wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 04:45 PM EDT

PDB ID	:	2YP1
Title	:	Crystallization of a 45 kDa peroxygenase- peroxidase from the mushroom Agrocybe aegerita and structure determination by SAD utilizing only the haem iron
Authors	:	Piontek, K.; Strittmatter, E.; Ullrich, R.; Plattner, D.A.; Hofrichter, M.
Deposited on	:	2012-10-29
Resolution	:	2.31 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*
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:

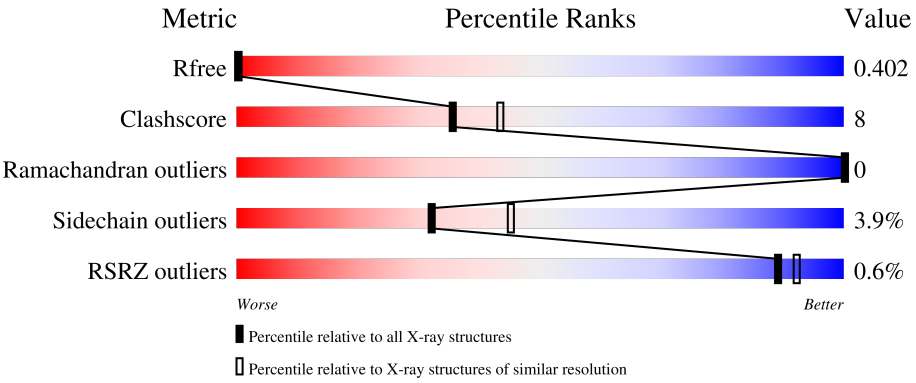
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	325	84% 14%
1	B	325	83% 15%
1	C	325	% 88% 11%
1	D	325	2% 78% 20%
2	E	6	33% 67%

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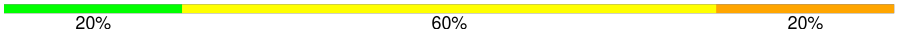
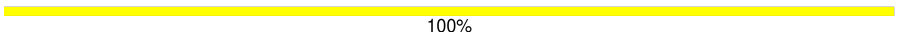
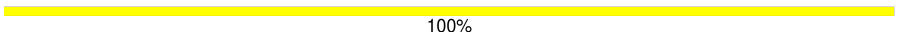
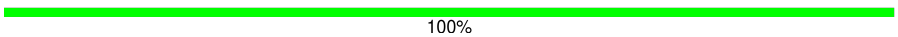
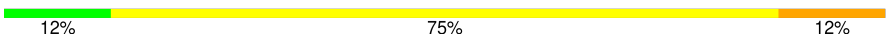
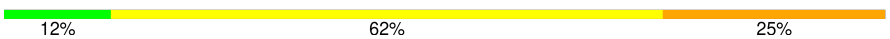
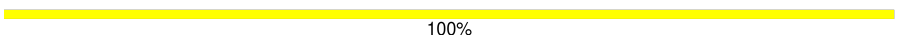
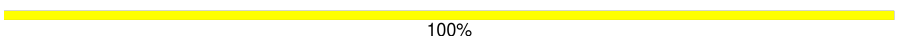
Mol	Chain	Length	Quality of chain
3	F	5	
3	J	5	
4	G	2	
4	I	2	
4	K	2	
4	L	2	
4	N	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
5	H	8	
5	M	8	
6	O	3	
6	T	3	

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
10	SO4	A	1331	-	-	X	-
10	SO4	B	1331	-	-	X	-
3	MAN	F	5	-	-	-	X
3	MAN	J	5	-	-	-	X
4	NAG	I	2	-	-	-	X
4	NAG	N	2	-	-	-	X
5	MAN	H	5	-	-	-	X
6	BMA	O	3	-	-	-	X

2 Entry composition (i)

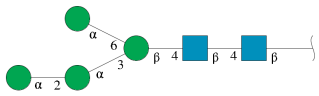
There are 12 unique types of molecules in this entry. The entry contains 12290 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 AROMATIC PEROXYGENASE.

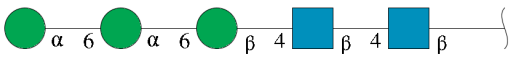
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	1	0
			2506	1589	434	475	8			
1	B	324	Total	C	N	O	S	0	4	0
			2537	1608	442	479	8			
1	C	325	Total	C	N	O	S	0	1	0
			2526	1599	440	479	8			
1	D	323	Total	C	N	O	S	0	1	0
			2507	1590	435	474	8			

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
2	E	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-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
3	F	5	Total	C	N	O	0	0	0
			61	34	2	25			

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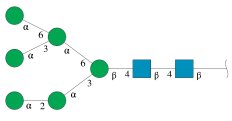
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	J	5	Total C N O 61 34 2 25	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	2	Total C N O 28 16 2 10	0	0	0
4	I	2	Total C N O 28 16 2 10	0	0	0
4	K	2	Total C N O 28 16 2 10	0	0	0
4	L	2	Total C N O 28 16 2 10	0	0	0
4	N	2	Total C N O 28 16 2 10	0	0	0
4	P	2	Total C N O 28 16 2 10	0	0	0
4	Q	2	Total C N O 28 16 2 10	0	0	0
4	R	2	Total C N O 28 16 2 10	0	0	0
4	S	2	Total C N O 28 16 2 10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]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	H	8	Total C N O 94 52 2 40	0	0	0

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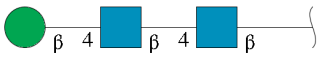
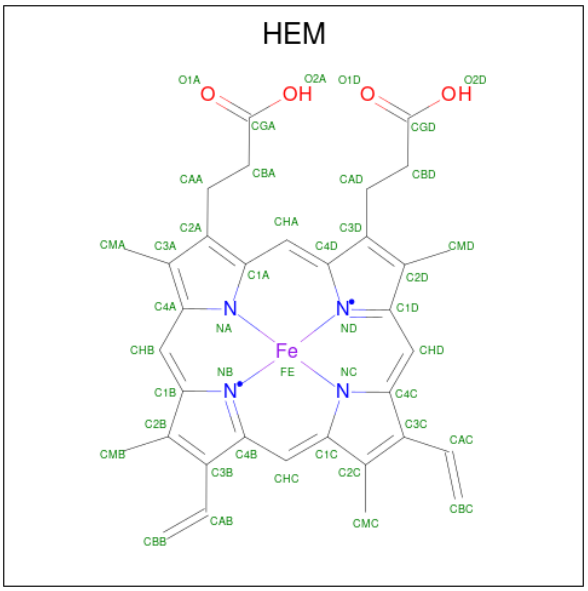
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	M	8	Total C N O 94 52 2 40	0	0	0

- Molecule 6 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
6	O	3	Total C N O 39 22 2 15	0	0	0
6	T	3	Total C N O 39 22 2 15	0	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C Fe N O 43 34 1 4 4	0	0
7	B	1	Total C Fe N O 43 34 1 4 4	0	0
7	C	1	Total C Fe N O 43 34 1 4 4	0	0

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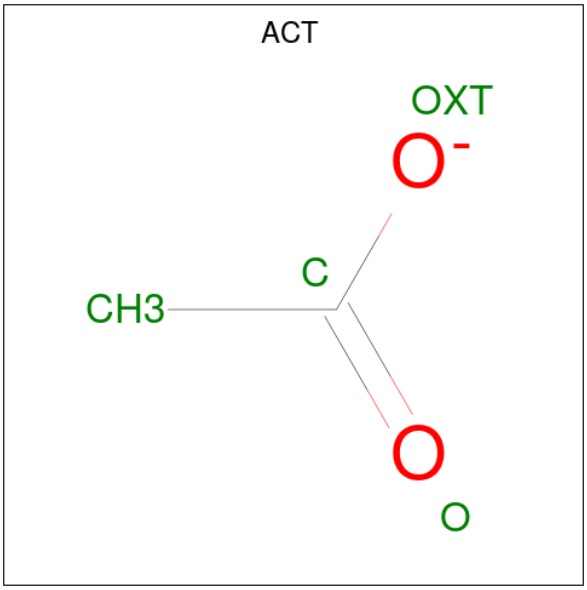
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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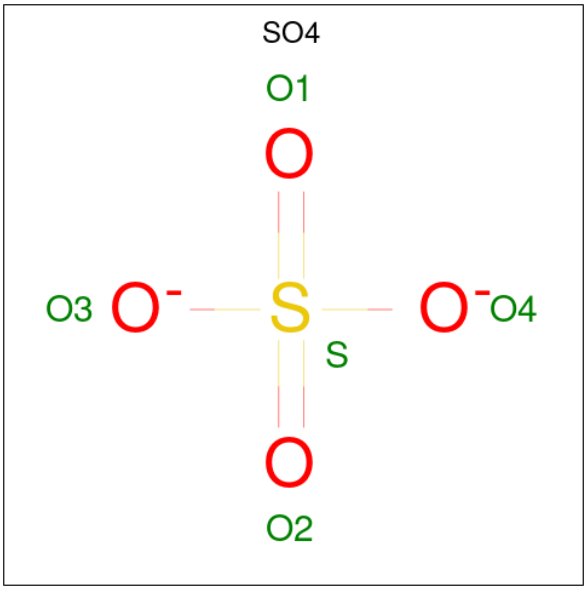
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	D	1	Total C O 4 2 2	0	0

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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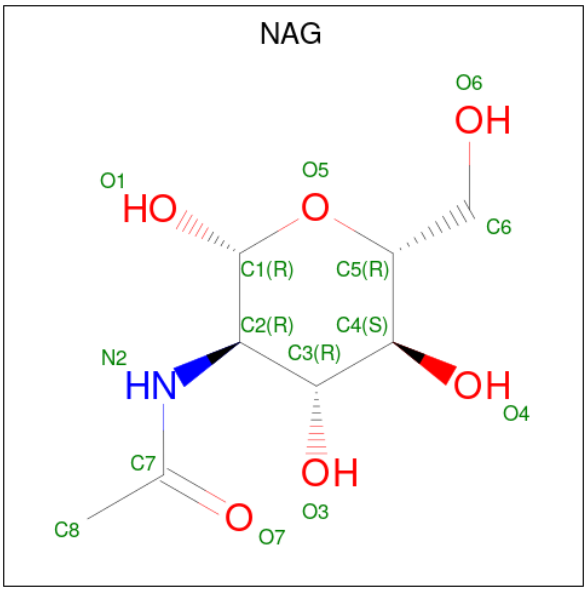
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0
10	D	1	Total O S 5 4 1	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	327	Total O 327 327	0	0
12	B	369	Total O 369 369	0	0

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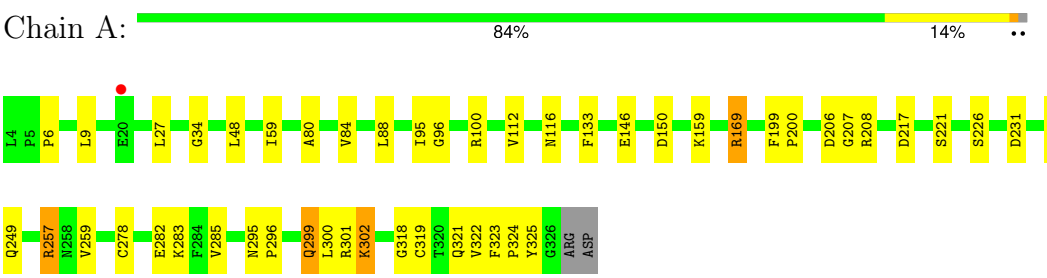
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	291	Total O 291 291	0	0
12	D	198	Total O 198 198	0	0

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.

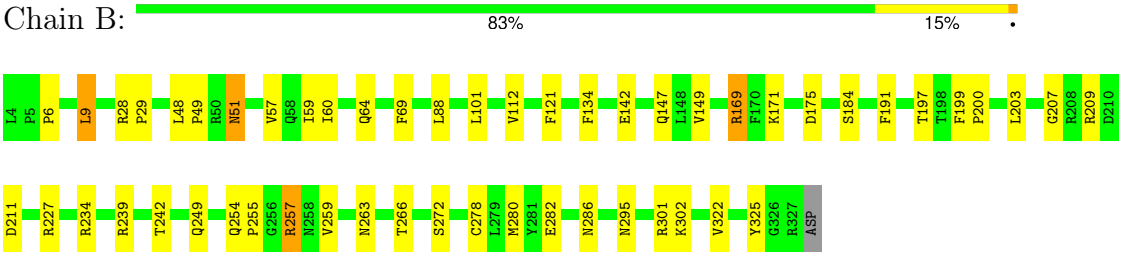
• Molecule 1: AROMATIC PEROXYGENASE

Chain A:



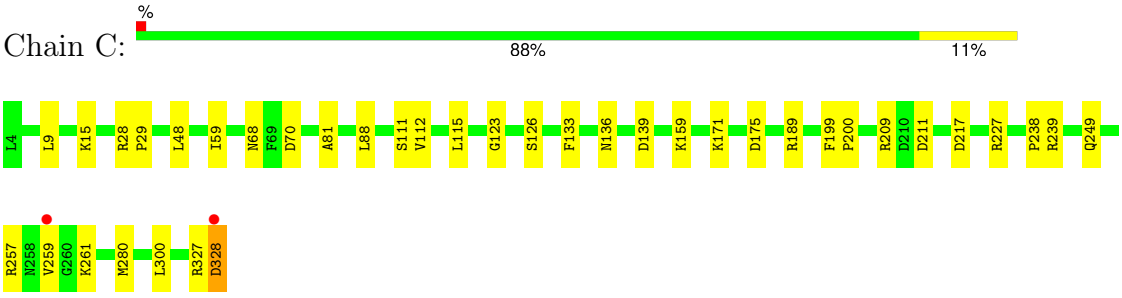
• Molecule 1: AROMATIC PEROXYGENASE

Chain B:



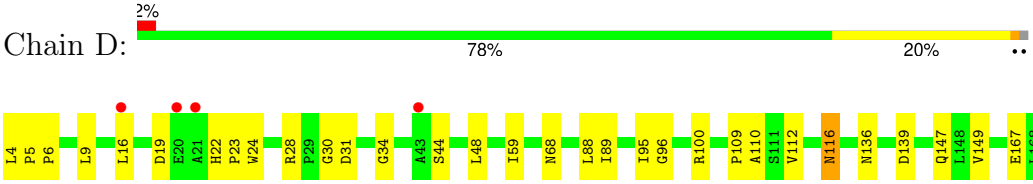
• Molecule 1: AROMATIC PEROXYGENASE

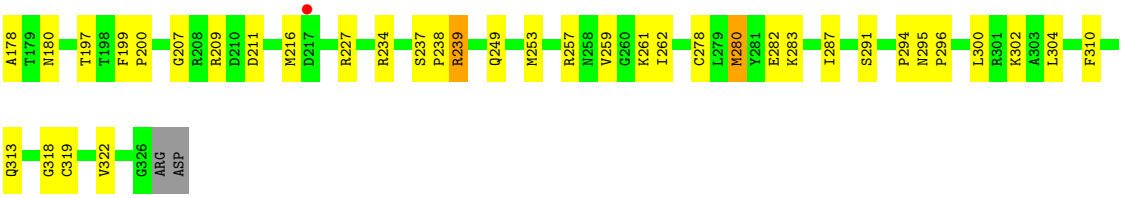
Chain C:



• Molecule 1: AROMATIC PEROXYGENASE

Chain D:



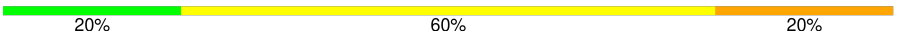


• Molecule 2: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

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

Chain G:

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

Chain I:

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

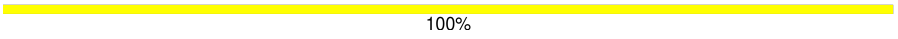
Chain K:

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

Chain L:

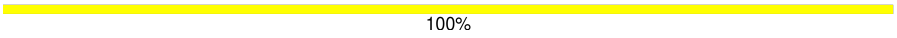
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



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

Chain P:

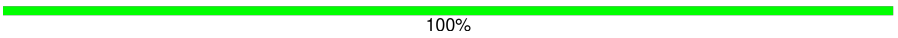


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

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

Chain R:

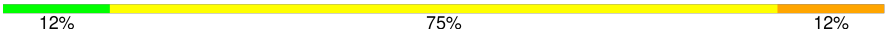


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

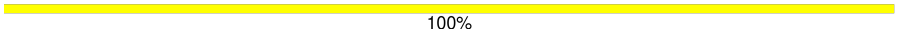


• Molecule 5: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

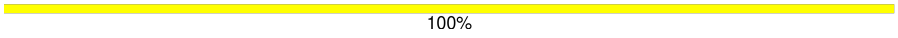
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	112.75Å 144.88Å 134.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.31 48.93 – 2.31	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.91-2.31) 99.4 (48.93-2.31)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.01 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.177 , 0.230 0.377 , 0.402	Depositor DCC
R_{free} test set	4851 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12290	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.95% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, ACT, SO4, HEM, MG, MAN

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	0.48	0/2579	0.56	0/3512
1	B	0.52	0/2619	0.57	0/3564
1	C	0.52	0/2599	0.53	0/3538
1	D	0.44	0/2580	0.51	0/3513
All	All	0.49	0/10377	0.54	0/14127

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	30	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2506	0	2386	40	0
1	B	2537	0	2426	41	0
1	C	2526	0	2405	20	0
1	D	2507	0	2390	52	0
2	E	72	0	61	2	0
3	F	61	0	52	2	0
3	J	61	0	52	2	0
4	G	28	0	25	3	0
4	I	28	0	25	3	0
4	K	28	0	25	2	0
4	L	28	0	25	0	0
4	N	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
5	H	94	0	79	4	0
5	M	94	0	79	2	0
6	O	39	0	34	0	0
6	T	39	0	34	0	0
7	A	43	0	30	5	0
7	B	43	0	30	3	0
7	C	43	0	30	3	0
7	D	43	0	30	3	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	4	0	3	0	0
9	B	4	0	3	0	0
9	C	8	0	6	0	0
9	D	4	0	3	0	0
10	A	20	0	0	2	0
10	B	15	0	0	2	0
10	C	20	0	0	0	0
10	D	10	0	0	2	0
11	C	14	0	13	1	0
11	D	42	0	39	0	0
12	A	327	0	0	9	0
12	B	369	0	0	13	0
12	C	291	0	0	5	0
12	D	198	0	0	6	0
All	All	12290	0	10410	174	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 8.

The worst 5 of 174 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)
7:D:350:HEM:HMC2	7:D:350:HEM:HBC2	1.29	1.11
1:A:259:VAL:HG23	1:A:259:VAL:O	1.68	0.94
1:A:299:GLN:HG2	12:A:2271:HOH:O	1.73	0.88
1:A:299:GLN:NE2	12:A:2273:HOH:O	2.07	0.88
1:D:89:ILE:HD11	1:D:300:LEU:HD13	1.56	0.88

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	322/325 (99%)	301 (94%)	21 (6%)	0	100	100
1	B	326/325 (100%)	307 (94%)	19 (6%)	0	100	100
1	C	324/325 (100%)	304 (94%)	20 (6%)	0	100	100
1	D	322/325 (99%)	298 (92%)	24 (8%)	0	100	100
All	All	1294/1300 (100%)	1210 (94%)	84 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	270/271 (100%)	258 (96%)	12 (4%)	28	39
1	B	274/271 (101%)	262 (96%)	12 (4%)	28	39
1	C	272/271 (100%)	261 (96%)	11 (4%)	31	44
1	D	270/271 (100%)	262 (97%)	8 (3%)	41	56
All	All	1086/1084 (100%)	1043 (96%)	43 (4%)	32	44

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	217	ASP
1	D	9	LEU
1	C	239	ARG
1	C	280	MET
1	D	169	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	61	ASN
1	C	249	GLN
1	D	263	ASN
1	D	116	ASN
1	A	299	GLN

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)

56 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	0.44	0	17,19,21	1.39	3 (17%)
2	NAG	E	2	2	14,14,15	0.46	0	17,19,21	1.12	1 (5%)
2	BMA	E	3	2	11,11,12	0.55	0	15,15,17	0.94	1 (6%)
2	MAN	E	4	2	11,11,12	0.52	0	15,15,17	0.94	0
2	MAN	E	5	2	11,11,12	0.58	0	15,15,17	0.73	0
2	MAN	E	6	2	11,11,12	0.54	0	15,15,17	1.14	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.69	0	17,19,21	1.26	2 (11%)
3	NAG	F	2	3	14,14,15	0.79	0	17,19,21	1.31	4 (23%)
3	BMA	F	3	3	11,11,12	0.56	0	15,15,17	1.00	0
3	MAN	F	4	3	11,11,12	0.59	0	15,15,17	0.88	1 (6%)
3	MAN	F	5	3	11,11,12	0.54	0	15,15,17	0.87	0
4	NAG	G	1	1,4	14,14,15	0.53	0	17,19,21	1.13	1 (5%)
4	NAG	G	2	4	14,14,15	0.53	0	17,19,21	1.55	4 (23%)
5	NAG	H	1	1,5	14,14,15	0.65	0	17,19,21	1.64	2 (11%)
5	NAG	H	2	5	14,14,15	0.69	0	17,19,21	1.15	1 (5%)
5	BMA	H	3	5	11,11,12	0.68	0	15,15,17	1.14	1 (6%)
5	MAN	H	4	5	11,11,12	0.58	0	15,15,17	1.08	1 (6%)
5	MAN	H	5	5	11,11,12	0.42	0	15,15,17	1.07	1 (6%)
5	MAN	H	6	5	11,11,12	0.57	0	15,15,17	0.83	0
5	MAN	H	7	5	11,11,12	0.53	0	15,15,17	0.87	0
5	MAN	H	8	5	11,11,12	0.57	0	15,15,17	1.12	1 (6%)
4	NAG	I	1	1,4	14,14,15	0.49	0	17,19,21	1.94	3 (17%)
4	NAG	I	2	4	14,14,15	0.49	0	17,19,21	0.90	1 (5%)
3	NAG	J	1	1,3	14,14,15	0.60	0	17,19,21	1.18	2 (11%)
3	NAG	J	2	3	14,14,15	0.42	0	17,19,21	2.01	5 (29%)
3	BMA	J	3	3	11,11,12	0.56	0	15,15,17	1.22	2 (13%)
3	MAN	J	4	3	11,11,12	0.59	0	15,15,17	1.14	2 (13%)
3	MAN	J	5	3	11,11,12	0.61	0	15,15,17	1.68	3 (20%)
4	NAG	K	1	1,4	14,14,15	0.55	0	17,19,21	1.80	4 (23%)
4	NAG	K	2	4	14,14,15	0.59	0	17,19,21	1.56	2 (11%)
4	NAG	L	1	1,4	14,14,15	0.77	0	17,19,21	1.28	1 (5%)
4	NAG	L	2	4	14,14,15	0.55	0	17,19,21	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	M	1	1,5	14,14,15	0.65	0	17,19,21	1.80	4 (23%)
5	NAG	M	2	5	14,14,15	0.74	0	17,19,21	1.17	2 (11%)
5	BMA	M	3	5	11,11,12	0.78	0	15,15,17	1.22	1 (6%)
5	MAN	M	4	5	11,11,12	0.64	0	15,15,17	1.09	1 (6%)
5	MAN	M	5	5	11,11,12	0.43	0	15,15,17	1.44	1 (6%)
5	MAN	M	6	5	11,11,12	0.52	0	15,15,17	1.96	4 (26%)
5	MAN	M	7	5	11,11,12	0.48	0	15,15,17	0.81	0
5	MAN	M	8	5	11,11,12	0.73	0	15,15,17	1.41	2 (13%)
4	NAG	N	1	1,4	14,14,15	0.57	0	17,19,21	0.90	1 (5%)
4	NAG	N	2	4	14,14,15	0.51	0	17,19,21	0.76	1 (5%)
6	NAG	O	1	6,1	14,14,15	0.59	0	17,19,21	0.85	1 (5%)
6	NAG	O	2	6	14,14,15	0.48	0	17,19,21	0.89	1 (5%)
6	BMA	O	3	6	11,11,12	0.51	0	15,15,17	1.80	3 (20%)
4	NAG	P	1	1,4	14,14,15	0.71	0	17,19,21	1.78	6 (35%)
4	NAG	P	2	4	14,14,15	0.51	0	17,19,21	1.03	1 (5%)
4	NAG	Q	1	1,4	14,14,15	0.56	0	17,19,21	1.59	3 (17%)
4	NAG	Q	2	4	14,14,15	0.49	0	17,19,21	0.77	0
4	NAG	R	1	1,4	14,14,15	0.59	0	17,19,21	0.74	0
4	NAG	R	2	4	14,14,15	0.57	0	17,19,21	0.70	0
4	NAG	S	1	1,4	14,14,15	0.66	0	17,19,21	1.24	3 (17%)
4	NAG	S	2	4	14,14,15	0.49	0	17,19,21	0.57	0
6	NAG	T	1	6,1	14,14,15	0.64	0	17,19,21	1.49	3 (17%)
6	NAG	T	2	6	14,14,15	0.57	0	17,19,21	0.90	1 (5%)
6	BMA	T	3	6	11,11,12	0.51	0	15,15,17	1.27	2 (13%)

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	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	2/2/19/22	0/1/1/1
2	MAN	E	4	2	-	0/2/19/22	0/1/1/1
2	MAN	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	0/2/19/22	1/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	1,3	-	1/6/23/26	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	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	MAN	F	5	3	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1
5	MAN	H	4	5	-	0/2/19/22	0/1/1/1
5	MAN	H	5	5	-	0/2/19/22	0/1/1/1
5	MAN	H	6	5	-	2/2/19/22	0/1/1/1
5	MAN	H	7	5	-	1/2/19/22	0/1/1/1
5	MAN	H	8	5	-	0/2/19/22	0/1/1/1
4	NAG	I	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	I	2	4	-	4/6/23/26	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	MAN	J	4	3	-	2/2/19/22	0/1/1/1
3	MAN	J	5	3	-	2/2/19/22	0/1/1/1
4	NAG	K	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	2/2/19/22	0/1/1/1
5	MAN	M	5	5	-	2/2/19/22	0/1/1/1
5	MAN	M	6	5	-	2/2/19/22	0/1/1/1
5	MAN	M	7	5	-	0/2/19/22	0/1/1/1
5	MAN	M	8	5	-	1/2/19/22	0/1/1/1
4	NAG	N	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	N	2	4	-	3/6/23/26	0/1/1/1
6	NAG	O	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	O	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BMA	O	3	6	-	0/2/19/22	0/1/1/1
4	NAG	P	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	4/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	S	2	4	-	0/6/23/26	0/1/1/1
6	NAG	T	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	T	2	6	-	0/6/23/26	0/1/1/1
6	BMA	T	3	6	-	2/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	2	NAG	C2-N2-C7	-5.23	115.89	122.90
4	I	1	NAG	C1-O5-C5	5.23	119.19	112.19
5	M	1	NAG	C1-O5-C5	4.94	118.81	112.19
4	K	2	NAG	O5-C1-C2	-4.69	104.04	111.29
3	J	5	MAN	C3-C4-C5	4.60	118.57	110.23

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	1	NAG	C3-C2-N2-C7
3	F	4	MAN	C4-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
3	J	4	MAN	C4-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

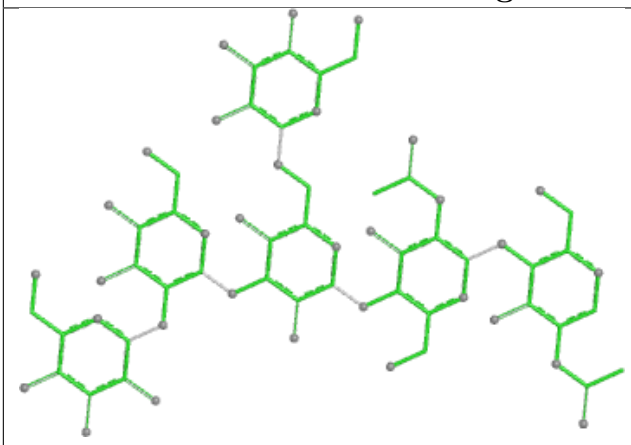
Mol	Chain	Res	Type	Atoms
2	E	6	MAN	C1-C2-C3-C4-C5-O5

19 monomers are involved in 20 short contacts:

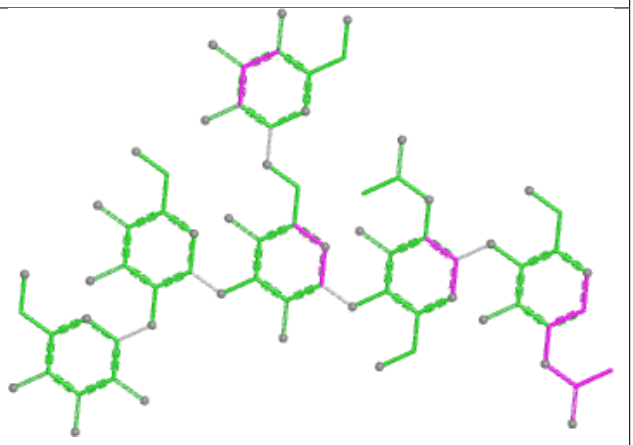
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	2	NAG	1	0
2	E	1	NAG	1	0
3	F	4	MAN	2	0
4	G	1	NAG	3	0
5	M	8	MAN	2	0
4	K	1	NAG	1	0
4	I	1	NAG	3	0
5	M	6	MAN	2	0
2	E	3	BMA	1	0
3	J	4	MAN	1	0
2	E	2	NAG	1	0
5	H	8	MAN	4	0
3	F	3	BMA	2	0
4	I	2	NAG	3	0
3	J	2	NAG	1	0
4	K	2	NAG	1	0
3	J	5	MAN	1	0
5	H	6	MAN	4	0
2	E	6	MAN	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.

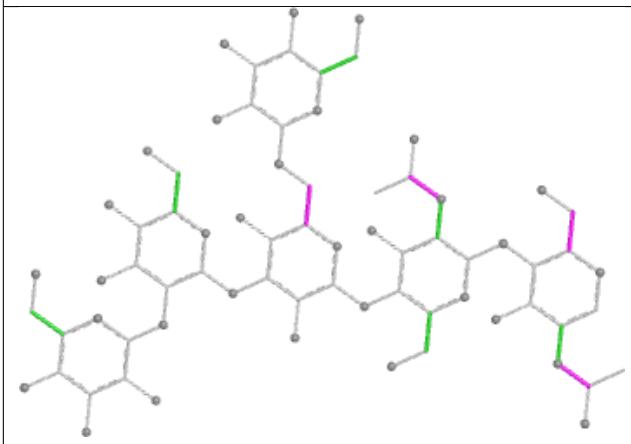
Oligosaccharide Chain E



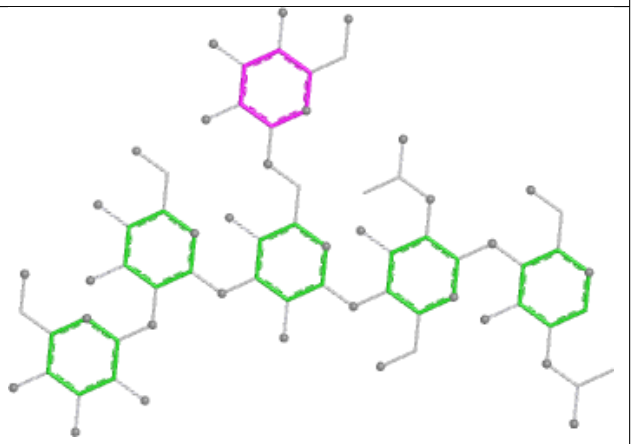
Bond lengths



Bond angles

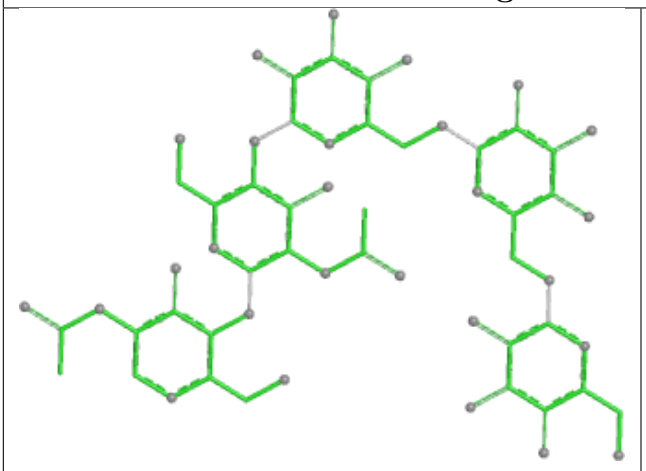


Torsions

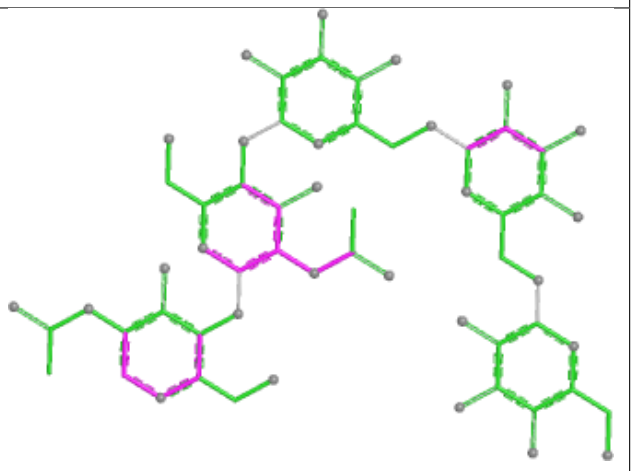


Rings

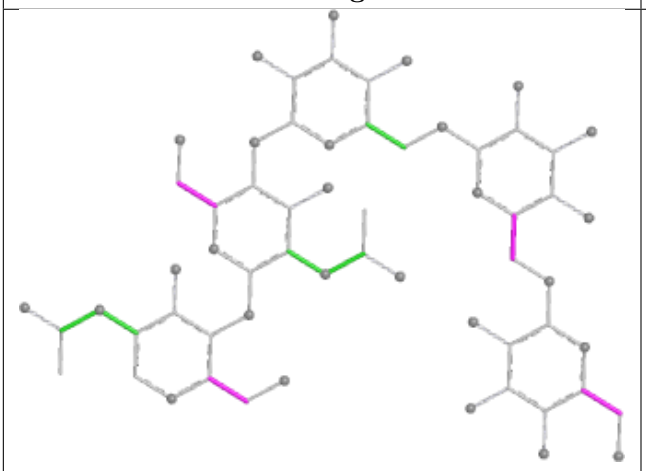
Oligosaccharide Chain F



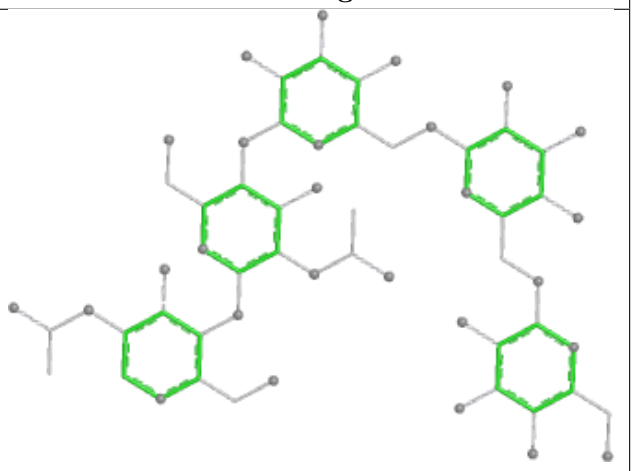
Bond lengths



Bond angles

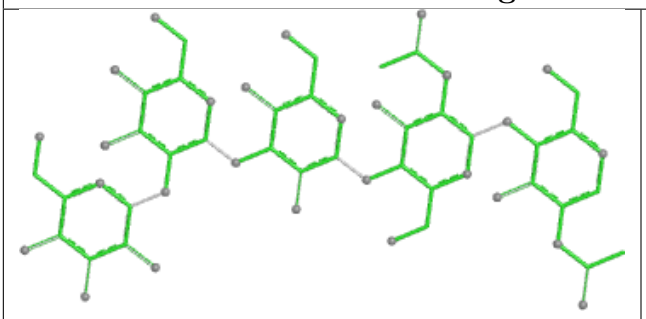


Torsions

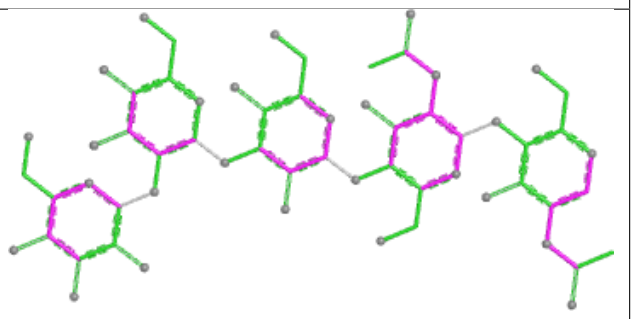


Rings

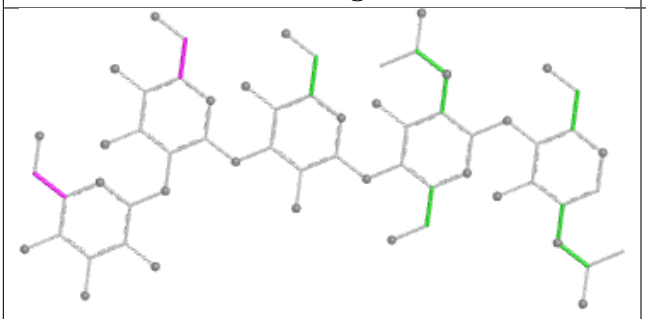
Oligosaccharide Chain J



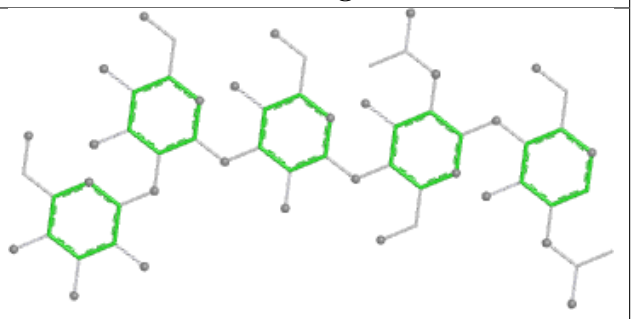
Bond lengths



Bond angles

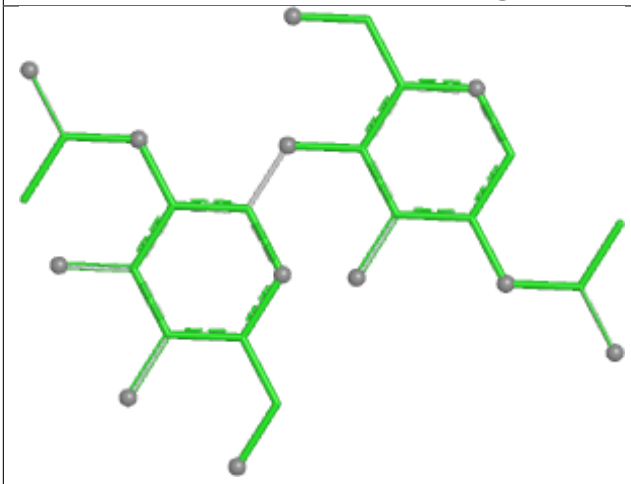


Torsions

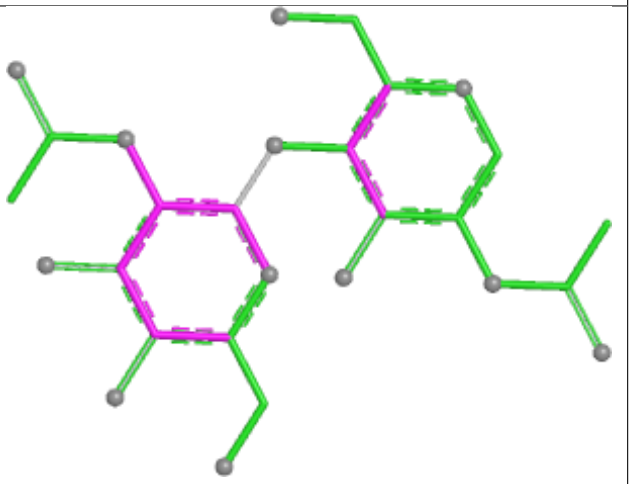


Rings

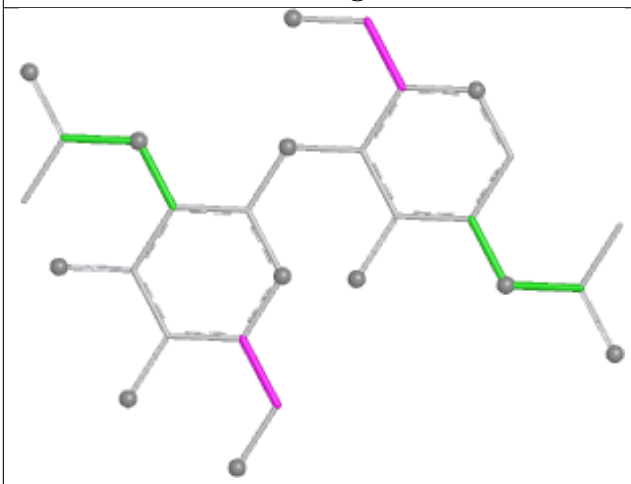
Oligosaccharide Chain G



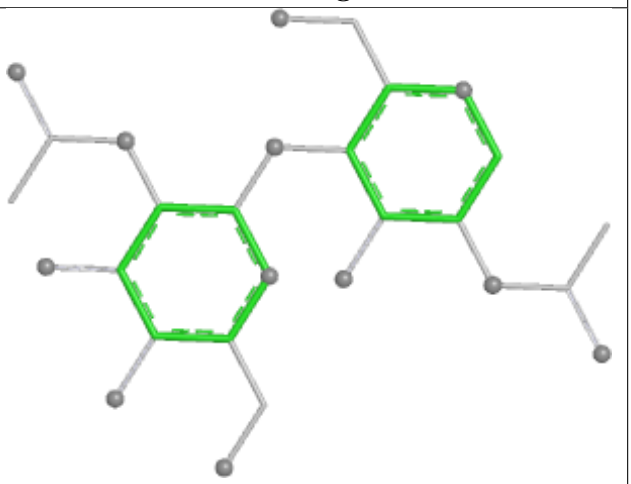
Bond lengths



Bond angles

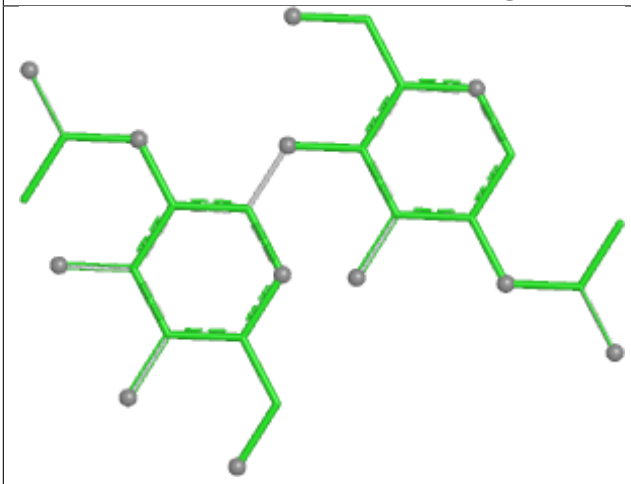


Torsions

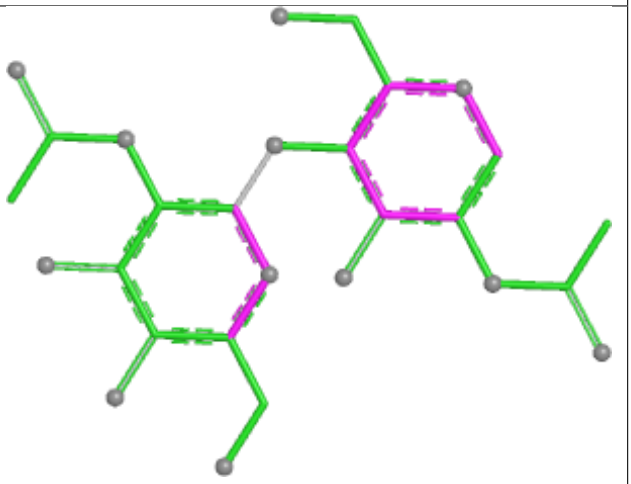


Rings

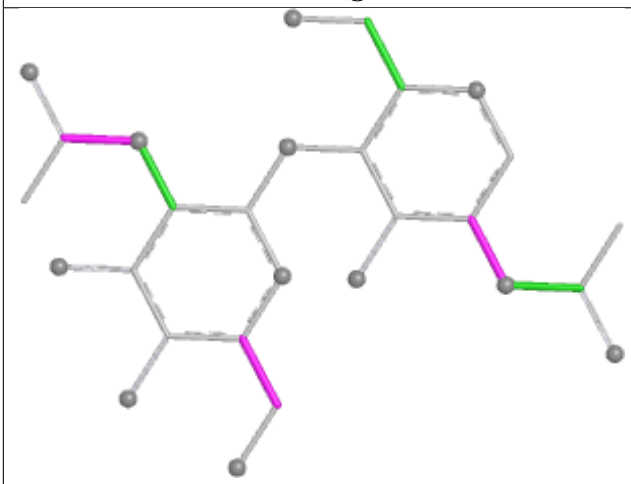
Oligosaccharide Chain I



Bond lengths



Bond angles



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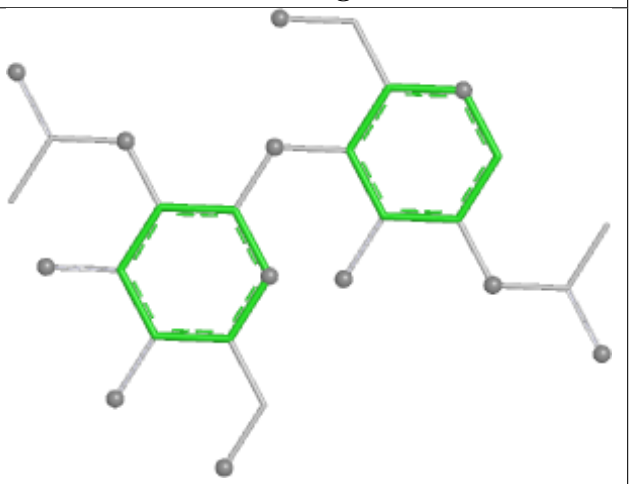
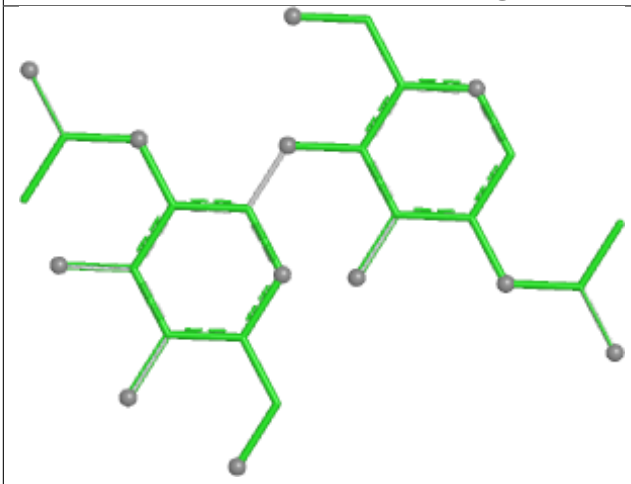
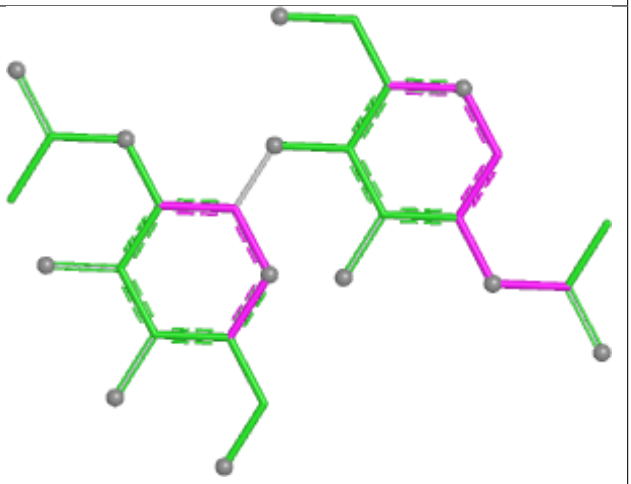


Rings

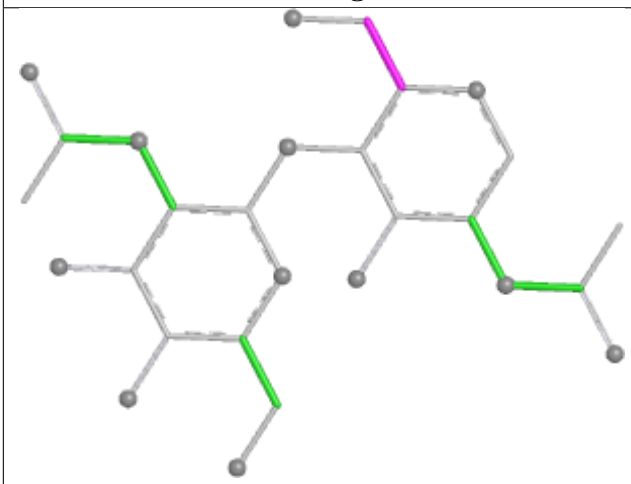
Oligosaccharide Chain K



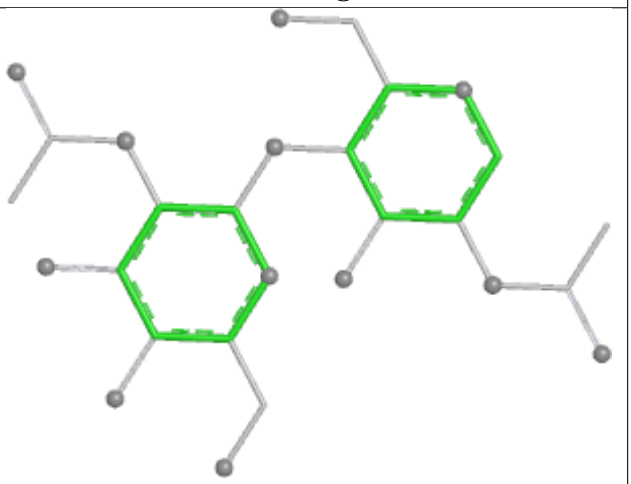
Bond lengths



Bond angles

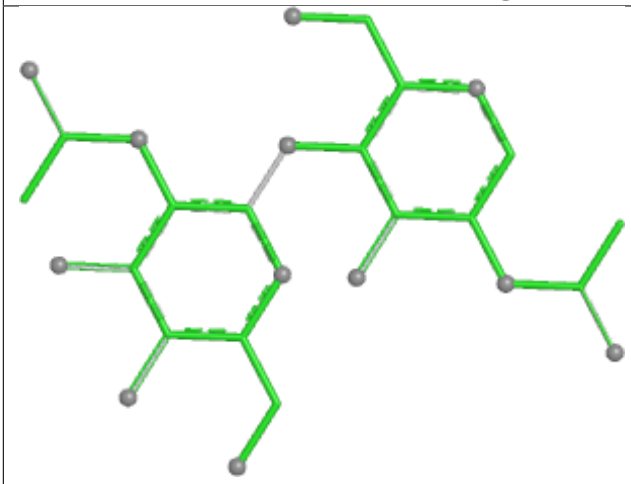


Torsions

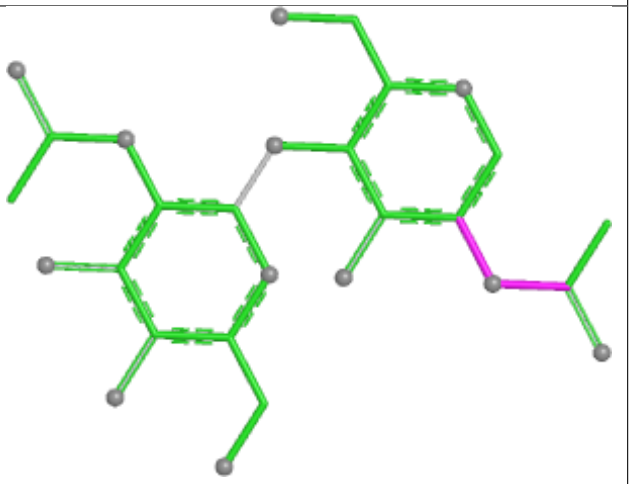


Rings

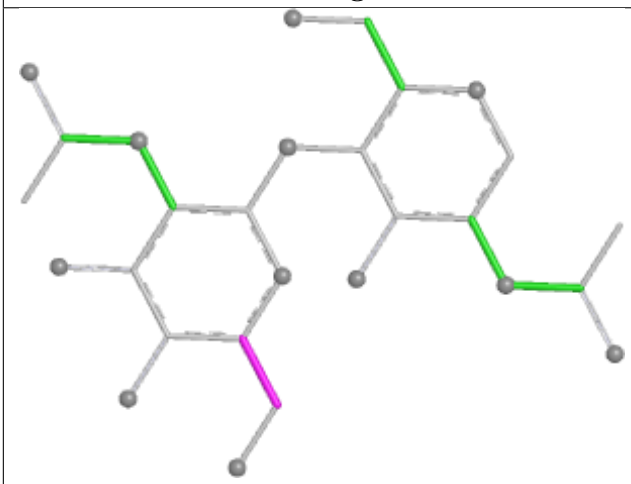
Oligosaccharide Chain L



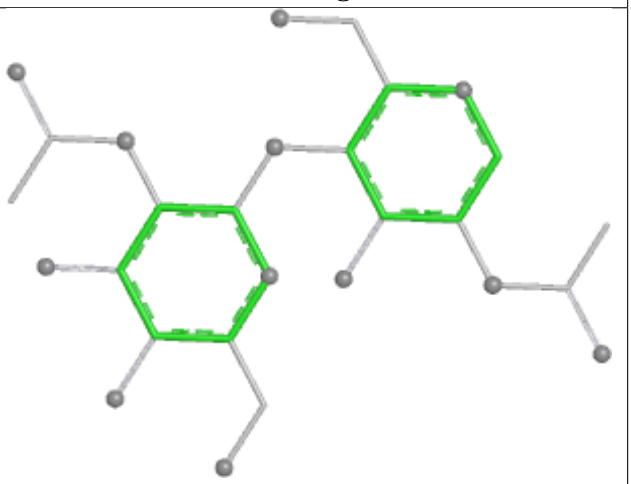
Bond lengths



Bond angles

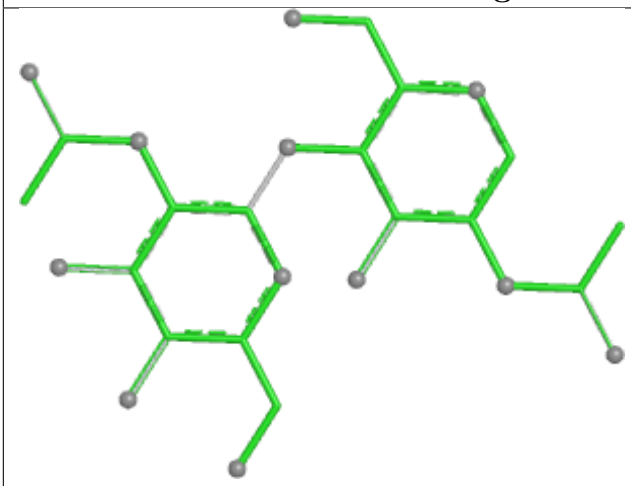


Torsions

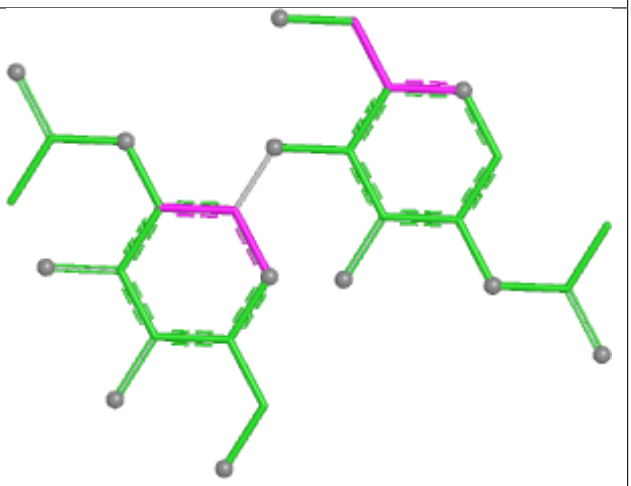


Rings

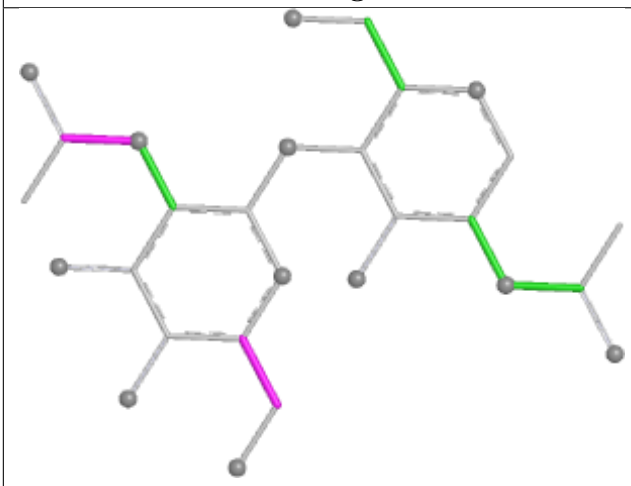
Oligosaccharide Chain N



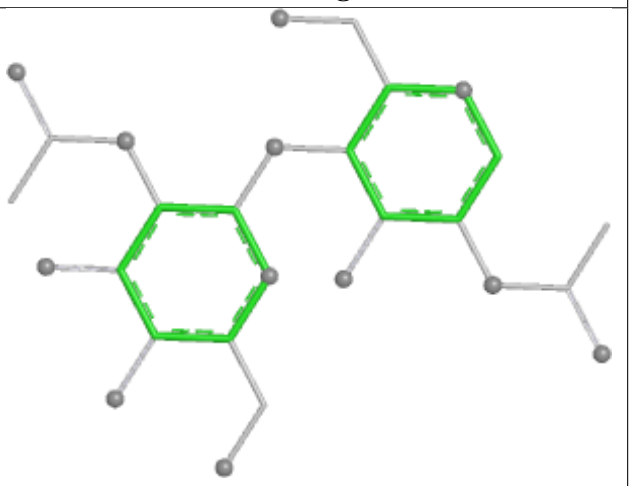
Bond lengths



Bond angles

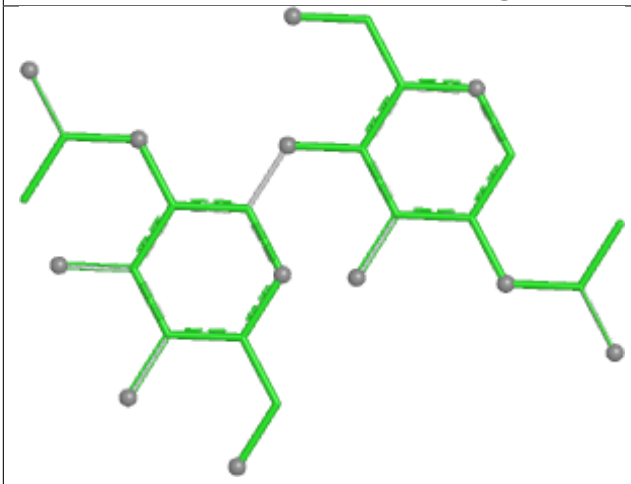


Torsions

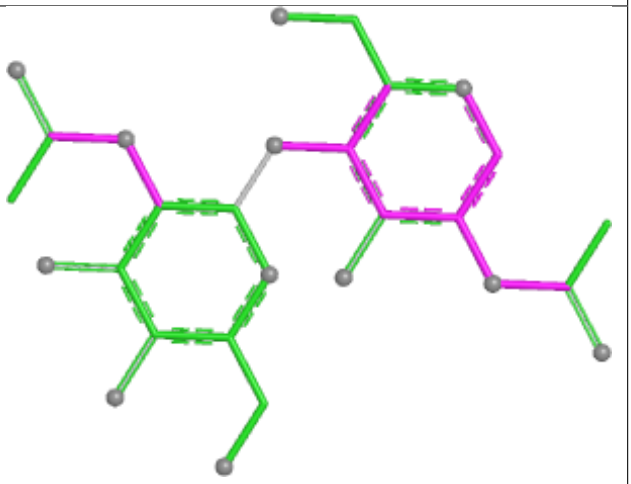


Rings

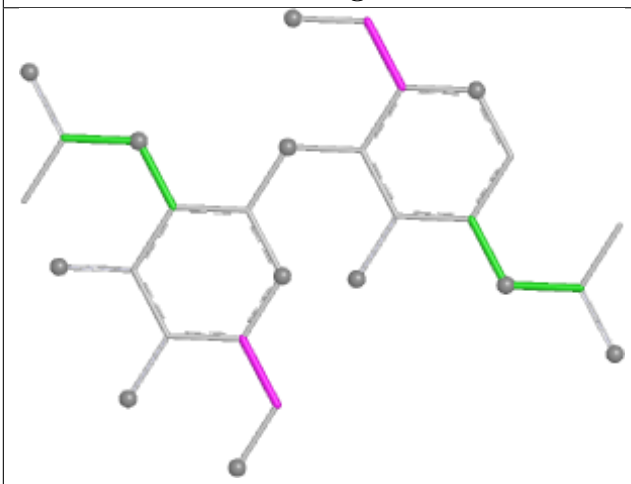
Oligosaccharide Chain P



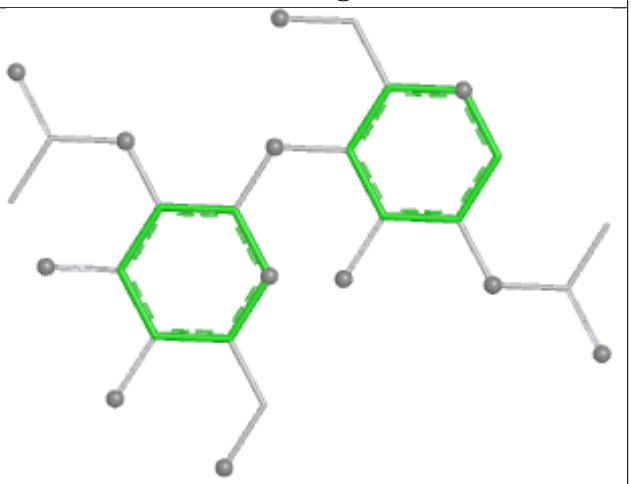
Bond lengths



Bond angles

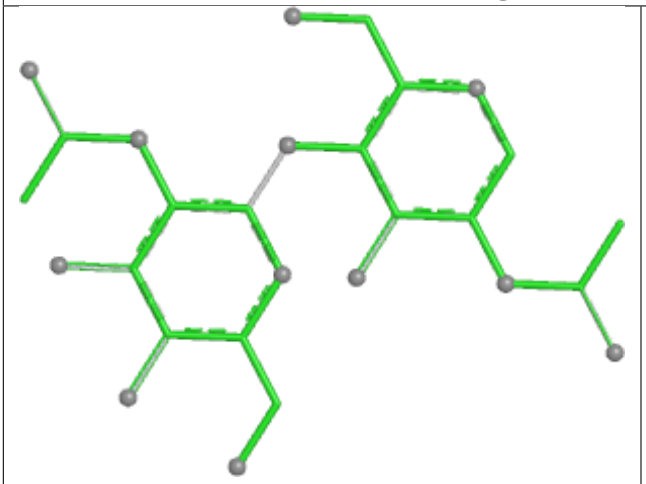


Torsions

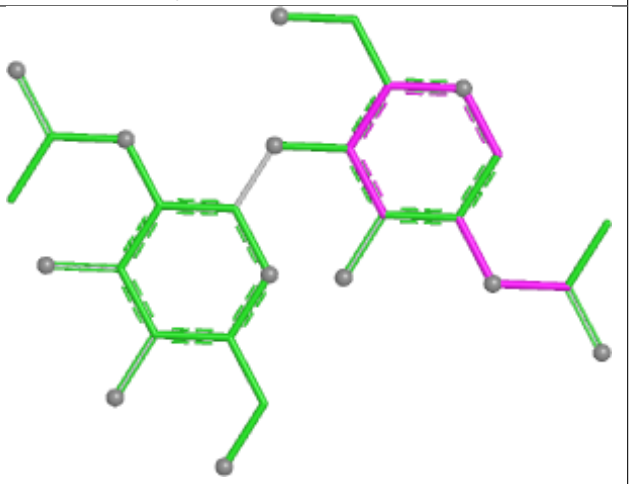


Rings

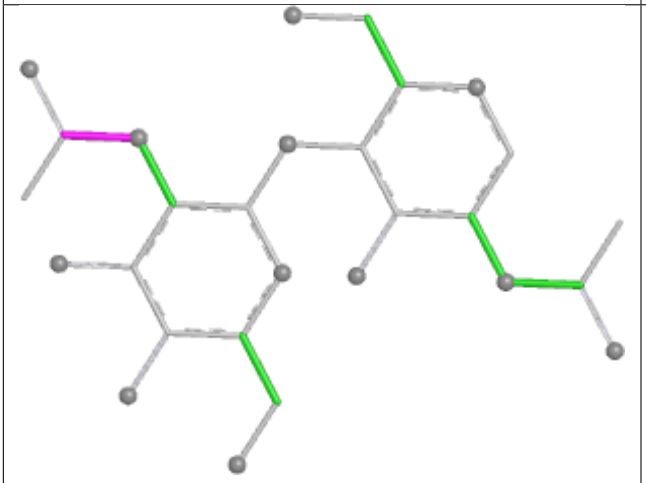
Oligosaccharide Chain Q



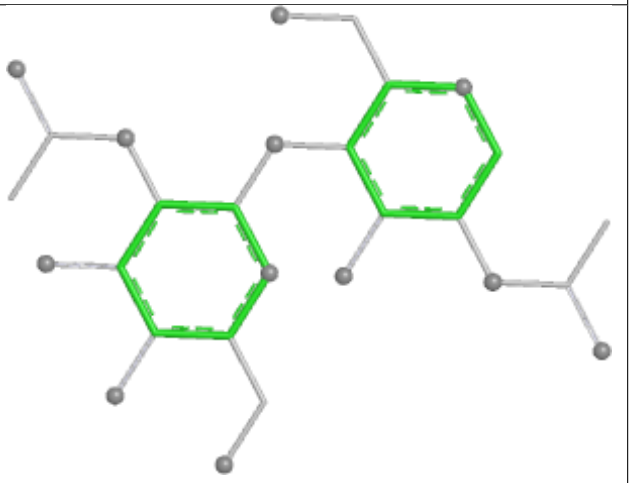
Bond lengths



Bond angles

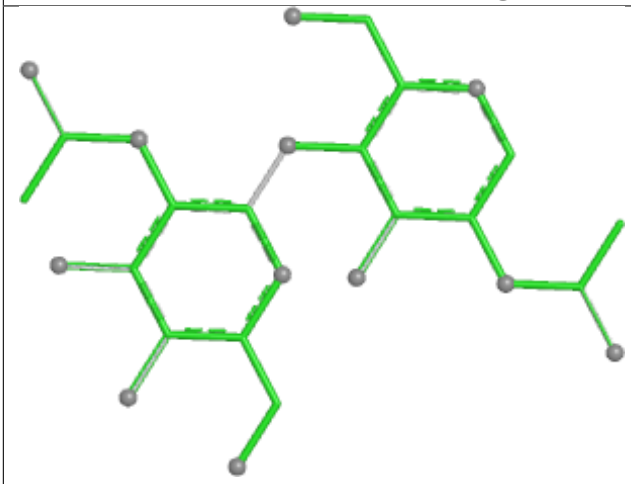


Torsions

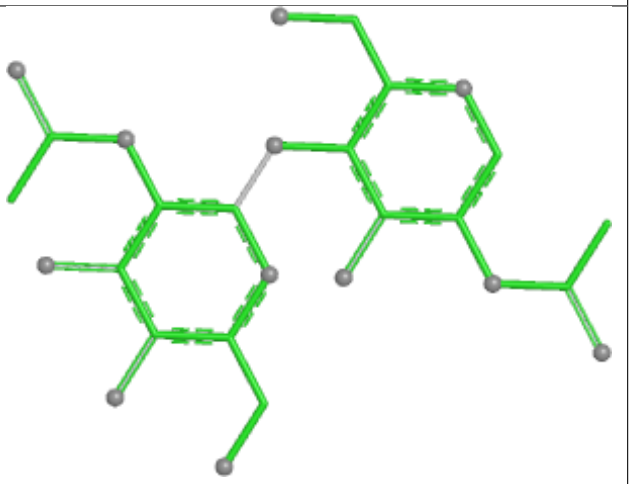


Rings

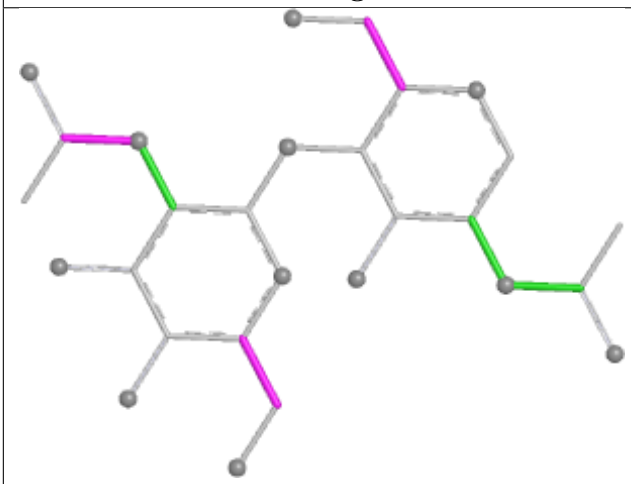
Oligosaccharide Chain R



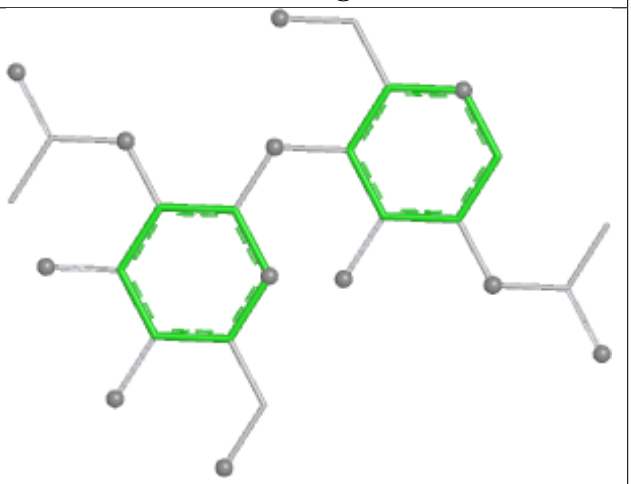
Bond lengths



Bond angles

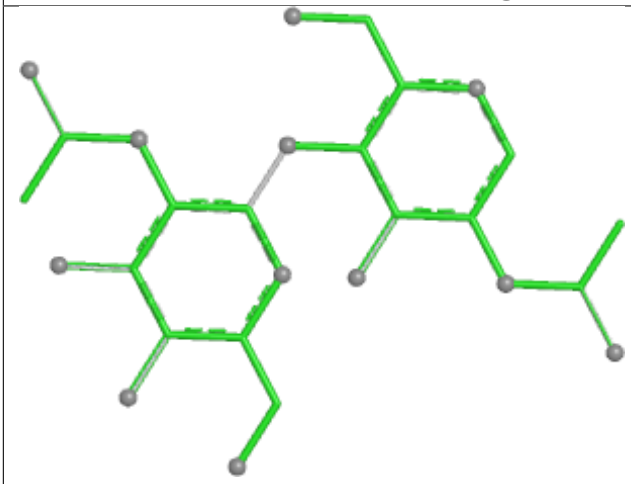


Torsions

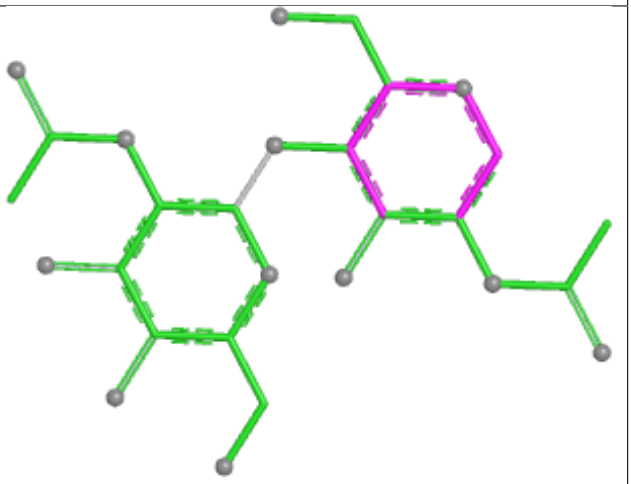


Rings

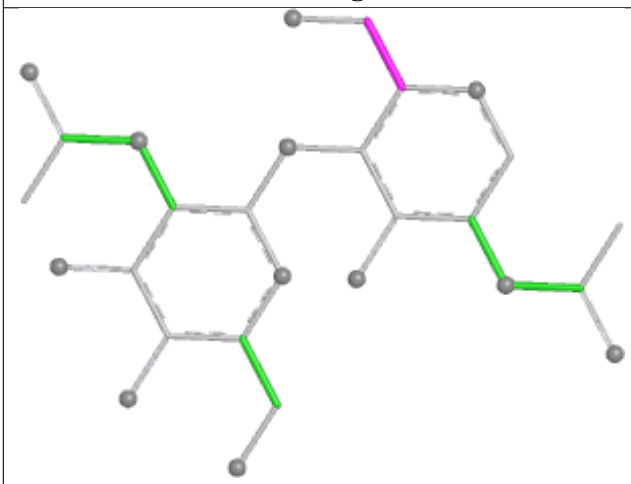
Oligosaccharide Chain S



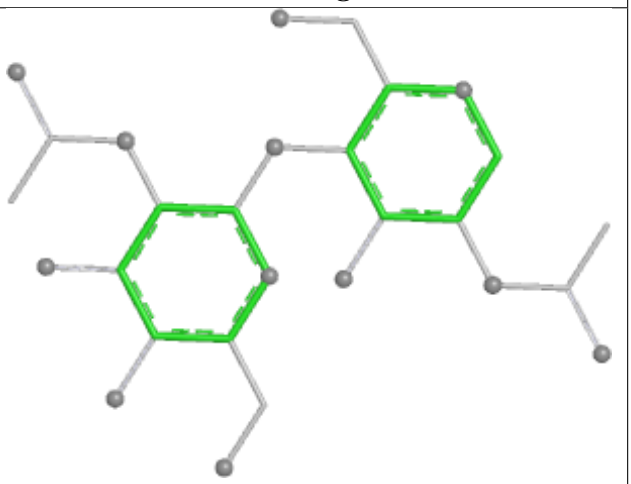
Bond lengths



Bond angles

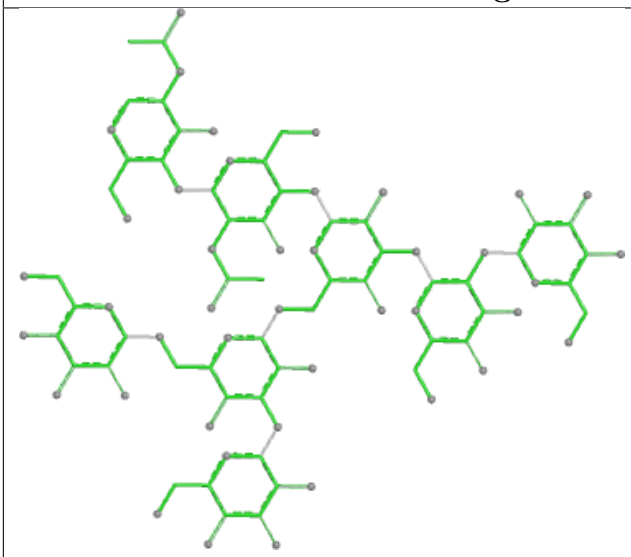


Torsions

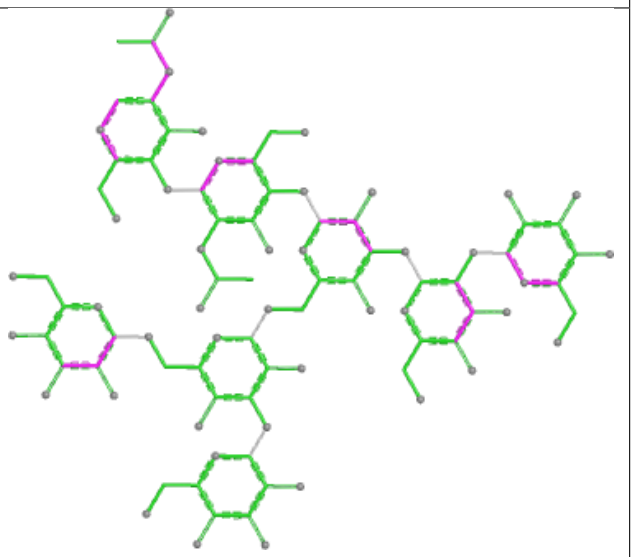


Rings

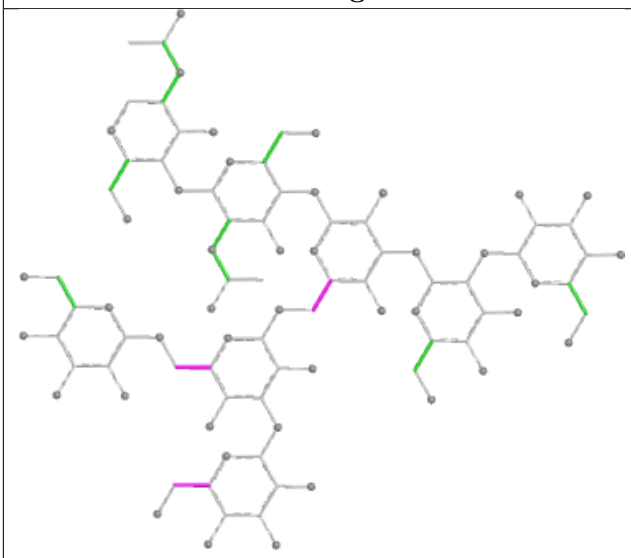
Oligosaccharide Chain H



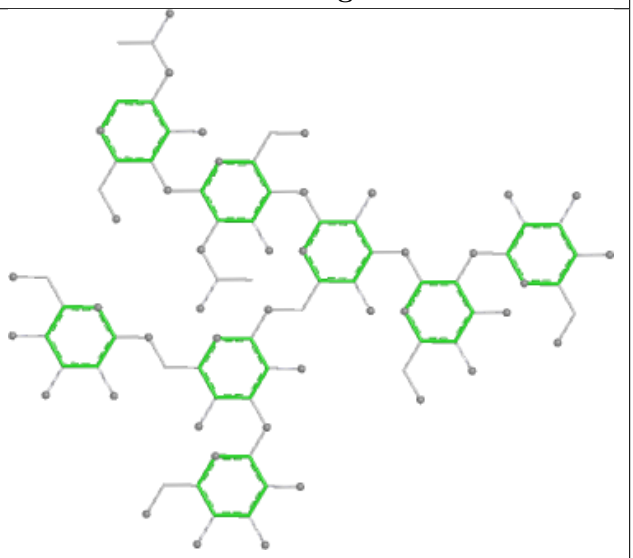
Bond lengths



Bond angles

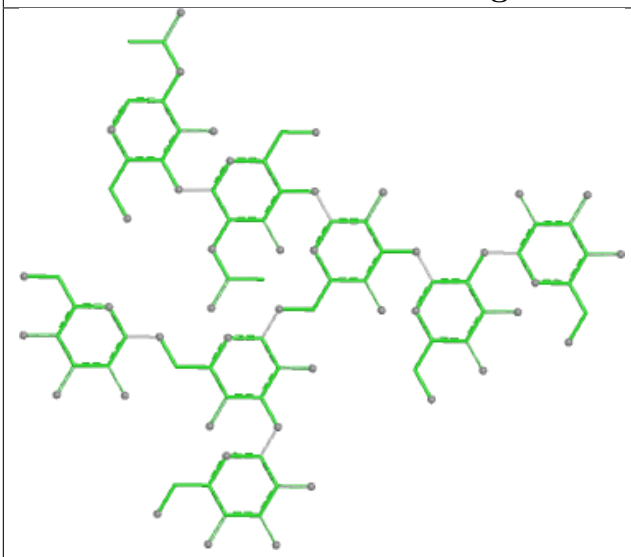


Torsions

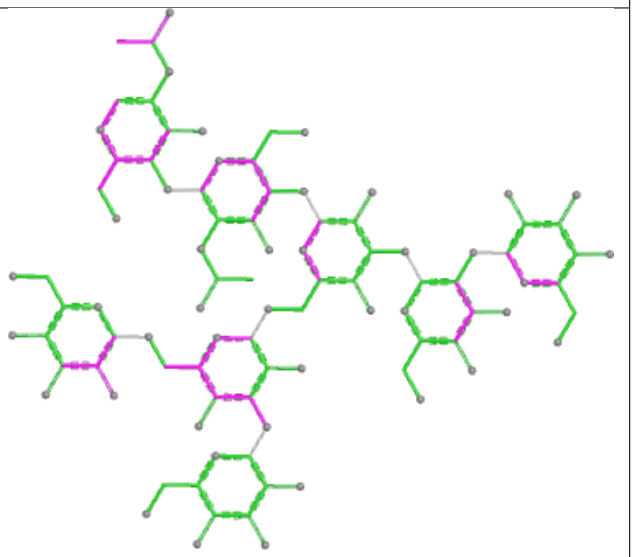


Rings

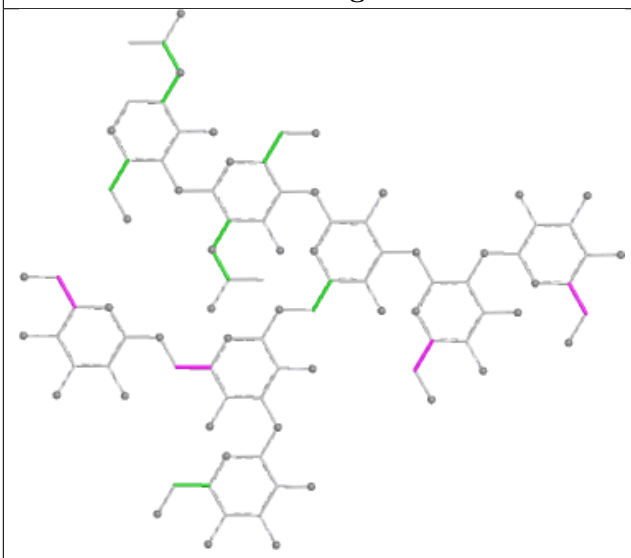
Oligosaccharide Chain M



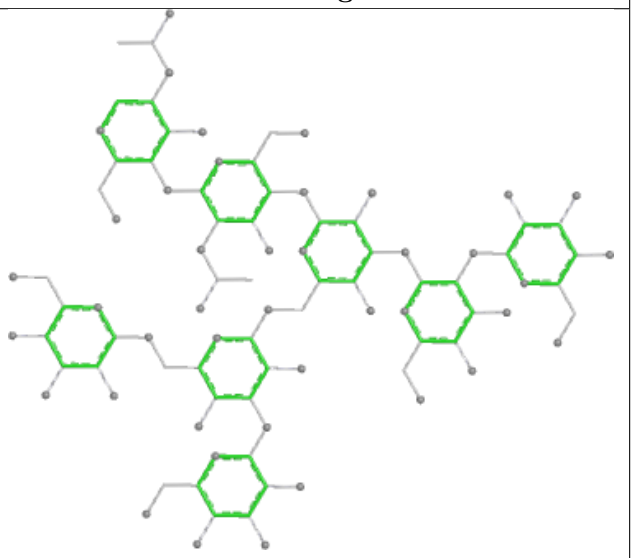
Bond lengths



Bond angles

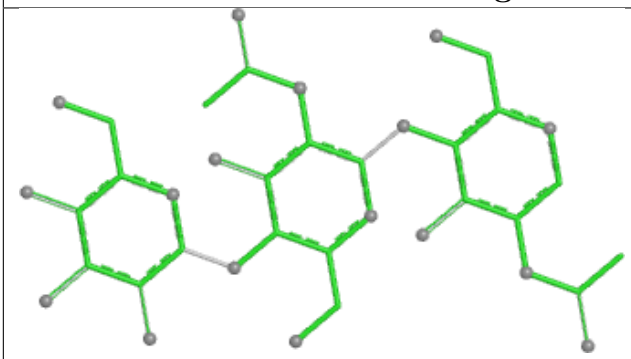


Torsions

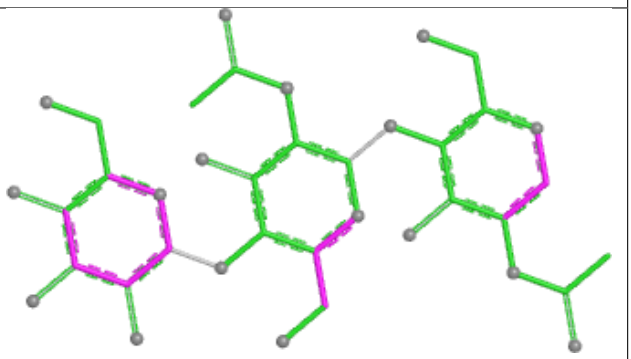


Rings

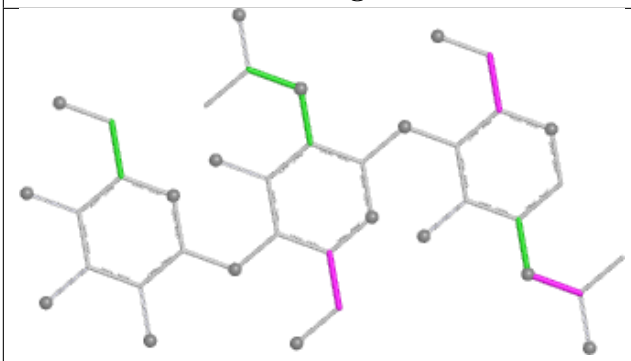
Oligosaccharide Chain O



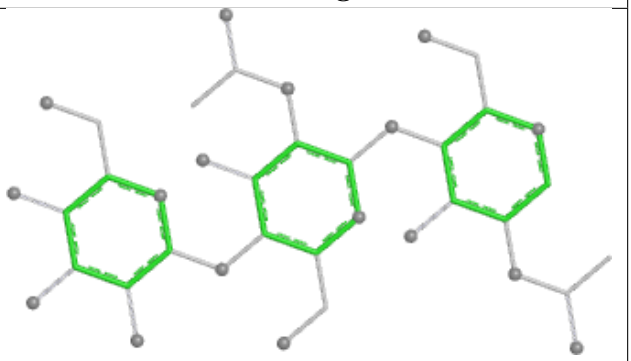
Bond lengths



Bond angles

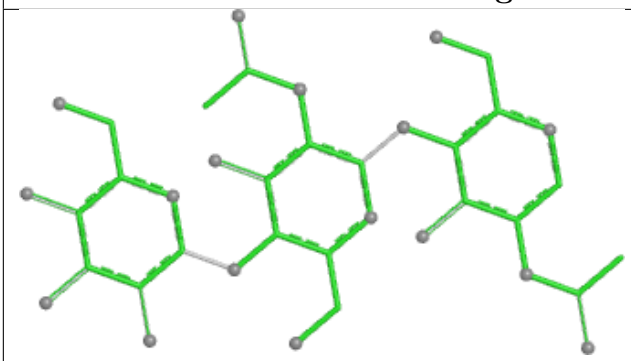


Torsions

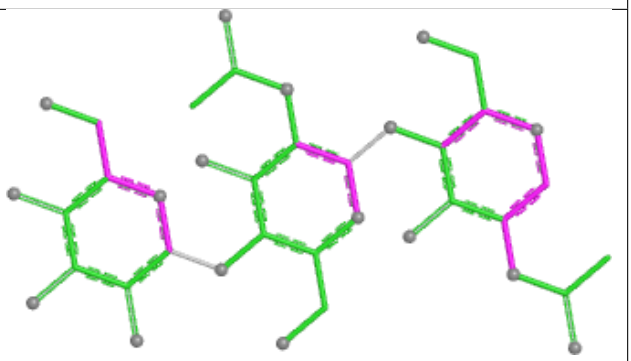


Rings

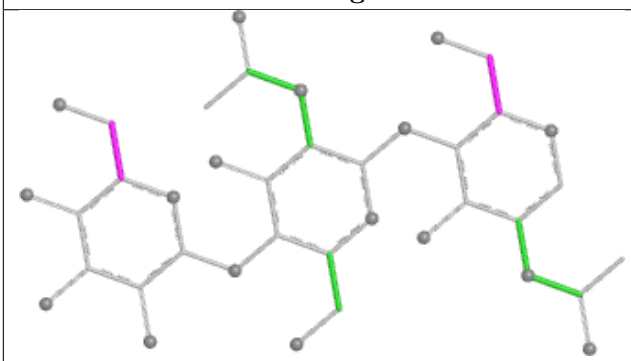
Oligosaccharide Chain T



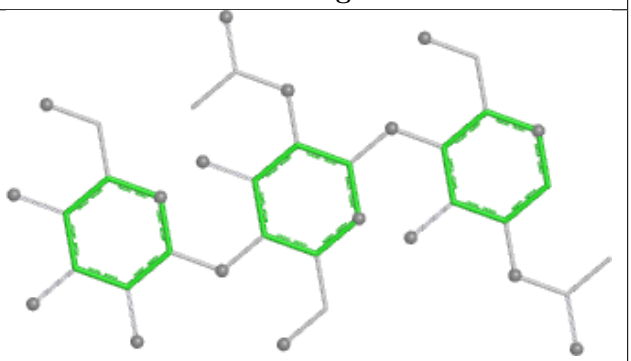
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 4 are monoatomic - leaving 26 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	$\#\|Z\| > 2$
10	SO4	A	1329	-	4,4,4	0.24	0	6,6,6	0.27	0
10	SO4	C	1331	-	4,4,4	0.24	0	6,6,6	0.13	0
9	ACT	C	1329	-	3,3,3	0.71	0	3,3,3	1.48	0
7	HEM	D	350	1,8	42,50,50	1.83	5 (11%)	46,82,82	1.69	10 (21%)
9	ACT	D	1327	-	3,3,3	0.71	0	3,3,3	1.39	0
11	NAG	D	411	1	14,14,15	0.55	0	17,19,21	0.83	0
10	SO4	C	1332	-	4,4,4	0.29	0	6,6,6	0.21	0
9	ACT	B	1328	7	3,3,3	0.80	0	3,3,3	1.25	0
7	HEM	C	350	1,8	42,50,50	1.87	8 (19%)	46,82,82	1.55	8 (17%)
11	NAG	C	381	1	14,14,15	0.63	0	17,19,21	1.37	2 (11%)
10	SO4	B	1331	-	4,4,4	0.27	0	6,6,6	0.19	0
10	SO4	B	1329	-	4,4,4	0.27	0	6,6,6	0.32	0
10	SO4	A	1328	-	4,4,4	0.31	0	6,6,6	0.19	0
10	SO4	B	1330	-	4,4,4	0.23	0	6,6,6	0.17	0
9	ACT	C	1334	-	3,3,3	0.76	0	3,3,3	1.35	0
10	SO4	A	1330	-	4,4,4	0.27	0	6,6,6	0.18	0
11	NAG	D	391	1	14,14,15	0.54	0	17,19,21	1.45	4 (23%)
9	ACT	A	1327	-	3,3,3	0.72	0	3,3,3	1.26	0
7	HEM	A	350	1,8	42,50,50	2.01	9 (21%)	46,82,82	1.46	5 (10%)
10	SO4	C	1333	-	4,4,4	0.21	0	6,6,6	0.07	0
7	HEM	B	350	1,9,8	42,50,50	1.96	5 (11%)	46,82,82	1.51	8 (17%)
10	SO4	A	1331	-	4,4,4	0.28	0	6,6,6	0.17	0
11	NAG	D	381	1	14,14,15	0.65	0	17,19,21	0.70	0
10	SO4	D	1328	-	4,4,4	0.20	0	6,6,6	0.28	0
10	SO4	D	1329	-	4,4,4	0.27	0	6,6,6	0.18	0
10	SO4	C	1330	-	4,4,4	0.22	0	6,6,6	0.21	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	NAG	D	381	1	-	0/6/23/26	0/1/1/1
7	HEM	B	350	1,9,8	-	3/12/54/54	-
7	HEM	D	350	1,8	-	3/12/54/54	-
11	NAG	D	411	1	-	0/6/23/26	0/1/1/1
11	NAG	D	391	1	-	2/6/23/26	0/1/1/1
11	NAG	C	381	1	-	2/6/23/26	0/1/1/1
7	HEM	A	350	1,8	-	4/12/54/54	-
7	HEM	C	350	1,8	-	4/12/54/54	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	350	HEM	C3D-C2D	7.43	1.52	1.36
7	A	350	HEM	C3D-C2D	7.41	1.52	1.36
7	D	350	HEM	C3D-C2D	7.29	1.52	1.36
7	B	350	HEM	C3D-C2D	6.88	1.51	1.36
7	A	350	HEM	C3C-C2C	-5.49	1.32	1.40

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	350	HEM	C4D-ND-C1D	4.56	110.60	105.21
7	D	350	HEM	C4D-ND-C1D	4.52	110.56	105.21
7	D	350	HEM	C4C-CHD-C1D	4.46	128.44	122.56
7	B	350	HEM	C4D-ND-C1D	4.40	110.42	105.21
7	C	350	HEM	C4D-ND-C1D	3.95	109.88	105.21

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	381	NAG	C4-C5-C6-O6
11	C	381	NAG	O5-C5-C6-O6
7	A	350	HEM	C2A-CAA-CBA-CGA
7	D	350	HEM	C2A-CAA-CBA-CGA
11	D	391	NAG	O5-C5-C6-O6

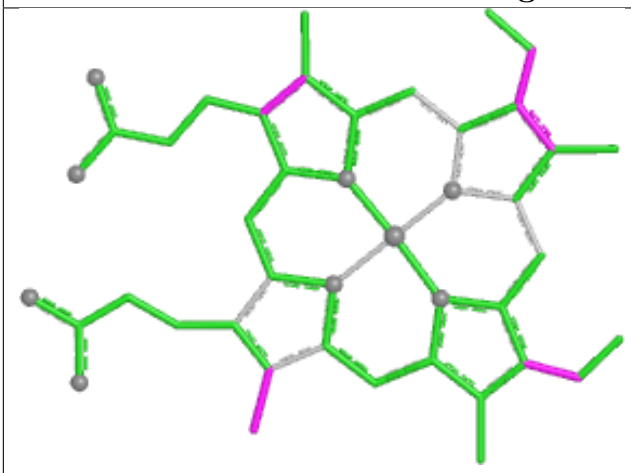
There are no ring outliers.

9 monomers are involved in 21 short contacts:

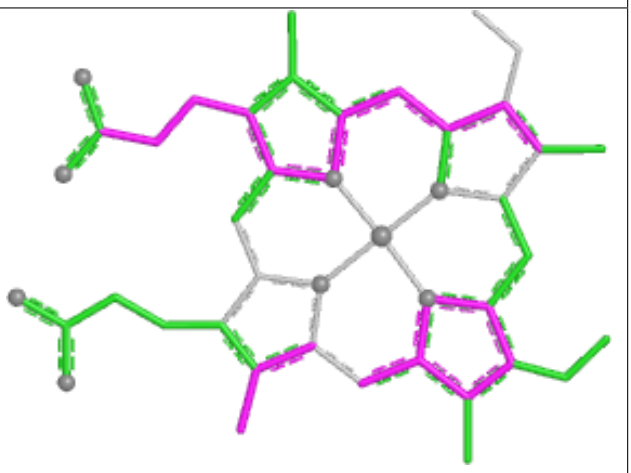
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	350	HEM	3	0
7	C	350	HEM	3	0
11	C	381	NAG	1	0
10	B	1331	SO4	2	0
7	A	350	HEM	5	0
7	B	350	HEM	3	0
10	A	1331	SO4	2	0
10	D	1328	SO4	1	0
10	D	1329	SO4	1	0

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.

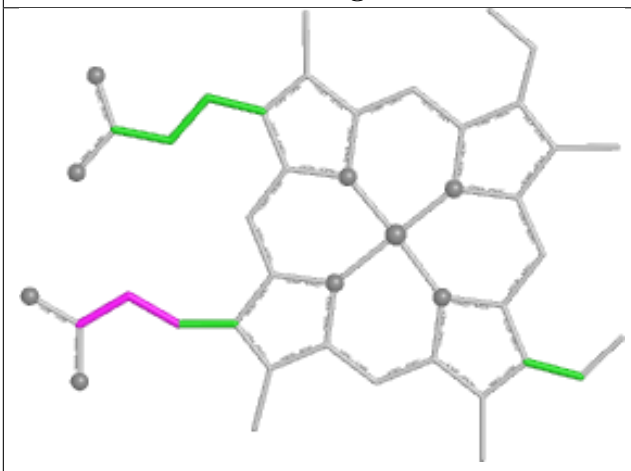
Ligand HEM D 350



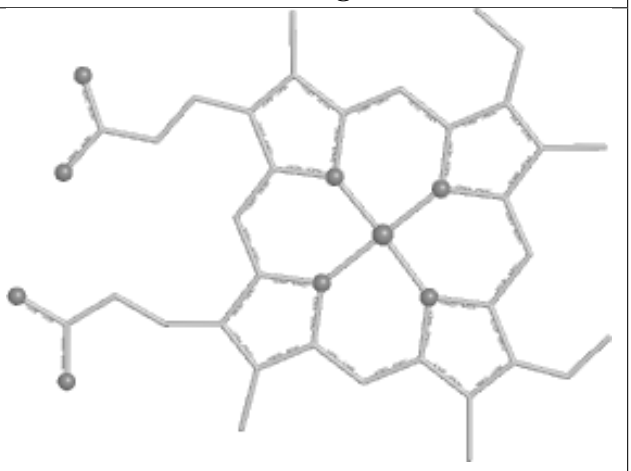
Bond lengths



Bond angles

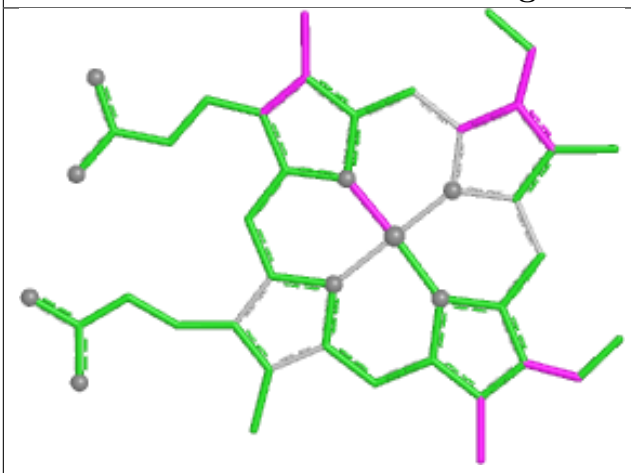


Torsions

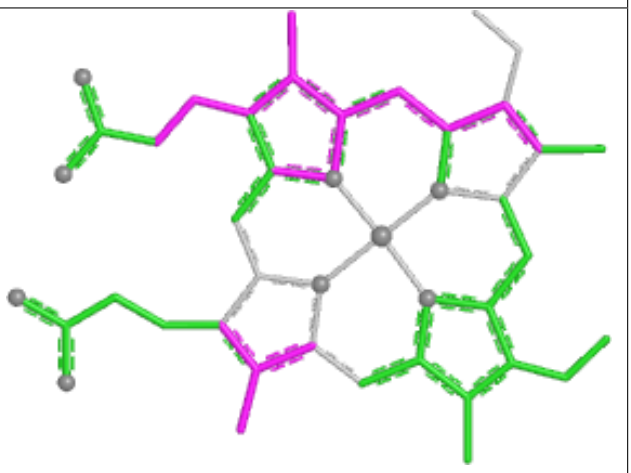


Rings

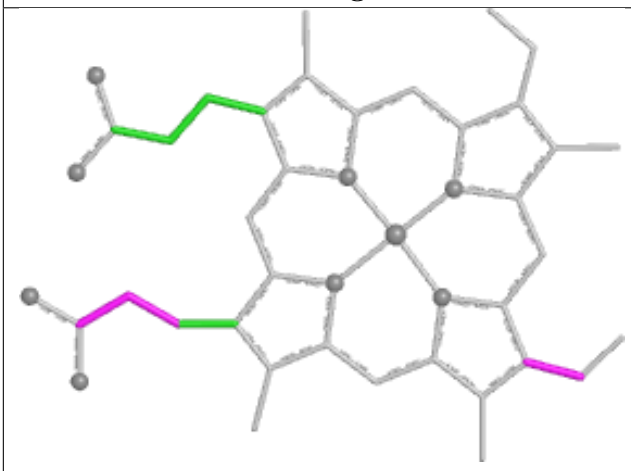
Ligand HEM C 350



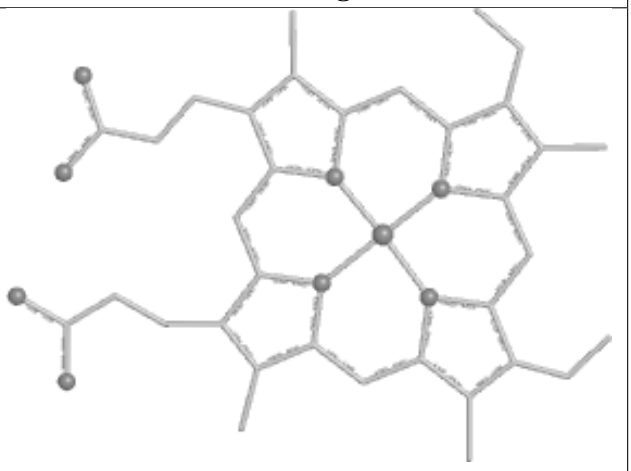
Bond lengths



Bond angles

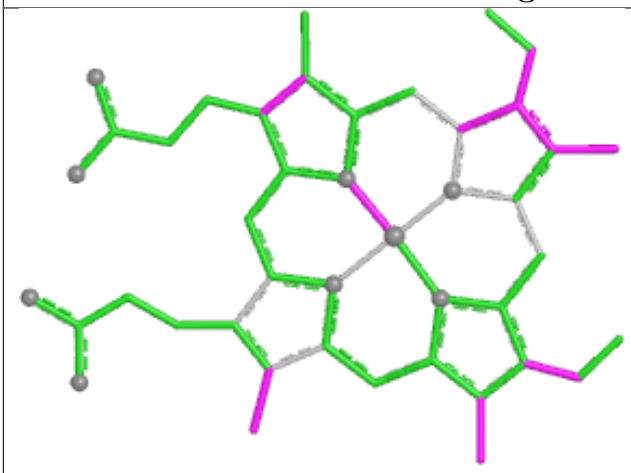


Torsions

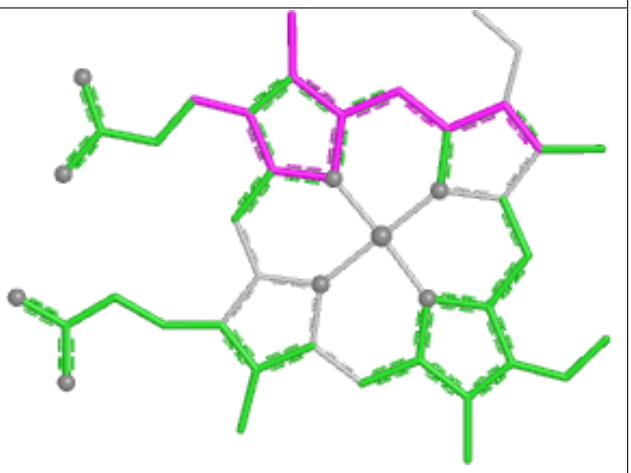


Rings

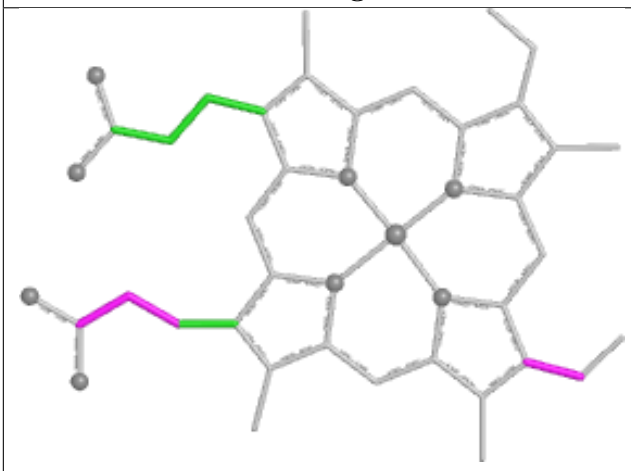
Ligand HEM A 350



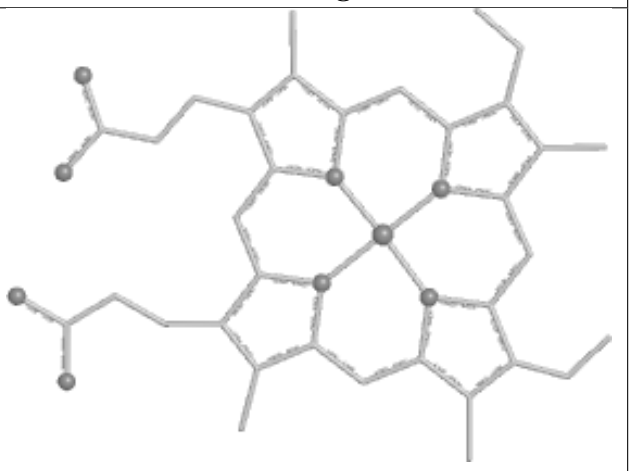
Bond lengths



Bond angles

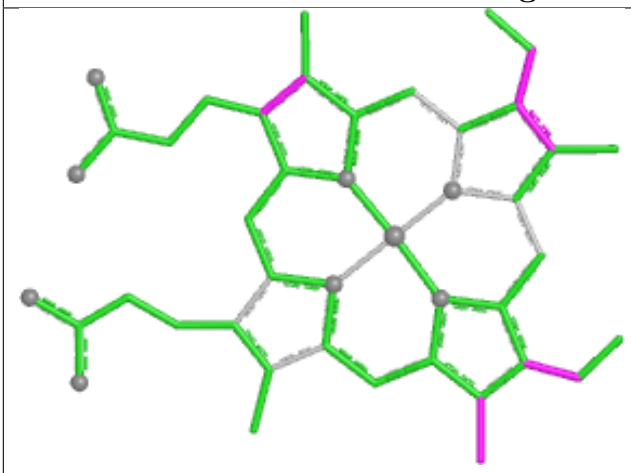


Torsions

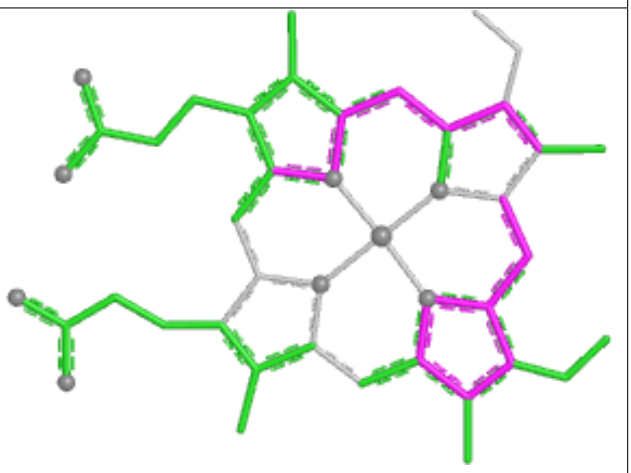


Rings

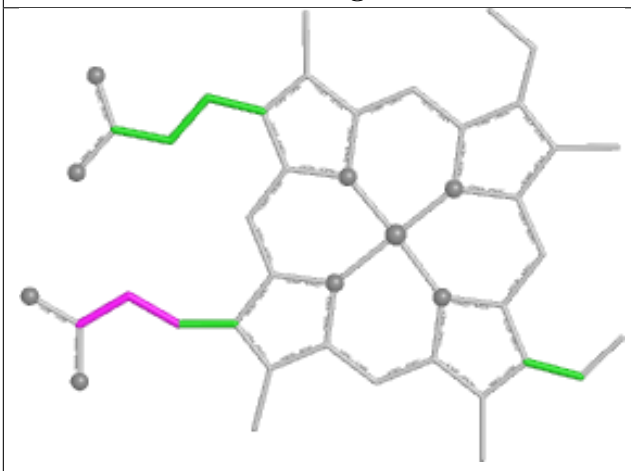
Ligand HEM B 350



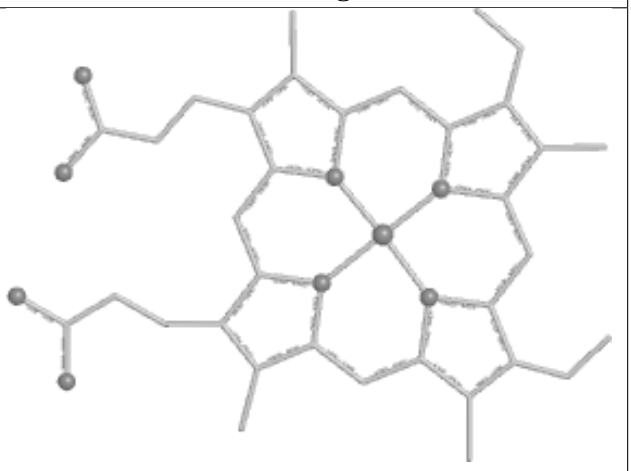
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	323/325 (99%)	-0.29	1 (0%) 94 96	12, 26, 42, 56	0
1	B	324/325 (99%)	-0.44	0 100 100	11, 21, 34, 53	0
1	C	325/325 (100%)	-0.32	2 (0%) 89 92	14, 24, 37, 68	0
1	D	323/325 (99%)	-0.06	5 (1%) 73 79	16, 32, 47, 59	0
All	All	1295/1300 (99%)	-0.28	8 (0%) 89 92	11, 26, 43, 68	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	328	ASP	3.8
1	D	20	GLU	3.7
1	A	20	GLU	2.9
1	C	259	VAL	2.5
1	D	217	ASP	2.5

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

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	J	5	11/12	0.42	0.46	78,80,81,81	0
3	BMA	J	3	11/12	0.65	0.32	59,62,64,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	H	5	11/12	0.69	0.41	58,64,65,65	0
3	MAN	F	4	11/12	0.71	0.38	79,81,84,88	0
2	MAN	E	6	11/12	0.71	0.24	64,65,66,67	0
6	BMA	O	3	11/12	0.71	0.48	75,78,79,79	0
6	BMA	T	3	11/12	0.71	0.25	58,60,62,62	0
3	BMA	F	3	11/12	0.72	0.33	56,58,68,74	0
3	MAN	J	4	11/12	0.75	0.30	67,69,72,75	0
3	MAN	F	5	11/12	0.76	0.52	88,90,90,91	0
3	NAG	J	2	14/15	0.76	0.26	45,50,52,56	0
4	NAG	I	2	14/15	0.77	0.51	75,78,81,81	0
2	MAN	E	5	11/12	0.78	0.35	66,68,70,71	0
4	NAG	N	2	14/15	0.80	0.61	74,77,79,81	0
4	NAG	G	2	14/15	0.81	0.26	57,61,65,66	0
5	MAN	H	8	11/12	0.81	0.25	60,61,63,64	0
4	NAG	P	2	14/15	0.81	0.23	47,53,55,58	0
4	NAG	S	2	14/15	0.81	0.35	60,62,65,66	0
4	NAG	R	2	14/15	0.82	0.48	73,76,77,78	0
4	NAG	L	2	14/15	0.82	0.30	57,59,63,64	0
5	MAN	H	6	11/12	0.84	0.20	46,49,55,59	0
4	NAG	K	2	14/15	0.85	0.20	43,49,52,53	0
4	NAG	Q	2	14/15	0.86	0.47	56,60,63,65	0
5	MAN	H	4	11/12	0.87	0.27	55,59,60,62	0
5	MAN	M	5	11/12	0.88	0.36	52,55,57,58	0
4	NAG	Q	1	14/15	0.88	0.21	31,42,48,51	0
3	NAG	F	2	14/15	0.88	0.14	37,42,46,52	0
2	BMA	E	3	11/12	0.89	0.23	49,54,59,62	0
2	MAN	E	4	11/12	0.89	0.23	51,54,58,63	0
4	NAG	R	1	14/15	0.89	0.28	55,60,64,69	0
2	NAG	E	2	14/15	0.90	0.23	40,46,53,56	0
5	MAN	M	8	11/12	0.90	0.21	47,50,52,52	0
4	NAG	I	1	14/15	0.91	0.30	56,64,68,70	0
6	NAG	T	2	14/15	0.91	0.18	48,52,58,58	0
6	NAG	O	2	14/15	0.91	0.32	58,61,65,70	0
4	NAG	N	1	14/15	0.92	0.26	51,57,62,69	0
6	NAG	O	1	14/15	0.93	0.22	41,46,49,54	0
5	NAG	H	1	14/15	0.93	0.20	34,39,42,43	0
5	MAN	M	4	11/12	0.93	0.16	40,43,45,50	0
4	NAG	S	1	14/15	0.93	0.22	50,54,56,59	0
5	MAN	H	7	11/12	0.93	0.21	52,53,54,55	0
5	BMA	H	3	11/12	0.94	0.12	40,44,47,48	0
6	NAG	T	1	14/15	0.94	0.11	26,34,39,43	0
2	NAG	E	1	14/15	0.95	0.16	33,36,41,41	0

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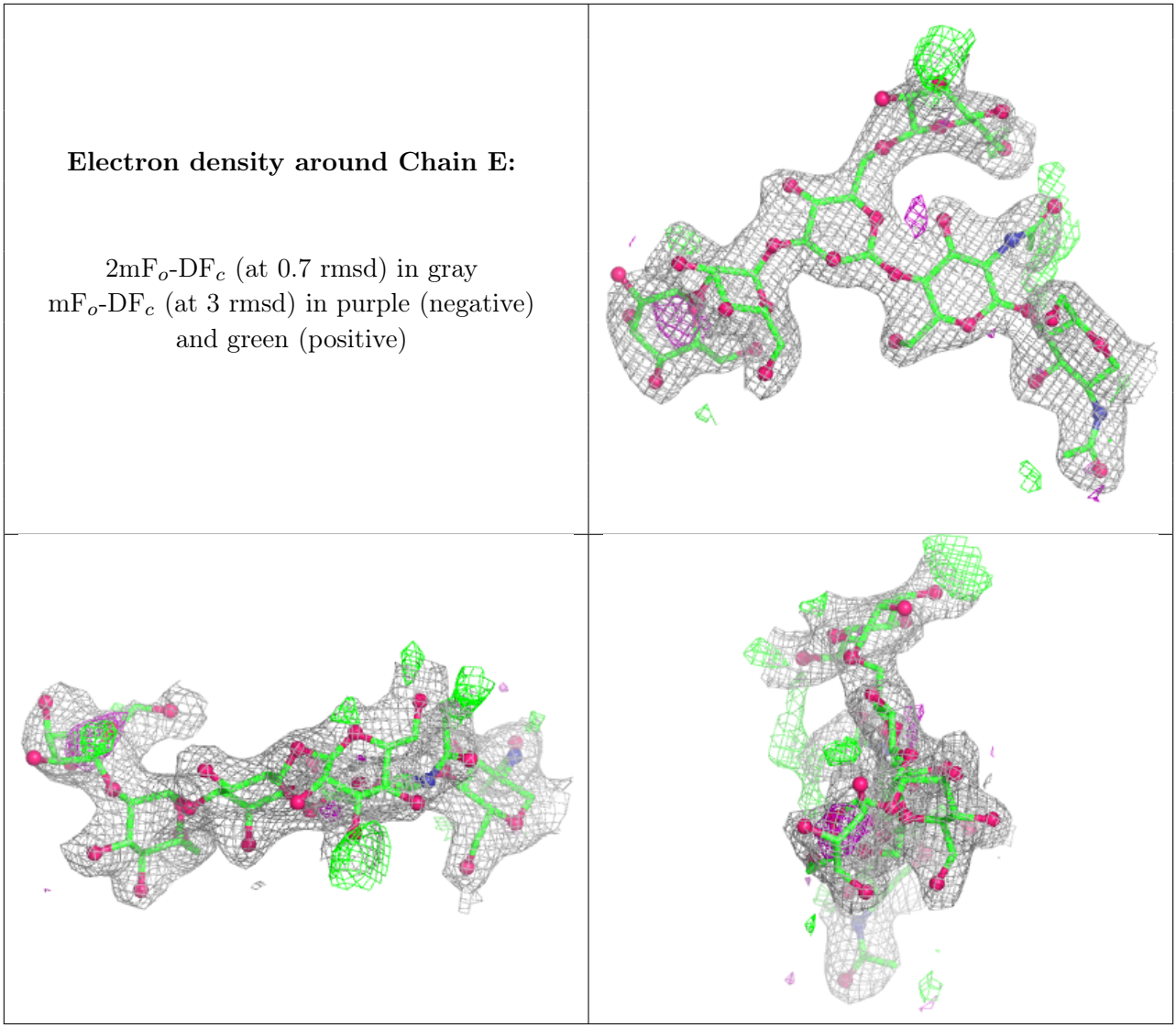
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	L	1	14/15	0.95	0.13	39,42,46,53	0
3	NAG	J	1	14/15	0.95	0.15	30,34,41,45	0
4	NAG	G	1	14/15	0.95	0.17	39,43,47,54	0
4	NAG	K	1	14/15	0.96	0.10	16,23,29,36	0
4	NAG	P	1	14/15	0.96	0.11	25,30,36,42	0
5	MAN	M	6	11/12	0.96	0.10	26,30,36,45	0
5	NAG	H	2	14/15	0.96	0.18	42,45,47,47	0
5	BMA	M	3	11/12	0.96	0.13	30,33,36,37	0
5	MAN	M	7	11/12	0.97	0.15	27,31,32,34	0
5	NAG	M	1	14/15	0.97	0.14	26,30,32,37	0
5	NAG	M	2	14/15	0.97	0.13	23,31,34,40	0
3	NAG	F	1	14/15	0.97	0.10	18,21,26,30	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.

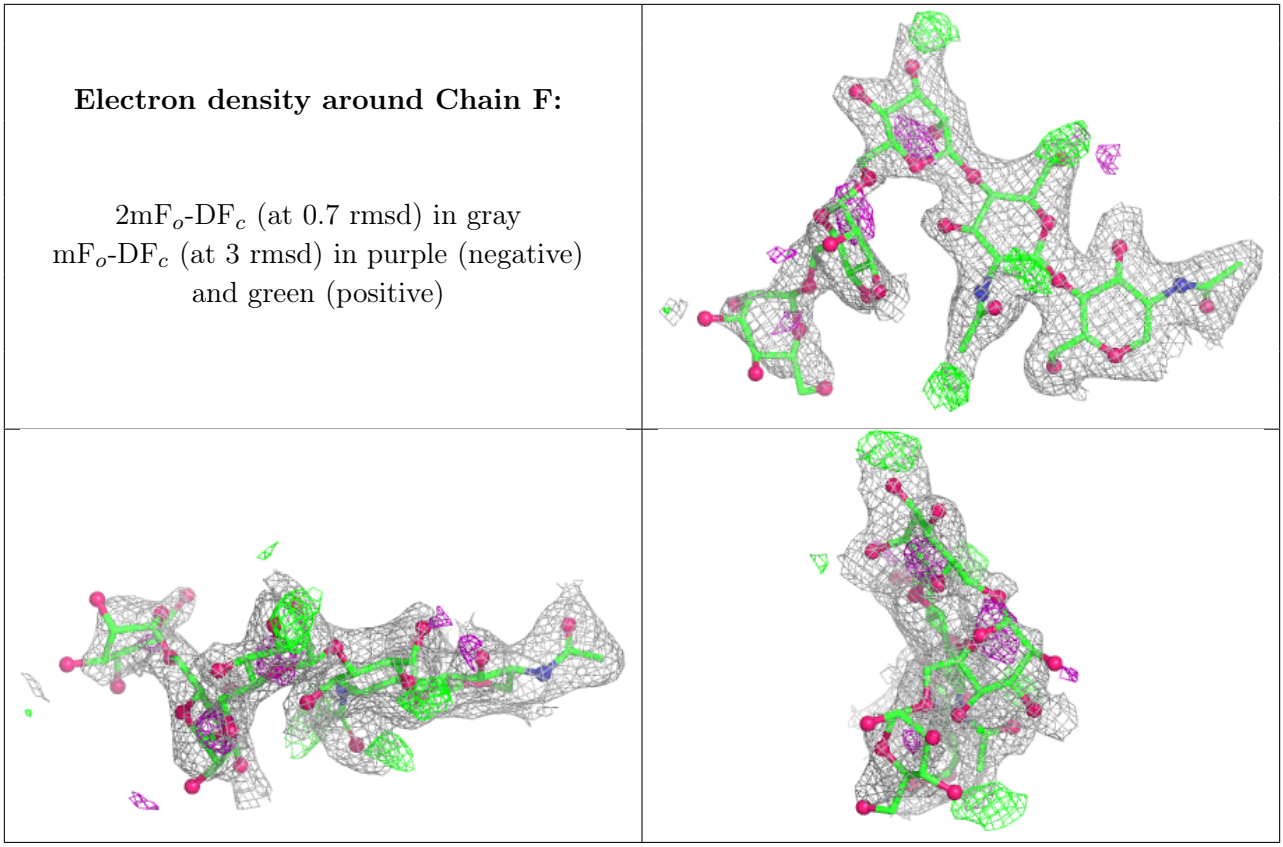
Electron density around Chain E:

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



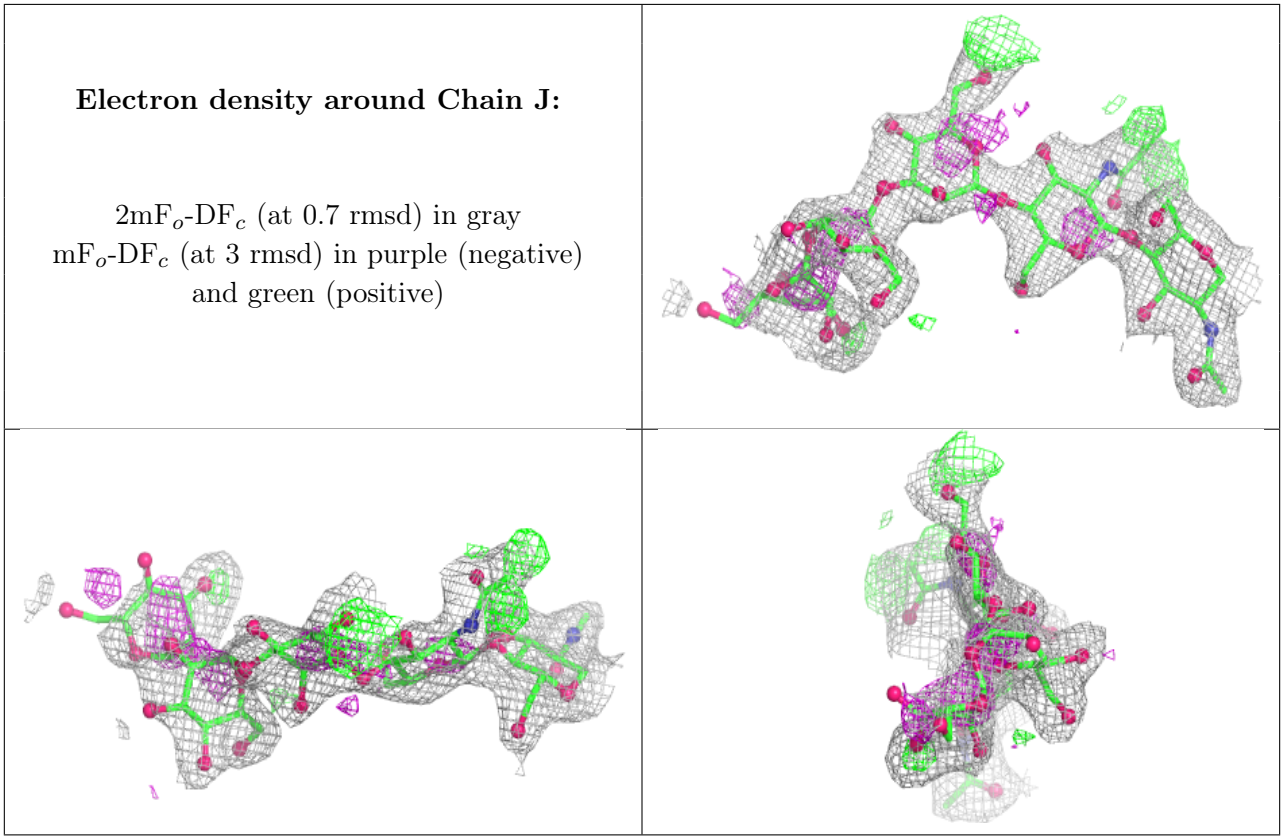
Electron density around Chain F:

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



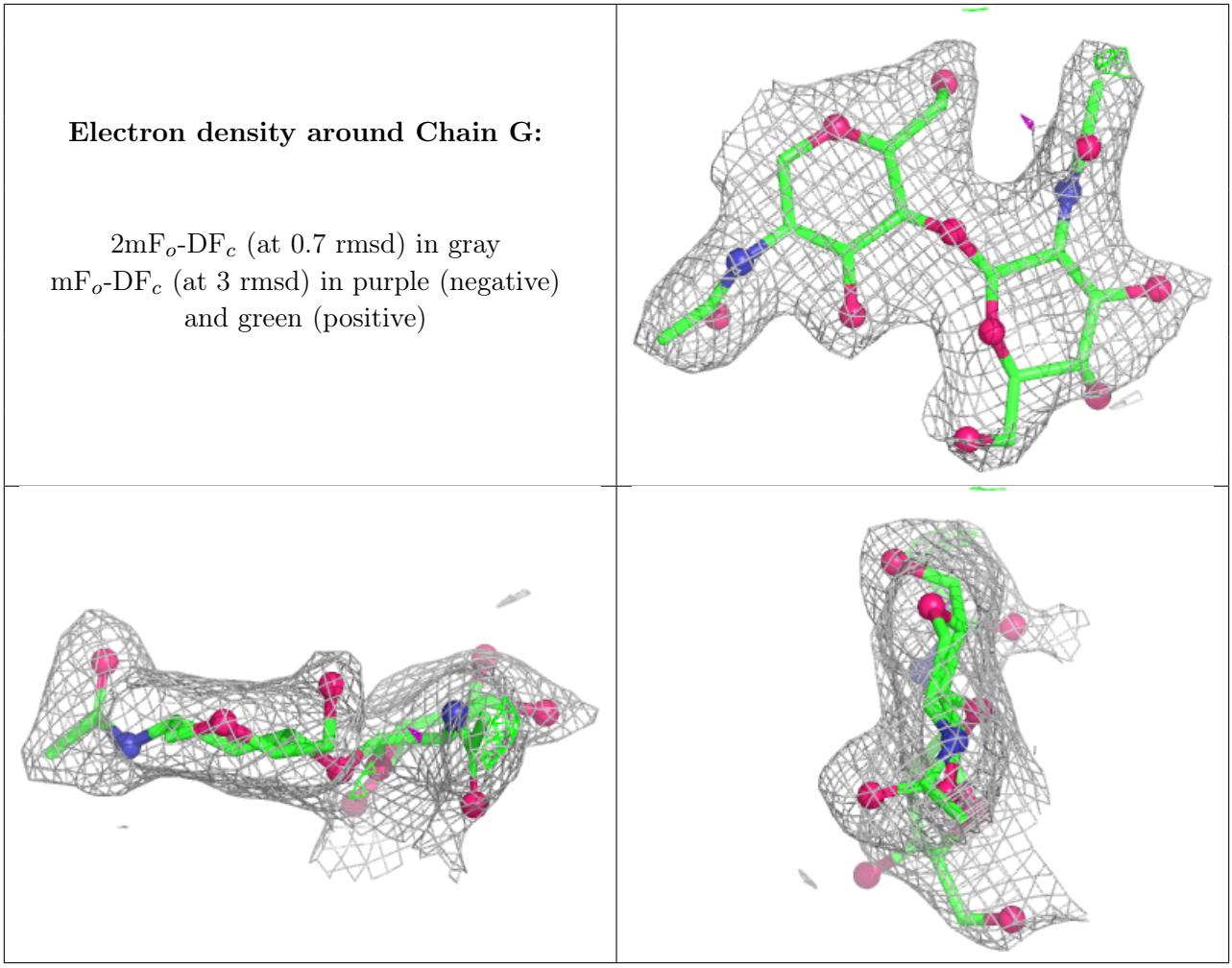
Electron density around Chain J:

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



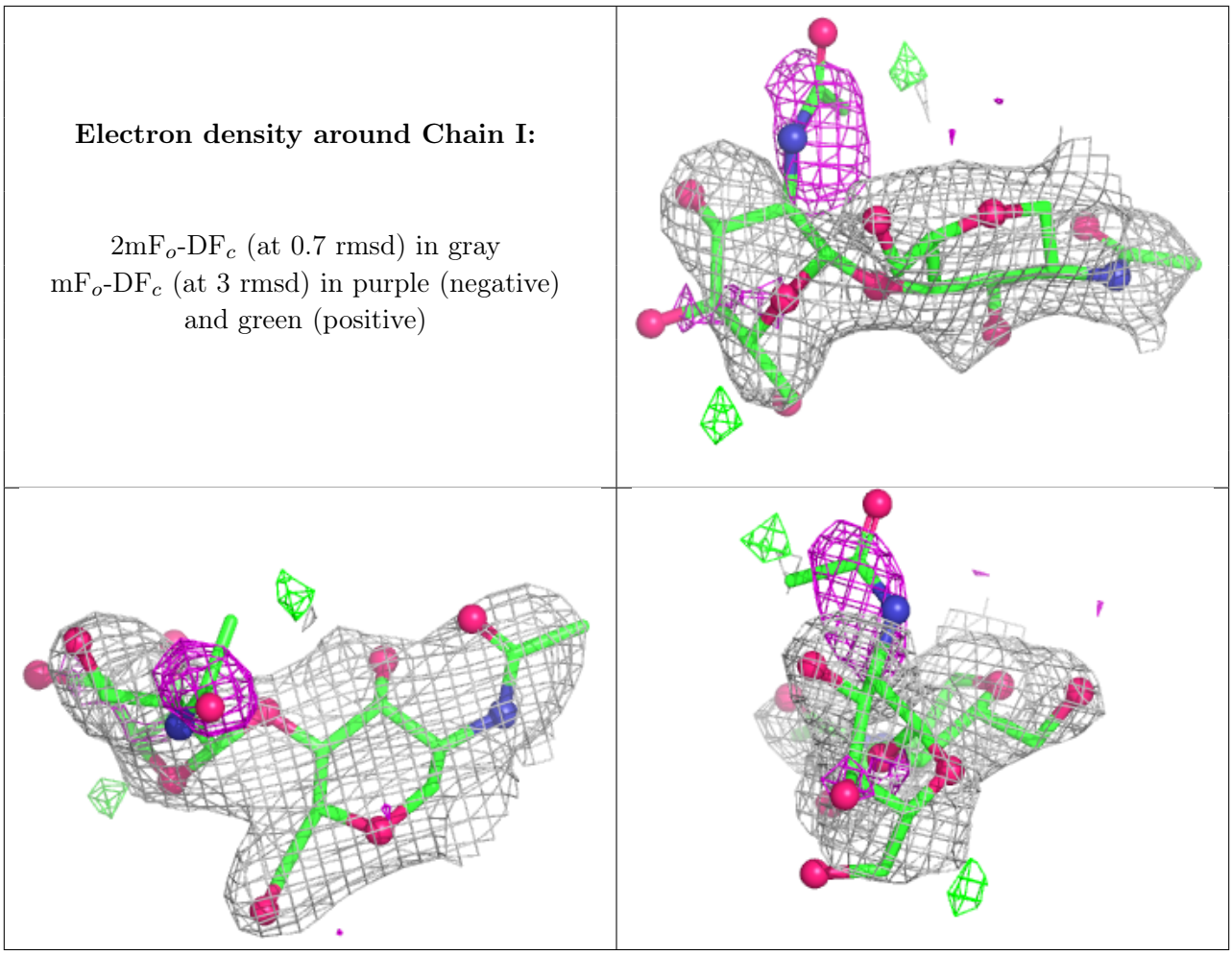
Electron density around Chain G:

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



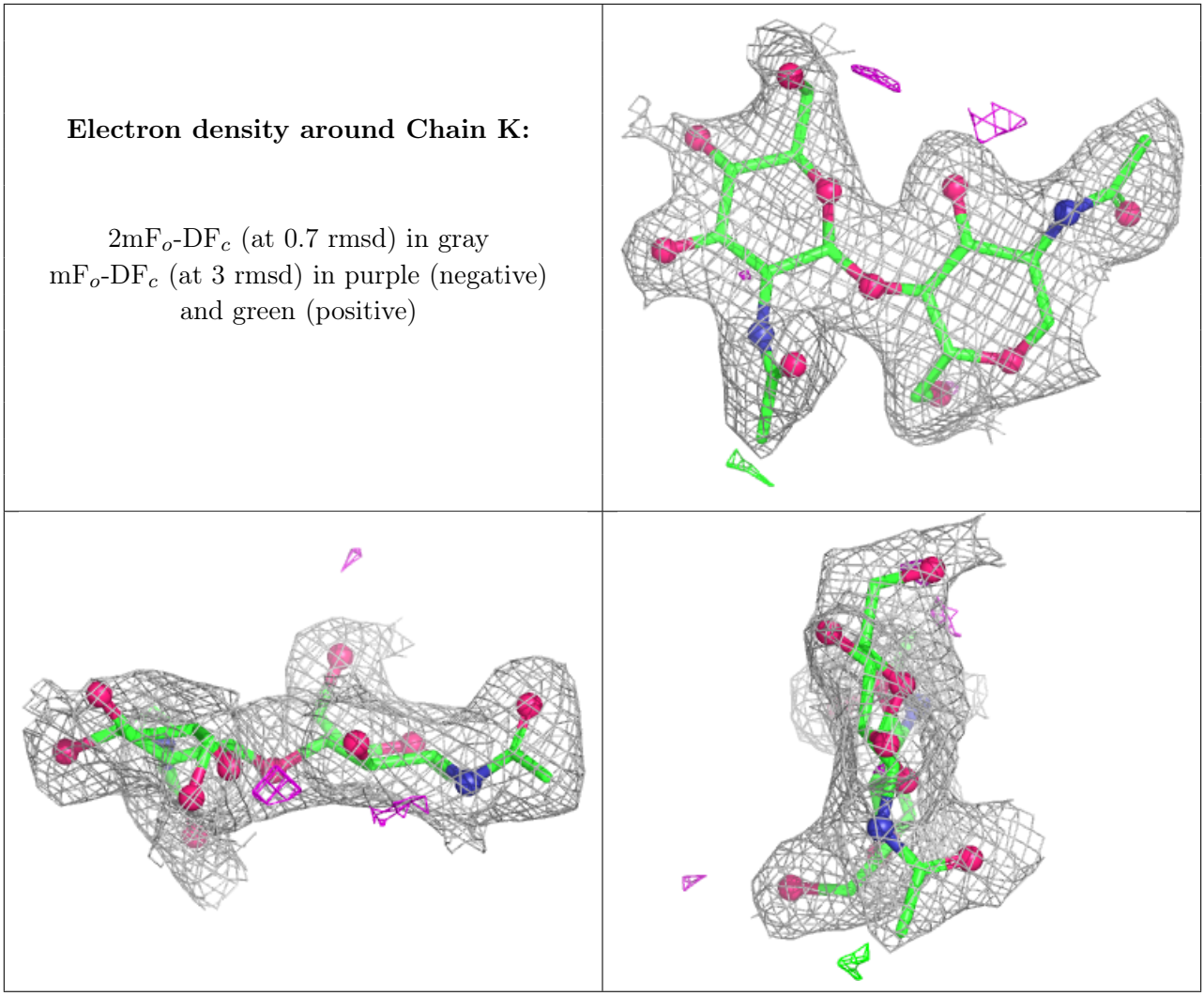
Electron density around Chain I:

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



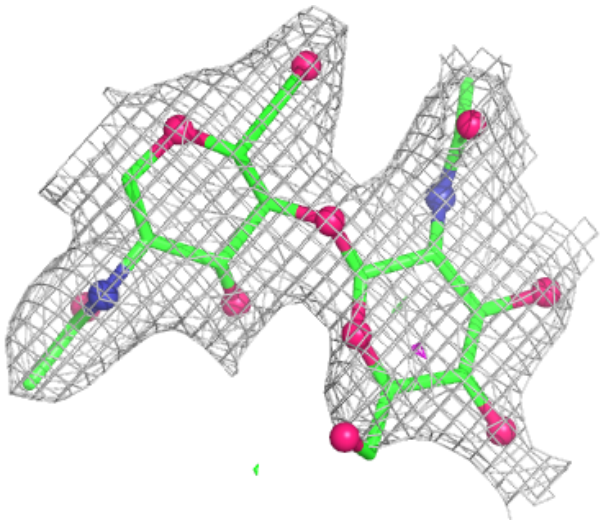
Electron density around Chain K:

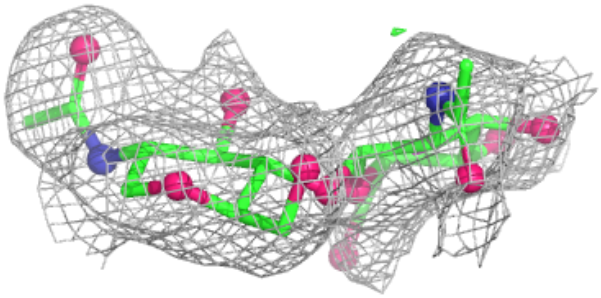
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

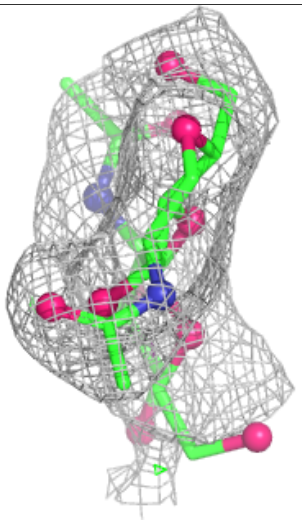


Electron density around Chain L:

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

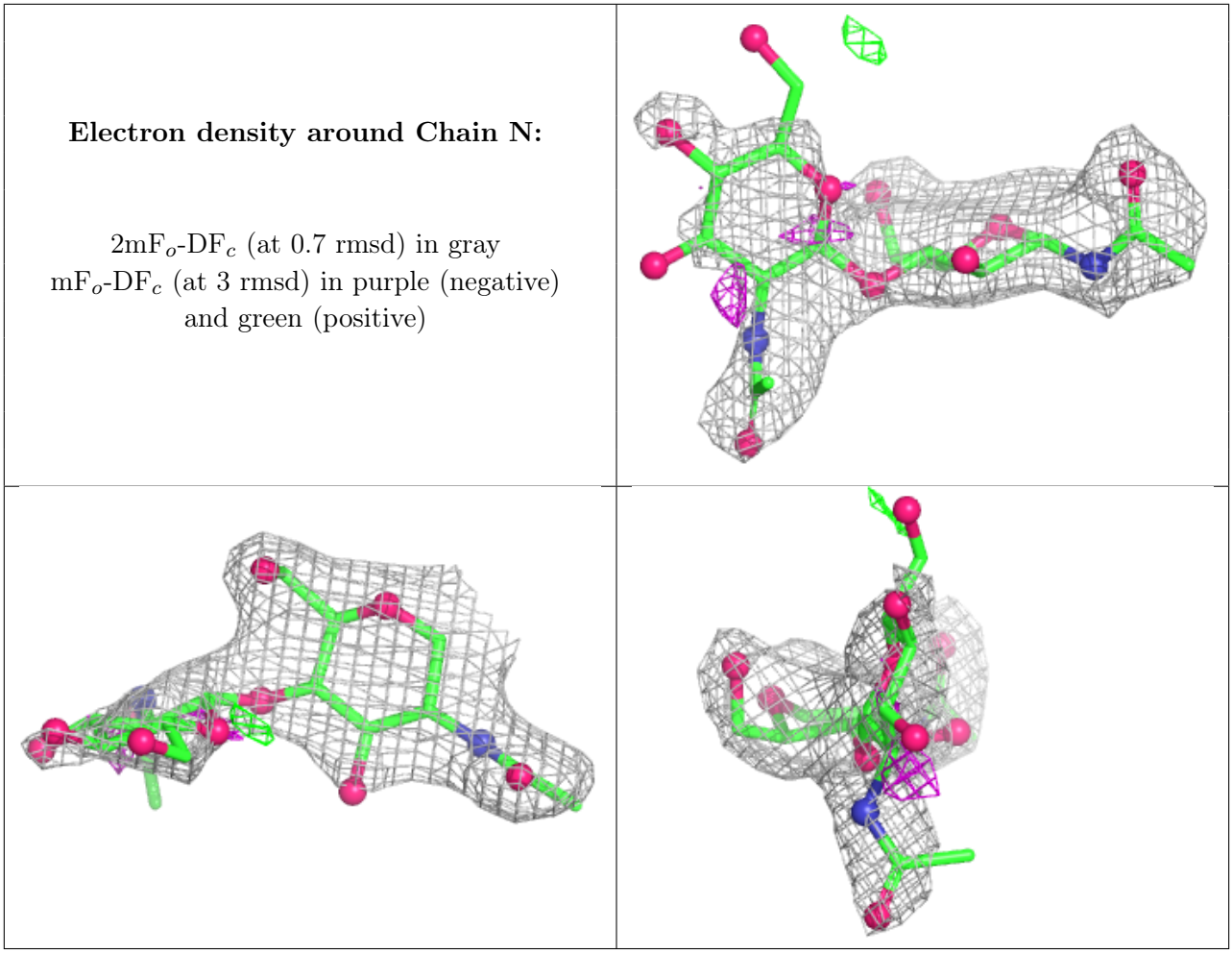






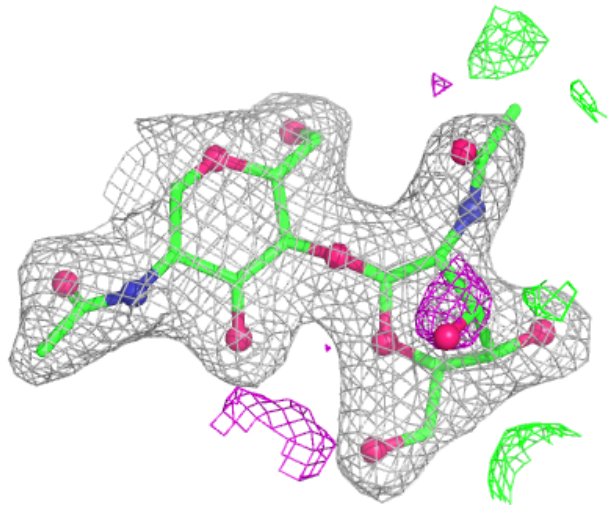
Electron density around Chain N:

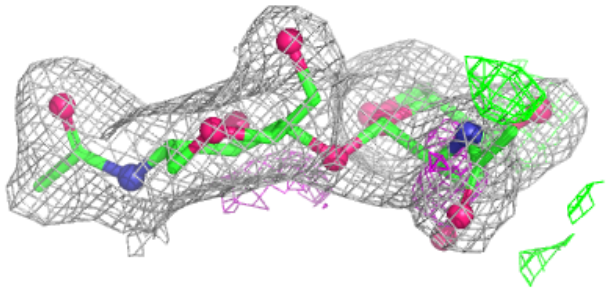
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

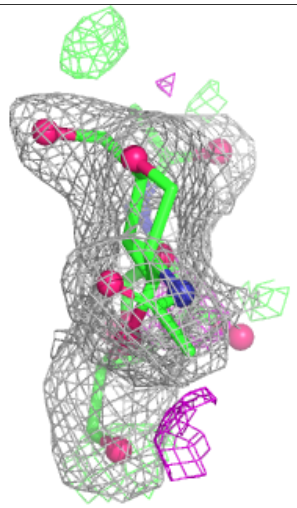


Electron density around Chain P:

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

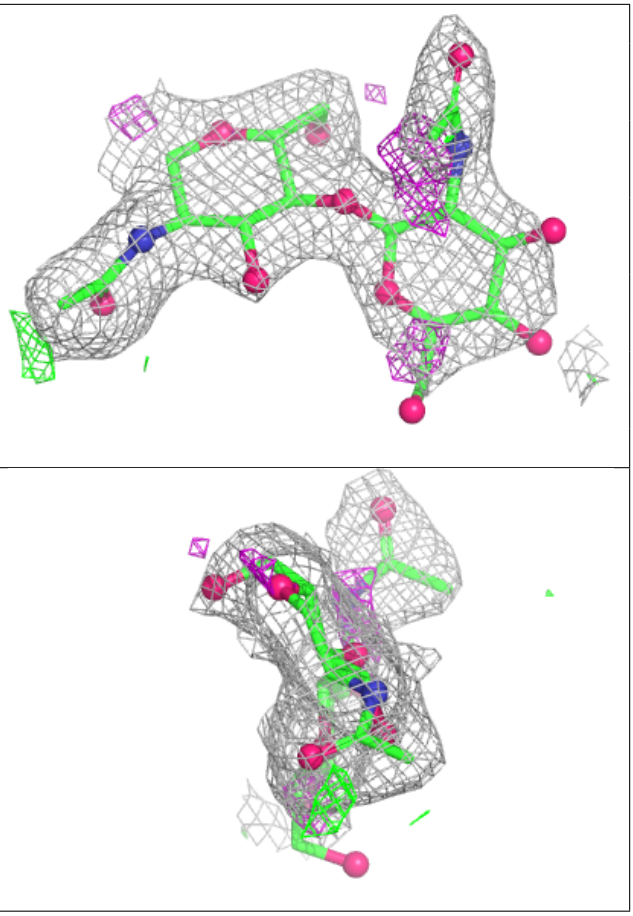






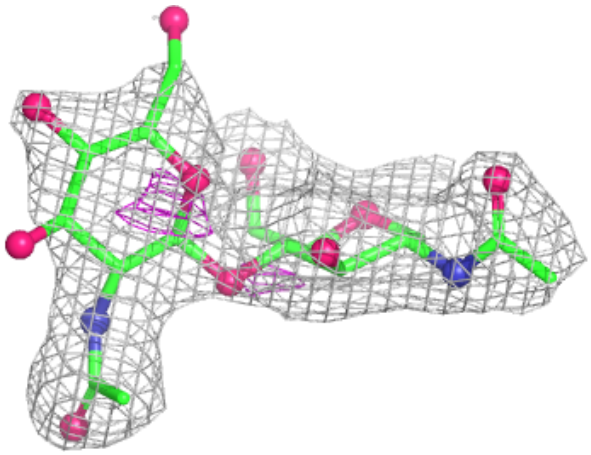
Electron density around Chain Q:

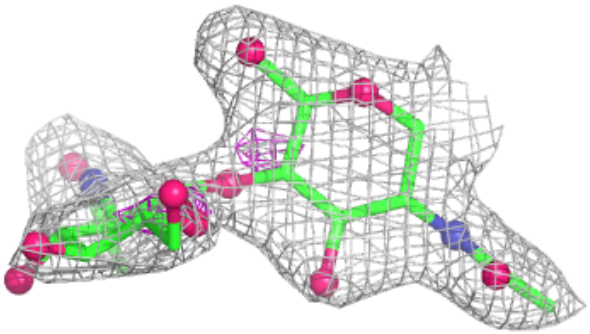
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

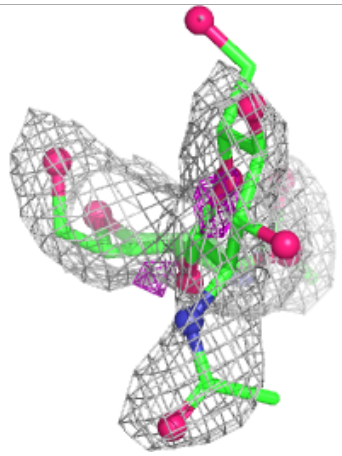


Electron density around Chain R:

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

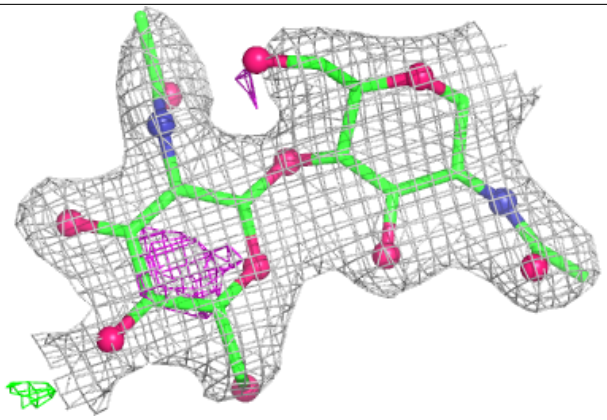


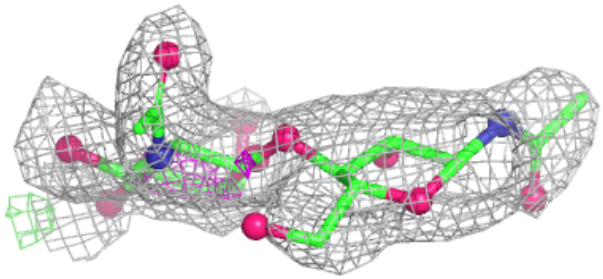


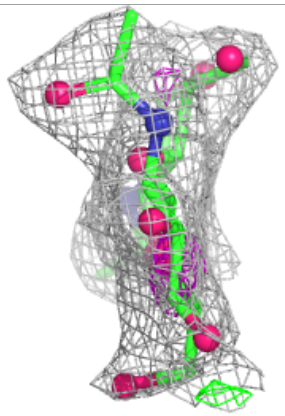


Electron density around Chain S:

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

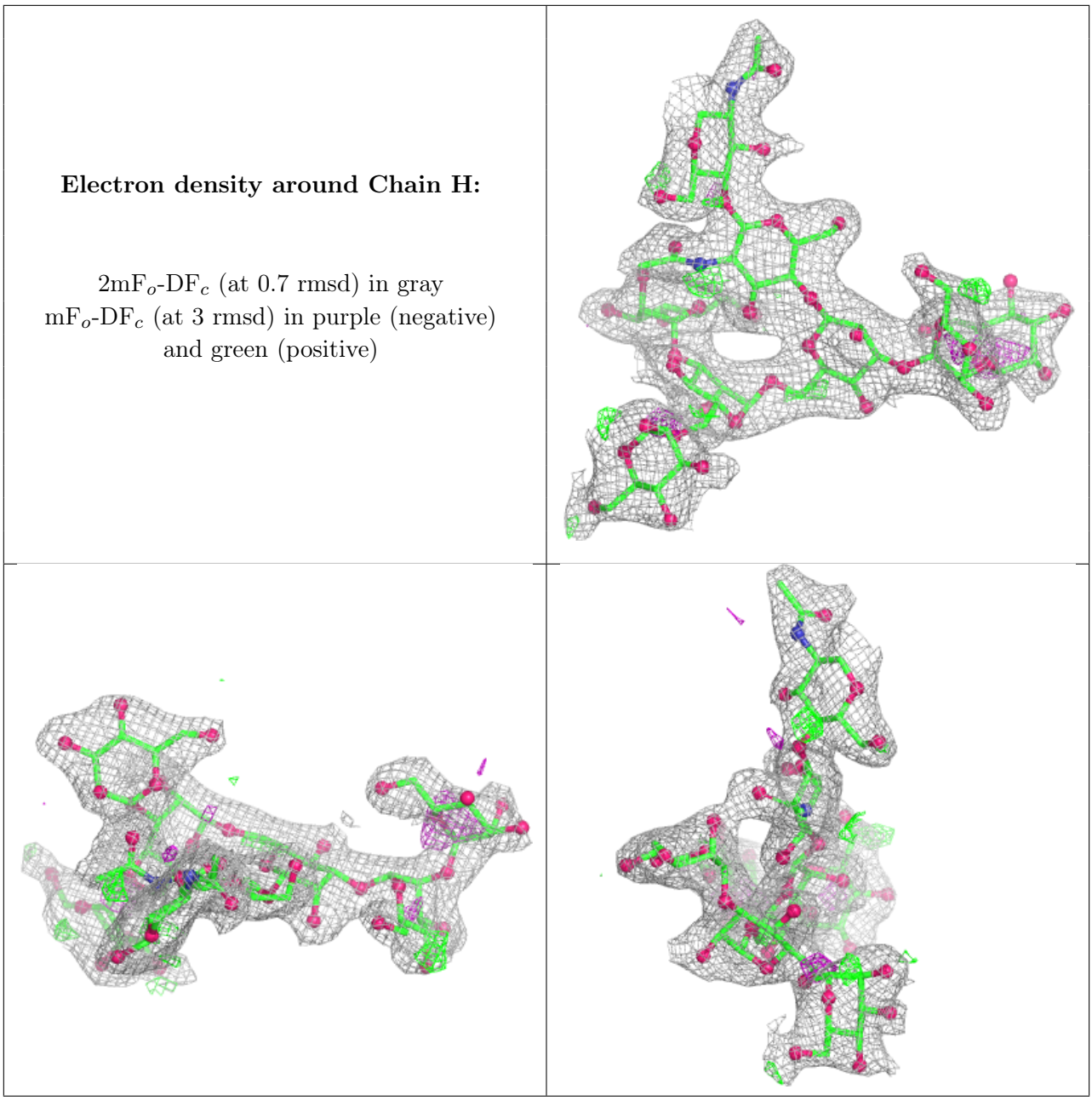






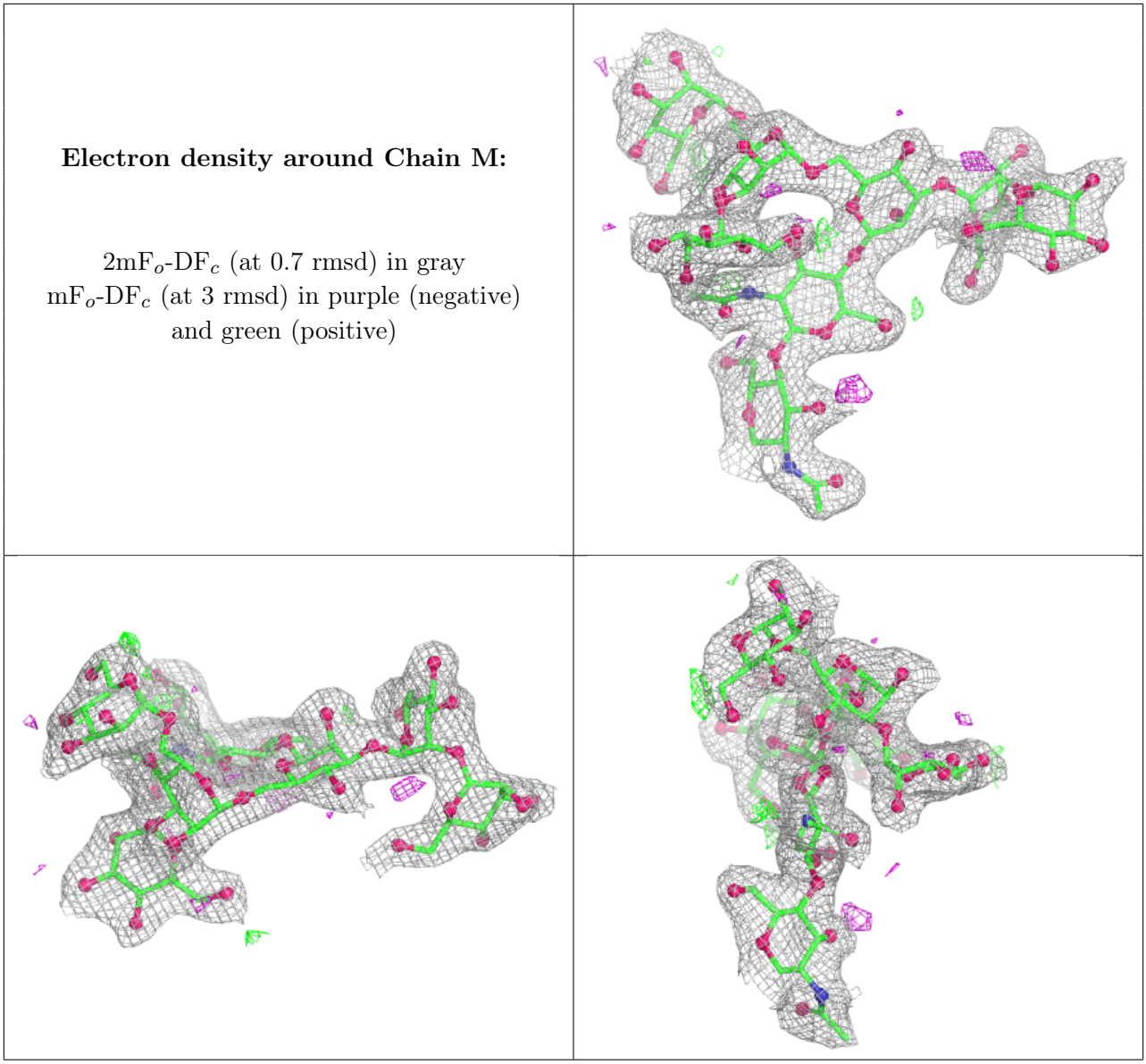
Electron density around Chain H:

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



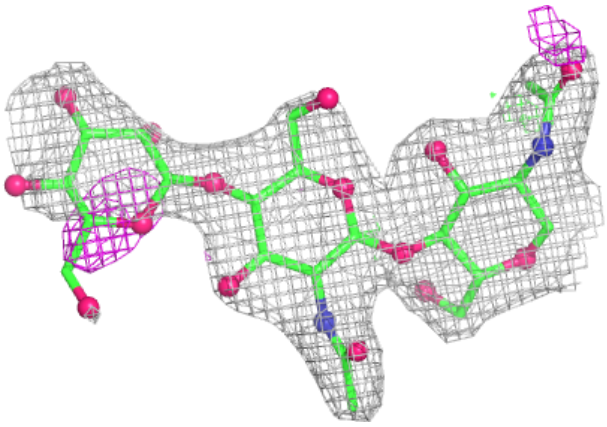
Electron density around Chain M:

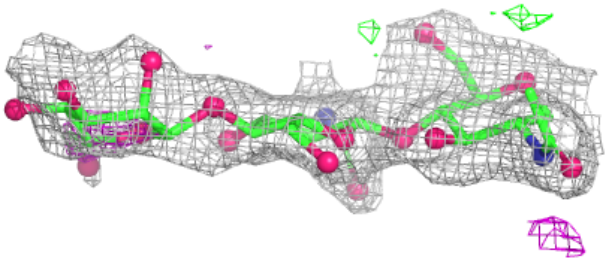
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

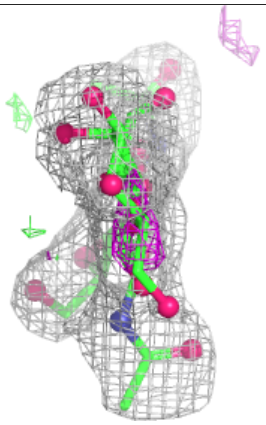


Electron density around Chain O:

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

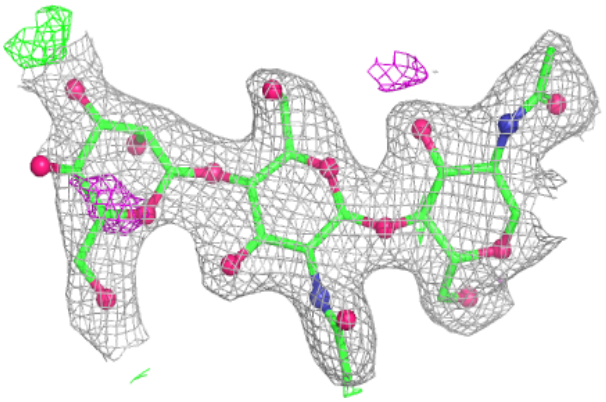


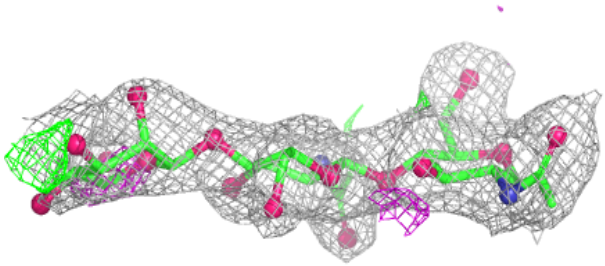


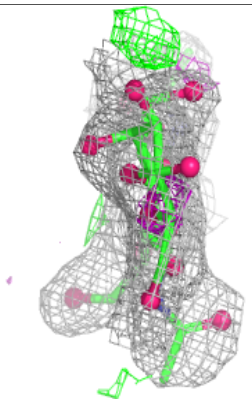


Electron density around Chain T:

$2mF_o$-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)

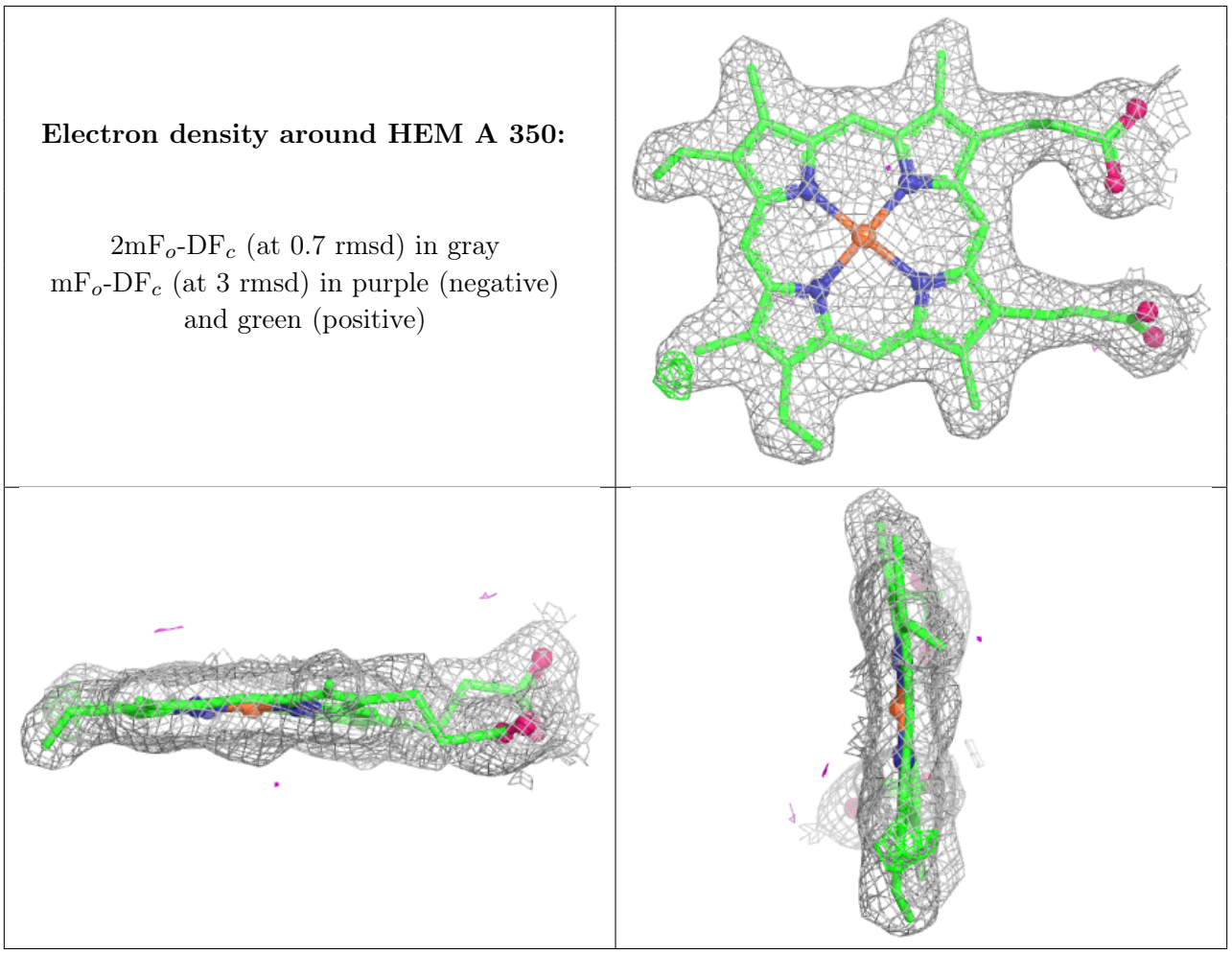
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	NAG	D	381	14/15	0.80	0.25	54,57,61,62	0
11	NAG	C	381	14/15	0.87	0.33	50,54,57,58	0
10	SO4	C	1331	5/5	0.89	0.20	87,88,88,89	0
11	NAG	D	391	14/15	0.89	0.25	46,48,51,53	0
10	SO4	B	1329	5/5	0.90	0.23	57,58,61,62	0
8	MG	D	353	1/1	0.92	0.06	26,26,26,26	0
10	SO4	B	1330	5/5	0.92	0.18	65,65,65,66	0
11	NAG	D	411	14/15	0.92	0.17	53,56,58,59	0
10	SO4	B	1331	5/5	0.93	0.19	68,69,69,71	0
9	ACT	A	1327	4/4	0.93	0.18	30,32,32,32	0
9	ACT	C	1329	4/4	0.94	0.19	31,34,37,38	0
10	SO4	C	1333	5/5	0.94	0.32	74,75,75,75	0
10	SO4	A	1329	5/5	0.95	0.18	70,71,71,72	0
10	SO4	C	1332	5/5	0.95	0.14	62,62,63,63	0
10	SO4	A	1330	5/5	0.95	0.15	59,62,63,63	0
10	SO4	D	1328	5/5	0.95	0.13	60,60,61,62	0
10	SO4	A	1331	5/5	0.95	0.21	60,60,61,63	0
9	ACT	B	1328	4/4	0.95	0.15	25,25,30,32	0
8	MG	A	353	1/1	0.95	0.06	18,18,18,18	0
9	ACT	D	1327	4/4	0.95	0.20	48,49,49,50	0
8	MG	C	353	1/1	0.96	0.03	19,19,19,19	0
10	SO4	D	1329	5/5	0.96	0.14	55,56,58,58	0
7	HEM	A	350	43/43	0.97	0.12	12,19,21,27	0
10	SO4	A	1328	5/5	0.97	0.14	56,56,58,59	0
10	SO4	C	1330	5/5	0.97	0.11	61,62,63,63	0
7	HEM	D	350	43/43	0.98	0.12	18,23,28,33	0
9	ACT	C	1334	4/4	0.98	0.11	24,27,29,30	0
7	HEM	B	350	43/43	0.98	0.11	6,13,16,22	0
7	HEM	C	350	43/43	0.98	0.13	13,17,22,26	0
8	MG	B	353	1/1	0.99	0.03	12,12,12,12	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.

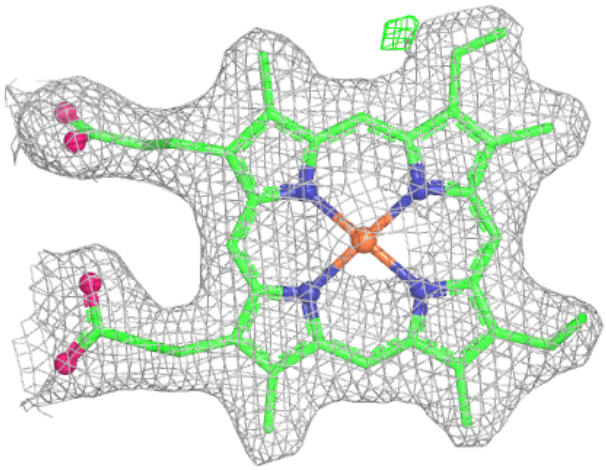
Electron density around HEM A 350:

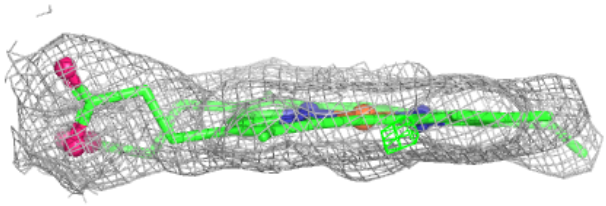
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

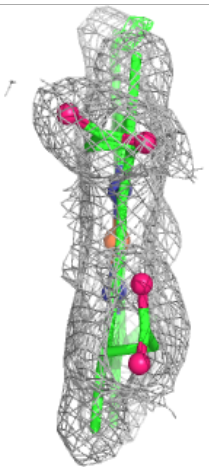


Electron density around HEM D 350:

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

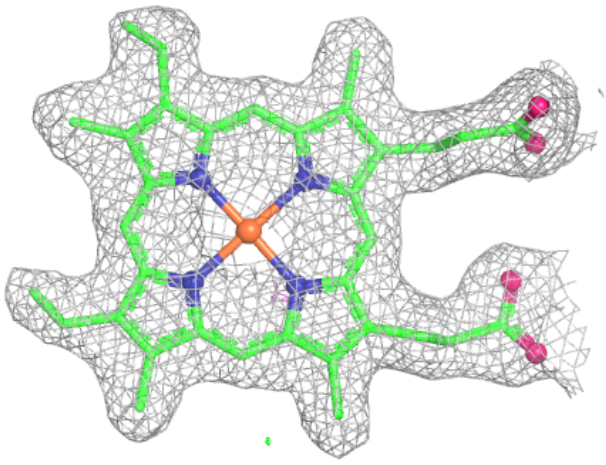


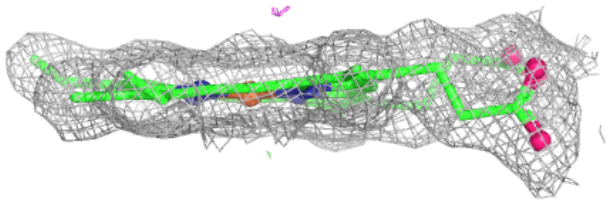


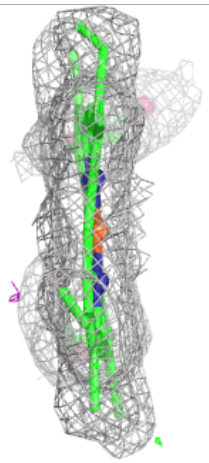


Electron density around HEM B 350:

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

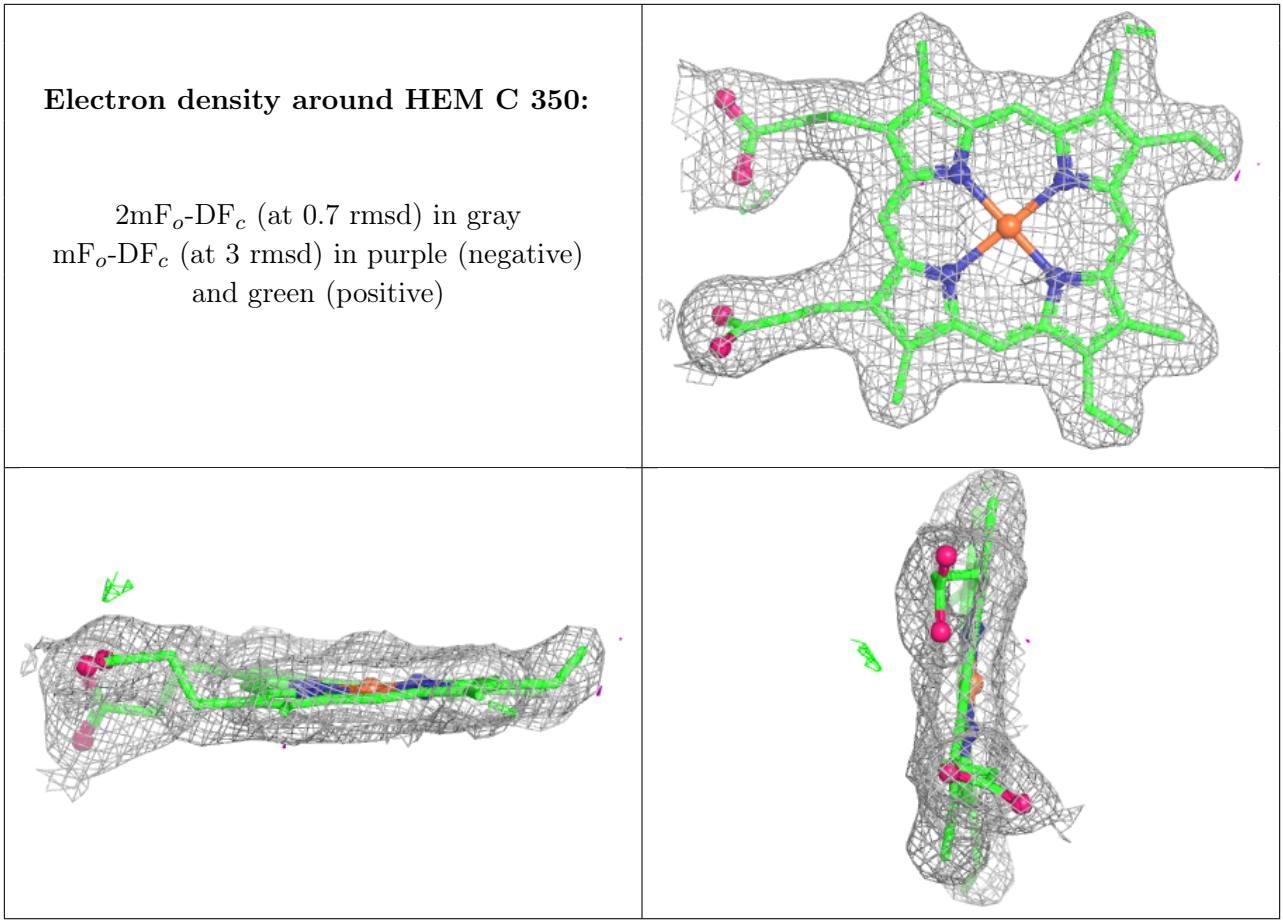






Electron density around HEM C 350:

$2mF_o$-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.