Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 12:49 PM EDT

PDB ID	:	6OF5
Title	:	The crystal structure of dodecyloxy(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.
Deposited on	:	2019-03-28
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

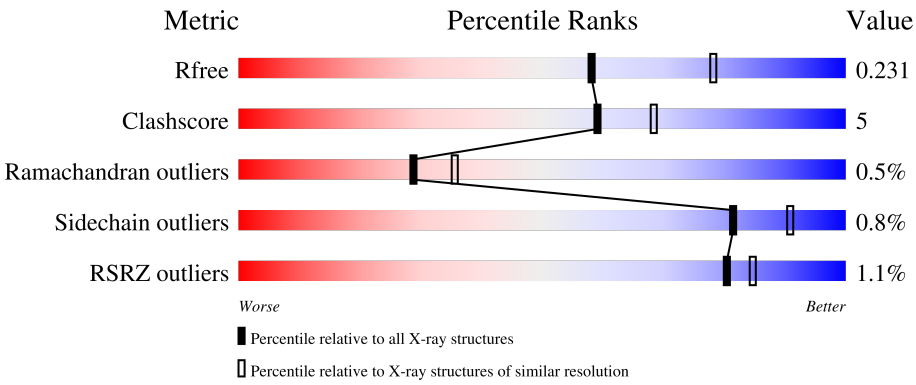
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	426	% 90% 9%
1	B	426	% 86% 13%
1	C	426	% 89% 10% •
1	D	426	% 89% 9% ••
2	E	3	67% 33%

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Mol	Chain	Length	Quality of chain
2	H	3	33% 67%
2	K	3	67% 33%
2	M	3	33% 33% 33%
3	F	4	25% 50% 25%
3	I	4	25% 75%
3	J	4	50% 50%
3	N	4	25% 75%
4	G	6	17% 83%
5	L	2	50% 50%

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
11	EDO	A	525	-	-	-	X
11	EDO	D	515	-	-	-	X
12	PGE	A	527	-	-	-	X
12	PGE	D	521	-	-	-	X
4	MAN	G	5	-	-	-	X
8	NAG	C	523	-	-	-	X
9	SO4	A	519	-	-	X	-
9	SO4	B	516	-	-	X	-
9	SO4	B	517	-	-	X	-
9	SO4	B	522	-	-	-	X

2 Entry composition (i)

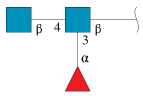
There are 15 unique types of molecules in this entry. The entry contains 15939 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

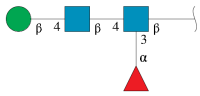
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	424	3507	2251	611	635	10	0	2	0
1	B	425	3531	2265	616	639	11	0	4	0
1	D	423	3491	2244	605	632	10	0	1	0
1	C	423	3487	2240	604	633	10	0	1	0

- 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.



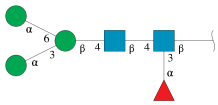
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	3	38	22	2	14	0	0	0
2	H	3	38	22	2	14	0	0	0
2	K	3	38	22	2	14	0	0	0
2	M	3	38	22	2	14	0	0	0

- 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
			Total	C	N	O			
3	F	4	49	28	2	19	0	0	0
3	I	4	49	28	2	19	0	0	0
3	J	4	49	28	2	19	0	0	0
3	N	4	49	28	2	19	0	0	0

- 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
			Total	C	N	O			
4	G	6	71	40	2	29	0	0	0

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	A	1	1	1	0	0

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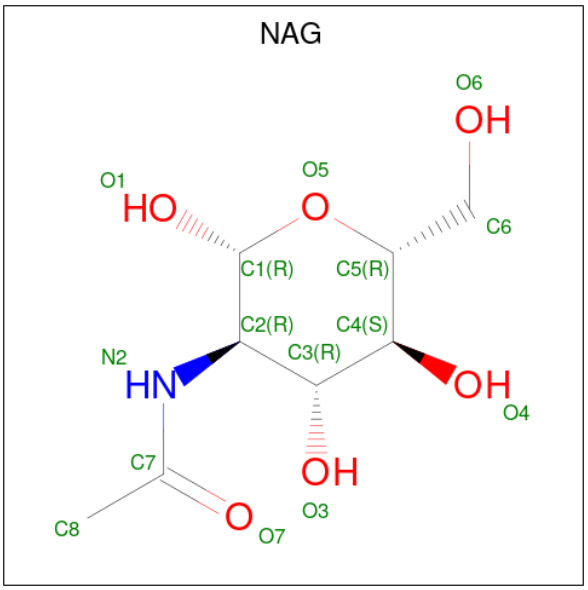
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Zn 1 1	0	0
6	D	1	Total Zn 1 1	0	0
6	C	1	Total Zn 1 1	0	0

- Molecule 7 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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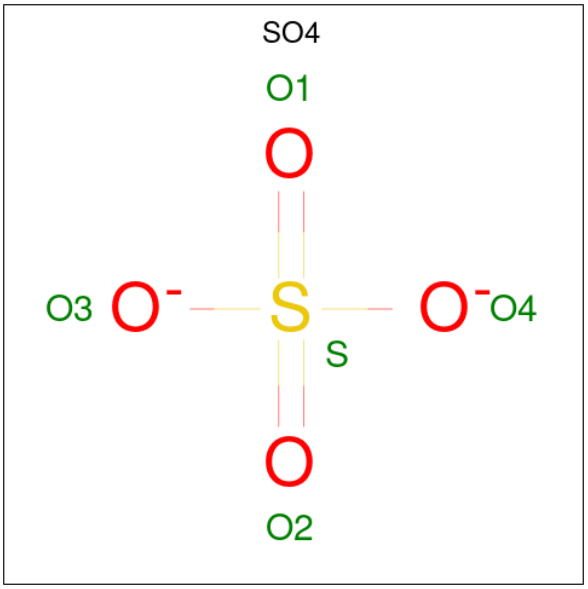
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total C N O 14 8 1 5	0	0
8	D	1	Total C N O 14 8 1 5	0	0
8	C	1	Total C N O 14 8 1 5	0	0
8	C	1	Total C N O 14 8 1 5	0	0
8	C	1	Total C N O 14 8 1 5	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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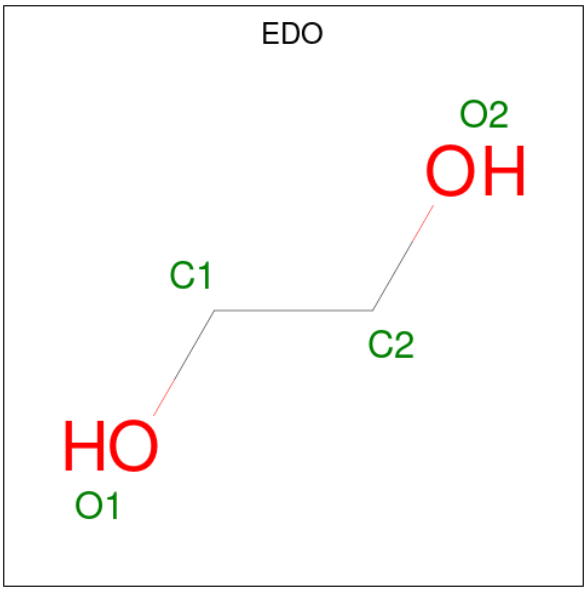
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	B	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	D	1	Total O S 5 4 1	0	0
9	C	1	Total O S 5 4 1	0	0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

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

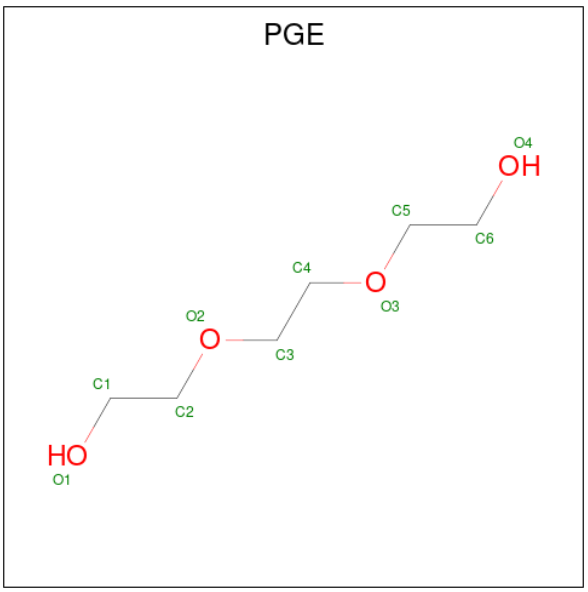
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	2	Total Na 2 2	0	0
10	D	1	Total Na 1 1	0	0
10	C	2	Total Na 2 2	0	0

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



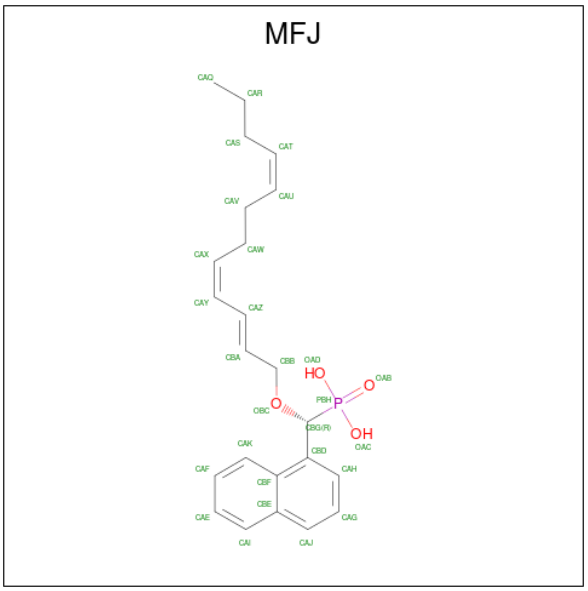
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
11	A	1	4	2	2	0	0
11	A	1	4	2	2	0	0
11	A	1	4	2	2	0	0
11	B	1	4	2	2	0	0
11	B	1	4	2	2	0	0
11	D	1	4	2	2	0	0
11	D	1	4	2	2	0	0
11	D	1	4	2	2	0	0
11	D	1	4	2	2	0	0
11	C	1	4	2	2	0	0
11	C	1	4	2	2	0	0
11	C	1	4	2	2	0	0
11	C	1	4	2	2	0	0
11	C	1	4	2	2	0	0

- Molecule 12 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



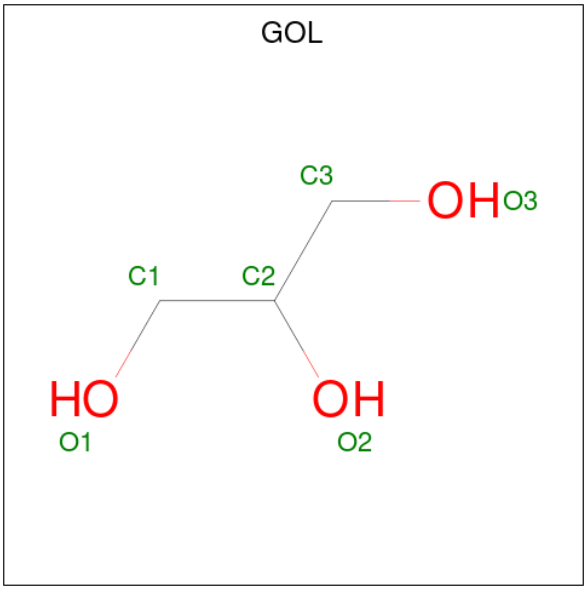
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
12	A	1	7	4	3	0	0
			Total	C	O		
12	A	1	10	6	4	0	0
			Total	C	O		
12	D	1	7	4	3	0	0
			Total	C	O		
12	D	1	4	2	2	0	0
			Total	C	O		
12	D	1	10	6	4	0	0

- Molecule 13 is [(R)-{[(2E,4Z,8Z)-dodeca-2,4,8-trien-1-yl]oxy}(naphthalen-1-yl)methyl]phosphonic acid (three-letter code: MFJ) (formula: $C_{23}H_{29}O_4P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
13	A	1	28	23	4	1	0	0

- Molecule 14 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 15 is water.

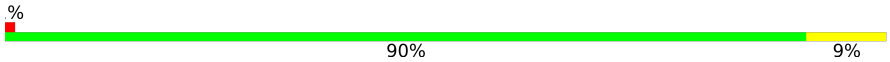
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
15	A	316	316	316	0	0
			Total	O		
15	B	265	265	265	0	0
			Total	O		
15	D	287	287	287	0	0
			Total	O		
15	C	278	278	278	0	0

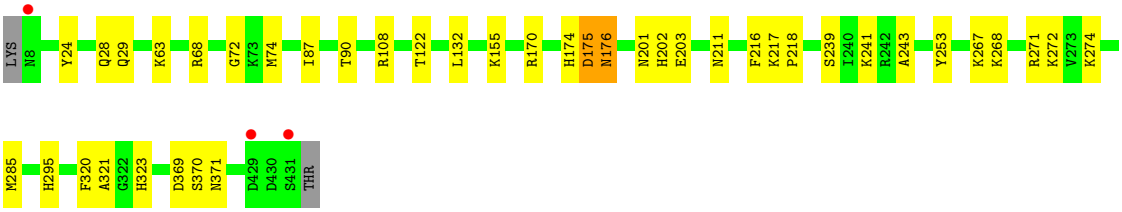
3 Residue-property plots (i)

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

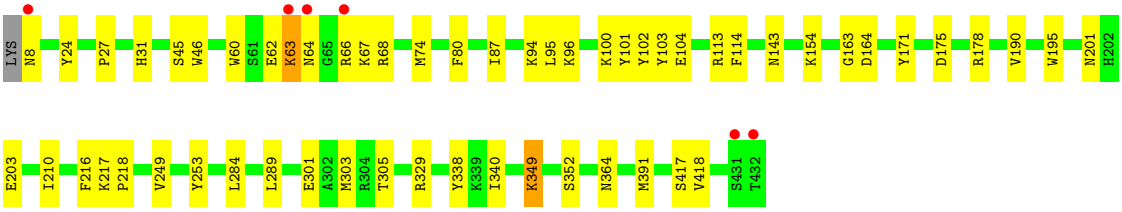
Chain A:





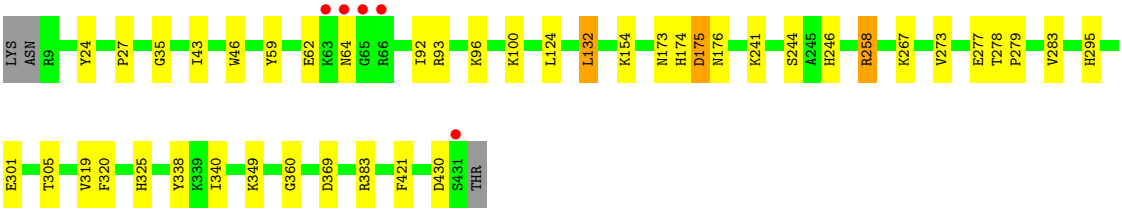
• Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

Chain B:



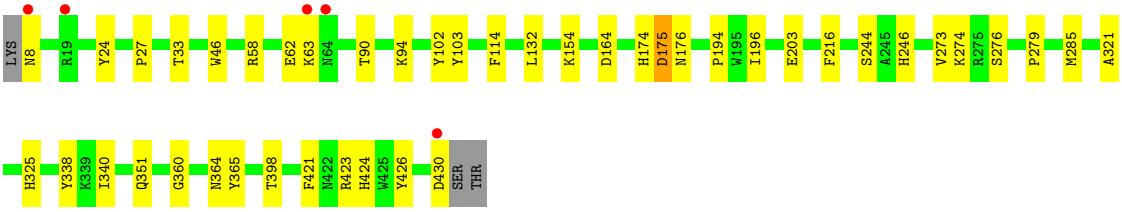
• Molecule 1: Fe(3+)-Zn(2+) purple acid phosphatase

Chain D:



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

Chain C:



• 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: 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 H: 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: 33% 33% 33%

• 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: 25% 50% 25%

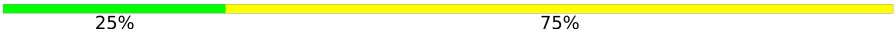
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 25% 75%

• 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:

• 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: 

• 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:

• Molecule 5: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	126.81Å 126.81Å 298.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (19.99-2.30) 97.8 (19.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.30Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.179 , 0.231 0.179 , 0.231	Depositor DCC
R_{free} test set	6057 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 53.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15939	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.46	0/3632	0.59	0/4938
1	B	0.43	0/3656	0.56	0/4969
1	C	0.47	0/3609	0.59	1/4909 (0.0%)
1	D	0.46	0/3613	0.58	1/4913 (0.0%)
All	All	0.45	0/14510	0.58	2/19729 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	132	LEU	CA-CB-CG	-6.27	100.87	115.30
1	C	132	LEU	CA-CB-CG	-5.68	102.24	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	3507	0	3327	33	0
1	B	3531	0	3353	33	0
1	C	3487	0	3296	28	0
1	D	3491	0	3313	31	0
2	E	38	0	34	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	38	0	34	2	0
2	K	38	0	34	0	0
2	M	38	0	34	1	0
3	F	49	0	43	1	0
3	I	49	0	43	0	0
3	J	49	0	43	0	0
3	N	49	0	43	1	0
4	G	71	0	61	0	0
5	L	24	0	22	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	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	14	0	13	0	0
8	B	14	0	13	1	0
8	C	42	0	39	0	0
8	D	28	0	26	0	0
9	A	20	0	0	2	0
9	B	40	0	0	4	0
9	C	20	0	0	1	0
9	D	15	0	0	1	0
10	A	2	0	0	0	0
10	C	2	0	0	0	0
10	D	1	0	0	0	0
11	A	12	0	18	0	0
11	B	8	0	12	0	0
11	C	20	0	30	0	0
11	D	16	0	24	1	0
12	A	17	0	23	4	0
12	D	21	0	27	1	0
13	A	28	0	0	7	0
14	D	6	0	8	1	0
15	A	316	0	0	5	1
15	B	265	0	0	5	0
15	C	278	0	0	6	0
15	D	287	0	0	9	0
All	All	15939	0	13913	135	1

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 5.

All (135) 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:A:68:ARG:NH1	9:A:519:SO4:O4	2.02	0.91
1:C:274:LYS:HE3	1:C:276:SER:H	1.34	0.89
1:D:154:LYS:NZ	15:D:601:HOH:O	2.04	0.89
1:B:96:LYS:NZ	15:B:603:HOH:O	2.19	0.74
15:C:601:HOH:O	2:M:2:FUC:O2	2.08	0.70
1:A:371:ASN:HB2	12:A:526:PGE:H4	1.74	0.70
1:A:370:SER:H	12:A:526:PGE:H3	1.59	0.67
1:C:351:GLN:NE2	1:C:423:ARG:HH12	1.92	0.67
9:B:517:SO4:O3	15:B:601:HOH:O	2.08	0.67
1:D:241:LYS:NZ	15:D:604:HOH:O	2.16	0.65
1:C:274:LYS:HE3	1:C:276:SER:N	2.11	0.64
1:D:277:GLU:OE1	15:D:603:HOH:O	2.14	0.64
9:B:516:SO4:O1	15:B:602:HOH:O	2.15	0.63
1:D:277:GLU:HG2	1:D:278:THR:HG23	1.82	0.62
13:A:528:MFJ:CAQ	1:D:258:ARG:HE	2.12	0.61
1:B:143:ASN:HD22	8:B:503:NAG:H83	1.67	0.59
1:D:301:GLU:O	1:D:305:THR:HG23	2.02	0.59
1:A:108:ARG:HB3	1:A:108:ARG:NH2	2.18	0.58
1:A:370:SER:N	12:A:526:PGE:H3	2.17	0.58
1:D:173:ASN:H	11:D:516:EDO:H22	1.67	0.58
1:A:241:LYS:NZ	15:A:601:HOH:O	2.13	0.56
1:D:27:PRO:HB3	1:D:46:TRP:CD1	2.41	0.56
1:D:421:PHE:CD2	1:D:430:ASP:HB3	2.41	0.56
13:A:528:MFJ:CAE	12:D:521:PGE:H3	2.37	0.55
1:A:371:ASN:ND2	15:A:611:HOH:O	2.41	0.54
1:D:258:ARG:NH1	15:D:612:HOH:O	2.38	0.54
1:A:211[A]:ASN:OD1	15:A:602:HOH:O	2.18	0.54
1:B:329:ARG:CZ	1:B:418:VAL:HG11	2.37	0.54
1:D:100:LYS:NZ	15:D:610:HOH:O	2.33	0.53
1:A:295:HIS:CE1	13:A:528:MFJ:CAK	2.92	0.52
1:C:27:PRO:HB3	1:C:46:TRP:CD1	2.44	0.52
1:C:424:HIS:HD2	15:C:850:HOH:O	1.92	0.52
1:A:108:ARG:HB3	1:A:108:ARG:HH21	1.73	0.52
1:A:268:LYS:HG2	1:A:272:LYS:HE3	1.92	0.52
1:C:8:ASN:ND2	15:C:608:HOH:O	2.43	0.51
1:B:104:GLU:HG2	1:B:113:ARG:HB2	1.93	0.51
1:B:249:VAL:HG22	1:B:284:LEU:HD12	1.92	0.51
1:C:364:ASN:OD1	1:C:365:TYR:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170[A]:ARG:NH2	15:A:609:HOH:O	2.39	0.50
1:C:421:PHE:CD2	1:C:430:ASP:HB3	2.47	0.49
1:C:103:TYR:CE1	1:C:114:PHE:HB2	2.48	0.49
1:D:267:LYS:HE2	15:D:853:HOH:O	2.12	0.49
1:B:66:ARG:HD2	1:B:68:ARG:NH2	2.28	0.49
1:D:62:GLU:HG3	1:D:100:LYS:HG2	1.95	0.48
1:A:295:HIS:HD1	1:A:369:ASP:CG	2.16	0.48
1:A:170[B]:ARG:NH1	12:A:527:PGE:H32	2.28	0.48
1:C:103:TYR:CZ	1:C:114:PHE:HB2	2.49	0.48
1:D:174:HIS:O	1:D:175:ASP:C	2.52	0.47
1:C:351:GLN:HE21	1:C:423:ARG:HH12	1.58	0.47
1:D:24:TYR:CD2	5:L:1:NAG:H82	2.48	0.47
1:D:349:LYS:NZ	15:D:617:HOH:O	2.47	0.47
1:A:63:LYS:HE3	1:A:63:LYS:HB2	1.53	0.47
1:A:72:GLY:HA3	1:A:90:THR:OG1	2.15	0.47
1:C:246:HIS:CE1	1:C:273:VAL:HG22	2.50	0.47
3:F:2:NAG:O5	3:F:4:FUC:H5	2.15	0.47
1:B:203:GLU:O	1:B:216:PHE:HA	2.14	0.47
1:C:62:GLU:HG3	1:C:102:TYR:HE2	1.79	0.47
1:A:201:ASN:HB3	1:A:253:TYR:CZ	2.51	0.46
1:C:24:TYR:CD2	3:N:1:NAG:H82	2.51	0.46
1:C:244:SER:HB2	1:C:279:PRO:HD2	1.97	0.46
1:C:285:MET:O	1:C:321:ALA:HA	2.16	0.46
1:B:349:LYS:CE	1:B:349:LYS:H	2.29	0.46
1:C:154:LYS:HE3	15:C:727:HOH:O	2.15	0.45
1:D:35:GLY:HA2	1:D:43:ILE:HG13	1.98	0.45
1:D:295:HIS:ND1	1:D:369:ASP:OD2	2.41	0.45
1:A:68:ARG:NH1	9:A:519:SO4:S	2.79	0.45
1:A:285:MET:O	1:A:321:ALA:HA	2.16	0.45
9:D:512:SO4:O3	15:D:606:HOH:O	2.21	0.45
1:C:90:THR:HA	9:C:515:SO4:O1	2.16	0.45
13:A:528:MFJ:OAB	13:A:528:MFJ:CAH	2.64	0.45
1:C:58:ARG:O	1:C:103:TYR:HA	2.16	0.45
1:B:289:LEU:HD21	1:B:303:MET:HG2	1.99	0.44
1:B:349:LYS:H	1:B:349:LYS:CD	2.31	0.44
9:B:517:SO4:O1	15:B:604:HOH:O	2.21	0.44
1:D:244:SER:HB2	1:D:279:PRO:HD2	1.99	0.44
1:A:203:GLU:O	1:A:216:PHE:HA	2.18	0.44
1:B:154:LYS:HB2	1:B:391[B]:MET:HE2	1.99	0.44
1:B:103:TYR:CZ	1:B:114:PHE:HB2	2.53	0.44
1:B:66:ARG:O	1:B:66:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:MET:HA	1:B:87:ILE:O	2.18	0.44
1:D:96:LYS:HD2	1:D:96:LYS:HA	1.81	0.44
1:A:174:HIS:O	1:A:175:ASP:C	2.57	0.43
1:A:211[B]:ASN:ND2	15:A:604:HOH:O	2.35	0.43
1:B:60:TRP:CD2	1:B:67:LYS:HE2	2.53	0.43
1:C:274:LYS:HA	1:C:274:LYS:HD2	1.82	0.43
1:A:28:GLN:HG3	1:A:29:GLN:HG3	2.00	0.43
1:C:398:THR:HG22	1:C:426:TYR:HB2	2.00	0.43
1:A:174:HIS:O	1:A:176:ASN:ND2	2.47	0.43
1:A:122:THR:HA	1:A:243:ALA:O	2.18	0.43
1:A:217:LYS:HB3	1:A:218:PRO:HD3	2.00	0.43
1:B:217:LYS:HB3	1:B:218:PRO:HD3	2.01	0.43
1:B:31:HIS:CD2	1:B:45:SER:HB2	2.54	0.42
1:B:171:TYR:CE1	1:B:178:ARG:HG3	2.54	0.42
1:B:349:LYS:N	1:B:349:LYS:HD3	2.33	0.42
1:C:33:THR:HA	1:C:194:PRO:HB3	2.01	0.42
1:A:267:LYS:HE2	1:A:271:ARG:NH1	2.34	0.42
1:B:95:LEU:HD22	1:B:101:TYR:CZ	2.53	0.42
1:B:301:GLU:O	1:B:305:THR:HG23	2.19	0.42
1:A:202:HIS:HE1	13:A:528:MFJ:CAZ	2.32	0.42
1:D:93:ARG:NH1	15:D:605:HOH:O	2.21	0.42
1:B:8:ASN:N	15:B:625:HOH:O	2.53	0.42
1:B:27:PRO:HB3	1:B:46:TRP:CD1	2.54	0.42
1:A:108:ARG:HH21	1:A:108:ARG:CB	2.31	0.42
1:D:132:LEU:HD13	1:D:320:PHE:CE1	2.54	0.42
1:A:74:MET:HA	1:A:87:ILE:O	2.20	0.42
1:C:338:TYR:CZ	1:C:340:ILE:HA	2.54	0.42
1:B:31:HIS:NE2	1:B:45:SER:HB2	2.35	0.41
1:B:201:ASN:HB3	1:B:253:TYR:CZ	2.55	0.41
1:B:338:TYR:CZ	1:B:340:ILE:HA	2.54	0.41
1:B:100:LYS:HE2	1:B:102:TYR:CZ	2.55	0.41
1:C:325:HIS:HA	1:C:360:GLY:O	2.20	0.41
1:B:80:PHE:CD1	1:B:210:ILE:HB	2.55	0.41
1:D:338:TYR:CZ	1:D:340:ILE:HA	2.55	0.41
2:H:2:FUC:H5	2:H:3:NAG:H83	2.02	0.41
1:B:163:GLY:O	1:B:164:ASP:HB2	2.21	0.41
1:C:196:ILE:HA	15:C:683:HOH:O	2.20	0.41
1:D:246:HIS:CE1	1:D:273:VAL:HG22	2.55	0.41
1:D:325:HIS:HA	1:D:360:GLY:O	2.20	0.41
1:D:383:ARG:HH21	14:D:518:GOL:H31	1.86	0.41
13:A:528:MFJ:CAR	1:D:258:ARG:HE	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLU:HB3	1:B:63:LYS:HE3	2.02	0.41
1:D:283:VAL:HB	1:D:319:VAL:HG22	2.01	0.41
1:C:174:HIS:O	1:C:175:ASP:C	2.58	0.41
1:A:24:TYR:CD2	2:E:1:NAG:H82	2.56	0.41
1:B:60:TRP:HB3	1:B:67:LYS:HA	2.02	0.41
1:D:24:TYR:CG	5:L:1:NAG:H82	2.55	0.41
1:D:59:TYR:CZ	1:D:92[A]:ILE:HG23	2.56	0.41
1:B:24:TYR:CD2	2:H:1:NAG:H82	2.56	0.41
1:A:132:LEU:HD22	1:A:320:PHE:CD1	2.56	0.40
1:B:190:VAL:HG23	1:B:195:TRP:CD1	2.56	0.40
1:D:124:LEU:HD12	1:D:279:PRO:HG3	2.03	0.40
1:C:203:GLU:O	1:C:216:PHE:HA	2.21	0.40
1:A:323:HIS:O	13:A:528:MFJ:OAD	2.39	0.40
1:C:94:LYS:HD3	15:C:798:HOH:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:795:HOH:O	15:A:859:HOH:O[5_554]	2.18	0.02

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	424/426 (100%)	400 (94%)	22 (5%)	2 (0%)	29	35
1	B	427/426 (100%)	405 (95%)	19 (4%)	3 (1%)	22	26
1	C	422/426 (99%)	402 (95%)	17 (4%)	3 (1%)	22	26
1	D	422/426 (99%)	403 (96%)	18 (4%)	1 (0%)	47	58
All	All	1695/1704 (100%)	1610 (95%)	76 (4%)	9 (0%)	29	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	175	ASP
1	A	175	ASP
1	B	64	ASN
1	B	175	ASP
1	B	364	ASN
1	D	175	ASP
1	A	155	LYS
1	C	63	LYS
1	C	164	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	375/375 (100%)	372 (99%)	3 (1%)	81 91
1	B	378/375 (101%)	373 (99%)	5 (1%)	69 82
1	C	372/375 (99%)	371 (100%)	1 (0%)	92 97
1	D	373/375 (100%)	370 (99%)	3 (1%)	81 91
All	All	1498/1500 (100%)	1486 (99%)	12 (1%)	81 91

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	A	239	SER
1	A	274	LYS
1	B	63	LYS
1	B	94	LYS
1	B	349	LYS
1	B	352	SER
1	B	417	SER
1	D	64	ASN
1	D	176	ASN
1	D	258	ARG

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Mol	Chain	Res	Type
1	C	176	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	ASN
1	C	29	GLN
1	C	351	GLN
1	C	424	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	0.65	0	17,19,21	1.08	1 (5%)
2	FUC	E	2	2	10,10,11	0.92	0	14,14,16	1.46	4 (28%)
2	NAG	E	3	2	14,14,15	0.79	1 (7%)	17,19,21	0.43	0
3	NAG	F	1	1,3	14,14,15	0.42	0	17,19,21	0.52	0
3	NAG	F	2	3	14,14,15	0.34	0	17,19,21	0.50	0
3	BMA	F	3	3	11,11,12	1.11	1 (9%)	15,15,17	0.78	0
3	FUC	F	4	3	10,10,11	0.94	0	14,14,16	1.31	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	G	1	4,1	14,14,15	0.33	0	17,19,21	0.71	1 (5%)
4	NAG	G	2	4	14,14,15	0.43	0	17,19,21	0.65	0
4	BMA	G	3	4	11,11,12	1.54	3 (27%)	15,15,17	1.01	0
4	MAN	G	4	4	11,11,12	0.87	1 (9%)	15,15,17	1.32	3 (20%)
4	MAN	G	5	4	11,11,12	1.54	3 (27%)	15,15,17	1.14	1 (6%)
4	FUC	G	6	4	10,10,11	0.92	1 (10%)	14,14,16	1.03	0
2	NAG	H	1	1,2	14,14,15	0.35	0	17,19,21	1.23	1 (5%)
2	FUC	H	2	2	10,10,11	0.69	0	14,14,16	1.62	4 (28%)
2	NAG	H	3	2	14,14,15	0.50	0	17,19,21	0.54	0
3	NAG	I	1	1,3	14,14,15	0.68	1 (7%)	17,19,21	1.54	2 (11%)
3	NAG	I	2	3	14,14,15	0.48	0	17,19,21	0.69	0
3	BMA	I	3	3	11,11,12	1.34	2 (18%)	15,15,17	0.97	1 (6%)
3	FUC	I	4	3	10,10,11	1.59	3 (30%)	14,14,16	1.84	3 (21%)
3	NAG	J	1	1,3	14,14,15	0.36	0	17,19,21	0.54	0
3	NAG	J	2	3	14,14,15	0.51	0	17,19,21	0.55	0
3	BMA	J	3	3	11,11,12	1.31	1 (9%)	15,15,17	0.96	0
3	FUC	J	4	3	10,10,11	1.04	0	14,14,16	1.49	3 (21%)
2	NAG	K	1	1,2	14,14,15	0.57	0	17,19,21	0.60	0
2	FUC	K	2	2	10,10,11	0.88	0	14,14,16	1.25	1 (7%)
2	NAG	K	3	2	14,14,15	0.37	0	17,19,21	0.63	0
5	NAG	L	1	5,1	14,14,15	0.31	0	17,19,21	0.81	1 (5%)
5	FUC	L	2	5	10,10,11	1.27	1 (10%)	14,14,16	1.12	1 (7%)
2	NAG	M	1	1,2	14,14,15	0.39	0	17,19,21	0.60	0
2	FUC	M	2	2	10,10,11	1.02	0	14,14,16	1.09	1 (7%)
2	NAG	M	3	2	14,14,15	0.63	1 (7%)	17,19,21	0.47	0
3	NAG	N	1	1,3	14,14,15	0.42	0	17,19,21	0.64	0
3	NAG	N	2	3	14,14,15	0.43	0	17,19,21	0.70	0
3	BMA	N	3	3	11,11,12	1.25	1 (9%)	15,15,17	1.43	2 (13%)
3	FUC	N	4	3	10,10,11	1.06	0	14,14,16	0.95	1 (7%)

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

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	N	3	BMA	C1-C2	3.28	1.59	1.52
3	I	4	FUC	O5-C1	-2.88	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3	BMA	C2-C3	2.81	1.56	1.52
4	G	3	BMA	C1-C2	2.74	1.58	1.52
4	G	5	MAN	C2-C3	2.54	1.56	1.52
3	J	3	BMA	C1-C2	2.45	1.57	1.52
3	I	3	BMA	C2-C3	2.40	1.56	1.52
4	G	5	MAN	C1-C2	2.40	1.57	1.52
4	G	4	MAN	C1-C2	2.37	1.57	1.52
3	I	3	BMA	C1-C2	2.34	1.57	1.52
3	I	1	NAG	O5-C1	2.32	1.47	1.43
3	I	4	FUC	C1-C2	2.27	1.57	1.52
3	F	3	BMA	C2-C3	2.25	1.55	1.52
2	E	3	NAG	O5-C1	2.24	1.47	1.43
5	L	2	FUC	O5-C5	2.24	1.48	1.43
3	I	4	FUC	C4-C5	2.20	1.57	1.52
4	G	5	MAN	O5-C5	2.18	1.47	1.43
4	G	3	BMA	C4-C3	2.16	1.57	1.52
2	M	3	NAG	C1-C2	2.09	1.55	1.52
4	G	6	FUC	C1-C2	2.04	1.56	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	1	NAG	O3-C3-C4	4.57	120.91	110.35
2	H	1	NAG	C1-O5-C5	4.46	118.24	112.19
3	I	4	FUC	O5-C1-C2	4.34	117.47	110.77
2	E	1	NAG	C1-O5-C5	3.83	117.39	112.19
3	N	3	BMA	C1-O5-C5	3.57	117.03	112.19
3	I	4	FUC	O2-C2-C1	3.56	116.44	109.15
3	I	1	NAG	C3-C4-C5	-3.38	104.21	110.24
2	E	2	FUC	C1-O5-C5	3.20	120.03	112.78
3	J	4	FUC	C1-C2-C3	-3.08	105.87	109.67
5	L	2	FUC	O2-C2-C1	2.98	115.26	109.15
2	K	2	FUC	C1-O5-C5	2.91	119.38	112.78
2	H	2	FUC	C1-C2-C3	-2.81	106.21	109.67
4	G	4	MAN	C1-O5-C5	2.79	115.97	112.19
3	J	4	FUC	O2-C2-C1	2.79	114.85	109.15
2	H	2	FUC	C1-O5-C5	2.73	118.95	112.78
2	H	2	FUC	O5-C5-C4	2.71	114.39	109.52
2	H	2	FUC	C2-C3-C4	-2.58	106.43	110.89
2	E	2	FUC	C2-C3-C4	-2.51	106.55	110.89
3	F	4	FUC	C2-C3-C4	-2.49	106.58	110.89
4	G	1	NAG	C1-O5-C5	2.49	115.56	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	4	FUC	C2-C3-C4	-2.40	106.74	110.89
5	L	1	NAG	C1-O5-C5	2.38	115.42	112.19
2	M	2	FUC	C1-O5-C5	2.38	118.17	112.78
3	I	4	FUC	O3-C3-C2	-2.32	105.55	109.99
3	I	3	BMA	C1-O5-C5	2.29	115.29	112.19
3	N	4	FUC	C1-O5-C5	2.21	117.78	112.78
4	G	4	MAN	O2-C2-C3	-2.19	105.75	110.14
4	G	4	MAN	C1-C2-C3	2.18	112.35	109.67
3	N	3	BMA	C1-C2-C3	2.15	112.31	109.67
2	E	2	FUC	O2-C2-C1	2.11	113.46	109.15
4	G	5	MAN	O2-C2-C1	2.04	113.34	109.15
2	E	2	FUC	O5-C5-C4	2.00	113.11	109.52

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	3	NAG	O5-C5-C6-O6
2	K	3	NAG	C4-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	M	3	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
2	E	3	NAG	C8-C7-N2-C2
2	E	3	NAG	O7-C7-N2-C2
2	H	3	NAG	C8-C7-N2-C2
2	H	3	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	N	2	NAG	C8-C7-N2-C2
3	N	2	NAG	O7-C7-N2-C2
2	M	3	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	E	3	NAG	O5-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
2	E	3	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
4	G	4	MAN	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
2	H	3	NAG	C4-C5-C6-O6

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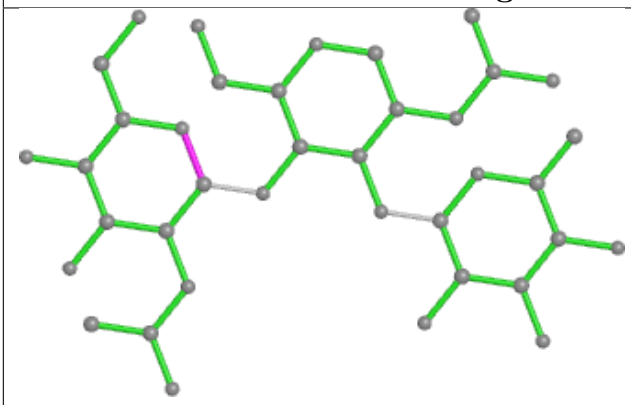
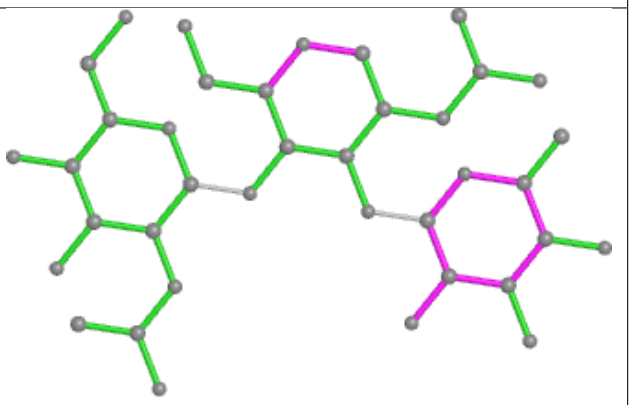
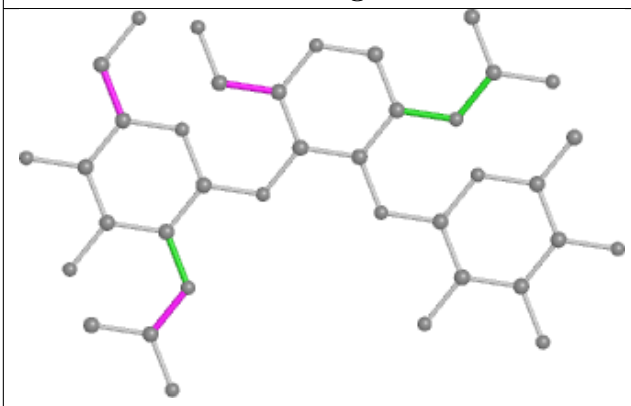
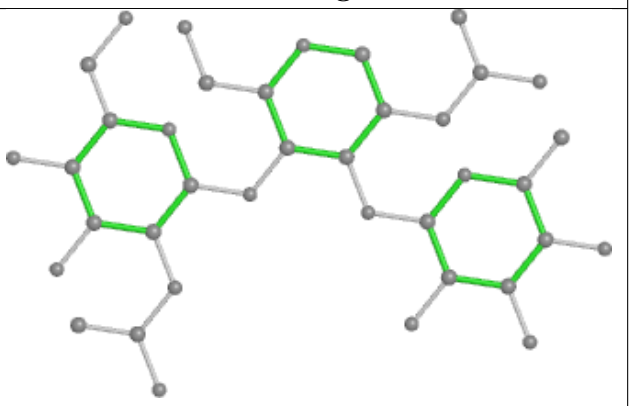
Mol	Chain	Res	Type	Atoms
2	H	3	NAG	O5-C5-C6-O6
5	L	1	NAG	C4-C5-C6-O6
5	L	1	NAG	O5-C5-C6-O6

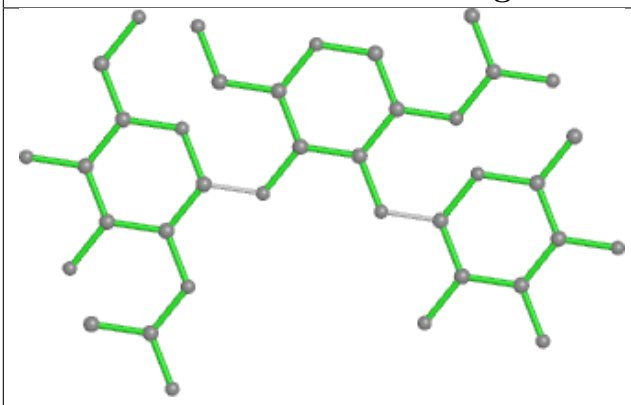
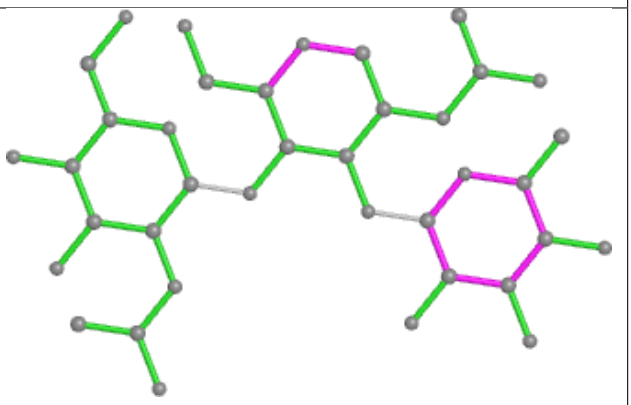
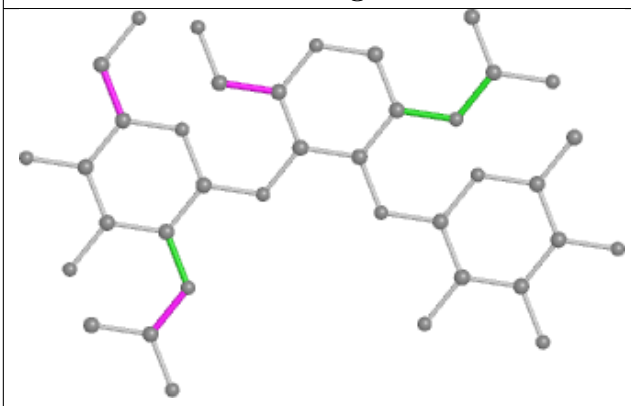
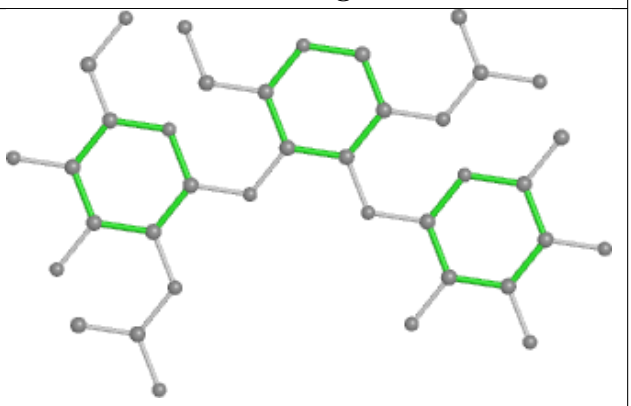
There are no ring outliers.

9 monomers are involved in 8 short contacts:

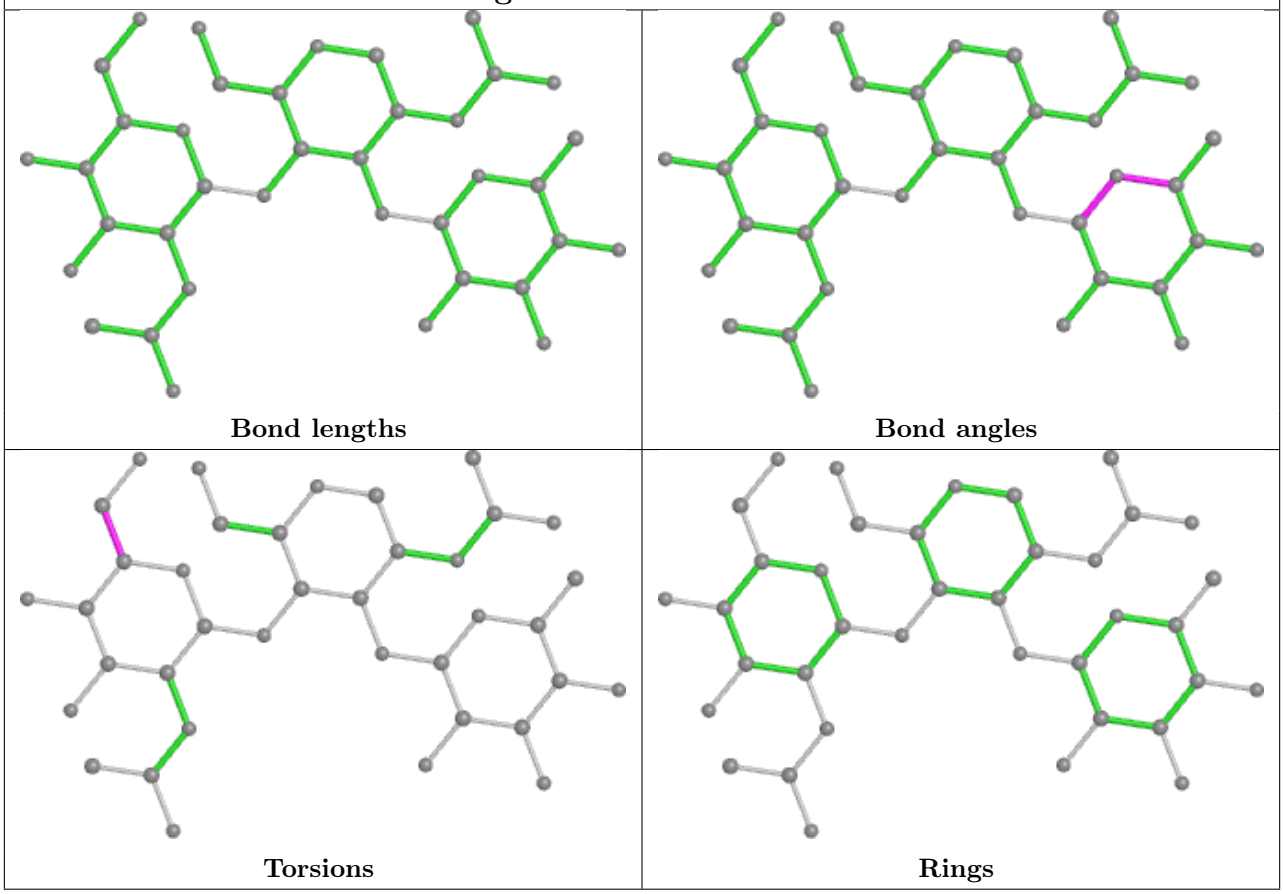
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	4	FUC	1	0
2	E	1	NAG	1	0
2	H	2	FUC	1	0
5	L	1	NAG	2	0
3	N	1	NAG	1	0
2	H	1	NAG	1	0
2	H	3	NAG	1	0
3	F	2	NAG	1	0
2	M	2	FUC	1	0

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

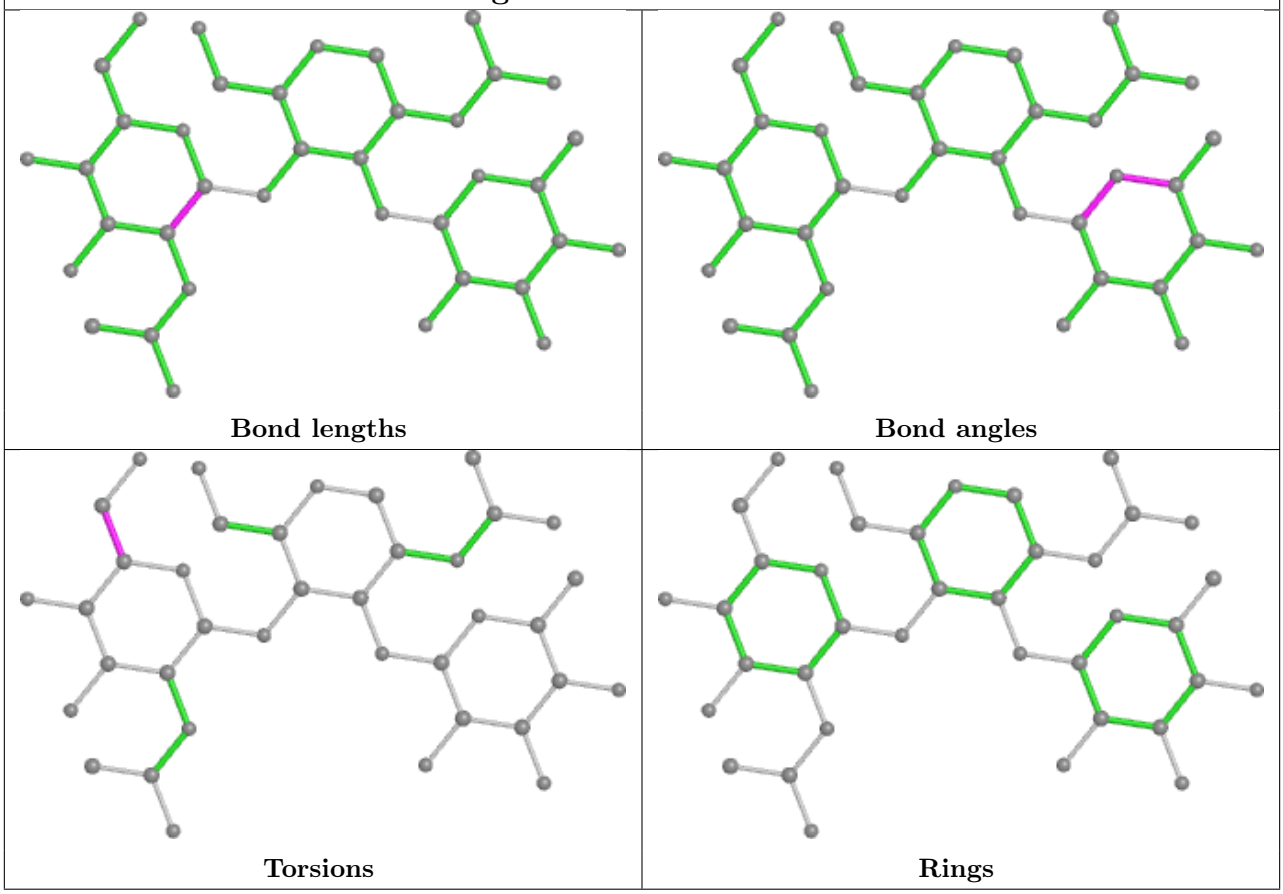
Oligosaccharide Chain E	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

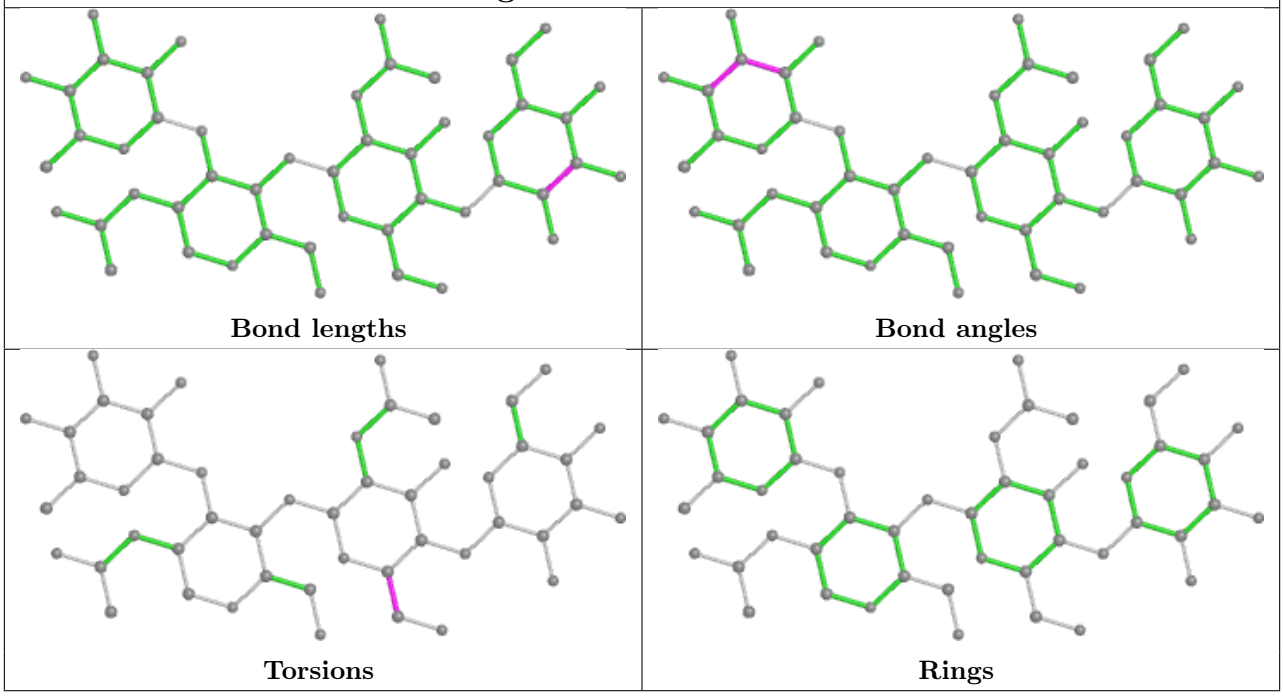
Oligosaccharide Chain K



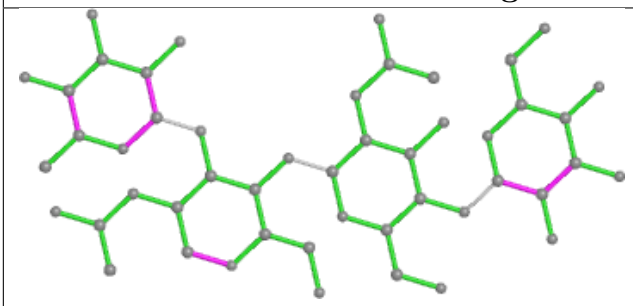
Oligosaccharide Chain M



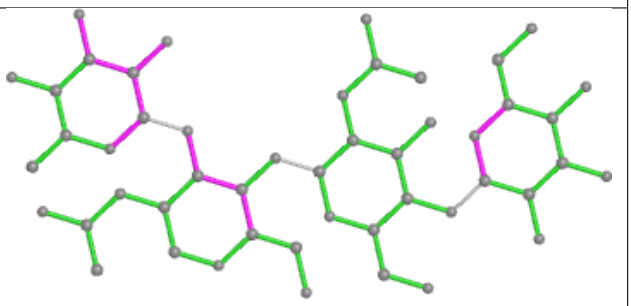
Oligosaccharide Chain F



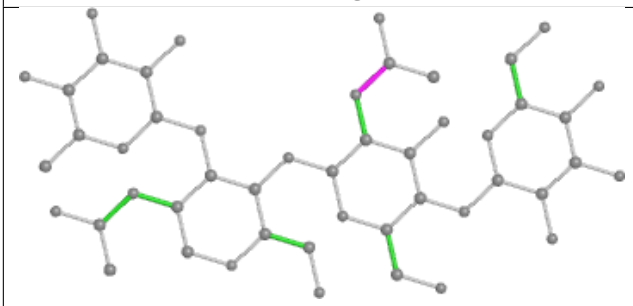
Oligosaccharide Chain I



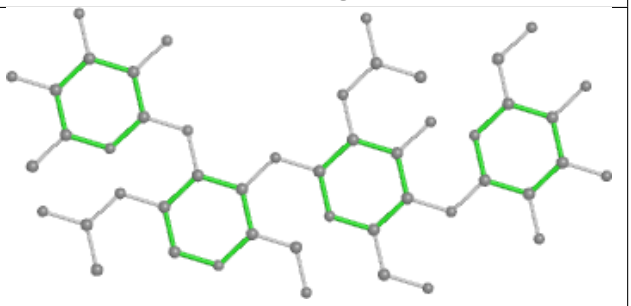
Bond lengths



Bond angles

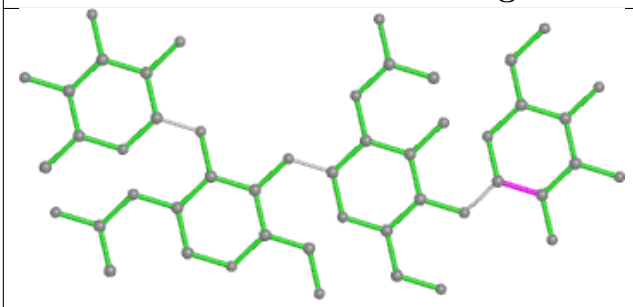


Torsions

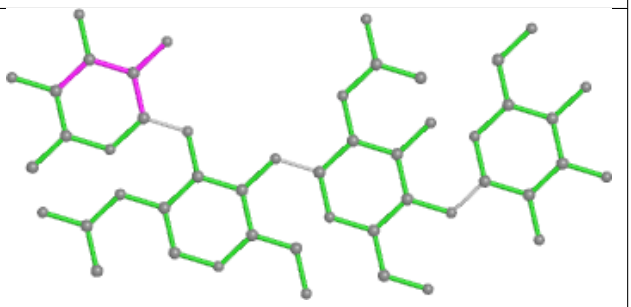


Rings

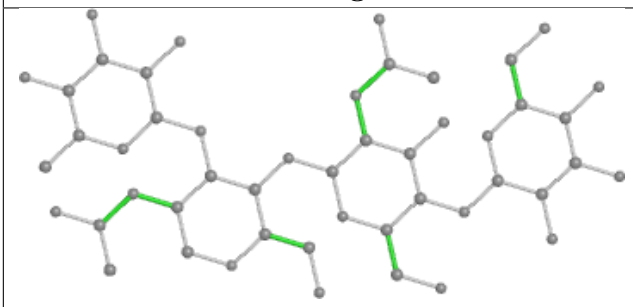
Oligosaccharide Chain J



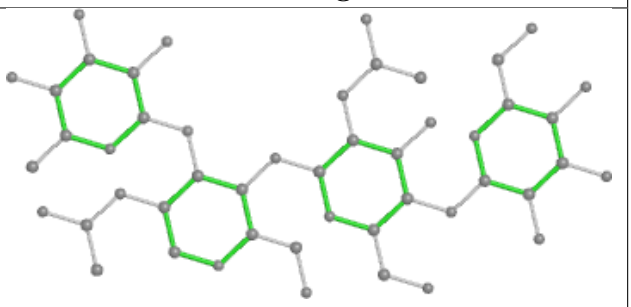
Bond lengths



Bond angles

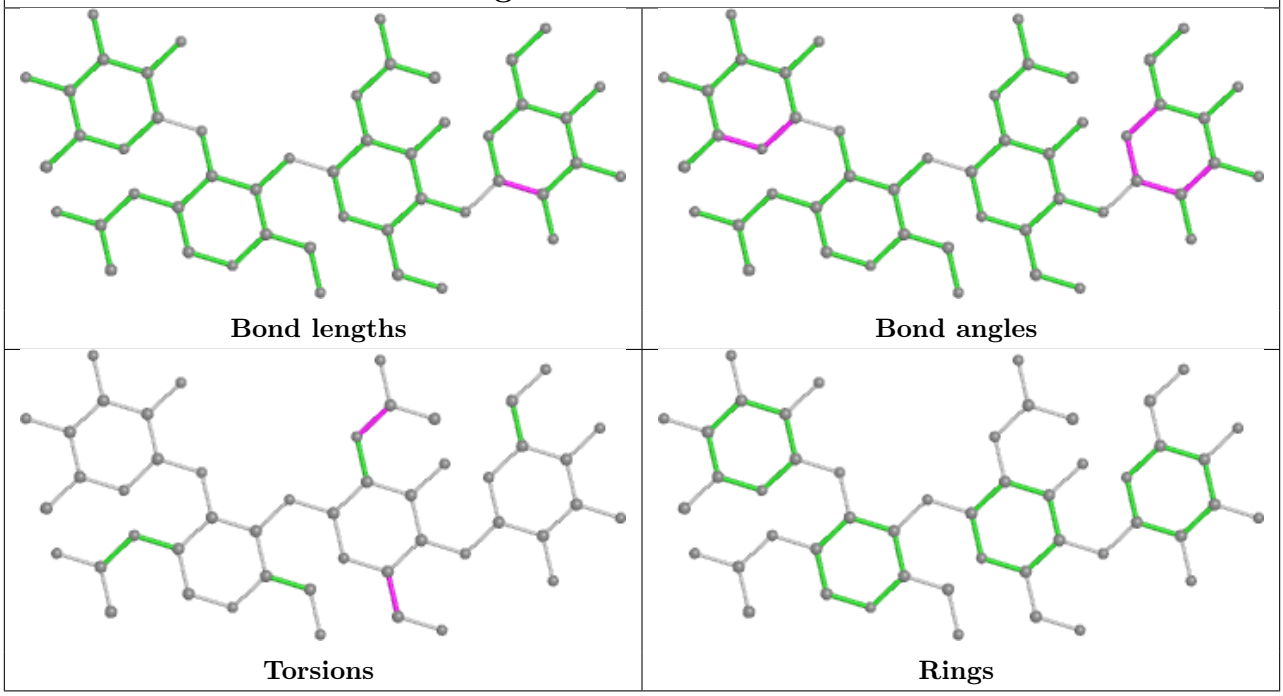


Torsions

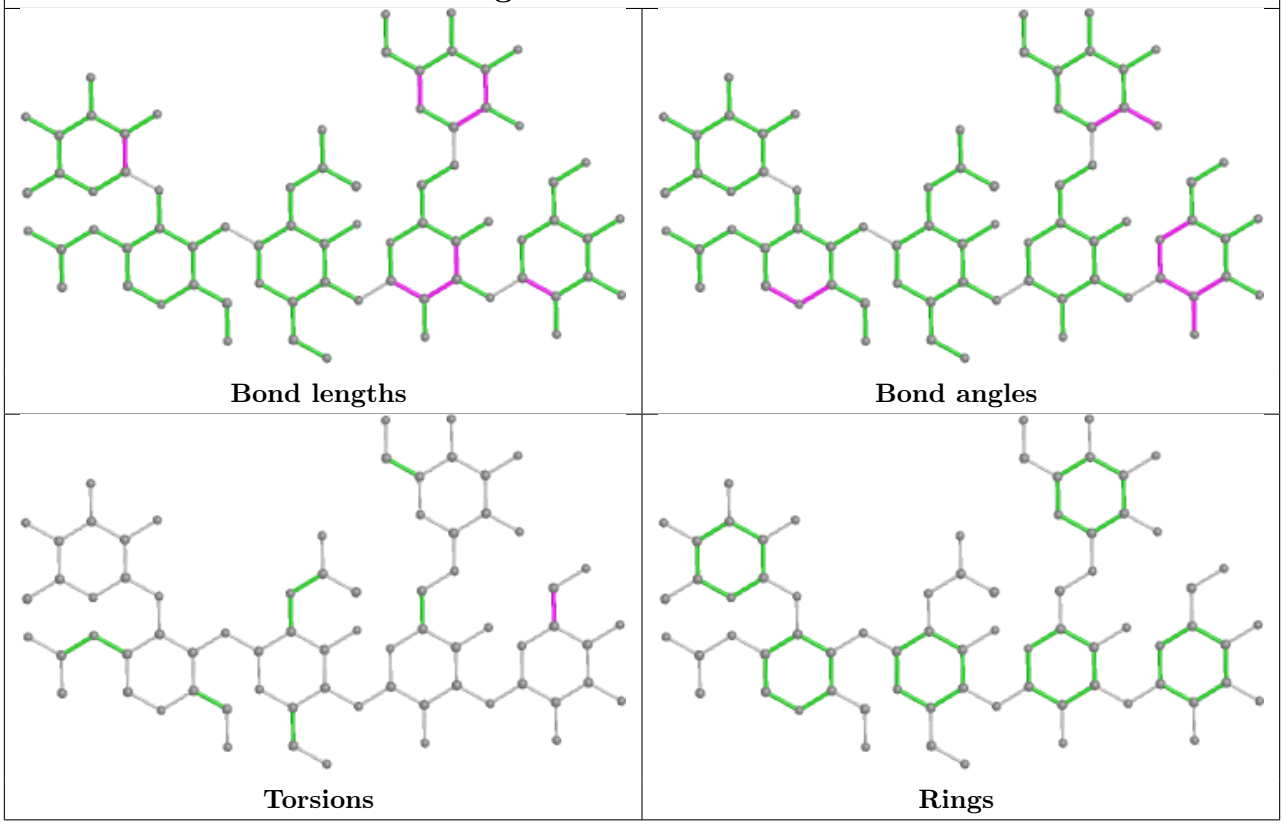


Rings

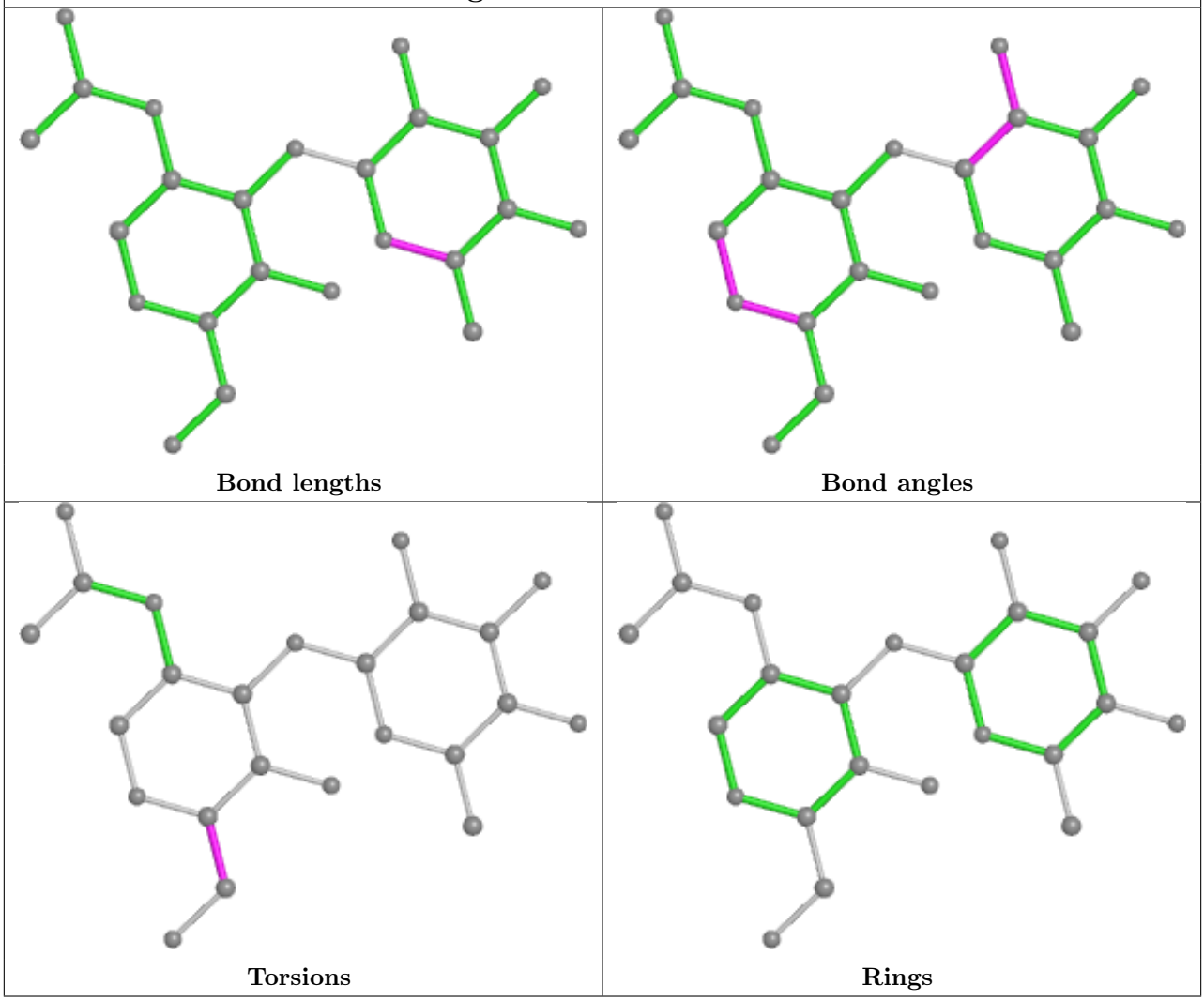
Oligosaccharide Chain N



Oligosaccharide Chain G



Oligosaccharide Chain L



5.6 Ligand geometry (i)

Of 60 ligands modelled in this entry, 13 are monoatomic - leaving 47 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	EDO	C	518	-	3,3,3	0.48	0	2,2,2	0.76	0
8	NAG	C	503	1	14,14,15	0.88	2 (14%)	17,19,21	0.80	0
11	EDO	A	525	-	3,3,3	0.69	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	PGE	A	527	-	9,9,9	0.39	0	8,8,8	0.37	0
9	SO4	C	512	-	4,4,4	0.19	0	6,6,6	0.28	0
11	EDO	D	504	-	3,3,3	0.60	0	2,2,2	0.26	0
11	EDO	D	517	-	3,3,3	0.61	0	2,2,2	0.56	0
8	NAG	D	503	1	14,14,15	0.42	0	17,19,21	0.54	0
8	NAG	B	503	1	14,14,15	0.38	0	17,19,21	0.78	1 (5%)
11	EDO	D	516	-	3,3,3	0.47	0	2,2,2	0.44	0
12	PGE	D	519	-	6,6,9	0.33	0	5,5,8	0.32	0
12	PGE	D	521	-	9,9,9	0.42	0	8,8,8	0.27	0
11	EDO	B	524	-	3,3,3	0.43	0	2,2,2	0.63	0
9	SO4	C	513	-	4,4,4	0.20	0	6,6,6	0.16	0
9	SO4	B	515	-	4,4,4	0.11	0	6,6,6	0.30	0
14	GOL	D	518	-	5,5,5	0.78	0	5,5,5	1.16	0
9	SO4	B	519	-	4,4,4	0.16	0	6,6,6	0.19	0
9	SO4	B	521	-	4,4,4	0.14	0	6,6,6	0.14	0
11	EDO	B	523	-	3,3,3	0.48	0	2,2,2	0.50	0
9	SO4	A	519	10	4,4,4	0.23	0	6,6,6	0.40	0
9	SO4	B	516	10	4,4,4	0.29	0	6,6,6	0.20	0
9	SO4	B	517	-	4,4,4	0.12	0	6,6,6	0.36	0
12	PGE	A	526	-	6,6,9	0.23	0	5,5,8	0.37	0
9	SO4	B	518	-	4,4,4	0.24	0	6,6,6	0.34	0
9	SO4	B	522	-	4,4,4	0.18	0	6,6,6	0.13	0
9	SO4	A	518	-	4,4,4	0.21	0	6,6,6	0.38	0
11	EDO	D	515	-	3,3,3	0.59	0	2,2,2	0.07	0
8	NAG	D	510	1	14,14,15	0.84	1 (7%)	17,19,21	0.77	1 (5%)
11	EDO	C	520	-	3,3,3	0.45	0	2,2,2	0.76	0
9	SO4	D	512	-	4,4,4	0.12	0	6,6,6	0.25	0
9	SO4	A	517	-	4,4,4	0.21	0	6,6,6	0.13	0
11	EDO	A	524	-	3,3,3	0.72	0	2,2,2	0.32	0
9	SO4	D	511	-	4,4,4	0.20	0	6,6,6	0.27	0
9	SO4	D	513	-	4,4,4	0.18	0	6,6,6	0.26	0
11	EDO	C	521	-	3,3,3	0.39	0	2,2,2	0.86	0
11	EDO	C	522	-	3,3,3	0.50	0	2,2,2	0.39	0
11	EDO	C	519	-	3,3,3	0.50	0	2,2,2	0.46	0
13	MFJ	A	528	6,7	27,29,29	2.05	7 (25%)	31,37,37	1.81	10 (32%)
8	NAG	A	503	1	14,14,15	0.54	0	17,19,21	0.70	1 (5%)
8	NAG	C	523	1	14,14,15	1.87	2 (14%)	17,19,21	1.64	4 (23%)
9	SO4	C	515	-	4,4,4	0.19	0	6,6,6	0.24	0
11	EDO	A	523	-	3,3,3	0.63	0	2,2,2	0.23	0
9	SO4	C	514	-	4,4,4	0.15	0	6,6,6	0.12	0
9	SO4	B	520	-	4,4,4	0.17	0	6,6,6	0.23	0
9	SO4	A	520	-	4,4,4	0.17	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	C	507	1	14,14,15	0.57	0	17,19,21	0.62	0
12	PGE	D	520	-	3,3,9	0.36	0	2,2,8	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	EDO	C	518	-	-	1/1/1/1	-
8	NAG	C	503	1	-	2/6/23/26	0/1/1/1
11	EDO	A	525	-	-	1/1/1/1	-
12	PGE	A	527	-	-	2/7/7/7	-
11	EDO	D	504	-	-	0/1/1/1	-
11	EDO	D	517	-	-	1/1/1/1	-
8	NAG	D	503	1	-	2/6/23/26	0/1/1/1
8	NAG	B	503	1	-	4/6/23/26	0/1/1/1
11	EDO	D	516	-	-	0/1/1/1	-
12	PGE	D	519	-	-	1/4/4/7	-
12	PGE	D	521	-	-	4/7/7/7	-
11	EDO	B	524	-	-	0/1/1/1	-
14	GOL	D	518	-	-	2/4/4/4	-
11	EDO	B	523	-	-	1/1/1/1	-
12	PGE	A	526	-	-	1/4/4/7	-
11	EDO	D	515	-	-	1/1/1/1	-
8	NAG	D	510	1	-	1/6/23/26	0/1/1/1
11	EDO	C	520	-	-	1/1/1/1	-
11	EDO	A	524	-	-	1/1/1/1	-
11	EDO	C	521	-	-	0/1/1/1	-
11	EDO	C	522	-	-	0/1/1/1	-
11	EDO	C	519	-	-	0/1/1/1	-
13	MFJ	A	528	6,7	-	9/20/23/23	0/2/2/2
8	NAG	A	503	1	-	0/6/23/26	0/1/1/1
8	NAG	C	523	1	-	4/6/23/26	0/1/1/1
11	EDO	A	523	-	-	1/1/1/1	-
8	NAG	C	507	1	-	0/6/23/26	0/1/1/1
12	PGE	D	520	-	-	1/1/1/7	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	528	MFJ	CAY-CAX	5.11	1.51	1.33
8	C	523	NAG	C1-C2	-5.04	1.44	1.52
13	A	528	MFJ	CAZ-CBA	4.54	1.49	1.33
13	A	528	MFJ	PBH-OAC	-4.23	1.48	1.54
13	A	528	MFJ	CBF-CBE	-3.95	1.35	1.43
8	C	523	NAG	C8-C7	3.91	1.58	1.50
13	A	528	MFJ	CAU-CAT	3.48	1.51	1.31
8	D	510	NAG	O5-C1	2.81	1.48	1.43
13	A	528	MFJ	OBC-CBB	-2.41	1.37	1.43
8	C	503	NAG	O5-C1	2.26	1.47	1.43
8	C	503	NAG	C1-C2	2.20	1.55	1.52
13	A	528	MFJ	CAZ-CAY	2.01	1.50	1.44

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	A	528	MFJ	CBG-CBD-CBF	3.81	124.26	119.75
8	C	523	NAG	C1-O5-C5	-3.37	107.63	112.19
13	A	528	MFJ	CAI-CBE-CBF	3.24	123.38	119.12
13	A	528	MFJ	OAD-PBH-OAB	-3.21	105.39	113.45
8	C	523	NAG	C2-N2-C7	3.06	127.26	122.90
13	A	528	MFJ	CBB-CBA-CAZ	-3.00	117.88	125.07
13	A	528	MFJ	CAJ-CAG-CAH	-2.95	116.28	120.99
13	A	528	MFJ	OAC-PBH-OAB	-2.82	106.37	113.45
13	A	528	MFJ	OBC-CBB-CBA	2.71	119.81	110.39
13	A	528	MFJ	CAJ-CBE-CAI	-2.50	117.34	123.19
8	C	523	NAG	C8-C7-N2	2.44	120.23	116.10
8	B	503	NAG	C1-O5-C5	2.41	115.46	112.19
8	C	523	NAG	C1-C2-N2	2.36	114.52	110.49
8	D	510	NAG	C1-O5-C5	2.23	115.22	112.19
13	A	528	MFJ	CAG-CAJ-CBE	2.23	123.93	120.44
8	A	503	NAG	C1-O5-C5	2.15	115.11	112.19
13	A	528	MFJ	OAD-PBH-OAC	-2.14	101.88	107.64

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	528	MFJ	CAX-CAY-CAZ-CBA
13	A	528	MFJ	CAH-CBD-CBG-OBC
13	A	528	MFJ	CAH-CBD-CBG-PBH
13	A	528	MFJ	CBD-CBG-PBH-OAB

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Mol	Chain	Res	Type	Atoms
13	A	528	MFJ	CBD-CBG-PBH-OAD
13	A	528	MFJ	OBC-CBG-PBH-OAB
14	D	518	GOL	O1-C1-C2-O2
14	D	518	GOL	O1-C1-C2-C3
8	C	523	NAG	C4-C5-C6-O6
8	C	503	NAG	C4-C5-C6-O6
12	A	527	PGE	C1-C2-O2-C3
8	C	523	NAG	O5-C5-C6-O6
8	B	503	NAG	C8-C7-N2-C2
8	B	503	NAG	O7-C7-N2-C2
8	C	523	NAG	C8-C7-N2-C2
8	C	523	NAG	O7-C7-N2-C2
12	D	521	PGE	O2-C3-C4-O3
12	D	521	PGE	O3-C5-C6-O4
8	C	503	NAG	O5-C5-C6-O6
12	A	527	PGE	O3-C5-C6-O4
12	D	520	PGE	O2-C3-C4-O3
8	D	503	NAG	C4-C5-C6-O6
11	D	515	EDO	O1-C1-C2-O2
12	D	521	PGE	C1-C2-O2-C3
8	D	503	NAG	O5-C5-C6-O6
13	A	528	MFJ	CBD-CBG-PBH-OAC
11	A	524	EDO	O1-C1-C2-O2
11	B	523	EDO	O1-C1-C2-O2
8	D	510	NAG	O5-C5-C6-O6
11	D	517	EDO	O1-C1-C2-O2
11	C	518	EDO	O1-C1-C2-O2
12	A	526	PGE	C6-C5-O3-C4
12	D	519	PGE	O2-C3-C4-O3
13	A	528	MFJ	CAV-CAW-CAX-CAY
12	D	521	PGE	C3-C4-O3-C5
11	A	525	EDO	O1-C1-C2-O2
13	A	528	MFJ	CAZ-CBA-CBB-OBC
11	A	523	EDO	O1-C1-C2-O2
8	B	503	NAG	O5-C5-C6-O6
11	C	520	EDO	O1-C1-C2-O2
8	B	503	NAG	C4-C5-C6-O6

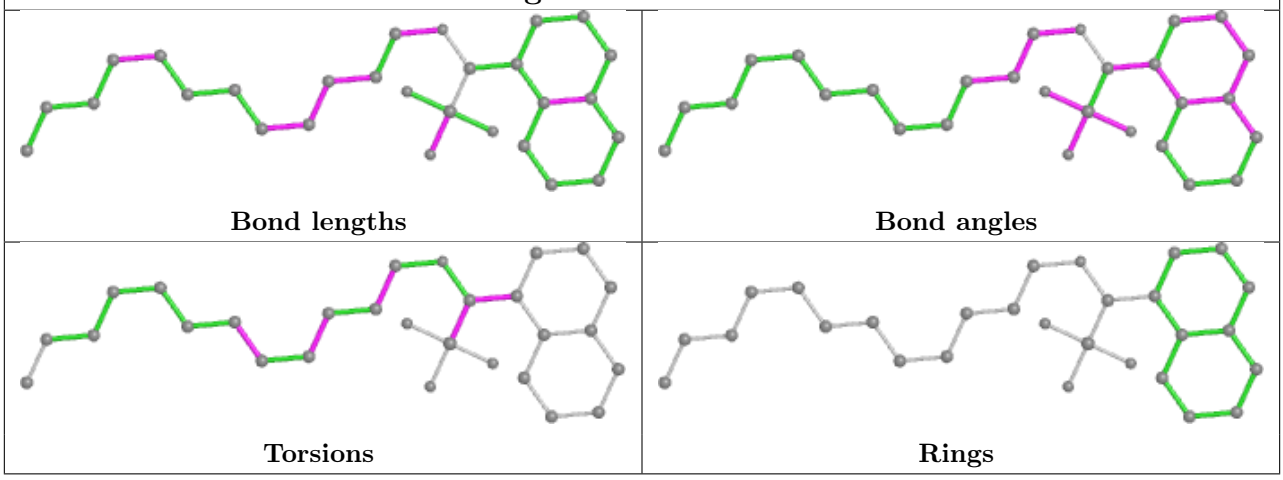
There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	527	PGE	1	0
8	B	503	NAG	1	0
11	D	516	EDO	1	0
12	D	521	PGE	1	0
14	D	518	GOL	1	0
9	A	519	SO4	2	0
9	B	516	SO4	2	0
9	B	517	SO4	2	0
12	A	526	PGE	3	0
9	D	512	SO4	1	0
13	A	528	MFJ	7	0
9	C	515	SO4	1	0

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

Ligand MFJ A 528



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	424/426 (99%)	-0.65	3 (0%)	87	91	22, 29, 42, 70	0
1	B	425/426 (99%)	-0.54	6 (1%)	75	80	24, 34, 47, 73	0
1	C	423/426 (99%)	-0.56	5 (1%)	79	83	23, 32, 45, 76	0
1	D	423/426 (99%)	-0.56	5 (1%)	79	83	24, 32, 45, 74	0
All	All	1695/1704 (99%)	-0.58	19 (1%)	80	85	22, 32, 45, 76	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	431	SER	6.6
1	B	432	THR	4.2
1	A	431	SER	3.8
1	C	8	ASN	3.7
1	B	63	LYS	3.7
1	D	64	ASN	3.5
1	B	431	SER	3.5
1	B	64	ASN	3.3
1	C	63	LYS	3.1
1	A	429	ASP	2.9
1	C	64	ASN	2.8
1	D	66	ARG	2.7
1	D	63	LYS	2.6
1	A	8	ASN	2.5
1	B	66	ARG	2.2
1	C	19	ARG	2.2
1	C	430	ASP	2.1
1	B	8	ASN	2.1
1	D	65	GLY	2.0

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

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

6.3 Carbohydrates (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
4	MAN	G	5	11/12	0.68	0.48	80,81,93,93	0
4	BMA	G	3	11/12	0.72	0.29	59,66,80,84	0
3	BMA	J	3	11/12	0.72	0.34	66,72,78,81	0
2	NAG	E	3	14/15	0.74	0.38	67,83,93,94	0
2	NAG	H	3	14/15	0.80	0.50	73,86,97,97	0
2	NAG	E	1	14/15	0.81	0.25	48,59,76,80	0
3	NAG	N	2	14/15	0.81	0.36	66,75,81,83	0
3	FUC	I	4	10/11	0.82	0.36	58,62,67,69	0
3	BMA	I	3	11/12	0.83	0.27	55,62,67,71	0
3	BMA	F	3	11/12	0.84	0.29	64,76,80,83	0
2	NAG	H	1	14/15	0.85	0.20	45,65,75,81	0
3	BMA	N	3	11/12	0.86	0.44	76,83,88,91	0
3	NAG	F	2	14/15	0.86	0.30	46,68,73,77	0
2	FUC	H	2	10/11	0.86	0.34	72,77,83,87	0
5	NAG	L	1	14/15	0.86	0.18	47,54,60,62	0
5	FUC	L	2	10/11	0.86	0.24	54,62,66,68	0
3	NAG	I	2	14/15	0.87	0.33	54,65,70,71	0
3	NAG	N	1	14/15	0.88	0.14	41,58,66,69	0
2	NAG	M	3	14/15	0.88	0.29	39,51,59,63	0
3	FUC	F	4	10/11	0.88	0.33	63,67,72,75	0
3	FUC	N	4	10/11	0.88	0.24	51,61,66,66	0
4	MAN	G	4	11/12	0.89	0.34	60,69,75,75	0
2	FUC	E	2	10/11	0.91	0.30	68,71,79,82	0
3	NAG	J	2	14/15	0.91	0.19	37,47,56,64	0
3	NAG	I	1	14/15	0.91	0.19	37,49,61,61	0
2	FUC	K	2	10/11	0.92	0.23	48,53,59,59	0
2	NAG	K	1	14/15	0.93	0.12	36,40,42,51	0
3	NAG	F	1	14/15	0.93	0.13	45,53,60,63	0
3	FUC	J	4	10/11	0.93	0.15	40,46,54,59	0
2	NAG	K	3	14/15	0.93	0.26	37,50,63,64	0
2	FUC	M	2	10/11	0.94	0.21	50,53,55,56	0
3	NAG	J	1	14/15	0.94	0.12	28,41,46,47	0

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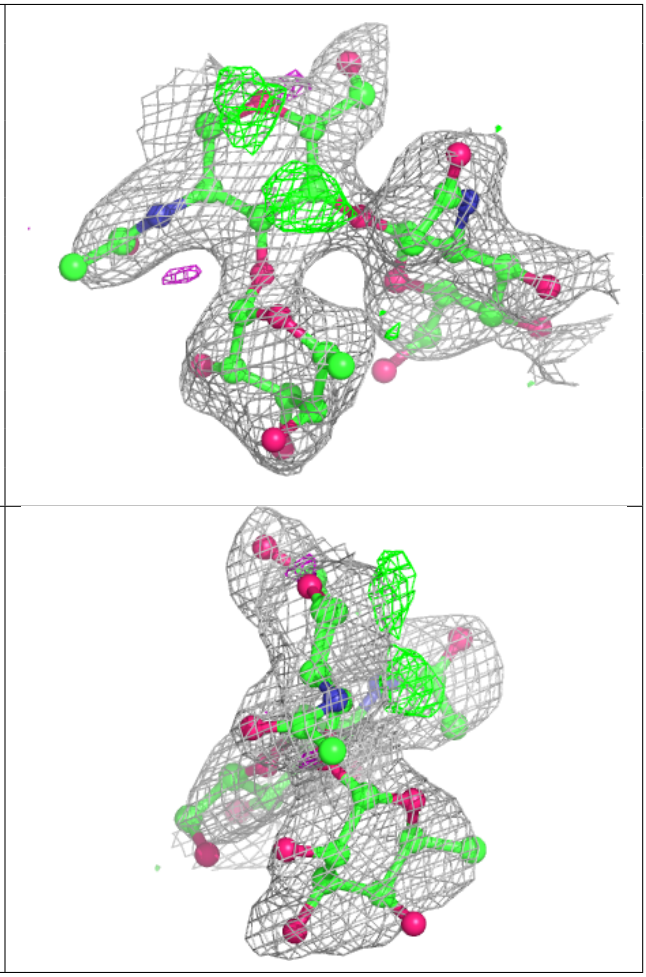
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	G	1	14/15	0.95	0.11	32,36,42,44	0
2	NAG	M	1	14/15	0.95	0.11	39,43,48,52	0
4	NAG	G	2	14/15	0.96	0.11	34,44,48,52	0
4	FUC	G	6	10/11	0.96	0.21	38,46,48,54	0

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.

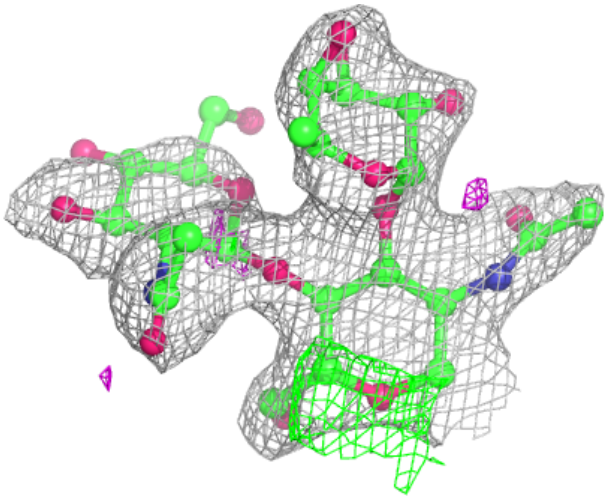
Electron density around Chain E:

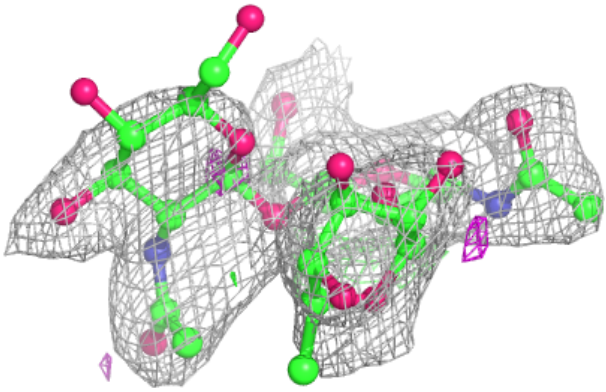
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

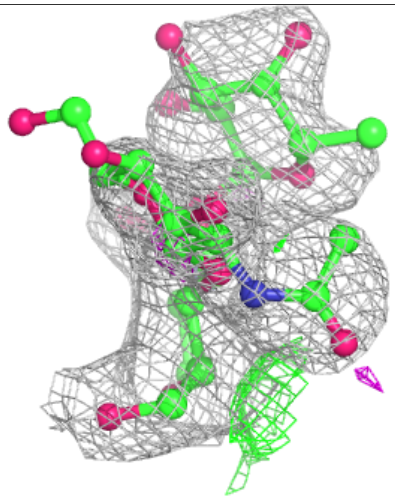


Electron density around Chain H:

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

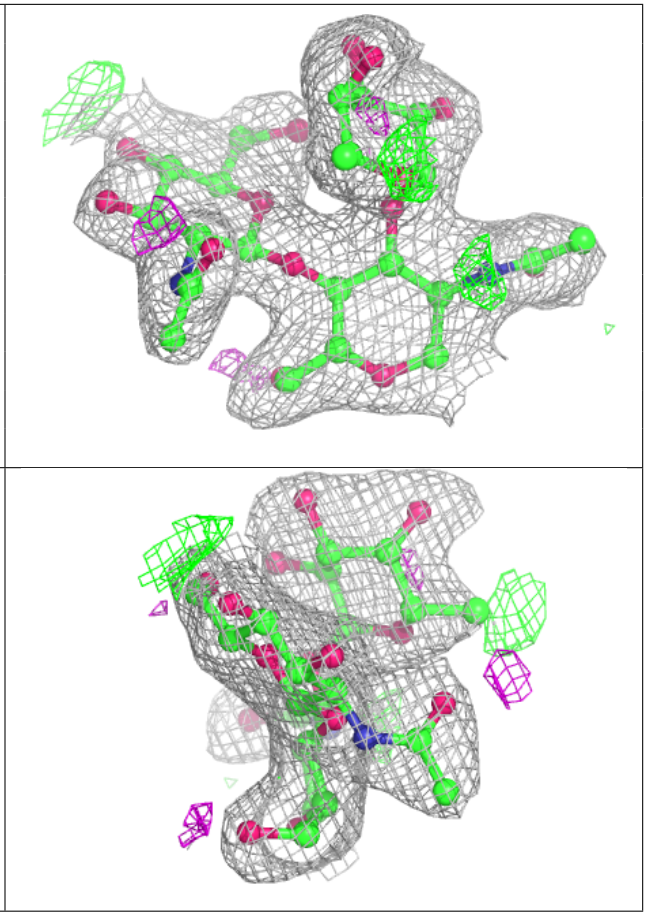






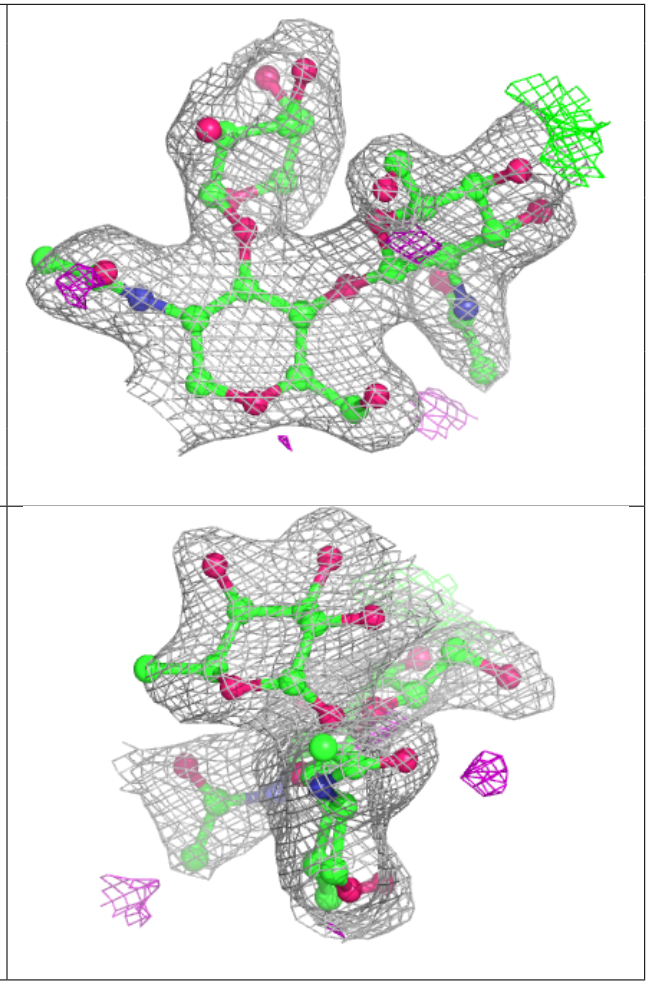
Electron density around Chain K:

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



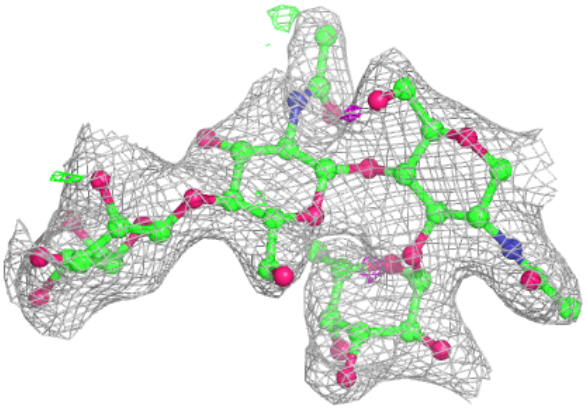
Electron density around Chain M:

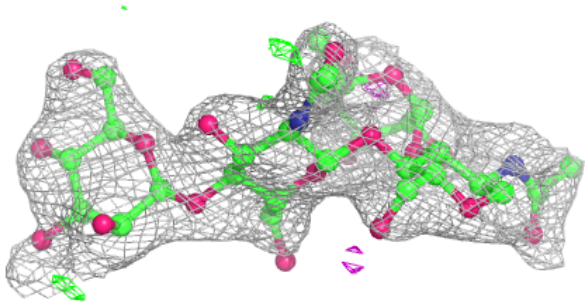
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

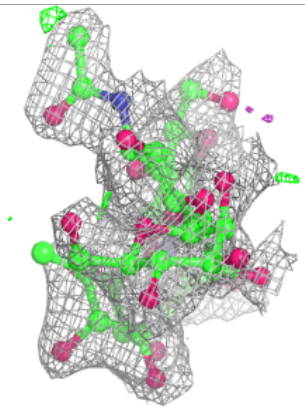


Electron density around Chain F:

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

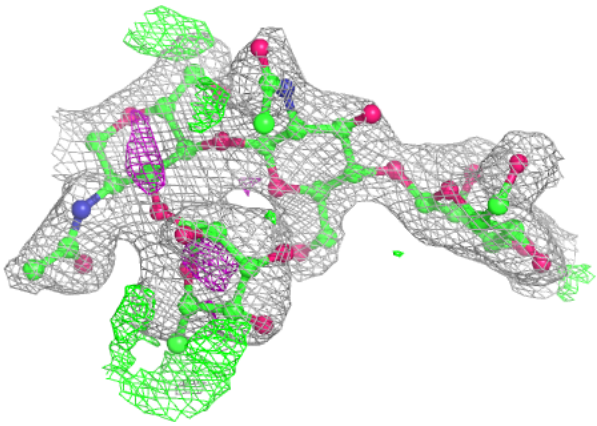


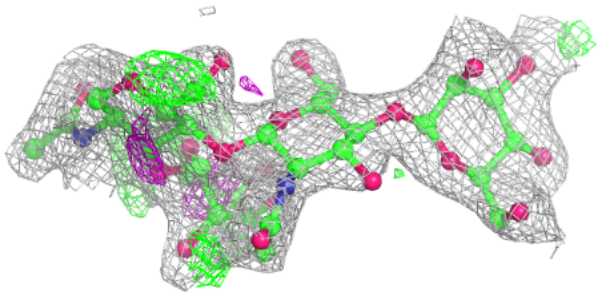


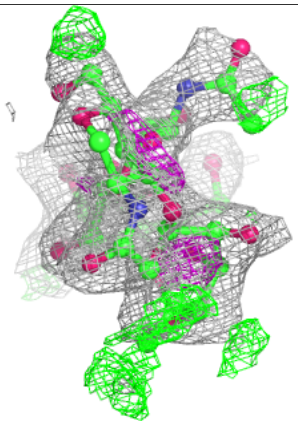


Electron density around Chain I:

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

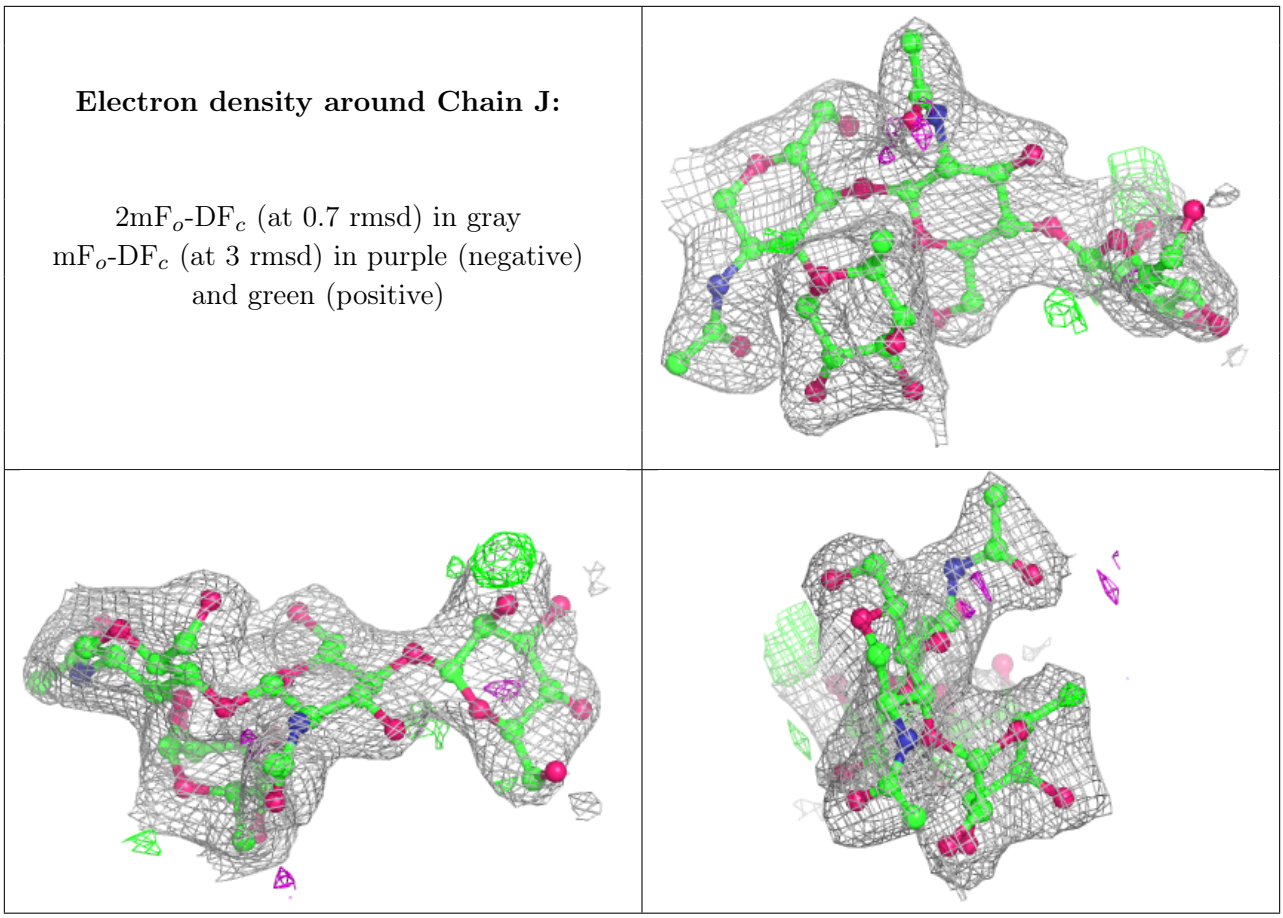






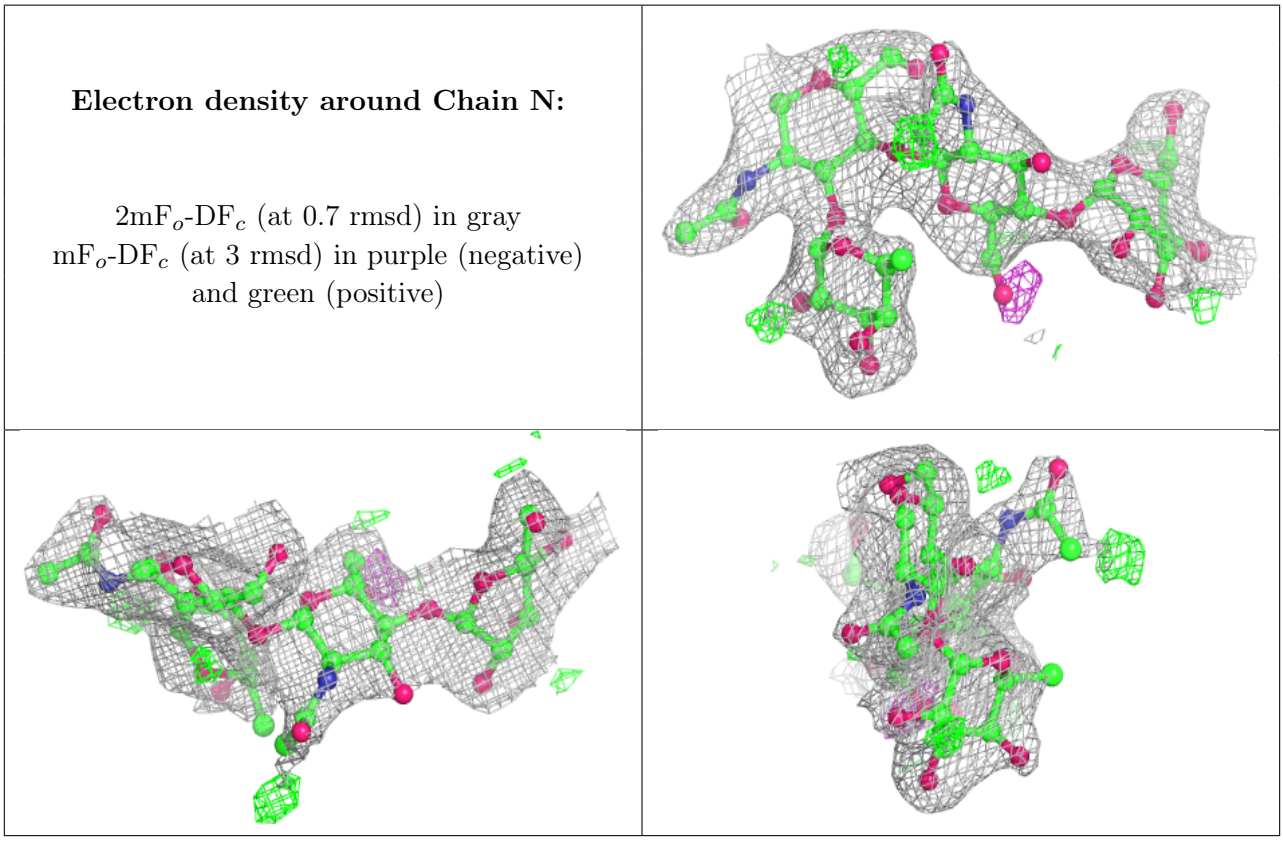
Electron density around Chain J:

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



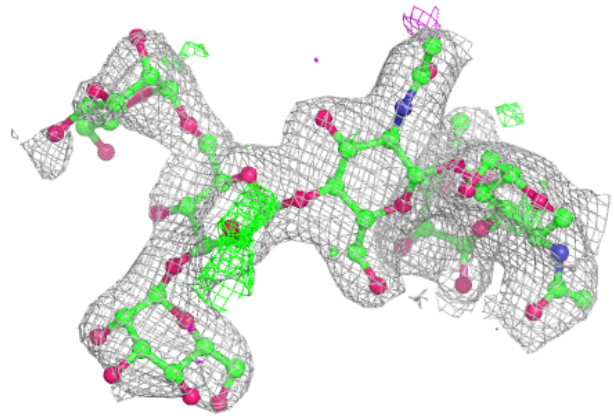
Electron density around Chain N:

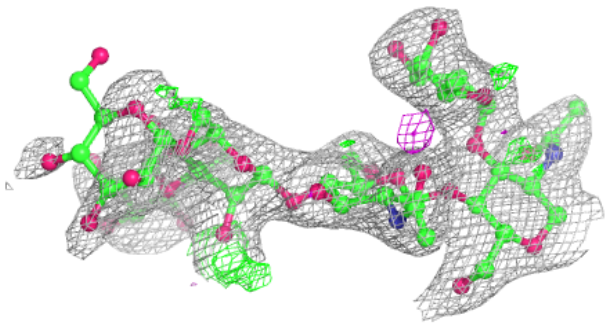
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

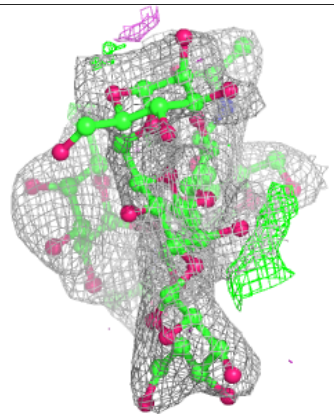


Electron density around Chain G:

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

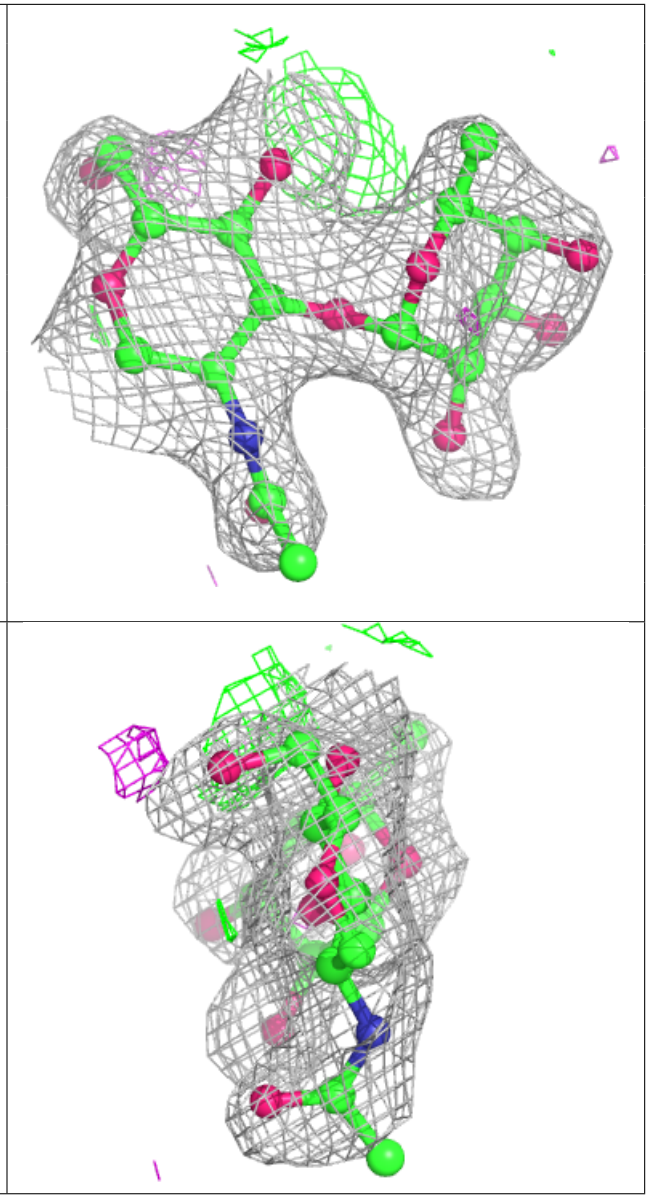






Electron density around Chain L:

$2mF_o$-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
11	EDO	A	525	4/4	0.55	0.49	58,67,69,70	0
8	NAG	C	523	14/15	0.56	0.49	77,90,99,110	0
12	PGE	D	521	10/10	0.61	0.54	62,80,88,91	0
11	EDO	D	515	4/4	0.63	0.46	69,69,69,71	0
12	PGE	A	527	10/10	0.73	0.51	57,64,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	SO4	B	522	5/5	0.76	0.44	93,94,121,123	0
12	PGE	D	520	4/10	0.79	0.14	48,48,56,57	0
11	EDO	A	523	4/4	0.80	0.21	45,51,60,64	0
11	EDO	D	504	4/4	0.86	0.20	39,45,48,53	0
9	SO4	C	513	5/5	0.87	0.41	85,88,112,112	0
9	SO4	C	512	5/5	0.88	0.26	80,87,97,108	0
11	EDO	C	522	4/4	0.88	0.10	40,49,54,58	0
12	PGE	A	526	7/10	0.88	0.20	36,47,58,65	0
11	EDO	C	518	4/4	0.89	0.23	53,54,55,63	0
12	PGE	D	519	7/10	0.89	0.29	47,47,54,55	0
9	SO4	B	521	5/5	0.89	0.38	85,97,109,110	0
9	SO4	A	518	5/5	0.89	0.26	36,39,49,56	5
9	SO4	D	513	5/5	0.90	0.38	78,80,93,95	0
14	GOL	D	518	6/6	0.90	0.18	39,47,49,51	0
11	EDO	C	519	4/4	0.91	0.28	43,50,53,65	0
9	SO4	B	518	5/5	0.91	0.23	44,45,55,59	5
11	EDO	D	516	4/4	0.91	0.15	44,45,53,54	0
9	SO4	D	512	5/5	0.91	0.35	48,64,85,89	0
11	EDO	D	517	4/4	0.92	0.11	36,40,41,45	0
9	SO4	A	520	5/5	0.92	0.33	71,72,94,96	0
8	NAG	C	503	14/15	0.92	0.19	36,42,52,57	0
11	EDO	C	520	4/4	0.92	0.16	37,39,51,55	0
11	EDO	C	521	4/4	0.92	0.20	31,40,43,55	0
11	EDO	B	524	4/4	0.92	0.24	46,55,55,57	0
8	NAG	D	510	14/15	0.93	0.17	39,52,55,56	0
11	EDO	B	523	4/4	0.93	0.30	50,53,54,55	0
13	MFJ	A	528	28/28	0.93	0.26	33,54,64,67	28
9	SO4	B	515	5/5	0.93	0.29	45,50,62,63	5
8	NAG	A	503	14/15	0.94	0.12	33,36,43,48	0
11	EDO	A	524	4/4	0.94	0.12	32,32,34,37	0
9	SO4	B	519	5/5	0.94	0.27	44,45,51,52	5
8	NAG	B	503	14/15	0.94	0.12	37,43,49,55	0
9	SO4	B	517	5/5	0.94	0.20	31,37,41,42	5
9	SO4	C	515	5/5	0.94	0.39	61,64,76,87	0
10	NA	C	516	1/1	0.94	0.09	33,33,33,33	0
9	SO4	D	511	5/5	0.95	0.12	34,35,36,44	5
9	SO4	B	520	5/5	0.95	0.26	51,58,64,75	0
8	NAG	C	507	14/15	0.95	0.14	37,44,48,50	0
8	NAG	D	503	14/15	0.95	0.15	32,41,49,51	0
9	SO4	A	517	5/5	0.96	0.16	41,47,54,55	5
7	FE	D	502	1/1	0.96	0.04	46,46,46,46	1
9	SO4	C	514	5/5	0.97	0.42	71,72,93,96	0

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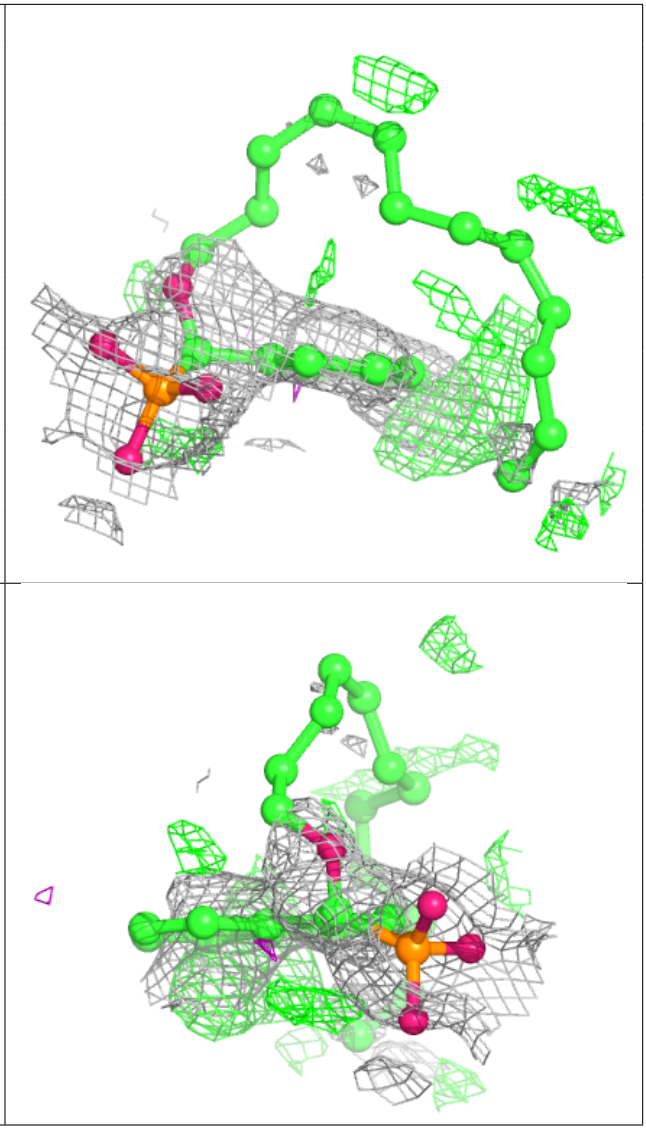
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	NA	A	522	1/1	0.98	0.07	35,35,35,35	0
9	SO4	B	516	5/5	0.98	0.21	20,27,29,33	5
10	NA	C	517	1/1	0.98	0.10	17,17,17,17	0
7	FE	B	502	1/1	0.98	0.05	38,38,38,38	1
9	SO4	A	519	5/5	0.99	0.06	37,40,48,53	0
6	ZN	B	501	1/1	0.99	0.02	39,39,39,39	0
10	NA	A	521	1/1	0.99	0.13	19,19,19,19	0
6	ZN	D	501	1/1	0.99	0.04	35,35,35,35	0
10	NA	D	514	1/1	0.99	0.14	21,21,21,21	0
7	FE	C	502	1/1	0.99	0.04	40,40,40,40	1
7	FE	A	502	1/1	0.99	0.08	30,30,30,30	1
6	ZN	A	501	1/1	1.00	0.04	28,28,28,28	1
6	ZN	C	501	1/1	1.00	0.05	31,31,31,31	1

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 MFJ A 528:

$2mF_o$-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.