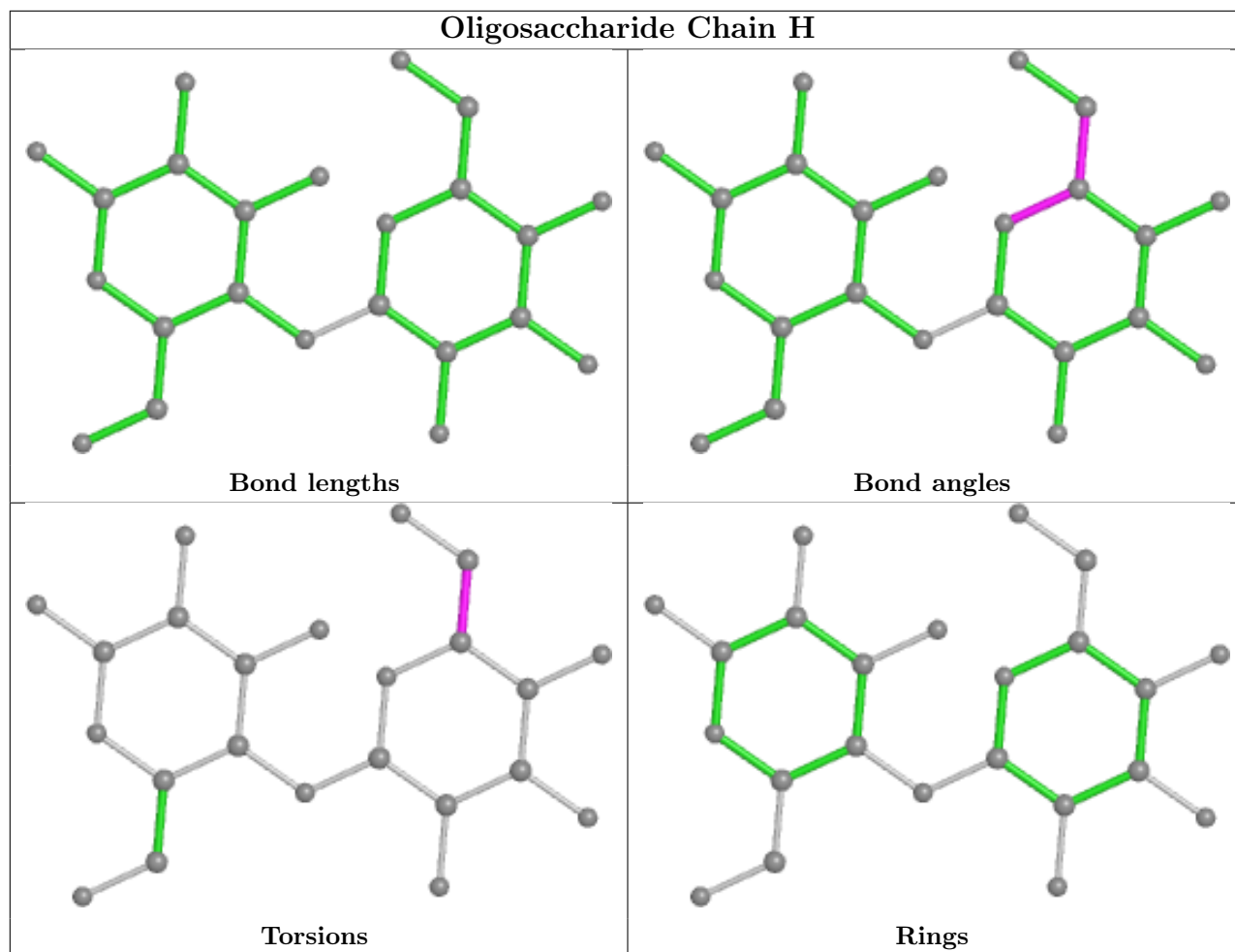| Mol	Chain	Res	Type	Atoms
2	H	2	GLC	C4-C5-C6-O6
2	L	1	GLC	C4-C5-C6-O6
2	L	1	GLC	O5-C5-C6-O6
2	I	2	GLC	C4-C5-C6-O6
2	H	2	GLC	O5-C5-C6-O6
2	N	1	GLC	C4-C5-C6-O6
2	K	2	GLC	C4-C5-C6-O6
2	N	2	GLC	C4-C5-C6-O6
2	N	1	GLC	O5-C5-C6-O6
2	K	2	GLC	O5-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

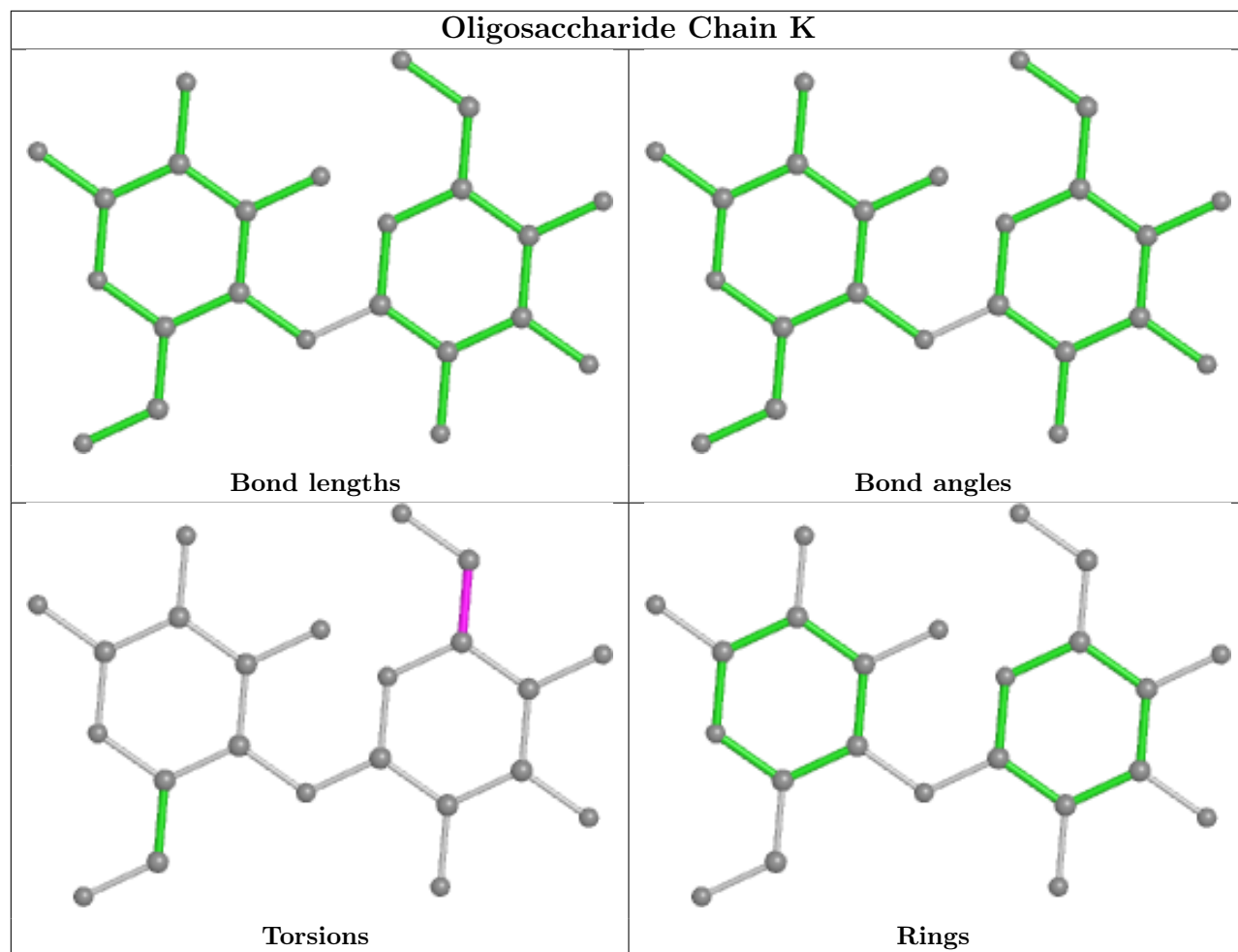| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1	GLC	1	0

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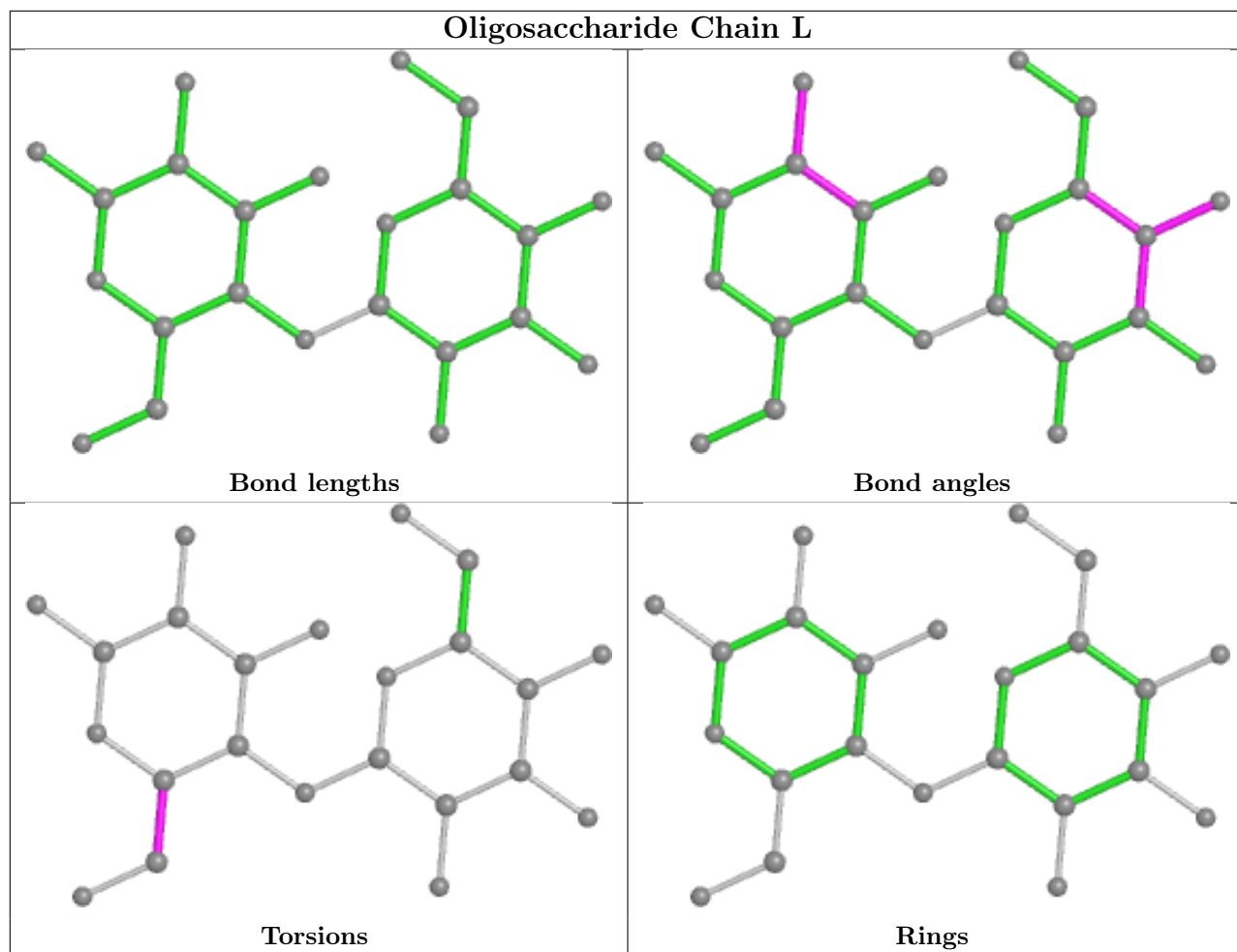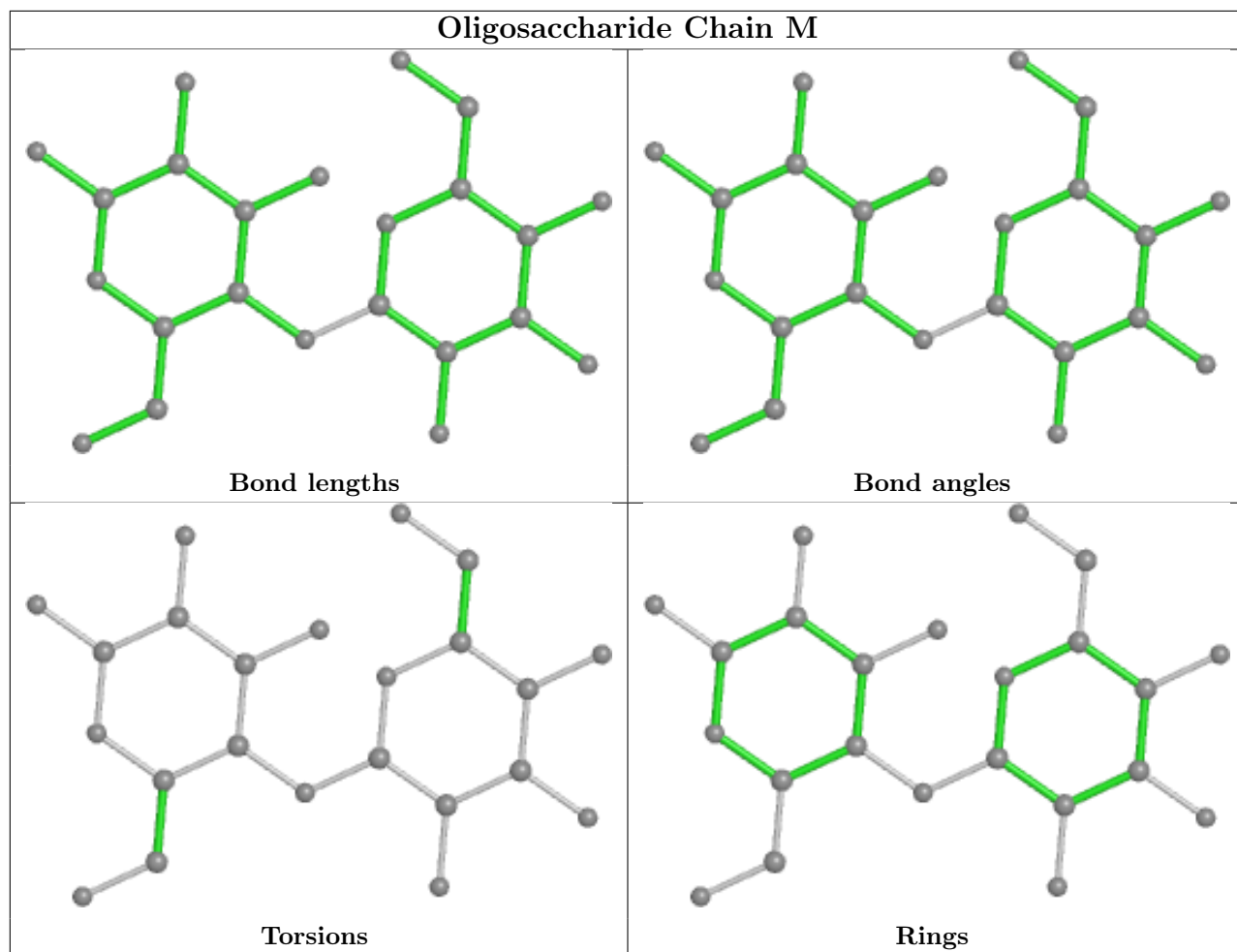
Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain I

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain J

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain K

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain L

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain M

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain N
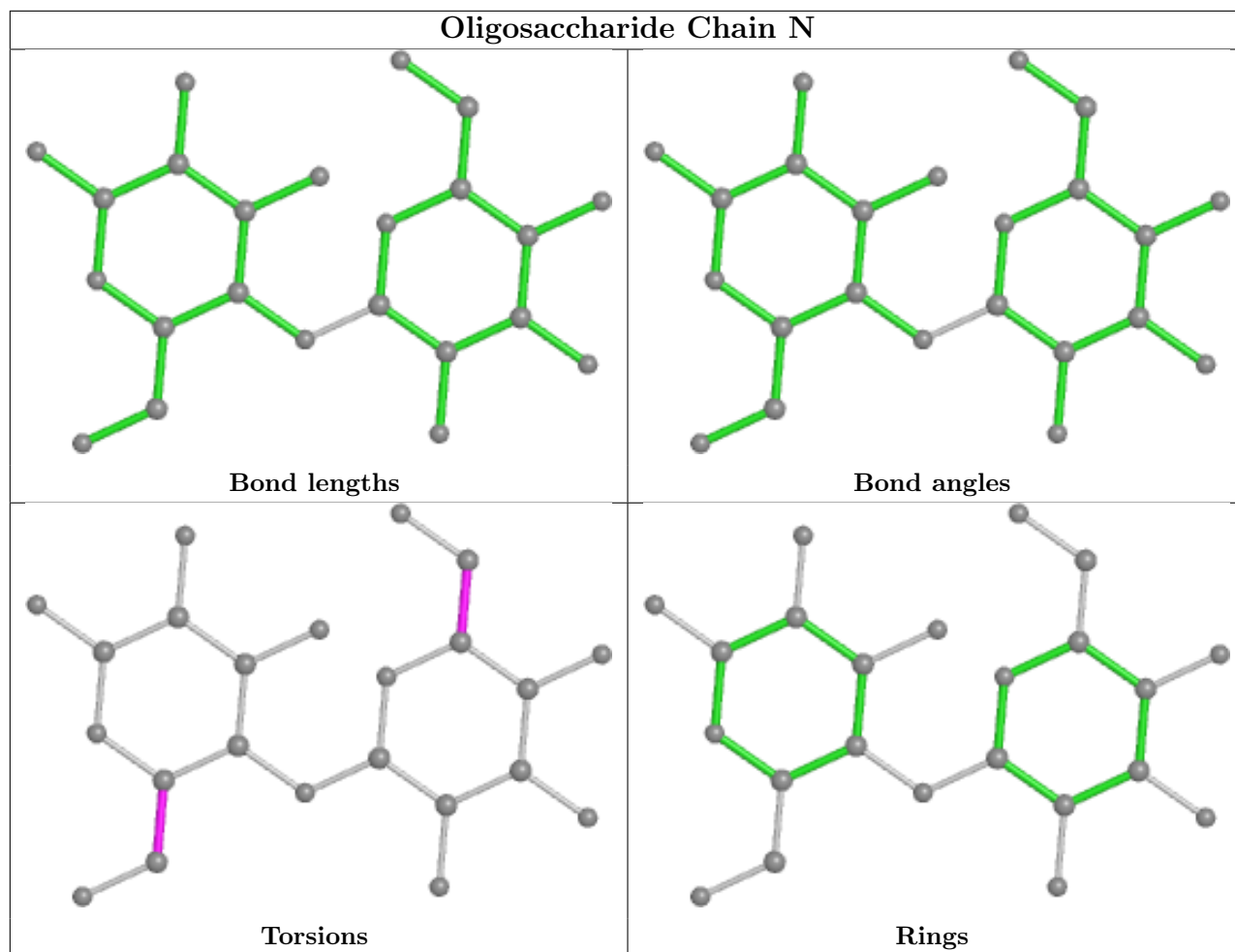

Bond lengths

Bond angles

Torsions

Rings

5.6 Ligand geometry ⓘ

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	D	501	-	12,12,12	0.93	1 (8%)	17,17,17	2.18	7 (41%)
4	PGE	A	504	-	9,9,9	0.71	0	8,8,8	0.82	0
3	GLC	E	501	-	12,12,12	0.74	0	17,17,17	2.11	6 (35%)
4	PGE	E	506	-	9,9,9	0.86	0	8,8,8	0.77	0
4	PGE	C	504	-	9,9,9	0.56	0	8,8,8	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	1PE	B	505	-	15,15,15	0.60	0	14,14,14	0.32	0
6	1PE	F	505	9	15,15,15	0.77	0	14,14,14	0.53	0
5	PEG	B	503	-	6,6,6	0.66	0	5,5,5	0.24	0
3	GLC	B	501	-	12,12,12	0.78	0	17,17,17	2.34	10 (58%)
8	P6G	C	502	9	18,18,18	0.77	0	17,17,17	0.93	0
7	PG4	B	506	-	12,12,12	0.68	0	11,11,11	0.37	0
3	GLC	A	501	-	12,12,12	0.75	0	17,17,17	2.39	9 (52%)
4	PGE	F	504	-	9,9,9	0.74	0	8,8,8	0.78	0
5	PEG	B	502	-	6,6,6	0.53	0	5,5,5	0.31	0
4	PGE	B	504	-	9,9,9	0.85	0	8,8,8	0.88	0
3	GLC	C	501	-	12,12,12	0.76	0	17,17,17	2.01	5 (29%)
4	PGE	D	503	-	9,9,9	0.57	0	8,8,8	0.56	0
4	PGE	A	505	-	9,9,9	0.78	0	8,8,8	0.89	0
3	GLC	F	501	-	12,12,12	0.72	0	17,17,17	2.22	6 (35%)
4	PGE	D	502	-	9,9,9	0.76	0	8,8,8	0.78	0
4	PGE	E	507	-	9,9,9	0.90	0	8,8,8	0.77	0
4	PGE	C	503	-	9,9,9	1.08	0	8,8,8	1.47	2 (25%)
8	P6G	E	508	-	18,18,18	0.81	0	17,17,17	0.98	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	D	501	-	-	1/2/22/22	0/1/1/1
4	PGE	A	504	-	-	4/7/7/7	-
3	GLC	E	501	-	-	0/2/22/22	0/1/1/1
4	PGE	E	506	-	-	2/7/7/7	-
4	PGE	C	504	-	-	2/7/7/7	-
6	1PE	B	505	-	-	6/13/13/13	-
6	1PE	F	505	9	-	7/13/13/13	-
5	PEG	B	503	-	-	2/4/4/4	-
3	GLC	B	501	-	-	0/2/22/22	0/1/1/1
8	P6G	C	502	9	-	7/16/16/16	-
7	PG4	B	506	-	-	2/10/10/10	-
3	GLC	A	501	-	-	2/2/22/22	0/1/1/1
4	PGE	F	504	-	-	7/7/7/7	-
5	PEG	B	502	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	B	504	-	-	2/7/7/7	-
3	GLC	C	501	-	-	2/2/22/22	0/1/1/1
4	PGE	D	503	-	-	5/7/7/7	-
4	PGE	A	505	-	-	1/7/7/7	-
3	GLC	F	501	-	-	0/2/22/22	0/1/1/1
4	PGE	D	502	-	-	5/7/7/7	-
4	PGE	E	507	-	-	4/7/7/7	-
4	PGE	C	503	-	-	5/7/7/7	-
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(^{o})	Ideal(^{o})
3	F	501	GLC	O5-C1-C2	-5.24	100.93	110.28
3	E	501	GLC	O5-C1-C2	-4.82	101.69	110.28
3	A	501	GLC	C4-C3-C2	4.36	118.44	110.82
3	D	501	GLC	O2-C2-C1	4.32	119.19	109.16
3	C	501	GLC	O5-C1-C2	-3.96	103.22	110.28
3	B	501	GLC	C4-C3-C2	3.79	117.44	110.82
3	D	501	GLC	C4-C3-C2	3.70	117.28	110.82
3	E	501	GLC	C3-C4-C5	3.62	116.69	110.24
3	F	501	GLC	C4-C3-C2	3.54	117.00	110.82
3	D	501	GLC	O3-C3-C2	-3.46	102.34	110.35
3	A	501	GLC	O5-C1-C2	-3.44	104.14	110.28
3	B	501	GLC	C3-C4-C5	3.38	116.28	110.24
3	A	501	GLC	C1-C2-C3	-3.36	103.33	110.31
3	E	501	GLC	O6-C6-C5	-3.26	100.10	111.29
3	B	501	GLC	O2-C2-C1	3.24	116.67	109.16
3	C	501	GLC	C4-C3-C2	3.17	116.36	110.82
3	F	501	GLC	C3-C4-C5	3.16	115.88	110.24
3	A	501	GLC	O2-C2-C1	3.08	116.31	109.16
3	B	501	GLC	O1-C1-C2	3.06	117.65	109.03
3	F	501	GLC	O6-C6-C5	-3.03	100.91	111.29
3	D	501	GLC	C3-C4-C5	3.02	115.62	110.24
3	A	501	GLC	C3-C4-C5	3.02	115.62	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	GLC	O1-C1-O5	-2.97	101.46	110.38
3	C	501	GLC	C3-C4-C5	2.86	115.34	110.24
3	A	501	GLC	O3-C3-C4	-2.81	103.85	110.35
3	B	501	GLC	C1-C2-C3	-2.75	104.60	110.31
3	E	501	GLC	O3-C3-C2	-2.66	104.20	110.35
3	B	501	GLC	O6-C6-C5	-2.59	102.41	111.29
3	C	501	GLC	O1-C1-C2	2.58	116.29	109.03
4	C	503	PGE	O2-C3-C4	2.56	121.93	110.39
3	B	501	GLC	O3-C3-C2	-2.51	104.54	110.35
3	A	501	GLC	O3-C3-C2	-2.45	104.69	110.35
3	F	501	GLC	C1-C2-C3	-2.41	105.31	110.31
3	E	501	GLC	C4-C3-C2	2.38	114.98	110.82
3	A	501	GLC	O6-C6-C5	-2.35	103.21	111.29
3	A	501	GLC	O5-C5-C4	2.32	113.91	109.69
4	C	503	PGE	C5-O3-C4	2.28	123.18	113.29
3	E	501	GLC	O4-C4-C5	-2.28	103.63	109.30
3	D	501	GLC	O1-C1-O5	-2.25	103.62	110.38
3	B	501	GLC	C1-O5-C5	-2.23	109.46	113.66
3	B	501	GLC	O5-C5-C4	2.18	113.66	109.69
3	D	501	GLC	O5-C5-C4	2.18	113.66	109.69
3	F	501	GLC	O3-C3-C2	-2.17	105.33	110.35
3	D	501	GLC	O6-C6-C5	-2.06	104.22	111.29
3	C	501	GLC	C1-O5-C5	-2.02	109.86	113.66

There are no chirality outliers.

All (76) 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	OH4-C13-C23-OH3
6	B	505	1PE	OH6-C15-C25-OH5
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
4	B	504	PGE	O3-C5-C6-O4
4	C	503	PGE	O3-C5-C6-O4
4	F	504	PGE	O3-C5-C6-O4
8	C	502	P6G	O13-C14-C15-O16
8	E	508	P6G	O10-C11-C12-O13
3	C	501	GLC	C4-C5-C6-O6

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

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Mol	Chain	Res	Type	Atoms
4	D	503	PGE	C6-C5-O3-C4
4	F	504	PGE	O1-C1-C2-O2
4	C	504	PGE	C1-C2-O2-C3
4	E	506	PGE	C3-C4-O3-C5
5	B	502	PEG	C4-C3-O2-C2
3	D	501	GLC	C4-C5-C6-O6
4	F	504	PGE	C6-C5-O3-C4
8	C	502	P6G	C18-C17-O16-C15
8	E	508	P6G	C18-C17-O16-C15
8	C	502	P6G	C11-C12-O13-C14
4	C	504	PGE	O1-C1-C2-O2
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

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	501	GLC	2	0
4	A	504	PGE	1	0
3	E	501	GLC	2	0
3	B	501	GLC	2	0
7	B	506	PG4	1	0
3	A	501	GLC	1	0
5	B	502	PEG	1	0
3	C	501	GLC	3	0
4	D	503	PGE	1	0
3	F	501	GLC	3	0
4	D	502	PGE	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 then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.
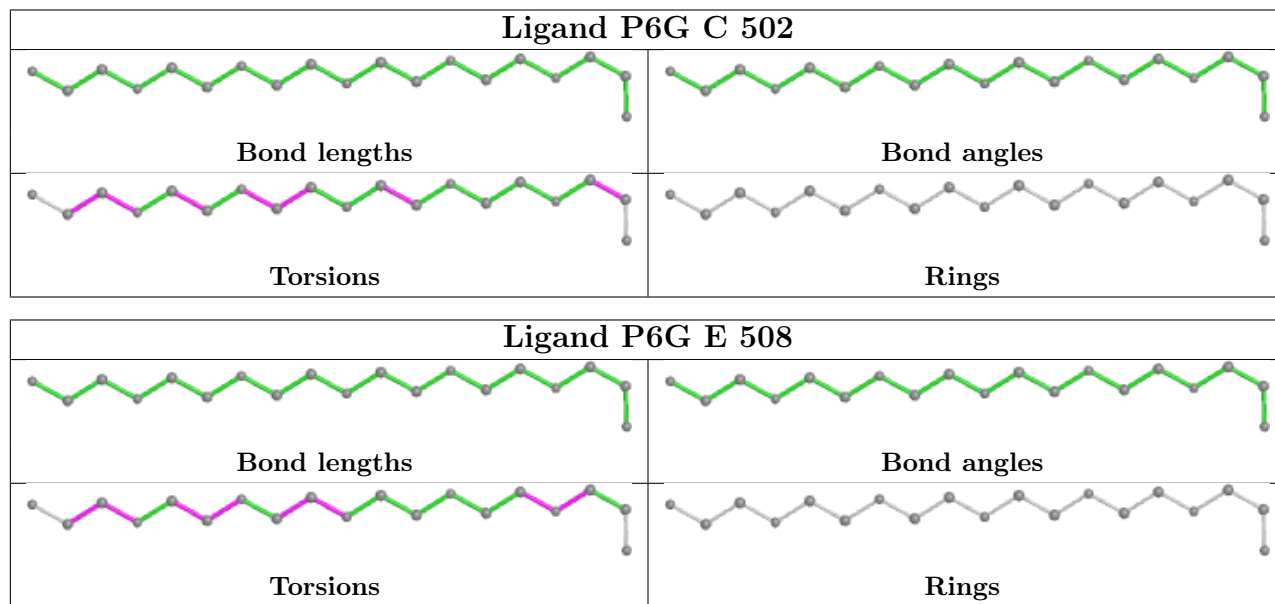
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6　Fit of model and data ⓘ

6.1　Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	421/447 (94%)	-0.20	13 (3%)	49	47	19, 31, 57, 86	0
1	B	421/447 (94%)	-0.20	13 (3%)	49	47	19, 28, 55, 90	0
1	C	421/447 (94%)	-0.10	16 (3%)	40	38	20, 33, 59, 94	1 (0%)
1	D	425/447 (95%)	-0.05	17 (4%)	38	36	19, 31, 63, 110	0
1	E	421/447 (94%)	-0.22	5 (1%)	79	77	17, 30, 57, 79	0
1	F	428/447 (95%)	-0.12	13 (3%)	50	48	20, 32, 60, 87	0
All	All	2537/2682 (94%)	-0.15	77 (3%)	50	48	17, 31, 59, 110	1 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	156	PRO	7.1
1	C	154	ASP	6.3
1	B	150	ALA	5.8
1	B	5	ALA	5.4
1	C	424	ASP	5.3
1	B	154	ASP	5.3
1	D	1	MET	5.3
1	B	4	THR	5.2
1	A	150	ALA	4.8
1	C	139	TYR	4.8
1	C	153	LYS	4.8
1	B	424	ASP	4.5
1	D	150	ALA	4.4
1	A	424	ASP	4.3
1	D	2	THR	4.2
1	E	424	ASP	4.2
1	A	154	ASP	4.1
1	D	3	LEU	4.1
1	C	155	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	373	ARG	3.7
1	B	151	GLU	3.7
1	D	151	GLU	3.6
1	A	149	ASN	3.6
1	D	154	ASP	3.5
1	C	4	THR	3.5
1	C	148	ASP	3.5
1	C	150	ALA	3.5
1	A	151	GLU	3.5
1	D	139	TYR	3.4
1	F	-3	GLU	3.4
1	A	250	GLU	3.4
1	D	155	ARG	3.4
1	B	156	PRO	3.3
1	C	152	PHE	3.2
1	A	139	TYR	3.2
1	D	227	GLU	3.1
1	F	371	ASN	3.1
1	F	424	ASP	3.0
1	A	156	PRO	3.0
1	B	152	PHE	3.0
1	F	154	ASP	2.9
1	D	226	ARG	2.8
1	A	226	ARG	2.8
1	D	253	LYS	2.7
1	B	337	ALA	2.7
1	D	152	PHE	2.7
1	F	156	PRO	2.7
1	A	227	GLU	2.7
1	B	139	TYR	2.6
1	D	251	ASP	2.6
1	C	149	ASN	2.6
1	A	153	LYS	2.6
1	D	156	PRO	2.5
1	F	152	PHE	2.5
1	B	155	ARG	2.5
1	E	150	ALA	2.5
1	F	399	ASP	2.5
1	F	153	LYS	2.4
1	E	4	THR	2.4
1	D	424	ASP	2.4
1	D	149	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	153	LYS	2.3
1	A	251	ASP	2.3
1	F	392	TRP	2.2
1	F	423	GLU	2.2
1	B	153	LYS	2.2
1	B	149	ASN	2.2
1	F	139	TYR	2.1
1	A	152	PHE	2.1
1	C	151	GLU	2.1
1	C	5	ALA	2.1
1	C	140	GLY	2.1
1	E	8	GLN	2.1
1	F	-2	GLY	2.0
1	E	423	GLU	2.0
1	F	151	GLU	2.0
1	C	157	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	J	1	12/12	0.68	0.38	75,91,99,110	0
2	GLC	J	2	11/12	0.74	0.52	89,97,104,106	0
2	GLC	L	2	11/12	0.78	0.26	33,39,42,44	11
2	GLC	I	1	12/12	0.79	0.28	58,67,73,73	0
2	GLC	G	1	12/12	0.79	0.23	55,58,64,66	0
2	GLC	I	2	11/12	0.80	0.37	63,73,80,81	0
2	GLC	K	2	11/12	0.81	0.28	59,67,76,84	0
2	GLC	G	2	11/12	0.82	0.22	49,57,63,66	0
2	GLC	H	2	11/12	0.84	0.45	64,76,82,85	0
2	GLC	H	1	12/12	0.86	0.33	52,72,84,103	0
2	GLC	M	2	11/12	0.86	0.22	49,56,58,59	0
2	GLC	N	2	11/12	0.86	0.34	61,68,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	N	1	12/12	0.87	0.42	58,66,73,78	0
2	GLC	L	1	12/12	0.87	0.22	28,41,44,46	12
2	GLC	M	1	12/12	0.89	0.19	47,53,58,59	0
2	GLC	K	1	12/12	0.89	0.28	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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
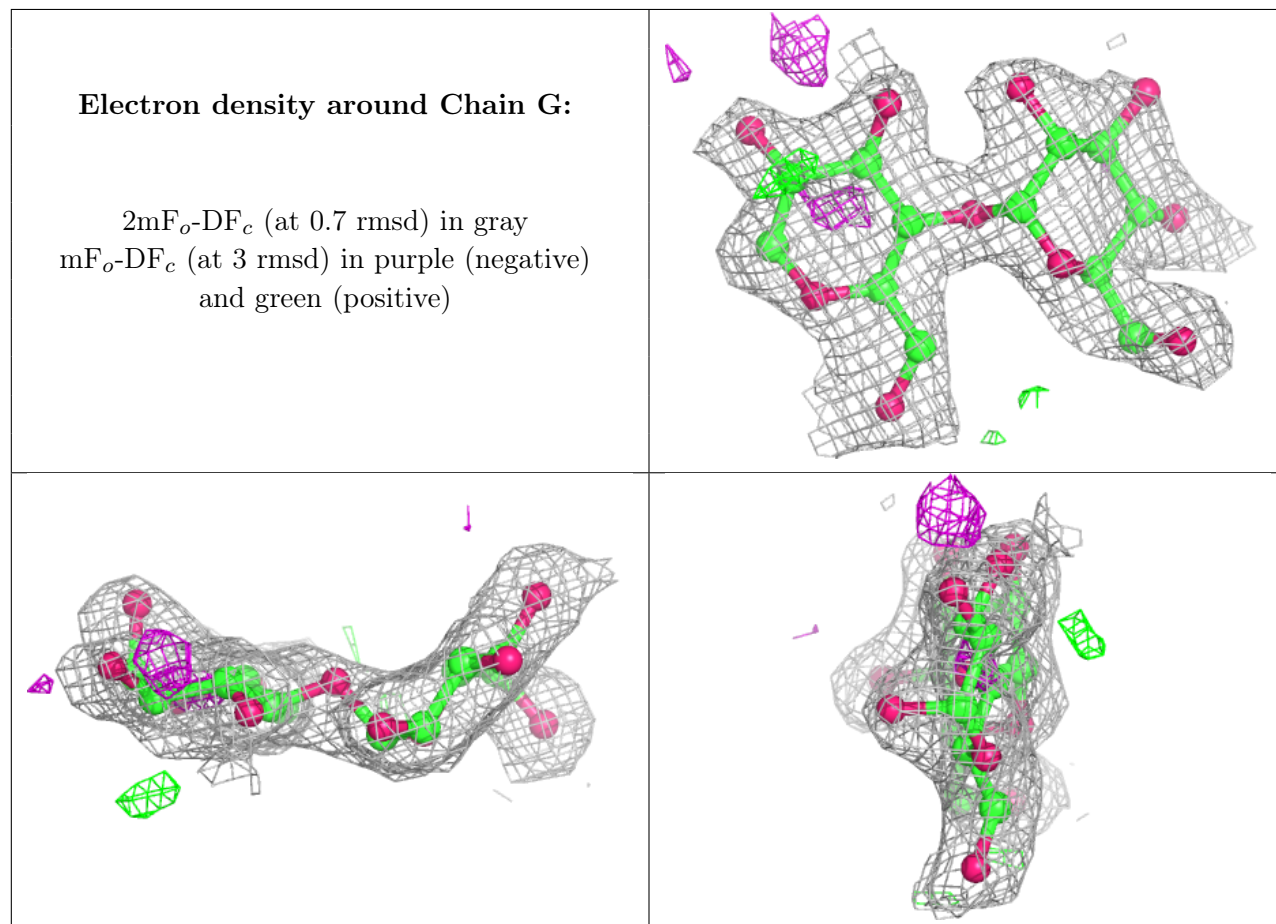
Electron density around Chain H:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
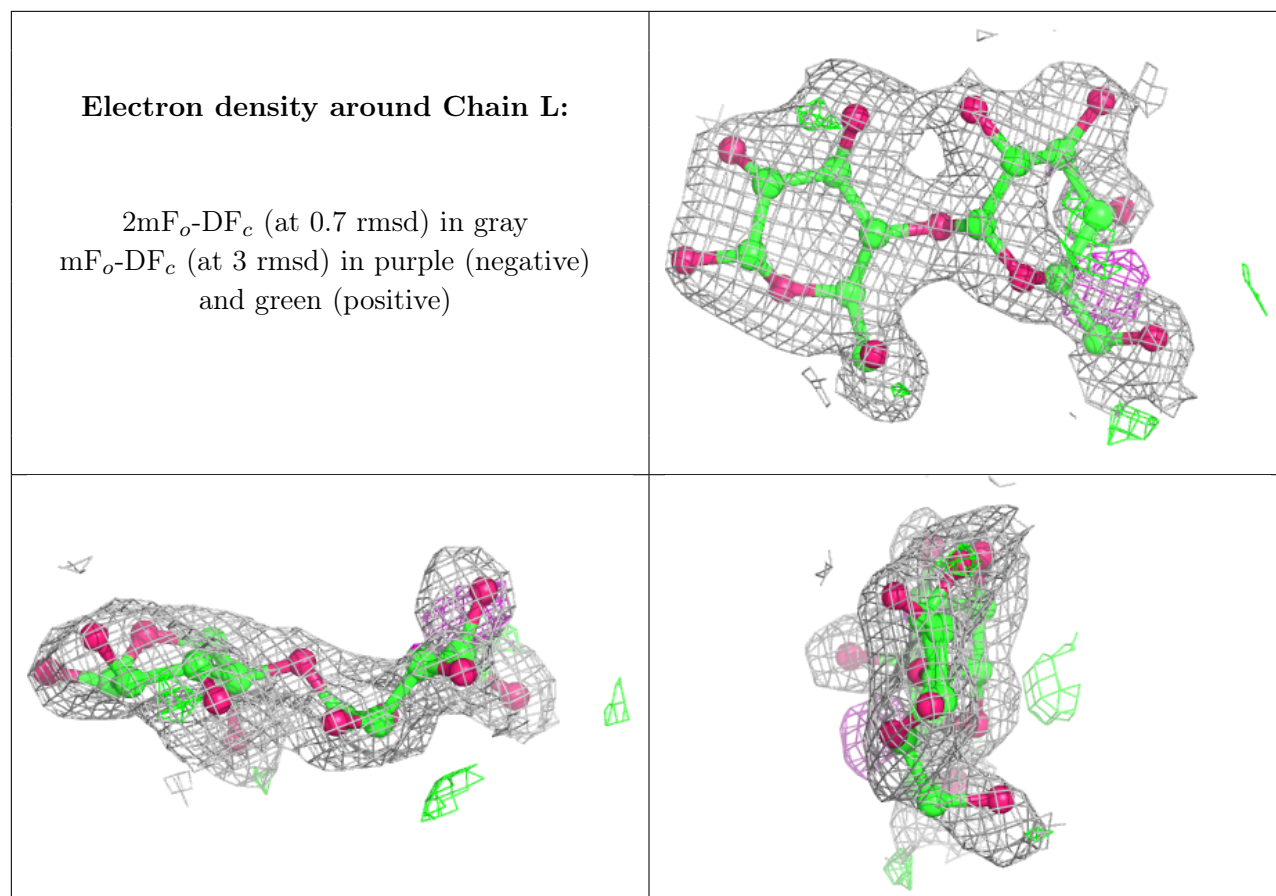mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
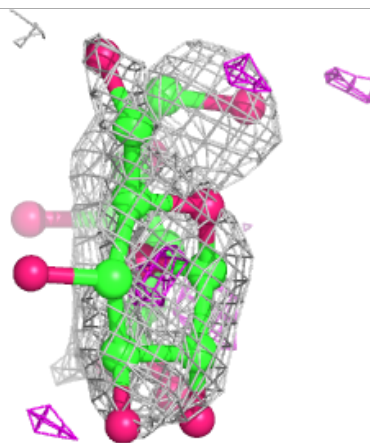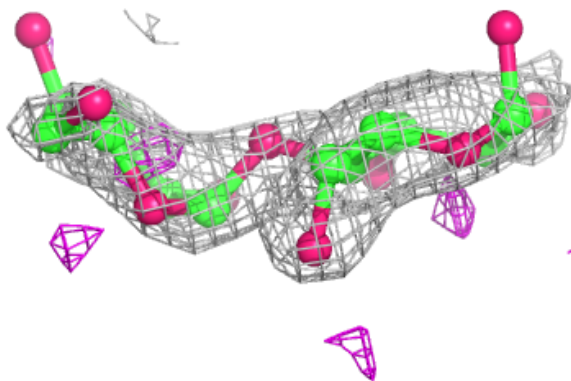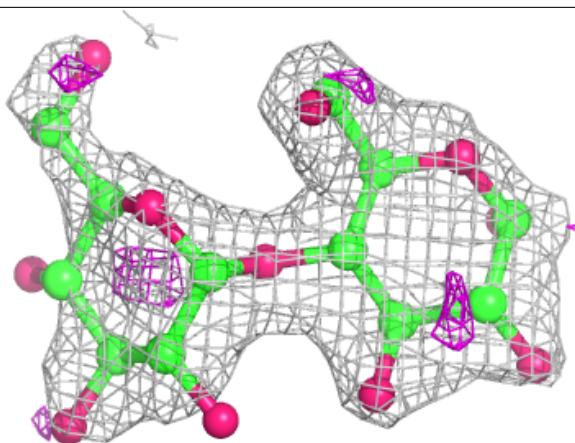
Electron density around Chain I:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
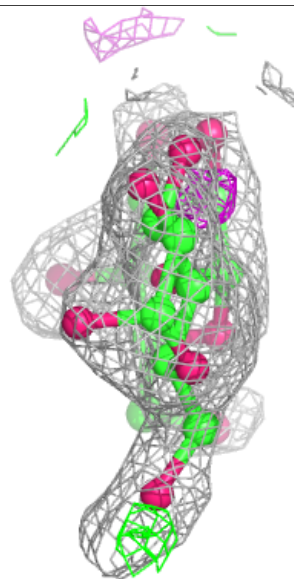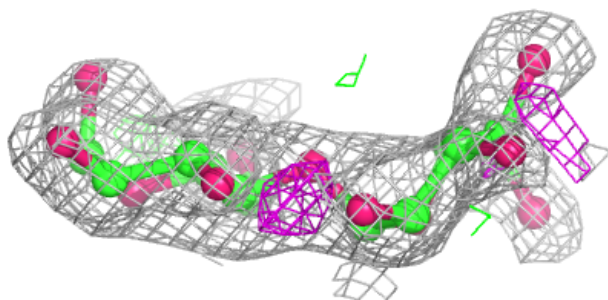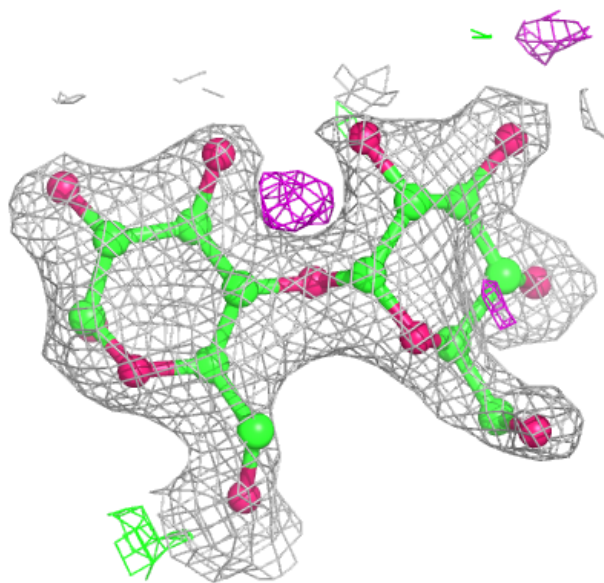
**Electron density around Chain J:**

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
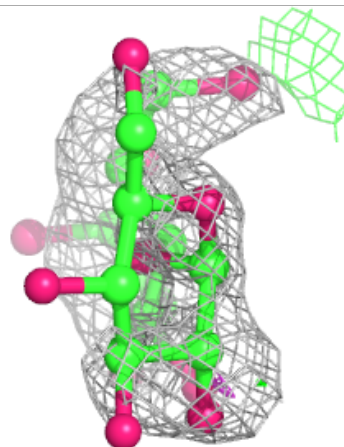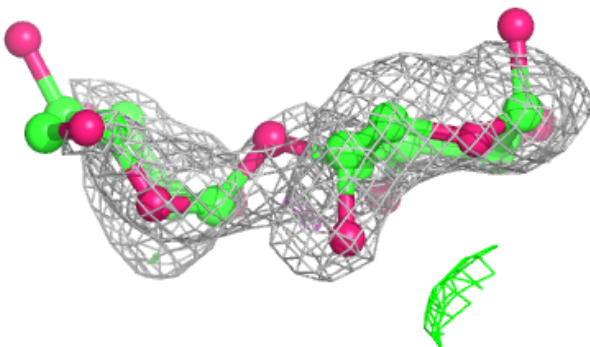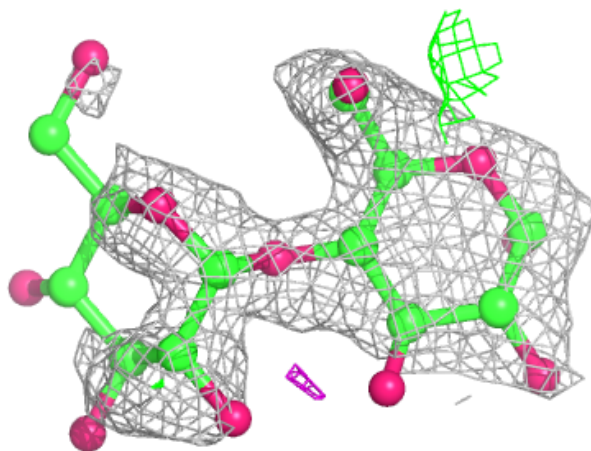
Electron density around Chain K:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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)
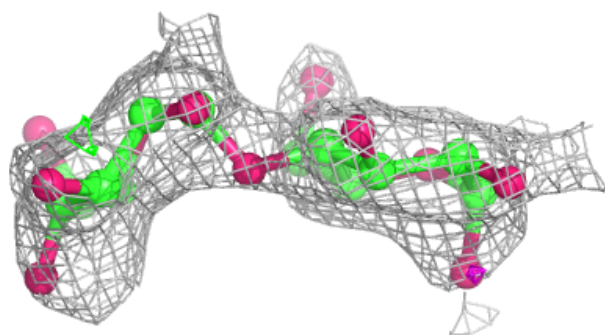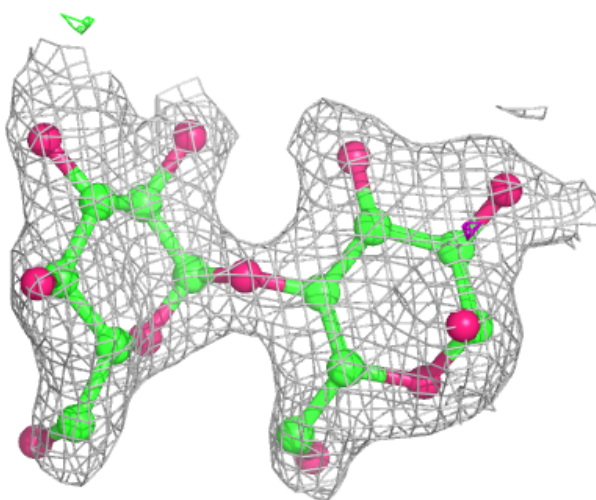
Electron density around Chain M:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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)
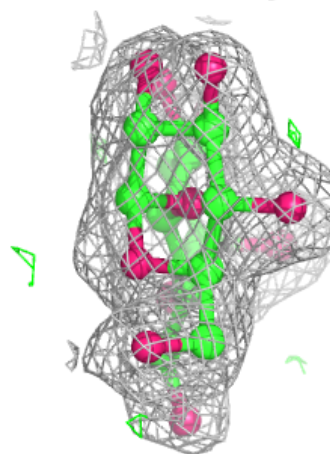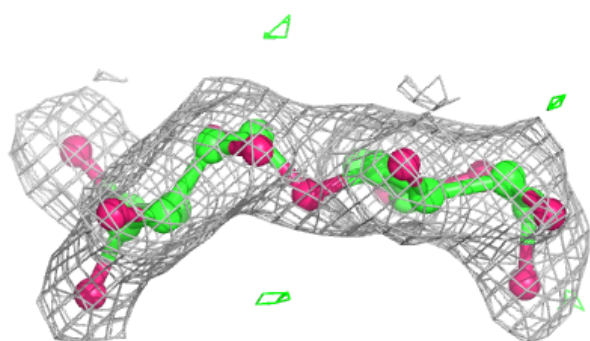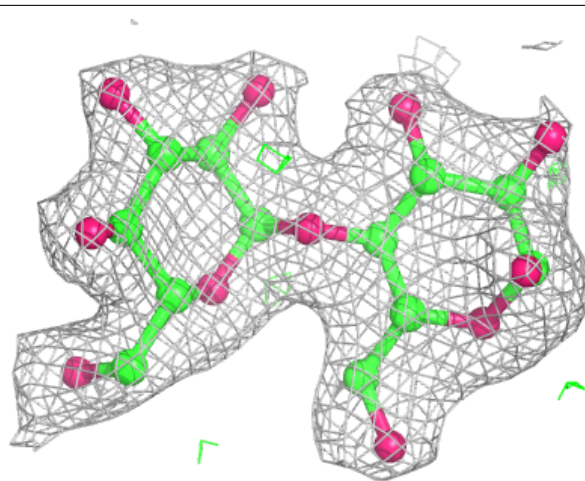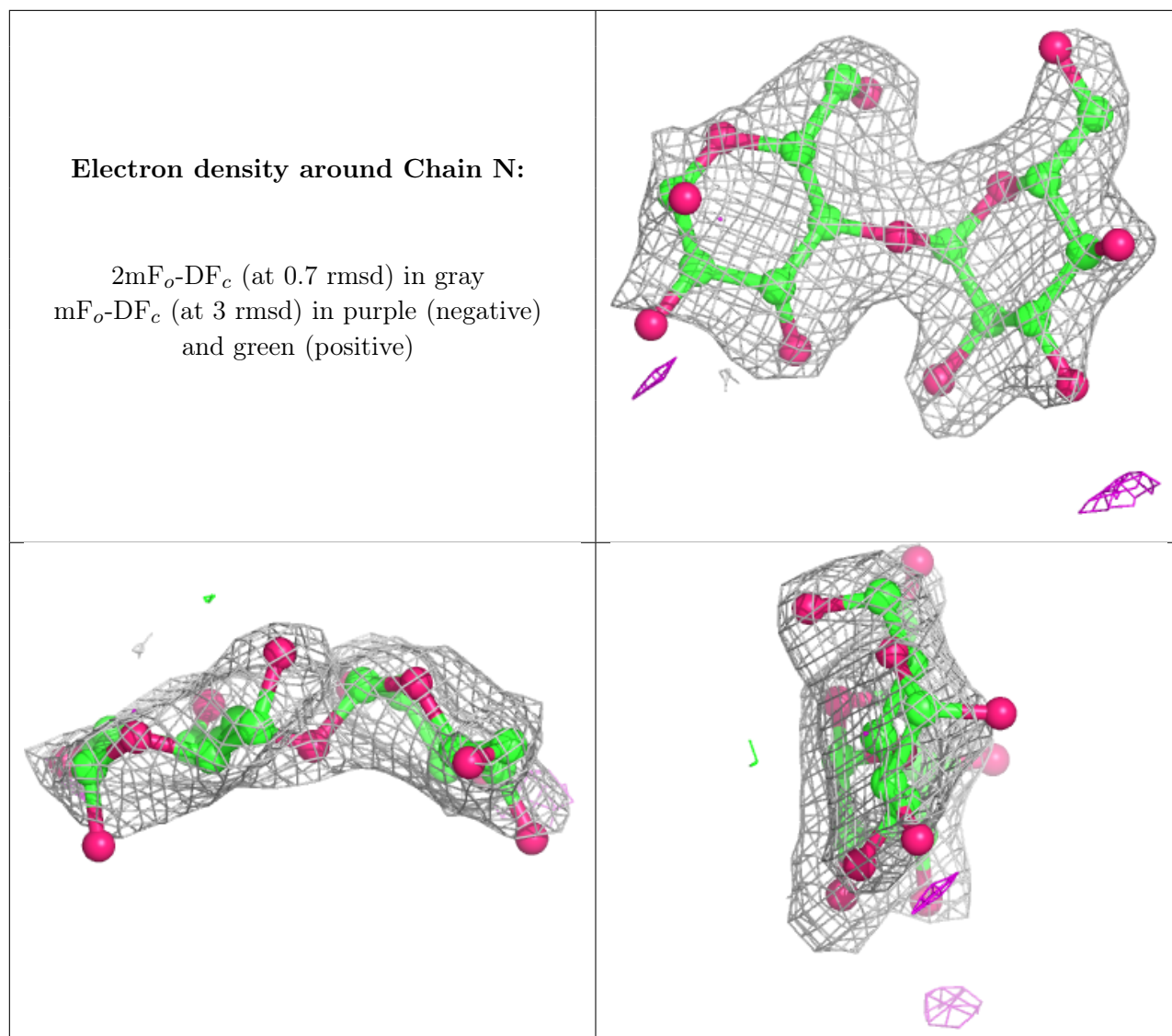
6.4 Ligands (i)

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
6	1PE	F	505	16/16	0.71	0.25	56,73,82,83	0
4	PGE	E	506	10/10	0.72	0.18	62,67,77,78	0
4	PGE	A	505	10/10	0.73	0.34	60,74,83,84	0
4	PGE	D	502	10/10	0.73	0.21	65,72,75,81	0
4	PGE	B	504	10/10	0.75	0.29	65,69,81,83	0
6	1PE	B	505	16/16	0.75	0.18	60,70,76,77	0
3	GLC	C	501	12/12	0.75	0.22	37,57,66,74	0

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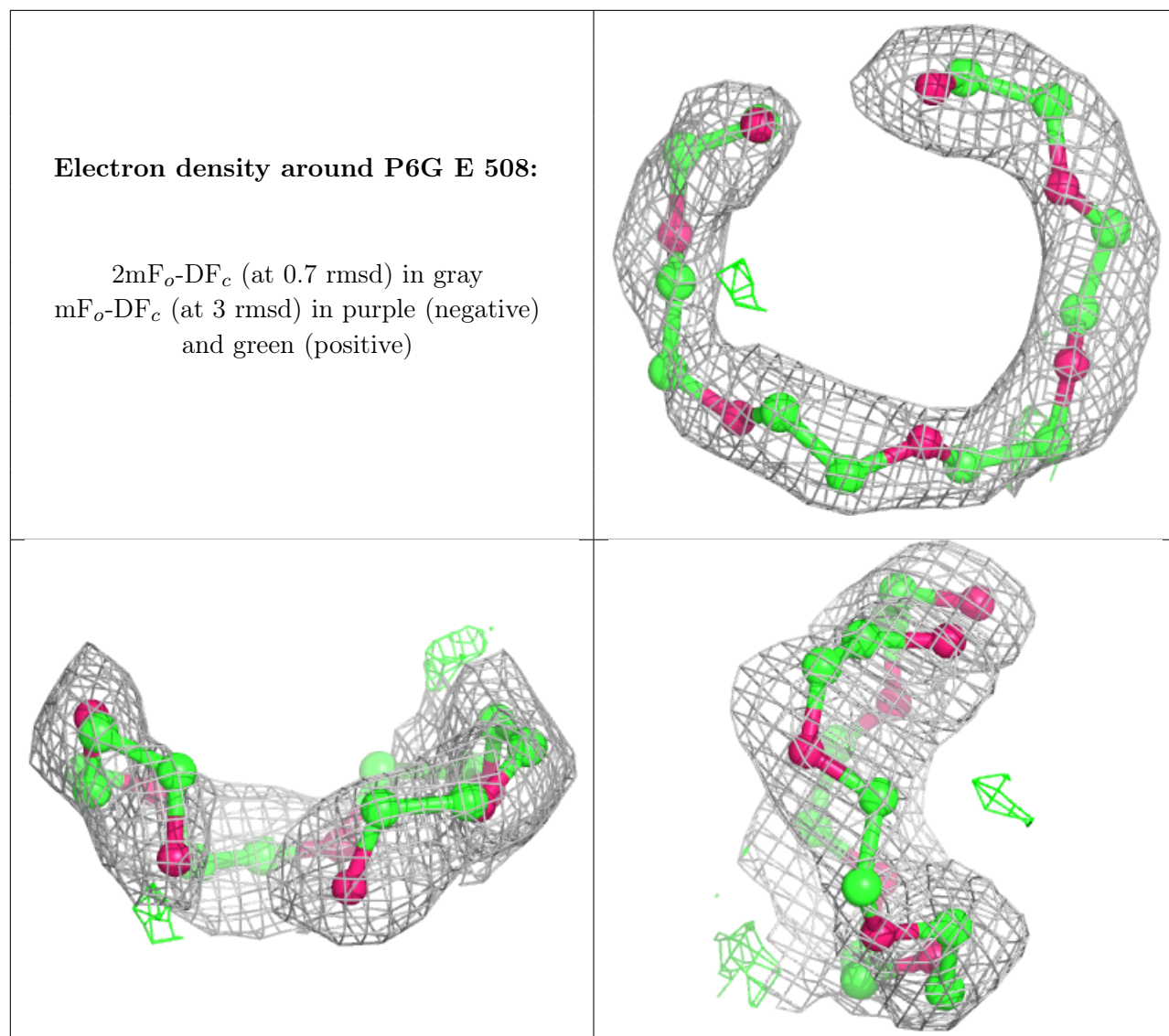
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
9	NA	C	505	1/1	0.75	0.23	69,69,69,69	0
9	NA	F	506	1/1	0.76	0.24	63,63,63,63	0
4	PGE	A	504	10/10	0.77	0.17	63,80,84,85	0
4	PGE	C	503	10/10	0.81	0.21	55,69,78,80	0
7	PG4	B	506	13/13	0.82	0.18	56,64,81,94	0
8	P6G	C	502	19/19	0.82	0.18	52,65,81,81	0
3	GLC	F	501	12/12	0.83	0.20	37,55,61,69	0
4	PGE	F	504	10/10	0.83	0.17	49,74,86,90	0
4	PGE	E	507	10/10	0.84	0.23	62,64,69,72	0
3	GLC	A	501	12/12	0.85	0.23	36,52,64,73	0
8	P6G	E	508	19/19	0.85	0.19	52,70,77,80	0
3	GLC	D	501	12/12	0.85	0.21	33,51,59,59	0
4	PGE	D	503	10/10	0.85	0.16	61,67,71,72	0
3	GLC	B	501	12/12	0.87	0.18	40,53,57,65	0
3	GLC	E	501	12/12	0.88	0.16	34,52,57,68	0
5	PEG	B	503	7/7	0.88	0.29	60,63,67,68	0
4	PGE	C	504	10/10	0.88	0.26	58,65,74,77	0
5	PEG	B	502	7/7	0.89	0.27	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 C 502:

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

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)

6.5 Other polymers ⓘ

There are no such residues in this entry.