



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 02:24 AM BST

PDB ID : 6OFD  
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

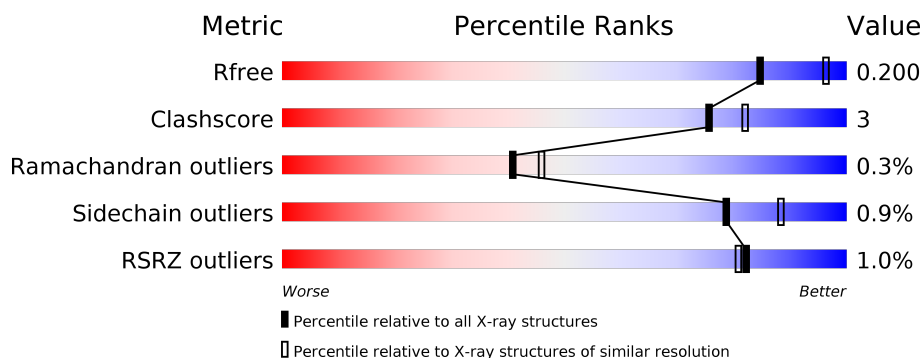
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>7%</div> </div> </div>
1	B	459	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>7%</div> </div> </div>
1	C	459	<div> <div></div> <div> <div>83%</div> <div>8%</div> <div>8%</div> </div> </div>
1	D	459	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>8%</div> </div> </div>
2	E	3	<div> <div></div> <div> <div>33%</div> <div>67%</div> </div> </div>
2	K	3	<div> <div></div> <div> <div>67%</div> <div>33%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	M	3	 100%
3	F	4	 50% 50%
3	H	4	 25% 50% 25%
3	J	4	 50% 50%
3	N	4	 25% 50% 25%
4	G	6	 33% 67%
5	I	3	 67% 33%
6	L	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
12	SO4	B	516	-	-	X	-
12	SO4	C	514	-	-	X	-
12	SO4	C	516	-	-	-	X

## 2 Entry composition [i](#)

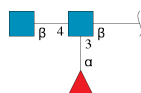
There are 17 unique types of molecules in this entry. The entry contains 16494 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

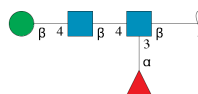
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	2	0
			3523	2261	614	638	10			
1	B	425	Total	C	N	O	S	0	2	0
			3515	2255	610	639	11			
1	D	424	Total	C	N	O	S	0	1	0
			3499	2248	607	634	10			
1	C	423	Total	C	N	O	S	0	1	0
			3487	2240	604	633	10			

- 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.



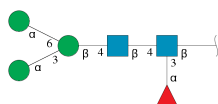
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	K	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	M	3	Total	C	N	O	0	0	0
			38	22	2	14			

- 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			

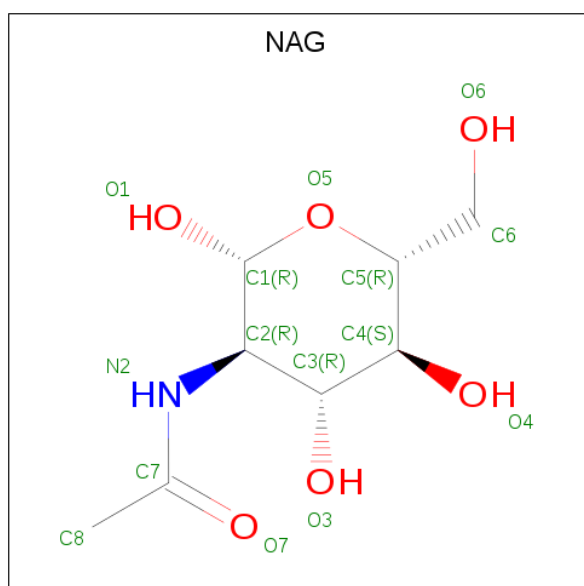
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Zn	0	0
			1	1		
7	A	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 (three-letter code: FE) (formula: Fe).

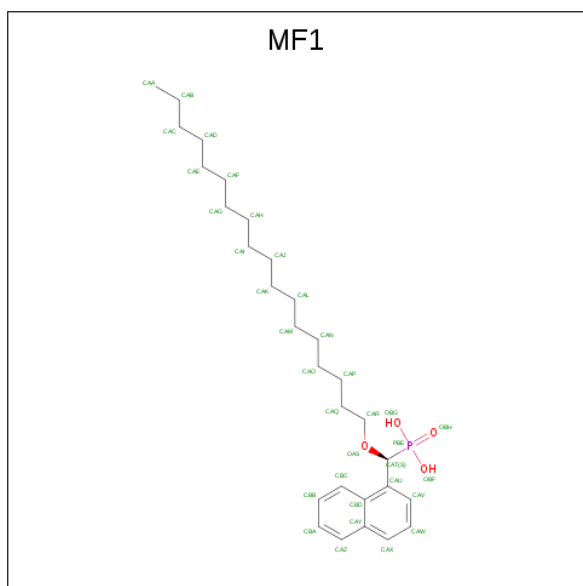
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Fe	0	0
			1	1		
8	A	1	Total	Fe	0	0
			1	1		
8	D	1	Total	Fe	0	0
			1	1		
8	C	1	Total	Fe	0	0
			1	1		

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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 (three-letter code: MF1) (formula: C<sub>29</sub>H<sub>47</sub>O<sub>4</sub>P).



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

- Molecule 11 is SODIUM ION (three-letter code: NA) (formula: Na).

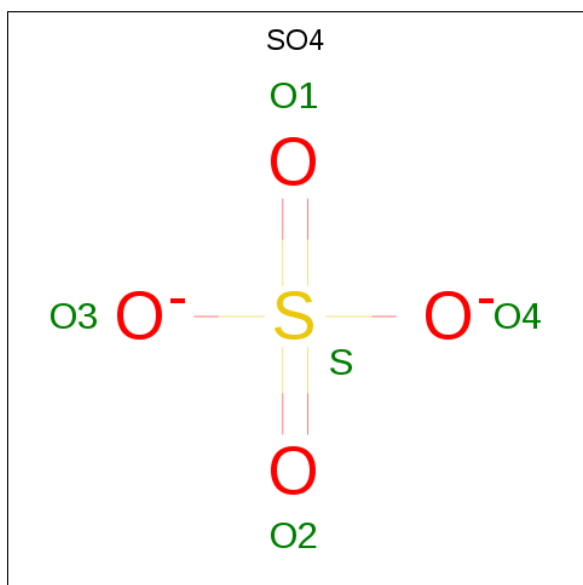
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Na	0	0
			2	2		

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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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

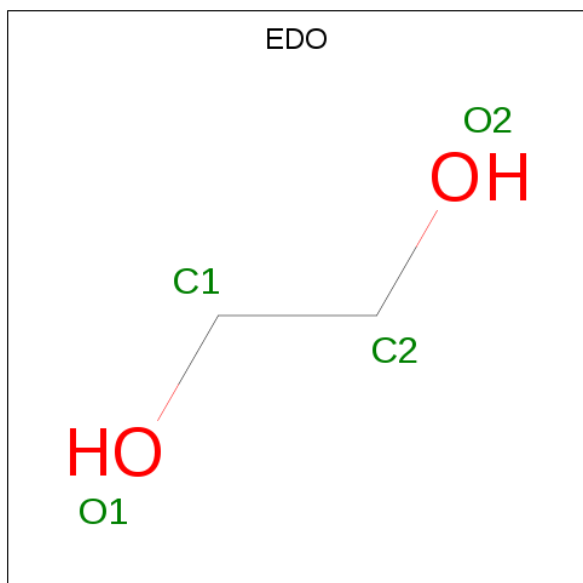
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	B	1	Total	O	S	0	0
			5	4	1		
12	D	1	Total	O	S	0	0
			5	4	1		
12	D	1	Total	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 (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



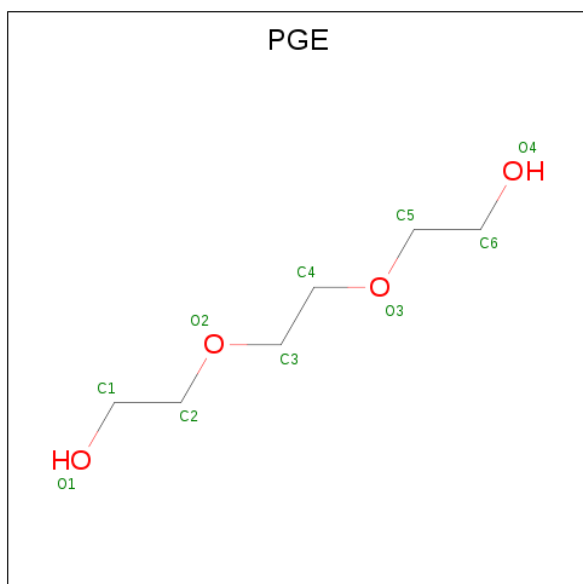
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	O	0	0
			4	2	2		

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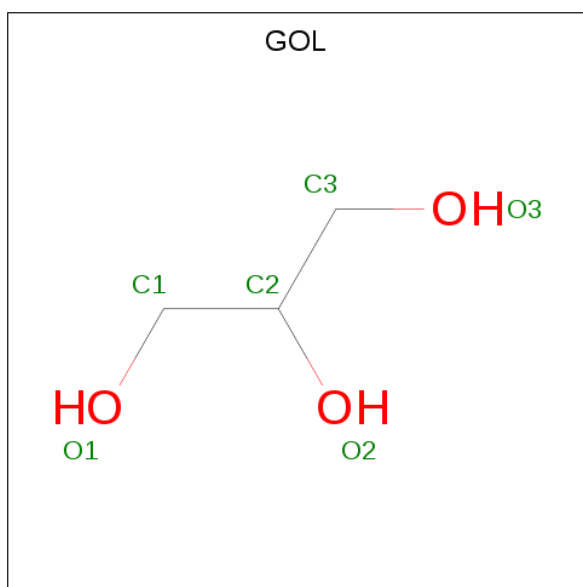
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	B	1	Total	C	O	0	0
			4	2	2		
13	D	1	Total	C	O	0	0
			4	2	2		
13	C	1	Total	C	O	0	0
			4	2	2		
13	C	1	Total	C	O	0	0
			4	2	2		
13	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 14 is TRIETHYLENE GLYCOL (three-letter code: 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 (three-letter code: 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 (three-letter code: CL) (formula: Cl).

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

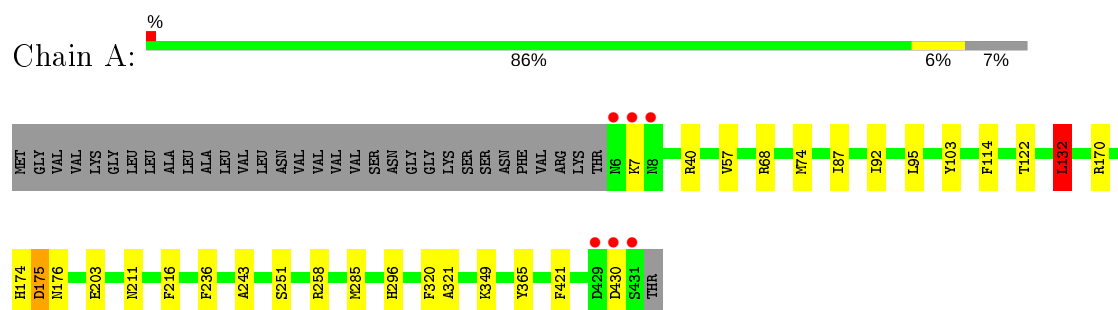
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	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		

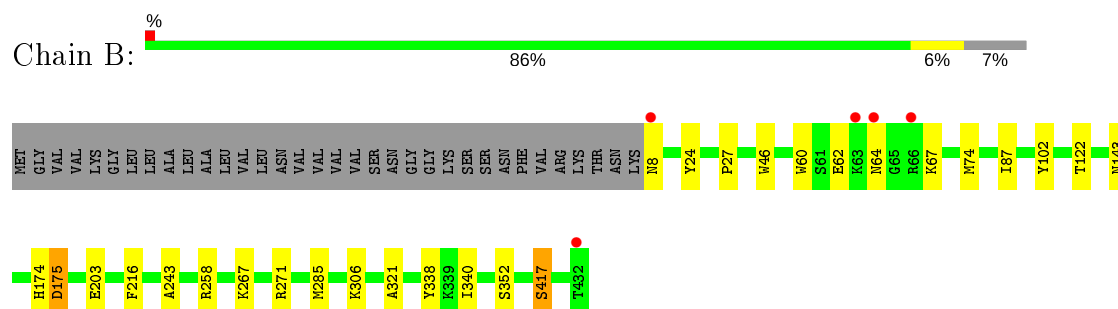
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

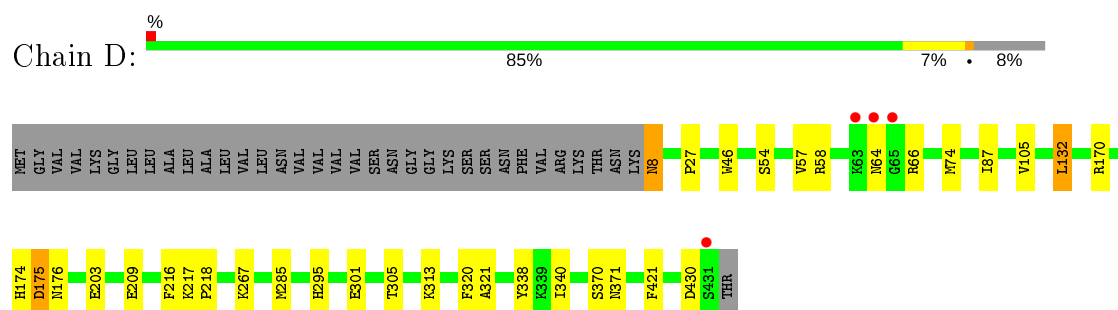
- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase



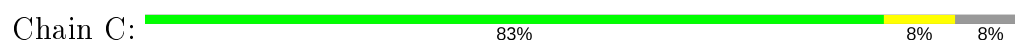
- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

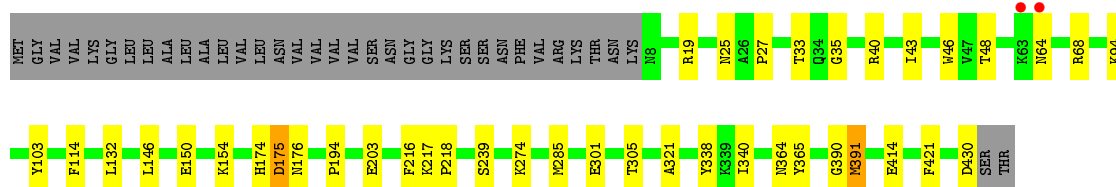


- Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase



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





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

Chain E: 33% 67%



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

Chain K: 67% 33%



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

Chain M: 100%



- 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 F: 50% 50%



- 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 H: 25% 50% 25%



- 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

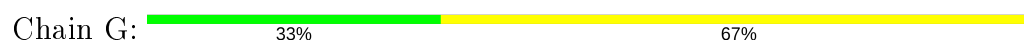
Chain J: 50% 50%



- 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 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



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.9 (20.05-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 2.19Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.155 , 0.199 0.155 , 0.200	Depositor DCC
$R_{free}$ test set	6987 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.5	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, ZN, BMA, NAG, CL, NA, EDO, FUC, MF1, PGE, SO4, MAN, FE

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	0.42	0/3649	0.56	1/4961 (0.0%)
1	B	0.42	0/3634	0.55	0/4941
1	C	0.43	0/3609	0.56	1/4909 (0.0%)
1	D	0.43	0/3621	0.57	1/4924 (0.0%)
All	All	0.43	0/14513	0.56	3/19735 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	LEU	CA-CB-CG	-7.82	97.30	115.30
1	D	132	LEU	CA-CB-CG	-6.79	99.68	115.30
1	A	132	LEU	CA-CB-CG	-6.53	100.28	115.30

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	21	0
1	B	3515	0	3327	17	0
1	C	3487	0	3297	23	0
1	D	3499	0	3319	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	38	0	34	0	0
2	K	38	0	34	0	0
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	3	0
17	B	435	0	0	5	0
17	C	402	0	0	1	0
17	D	403	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16494	0	13836	89	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.

The worst 5 of 89 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

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%)	47	55
1	B	425/459 (93%)	406 (96%)	17 (4%)	2 (0%)	29	31
1	C	422/459 (92%)	401 (95%)	20 (5%)	1 (0%)	47	55
1	D	423/459 (92%)	401 (95%)	21 (5%)	1 (0%)	47	55
All	All	1696/1836 (92%)	1616 (95%)	75 (4%)	5 (0%)	41	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	ASN

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

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	377/402 (94%)	374 (99%)	3 (1%)	81	90
1	B	376/402 (94%)	374 (100%)	2 (0%)	88	94
1	C	372/402 (92%)	368 (99%)	4 (1%)	73	85
1	D	374/402 (93%)	370 (99%)	4 (1%)	73	85
All	All	1499/1608 (93%)	1486 (99%)	13 (1%)	78	88

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	8	ASN
1	D	54	SER
1	C	239	SER
1	B	417	SER
1	C	176	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	64	ASN

### 5.3.3 RNA [i](#)

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	1,2	14,14,15	0.27	0	17,19,21	0.90	1 (5%)
2	FUC	E	2	2	10,10,11	1.01	1 (10%)	14,14,16	1.55	4 (28%)
2	NAG	E	3	2	14,14,15	0.34	0	17,19,21	0.39	0
3	NAG	F	1	1,3	14,14,15	0.36	0	17,19,21	0.50	0
3	NAG	F	2	3	14,14,15	0.50	0	17,19,21	0.66	0
3	BMA	F	3	3	11,11,12	1.68	2 (18%)	15,15,17	0.95	2 (13%)
3	FUC	F	4	3	10,10,11	1.30	2 (20%)	14,14,16	1.11	2 (14%)
4	NAG	G	1	1,4	14,14,15	0.47	0	17,19,21	0.76	1 (5%)
4	NAG	G	2	4	14,14,15	0.42	0	17,19,21	0.51	0
4	BMA	G	3	4	11,11,12	1.66	3 (27%)	15,15,17	1.13	0
4	MAN	G	4	4	11,11,12	1.01	0	15,15,17	1.27	1 (6%)
4	MAN	G	5	4	11,11,12	1.37	2 (18%)	15,15,17	1.00	0
4	FUC	G	6	4	10,10,11	0.87	0	14,14,16	1.03	0
3	NAG	H	1	1,3	14,14,15	0.50	0	17,19,21	0.80	1 (5%)
3	NAG	H	2	3	14,14,15	0.24	0	17,19,21	0.54	0
3	BMA	H	3	3	11,11,12	1.52	4 (36%)	15,15,17	1.40	1 (6%)
3	FUC	H	4	3	10,10,11	0.80	0	14,14,16	1.23	3 (21%)
5	NAG	I	1	1,5	14,14,15	0.60	0	17,19,21	0.63	0
5	NAG	I	2	5	14,14,15	0.28	0	17,19,21	0.44	0
5	BMA	I	3	5	11,11,12	1.69	4 (36%)	15,15,17	1.06	1 (6%)
3	NAG	J	1	1,3	14,14,15	0.39	0	17,19,21	0.69	1 (5%)
3	NAG	J	2	3	14,14,15	0.41	0	17,19,21	0.53	0
3	BMA	J	3	3	11,11,12	1.55	2 (18%)	15,15,17	1.07	1 (6%)
3	FUC	J	4	3	10,10,11	0.75	0	14,14,16	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	K	1	1,2	14,14,15	0.53	0	17,19,21	0.54	0
2	FUC	K	2	2	10,10,11	0.93	1 (10%)	14,14,16	0.94	0
2	NAG	K	3	2	14,14,15	0.45	0	17,19,21	0.46	0
6	NAG	L	1	1,6	14,14,15	0.36	0	17,19,21	0.67	0
6	FUC	L	2	6	10,10,11	1.19	0	14,14,16	0.79	0
2	NAG	M	1	1,2	14,14,15	0.48	0	17,19,21	0.52	0
2	FUC	M	2	2	10,10,11	1.15	0	14,14,16	0.86	0
2	NAG	M	3	2	14,14,15	0.54	0	17,19,21	0.59	0
3	NAG	N	1	1,3	14,14,15	0.37	0	17,19,21	0.62	0
3	NAG	N	2	3	14,14,15	0.36	0	17,19,21	0.78	1 (5%)
3	BMA	N	3	3	11,11,12	1.56	2 (18%)	15,15,17	1.44	1 (6%)
3	FUC	N	4	3	10,10,11	0.80	0	14,14,16	0.92	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	1,2	-	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	1,3	-	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
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	1,3	-	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	1,5	-	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	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1,2	-	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	-	0/6/23/26	0/1/1/1
6	FUC	L	2	6	-	-	0/1/1/1
2	NAG	M	1	1,2	-	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	1,3	-	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

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3	BMA	C2-C3	4.06	1.58	1.52
3	N	3	BMA	C1-C2	3.18	1.59	1.52
3	F	3	BMA	C1-C2	3.16	1.59	1.52
3	J	3	BMA	C1-C2	3.03	1.59	1.52
5	I	3	BMA	C1-C2	2.81	1.58	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3	BMA	C1-O5-C5	4.33	118.06	112.19
3	N	3	BMA	C1-O5-C5	4.24	117.94	112.19
4	G	4	MAN	C1-O5-C5	3.61	117.08	112.19
2	E	2	FUC	C1-O5-C5	3.11	119.82	112.78
2	E	1	NAG	C1-O5-C5	3.11	116.40	112.19

There are no chirality outliers.

5 of 24 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	H	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	N	2	NAG	O5-C5-C6-O6
2	K	3	NAG	C4-C5-C6-O6

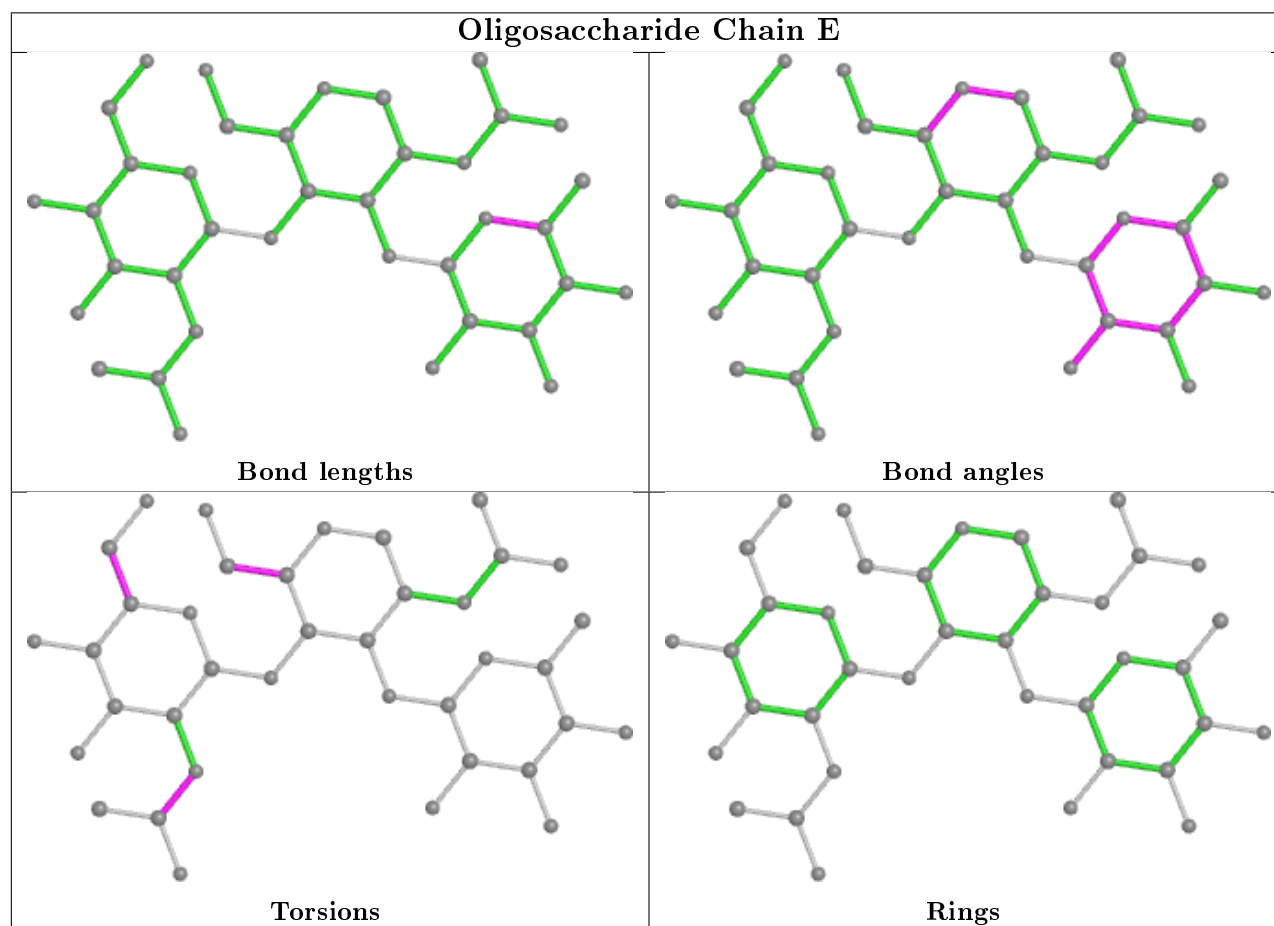
All (1) ring outliers are listed below:

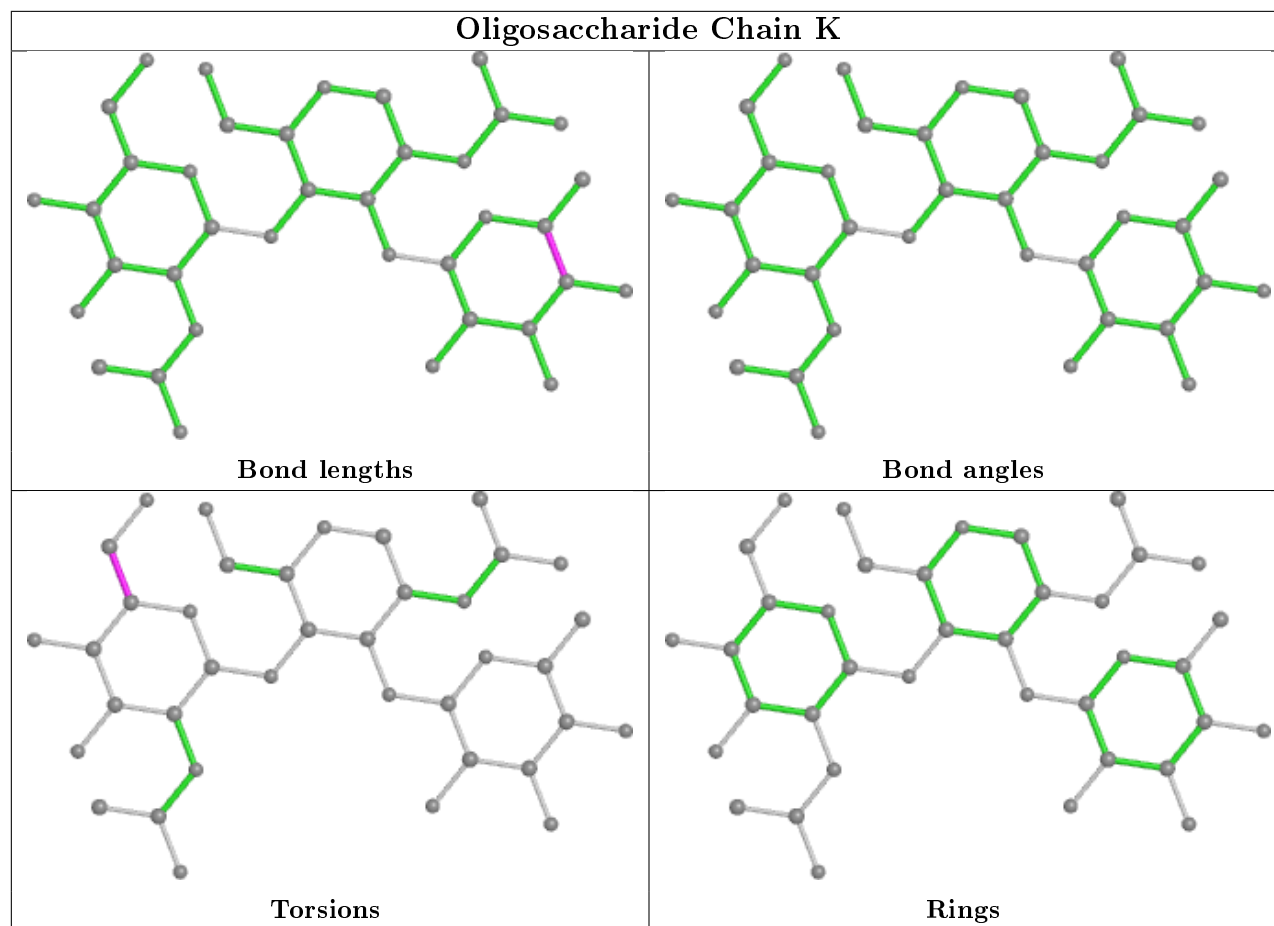
Mol	Chain	Res	Type	Atoms
3	H	3	BMA	C1-C2-C3-C4-C5-O5

3 monomers are involved in 2 short contacts:

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

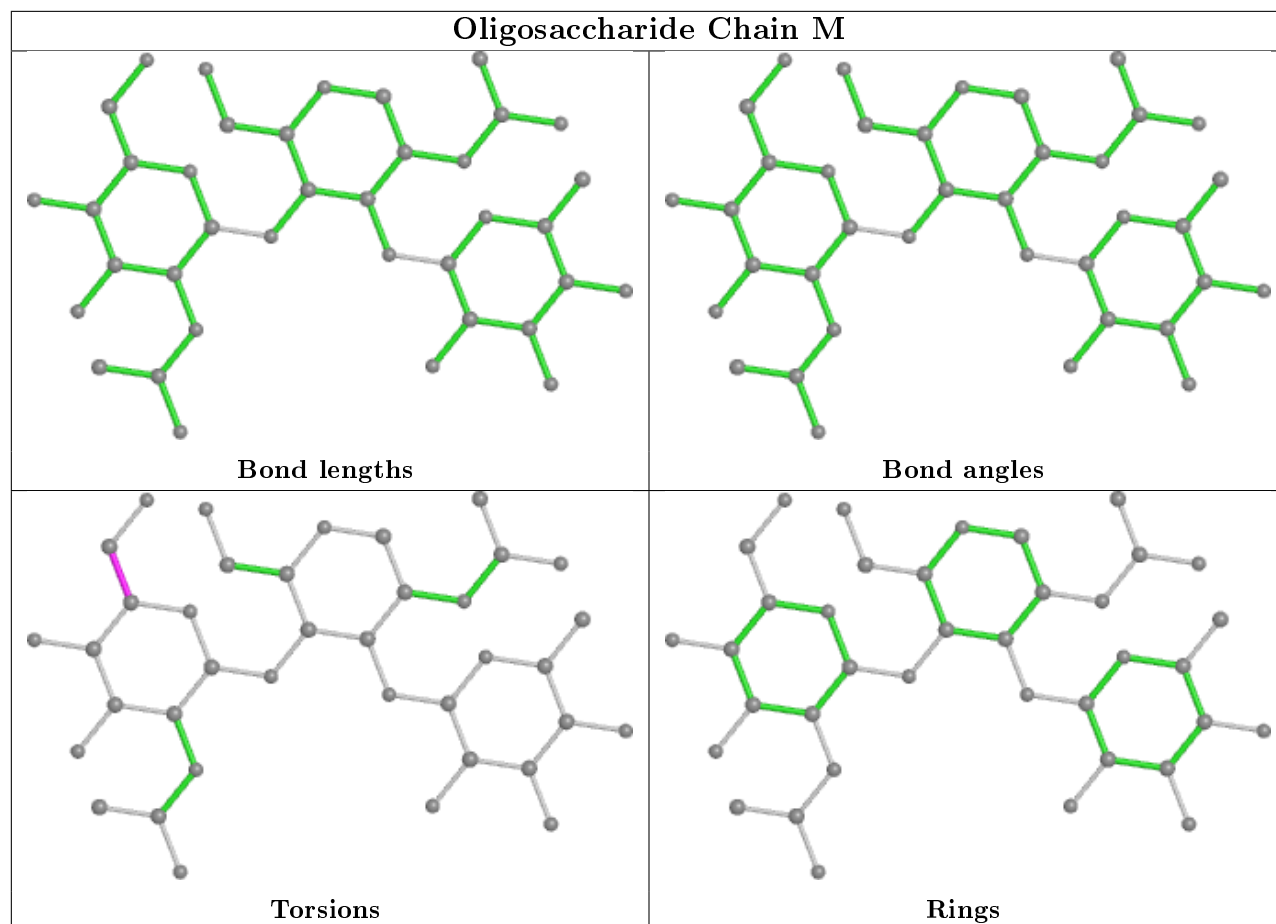
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



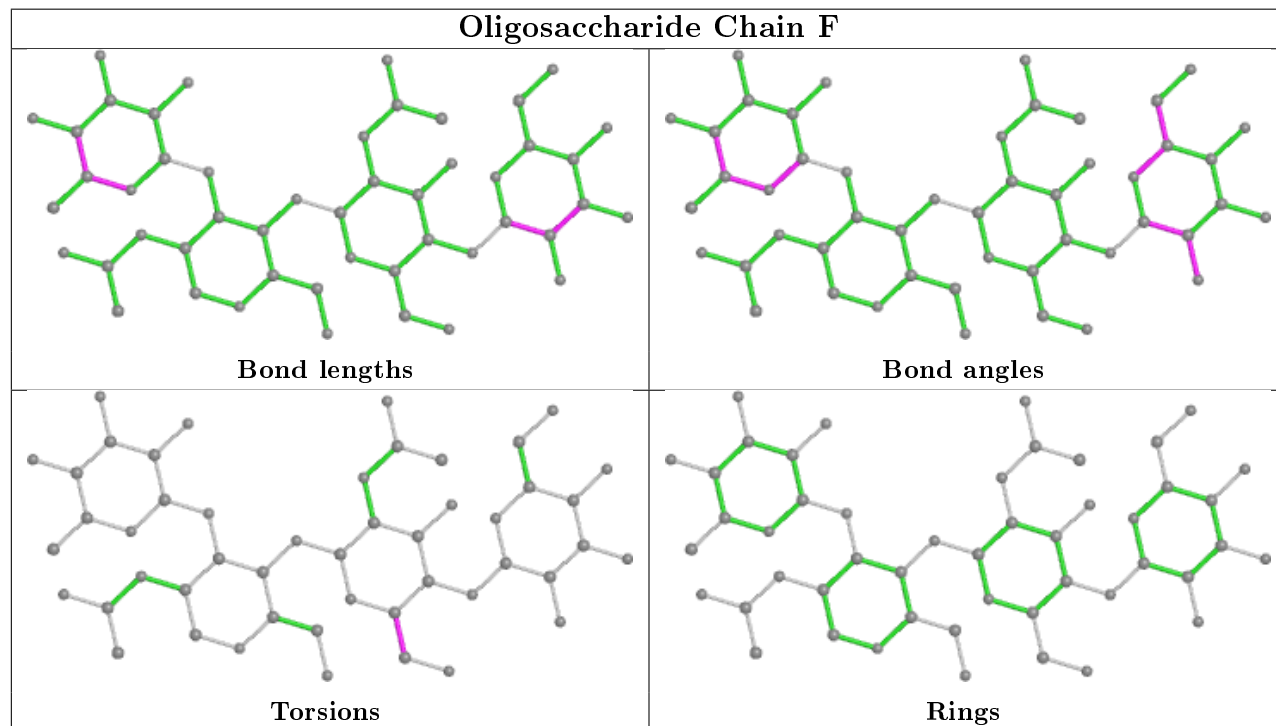




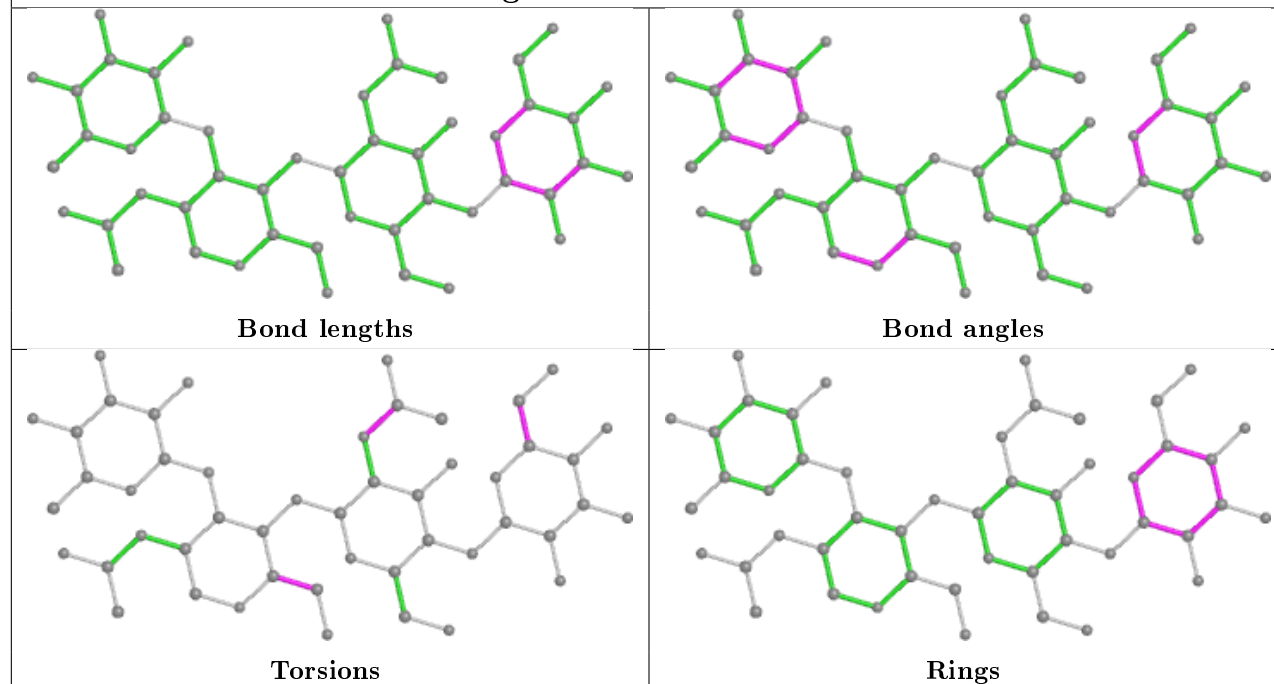
## Oligosaccharide Chain M



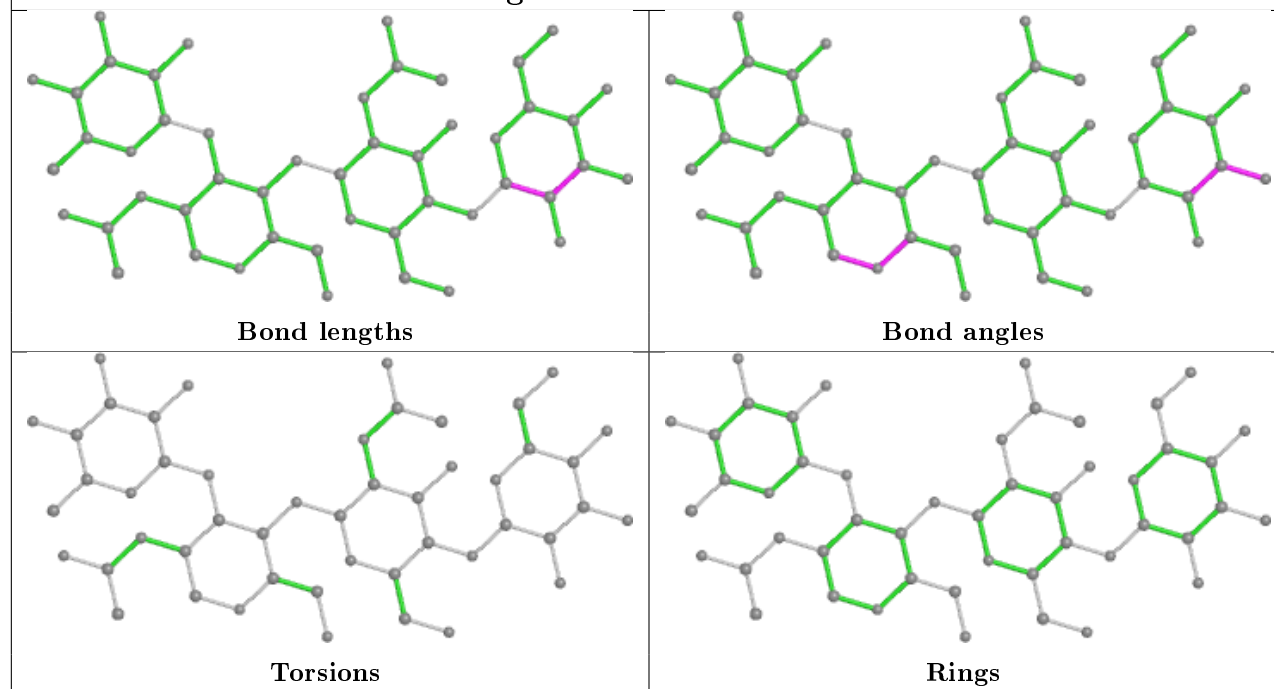
## Oligosaccharide Chain F



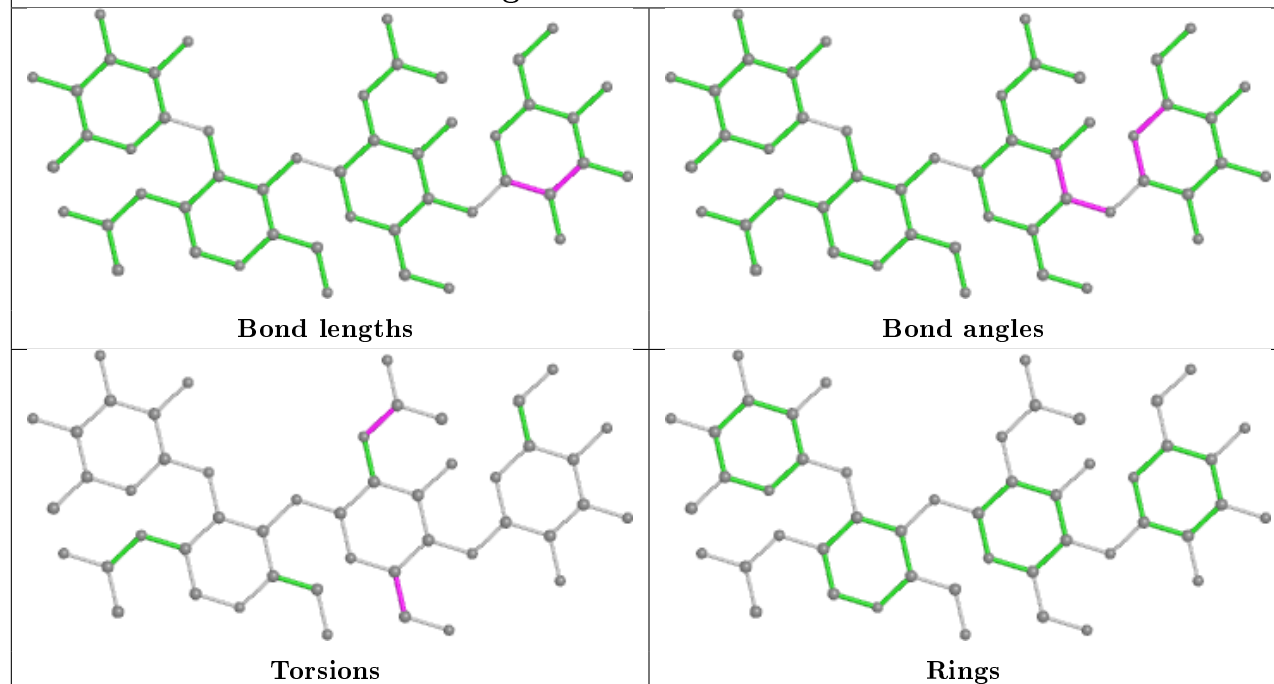
## Oligosaccharide Chain H



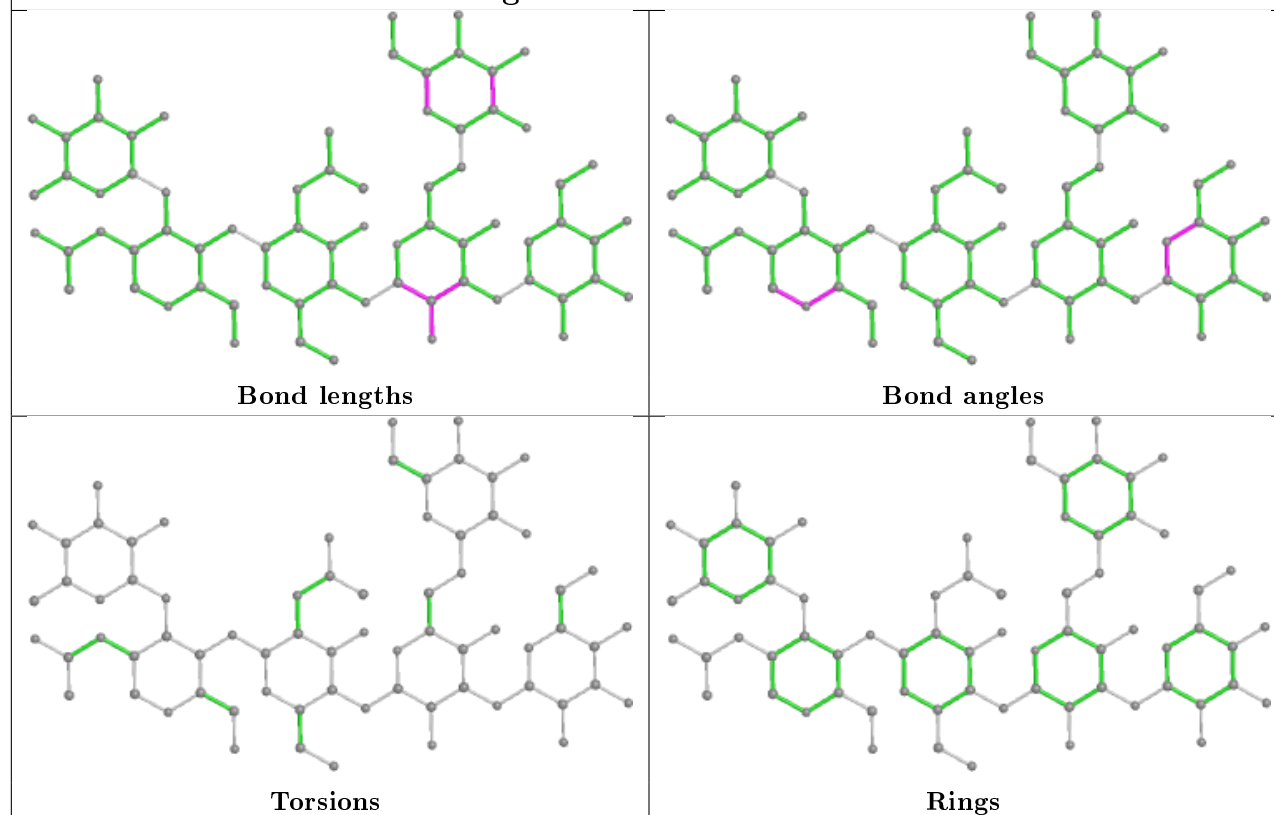
## Oligosaccharide Chain J

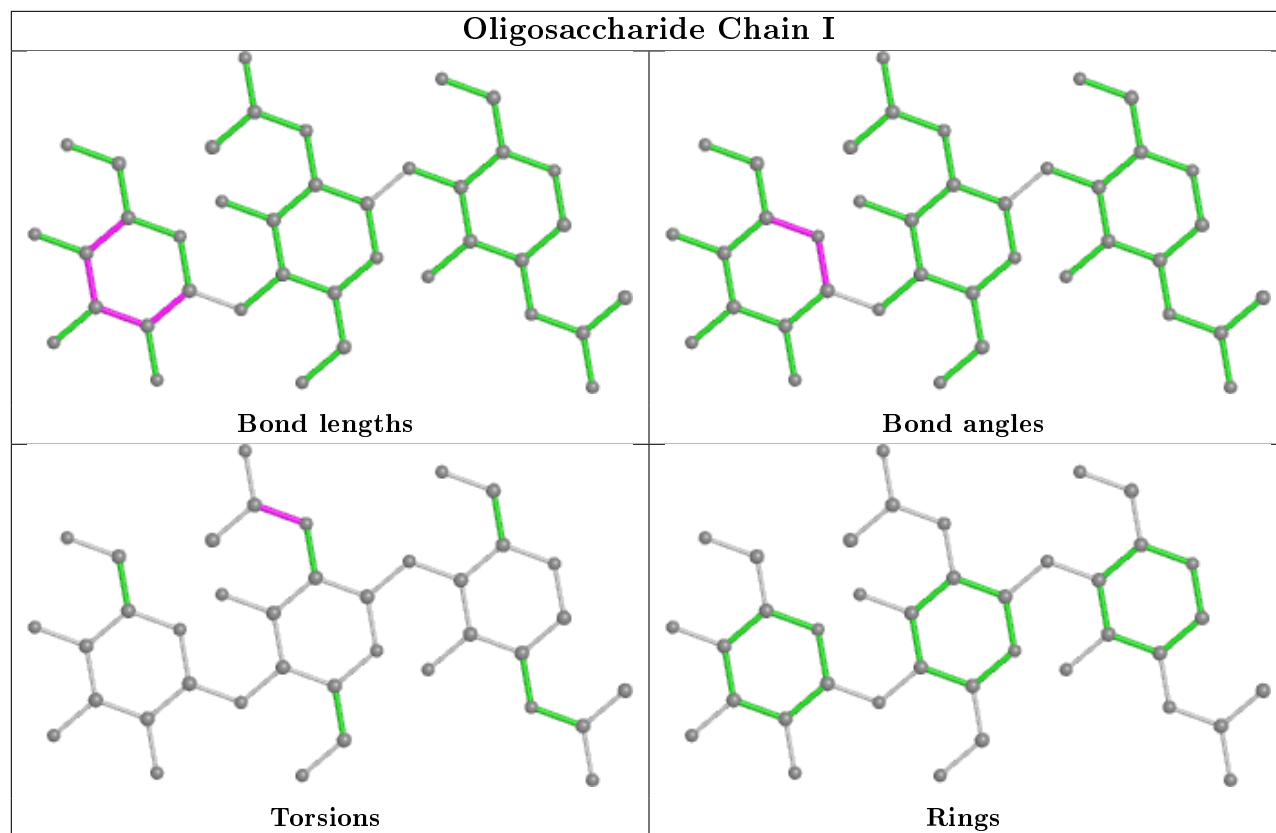


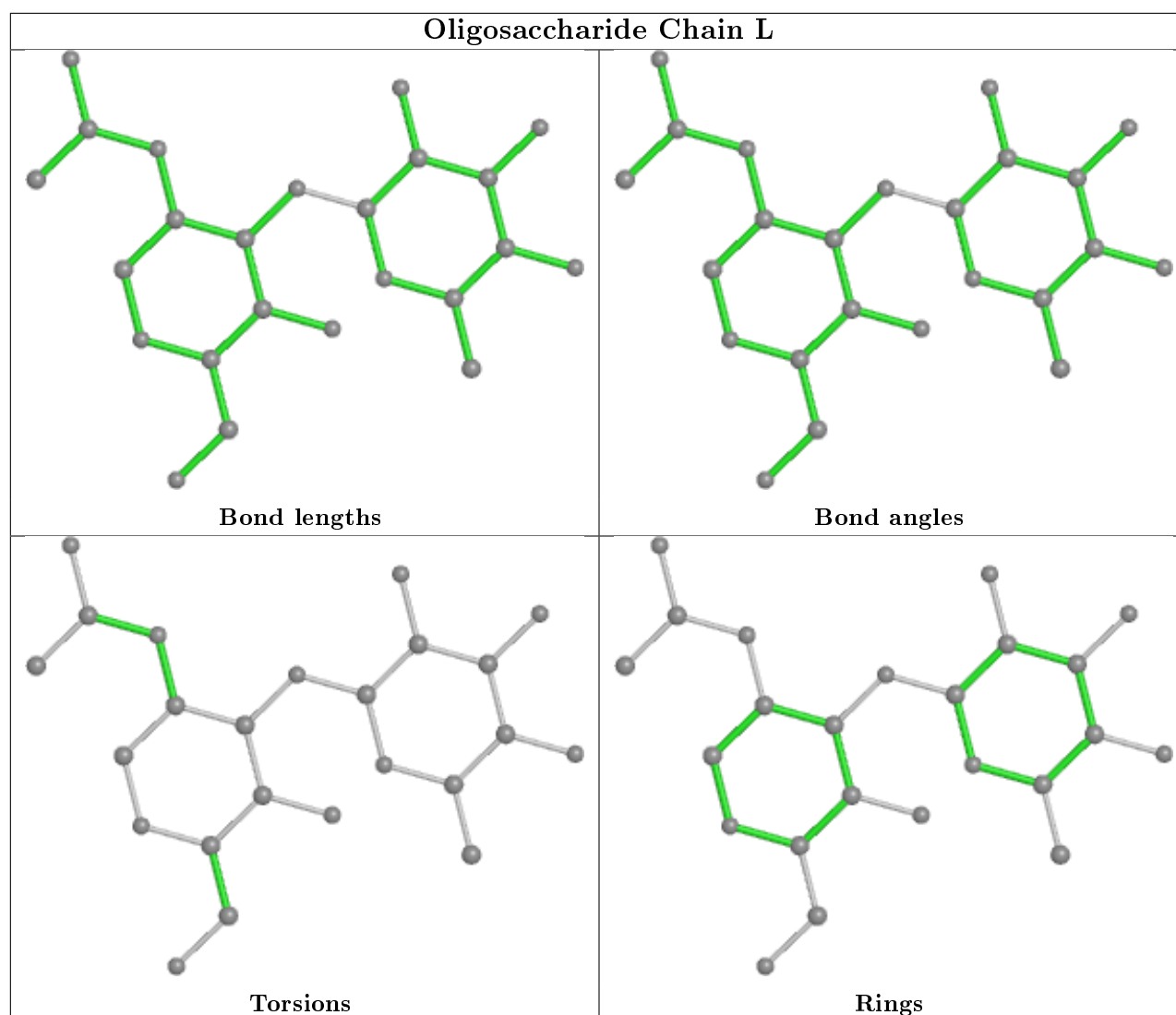
## Oligosaccharide Chain N



## 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	$\# Z  > 2$
9	NAG	D	503	1	14,14,15	0.45	0	17,19,21	0.48	0
14	PGE	D	515	-	6,6,9	0.36	0	5,5,8	0.39	0
9	NAG	B	503	1	14,14,15	0.41	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	GOL	D	514	-	5,5,5	1.26	1 (20%)	5,5,5	1.03	0
9	NAG	C	503	1	14,14,15	0.65	0	17,19,21	0.61	0
12	SO4	B	517	-	4,4,4	0.15	0	6,6,6	0.11	0
12	SO4	C	515	-	4,4,4	0.19	0	6,6,6	0.09	0
14	PGE	A	527	-	6,6,9	0.40	0	5,5,8	0.19	0
14	PGE	D	516	-	3,3,9	0.35	0	2,2,8	0.43	0
12	SO4	A	524	-	4,4,4	0.16	0	6,6,6	0.17	0
13	EDO	D	504	-	3,3,3	0.53	0	2,2,2	0.40	0
10	MF1	A	517[B]	-	33,35,35	2.11	3 (9%)	37,43,43	1.63	8 (21%)
10	MF1	A	517[C]	-	33,35,35	1.68	3 (9%)	37,43,43	1.75	8 (21%)
12	SO4	B	522	-	4,4,4	0.17	0	6,6,6	0.23	0
13	EDO	C	518	-	3,3,3	0.52	0	2,2,2	0.22	0
12	SO4	D	512	11	4,4,4	0.23	0	6,6,6	0.18	0
12	SO4	D	513	-	4,4,4	0.15	0	6,6,6	0.25	0
13	EDO	C	517	-	3,3,3	0.50	0	2,2,2	0.58	0
12	SO4	B	520	-	4,4,4	0.17	0	6,6,6	0.28	0
13	EDO	C	519	-	3,3,3	0.43	0	2,2,2	0.48	0
9	NAG	C	521	1	14,14,15	0.52	0	17,19,21	0.64	0
9	NAG	A	503	1	14,14,15	0.34	0	17,19,21	0.60	0
9	NAG	C	507	1	14,14,15	0.41	0	17,19,21	0.55	0
12	SO4	A	522	11	4,4,4	0.15	0	6,6,6	0.25	0
12	SO4	A	525	-	4,4,4	0.32	0	6,6,6	0.09	0
9	NAG	D	510	1	14,14,15	0.80	1 (7%)	17,19,21	0.84	1 (5%)
13	EDO	C	520	-	3,3,3	0.40	0	2,2,2	0.55	0
13	EDO	A	526	-	3,3,3	0.58	0	2,2,2	0.11	0
12	SO4	B	521	-	4,4,4	0.11	0	6,6,6	0.20	0
12	SO4	A	523	-	4,4,4	0.14	0	6,6,6	0.13	0
12	SO4	A	520	-	4,4,4	0.15	0	6,6,6	0.05	0
12	SO4	B	515	-	4,4,4	0.10	0	6,6,6	0.18	0
12	SO4	C	516	-	4,4,4	0.18	0	6,6,6	0.15	0
12	SO4	B	516	11	4,4,4	0.24	0	6,6,6	0.20	0
12	SO4	B	518	-	4,4,4	0.18	0	6,6,6	0.41	0
12	SO4	B	519	-	4,4,4	0.14	0	6,6,6	0.25	0
12	SO4	A	521	-	4,4,4	0.19	0	6,6,6	0.30	0
13	EDO	B	523	-	3,3,3	0.57	0	2,2,2	0.29	0
12	SO4	C	514	-	4,4,4	0.15	0	6,6,6	0.25	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	D	504	-	-	0/1/1/1	-
15	GOL	D	514	-	-	0/4/4/4	-
10	MF1	A	517[B]	-	-	8/26/29/29	0/2/2/2
9	NAG	C	521	1	-	4/6/23/26	0/1/1/1
10	MF1	A	517[C]	-	-	2/26/29/29	0/2/2/2
9	NAG	A	503	1	-	2/6/23/26	0/1/1/1
9	NAG	D	503	1	-	2/6/23/26	0/1/1/1
14	PGE	D	515	-	-	1/4/4/7	-
9	NAG	B	503	1	-	2/6/23/26	0/1/1/1
9	NAG	D	510	1	-	1/6/23/26	0/1/1/1
9	NAG	C	503	1	-	2/6/23/26	0/1/1/1
13	EDO	A	526	-	-	1/1/1/1	-
13	EDO	C	517	-	-	1/1/1/1	-
14	PGE	A	527	-	-	1/4/4/7	-
14	PGE	D	516	-	-	0/1/1/7	-
9	NAG	C	507	1	-	0/6/23/26	0/1/1/1
13	EDO	B	523	-	-	0/1/1/1	-
13	EDO	C	518	-	-	0/1/1/1	-
13	EDO	C	519	-	-	1/1/1/1	-
13	EDO	C	520	-	-	1/1/1/1	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	517[B]	MF1	CAU-CAT	-10.15	1.41	1.51
10	A	517[C]	MF1	CAU-CAT	-6.99	1.44	1.51
10	A	517[C]	MF1	PBE-OBF	-3.99	1.48	1.54
10	A	517[B]	MF1	PBE-OBF	-3.98	1.48	1.54
10	A	517[C]	MF1	PBE-OBG	3.91	1.61	1.54

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	517[C]	MF1	CAT-CAU-CBD	5.49	126.24	119.75
10	A	517[B]	MF1	CAT-CAU-CBD	4.85	125.49	119.75
10	A	517[C]	MF1	CAF-CAE-CAD	-3.22	98.08	114.42
10	A	517[B]	MF1	CAV-CAU-CAT	-3.22	115.03	119.60
10	A	517[C]	MF1	CAV-CAU-CAT	-2.89	115.49	119.60

There are no chirality outliers.

5 of 29 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

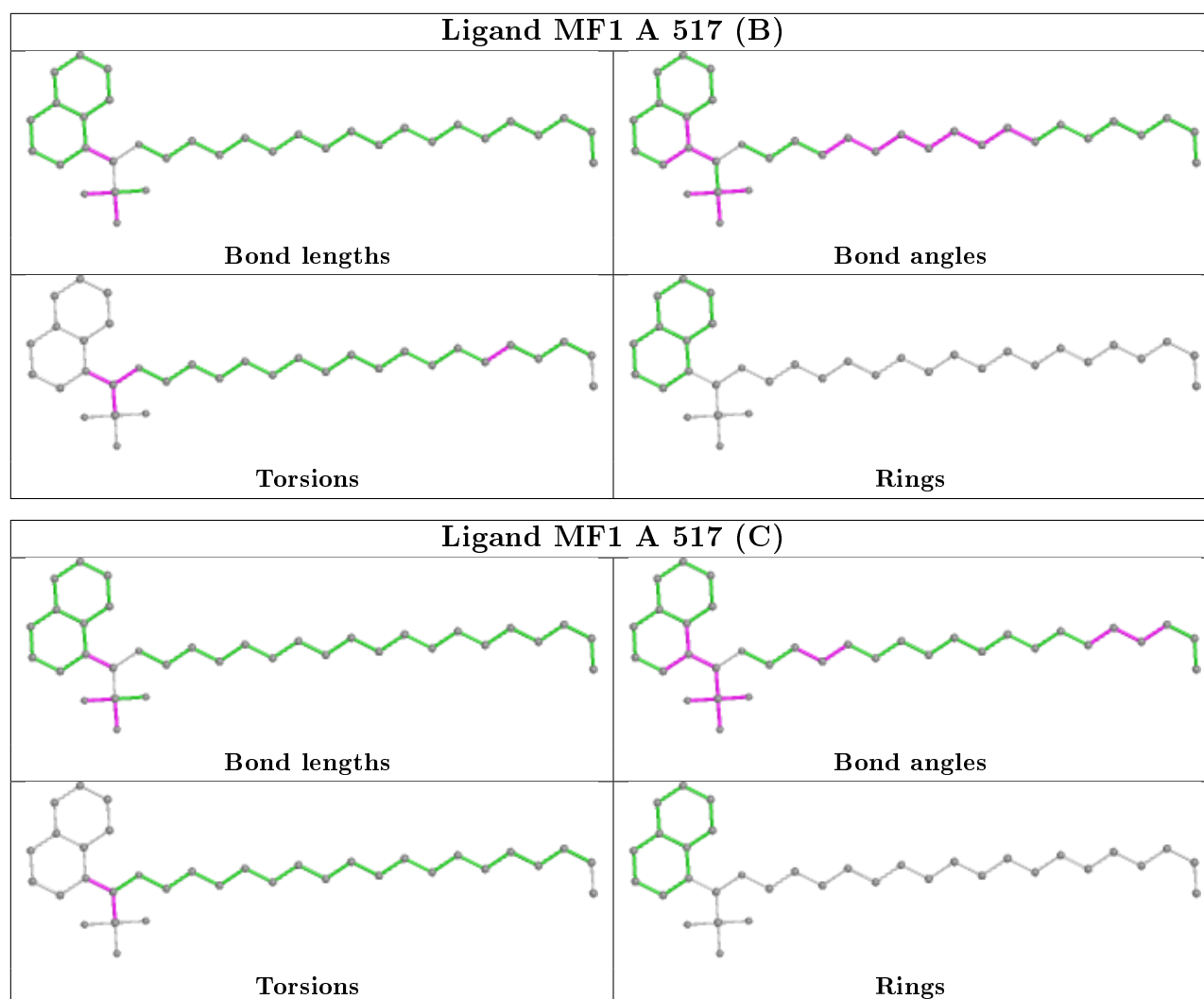
There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	D	515	PGE	4	0
9	B	503	NAG	1	0
15	D	514	GOL	1	0
14	A	527	PGE	1	0
10	A	517[B]	MF1	3	0
10	A	517[C]	MF1	3	0
12	D	513	SO4	1	0
12	A	522	SO4	1	0
12	B	516	SO4	3	0
12	C	514	SO4	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	426/459 (92%)	-0.83	6 (1%) 75 73	18, 25, 38, 91	0
1	B	425/459 (92%)	-0.78	5 (1%) 79 77	19, 28, 40, 73	0
1	C	423/459 (92%)	-0.77	2 (0%) 91 90	20, 27, 42, 71	0
1	D	424/459 (92%)	-0.79	4 (0%) 84 83	18, 26, 42, 68	0
All	All	1698/1836 (92%)	-0.79	17 (1%) 82 81	18, 27, 41, 91	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ASN	6.9
1	D	431	SER	4.4
1	B	63	LYS	3.8
1	A	7	LYS	3.4
1	A	431	SER	3.1

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	BMA	I	3	11/12	0.67	0.26	48,61,65,70	0
3	BMA	J	3	11/12	0.75	0.24	47,51,56,59	0

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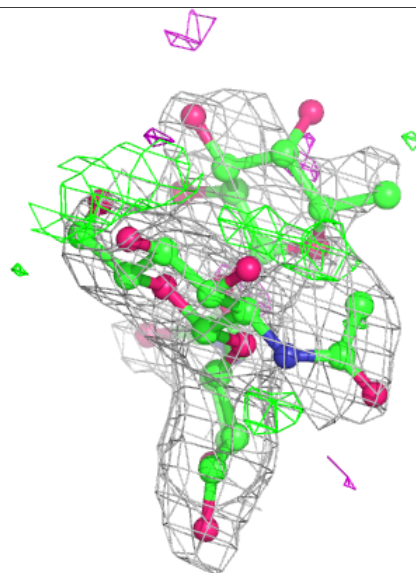
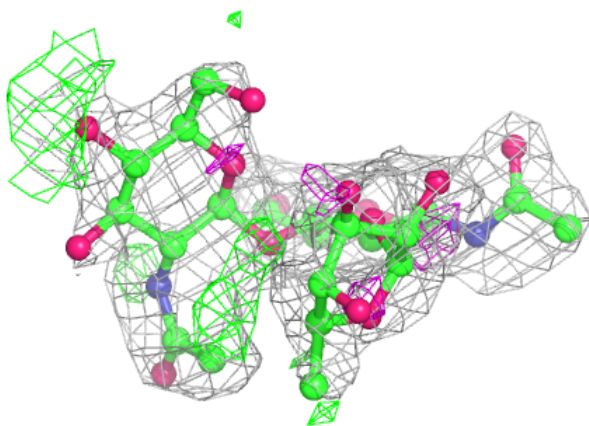
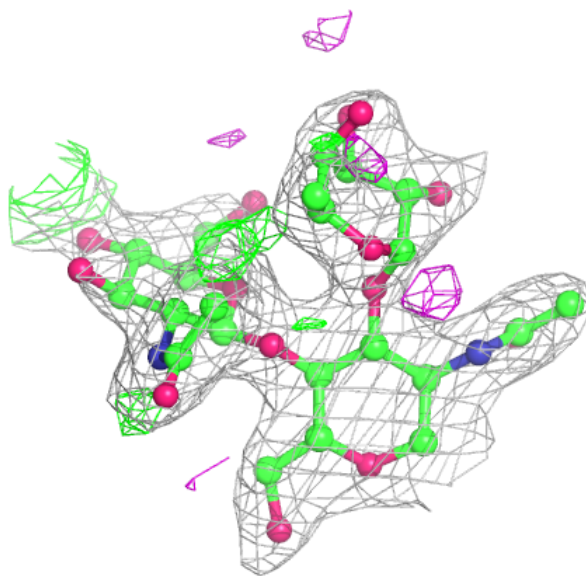
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BMA	N	3	11/12	0.77	0.39	65,79,86,90	0
3	BMA	F	3	11/12	0.78	0.25	61,68,71,77	0
6	FUC	L	2	10/11	0.79	0.33	46,63,64,65	0
3	FUC	H	4	10/11	0.80	0.29	67,72,75,79	0
5	NAG	I	2	14/15	0.80	0.29	55,60,63,67	0
2	NAG	E	3	14/15	0.80	0.29	67,73,75,76	0
3	NAG	N	2	14/15	0.81	0.37	62,74,79,80	0
3	BMA	H	3	11/12	0.82	0.45	83,96,101,101	0
2	FUC	E	2	10/11	0.82	0.34	65,71,79,87	0
3	FUC	F	4	10/11	0.85	0.34	52,60,65,65	0
2	NAG	K	3	14/15	0.86	0.31	39,56,64,67	0
3	NAG	H	2	14/15	0.87	0.41	73,80,92,99	0
2	FUC	M	2	10/11	0.87	0.22	45,49,56,56	0
2	NAG	M	3	14/15	0.87	0.27	35,52,60,62	0
5	NAG	I	1	14/15	0.87	0.17	38,47,54,57	0
2	FUC	K	2	10/11	0.88	0.24	53,55,60,62	0
6	NAG	L	1	14/15	0.90	0.21	42,51,57,58	0
3	NAG	F	2	14/15	0.90	0.24	40,55,61,64	0
2	NAG	E	1	14/15	0.90	0.15	40,50,69,73	0
4	BMA	G	3	11/12	0.91	0.22	37,47,53,54	0
3	NAG	H	1	14/15	0.91	0.18	43,55,71,74	0
3	FUC	N	4	10/11	0.92	0.27	52,60,61,64	0
3	NAG	F	1	14/15	0.93	0.15	40,43,49,55	0
4	MAN	G	5	11/12	0.93	0.33	55,63,69,71	0
3	NAG	N	1	14/15	0.93	0.16	39,53,59,63	0
2	NAG	K	1	14/15	0.94	0.08	35,40,46,55	0
3	NAG	J	2	14/15	0.95	0.12	28,36,41,46	0
2	NAG	M	1	14/15	0.95	0.08	30,38,42,44	0
4	NAG	G	1	14/15	0.95	0.09	28,32,36,37	0
4	NAG	G	2	14/15	0.95	0.11	30,36,43,46	0
3	FUC	J	4	10/11	0.95	0.09	31,35,38,42	0
4	FUC	G	6	10/11	0.96	0.17	34,40,44,45	0
4	MAN	G	4	11/12	0.96	0.25	44,49,51,52	0
3	NAG	J	1	14/15	0.97	0.08	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.

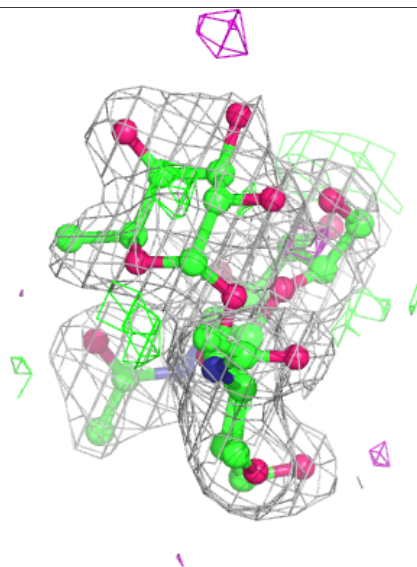
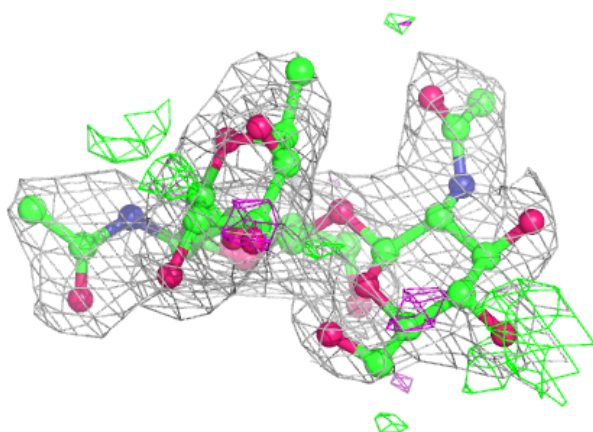
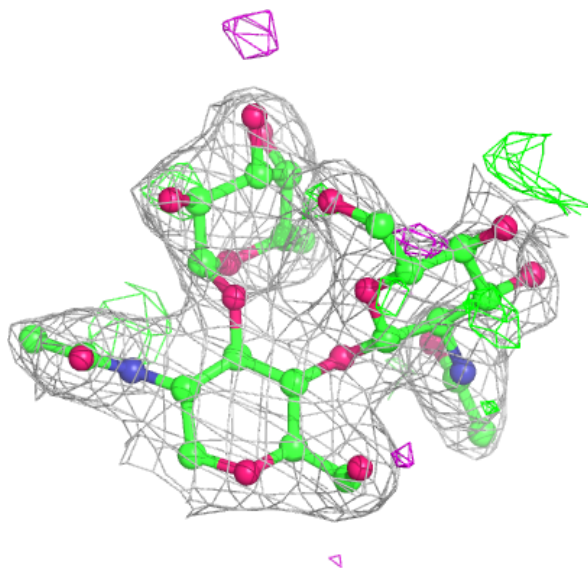
**Electron density around Chain E:**

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



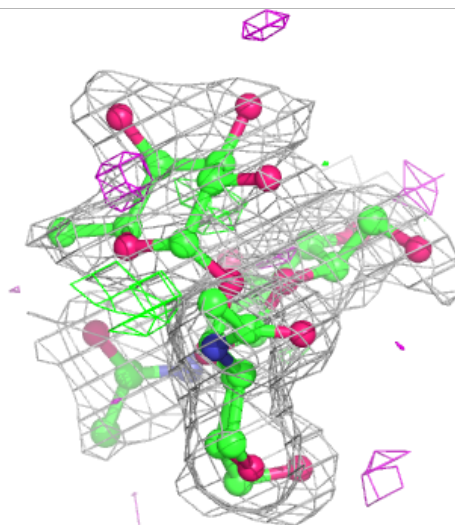
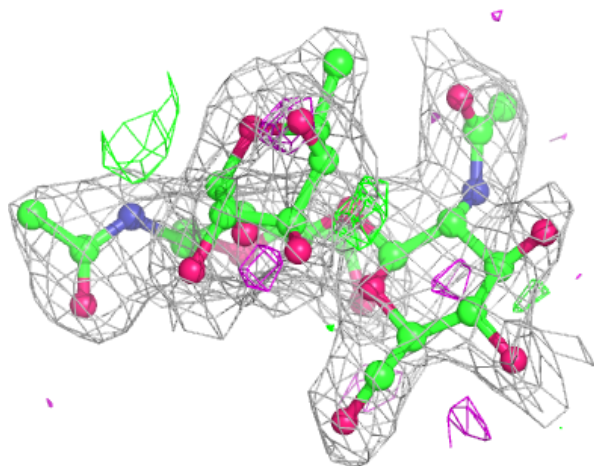
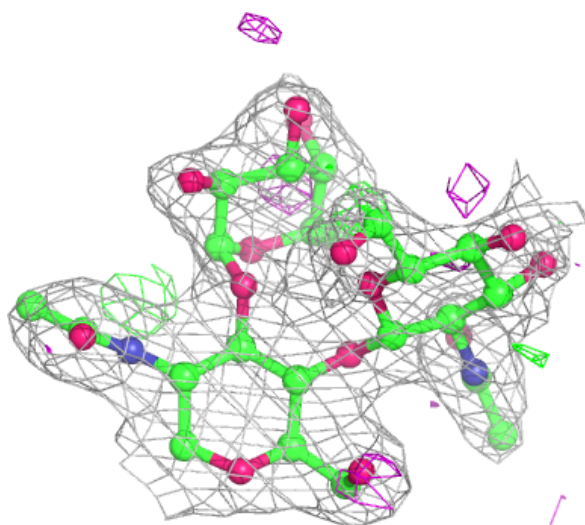
**Electron density around Chain K:**

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



**Electron density around Chain M:**

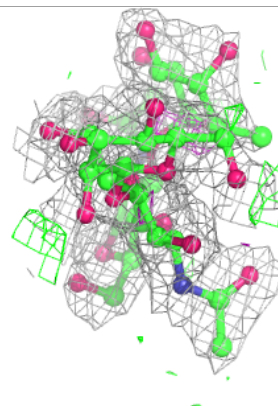
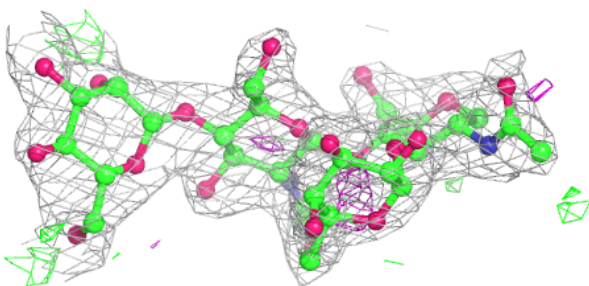
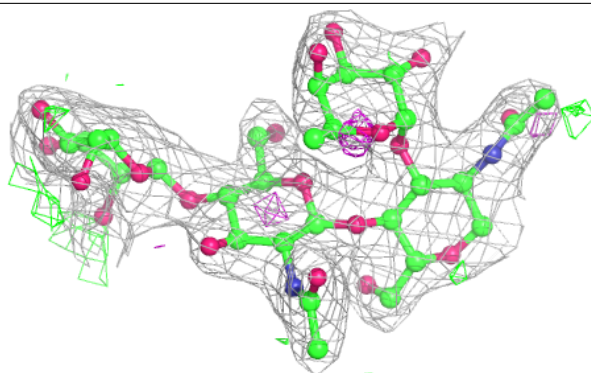
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



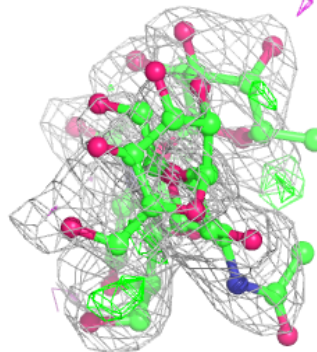
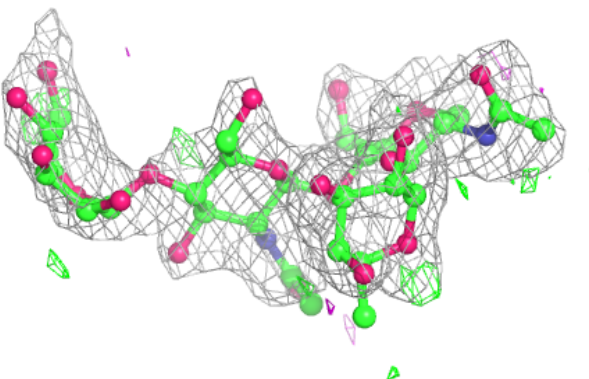
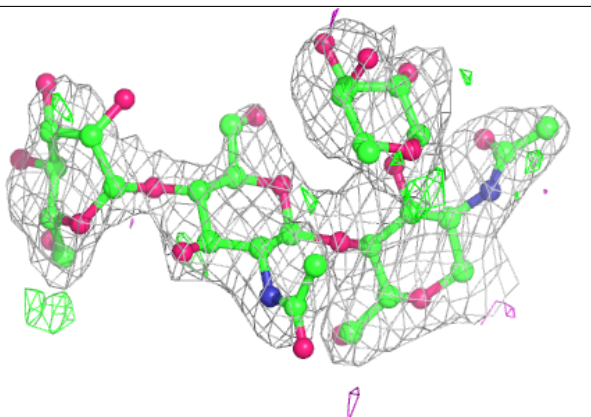


**Electron density around Chain F:**

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

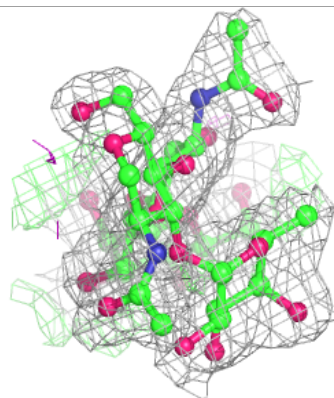
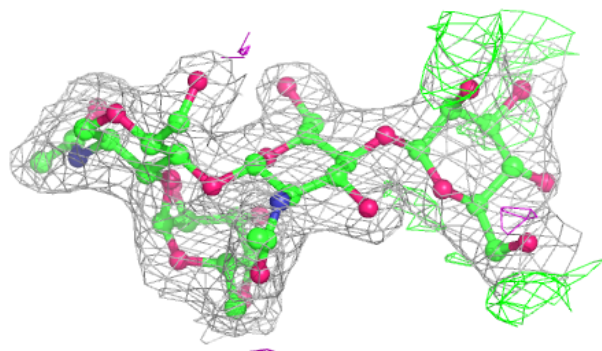
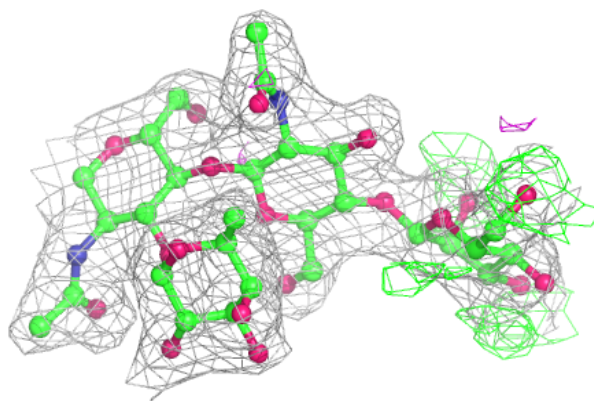
**Electron density around Chain H:**

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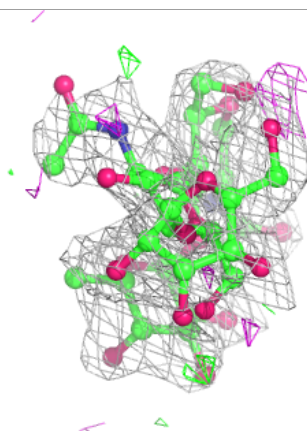
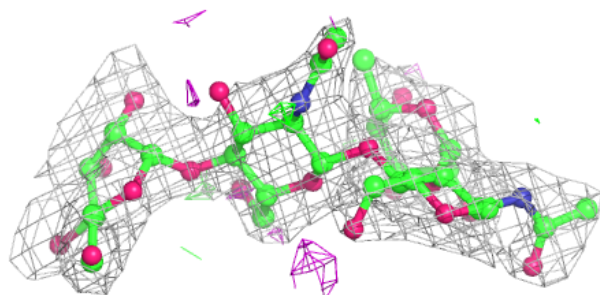
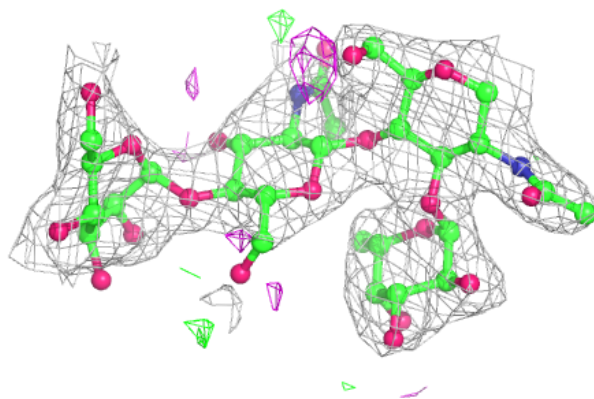


**Electron density around Chain J:**

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

**Electron density around Chain N:**

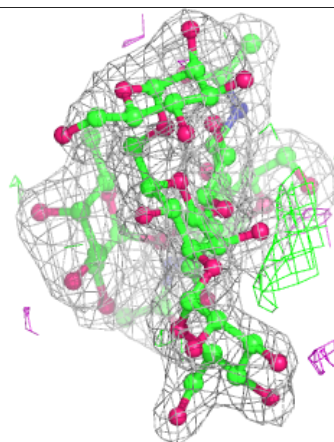
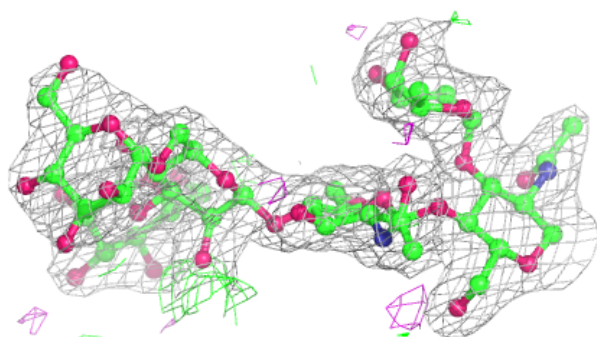
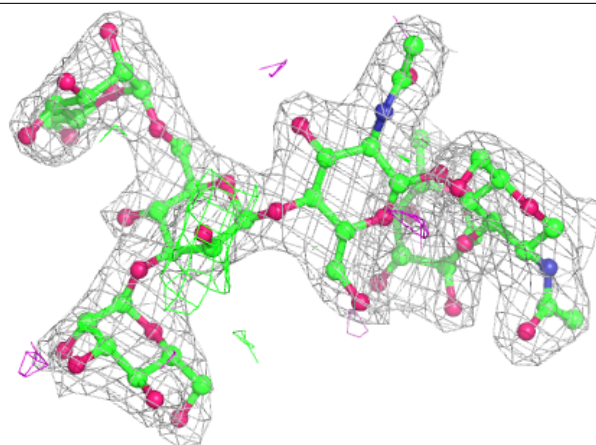
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



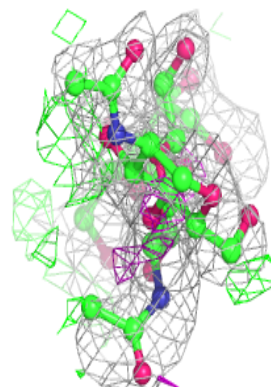
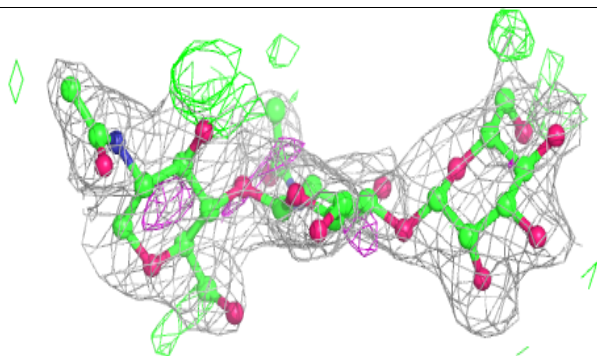
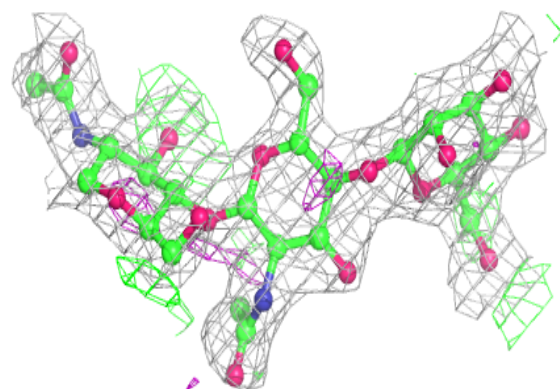


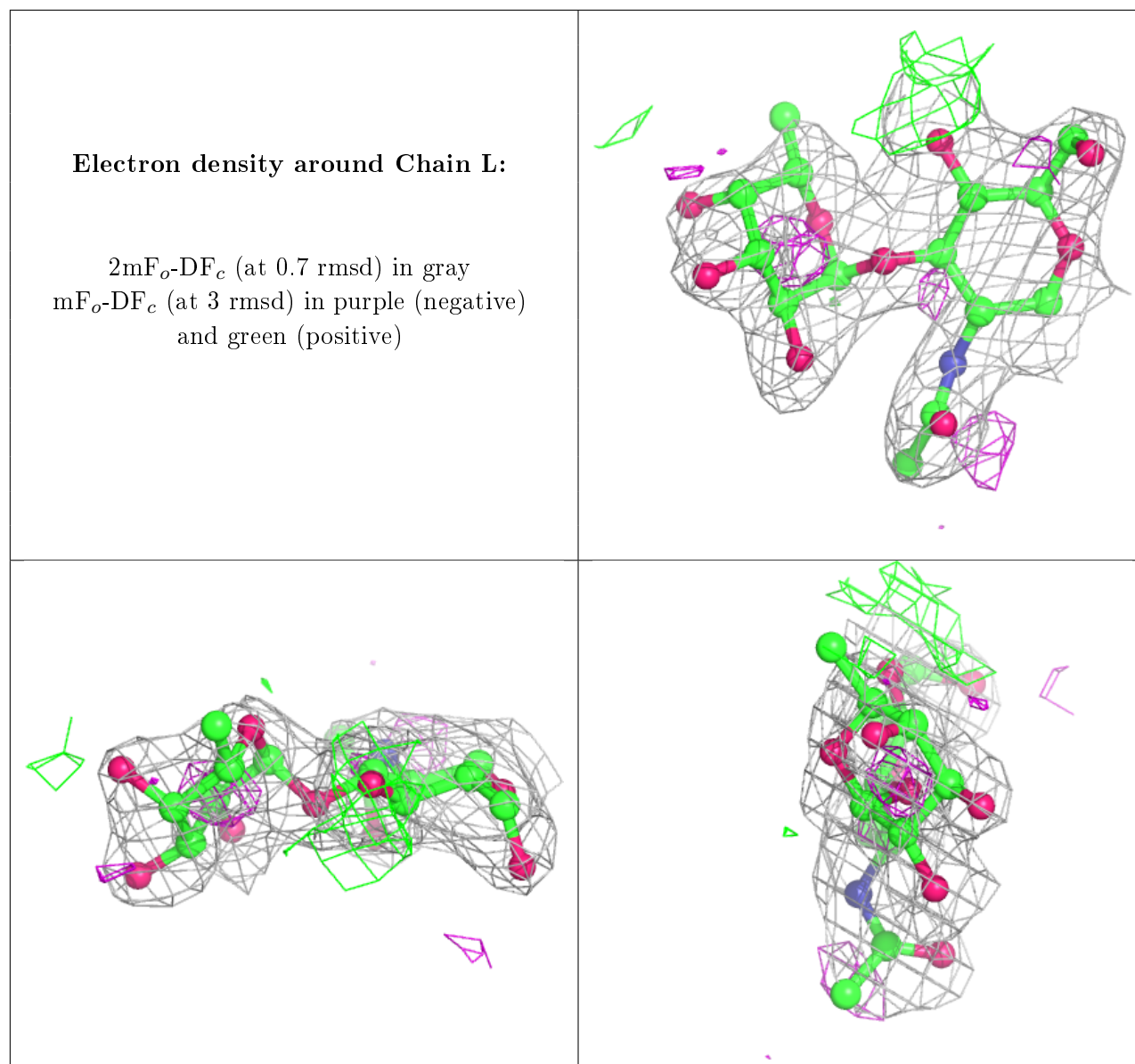
**Electron density around Chain G:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
10	MF1	A	517[B]	34/34	0.77	0.37	45,51,72,72	34
10	MF1	A	517[C]	34/34	0.77	0.37	38,52,72,72	34
12	SO4	C	514	5/5	0.77	0.29	72,81,90,103	0
12	SO4	C	516	5/5	0.79	0.46	60,75,94,105	0
12	SO4	A	525	5/5	0.80	0.61	100,101,106,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
12	SO4	B	522	5/5	0.82	0.29	57,69,94,98	0
13	EDO	C	517	4/4	0.84	0.18	40,47,48,58	0
13	EDO	D	504	4/4	0.84	0.32	41,42,55,57	0
14	PGE	A	527	7/10	0.87	0.27	31,45,49,51	0
13	EDO	B	523	4/4	0.87	0.33	38,41,43,43	0
9	NAG	C	521	14/15	0.87	0.29	50,59,60,60	0
12	SO4	A	523	5/5	0.88	0.39	64,73,92,93	0
14	PGE	D	516	4/10	0.89	0.24	43,51,55,68	0
15	GOL	D	514	6/6	0.89	0.18	33,40,43,51	0
9	NAG	D	510	14/15	0.89	0.14	46,51,57,61	0
12	SO4	B	521	5/5	0.89	0.31	55,79,84,85	0
12	SO4	C	515	5/5	0.90	0.40	70,75,94,96	0
12	SO4	B	518	5/5	0.90	0.14	33,40,57,57	5
12	SO4	D	513	5/5	0.90	0.24	44,58,73,79	0
9	NAG	C	503	14/15	0.90	0.21	40,49,58,65	0
12	SO4	A	521	5/5	0.91	0.14	32,32,46,46	5
9	NAG	B	503	14/15	0.92	0.15	30,38,50,51	0
14	PGE	D	515	7/10	0.92	0.22	25,37,49,56	0
13	EDO	C	518	4/4	0.92	0.26	36,39,42,45	0
12	SO4	B	515	5/5	0.93	0.27	36,48,50,56	5
13	EDO	C	519	4/4	0.94	0.22	35,37,40,49	0
9	NAG	A	503	14/15	0.94	0.12	28,36,41,49	0
13	EDO	A	526	4/4	0.94	0.12	37,44,47,49	0
12	SO4	A	520	5/5	0.95	0.16	33,39,45,46	5
12	SO4	A	524	5/5	0.95	0.32	39,51,56,60	0
9	NAG	D	503	14/15	0.95	0.14	29,32,42,45	0
11	NA	D	511	1/1	0.95	0.29	55,55,55,55	0
13	EDO	C	520	4/4	0.96	0.18	27,35,45,48	0
9	NAG	C	507	14/15	0.97	0.14	33,36,44,50	0
11	NA	A	519	1/1	0.97	0.05	34,34,34,34	0
12	SO4	B	517	5/5	0.97	0.10	23,33,36,37	5
11	NA	C	508	1/1	0.97	0.14	28,28,28,28	0
12	SO4	B	520	5/5	0.97	0.36	58,59,65,66	0
12	SO4	B	519	5/5	0.98	0.12	29,34,35,41	5
12	SO4	D	512	5/5	0.98	0.10	27,33,37,39	5
12	SO4	A	522	5/5	0.99	0.07	36,37,41,43	0
11	NA	C	509	1/1	0.99	0.14	15,15,15,15	0
12	SO4	B	516	5/5	0.99	0.16	8,27,29,30	5
8	FE	B	502	1/1	1.00	0.02	28,28,28,28	1
16	CL	D	517	1/1	1.00	0.07	26,26,26,26	0
8	FE	C	502	1/1	1.00	0.02	25,25,25,25	1
8	FE	D	502	1/1	1.00	0.03	28,28,28,28	1

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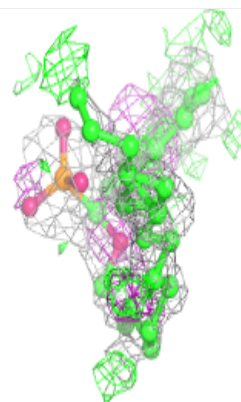
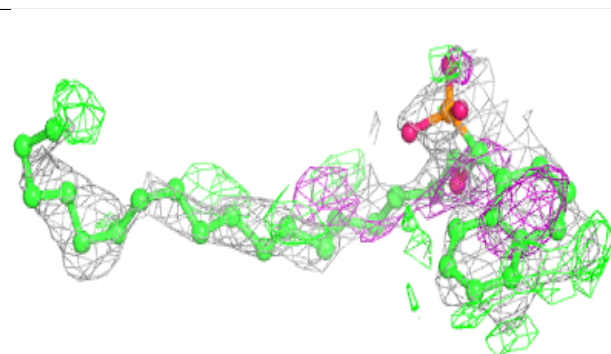
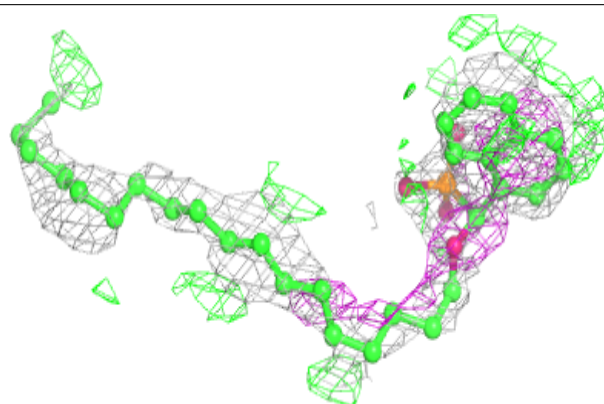
*Continued from previous page...*

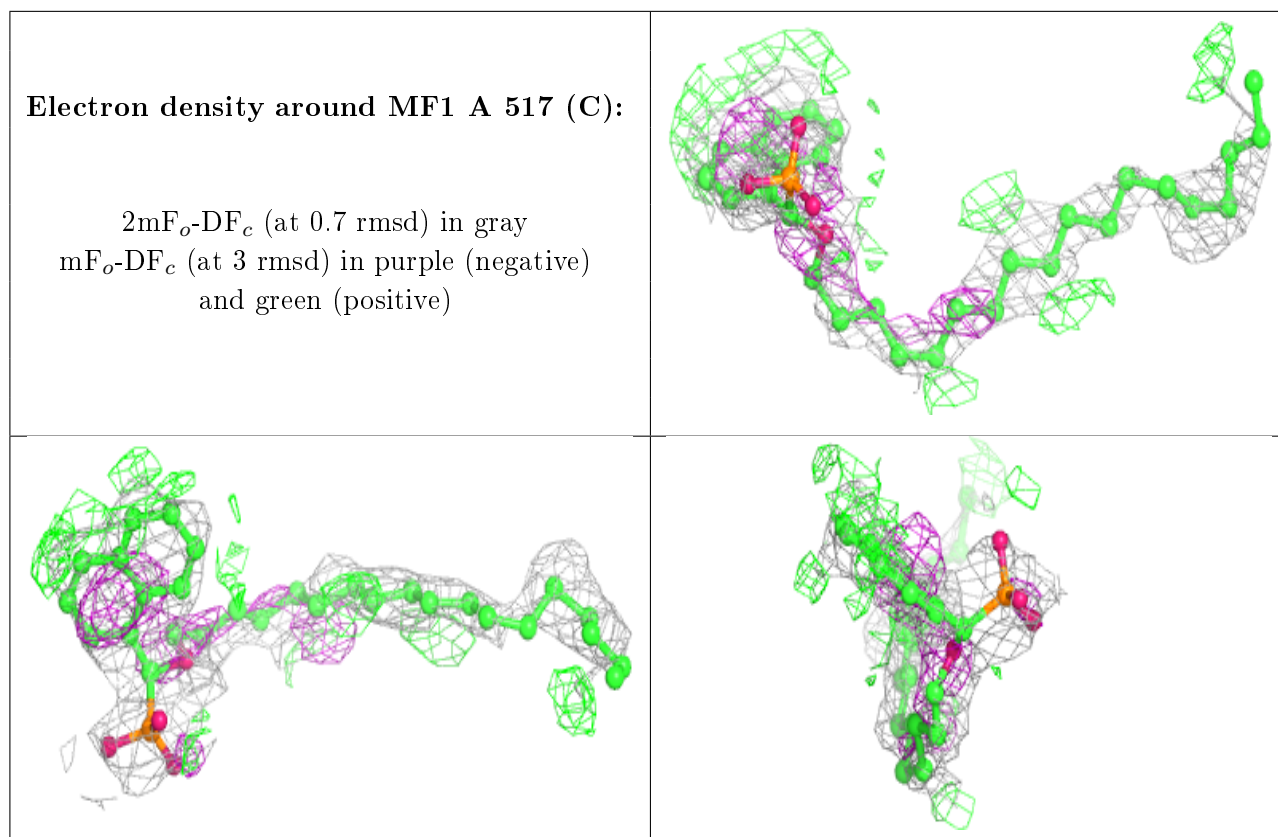
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	ZN	B	501	1/1	1.00	0.02	27,27,27,27	0
7	ZN	D	501	1/1	1.00	0.03	22,22,22,22	0
8	FE	A	502	1/1	1.00	0.02	27,27,27,27	1
11	NA	A	518	1/1	1.00	0.14	16,16,16,16	0
7	ZN	A	501	1/1	1.00	0.03	26,26,26,26	0
7	ZN	C	501	1/1	1.00	0.03	26,26,26,26	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 (B):**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.