



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:38 AM UTC

PDB ID : 6OFD / pdb_00006ofd
Title : The crystal structure of octadecyloxy(naphthalen-1-yl)methylphosphonic acid in complex with red kidney bean purple acid phosphatase
Authors : Feder, D.; Schenk, G.; Guddat, L.W.; Hussein, W.M.; McGeary, R.P.; Kan, M.W.
Deposited on : 2019-03-29
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

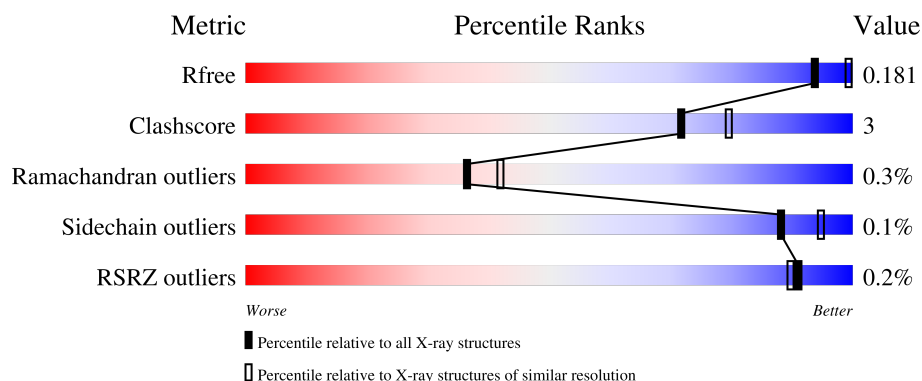
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

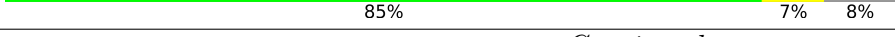
The reported resolution of this entry is 2.20 Å.

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	459	 86% 7% 7%
1	B	459	 87% 5% 7%
1	C	459	 83% 9% 8%
1	D	459	 85% 7% 8%

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Mol	Chain	Length	Quality of chain
2	E	3	
2	K	3	
2	M	3	
3	F	4	
3	H	4	
3	J	4	
3	N	4	
4	G	6	
5	I	3	
6	L	2	

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
12	SO4	B	516	-	-	X	-
12	SO4	C	514	-	-	X	-

2 Entry composition [i](#)

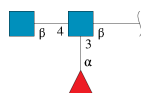
There are 17 unique types of molecules in this entry. The entry contains 16494 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fe(3+)-Zn(2+) purple acid phosphatase.

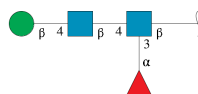
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	2	0
			3523	2261	614	638	10			
1	B	425	Total	C	N	O	S	0	2	0
			3515	2255	610	639	11			
1	D	424	Total	C	N	O	S	0	1	0
			3499	2248	607	634	10			
1	C	423	Total	C	N	O	S	0	1	0
			3487	2240	604	633	10			

- Molecule 2 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose.



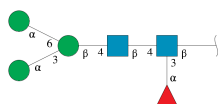
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	K	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	M	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



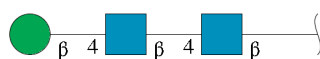
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	4	Total	C	N	O	0	0	0
			49	28	2	19			
3	H	4	Total	C	N	O	0	0	0
			49	28	2	19			
3	J	4	Total	C	N	O	0	0	0
			49	28	2	19			
3	N	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	6	Total	C	N	O	0	0	0
			71	40	2	29			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	L	2	Total	C	N	O	0	0	0
			24	14	1	9			

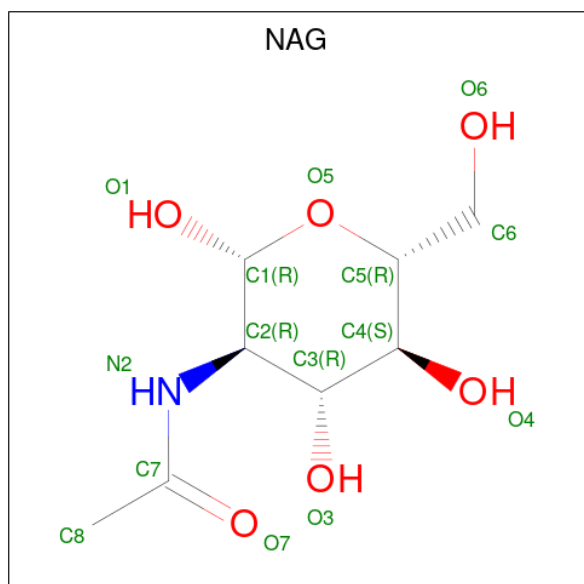
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Zn	0	0
			1	1		
7	B	1	Total	Zn	0	0
			1	1		
7	D	1	Total	Zn	0	0
			1	1		
7	C	1	Total	Zn	0	0
			1	1		

- Molecule 8 is FE (III) ION (CCD ID: FE) (formula: Fe).

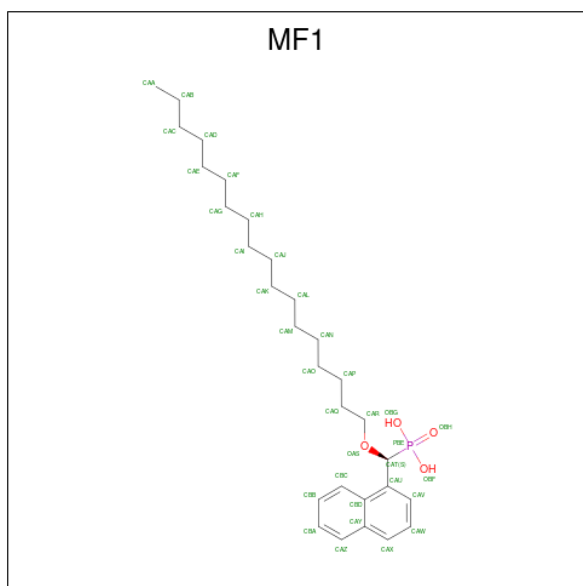
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Fe	0	0
			1	1		
8	B	1	Total	Fe	0	0
			1	1		
8	D	1	Total	Fe	0	0
			1	1		
8	C	1	Total	Fe	0	0
			1	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	1	Total	C	N	O	0	0
			14	8	1	5		
9	B	1	Total	C	N	O	0	0
			14	8	1	5		
9	D	1	Total	C	N	O	0	0
			14	8	1	5		
9	D	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		
9	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 10 is [(S)-(naphthalen-1-yl)(octadecyloxy)methyl]phosphonic acid (CCD ID: MF1) (formula: C₂₉H₄₇O₄P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O	P	0	1
			68	58	8	2		

- Molecule 11 is SODIUM ION (CCD ID: NA) (formula: Na).

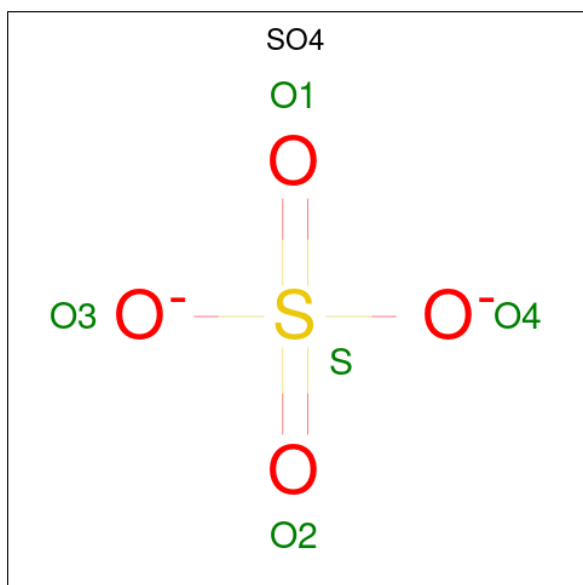
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Na	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	1	Total	Na	0	0
			1	1		
11	C	2	Total	Na	0	0
			2	2		

- Molecule 12 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



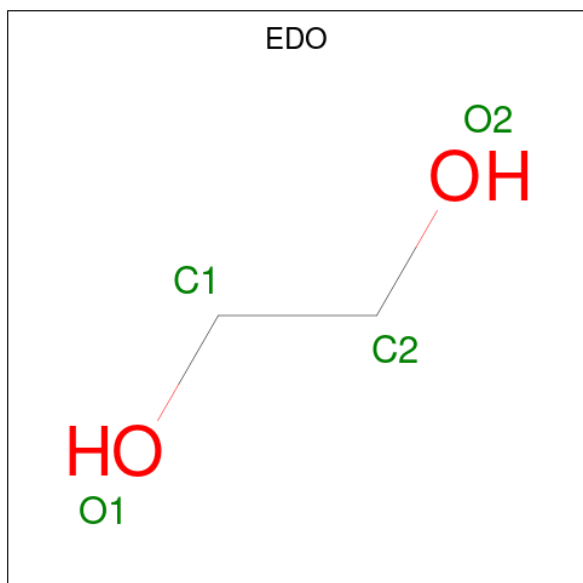
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	O	S	0	0
			5	4	1		
12	A	1	Total	O	S	0	0
			5	4	1		
12	A	1	Total	O	S	0	0
			5	4	1		
12	A	1	Total	O	S	0	0
			5	4	1		
12	A	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	D	1	Total	O	S	0	0
			5	4	1		
12	D	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		
12	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 13 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



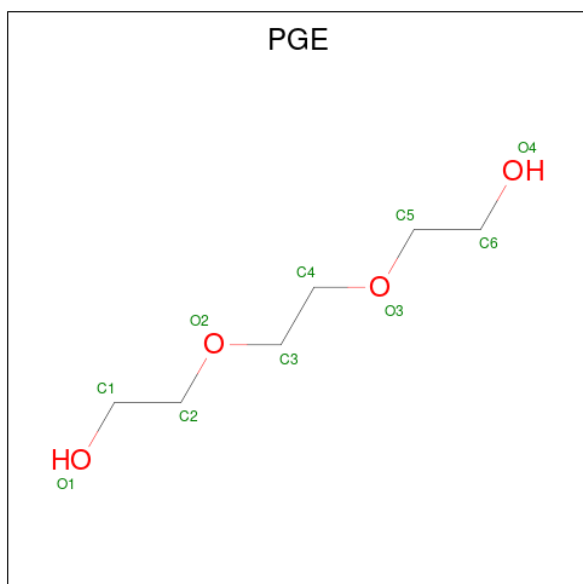
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			4	2	2		

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	A	1	Total	C	O	0	0
			7	4	3		
14	D	1	Total	C	O	0	0
			7	4	3		
14	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 15 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	D	1	Total	C	O	0	0
			6	3	3		

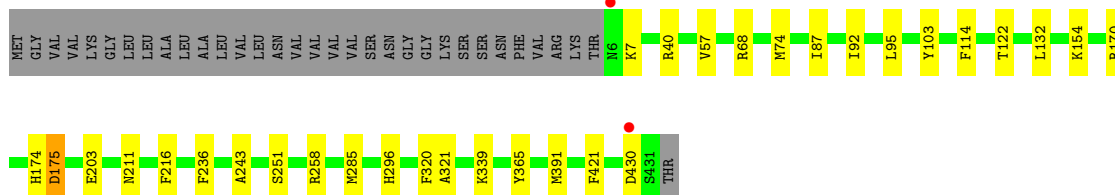
- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

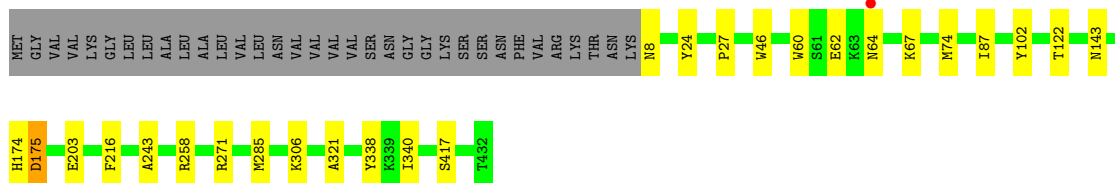
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	459	Total	O	0	0
			459	459		
17	B	435	Total	O	0	0
			435	435		
17	D	403	Total	O	0	0
			403	403		
17	C	402	Total	O	0	0
			402	402		

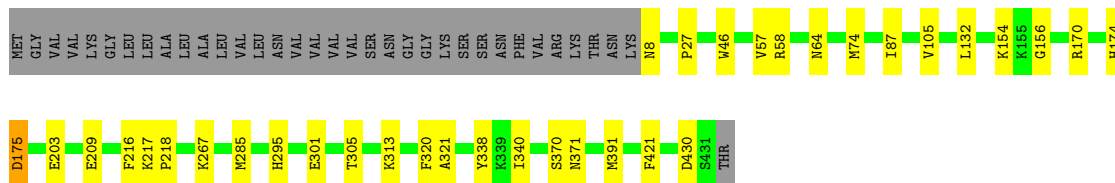
- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

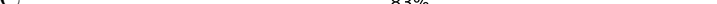


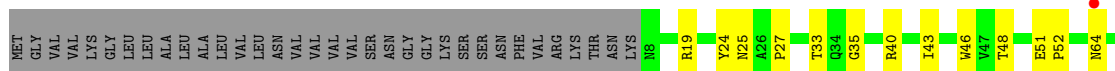
Chain B: 87% 5% 7%

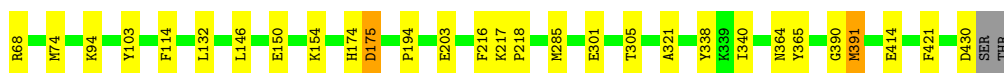


Chain D: 85% 7% 8%

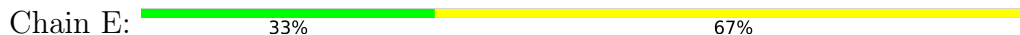


Chain C:  83% 9% 8%





- Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose



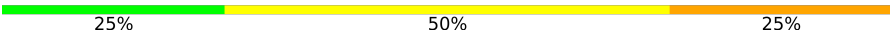
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

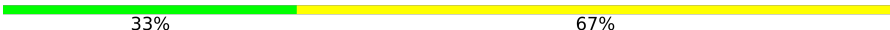


- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  25% 50% 25%

MAG1
MAG2
BMA3
FUC4

- Molecule 4: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  33% 67%

MAG1
MAG2
BMA3
MAN4
MAN5
FUC6

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  67% 33%

MAG1
MAG2
BMA3

- Molecule 6: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  50% 50%

MAG1
FUC2

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	126.17Å 126.17Å 298.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.05 – 2.20 20.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.05-2.20) 99.7 (20.05-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.19Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.155 , 0.199 (Not available) , 0.181	Depositor DCC
R_{free} test set	6987 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16494	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MF1, NAG, BMA, NA, SO4, MAN, GOL, CL, FUC, ZN, FE, PGE, EDO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/3649	0.53	0/4961
1	B	0.34	0/3634	0.50	0/4941
1	C	0.34	0/3609	0.52	1/4909 (0.0%)
1	D	0.35	0/3621	0.51	0/4924
All	All	0.34	0/14513	0.52	1/19735 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	LEU	CA-CB-CG	-5.43	97.30	116.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3523	0	3340	23	0
1	B	3515	0	3327	16	0
1	C	3487	0	3297	25	0
1	D	3499	0	3319	25	0
2	E	38	0	34	0	0
2	K	38	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	38	0	34	0	0
3	F	49	0	43	0	0
3	H	49	0	43	1	0
3	J	49	0	43	0	0
3	N	49	0	43	1	0
4	G	71	0	61	0	0
5	I	39	0	34	0	0
6	L	24	0	22	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	14	0	13	0	0
9	B	14	0	13	1	0
9	C	42	0	39	0	0
9	D	28	0	26	0	0
10	A	68	0	0	6	0
11	A	2	0	0	0	0
11	C	2	0	0	0	0
11	D	1	0	0	0	0
12	A	30	0	0	1	0
12	B	40	0	0	3	0
12	C	15	0	0	2	0
12	D	10	0	0	1	0
13	A	4	0	6	0	0
13	B	4	0	6	0	0
13	C	16	0	24	0	0
13	D	4	0	6	0	0
14	A	7	0	9	1	0
14	D	11	0	13	4	0
15	D	6	0	7	1	0
16	D	1	0	0	0	0
17	A	459	0	0	4	0
17	B	435	0	0	4	0
17	C	402	0	0	1	0
17	D	403	0	0	10	0
All	All	16494	0	13836	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 3.

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:B:271:ARG:NH2	17:B:601:HOH:O	2.05	0.89
1:D:64:ASN:ND2	17:D:604:HOH:O	2.19	0.75
1:D:267:LYS:NZ	17:D:605:HOH:O	2.20	0.73
1:C:19:ARG:NH1	17:C:601:HOH:O	2.21	0.73
12:D:513:SO4:O3	17:D:601:HOH:O	2.06	0.72
1:A:421:PHE:CD2	1:A:430:ASP:HB3	2.30	0.67
1:A:154:LYS:HB2	1:A:391:MET:HE3	1.76	0.66
1:A:68:ARG:NH1	12:A:522:SO4:O4	2.27	0.65
1:B:306:LYS:NZ	12:B:516:SO4:O3	2.31	0.62
1:B:143:ASN:HD22	9:B:503:NAG:H83	1.65	0.62
1:B:8:ASN:N	17:B:605:HOH:O	2.34	0.60
1:B:62:GLU:HG3	1:B:102:TYR:HE2	1.67	0.60
15:D:514:GOL:H31	17:D:623:HOH:O	2.02	0.59
1:D:154:LYS:HB2	1:D:391:MET:HE3	1.85	0.59
1:C:421:PHE:CD2	1:C:430:ASP:HB3	2.38	0.58
1:C:64:ASN:ND2	12:C:514:SO4:O2	2.37	0.58
1:D:58:ARG:NH2	17:D:607:HOH:O	2.32	0.57
1:D:217:LYS:HB3	1:D:218:PRO:HD3	1.87	0.56
1:A:132:LEU:HD22	1:A:320:PHE:CD1	2.40	0.56
1:A:170:ARG:HE	10:A:517[C]:MF1:CAO	2.18	0.56
1:D:421:PHE:CD2	1:D:430:ASP:HB3	2.40	0.56
1:A:170:ARG:HE	10:A:517[B]:MF1:CAO	2.19	0.55
1:A:7:LYS:HE3	10:A:517[C]:MF1:CAJ	2.37	0.53
12:B:516:SO4:O1	17:B:602:HOH:O	2.18	0.53
1:D:370:SER:H	14:D:515:PGE:H5	1.74	0.53
1:A:170:ARG:HH21	10:A:517[B]:MF1:CAN	2.23	0.51
1:D:370:SER:N	14:D:515:PGE:H5	2.25	0.51
1:D:430:ASP:OD1	17:D:602:HOH:O	2.19	0.51
1:D:209:GLU:OE2	17:D:603:HOH:O	2.19	0.51
1:D:295:HIS:HB2	14:D:515:PGE:H42	1.93	0.51
1:C:203:GLU:O	1:C:216:PHE:HA	2.10	0.51
1:C:301:GLU:O	1:C:305:THR:HG23	2.11	0.50
1:B:258:ARG:N	12:B:516:SO4:O4	2.44	0.50
1:A:421:PHE:HD2	1:A:430:ASP:HB3	1.78	0.49
1:C:146:LEU:O	1:C:150:GLU:HG3	2.12	0.49
1:B:174:HIS:O	1:B:175:ASP:C	2.55	0.49
1:C:174:HIS:O	1:C:175:ASP:C	2.55	0.48
1:D:8:ASN:N	17:D:614:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:TYR:CZ	1:C:114:PHE:HB2	2.49	0.47
1:D:313:LYS:NZ	17:D:615:HOH:O	2.46	0.47
1:A:339:LYS:NZ	17:A:608:HOH:O	2.47	0.47
1:A:57:VAL:HG11	1:A:92:ILE:HD11	1.97	0.47
1:B:338:TYR:CZ	1:B:340:ILE:HA	2.50	0.46
1:D:203:GLU:O	1:D:216:PHE:HA	2.15	0.46
1:A:40:ARG:NH1	1:A:95:LEU:O	2.48	0.46
1:B:203:GLU:O	1:B:216:PHE:HA	2.16	0.46
1:D:174:HIS:O	1:D:175:ASP:C	2.58	0.46
1:C:285:MET:O	1:C:321:ALA:HA	2.15	0.46
1:A:174:HIS:O	1:A:175:ASP:C	2.60	0.45
3:N:2:NAG:H83	3:N:4:FUC:H61	1.96	0.45
1:C:40:ARG:HH12	1:C:94:LYS:HD2	1.81	0.45
1:A:258:ARG:HD3	17:A:665:HOH:O	2.16	0.45
1:D:57:VAL:HG22	1:D:105:VAL:HG12	1.98	0.45
1:D:371:ASN:CG	14:D:515:PGE:H62	2.42	0.45
1:A:236:PHE:O	1:A:251:SER:HB2	2.17	0.45
1:A:285:MET:O	1:A:321:ALA:HA	2.16	0.45
1:C:33:THR:HA	1:C:194:PRO:HB3	1.98	0.45
1:D:156:GLY:N	1:D:391:MET:HE1	2.32	0.44
1:C:217:LYS:HB3	1:C:218:PRO:HD3	1.99	0.44
1:D:285:MET:O	1:D:321:ALA:HA	2.17	0.44
1:A:365:TYR:OH	10:A:517[B]:MF1:OBG	2.30	0.44
1:D:27:PRO:HB3	1:D:46:TRP:CD1	2.53	0.44
1:B:27:PRO:HB3	1:B:46:TRP:CD1	2.53	0.44
1:B:74:MET:HA	1:B:87:ILE:O	2.18	0.44
1:D:132:LEU:HD22	1:D:320:PHE:CD1	2.53	0.43
1:B:285:MET:O	1:B:321:ALA:HA	2.18	0.43
1:C:27:PRO:HB3	1:C:46:TRP:CD1	2.53	0.43
1:C:40:ARG:NH1	1:C:94:LYS:HD2	2.34	0.43
1:C:391:MET:HE3	1:C:391:MET:HB2	1.83	0.43
1:A:203:GLU:O	1:A:216:PHE:HA	2.19	0.42
1:D:338:TYR:CZ	1:D:340:ILE:HA	2.54	0.42
1:B:417:SER:OG	17:B:603:HOH:O	2.21	0.42
1:C:52:PRO:HB3	1:C:74:MET:HE2	2.01	0.42
1:A:122:THR:HA	1:A:243:ALA:O	2.20	0.42
1:A:103:TYR:CZ	1:A:114:PHE:HB2	2.54	0.42
1:A:74:MET:HA	1:A:87:ILE:O	2.19	0.42
1:A:211[A]:ASN:ND2	17:A:605:HOH:O	2.37	0.42
1:C:24:TYR:OH	1:C:51:GLU:OE2	2.33	0.42
1:C:154:LYS:HE2	1:C:414:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:MET:HA	1:D:87:ILE:O	2.20	0.41
1:A:296:HIS:NE2	10:A:517[C]:MF1:OBF	2.33	0.41
14:A:527:PGE:H3	17:A:708:HOH:O	2.20	0.41
1:C:35:GLY:HA2	1:C:43:ILE:HG13	2.03	0.41
1:D:170:ARG:NH1	17:D:609:HOH:O	2.42	0.41
1:B:122:THR:HG22	1:B:243:ALA:O	2.21	0.41
1:B:24:TYR:CD2	3:H:1:NAG:H82	2.56	0.40
1:C:25:ASN:OD1	1:C:48:THR:HB	2.20	0.40
1:C:103:TYR:CE1	1:C:114:PHE:HB2	2.56	0.40
1:C:338:TYR:CZ	1:C:340:ILE:HA	2.55	0.40
1:C:390:GLY:O	1:C:391:MET:HE2	2.22	0.40
1:C:68:ARG:NH1	12:C:514:SO4:O4	2.45	0.40
1:C:364:ASN:OD1	1:C:365:TYR:N	2.51	0.40
1:B:60:TRP:HB3	1:B:67:LYS:HA	2.03	0.40
1:D:301:GLU:O	1:D:305:THR:HG23	2.21	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	426/459 (93%)	408 (96%)	17 (4%)	1 (0%)	43	51
1	B	425/459 (93%)	406 (96%)	17 (4%)	2 (0%)	24	27
1	C	422/459 (92%)	401 (95%)	20 (5%)	1 (0%)	43	51
1	D	423/459 (92%)	401 (95%)	21 (5%)	1 (0%)	43	51
All	All	1696/1836 (92%)	1616 (95%)	75 (4%)	5 (0%)	36	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	ASN
1	A	175	ASP
1	B	175	ASP
1	D	175	ASP
1	C	175	ASP

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	377/402 (94%)	377 (100%)	0	100	100
1	B	376/402 (94%)	376 (100%)	0	100	100
1	C	372/402 (92%)	371 (100%)	1 (0%)	86	93
1	D	374/402 (93%)	374 (100%)	0	100	100
All	All	1499/1608 (93%)	1498 (100%)	1 (0%)	88	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	391	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	A	193	GLN
1	A	405	ASN
1	B	8	ASN
1	B	173	ASN
1	B	176	ASN
1	B	193	GLN
1	B	405	ASN
1	D	173	ASN
1	D	401	HIS
1	D	405	ASN

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Mol	Chain	Res	Type
1	C	64	ASN
1	C	173	ASN
1	C	193	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

36 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	NAG	E	1	2,1	14,14,15	0.28	0	17,19,21	0.92	1 (5%)
2	FUC	E	2	2	10,10,11	1.03	1 (10%)	14,14,16	1.46	3 (21%)
2	NAG	E	3	2	14,14,15	0.36	0	17,19,21	0.40	0
3	NAG	F	1	3,1	14,14,15	0.37	0	17,19,21	0.51	0
3	NAG	F	2	3	14,14,15	0.51	0	17,19,21	0.66	0
3	BMA	F	3	3	11,11,12	1.65	2 (18%)	15,15,17	0.81	0
3	FUC	F	4	3	10,10,11	1.32	2 (20%)	14,14,16	1.05	1 (7%)
4	NAG	G	1	1,4	14,14,15	0.51	0	17,19,21	0.78	1 (5%)
4	NAG	G	2	4	14,14,15	0.43	0	17,19,21	0.53	0
4	BMA	G	3	4	11,11,12	1.63	2 (18%)	15,15,17	1.05	0
4	MAN	G	4	4	11,11,12	1.00	0	15,15,17	1.22	1 (6%)
4	MAN	G	5	4	11,11,12	1.36	2 (18%)	15,15,17	0.94	0
4	FUC	G	6	4	10,10,11	0.87	0	14,14,16	0.97	0
3	NAG	H	1	3,1	14,14,15	0.51	0	17,19,21	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	H	2	3	14,14,15	0.24	0	17,19,21	0.56	0
3	BMA	H	3	3	11,11,12	1.50	3 (27%)	15,15,17	1.34	1 (6%)
3	FUC	H	4	3	10,10,11	0.81	0	14,14,16	1.11	0
5	NAG	I	1	5,1	14,14,15	0.63	0	17,19,21	0.62	0
5	NAG	I	2	5	14,14,15	0.28	0	17,19,21	0.46	0
5	BMA	I	3	5	11,11,12	1.66	4 (36%)	15,15,17	0.96	1 (6%)
3	NAG	J	1	3,1	14,14,15	0.37	0	17,19,21	0.70	1 (5%)
3	NAG	J	2	3	14,14,15	0.40	0	17,19,21	0.54	0
3	BMA	J	3	3	11,11,12	1.51	2 (18%)	15,15,17	0.95	0
3	FUC	J	4	3	10,10,11	0.76	0	14,14,16	0.85	0
2	NAG	K	1	2,1	14,14,15	0.54	0	17,19,21	0.55	0
2	FUC	K	2	2	10,10,11	0.93	1 (10%)	14,14,16	0.90	0
2	NAG	K	3	2	14,14,15	0.48	0	17,19,21	0.47	0
6	NAG	L	1	1,6	14,14,15	0.37	0	17,19,21	0.68	1 (5%)
6	FUC	L	2	6	10,10,11	1.17	0	14,14,16	0.70	0
2	NAG	M	1	2,1	14,14,15	0.51	0	17,19,21	0.52	0
2	FUC	M	2	2	10,10,11	1.15	0	14,14,16	0.78	0
2	NAG	M	3	2	14,14,15	0.53	0	17,19,21	0.60	0
3	NAG	N	1	3,1	14,14,15	0.39	0	17,19,21	0.63	0
3	NAG	N	2	3	14,14,15	0.38	0	17,19,21	0.78	1 (5%)
3	BMA	N	3	3	11,11,12	1.52	2 (18%)	15,15,17	1.38	1 (6%)
3	FUC	N	4	3	10,10,11	0.81	0	14,14,16	0.86	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	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	E	2	2	-	-	0/1/1/1
2	NAG	E	3	2	-	4/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	FUC	F	4	3	-	-	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	G	5	4	-	0/2/19/22	0/1/1/1
4	FUC	G	6	4	-	-	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	BMA	H	3	3	-	2/2/19/22	1/1/1/1
3	FUC	H	4	3	-	-	0/1/1/1
5	NAG	I	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	2/6/23/26	0/1/1/1
5	BMA	I	3	5	-	0/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
3	FUC	J	4	3	-	-	0/1/1/1
2	NAG	K	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	K	2	2	-	-	0/1/1/1
2	NAG	K	3	2	-	2/6/23/26	0/1/1/1
6	NAG	L	1	1,6	-	1/6/23/26	0/1/1/1
6	FUC	L	2	6	-	-	0/1/1/1
2	NAG	M	1	2,1	-	0/6/23/26	0/1/1/1
2	FUC	M	2	2	-	-	0/1/1/1
2	NAG	M	3	2	-	2/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	4/6/23/26	0/1/1/1
3	BMA	N	3	3	-	0/2/19/22	0/1/1/1
3	FUC	N	4	3	-	-	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3	BMA	C2-C3	3.92	1.58	1.52
3	N	3	BMA	C1-C2	3.03	1.59	1.52
3	F	3	BMA	C1-C2	3.01	1.59	1.52
3	J	3	BMA	C1-C2	2.89	1.59	1.52
3	H	3	BMA	O5-C5	2.69	1.48	1.43
5	I	3	BMA	C1-C2	2.68	1.58	1.52
4	G	3	BMA	O2-C2	2.67	1.48	1.43
3	H	3	BMA	C1-C2	2.66	1.58	1.52
3	N	3	BMA	C2-C3	2.65	1.56	1.52
3	F	4	FUC	O5-C5	2.62	1.48	1.43
4	G	5	MAN	O5-C5	2.58	1.48	1.43
5	I	3	BMA	C2-C3	2.32	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	BMA	C2-C3	2.21	1.55	1.52
2	E	2	FUC	O5-C5	2.21	1.47	1.43
5	I	3	BMA	C4-C3	2.16	1.57	1.52
3	H	3	BMA	O5-C1	2.12	1.47	1.43
2	K	2	FUC	C4-C5	2.09	1.57	1.52
3	F	4	FUC	C4-C5	2.08	1.57	1.52
4	G	5	MAN	C2-C3	2.04	1.55	1.52
5	I	3	BMA	C4-C5	2.02	1.57	1.53
3	J	3	BMA	C2-C3	2.01	1.55	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	BMA	C1-O5-C5	4.39	118.06	112.19
3	N	3	BMA	C1-O5-C5	4.29	117.94	112.19
4	G	4	MAN	C1-O5-C5	3.65	117.08	112.19
2	E	1	NAG	C1-O5-C5	3.14	116.40	112.19
2	E	2	FUC	O5-C5-C4	2.94	114.85	109.55
2	E	2	FUC	C1-O5-C5	2.90	119.82	112.97
4	G	1	NAG	C1-O5-C5	2.52	115.56	112.19
3	H	1	NAG	C1-O5-C5	2.51	115.55	112.19
3	F	4	FUC	O5-C5-C4	2.44	113.95	109.55
5	I	3	BMA	C1-O5-C5	2.37	115.36	112.19
2	E	2	FUC	C2-C3-C4	-2.32	106.78	110.86
3	J	1	NAG	C1-O5-C5	2.30	115.26	112.19
3	N	2	NAG	O4-C4-C3	2.08	115.28	110.38
6	L	1	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	2	NAG	C4-C5-C6-O6
2	K	3	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
2	K	3	NAG	C4-C5-C6-O6
2	E	3	NAG	O5-C5-C6-O6
3	H	3	BMA	O5-C5-C6-O6
2	E	3	NAG	C8-C7-N2-C2
2	E	3	NAG	O7-C7-N2-C2
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
2	E	3	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
2	M	3	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	H	3	BMA	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	M	3	NAG	O5-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6

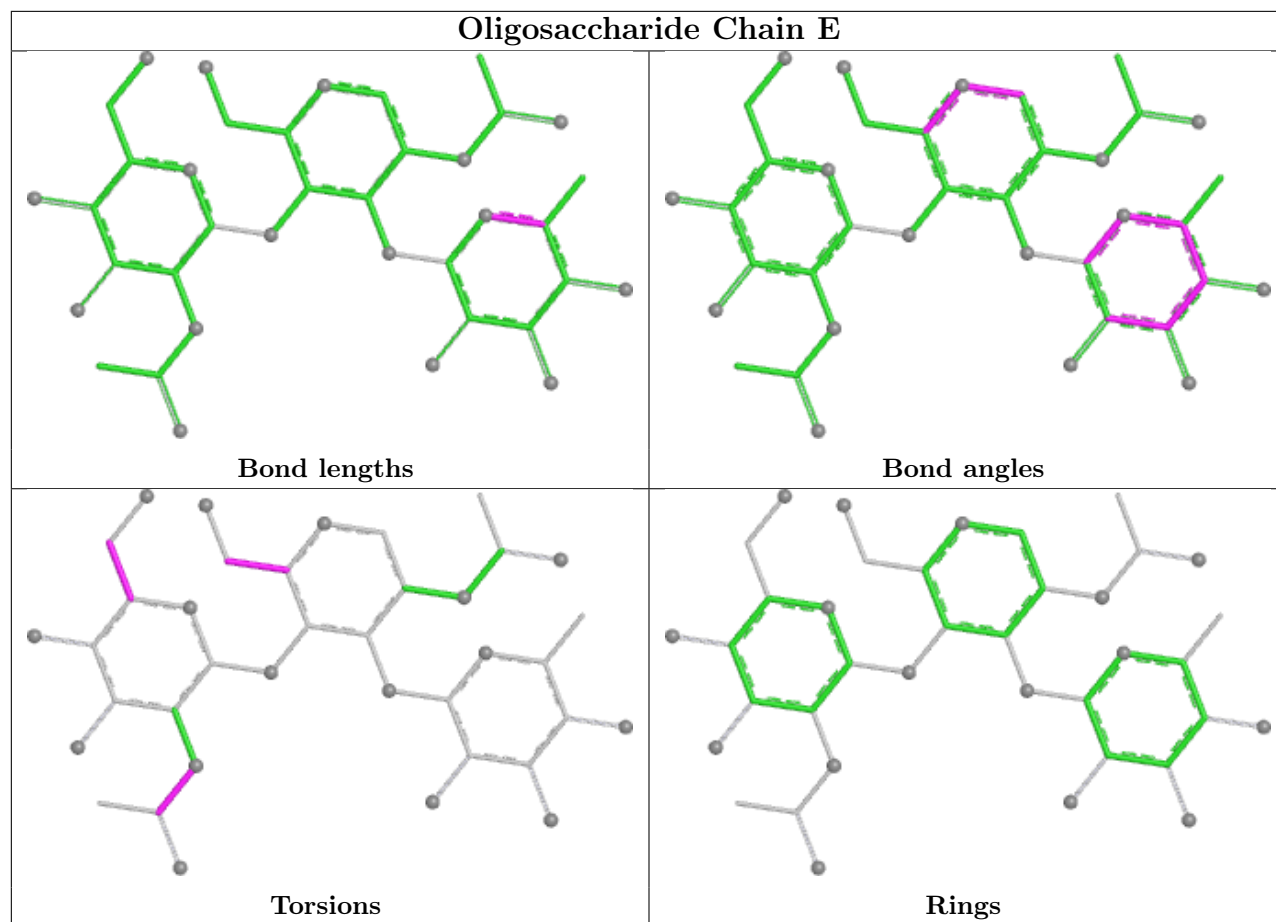
All (1) ring outliers are listed below:

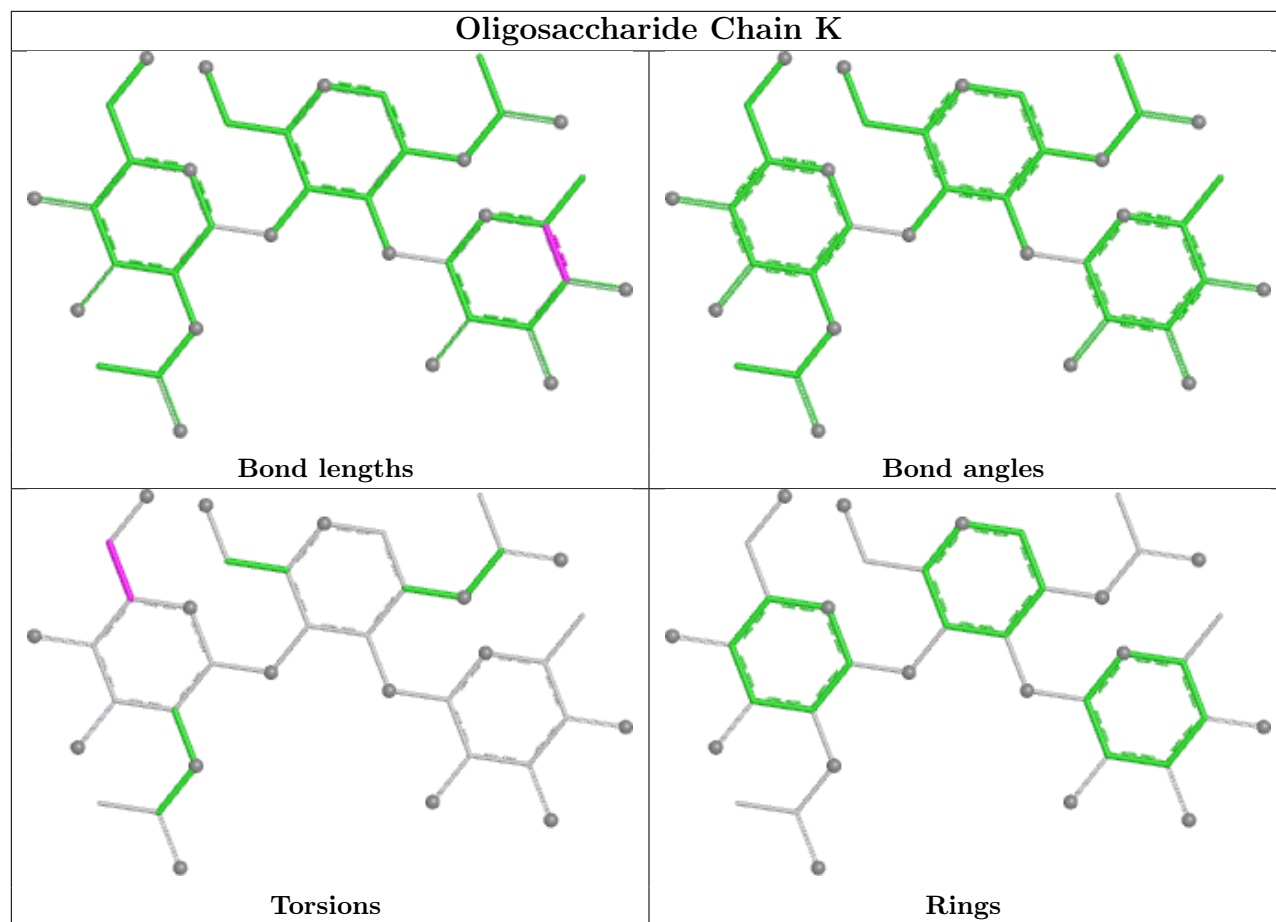
Mol	Chain	Res	Type	Atoms
3	H	3	BMA	C1-C2-C3-C4-C5-O5

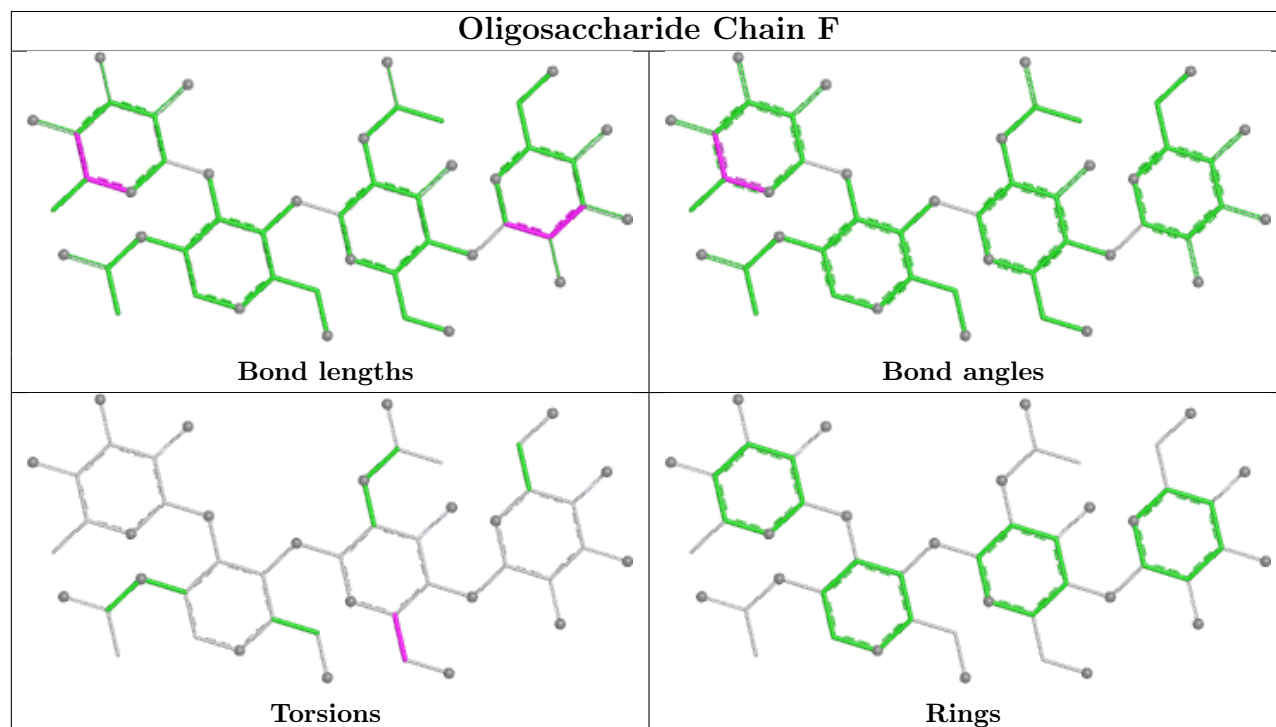
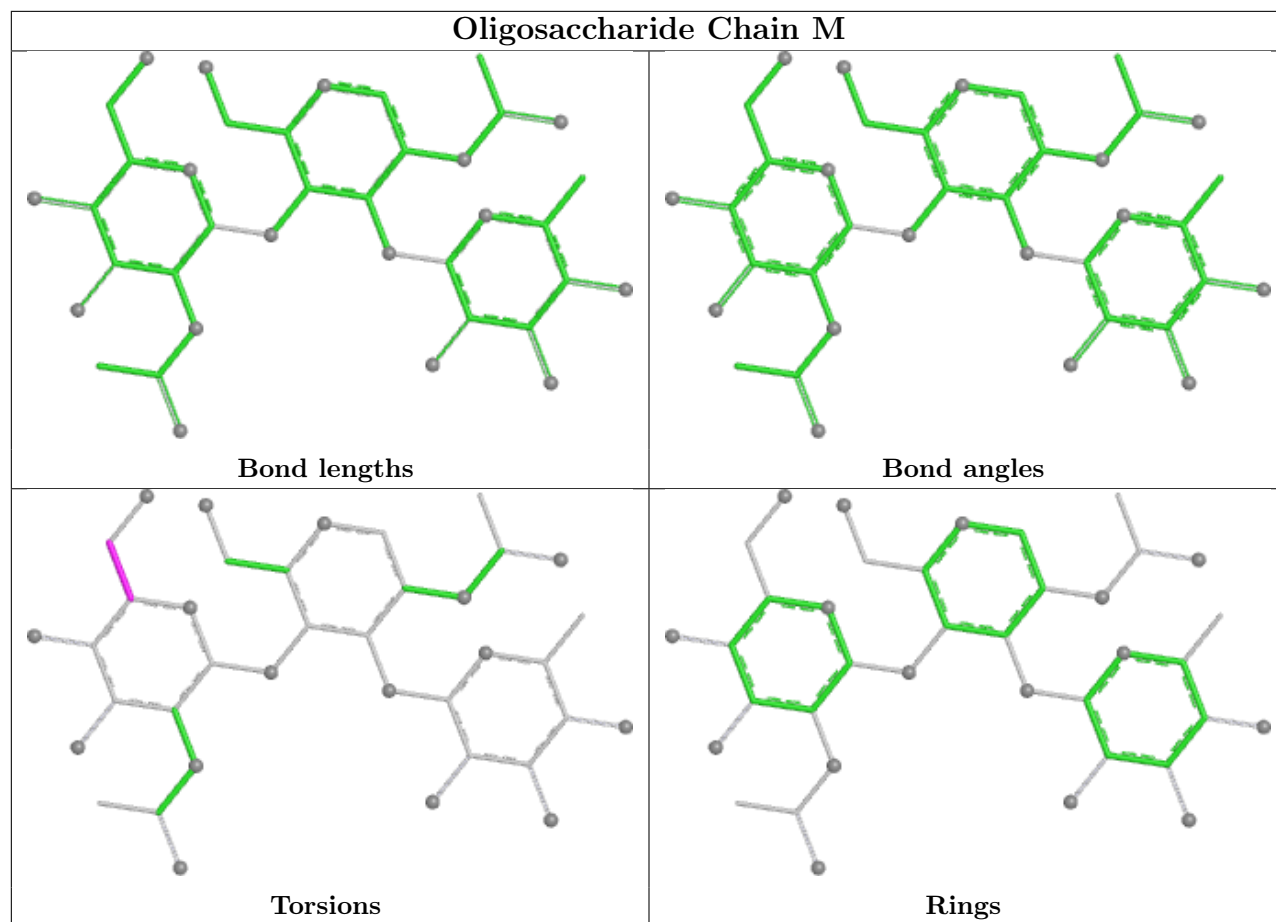
3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	4	FUC	1	0
3	H	1	NAG	1	0
3	N	2	NAG	1	0

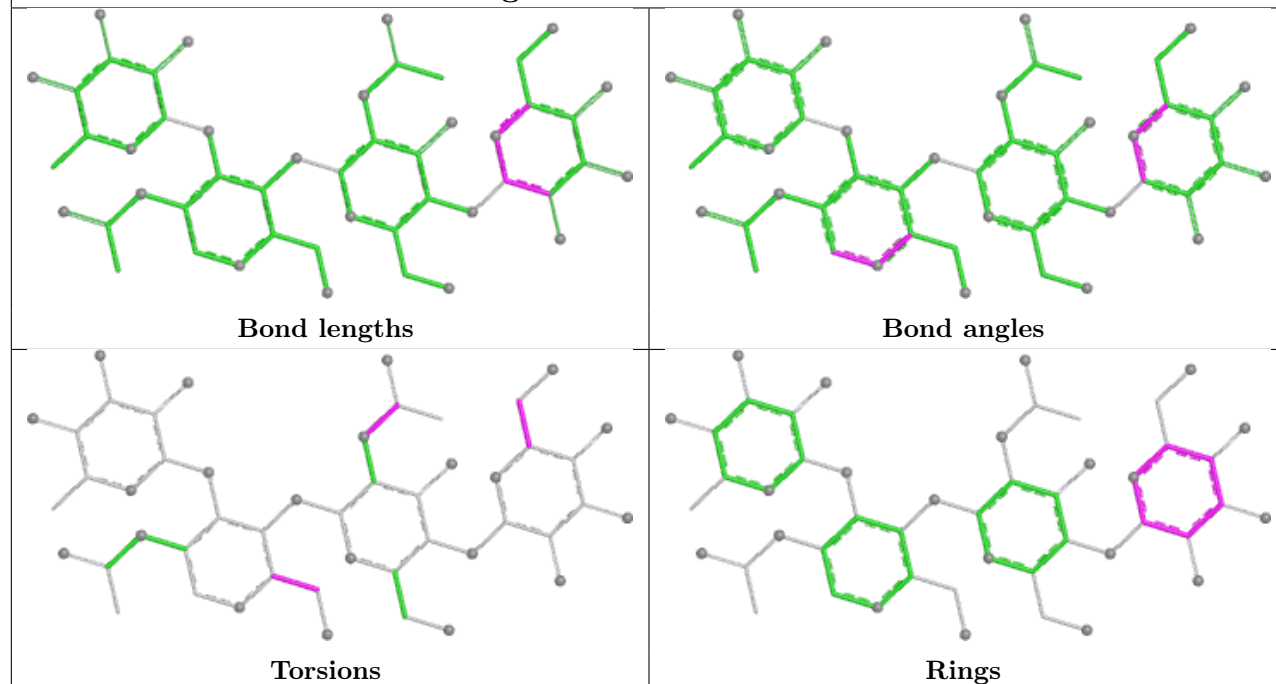
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



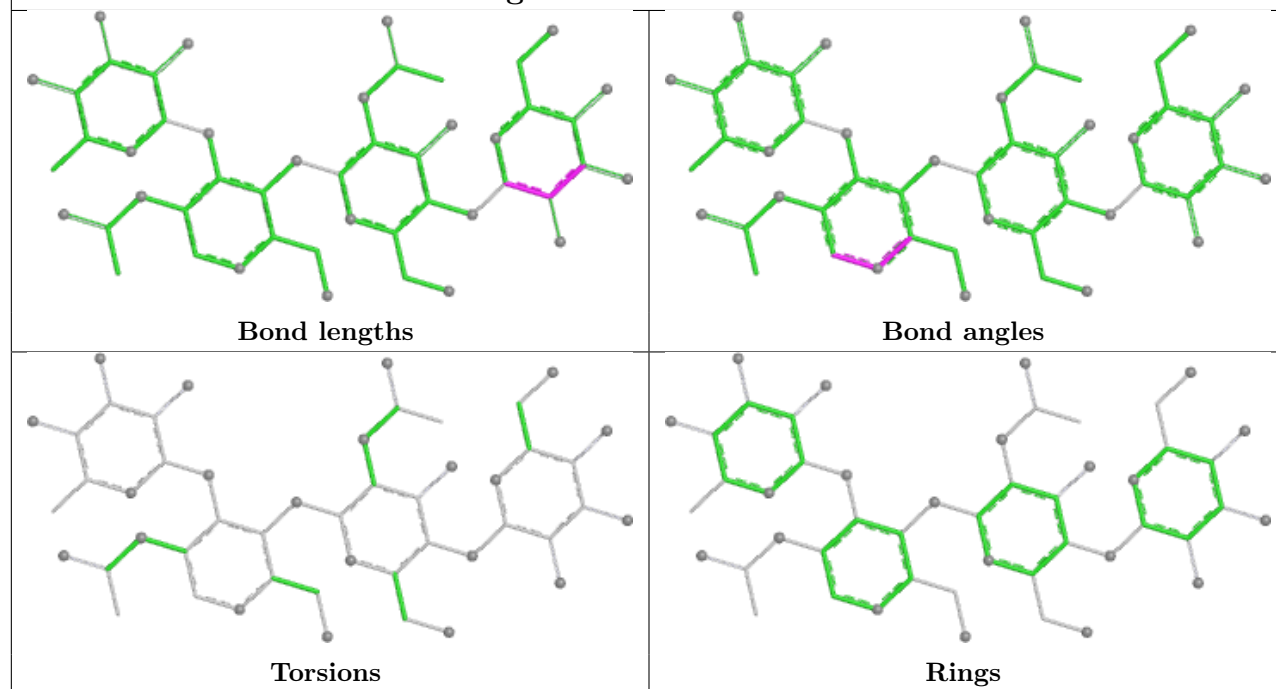




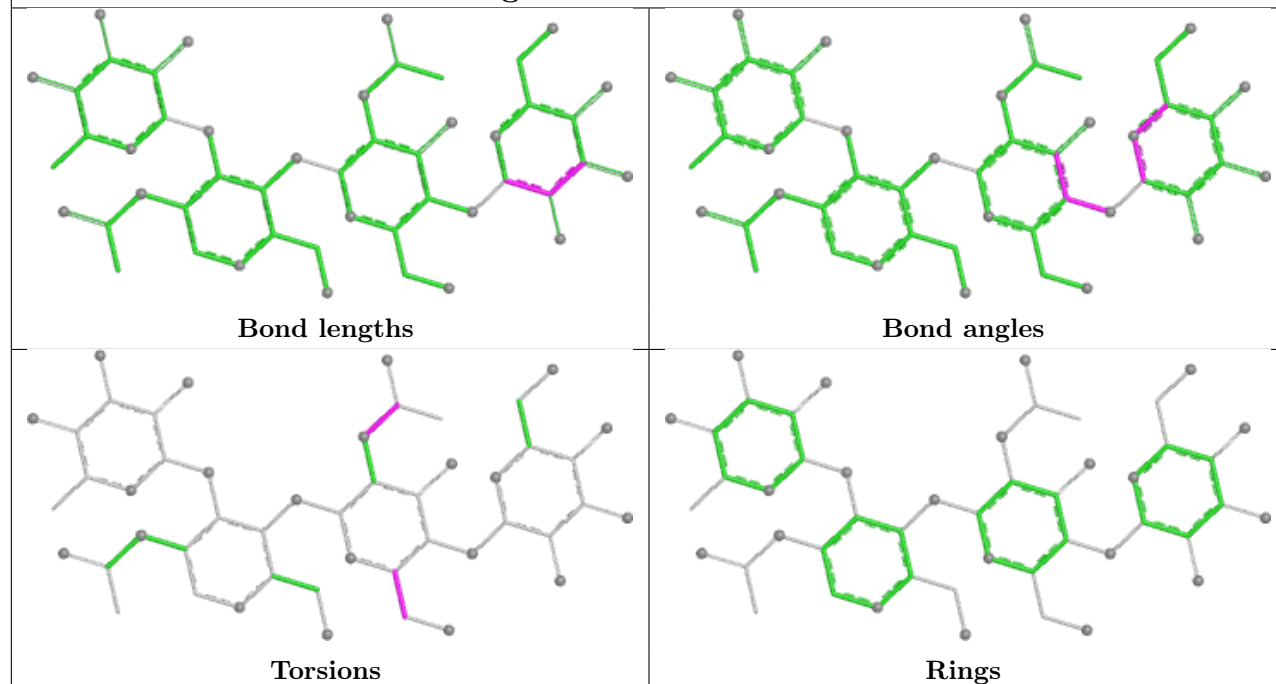
Oligosaccharide Chain H



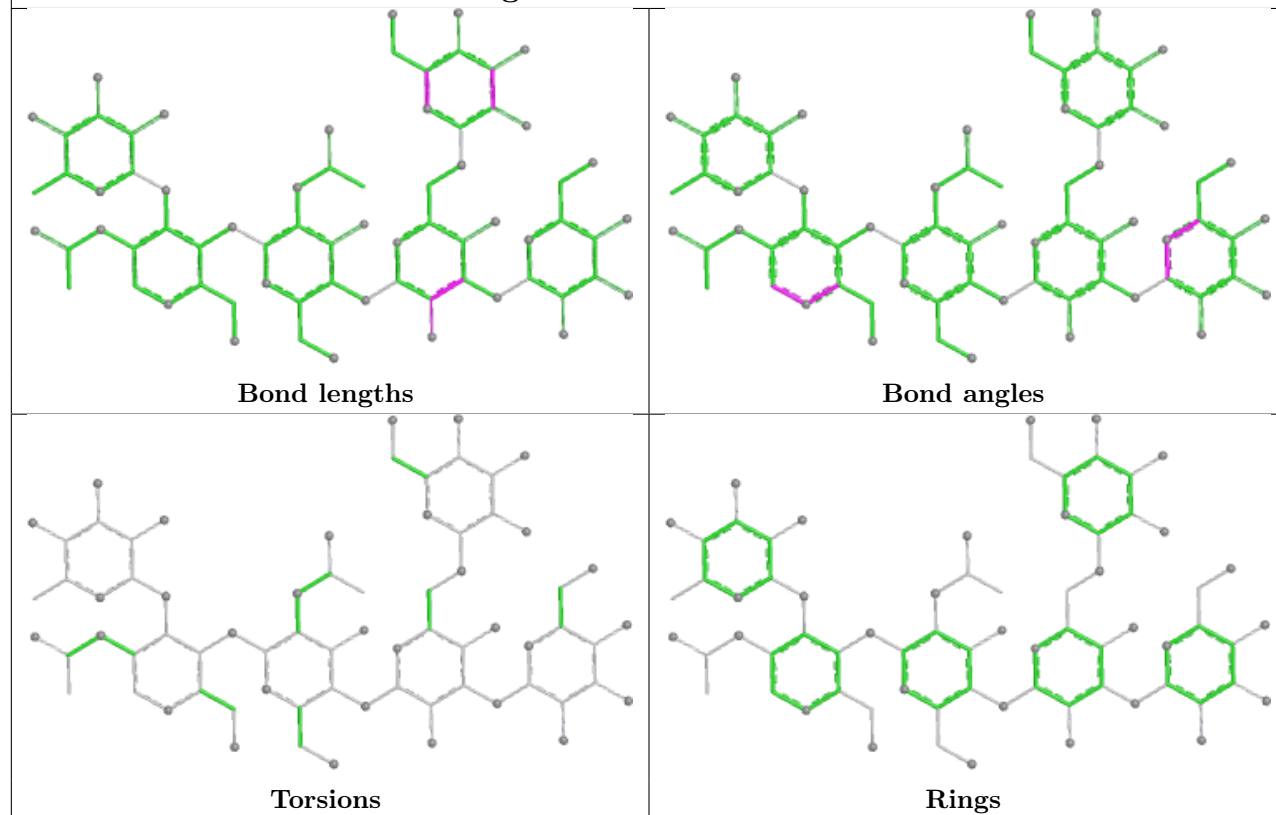
Oligosaccharide Chain J

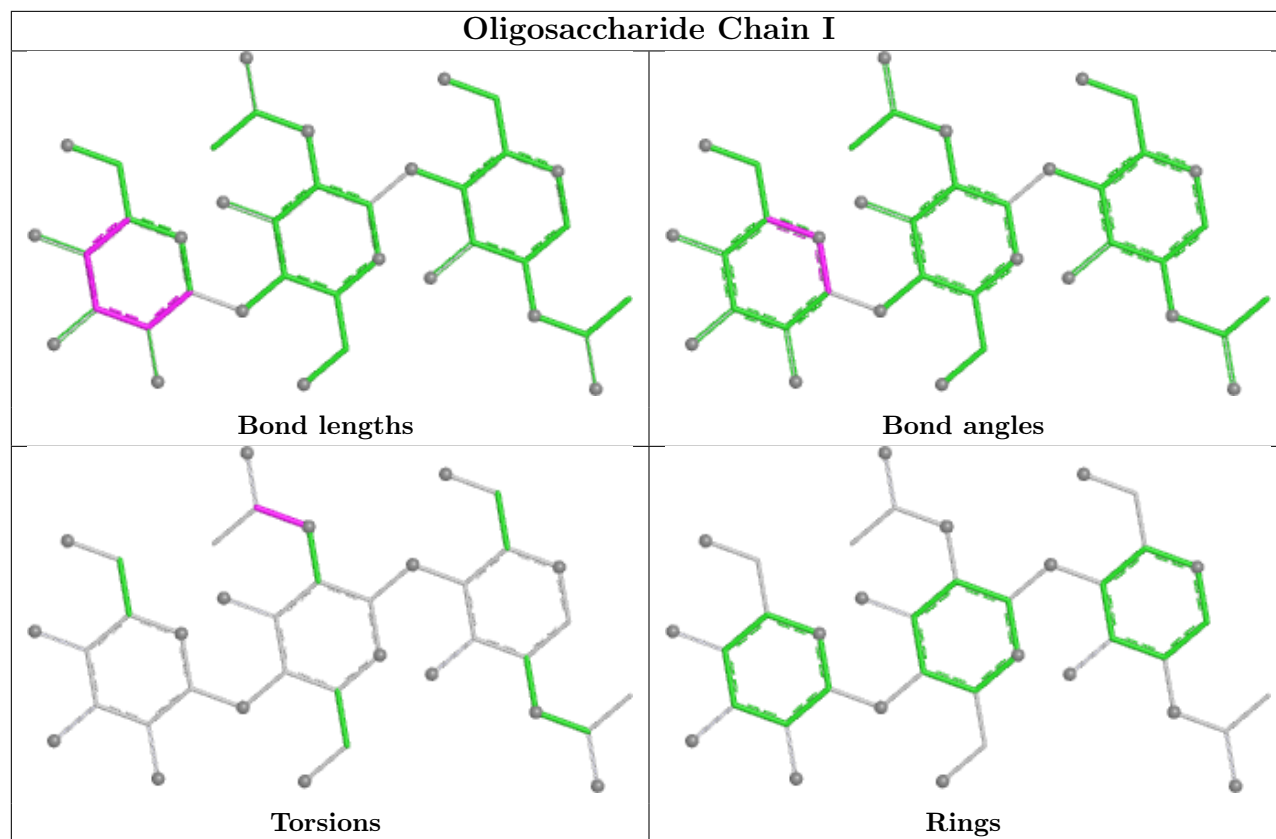


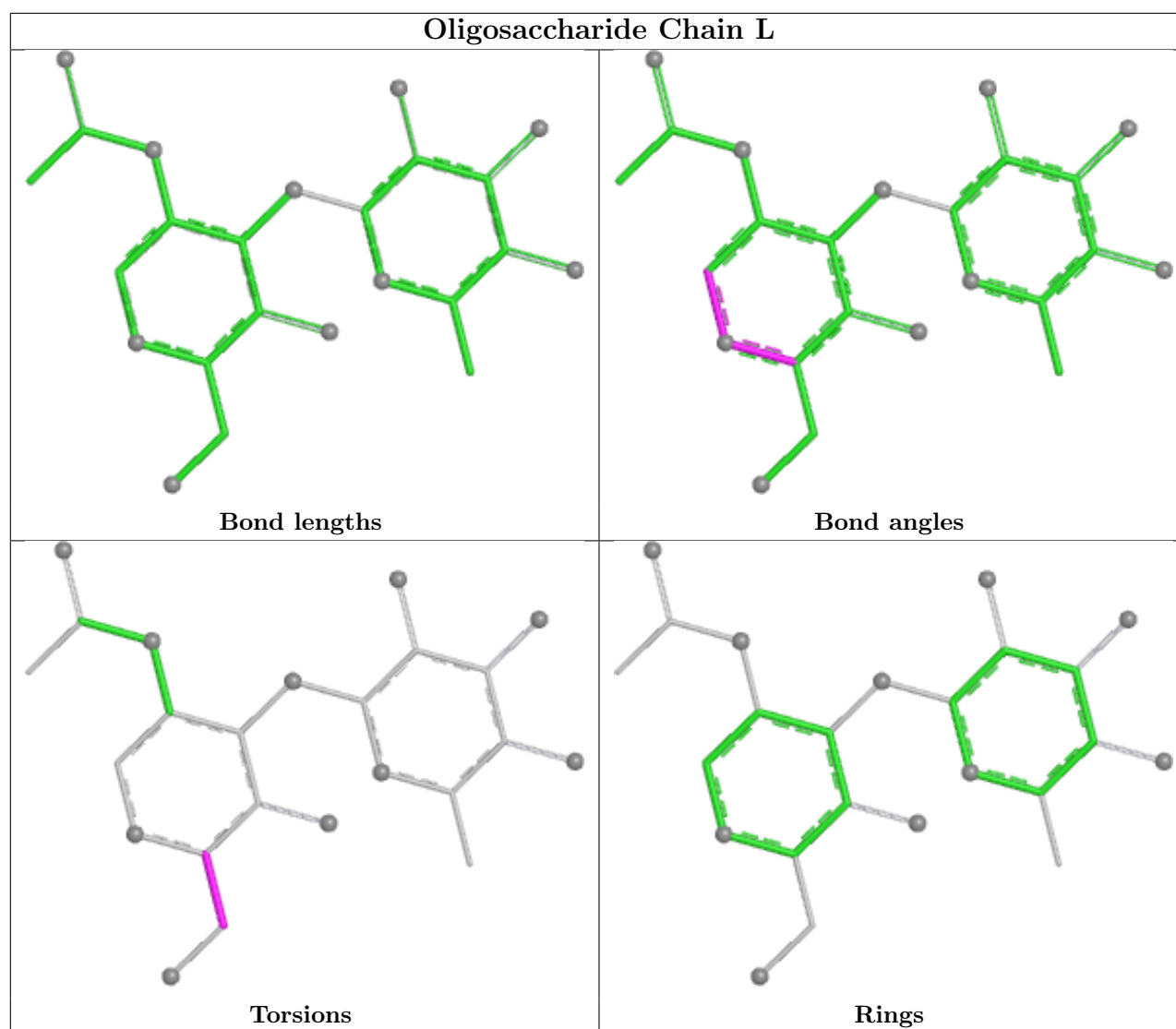
Oligosaccharide Chain N



Oligosaccharide Chain G







5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 14 are monoatomic - leaving 39 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	EDO	C	517	-	3,3,3	0.47	0	2,2,2	0.61	0
13	EDO	B	523	-	3,3,3	0.53	0	2,2,2	0.33	0
12	SO4	B	515	-	4,4,4	0.19	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	SO4	A	520	-	4,4,4	0.25	0	6,6,6	0.05	0
12	SO4	D	513	-	4,4,4	0.26	0	6,6,6	0.26	0
14	PGE	D	515	-	6,6,9	0.37	0	5,5,8	0.39	0
12	SO4	B	520	-	4,4,4	0.28	0	6,6,6	0.26	0
14	PGE	A	527	-	6,6,9	0.41	0	5,5,8	0.20	0
12	SO4	C	515	-	4,4,4	0.30	0	6,6,6	0.13	0
12	SO4	A	524	-	4,4,4	0.27	0	6,6,6	0.19	0
12	SO4	B	521	-	4,4,4	0.22	0	6,6,6	0.21	0
12	SO4	C	514	-	4,4,4	0.27	0	6,6,6	0.21	0
10	MF1	A	517[B]	-	33,35,35	2.16	3 (9%)	37,43,43	1.42	7 (18%)
9	NAG	B	503	1	14,14,15	0.43	0	17,19,21	0.59	0
12	SO4	B	516	11	4,4,4	0.27	0	6,6,6	0.17	0
9	NAG	A	503	1	14,14,15	0.34	0	17,19,21	0.62	0
12	SO4	A	522	11	4,4,4	0.26	0	6,6,6	0.26	0
13	EDO	C	518	-	3,3,3	0.49	0	2,2,2	0.27	0
9	NAG	D	510	1	14,14,15	0.79	1 (7%)	17,19,21	0.86	1 (5%)
9	NAG	C	521	1	14,14,15	0.53	0	17,19,21	0.65	1 (5%)
12	SO4	B	519	-	4,4,4	0.22	0	6,6,6	0.24	0
12	SO4	B	522	-	4,4,4	0.29	0	6,6,6	0.20	0
14	PGE	D	516	-	3,3,9	0.31	0	2,2,8	0.47	0
12	SO4	A	523	-	4,4,4	0.26	0	6,6,6	0.14	0
12	SO4	C	516	-	4,4,4	0.30	0	6,6,6	0.18	0
10	MF1	A	517[C]	-	33,35,35	1.72	3 (9%)	37,43,43	1.52	7 (18%)
15	GOL	D	514	-	5,5,5	1.31	1 (20%)	5,5,5	1.11	0
12	SO4	D	512	11	4,4,4	0.31	0	6,6,6	0.21	0
13	EDO	A	526	-	3,3,3	0.56	0	2,2,2	0.15	0
12	SO4	A	525	-	4,4,4	0.43	0	6,6,6	0.05	0
13	EDO	C	520	-	3,3,3	0.37	0	2,2,2	0.58	0
12	SO4	B	518	-	4,4,4	0.27	0	6,6,6	0.40	0
9	NAG	C	503	1	14,14,15	0.66	0	17,19,21	0.63	0
9	NAG	C	507	1	14,14,15	0.43	0	17,19,21	0.57	0
13	EDO	C	519	-	3,3,3	0.40	0	2,2,2	0.52	0
9	NAG	D	503	1	14,14,15	0.46	0	17,19,21	0.48	0
13	EDO	D	504	-	3,3,3	0.50	0	2,2,2	0.44	0
12	SO4	A	521	-	4,4,4	0.30	0	6,6,6	0.25	0
12	SO4	B	517	-	4,4,4	0.23	0	6,6,6	0.08	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
13	EDO	C	517	-	-	1/1/1/1	-
13	EDO	B	523	-	-	0/1/1/1	-
14	PGE	D	515	-	-	1/4/4/7	-
14	PGE	A	527	-	-	2/4/4/7	-
10	MF1	A	517[B]	-	-	8/26/29/29	0/2/2/2
9	NAG	B	503	1	-	2/6/23/26	0/1/1/1
9	NAG	A	503	1	-	2/6/23/26	0/1/1/1
13	EDO	C	518	-	-	0/1/1/1	-
9	NAG	D	510	1	-	1/6/23/26	0/1/1/1
9	NAG	C	521	1	-	4/6/23/26	0/1/1/1
14	PGE	D	516	-	-	0/1/1/7	-
10	MF1	A	517[C]	-	-	3/26/29/29	0/2/2/2
15	GOL	D	514	-	-	0/4/4/4	-
13	EDO	A	526	-	-	1/1/1/1	-
13	EDO	C	520	-	-	1/1/1/1	-
9	NAG	C	503	1	-	3/6/23/26	0/1/1/1
13	EDO	C	519	-	-	1/1/1/1	-
9	NAG	C	507	1	-	0/6/23/26	0/1/1/1
9	NAG	D	503	1	-	2/6/23/26	0/1/1/1
13	EDO	D	504	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	517[B]	MF1	CAU-CAT	-10.39	1.41	1.51
10	A	517[C]	MF1	CAU-CAT	-7.15	1.44	1.51
10	A	517[C]	MF1	PBE-OBF	-4.00	1.48	1.54
10	A	517[B]	MF1	PBE-OBF	-3.99	1.48	1.54
10	A	517[C]	MF1	PBE-OBG	3.91	1.61	1.54
10	A	517[B]	MF1	PBE-OBG	3.54	1.60	1.54
9	D	510	NAG	O5-C1	2.57	1.48	1.43
15	D	514	GOL	O2-C2	-2.27	1.36	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	517[C]	MF1	CAF-CAE-CAD	-3.22	98.08	114.37
10	A	517[B]	MF1	CAV-CAU-CAT	-3.15	115.03	119.81
10	A	517[C]	MF1	OBH-PBE-CAT	-3.09	107.61	113.40
10	A	517[B]	MF1	CAN-CAM-CAL	-2.89	99.75	114.37
10	A	517[C]	MF1	CAV-CAU-CAT	-2.85	115.49	119.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	510	NAG	C1-O5-C5	2.83	115.98	112.19
10	A	517[C]	MF1	CAE-CAD-CAC	-2.74	100.54	114.37
10	A	517[B]	MF1	OBf-PBE-OBH	2.69	120.18	113.45
10	A	517[C]	MF1	OBG-PBE-OBH	-2.46	107.28	113.45
10	A	517[B]	MF1	CAL-CAK-CAJ	-2.36	102.44	114.37
10	A	517[B]	MF1	CAP-CAO-CAN	-2.22	103.13	114.37
10	A	517[B]	MF1	CAJ-CAI-CAH	-2.16	103.44	114.37
10	A	517[C]	MF1	OBf-PBE-OBH	2.07	118.64	113.45
10	A	517[B]	MF1	OBG-PBE-OBH	-2.05	108.32	113.45
9	C	521	NAG	C1-O5-C5	2.02	114.90	112.19
10	A	517[C]	MF1	CAQ-CAP-CAO	-2.02	104.17	114.37

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	517[B]	MF1	CAU-CAT-PBE-OBf
10	A	517[B]	MF1	CAU-CAT-PBE-OBG
10	A	517[B]	MF1	CAU-CAT-PBE-OBH
10	A	517[B]	MF1	OAS-CAT-PBE-OBH
10	A	517[C]	MF1	OAS-CAT-CAU-CBD
9	C	503	NAG	C4-C5-C6-O6
9	C	503	NAG	O5-C5-C6-O6
9	B	503	NAG	C8-C7-N2-C2
9	B	503	NAG	O7-C7-N2-C2
9	C	521	NAG	C8-C7-N2-C2
9	C	521	NAG	O7-C7-N2-C2
9	D	510	NAG	O5-C5-C6-O6
9	D	503	NAG	C4-C5-C6-O6
9	D	503	NAG	O5-C5-C6-O6
9	C	521	NAG	C4-C5-C6-O6
9	C	521	NAG	O5-C5-C6-O6
10	A	517[C]	MF1	OAS-CAT-PBE-OBH
13	C	520	EDO	O1-C1-C2-O2
14	A	527	PGE	C6-C5-O3-C4
9	C	503	NAG	C1-C2-N2-C7
9	A	503	NAG	C4-C5-C6-O6
9	A	503	NAG	O5-C5-C6-O6
10	A	517[B]	MF1	CAD-CAE-CAF-CAG
13	A	526	EDO	O1-C1-C2-O2
13	C	519	EDO	O1-C1-C2-O2
14	D	515	PGE	O2-C3-C4-O3

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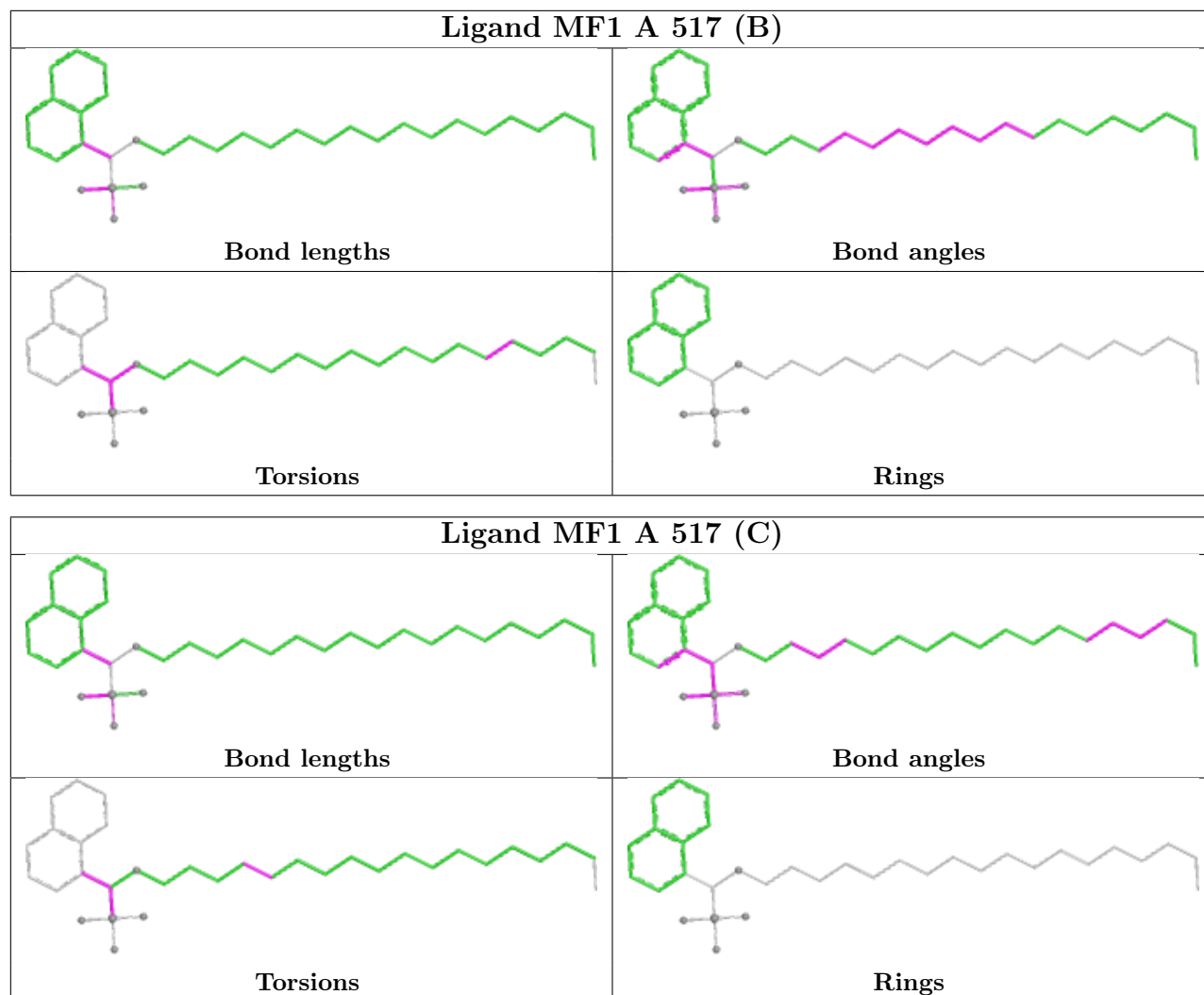
Mol	Chain	Res	Type	Atoms
10	A	517[B]	MF1	OAS-CAT-CAU-CBD
13	C	517	EDO	O1-C1-C2-O2
10	A	517[B]	MF1	CAU-CAT-OAS-CAR
10	A	517[B]	MF1	OAS-CAT-CAU-CAV
14	A	527	PGE	O2-C3-C4-O3
10	A	517[C]	MF1	CAM-CAN-CAO-CAP

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	513	SO4	1	0
14	D	515	PGE	4	0
14	A	527	PGE	1	0
12	C	514	SO4	2	0
10	A	517[B]	MF1	3	0
9	B	503	NAG	1	0
12	B	516	SO4	3	0
12	A	522	SO4	1	0
10	A	517[C]	MF1	3	0
15	D	514	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	426/459 (92%)	-0.87	2 (0%) 87 85	18, 25, 38, 91	2 (0%)
1	B	425/459 (92%)	-0.79	1 (0%) 91 90	14, 27, 40, 73	2 (0%)
1	C	423/459 (92%)	-0.78	1 (0%) 91 90	20, 27, 42, 71	1 (0%)
1	D	424/459 (92%)	-0.82	0 100 100	18, 26, 42, 68	1 (0%)
All	All	1698/1836 (92%)	-0.82	4 (0%) 91 90	14, 26, 41, 91	6 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ASN	2.6
1	B	64	ASN	2.2
1	C	64	ASN	2.1
1	A	430	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	BMA	H	3	11/12	0.47	0.14	83,96,101,101	0
3	BMA	N	3	11/12	0.62	0.13	65,79,86,90	0
2	NAG	E	3	14/15	0.64	0.13	67,73,75,76	0

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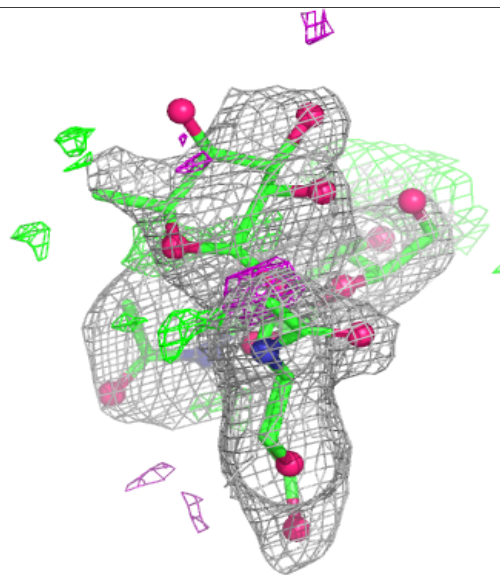
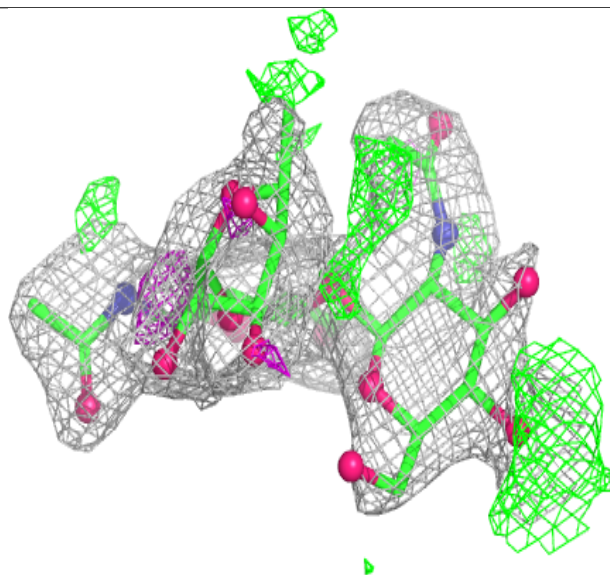
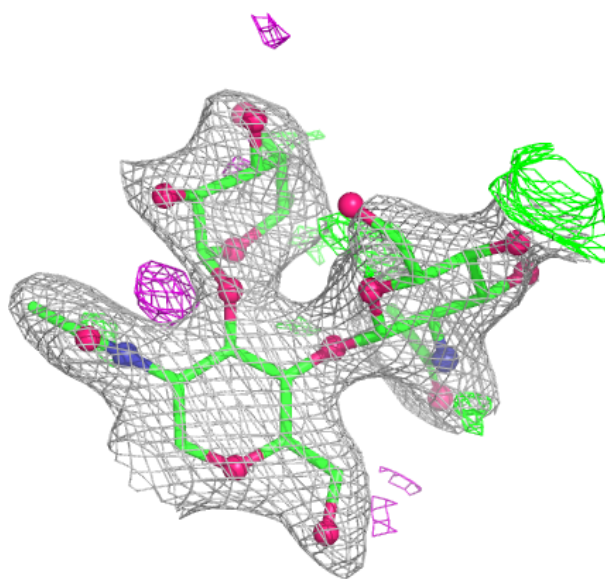
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FUC	E	2	10/11	0.68	0.15	65,71,79,87	0
3	BMA	F	3	11/12	0.68	0.14	61,68,71,77	0
3	FUC	H	4	10/11	0.69	0.15	67,72,75,79	0
3	BMA	J	3	11/12	0.71	0.12	47,51,56,59	0
5	BMA	I	3	11/12	0.71	0.13	48,61,65,70	0
3	NAG	H	2	14/15	0.74	0.12	73,80,92,99	0
3	NAG	N	2	14/15	0.76	0.13	62,74,79,80	0
5	NAG	I	2	14/15	0.77	0.14	55,60,63,67	0
5	NAG	I	1	14/15	0.77	0.12	38,47,54,57	0
2	NAG	K	3	14/15	0.82	0.11	39,56,64,67	0
2	FUC	M	2	10/11	0.82	0.12	45,49,56,56	0
6	FUC	L	2	10/11	0.82	0.13	46,63,64,65	0
2	FUC	K	2	10/11	0.83	0.11	53,55,60,62	0
4	MAN	G	5	11/12	0.83	0.10	55,63,69,71	0
6	NAG	L	1	14/15	0.84	0.11	42,51,57,58	0
3	FUC	F	4	10/11	0.84	0.11	52,60,65,65	0
2	NAG	M	3	14/15	0.86	0.10	35,52,60,62	0
3	NAG	F	2	14/15	0.87	0.09	40,55,61,64	0
3	NAG	H	1	14/15	0.88	0.09	43,55,71,74	0
4	BMA	G	3	11/12	0.88	0.09	37,47,53,54	0
3	FUC	N	4	10/11	0.89	0.10	52,60,61,64	0
2	NAG	E	1	14/15	0.89	0.09	40,50,69,73	0
3	NAG	N	1	14/15	0.90	0.08	39,53,59,63	0
4	FUC	G	6	10/11	0.93	0.07	34,40,44,45	0
3	NAG	F	1	14/15	0.93	0.08	40,43,49,55	0
4	NAG	G	2	14/15	0.94	0.06	30,36,43,46	0
3	NAG	J	2	14/15	0.95	0.06	28,36,41,46	0
2	NAG	K	1	14/15	0.95	0.07	35,40,46,55	0
3	FUC	J	4	10/11	0.95	0.06	31,35,38,42	0
2	NAG	M	1	14/15	0.95	0.07	30,38,42,44	0
4	MAN	G	4	11/12	0.96	0.07	44,49,51,52	0
4	NAG	G	1	14/15	0.96	0.07	28,32,36,37	0
3	NAG	J	1	14/15	0.97	0.05	25,29,31,34	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.

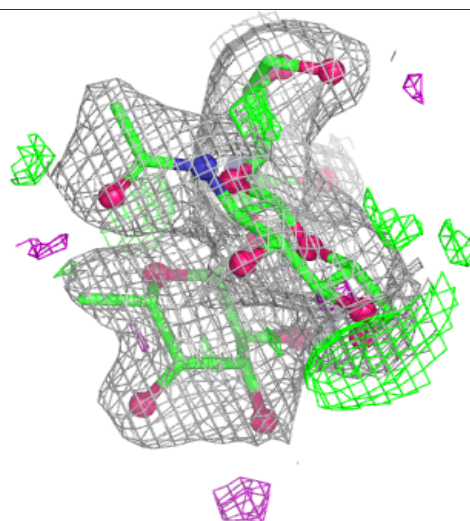
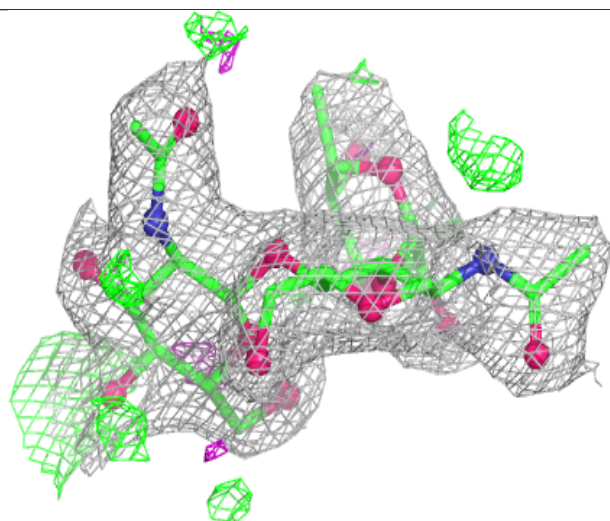
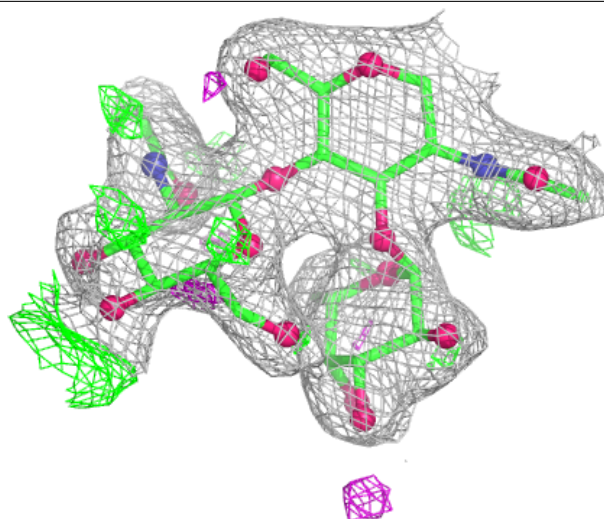
Electron density around Chain E:

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



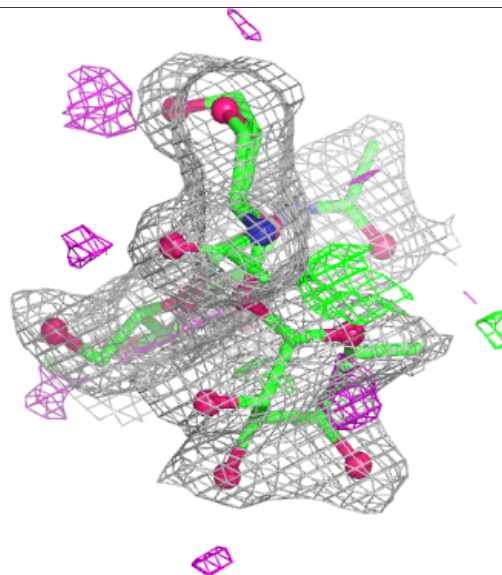
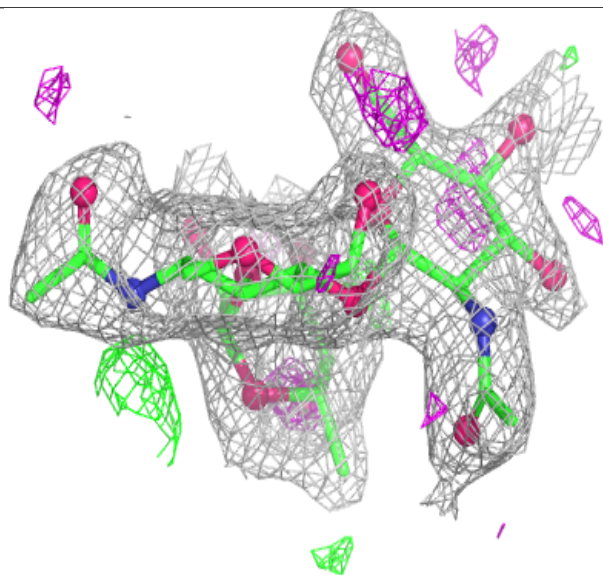
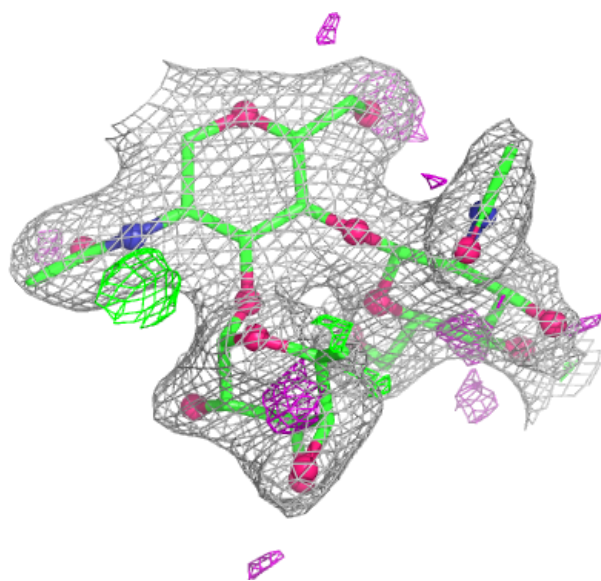
Electron density around Chain K:

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



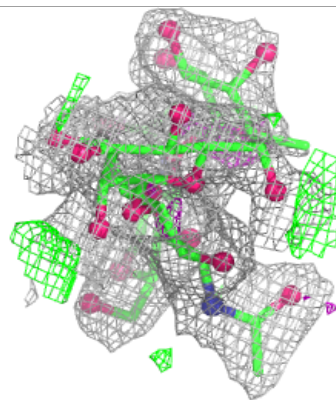
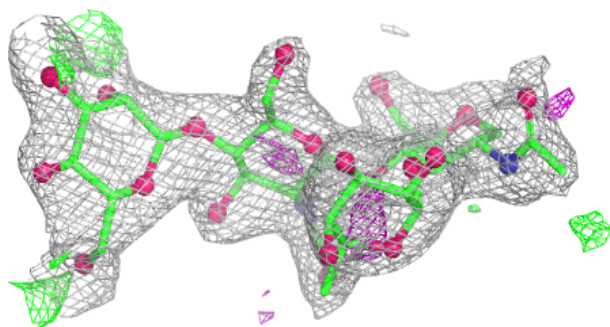
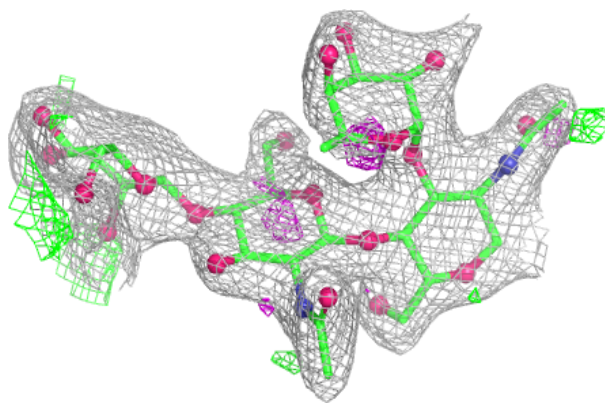
Electron density around Chain M:

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

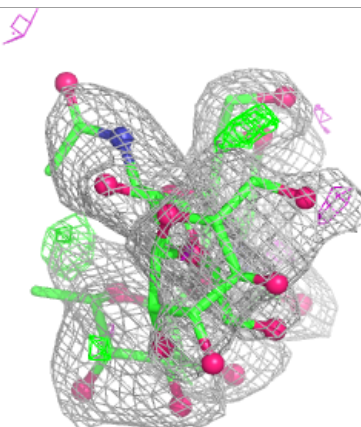
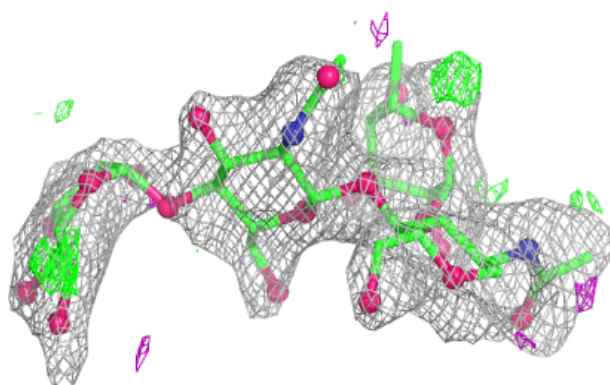
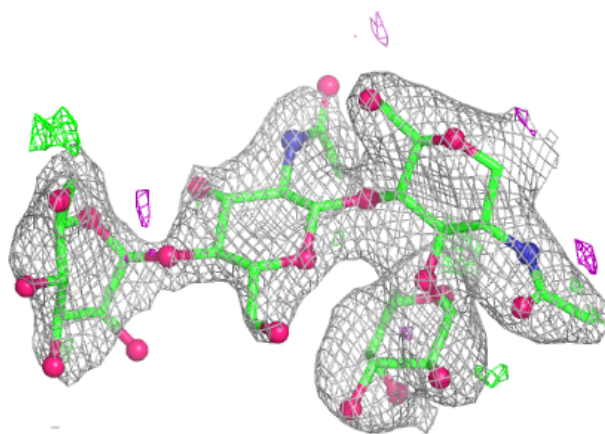


Electron density around Chain F:

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

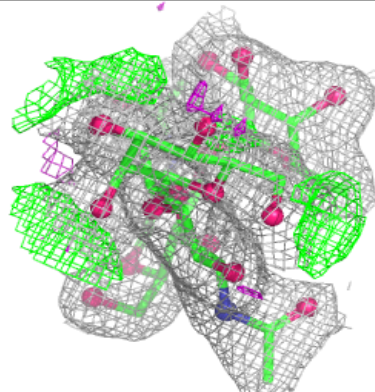
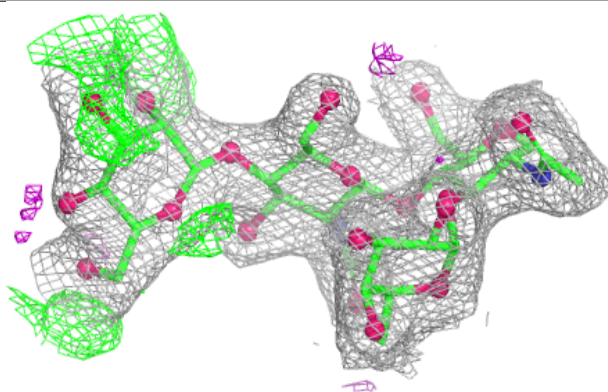
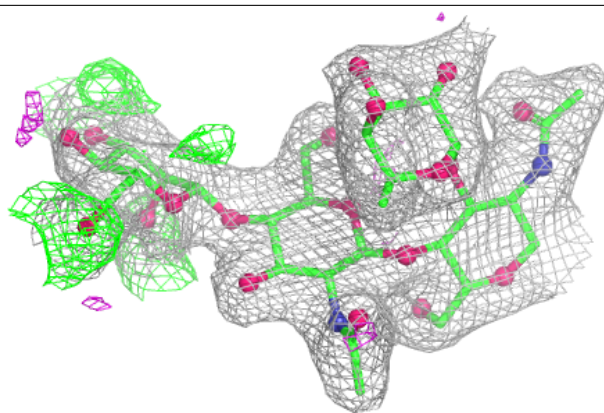
**Electron density around Chain H:**

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

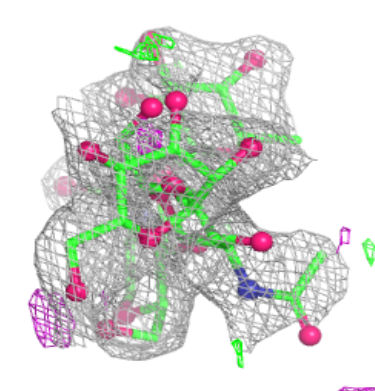
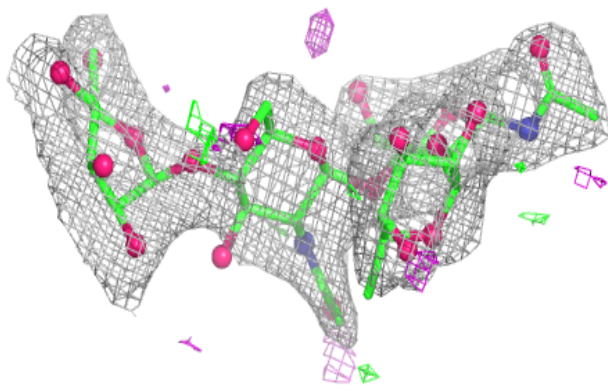
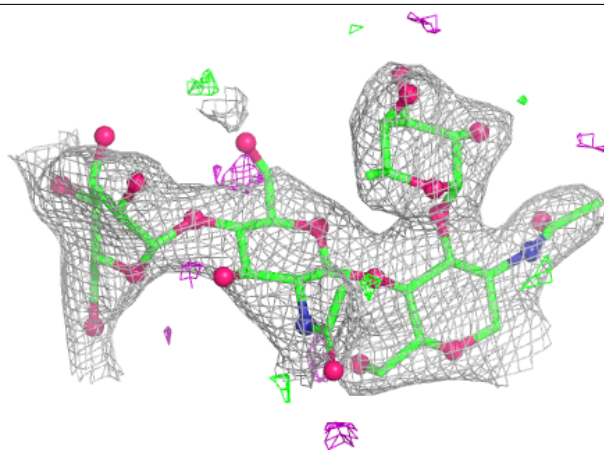


Electron density around Chain J:

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

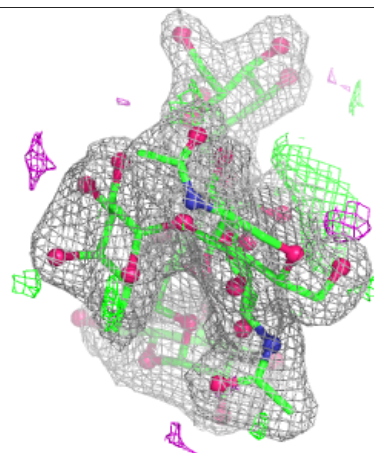
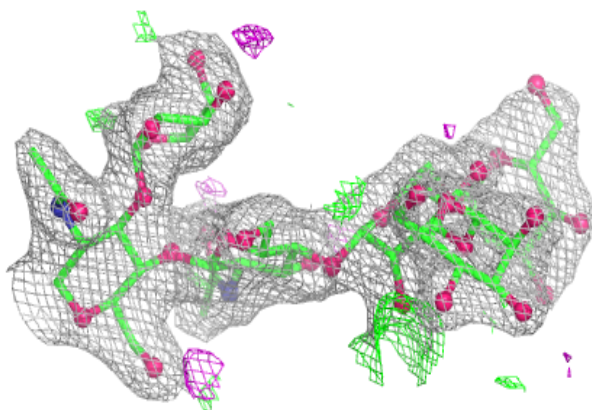
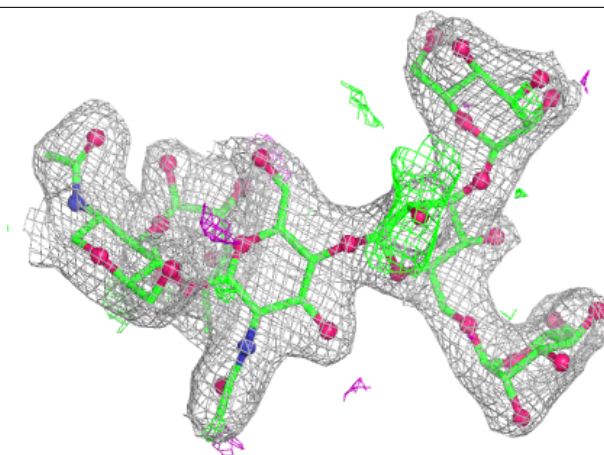
**Electron density around Chain N:**

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

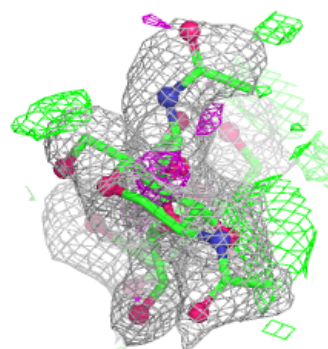
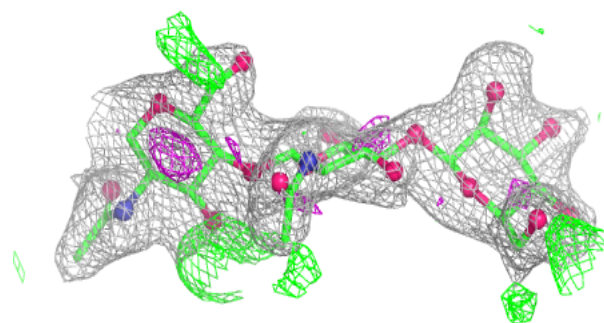
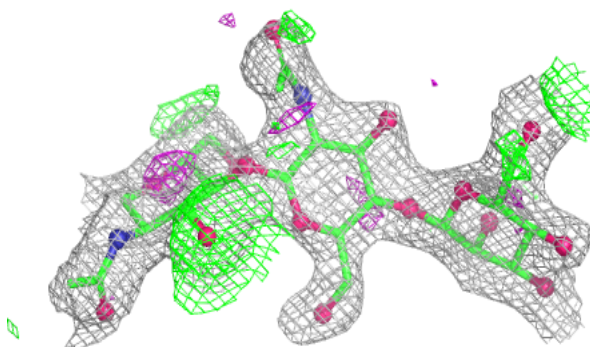


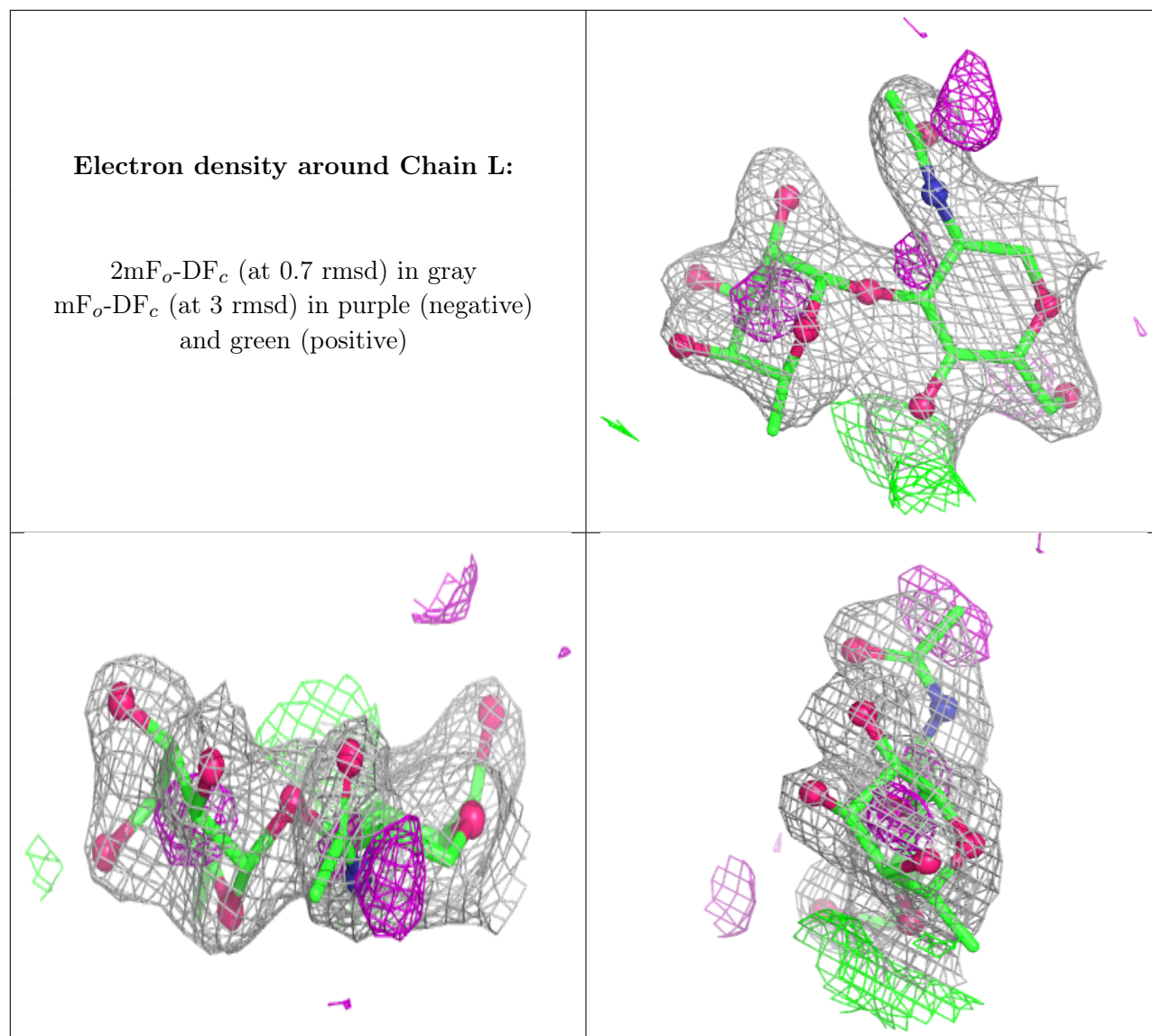
Electron density around Chain G:

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

**Electron density around Chain I:**

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	SO4	A	525	5/5	0.19	0.14	100,101,106,125	0
10	MF1	A	517[C]	34/34	0.59	0.25	38,52,72,72	34
10	MF1	A	517[B]	34/34	0.59	0.25	45,51,72,72	34
12	SO4	C	514	5/5	0.68	0.12	72,81,90,103	0
9	NAG	C	521	14/15	0.78	0.11	50,59,60,60	0
12	SO4	A	523	5/5	0.79	0.16	64,73,92,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	SO4	B	521	5/5	0.80	0.14	55,79,84,85	0
12	SO4	B	518	5/5	0.83	0.10	33,40,57,57	5
12	SO4	C	516	5/5	0.83	0.21	60,75,94,105	0
14	PGE	D	516	4/10	0.83	0.13	43,51,55,68	0
12	SO4	B	522	5/5	0.84	0.15	57,69,94,98	0
9	NAG	C	503	14/15	0.86	0.10	40,49,58,65	0
13	EDO	D	504	4/4	0.86	0.16	41,42,55,57	0
12	SO4	C	515	5/5	0.86	0.14	70,75,94,96	0
12	SO4	D	513	5/5	0.87	0.14	44,58,73,79	0
13	EDO	C	517	4/4	0.87	0.11	40,47,48,58	0
9	NAG	D	510	14/15	0.87	0.10	46,51,57,61	0
14	PGE	A	527	7/10	0.89	0.15	31,45,49,51	0
13	EDO	C	518	4/4	0.90	0.09	36,39,42,45	0
12	SO4	A	524	5/5	0.90	0.27	39,51,56,60	0
12	SO4	B	520	5/5	0.90	0.26	58,59,65,66	0
15	GOL	D	514	6/6	0.90	0.11	33,40,43,51	0
9	NAG	B	503	14/15	0.91	0.09	30,38,50,51	0
14	PGE	D	515	7/10	0.91	0.12	25,37,49,56	0
9	NAG	A	503	14/15	0.92	0.07	28,36,41,49	0
13	EDO	C	519	4/4	0.92	0.09	35,37,40,49	0
13	EDO	A	526	4/4	0.92	0.09	37,44,47,49	0
13	EDO	B	523	4/4	0.92	0.17	38,41,43,43	0
11	NA	D	511	1/1	0.92	0.12	55,55,55,55	0
9	NAG	D	503	14/15	0.92	0.08	29,32,42,45	0
12	SO4	A	521	5/5	0.93	0.08	32,32,46,46	5
9	NAG	C	507	14/15	0.93	0.07	33,36,44,50	0
12	SO4	B	515	5/5	0.93	0.09	36,48,50,56	5
12	SO4	A	520	5/5	0.94	0.10	33,39,45,46	5
13	EDO	C	520	4/4	0.96	0.09	27,35,45,48	0
12	SO4	D	512	5/5	0.97	0.07	27,33,37,39	5
11	NA	A	519	1/1	0.97	0.07	34,34,34,34	0
12	SO4	A	522	5/5	0.98	0.04	36,37,41,43	0
12	SO4	B	519	5/5	0.98	0.06	29,34,35,41	5
12	SO4	B	517	5/5	0.98	0.06	23,33,36,37	5
11	NA	A	518	1/1	0.99	0.04	16,16,16,16	0
12	SO4	B	516	5/5	0.99	0.12	8,27,29,30	5
11	NA	C	508	1/1	0.99	0.12	28,28,28,28	0
11	NA	C	509	1/1	0.99	0.05	15,15,15,15	0
8	FE	A	502	1/1	1.00	0.04	27,27,27,27	1
8	FE	B	502	1/1	1.00	0.03	28,28,28,28	1
8	FE	D	502	1/1	1.00	0.01	28,28,28,28	1
8	FE	C	502	1/1	1.00	0.02	25,25,25,25	1

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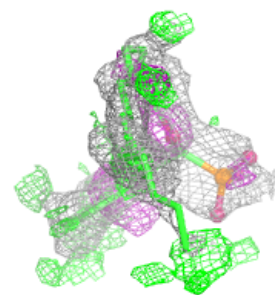
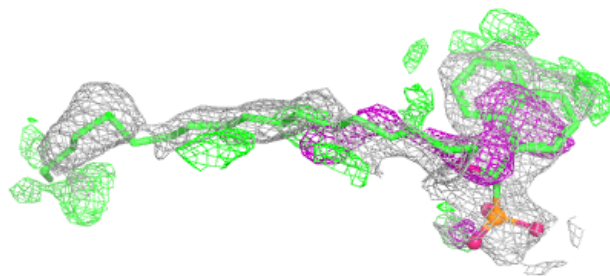
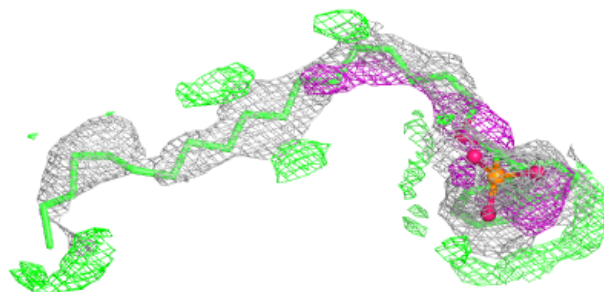
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	ZN	A	501	1/1	1.00	0.01	26,26,26,26	0
7	ZN	B	501	1/1	1.00	0.01	27,27,27,27	0
7	ZN	D	501	1/1	1.00	0.01	22,22,22,22	0
7	ZN	C	501	1/1	1.00	0.01	26,26,26,26	0
16	CL	D	517	1/1	1.00	0.01	26,26,26,26	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.

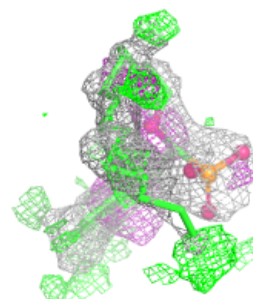
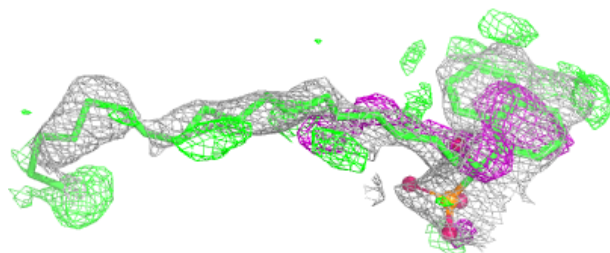
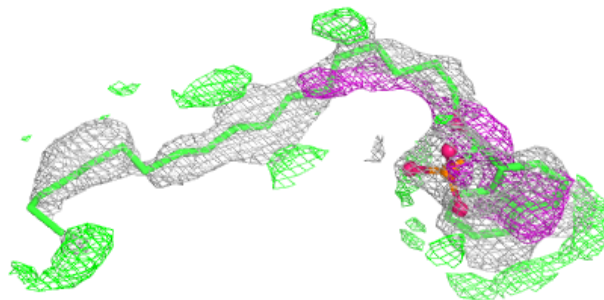
Electron density around MF1 A 517 (C):

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 MF1 A 517 (B):

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



6.5 Other polymers [i](#)

There are no such residues in this entry.