wwPDB X-ray Structure Validation Summary Report (i)

Aug 15, 2022 – 10:32 am BST

PDB ID	:	7OIH
Title	:	Glycosylation in the crystal structure of neutrophil myeloperoxidase
Authors	:	Krawczyk, L.; Semwal, S.; Bouckaert, J.
Deposited on	:	2021-05-11
Resolution	:	2.60 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:

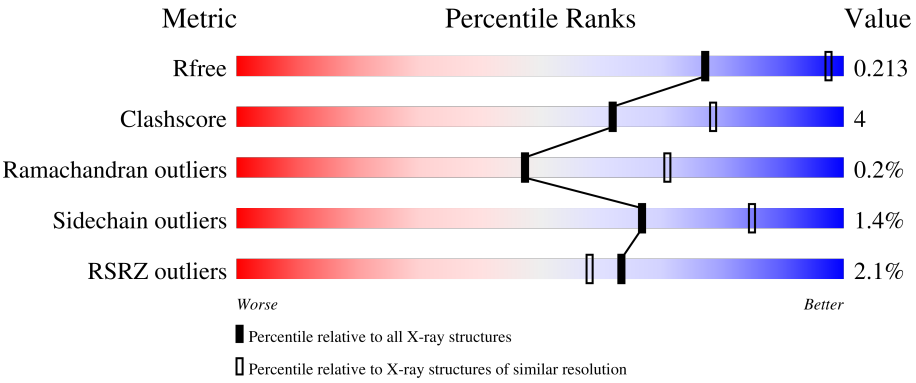
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	579	2% 89% 9% ••
1	B	579	3% 88% 9% ••
1	C	579	3% 88% 10% •
1	D	579	2% 90% 8% ••
1	E	579	3% 88% 10% •

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Mol	Chain	Length	Quality of chain
1	F	579	2% 88% 10%
1	G	579	2% 88% 10%
1	H	579	2% 88% 10%
2	I	3	67% 33%
2	J	3	100%
2	Y	3	100%
2	b	3	100%
2	e	3	100%
3	L	7	100%
3	c	7	100%
3	g	7	100%
4	K	6	17% 67% 17%
4	R	6	100%
5	M	2	100%
5	O	2	100%
5	S	2	100%
5	V	2	50% 50%
5	d	2	100%
5	f	2	100%
6	N	6	33% 67%
6	Q	6	100%
6	T	6	100%
6	W	6	100%
6	Z	6	33% 50% 17%
7	P	4	25% 50% 25%

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Mol	Chain	Length	Quality of chain
8	U	4	50% 50%
8	X	4	100%
9	a	6	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	8PR	F	807	-	-	-	X
14	8PR	H	807	-	-	-	X
15	PO4	B	812	-	-	-	X
15	PO4	C	810	-	-	-	X
15	PO4	G	810	-	-	-	X
15	PO4	H	810	-	-	-	X
16	NAG	B	805	-	-	-	X
16	NAG	C	804	-	-	-	X
16	NAG	D	804	-	-	-	X
2	NAG	Y	2	X	-	-	-
4	NAG	R	2	X	-	-	-
5	NAG	S	2	X	-	-	-
5	NAG	d	1	-	-	-	X
5	NAG	d	2	-	-	-	X
7	NAG	P	1	X	-	-	-
7	NAG	P	2	X	-	-	-
8	MAN	X	4	-	-	-	X

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 41050 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 Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	0	0
			4592	2893	841	826	32			
1	B	570	Total	C	N	O	S	0	0	0
			4571	2881	835	823	32			
1	C	570	Total	C	N	O	S	0	1	0
			4577	2884	836	824	33			
1	D	571	Total	C	N	O	S	0	0	0
			4574	2883	836	823	32			
1	E	572	Total	C	N	O	S	0	1	0
			4589	2892	838	826	33			
1	F	571	Total	C	N	O	S	0	1	0
			4585	2888	840	825	32			
1	G	569	Total	C	N	O	S	0	0	0
			4562	2875	834	821	32			
1	H	571	Total	C	N	O	S	0	1	0
			4579	2887	836	823	33			

- Molecule 2 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
2	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	Y	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	b	3	Total	C	N	O	0	0	0
			39	22	2	15			

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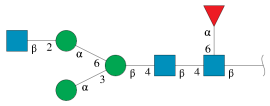
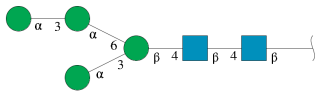
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	e	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	c	7	Total	C	N	O	0	0	0
			85	48	3	34			
3	g	7	Total	C	N	O	0	0	0
			85	48	3	34			
3	L	7	Total	C	N	O	0	0	0
			85	48	3	34			

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

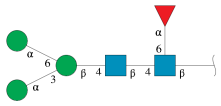


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	K	6	Total	C	N	O	0	0	0
			72	40	2	30			
4	R	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 5 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
5	M	2	Total C N O 28 16 2 10	0	0	0
5	O	2	Total C N O 28 16 2 10	0	0	0
5	V	2	Total C N O 28 16 2 10	0	0	0
5	d	2	Total C N O 28 16 2 10	0	0	0
5	f	2	Total C N O 28 16 2 10	0	0	0
5	S	2	Total C N O 28 16 2 10	0	0	0

- Molecule 6 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-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	N	6	Total C N O 71 40 2 29	0	0	0
6	Q	6	Total C N O 71 40 2 29	0	0	0
6	T	6	Total C N O 71 40 2 29	0	0	0
6	W	6	Total C N O 71 40 2 29	0	0	0
6	Z	6	Total C N O 71 40 2 29	0	0	0

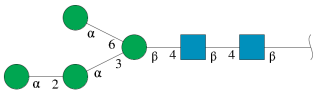
- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	P	4	Total C N O 50 28 2 20	0	0	0

- Molecule 8 is an oligosaccharide called 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
8	U	4	Total C N O 50 28 2 20	0	0	0
8	X	4	Total C N O 50 28 2 20	0	0	0

- Molecule 9 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
9	a	6	Total C N O 72 40 2 30	0	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	5	Total Cl 5 5	0	0
10	B	5	Total Cl 5 5	0	0
10	C	4	Total Cl 4 4	0	0
10	D	4	Total Cl 4 4	0	0
10	E	4	Total Cl 4 4	0	0

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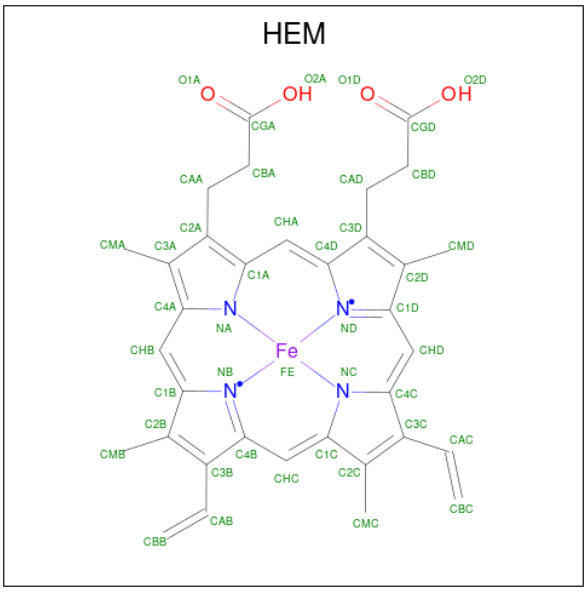
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	F	5	Total Cl 5 5	0	0
10	G	5	Total Cl 5 5	0	0
10	H	4	Total Cl 4 4	0	0

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

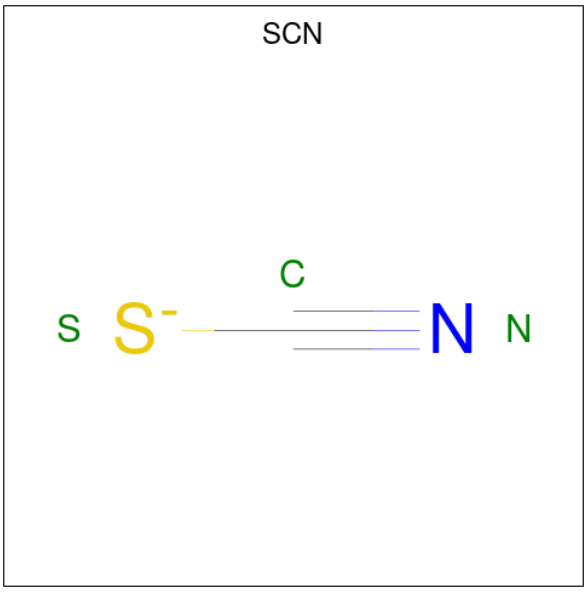
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total Ca 1 1	0	0
11	B	1	Total Ca 1 1	0	0
11	C	1	Total Ca 1 1	0	0
11	D	1	Total Ca 1 1	0	0
11	E	1	Total Ca 1 1	0	0
11	F	1	Total Ca 1 1	0	0
11	G	1	Total Ca 1 1	0	0
11	H	1	Total Ca 1 1	0	0

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



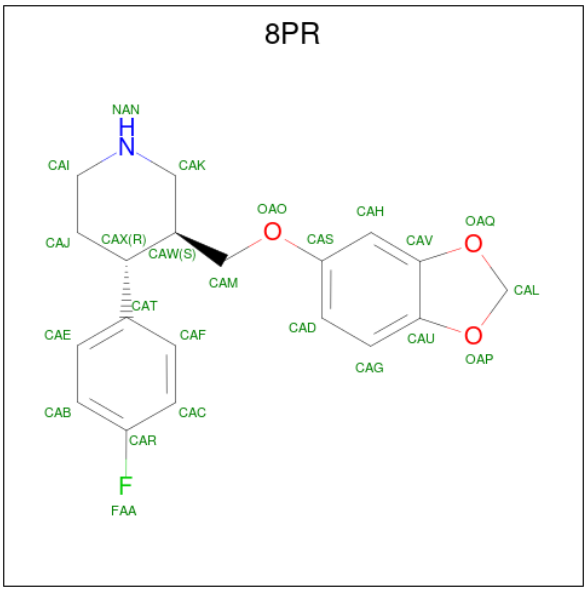
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



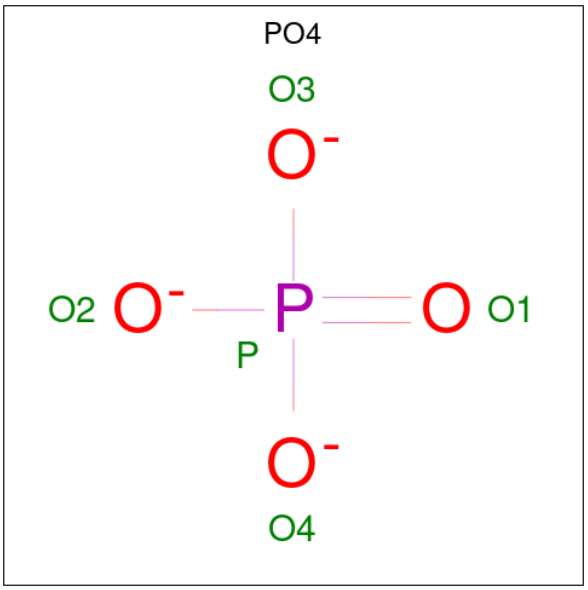
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	N	S	0	0
			3	1	1	1		
13	B	1	Total	C	N	S	0	0
			3	1	1	1		
13	B	1	Total	C	N	S	0	0
			3	1	1	1		
13	C	1	Total	C	N	S	0	0
			3	1	1	1		
13	D	1	Total	C	N	S	0	0
			3	1	1	1		
13	D	1	Total	C	N	S	0	0
			3	1	1	1		
13	E	1	Total	C	N	S	0	0
			3	1	1	1		
13	F	1	Total	C	N	S	0	0
			3	1	1	1		
13	G	1	Total	C	N	S	0	0
			3	1	1	1		
13	H	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 14 is Paroxetine (three-letter code: 8PR) (formula: $C_{19}H_{20}FNO_3$) (labeled as "Ligand of Interest" by depositor).



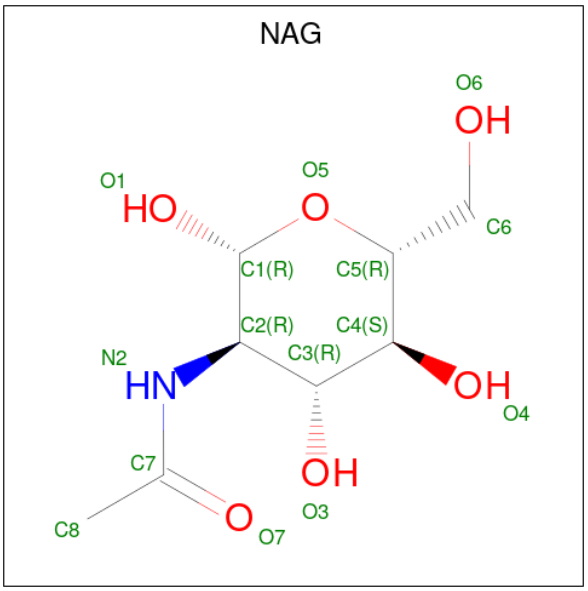
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	A	1	Total	C	F	N	O	0	0
			24	19	1	1	3		
14	D	1	Total	C	F	N	O	0	0
			24	19	1	1	3		
14	F	1	Total	C	F	N	O	0	0
			24	19	1	1	3		
14	H	1	Total	C	F	N	O	0	0
			24	19	1	1	3		

- Molecule 15 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total O P 5 4 1	0	0
15	B	1	Total O P 5 4 1	0	0
15	B	1	Total O P 5 4 1	0	0
15	C	1	Total O P 5 4 1	0	0
15	C	1	Total O P 5 4 1	0	0
15	D	1	Total O P 5 4 1	0	0
15	D	1	Total O P 5 4 1	0	0
15	D	1	Total O P 5 4 1	0	0
15	E	1	Total O P 5 4 1	0	0
15	F	1	Total O P 5 4 1	0	0
15	G	1	Total O P 5 4 1	0	0
15	G	1	Total O P 5 4 1	0	0
15	H	1	Total O P 5 4 1	0	0
15	H	1	Total O P 5 4 1	0	0

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	355	Total O 355 355	0	0
17	B	308	Total O 308 308	0	0
17	C	258	Total O 258 258	0	0
17	D	272	Total O 272 272	0	0
17	E	288	Total O 288 288	0	0
17	F	311	Total O 311 311	0	0
17	G	324	Total O 324 324	0	0

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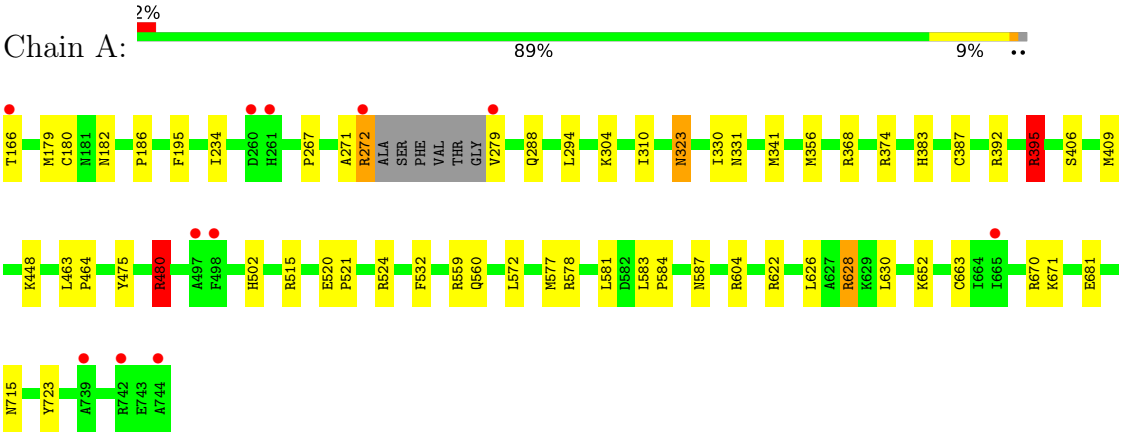
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	312	Total 312	O 312	0	0

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.

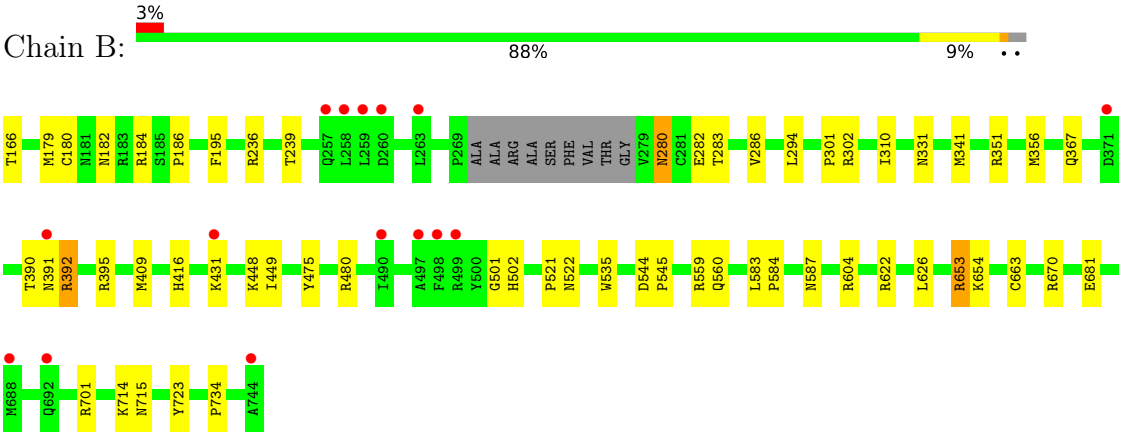
• Molecule 1: Myeloperoxidase

Chain A:



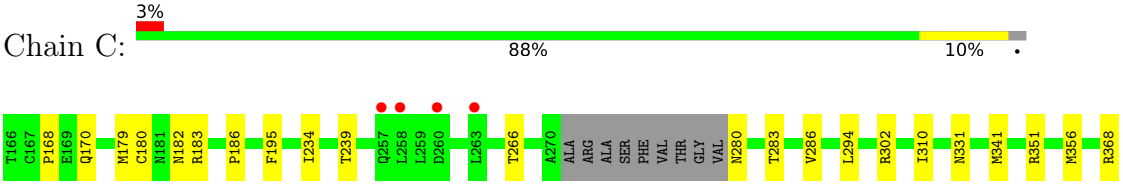
• Molecule 1: Myeloperoxidase

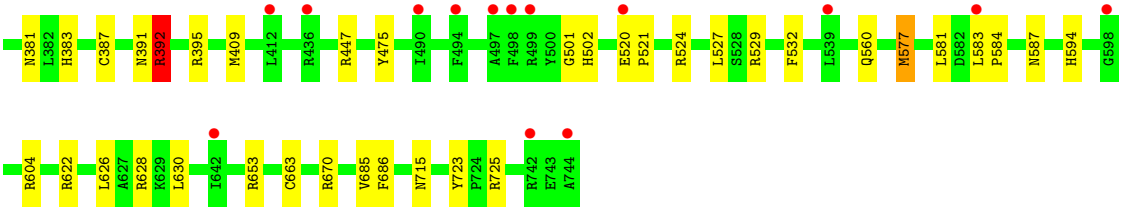
Chain B:



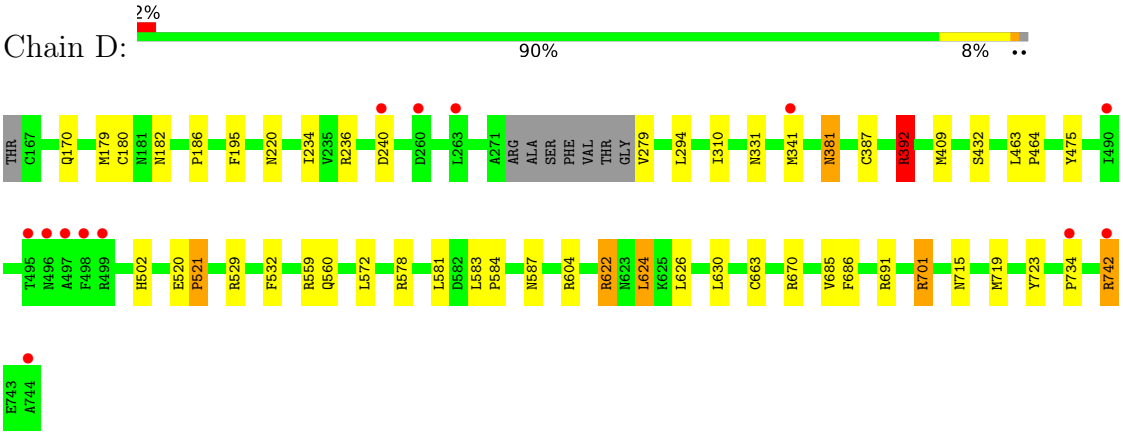
• Molecule 1: Myeloperoxidase

Chain C:

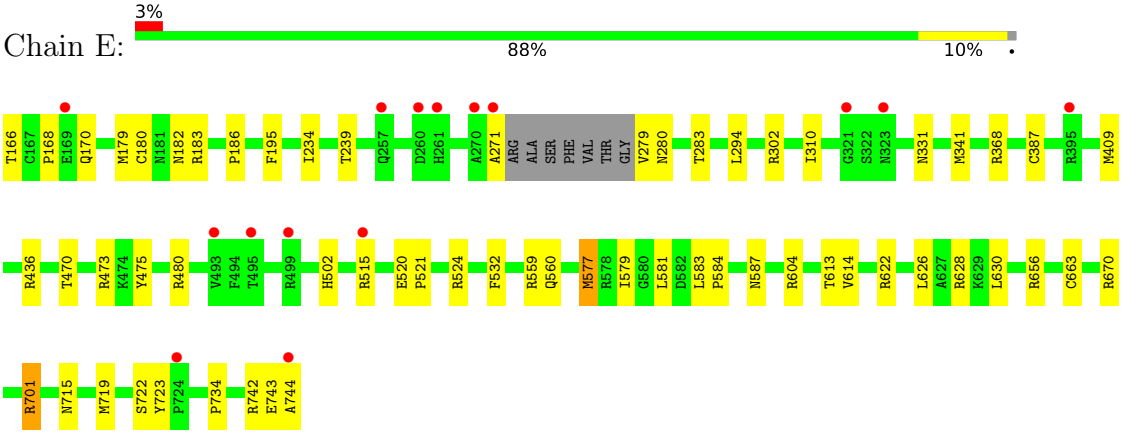




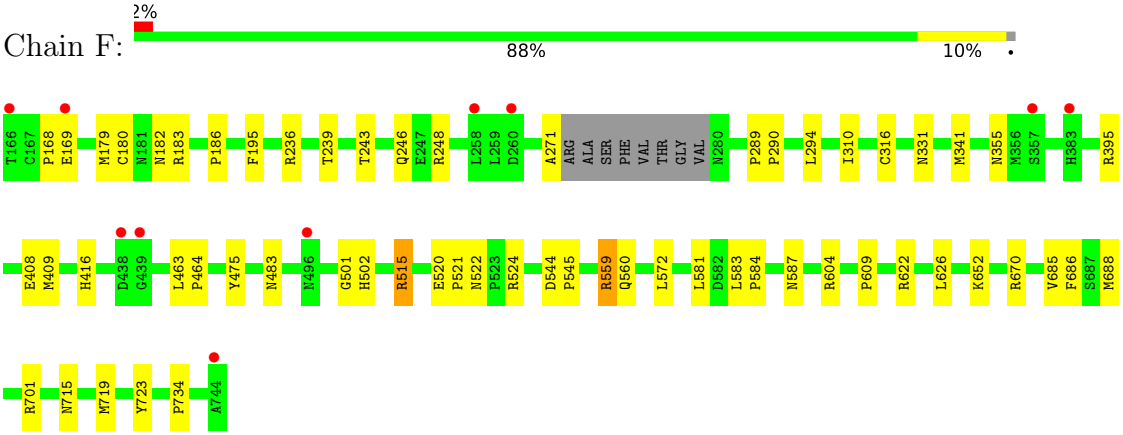
• Molecule 1: Myeloperoxidase



• Molecule 1: Myeloperoxidase

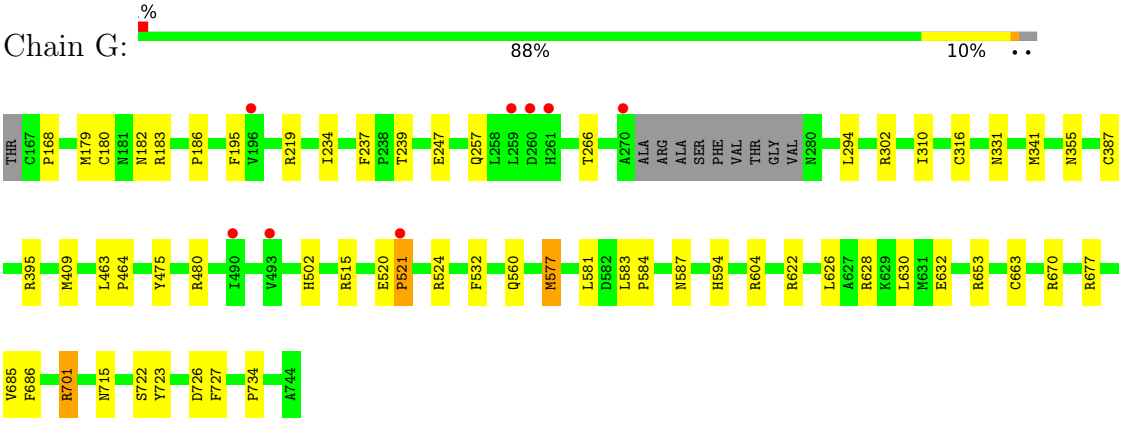


• Molecule 1: Myeloperoxidase



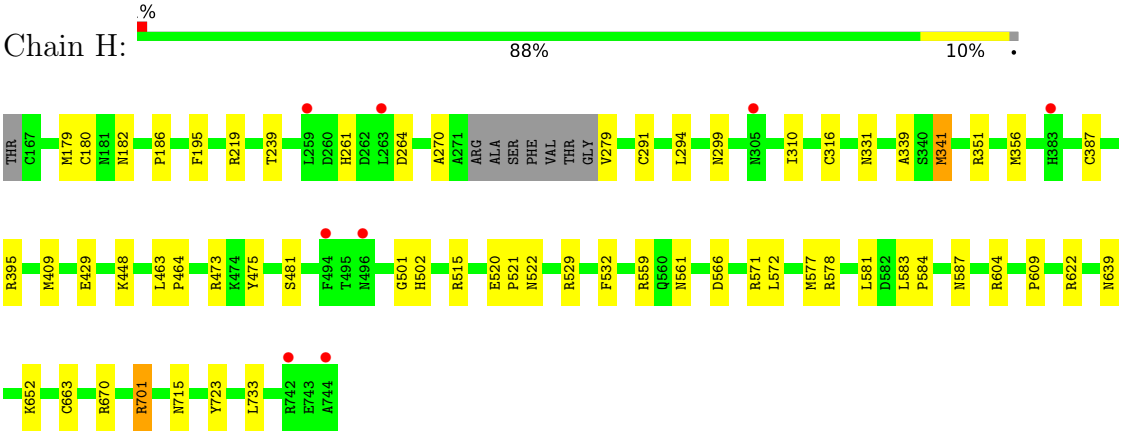
• Molecule 1: Myeloperoxidase

Chain G:



• Molecule 1: Myeloperoxidase

Chain H:

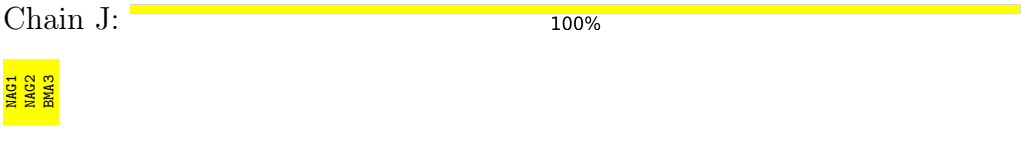


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

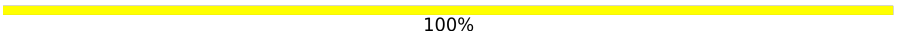
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



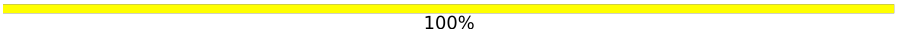
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



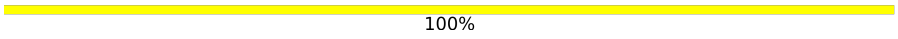
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



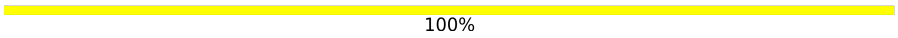
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



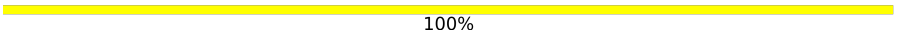
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



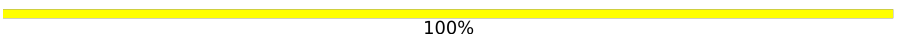
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



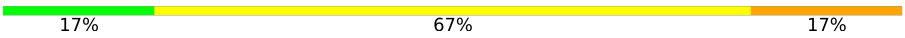
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

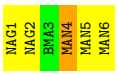
Chain L:



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

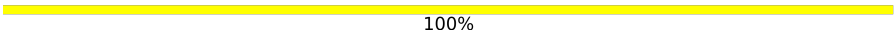
Chain K:





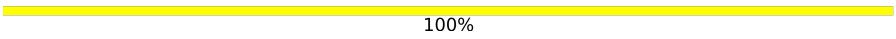
• Molecule 4: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



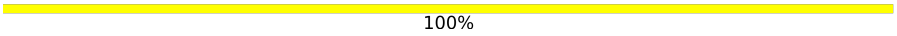
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain O:

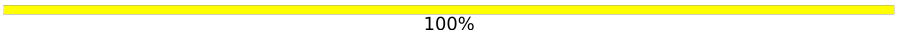


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

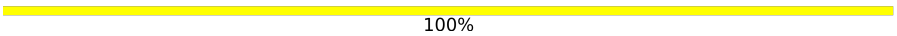
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



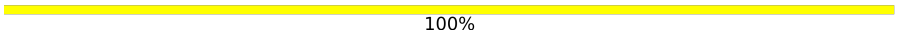
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



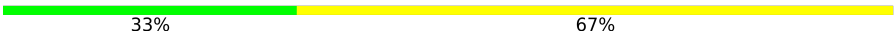
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

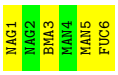
Chain S:



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

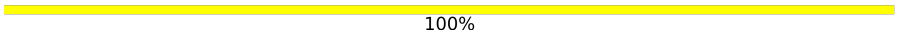
Chain N:





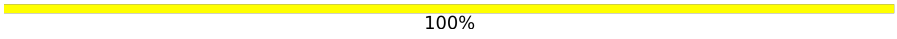
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



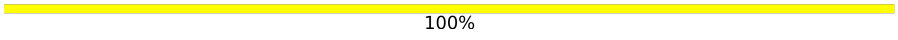
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



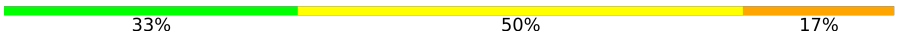
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

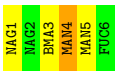
Chain W:



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

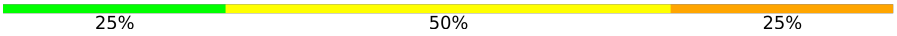
Chain Z:





• Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

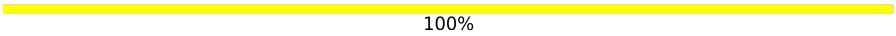


• Molecule 8: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

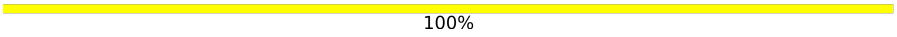
• Molecule 8: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



• Molecule 9: 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 a:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	155.91Å 144.63Å 236.45Å 90.00° 91.53° 90.00°	Depositor
Resolution (Å)	38.99 – 2.60 38.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (38.99-2.60) 89.7 (38.96-2.60)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0349, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.179 , 0.220 0.172 , 0.213	Depositor DCC
R_{free} test set	1826 reflections (1.27%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.098 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	41050	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: CSO, PO4, CA, NAG, CL, BMA, 8PR, FUC, MAN, HEM, SCN

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	0.40	0/4695	0.69	1/6373 (0.0%)
1	B	0.38	0/4674	0.69	1/6345 (0.0%)
1	C	0.37	0/4680	0.69	1/6352 (0.0%)
1	D	0.39	0/4677	0.69	1/6349 (0.0%)
1	E	0.38	0/4692	0.68	0/6369
1	F	0.38	0/4688	0.68	0/6363
1	G	0.39	0/4665	0.68	0/6332
1	H	0.38	0/4685	0.68	1/6359 (0.0%)
All	All	0.38	0/37456	0.68	5/50842 (0.0%)

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	A	0	12
1	B	0	11
1	C	0	14
1	D	0	10
1	E	0	14
1	F	0	10
1	G	0	12
1	H	0	11
All	All	0	94

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	323	ASN	CB-CA-C	-7.04	96.31	110.40
1	D	529	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	B	521	PRO	N-CA-CB	-5.63	96.41	102.60
1	C	447	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	H	701	ARG	CG-CD-NE	5.19	122.70	111.80

There are no chirality outliers.

5 of 94 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	368	ARG	Sidechain
1	A	395	ARG	Sidechain
1	A	480	ARG	Sidechain
1	A	515	ARG	Sidechain
1	A	520	GLU	Peptide

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	4592	0	4545	42	1
1	B	4571	0	4520	34	0
1	C	4577	0	4525	37	0
1	D	4574	0	4524	38	0
1	E	4589	0	4540	33	1
1	F	4585	0	4536	45	0
1	G	4562	0	4511	38	0
1	H	4579	0	4533	47	0
2	I	39	0	34	2	0
2	J	39	0	34	0	0
2	Y	39	0	34	0	0
2	b	39	0	34	0	0
2	e	39	0	34	0	0
3	L	85	0	73	0	0
3	c	85	0	73	0	0
3	g	85	0	73	0	0
4	K	72	0	61	0	1
4	R	72	0	61	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	28	0	25	0	0
5	O	28	0	25	0	0
5	S	28	0	25	0	0
5	V	28	0	25	1	0
5	d	28	0	25	0	0
5	f	28	0	25	0	0
6	N	71	0	61	1	0
6	Q	71	0	61	0	0
6	T	71	0	61	0	0
6	W	71	0	61	0	0
6	Z	71	0	61	4	0
7	P	50	0	42	6	0
8	U	50	0	43	1	0
8	X	50	0	43	1	0
9	a	72	0	61	0	0
10	A	5	0	0	0	0
10	B	5	0	0	0	0
10	C	4	0	0	0	0
10	D	4	0	0	0	0
10	E	4	0	0	0	0
10	F	5	0	0	0	0
10	G	5	0	0	0	0
10	H	4	0	0	0	0
11	A	1	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	F	1	0	0	0	0
11	G	1	0	0	0	0
11	H	1	0	0	0	0
12	A	43	0	30	8	0
12	B	43	0	30	10	0
12	C	43	0	30	8	0
12	D	43	0	30	7	0
12	E	43	0	30	6	0
12	F	43	0	30	10	0
12	G	43	0	30	7	0
12	H	43	0	30	9	0
13	A	3	0	0	0	0
13	B	6	0	0	0	0
13	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	D	6	0	0	0	0
13	E	3	0	0	0	0
13	F	3	0	0	0	0
13	G	3	0	0	0	0
13	H	3	0	0	0	0
14	A	24	0	20	0	0
14	D	24	0	20	1	0
14	F	24	0	20	0	0
14	H	24	0	20	0	0
15	A	5	0	0	0	0
15	B	10	0	0	0	0
15	C	10	0	0	0	0
15	D	15	0	0	0	0
15	E	5	0	0	0	0
15	F	5	0	0	0	0
15	G	10	0	0	1	0
15	H	10	0	0	1	0
16	B	28	0	26	1	0
16	C	28	0	26	0	0
16	D	14	0	13	0	0
17	A	355	0	0	12	0
17	B	308	0	0	11	1
17	C	258	0	0	4	0
17	D	272	0	0	7	1
17	E	288	0	0	7	0
17	F	311	0	0	14	0
17	G	324	0	0	11	1
17	H	312	0	0	17	0
All	All	41050	0	37774	326	3

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 4.

The worst 5 of 326 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:F:483:ASN:ND2	6:Z:1:NAG:C1	1.75	1.48
1:C:391:ASN:HD21	7:P:1:NAG:C1	1.45	1.27
1:F:409:MET:SD	12:F:805:HEM:CBB	2.26	1.23
1:G:409:MET:SD	12:G:806:HEM:HBB1	1.80	1.22
1:E:239:THR:HG23	17:E:1076:HOH:O	1.39	1.21

All (3) 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)
17:D:1017:HOH:O	17:G:1117:HOH:O[3_555]	1.88	0.32
1:A:622:ARG:NH1	1:E:283:THR:O[3_545]	2.05	0.15
4:K:4:MAN:O6	17:B:1164:HOH:O[3_445]	2.19	0.01

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	568/579 (98%)	554 (98%)	13 (2%)	1 (0%)	47	71
1	B	565/579 (98%)	547 (97%)	15 (3%)	3 (0%)	29	52
1	C	566/579 (98%)	552 (98%)	13 (2%)	1 (0%)	47	71
1	D	566/579 (98%)	551 (97%)	14 (2%)	1 (0%)	47	71
1	E	568/579 (98%)	552 (97%)	14 (2%)	2 (0%)	34	57
1	F	567/579 (98%)	553 (98%)	13 (2%)	1 (0%)	47	71
1	G	564/579 (97%)	549 (97%)	14 (2%)	1 (0%)	47	71
1	H	567/579 (98%)	553 (98%)	13 (2%)	1 (0%)	47	71
All	All	4531/4632 (98%)	4411 (97%)	109 (2%)	11 (0%)	47	71

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	392	ARG
1	E	280	ASN
1	C	521	PRO
1	E	521	PRO
1	F	521	PRO

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	502/506 (99%)	493 (98%)	9 (2%)	59 80
1	B	501/506 (99%)	493 (98%)	8 (2%)	62 82
1	C	501/506 (99%)	493 (98%)	8 (2%)	62 82
1	D	500/506 (99%)	489 (98%)	11 (2%)	52 76
1	E	502/506 (99%)	496 (99%)	6 (1%)	71 87
1	F	501/506 (99%)	497 (99%)	4 (1%)	81 92
1	G	499/506 (99%)	494 (99%)	5 (1%)	76 90
1	H	501/506 (99%)	497 (99%)	4 (1%)	81 92
All	All	4007/4048 (99%)	3952 (99%)	55 (1%)	67 85

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	341	MET
1	D	742	ARG
1	H	663	CYS
1	G	577	MET
1	D	381	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	416	HIS
1	H	689	GLN
1	E	367	GLN
1	E	633	GLN
1	F	633	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)

8 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	D	316	1	3,6,7	0.88	0	0,6,8	-	-
1	CSO	F	316	1	3,6,7	1.19	0	0,6,8	-	-
1	CSO	G	316	1	3,6,7	1.08	0	0,6,8	-	-
1	CSO	A	316	1	3,6,7	1.13	0	0,6,8	-	-
1	CSO	H	316	1	3,6,7	1.03	0	0,6,8	-	-
1	CSO	B	316	1	3,6,7	0.67	0	0,6,8	-	-
1	CSO	C	316	1	3,6,7	0.84	0	0,6,8	-	-
1	CSO	E	316	1	3,6,7	0.79	0	0,6,8	-	-

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
1	CSO	D	316	1	-	0/1/5/7	-
1	CSO	F	316	1	-	0/1/5/7	-
1	CSO	G	316	1	-	0/1/5/7	-
1	CSO	A	316	1	-	0/1/5/7	-
1	CSO	H	316	1	-	0/1/5/7	-
1	CSO	B	316	1	-	0/1/5/7	-
1	CSO	C	316	1	-	0/1/5/7	-
1	CSO	E	316	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	316	CSO	1	0

5.5 Carbohydrates (i)

108 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	I	1	1,2	14,14,15	0.38	0	17,19,21	0.62	0
2	NAG	I	2	2	14,14,15	0.38	0	17,19,21	0.54	0
2	BMA	I	3	2	11,11,12	0.25	0	15,15,17	0.65	0
2	NAG	J	1	1,2	14,14,15	0.60	0	17,19,21	1.55	2 (11%)
2	NAG	J	2	2	14,14,15	0.91	0	17,19,21	1.05	2 (11%)
2	BMA	J	3	2	11,11,12	1.43	2 (18%)	15,15,17	1.48	2 (13%)
4	NAG	K	1	4,1	14,14,15	0.62	0	17,19,21	1.58	3 (17%)
4	NAG	K	2	4	14,14,15	1.21	1 (7%)	17,19,21	1.47	3 (17%)
4	BMA	K	3	4	11,11,12	0.65	0	15,15,17	0.84	0
4	MAN	K	4	4	11,11,12	0.42	0	15,15,17	1.64	3 (20%)
4	MAN	K	5	4	11,11,12	0.87	0	15,15,17	1.67	4 (26%)
4	MAN	K	6	4	11,11,12	1.25	1 (9%)	15,15,17	2.14	6 (40%)
3	NAG	L	1	1,3	14,14,15	0.82	0	17,19,21	1.47	2 (11%)
3	NAG	L	2	3	14,14,15	0.81	0	17,19,21	1.43	3 (17%)
3	BMA	L	3	3	11,11,12	0.58	0	15,15,17	1.94	2 (13%)
3	MAN	L	4	3	11,11,12	0.46	0	15,15,17	1.81	3 (20%)
3	NAG	L	5	3	14,14,15	1.28	2 (14%)	17,19,21	2.03	4 (23%)
3	MAN	L	6	3	11,11,12	0.93	1 (9%)	15,15,17	2.33	6 (40%)
3	FUC	L	7	3	10,10,11	0.65	0	14,14,16	1.88	4 (28%)
5	NAG	M	1	5,1	14,14,15	0.93	0	17,19,21	1.39	2 (11%)
5	NAG	M	2	5	14,14,15	1.11	1 (7%)	17,19,21	1.76	4 (23%)
6	NAG	N	1	6,1	14,14,15	0.93	1 (7%)	17,19,21	1.70	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	N	2	6	14,14,15	0.39	0	17,19,21	0.54	0
6	BMA	N	3	6	11,11,12	0.43	0	15,15,17	1.12	1 (6%)
6	MAN	N	4	6	11,11,12	0.23	0	15,15,17	0.66	0
6	MAN	N	5	6	11,11,12	0.32	0	15,15,17	0.54	0
6	FUC	N	6	6	10,10,11	0.59	0	14,14,16	1.67	4 (28%)
5	NAG	O	1	5,1	14,14,15	0.65	0	17,19,21	1.52	3 (17%)
5	NAG	O	2	5	14,14,15	0.82	0	17,19,21	1.81	3 (17%)
7	NAG	P	1	7	14,14,15	3.06	1 (7%)	17,19,21	2.36	2 (11%)
7	NAG	P	2	7	14,14,15	0.40	0	17,19,21	0.52	0
7	BMA	P	3	7	11,11,12	0.35	0	15,15,17	0.76	0
7	MAN	P	4	7	11,11,12	0.23	0	15,15,17	0.62	0
6	NAG	Q	1	6,1	14,14,15	0.86	1 (7%)	17,19,21	1.56	3 (17%)
6	NAG	Q	2	6	14,14,15	0.69	0	17,19,21	1.39	3 (17%)
6	BMA	Q	3	6	11,11,12	0.92	0	15,15,17	1.69	5 (33%)
6	MAN	Q	4	6	11,11,12	0.93	0	15,15,17	2.29	6 (40%)
6	MAN	Q	5	6	11,11,12	1.48	2 (18%)	15,15,17	2.57	9 (60%)
6	FUC	Q	6	6	10,10,11	1.01	0	14,14,16	2.22	6 (42%)
4	NAG	R	1	4,1	14,14,15	1.55	1 (7%)	17,19,21	3.97	5 (29%)
4	NAG	R	2	4	14,14,15	1.15	2 (14%)	17,19,21	1.96	4 (23%)
4	BMA	R	3	4	11,11,12	0.96	1 (9%)	15,15,17	1.83	5 (33%)
4	MAN	R	4	4	11,11,12	1.27	2 (18%)	15,15,17	2.16	7 (46%)
4	MAN	R	5	4	11,11,12	1.13	1 (9%)	15,15,17	1.35	2 (13%)
4	MAN	R	6	4	11,11,12	0.94	1 (9%)	15,15,17	1.51	4 (26%)
5	NAG	S	1	5,1	14,14,15	1.52	1 (7%)	17,19,21	3.94	5 (29%)
5	NAG	S	2	5	14,14,15	0.81	1 (7%)	17,19,21	1.54	4 (23%)
6	NAG	T	1	6,1	14,14,15	0.70	0	17,19,21	1.51	3 (17%)
6	NAG	T	2	6	14,14,15	0.97	1 (7%)	17,19,21	1.53	3 (17%)
6	BMA	T	3	6	11,11,12	0.71	0	15,15,17	1.90	3 (20%)
6	MAN	T	4	6	11,11,12	0.72	0	15,15,17	1.74	3 (20%)
6	MAN	T	5	6	11,11,12	1.07	1 (9%)	15,15,17	2.16	3 (20%)
6	FUC	T	6	6	10,10,11	0.66	0	14,14,16	2.41	5 (35%)
8	NAG	U	1	8,1	14,14,15	0.86	0	17,19,21	1.70	5 (29%)
8	NAG	U	2	8	14,14,15	1.24	1 (7%)	17,19,21	2.24	7 (41%)
8	BMA	U	3	8	11,11,12	0.72	0	15,15,17	2.12	6 (40%)
8	MAN	U	4	8	11,11,12	1.33	2 (18%)	15,15,17	3.95	8 (53%)
5	NAG	V	1	5,1	14,14,15	0.87	0	17,19,21	1.70	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	V	2	5	14,14,15	1.45	2 (14%)	17,19,21	3.10	5 (29%)
6	NAG	W	1	6,1	14,14,15	1.05	2 (14%)	17,19,21	1.66	4 (23%)
6	NAG	W	2	6	14,14,15	0.84	0	17,19,21	1.92	3 (17%)
6	BMA	W	3	6	11,11,12	0.60	0	15,15,17	1.18	1 (6%)
6	MAN	W	4	6	11,11,12	0.66	0	15,15,17	2.03	5 (33%)
6	MAN	W	5	6	11,11,12	0.86	0	15,15,17	1.66	4 (26%)
6	FUC	W	6	6	10,10,11	0.35	0	14,14,16	1.28	3 (21%)
8	NAG	X	1	8,1	14,14,15	0.65	0	17,19,21	1.44	4 (23%)
8	NAG	X	2	8	14,14,15	0.77	0	17,19,21	0.98	0
8	BMA	X	3	8	11,11,12	0.73	0	15,15,17	1.08	1 (6%)
8	MAN	X	4	8	11,11,12	1.00	1 (9%)	15,15,17	2.07	5 (33%)
2	NAG	Y	1	1,2	14,14,15	2.48	1 (7%)	17,19,21	2.71	3 (17%)
2	NAG	Y	2	2	14,14,15	0.67	0	17,19,21	2.44	9 (52%)
2	BMA	Y	3	2	11,11,12	1.21	0	15,15,17	1.36	2 (13%)
6	NAG	Z	1	6	14,14,15	0.39	0	17,19,21	0.64	0
6	NAG	Z	2	6	14,14,15	0.39	0	17,19,21	0.46	0
6	BMA	Z	3	6	11,11,12	0.90	0	15,15,17	2.33	4 (26%)
6	MAN	Z	4	6	11,11,12	0.78	0	15,15,17	1.77	4 (26%)
6	MAN	Z	5	6	11,11,12	0.56	0	15,15,17	1.48	3 (20%)
6	FUC	Z	6	6	10,10,11	0.34	0	14,14,16	0.36	0
9	NAG	a	1	1,9	14,14,15	0.83	0	17,19,21	1.69	5 (29%)
9	NAG	a	2	9	14,14,15	0.80	0	17,19,21	1.28	1 (5%)
9	BMA	a	3	9	11,11,12	0.49	0	15,15,17	1.75	4 (26%)
9	MAN	a	4	9	11,11,12	0.84	0	15,15,17	1.45	3 (20%)
9	MAN	a	5	9	11,11,12	0.96	0	15,15,17	1.47	3 (20%)
9	MAN	a	6	9	11,11,12	0.86	0	15,15,17	1.41	2 (13%)
2	NAG	b	1	1,2	14,14,15	0.64	0	17,19,21	1.74	4 (23%)
2	NAG	b	2	2	14,14,15	1.10	1 (7%)	17,19,21	1.64	3 (17%)
2	BMA	b	3	2	11,11,12	1.17	1 (9%)	15,15,17	1.24	1 (6%)
3	NAG	c	1	1,3	14,14,15	0.77	0	17,19,21	1.23	2 (11%)
3	NAG	c	2	3	14,14,15	0.69	0	17,19,21	1.48	5 (29%)
3	BMA	c	3	3	11,11,12	0.77	0	15,15,17	1.41	3 (20%)
3	MAN	c	4	3	11,11,12	0.92	0	15,15,17	1.83	4 (26%)
3	NAG	c	5	3	14,14,15	1.43	2 (14%)	17,19,21	2.43	7 (41%)
3	MAN	c	6	3	11,11,12	0.62	0	15,15,17	1.67	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FUC	c	7	3	10,10,11	0.76	1 (10%)	14,14,16	1.82	4 (28%)
5	NAG	d	1	5,1	14,14,15	0.79	0	17,19,21	1.47	3 (17%)
5	NAG	d	2	5	14,14,15	0.94	1 (7%)	17,19,21	1.47	3 (17%)
2	NAG	e	1	1,2	14,14,15	0.84	0	17,19,21	1.37	4 (23%)
2	NAG	e	2	2	14,14,15	0.72	0	17,19,21	1.27	3 (17%)
2	BMA	e	3	2	11,11,12	1.02	0	15,15,17	2.06	5 (33%)
5	NAG	f	1	5,1	14,14,15	0.80	0	17,19,21	1.69	4 (23%)
5	NAG	f	2	5	14,14,15	0.80	0	17,19,21	1.04	1 (5%)
3	NAG	g	1	1,3	14,14,15	0.61	0	17,19,21	1.21	2 (11%)
3	NAG	g	2	3	14,14,15	0.79	0	17,19,21	1.54	2 (11%)
3	BMA	g	3	3	11,11,12	0.74	0	15,15,17	1.11	1 (6%)
3	MAN	g	4	3	11,11,12	0.67	0	15,15,17	1.45	3 (20%)
3	NAG	g	5	3	14,14,15	1.29	1 (7%)	17,19,21	1.95	6 (35%)
3	MAN	g	6	3	11,11,12	0.62	0	15,15,17	1.75	4 (26%)
3	FUC	g	7	3	10,10,11	0.47	0	14,14,16	1.72	5 (35%)

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	I	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	BMA	I	3	2	-	0/2/19/22	0/1/1/1
2	NAG	J	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	J	2	2	-	0/6/23/26	0/1/1/1
2	BMA	J	3	2	-	0/2/19/22	0/1/1/1
4	NAG	K	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	BMA	K	3	4	-	2/2/19/22	0/1/1/1
4	MAN	K	4	4	-	2/2/19/22	0/1/1/1
4	MAN	K	5	4	-	0/2/19/22	0/1/1/1
4	MAN	K	6	4	-	2/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
3	MAN	L	4	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	L	5	3	-	2/6/23/26	0/1/1/1
3	MAN	L	6	3	-	2/2/19/22	0/1/1/1
3	FUC	L	7	3	-	-	0/1/1/1
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
6	NAG	N	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1
6	MAN	N	4	6	-	0/2/19/22	0/1/1/1
6	MAN	N	5	6	-	0/2/19/22	0/1/1/1
6	FUC	N	6	6	-	-	0/1/1/1
5	NAG	O	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
7	NAG	P	1	7	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	P	2	7	1/1/5/7	0/6/23/26	0/1/1/1
7	BMA	P	3	7	-	1/2/19/22	0/1/1/1
7	MAN	P	4	7	-	0/2/19/22	0/1/1/1
6	NAG	Q	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	5	6	-	2/2/19/22	0/1/1/1
6	FUC	Q	6	6	-	-	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	1/1/5/7	1/6/23/26	0/1/1/1
4	BMA	R	3	4	-	1/2/19/22	0/1/1/1
4	MAN	R	4	4	-	2/2/19/22	0/1/1/1
4	MAN	R	5	4	-	0/2/19/22	0/1/1/1
4	MAN	R	6	4	-	0/2/19/22	0/1/1/1
5	NAG	S	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	S	2	5	1/1/5/7	2/6/23/26	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	-	0/2/19/22	0/1/1/1
6	MAN	T	4	6	-	0/2/19/22	0/1/1/1
6	MAN	T	5	6	-	0/2/19/22	0/1/1/1
6	FUC	T	6	6	-	-	0/1/1/1
8	NAG	U	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	U	2	8	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BMA	U	3	8	-	2/2/19/22	0/1/1/1
8	MAN	U	4	8	-	0/2/19/22	0/1/1/1
5	NAG	V	1	5,1	-	1/6/23/26	0/1/1/1
5	NAG	V	2	5	-	3/6/23/26	0/1/1/1
6	NAG	W	1	6,1	-	1/6/23/26	0/1/1/1
6	NAG	W	2	6	-	1/6/23/26	0/1/1/1
6	BMA	W	3	6	-	0/2/19/22	0/1/1/1
6	MAN	W	4	6	-	0/2/19/22	0/1/1/1
6	MAN	W	5	6	-	2/2/19/22	0/1/1/1
6	FUC	W	6	6	-	-	0/1/1/1
8	NAG	X	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	X	2	8	-	2/6/23/26	0/1/1/1
8	BMA	X	3	8	-	2/2/19/22	0/1/1/1
8	MAN	X	4	8	-	2/2/19/22	0/1/1/1
2	NAG	Y	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	Y	2	2	1/1/5/7	4/6/23/26	0/1/1/1
2	BMA	Y	3	2	-	0/2/19/22	0/1/1/1
6	NAG	Z	1	6	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Z	3	6	-	0/2/19/22	0/1/1/1
6	MAN	Z	4	6	-	2/2/19/22	0/1/1/1
6	MAN	Z	5	6	-	2/2/19/22	0/1/1/1
6	FUC	Z	6	6	-	-	0/1/1/1
9	NAG	a	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	a	2	9	-	2/6/23/26	0/1/1/1
9	BMA	a	3	9	-	1/2/19/22	0/1/1/1
9	MAN	a	4	9	-	2/2/19/22	0/1/1/1
9	MAN	a	5	9	-	0/2/19/22	0/1/1/1
9	MAN	a	6	9	-	1/2/19/22	0/1/1/1
2	NAG	b	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	b	2	2	-	2/6/23/26	0/1/1/1
2	BMA	b	3	2	-	2/2/19/22	0/1/1/1
3	NAG	c	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	c	2	3	-	0/6/23/26	0/1/1/1
3	BMA	c	3	3	-	0/2/19/22	0/1/1/1
3	MAN	c	4	3	-	0/2/19/22	0/1/1/1
3	NAG	c	5	3	-	3/6/23/26	0/1/1/1
3	MAN	c	6	3	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	c	7	3	-	-	0/1/1/1
5	NAG	d	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	d	2	5	-	2/6/23/26	0/1/1/1
2	NAG	e	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	e	2	2	-	2/6/23/26	0/1/1/1
2	BMA	e	3	2	-	0/2/19/22	0/1/1/1
5	NAG	f	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	f	2	5	-	2/6/23/26	0/1/1/1
3	NAG	g	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	BMA	g	3	3	-	0/2/19/22	0/1/1/1
3	MAN	g	4	3	-	2/2/19/22	0/1/1/1
3	NAG	g	5	3	-	2/6/23/26	0/1/1/1
3	MAN	g	6	3	-	0/2/19/22	0/1/1/1
3	FUC	g	7	3	-	-	0/1/1/1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	P	1	NAG	O4-C4	-11.38	1.16	1.43
2	Y	1	NAG	O4-C4	-9.09	1.21	1.43
4	R	1	NAG	O4-C4	-5.30	1.30	1.43
5	S	1	NAG	O4-C4	-4.53	1.32	1.43
3	c	5	NAG	C1-C2	3.85	1.58	1.52

The worst 5 of 350 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	R	1	NAG	O4-C4-C3	-15.12	75.40	110.35
5	S	1	NAG	O4-C4-C3	-13.59	78.92	110.35
5	V	2	NAG	C1-C2-N2	9.43	126.60	110.49
2	Y	1	NAG	O4-C4-C3	-8.27	91.22	110.35
7	P	1	NAG	O4-C4-C3	8.24	129.40	110.35

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	Y	2	NAG	C1
4	R	2	NAG	C1
5	S	2	NAG	C1

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Mol	Chain	Res	Type	Atom
7	P	1	NAG	C4
7	P	2	NAG	C1

5 of 108 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
3	c	5	NAG	C3-C2-N2-C7
8	X	3	BMA	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6

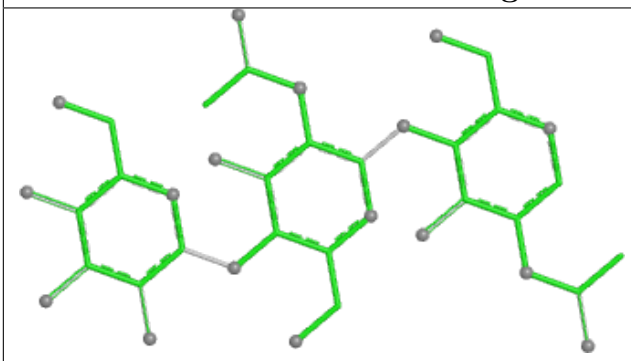
There are no ring outliers.

12 monomers are involved in 17 short contacts:

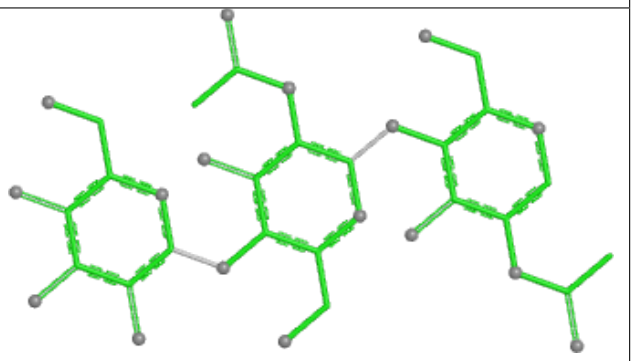
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	X	2	NAG	1	0
6	Z	4	MAN	1	0
7	P	3	BMA	1	0
7	P	4	MAN	1	0
4	K	4	MAN	0	1
6	N	5	MAN	1	0
2	I	1	NAG	2	0
8	U	3	BMA	1	0
6	Z	1	NAG	3	0
5	V	2	NAG	1	0
8	U	2	NAG	1	0
7	P	1	NAG	5	0

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

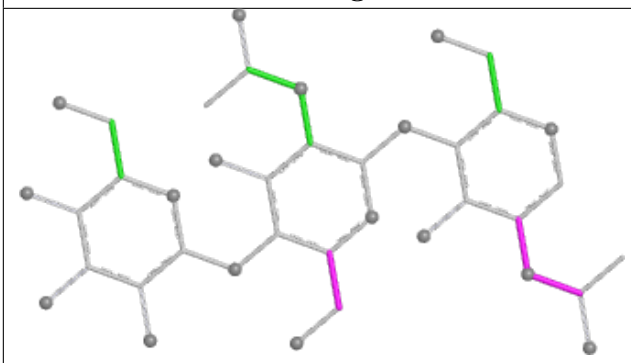
Oligosaccharide Chain I



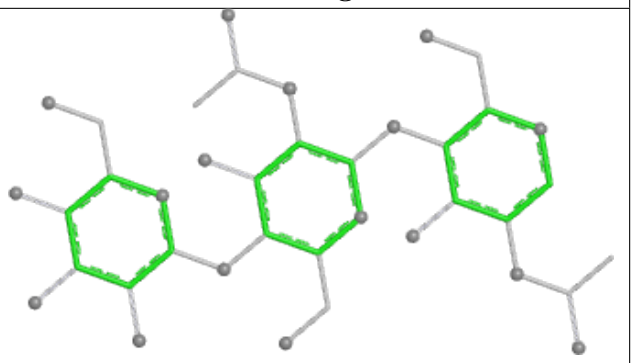
Bond lengths



Bond angles

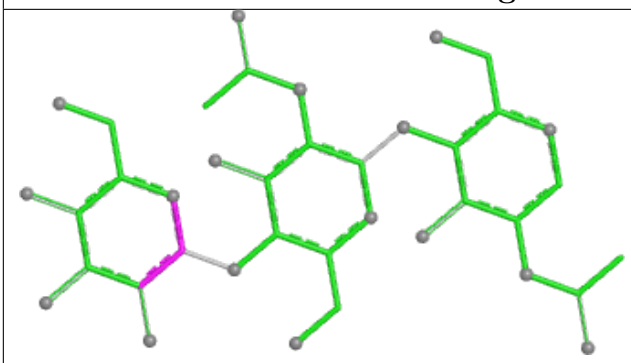


Torsions

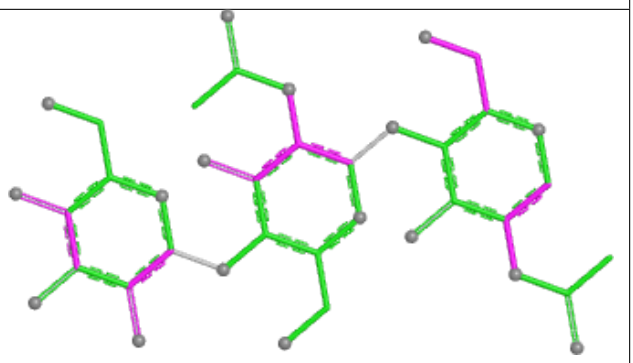


Rings

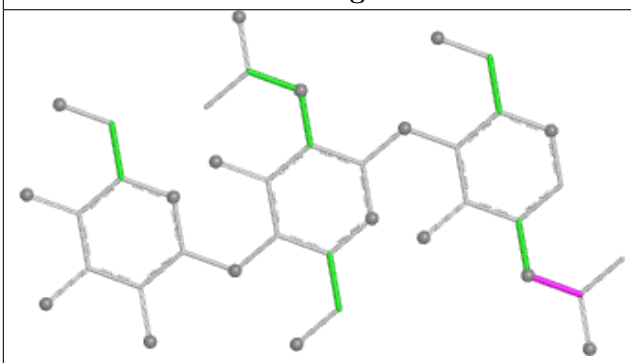
Oligosaccharide Chain J



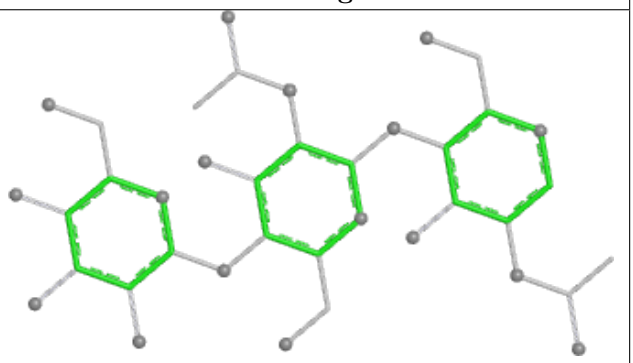
Bond lengths



Bond angles

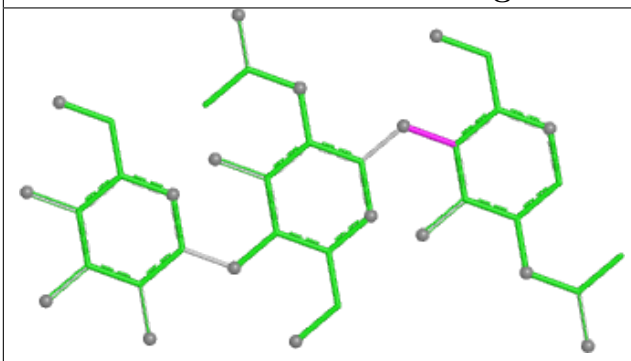


Torsions

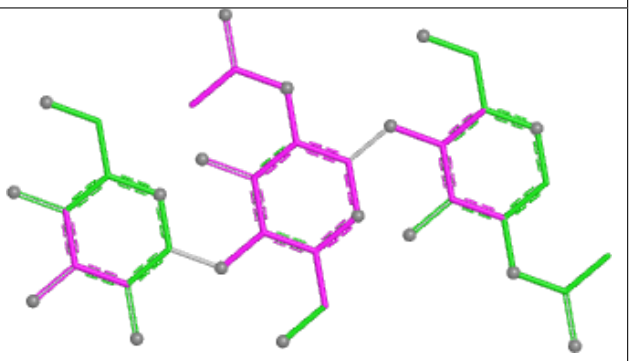


Rings

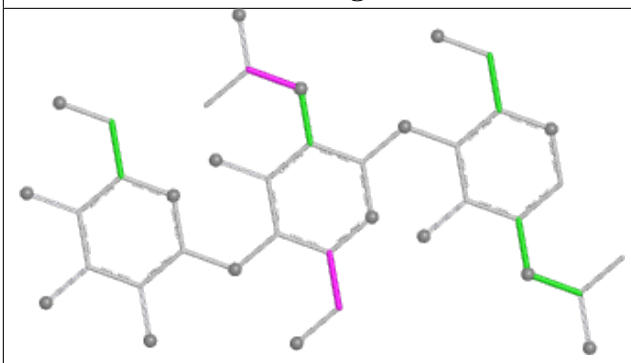
Oligosaccharide Chain Y



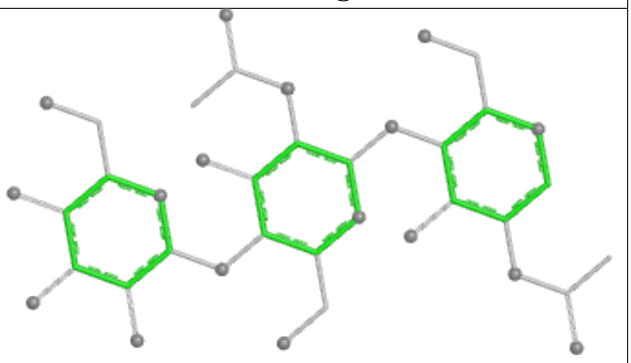
Bond lengths



Bond angles

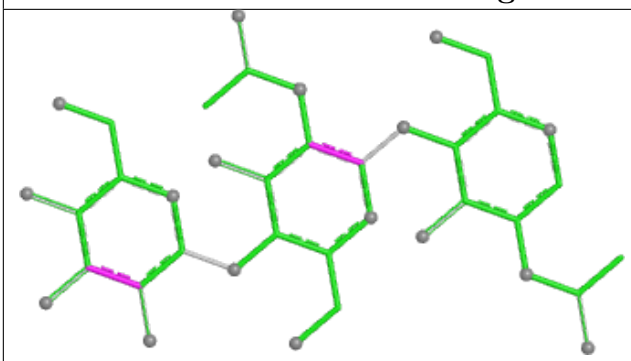


Torsions

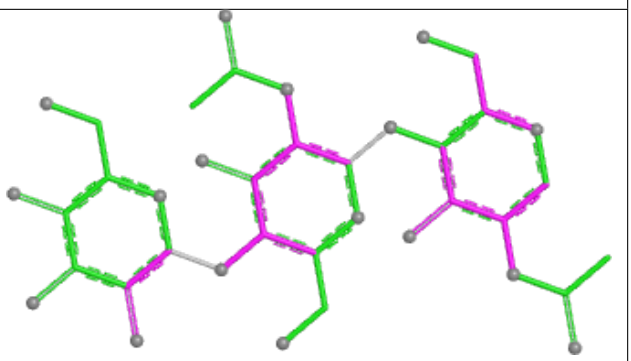


Rings

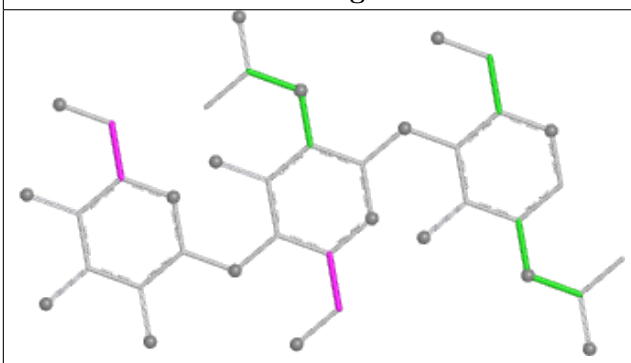
Oligosaccharide Chain b



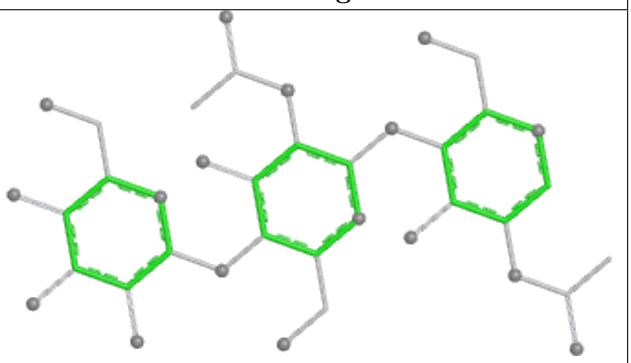
Bond lengths



Bond angles

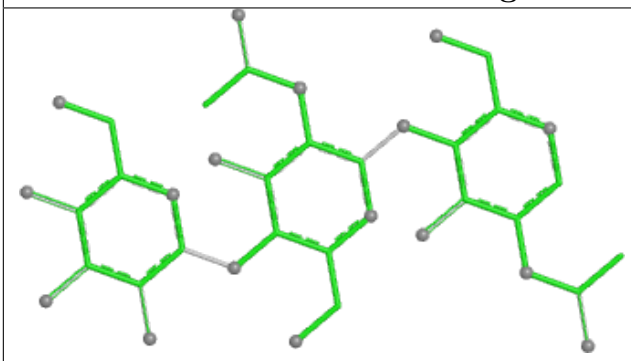


Torsions

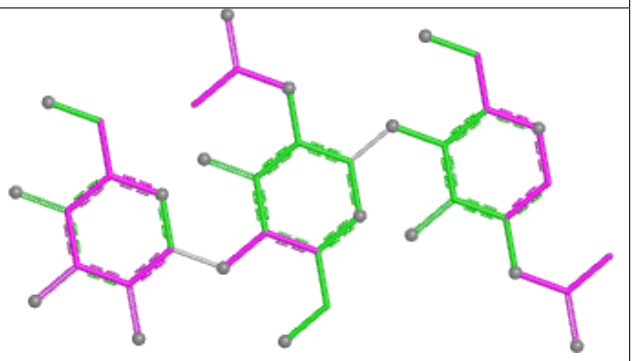


Rings

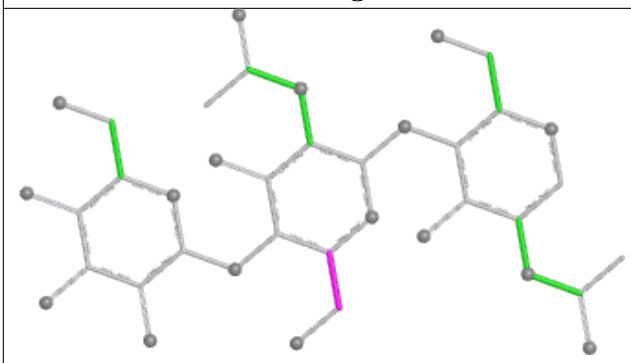
Oligosaccharide Chain e



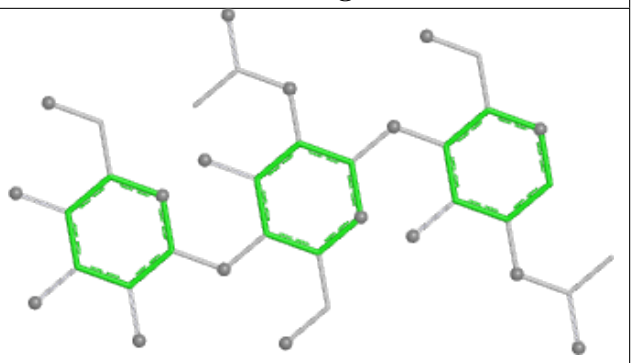
Bond lengths



Bond angles

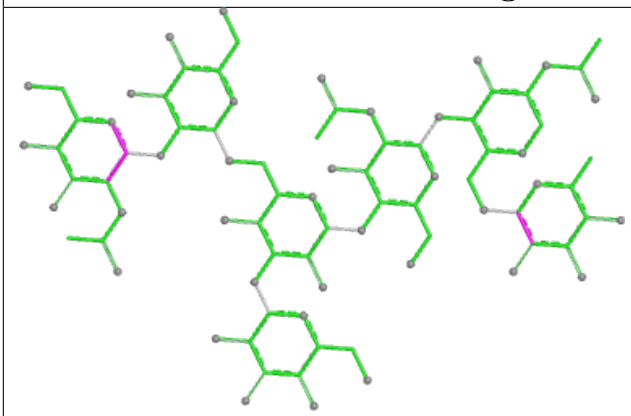


Torsions

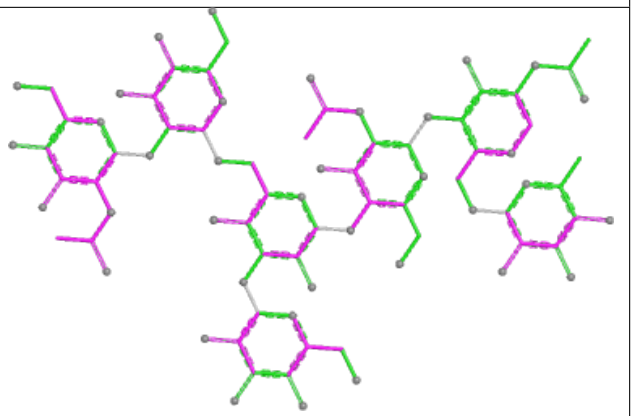


Rings

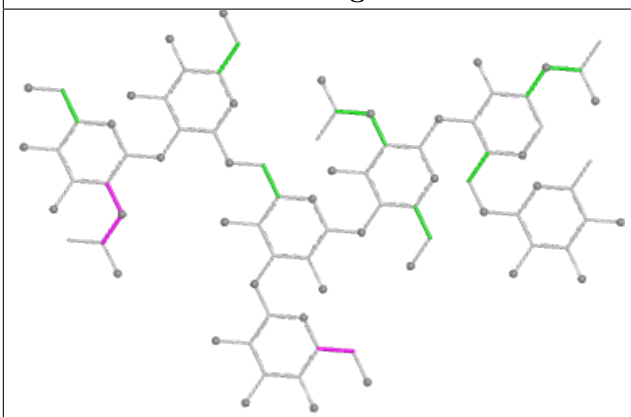
Oligosaccharide Chain c



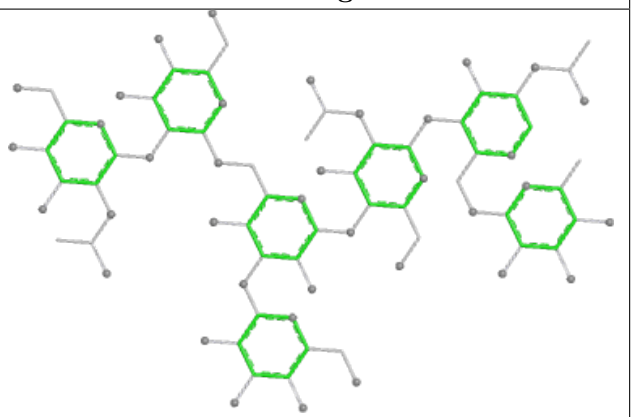
Bond lengths



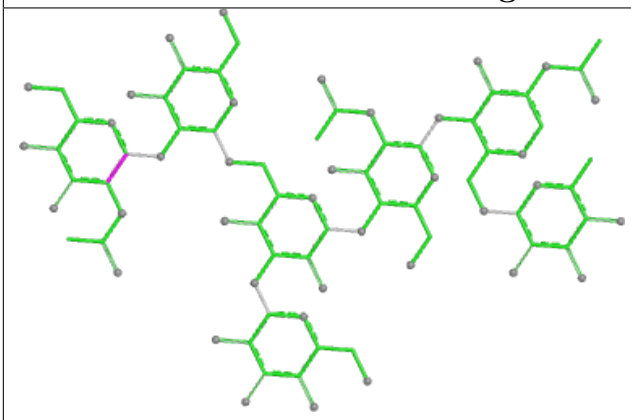
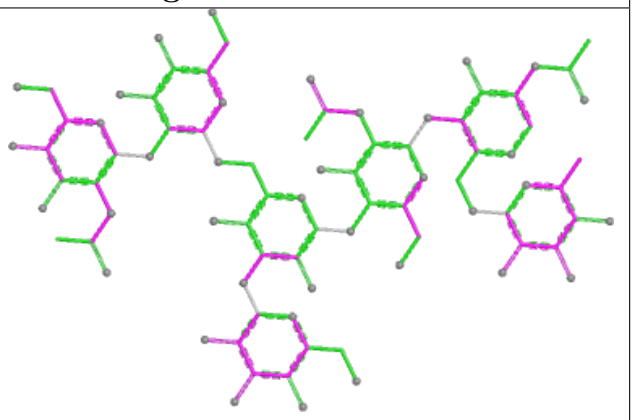
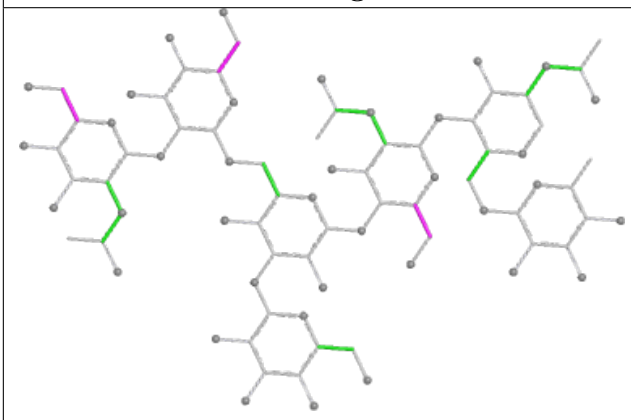
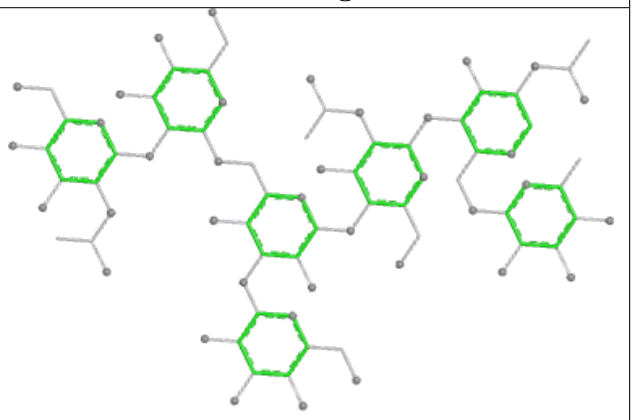
Bond angles

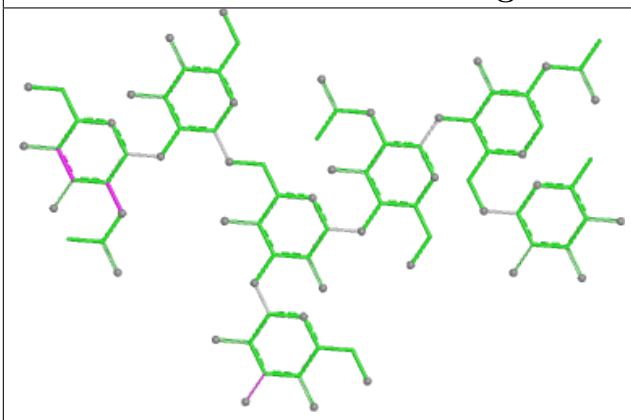
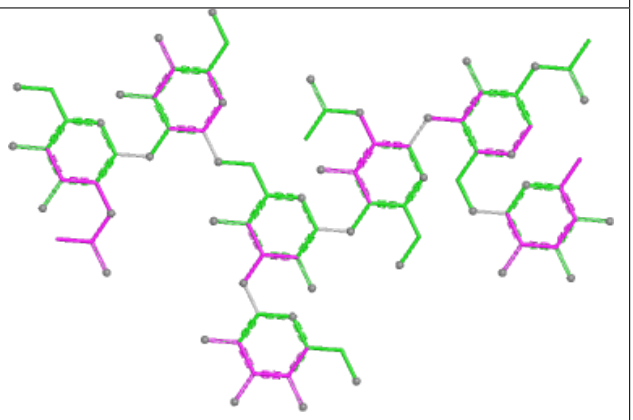
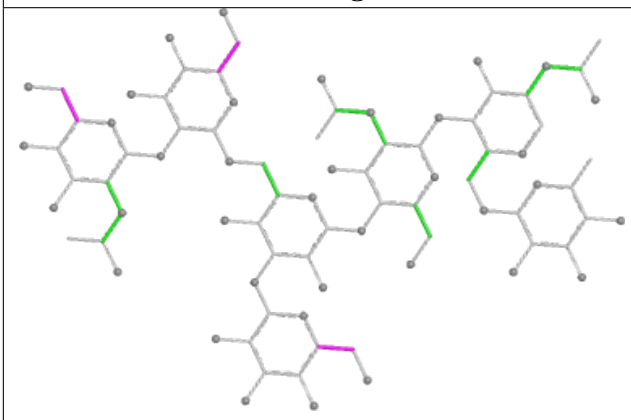
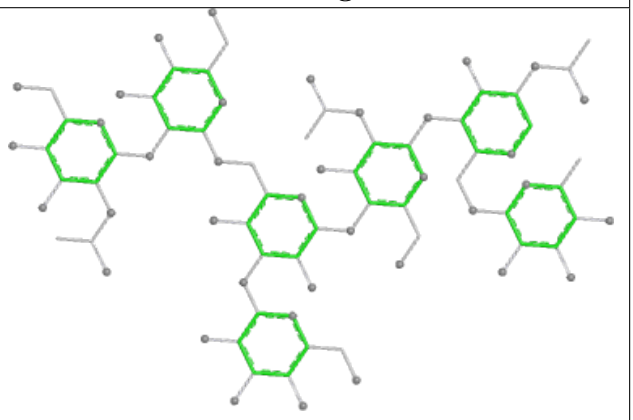


Torsions

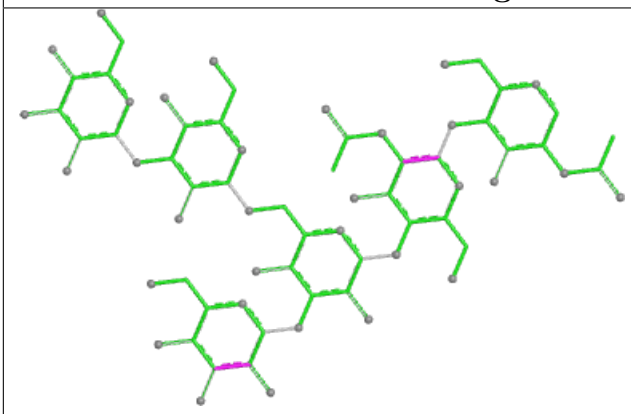


Rings

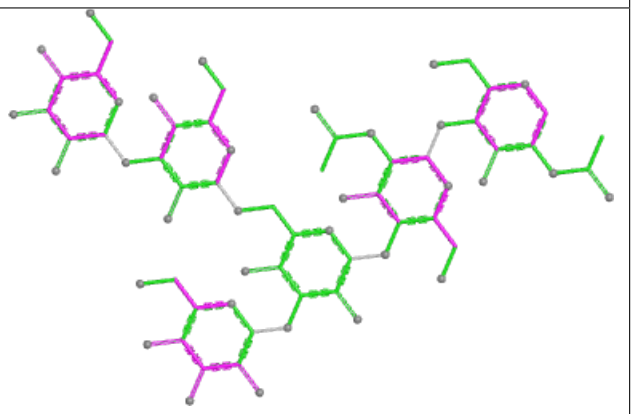
Oligosaccharide Chain g	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Oligosaccharide Chain L	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

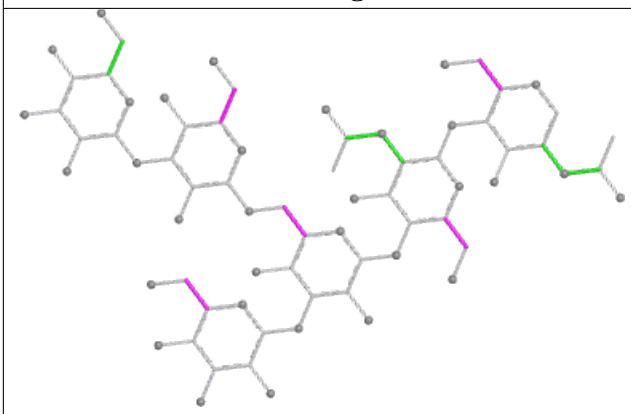
Oligosaccharide Chain K



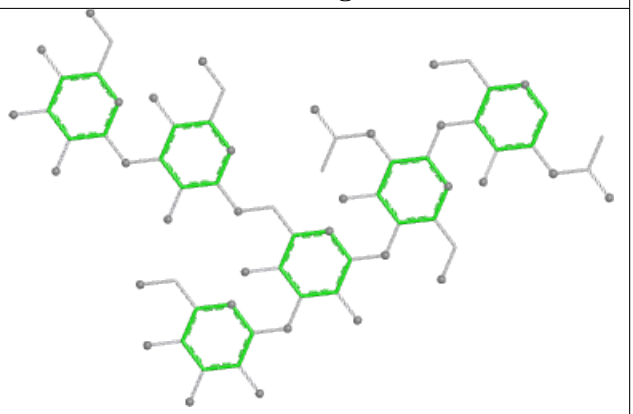
Bond lengths



Bond angles

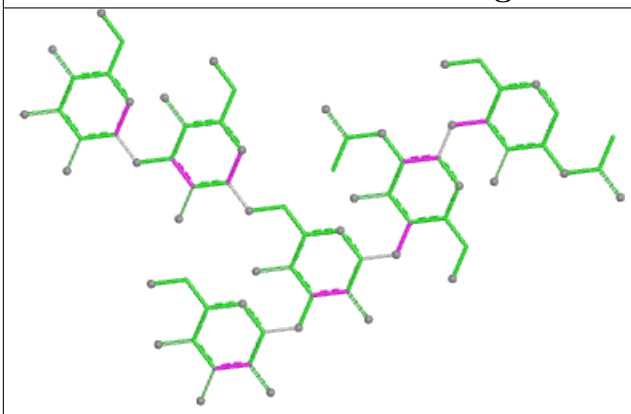


Torsions



Rings

Oligosaccharide Chain R



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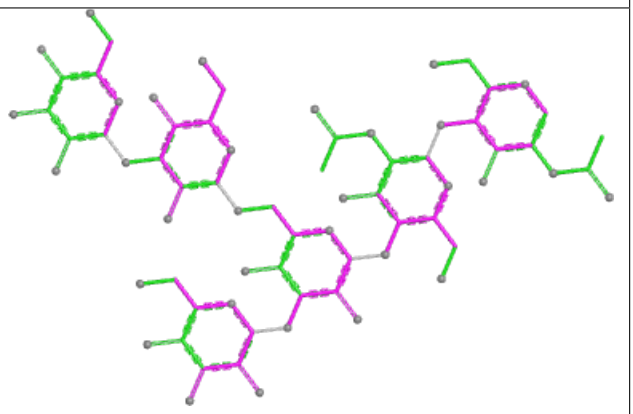
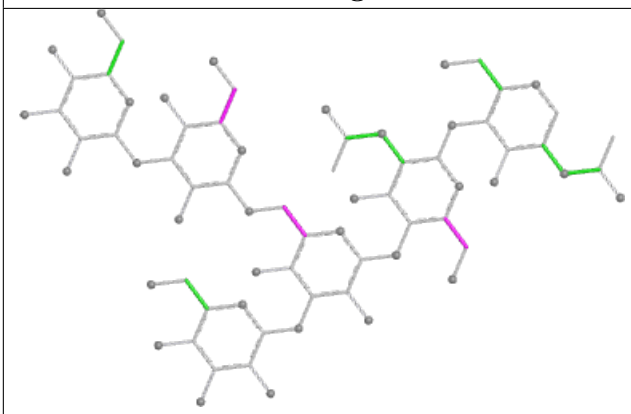
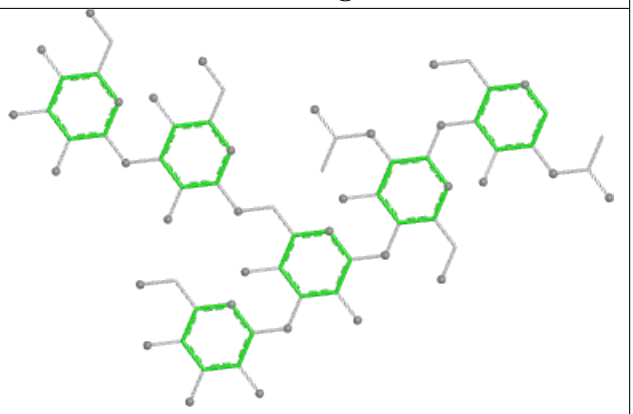


Bond angles

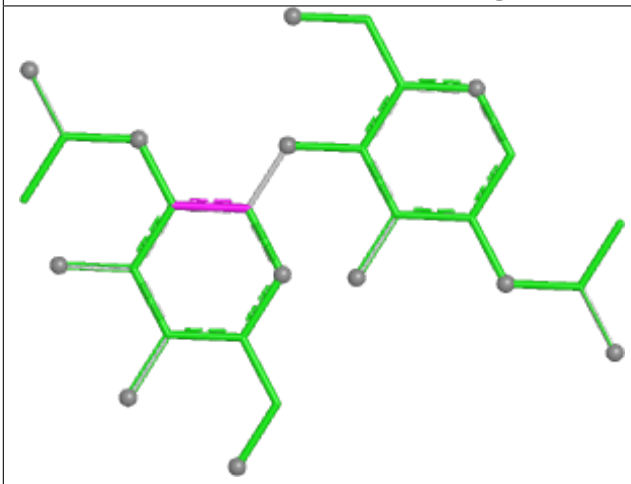


Torsions

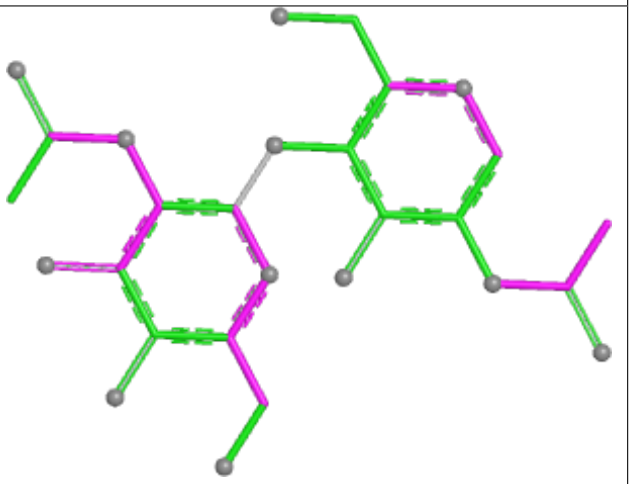


Rings

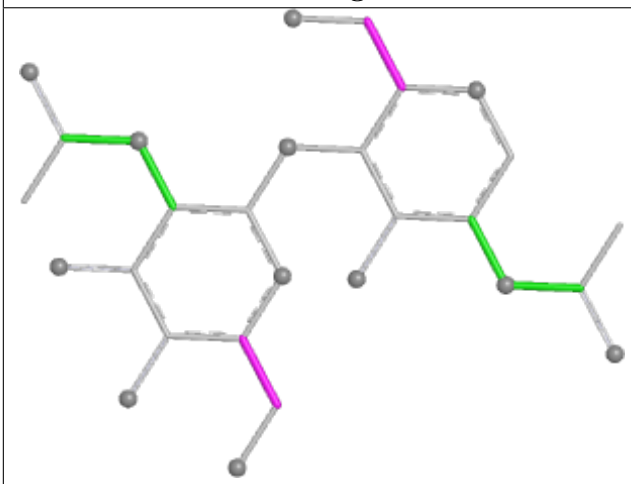
Oligosaccharide Chain M



Bond lengths



Bond angles



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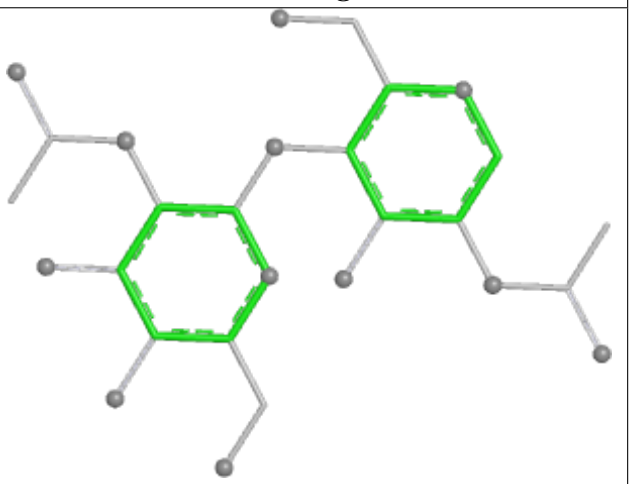
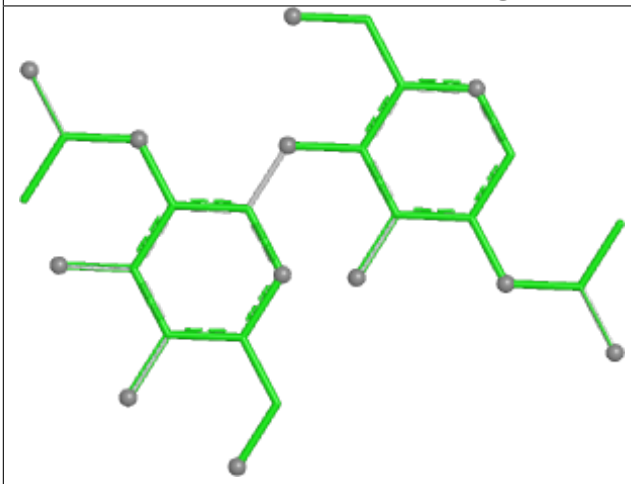


Rings

Oligosaccharide Chain O



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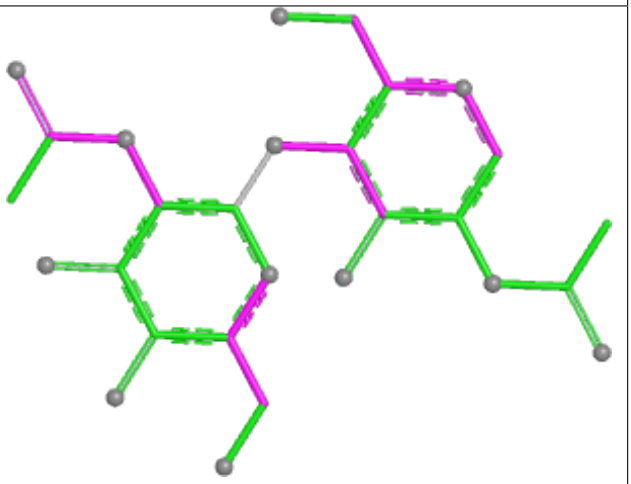
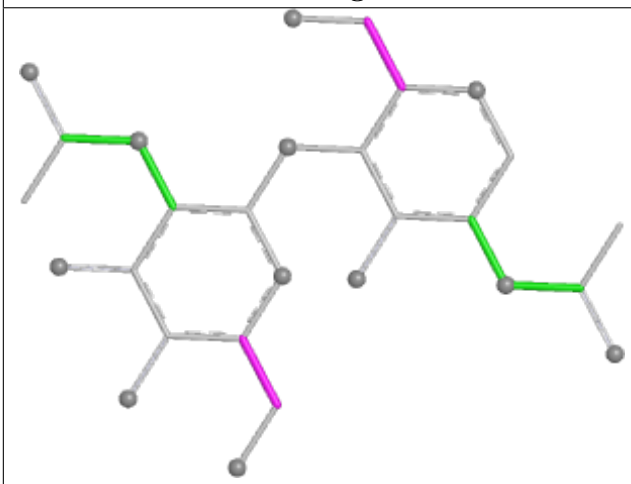
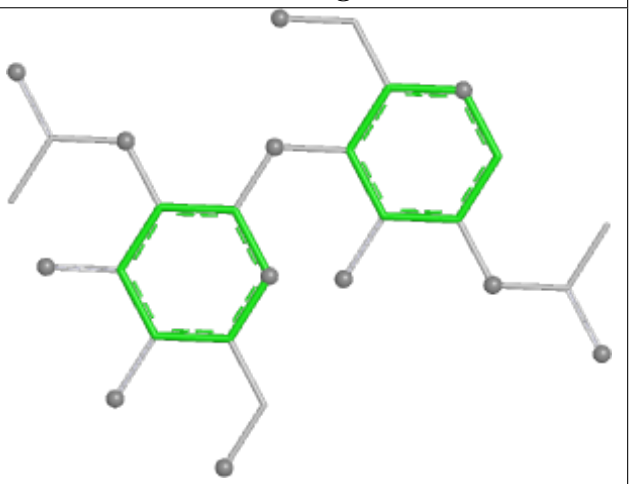


Bond angles

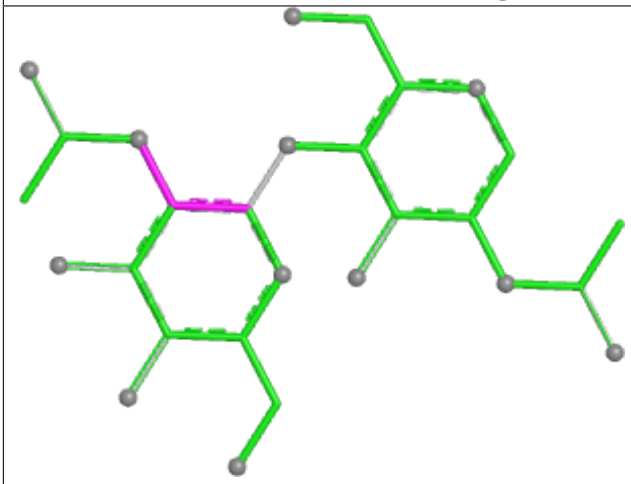


Torsions



Rings

Oligosaccharide Chain V



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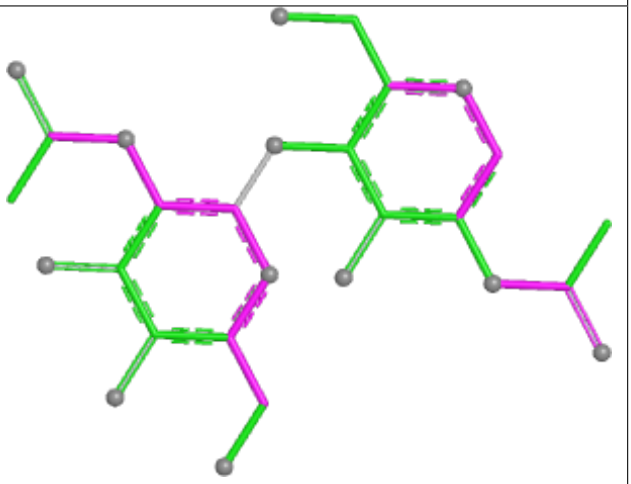
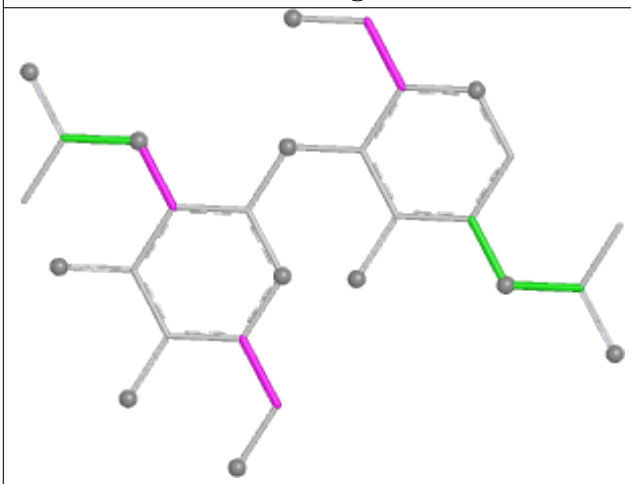


Bond angles



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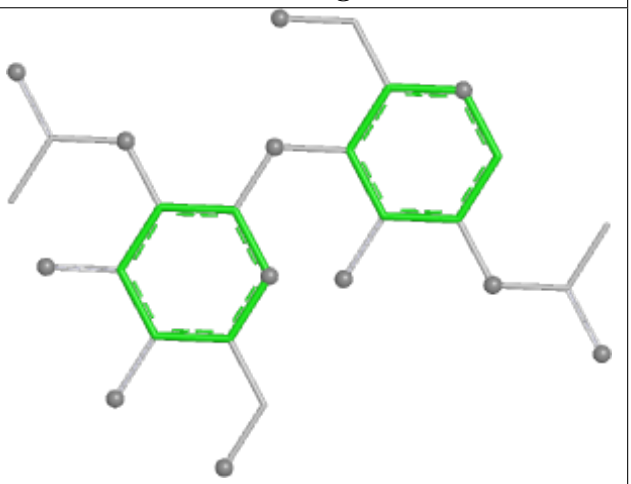
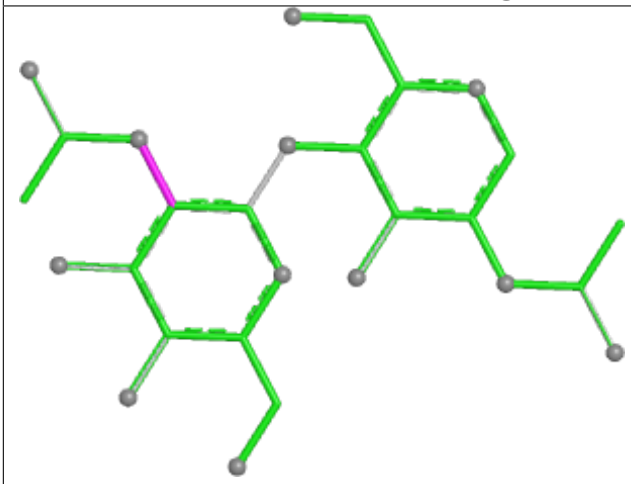


Rings

Oligosaccharide Chain d



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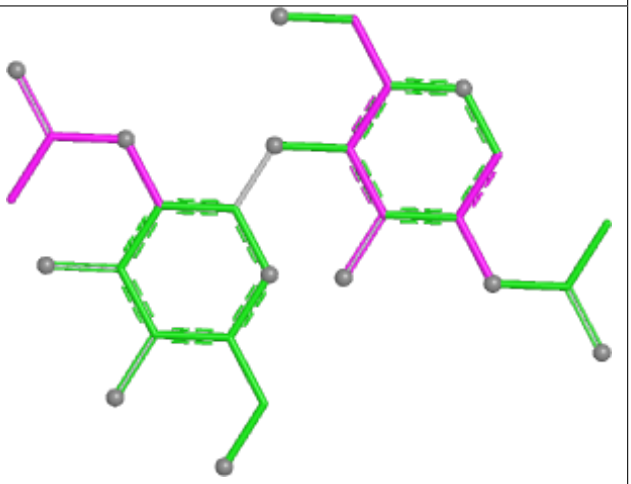
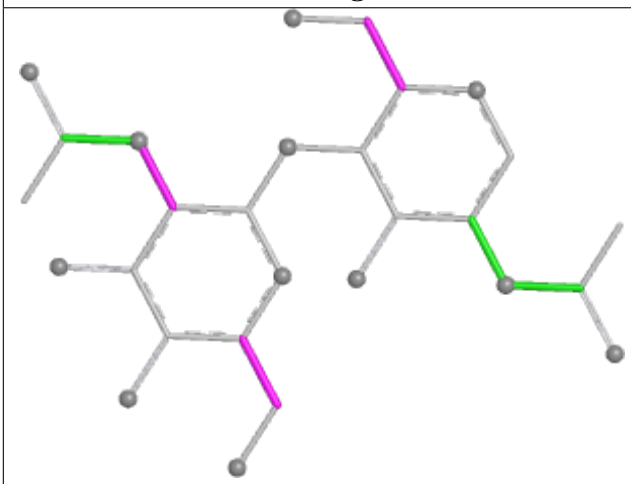


Bond angles



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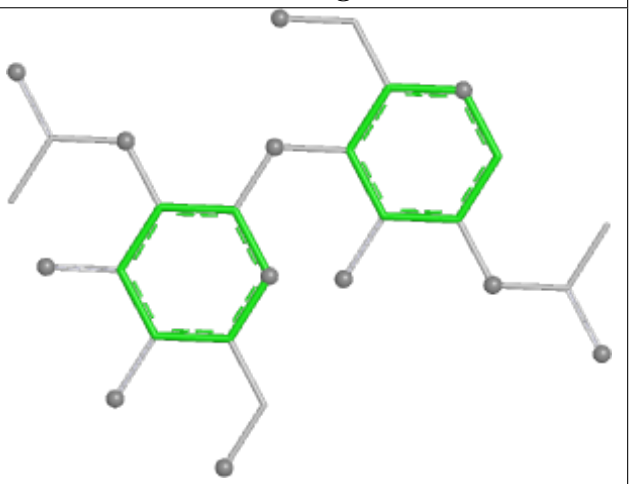
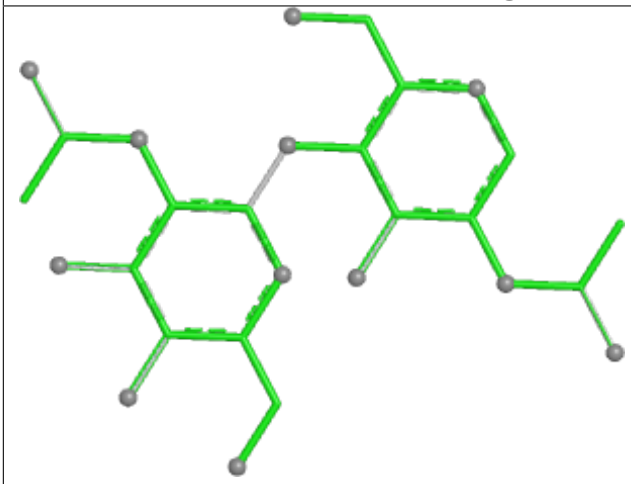


Rings

Oligosaccharide Chain f



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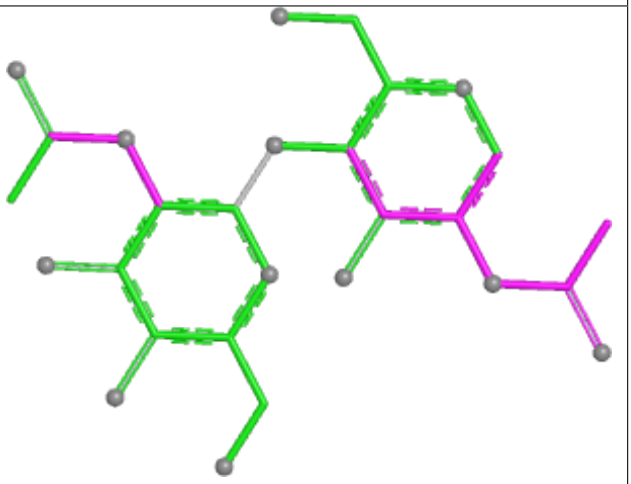
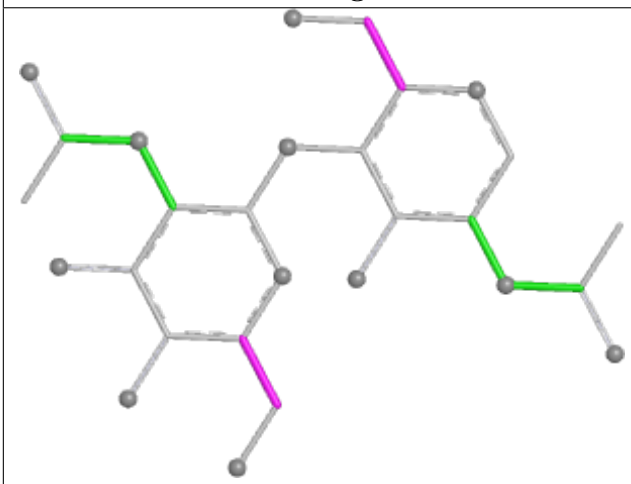


Bond angles



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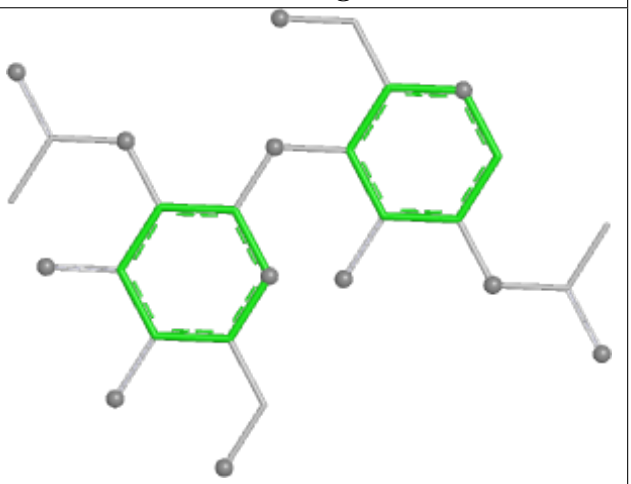
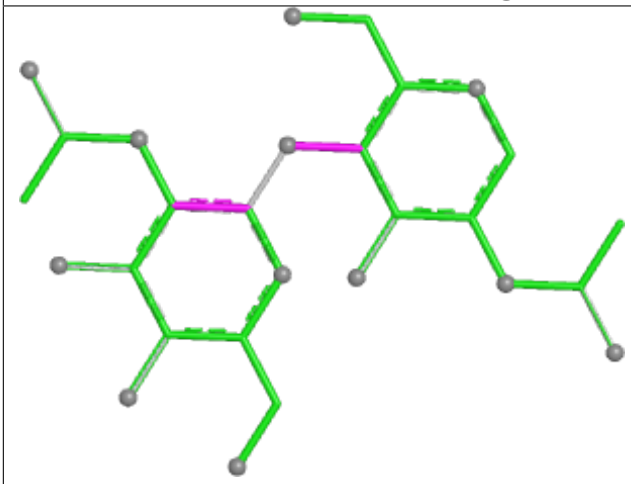


Rings

Oligosaccharide Chain S



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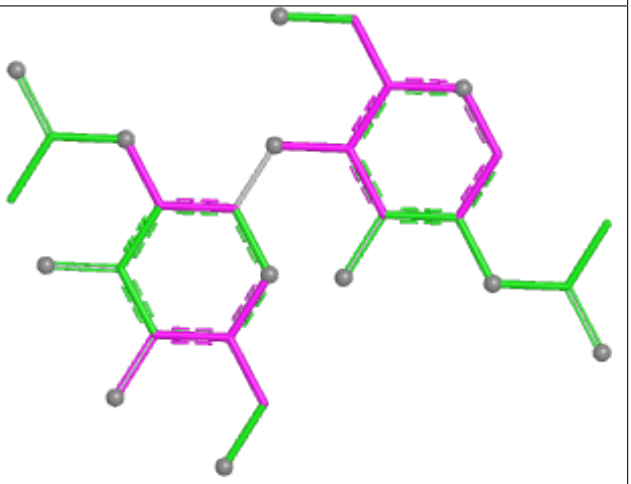
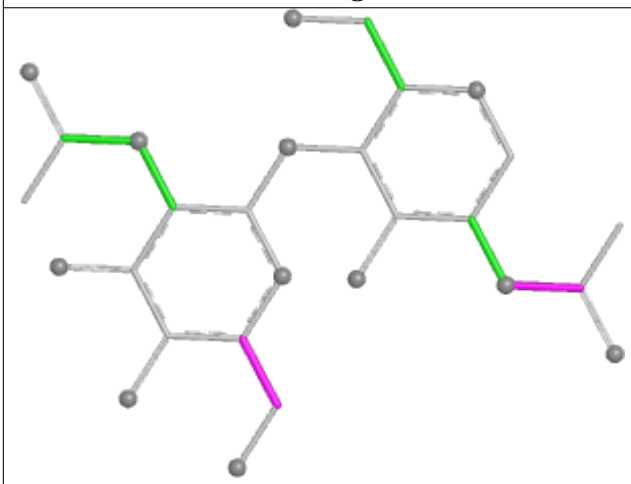


Bond angles



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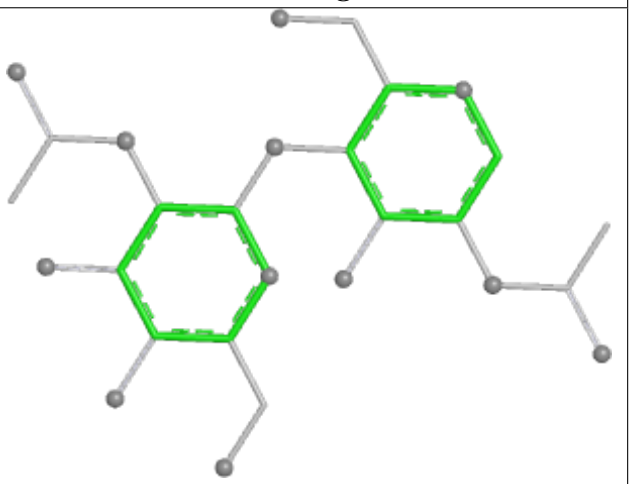
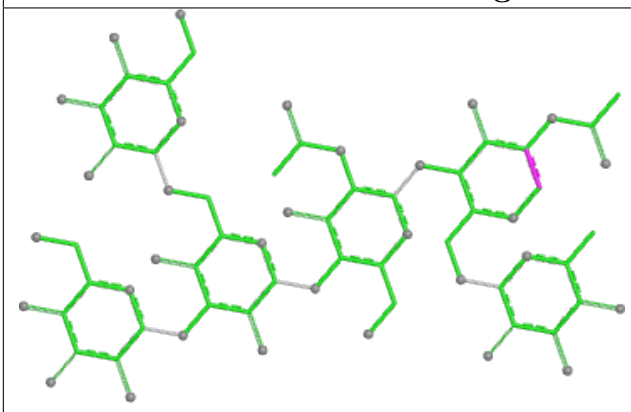


Rings

Oligosaccharide Chain N



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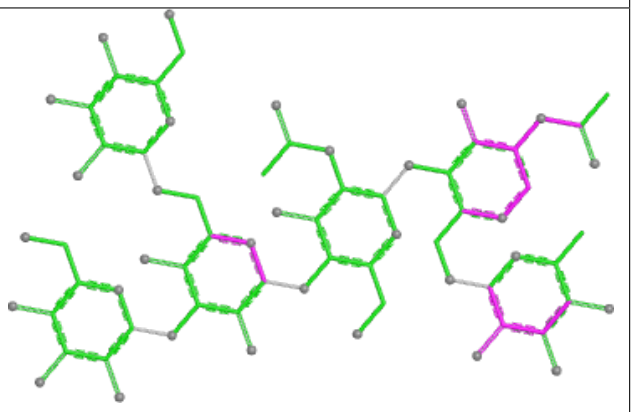
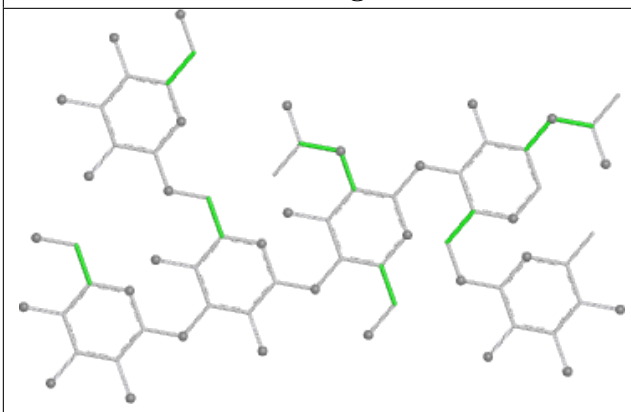


Bond angles



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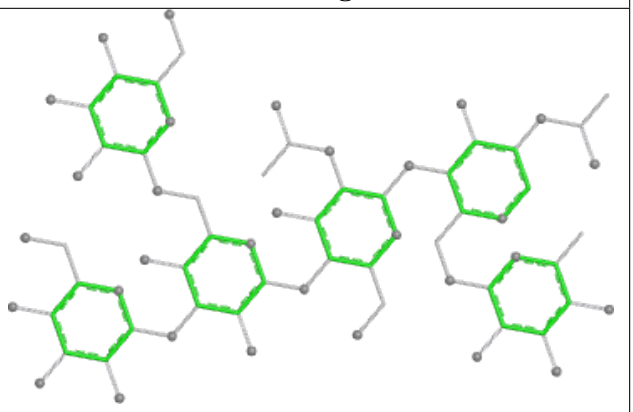
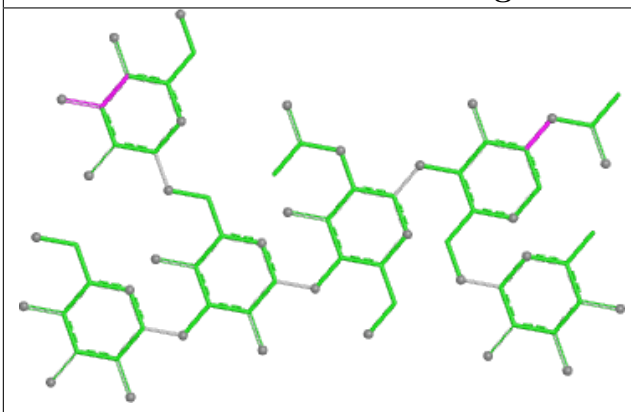
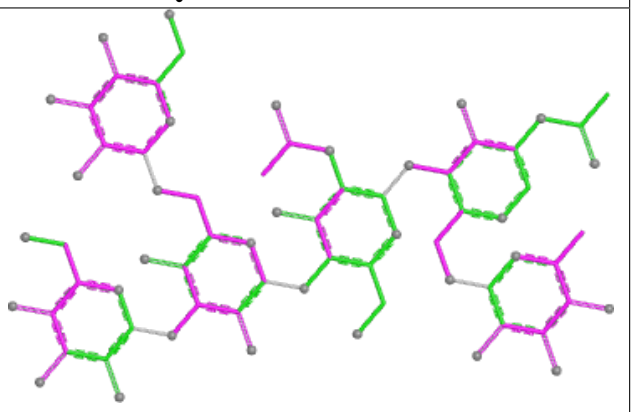
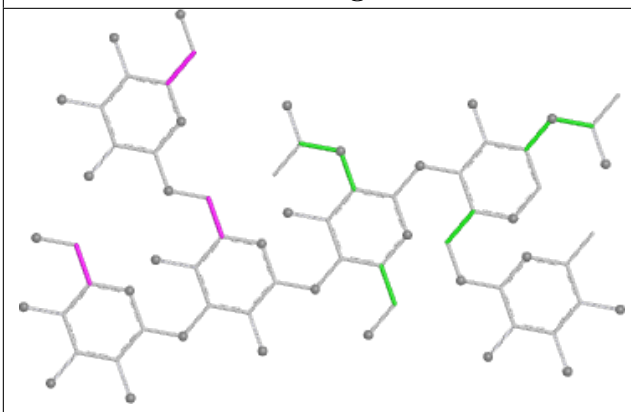
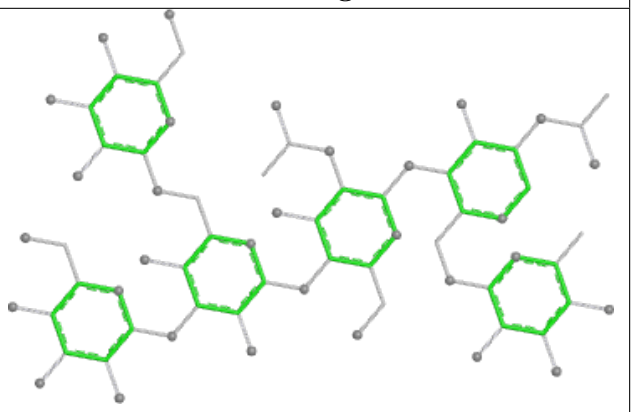
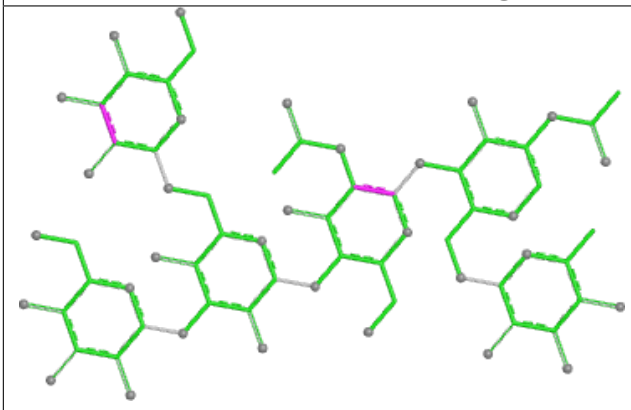


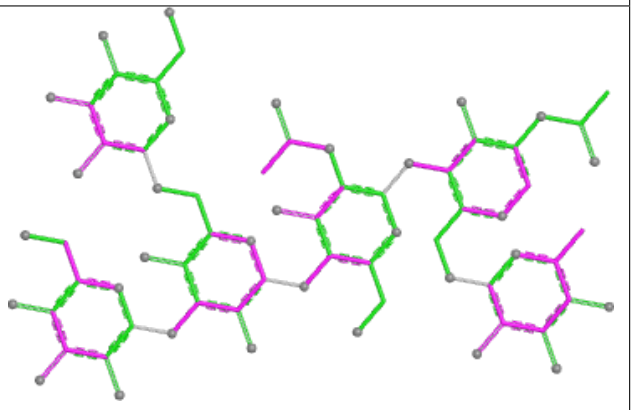
Rings

Oligosaccharide Chain Q	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

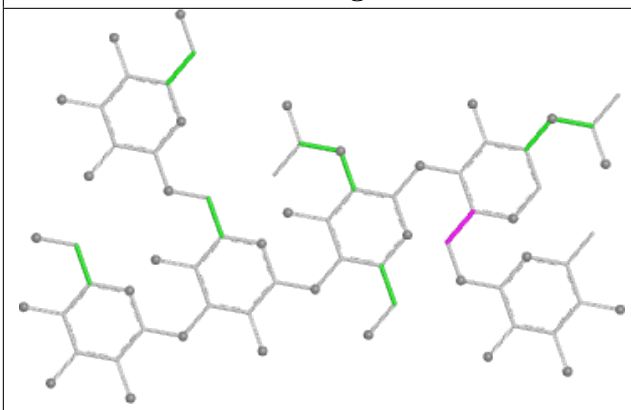
Oligosaccharide Chain T



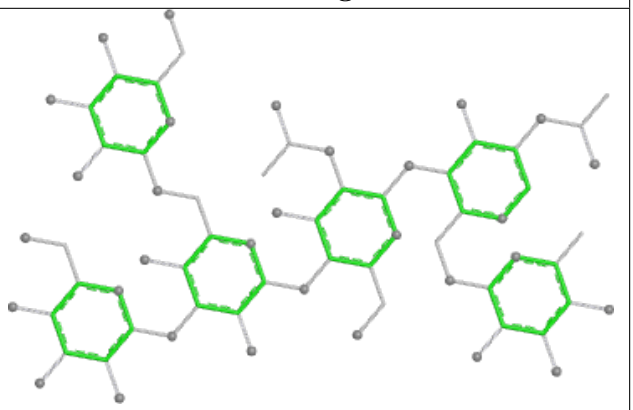
Bond lengths



Bond angles

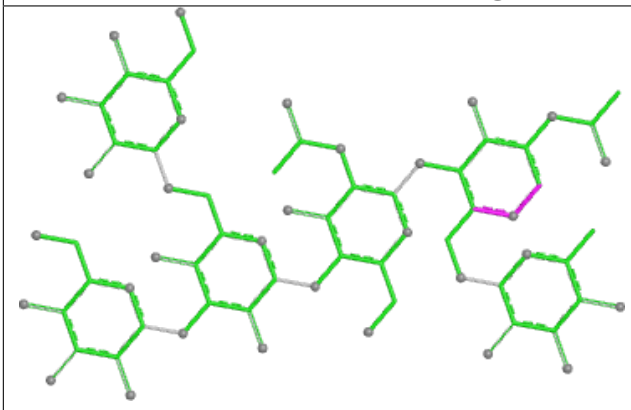


Torsions

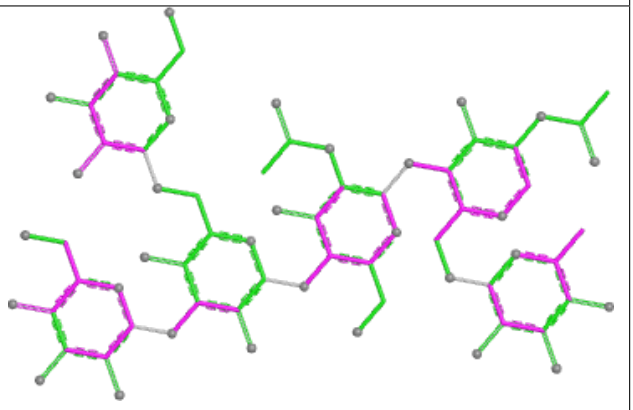


Rings

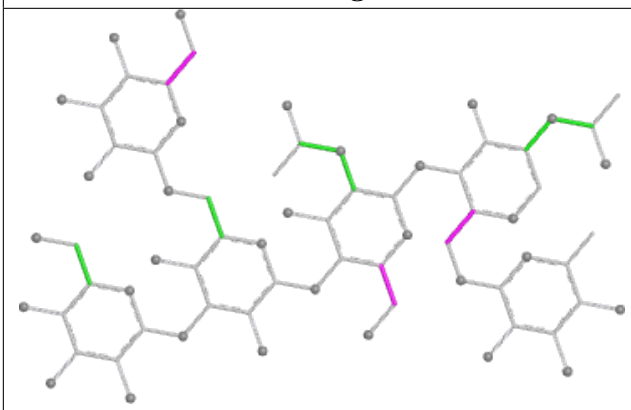
Oligosaccharide Chain W



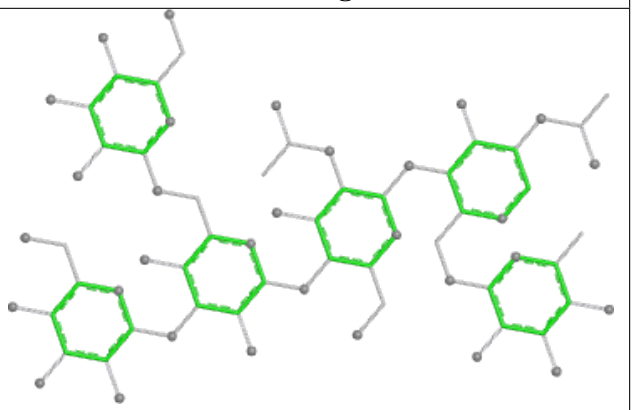
Bond lengths



Bond angles

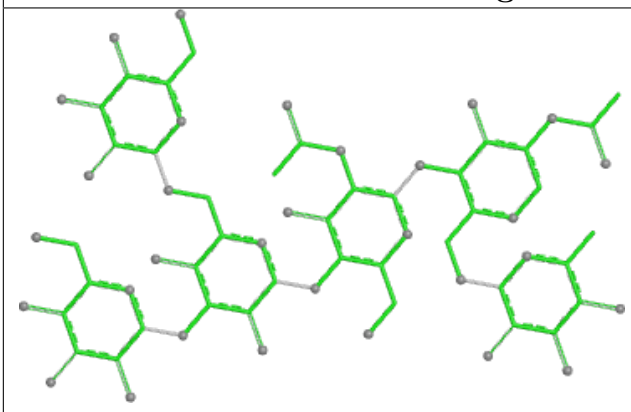


Torsions

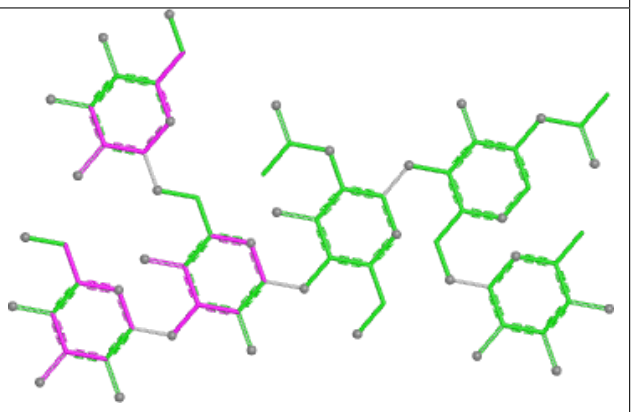


Rings

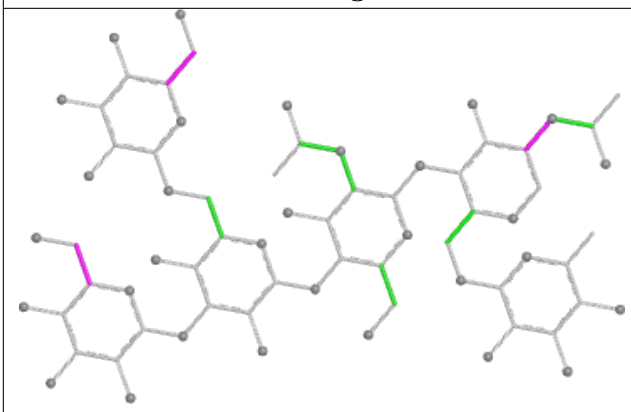
Oligosaccharide Chain Z



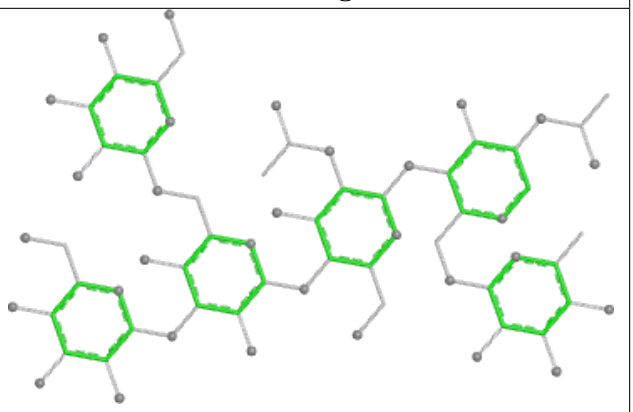
Bond lengths



Bond angles

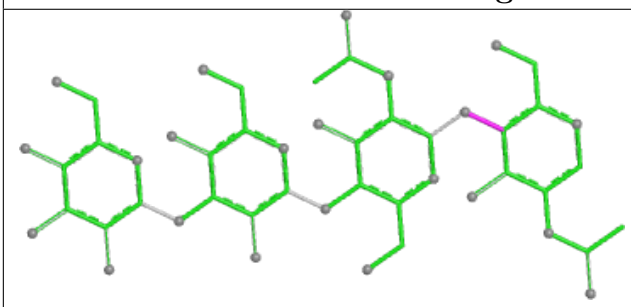


Torsions

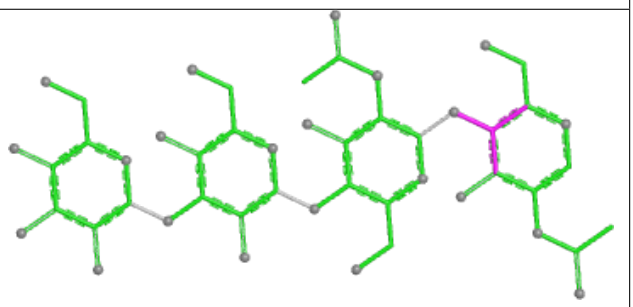


Rings

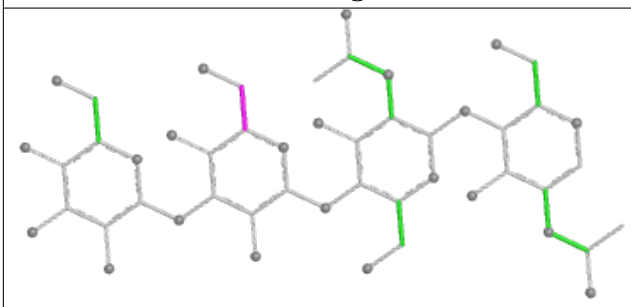
Oligosaccharide Chain P



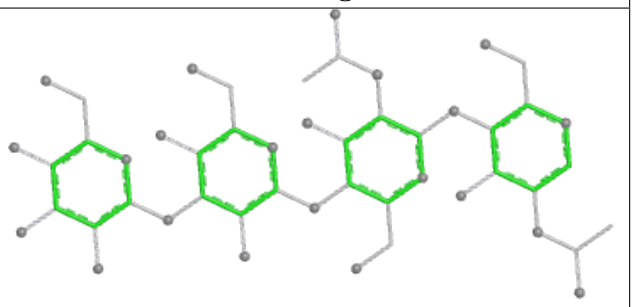
Bond lengths



Bond angles

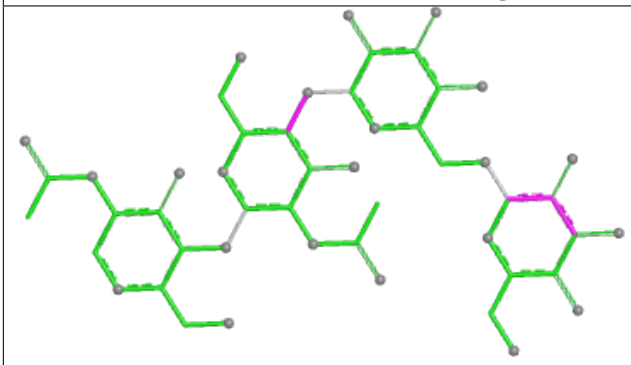


Torsions

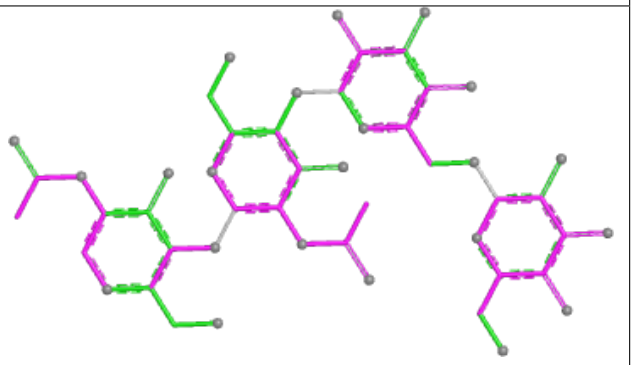


Rings

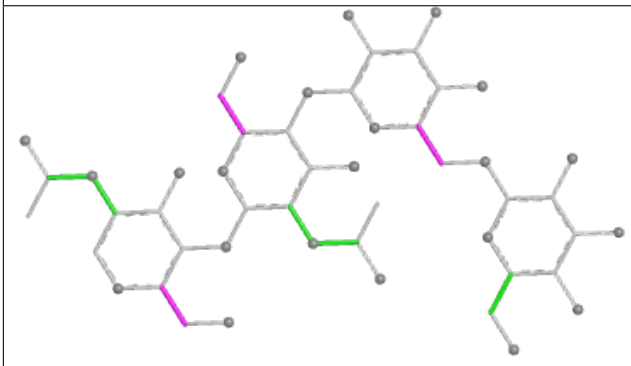
Oligosaccharide Chain U



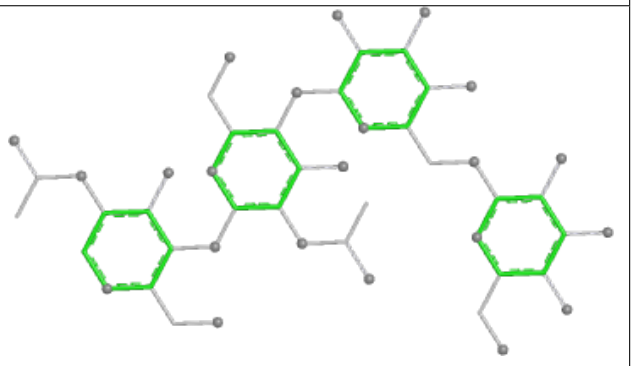
Bond lengths



Bond angles

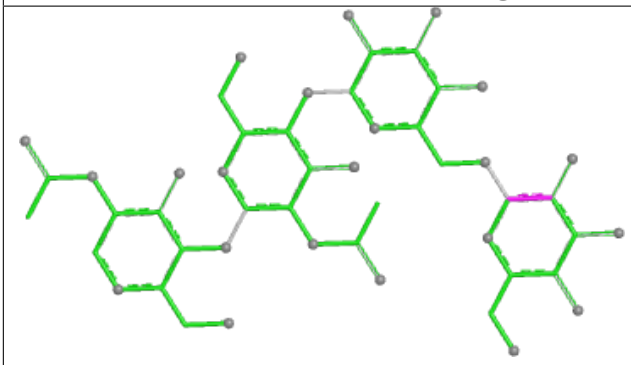


Torsions

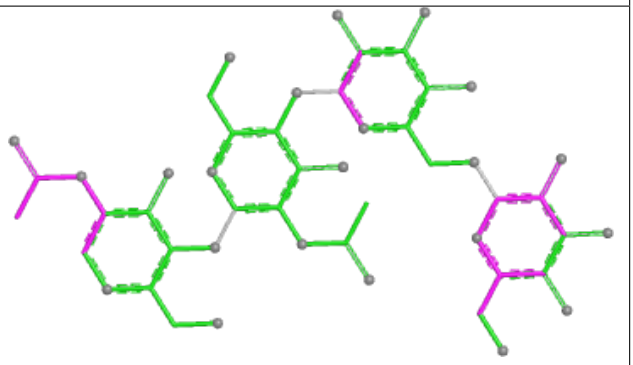


Rings

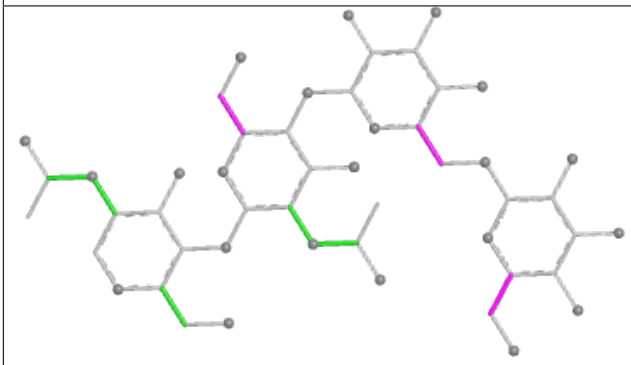
Oligosaccharide Chain X



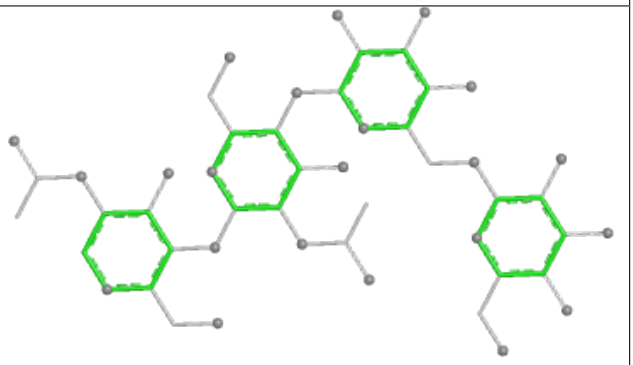
Bond lengths



Bond angles

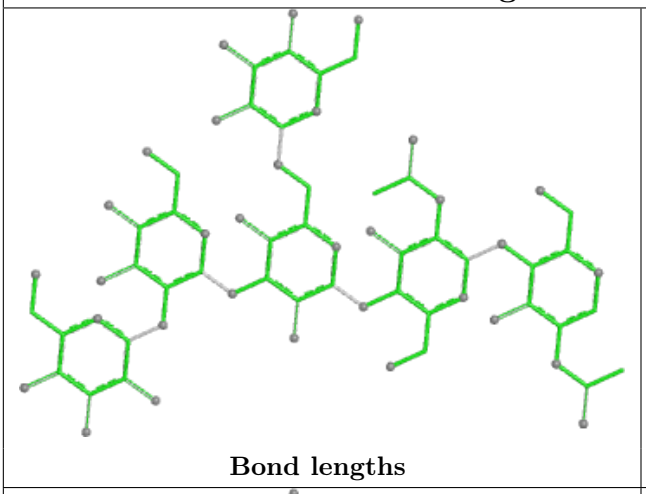


Torsions

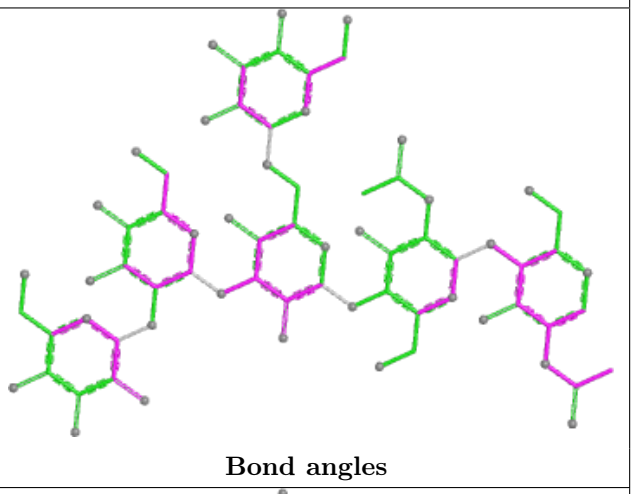


Rings

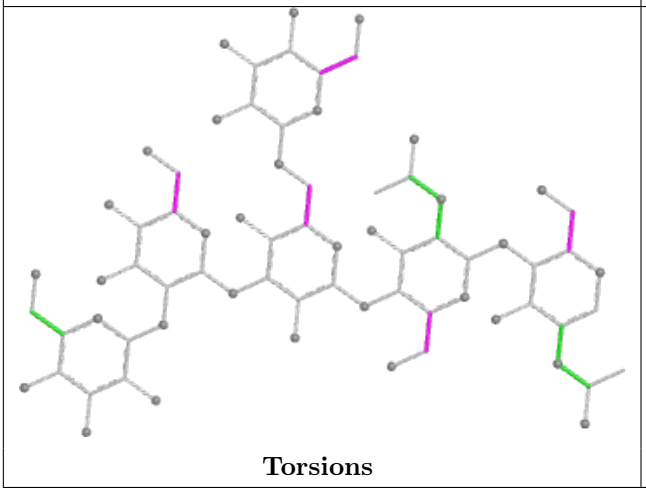
Oligosaccharide Chain a



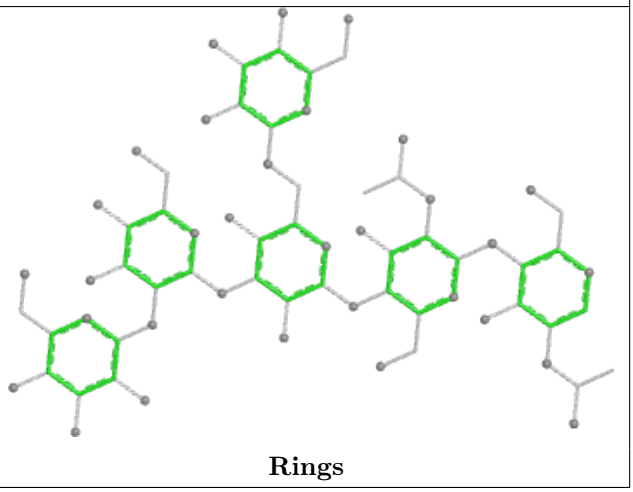
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

Of 85 ligands modelled in this entry, 44 are monoatomic - leaving 41 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	SCN	G	807	-	1,2,2	1.21	0	0,1,1	-	-
13	SCN	C	807	-	1,2,2	0.82	0	0,1,1	-	-
15	PO4	D	812	-	4,4,4	0.77	0	6,6,6	0.42	0
12	HEM	G	806	1,17	41,50,50	1.47	7 (17%)	45,82,82	1.83	13 (28%)
16	NAG	C	805	1	14,14,15	1.63	3 (21%)	17,19,21	2.18	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	HEM	D	805	1,17	41,50,50	1.50	8 (19%)	45,82,82	2.13	18 (40%)
12	HEM	F	805	1,17	41,50,50	1.42	7 (17%)	45,82,82	2.03	11 (24%)
14	8PR	H	807	-	26,27,27	0.40	0	33,37,37	0.50	0
14	8PR	A	807	-	26,27,27	0.48	0	33,37,37	1.00	2 (6%)
12	HEM	H	805	1,17	41,50,50	1.37	7 (17%)	45,82,82	1.95	14 (31%)
13	SCN	D	801	-	1,2,2	0.96	0	0,1,1	-	-
13	SCN	B	809	-	1,2,2	0.28	0	0,1,1	-	-
15	PO4	B	813	-	4,4,4	0.76	0	6,6,6	0.48	0
15	PO4	F	810	-	4,4,4	0.73	0	6,6,6	0.64	0
14	8PR	F	807	-	26,27,27	0.49	0	33,37,37	0.63	0
16	NAG	C	804	1	14,14,15	1.42	1 (7%)	17,19,21	1.93	4 (23%)
15	PO4	C	811	-	4,4,4	0.62	0	6,6,6	0.59	0
13	SCN	D	806	-	1,2,2	1.49	0	0,1,1	-	-
14	8PR	D	807	-	26,27,27	0.42	0	33,37,37	0.64	0
12	HEM	E	805	1,17	41,50,50	1.49	7 (17%)	45,82,82	1.98	16 (35%)
13	SCN	A	806	-	1,2,2	0.80	0	0,1,1	-	-
16	NAG	D	804	1	14,14,15	0.81	0	17,19,21	1.78	5 (29%)
15	PO4	A	810	-	4,4,4	0.68	0	6,6,6	0.46	0
13	SCN	H	806	-	1,2,2	0.56	0	0,1,1	-	-
15	PO4	H	810	-	4,4,4	0.63	0	6,6,6	0.54	0
16	NAG	B	805	1	14,14,15	1.32	2 (14%)	17,19,21	2.26	5 (29%)
15	PO4	E	808	-	4,4,4	0.72	0	6,6,6	0.47	0
13	SCN	E	806	-	1,2,2	0.60	0	0,1,1	-	-
15	PO4	B	812	-	4,4,4	0.77	0	6,6,6	0.48	0
12	HEM	C	806	1,17	41,50,50	1.41	5 (12%)	45,82,82	1.99	12 (26%)
15	PO4	C	810	-	4,4,4	0.86	0	6,6,6	0.38	0
15	PO4	D	811	-	4,4,4	1.12	1 (25%)	6,6,6	0.50	0
15	PO4	G	809	-	4,4,4	0.98	0	6,6,6	0.36	0
12	HEM	B	807	1,17	41,50,50	1.32	4 (9%)	45,82,82	2.20	16 (35%)
13	SCN	F	806	-	1,2,2	0.46	0	0,1,1	-	-
15	PO4	G	810	-	4,4,4	0.53	0	6,6,6	0.47	0
15	PO4	D	813	-	4,4,4	0.85	0	6,6,6	0.57	0
12	HEM	A	805	1,17	41,50,50	1.59	7 (17%)	45,82,82	1.74	15 (33%)
16	NAG	B	806	1	14,14,15	1.66	2 (14%)	17,19,21	2.87	6 (35%)
15	PO4	H	809	-	4,4,4	0.51	0	6,6,6	0.47	0
13	SCN	B	808	-	1,2,2	0.89	0	0,1,1	-	-

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
12	HEM	E	805	1,17	-	5/12/54/54	-
16	NAG	B	806	1	-	1/6/23/26	0/1/1/1
14	8PR	F	807	-	-	2/9/26/26	0/4/4/4
14	8PR	A	807	-	-	2/9/26/26	0/4/4/4
14	8PR	H	807	-	-	2/9/26/26	0/4/4/4
12	HEM	H	805	1,17	-	4/12/54/54	-
16	NAG	C	804	1	-	2/6/23/26	0/1/1/1
16	NAG	D	804	1	-	3/6/23/26	0/1/1/1
16	NAG	B	805	1	-	0/6/23/26	0/1/1/1
12	HEM	G	806	1,17	-	5/12/54/54	-
12	HEM	C	806	1,17	-	5/12/54/54	-
12	HEM	A	805	1,17	-	5/12/54/54	-
16	NAG	C	805	1	-	0/6/23/26	0/1/1/1
12	HEM	D	805	1,17	-	4/12/54/54	-
12	HEM	B	807	1,17	-	4/12/54/54	-
12	HEM	F	805	1,17	-	4/12/54/54	-
14	8PR	D	807	-	-	2/9/26/26	0/4/4/4

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	806	NAG	C1-C2	4.41	1.58	1.52
12	E	805	HEM	C1B-NB	-4.20	1.33	1.40
12	F	805	HEM	C4D-ND	-3.93	1.33	1.40
12	A	805	HEM	C3B-C4B	3.88	1.52	1.44
16	C	805	NAG	C1-C2	3.87	1.58	1.52

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	806	NAG	C1-C2-N2	7.27	122.90	110.49
16	B	806	NAG	C2-N2-C7	6.99	132.86	122.90
12	F	805	HEM	CHC-C4B-NB	6.36	131.34	124.43
12	B	807	HEM	CHC-C4B-NB	6.09	131.05	124.43
16	B	805	NAG	C2-N2-C7	5.17	130.27	122.90

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	807	8PR	OAO-CAM-CAW-CAK
14	A	807	8PR	OAO-CAM-CAW-CAX
14	D	807	8PR	OAO-CAM-CAW-CAK
14	D	807	8PR	OAO-CAM-CAW-CAX
14	F	807	8PR	OAO-CAM-CAW-CAK

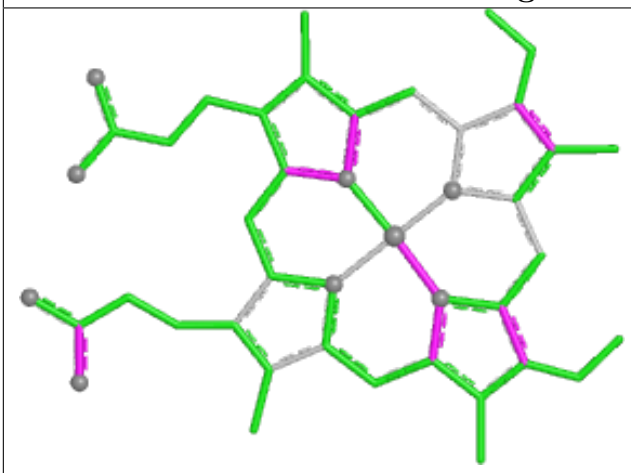
There are no ring outliers.

12 monomers are involved in 69 short contacts:

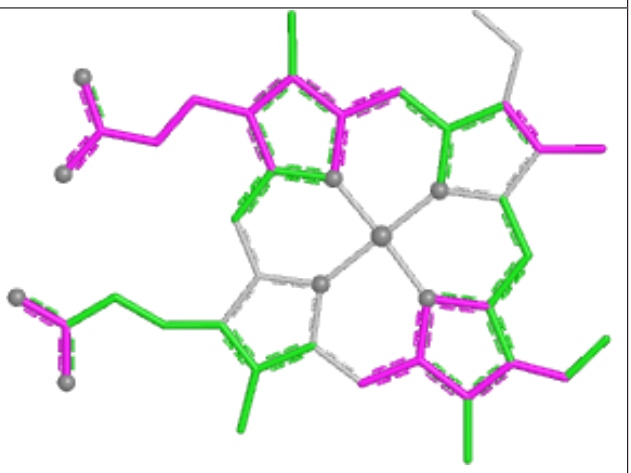
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	806	HEM	7	0
12	D	805	HEM	7	0
12	F	805	HEM	10	0
12	H	805	HEM	9	0
14	D	807	8PR	1	0
12	E	805	HEM	6	0
15	H	810	PO4	1	0
12	C	806	HEM	8	0
15	G	809	PO4	1	0
12	B	807	HEM	10	0
12	A	805	HEM	8	0
16	B	806	NAG	1	0

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

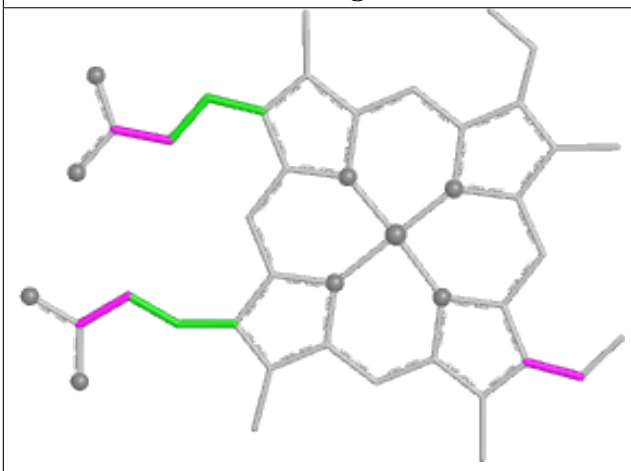
Ligand HEM G 806



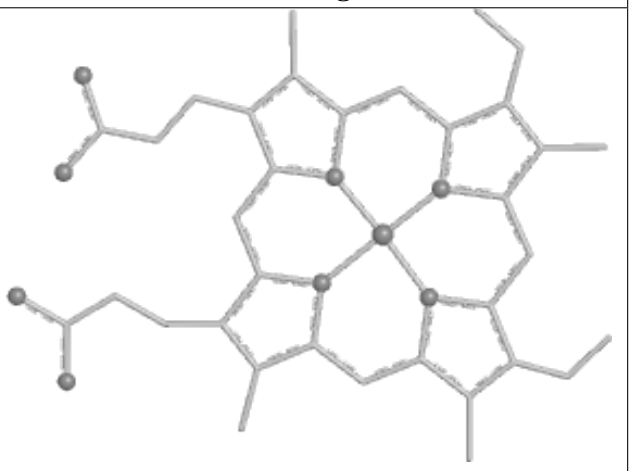
Bond lengths



Bond angles

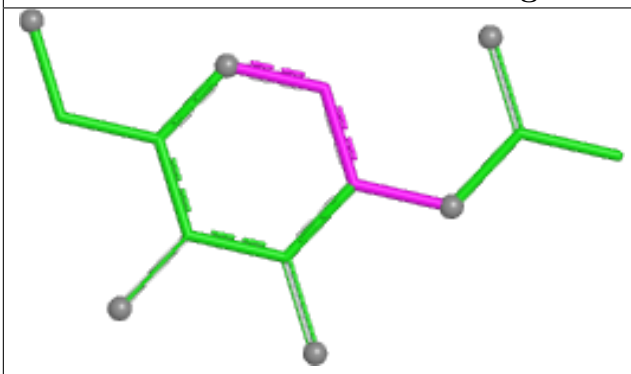


Torsions

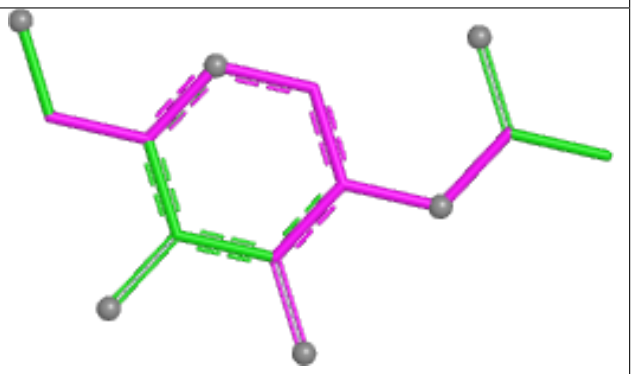


Rings

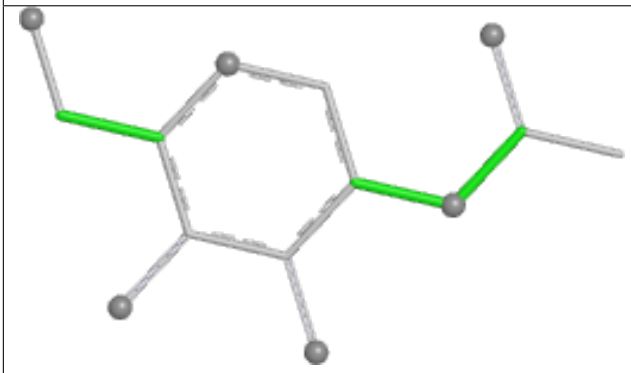
Ligand NAG C 805



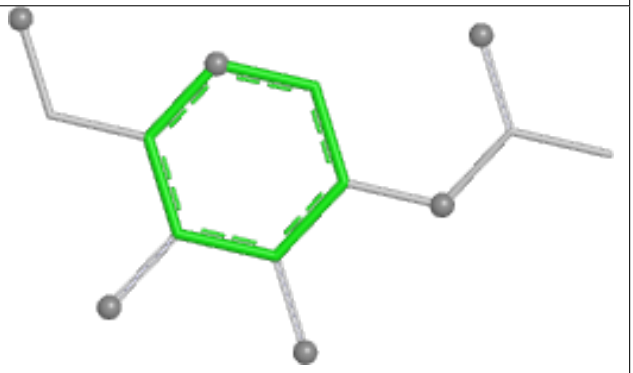
Bond lengths



Bond angles

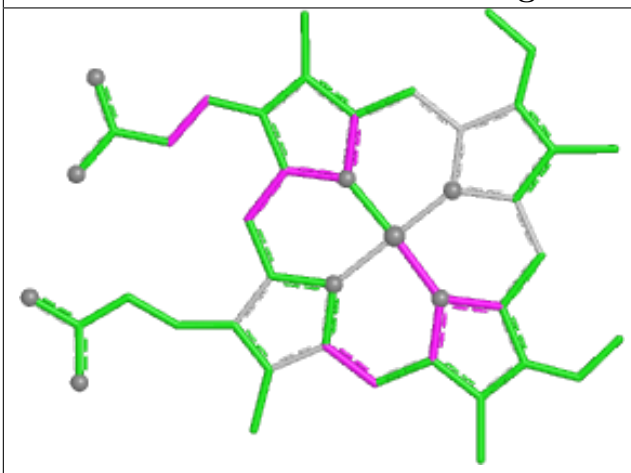


Torsions

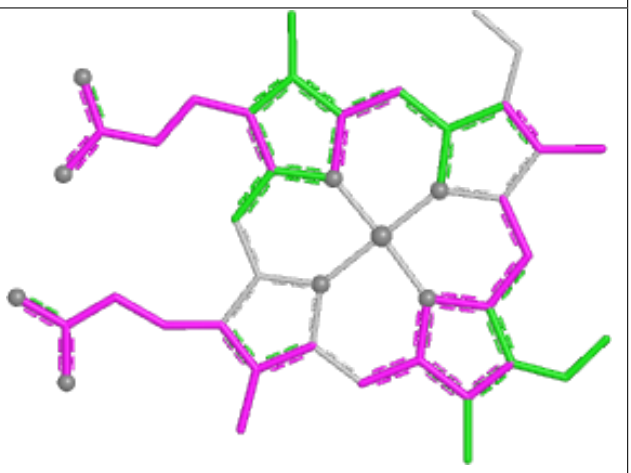


Rings

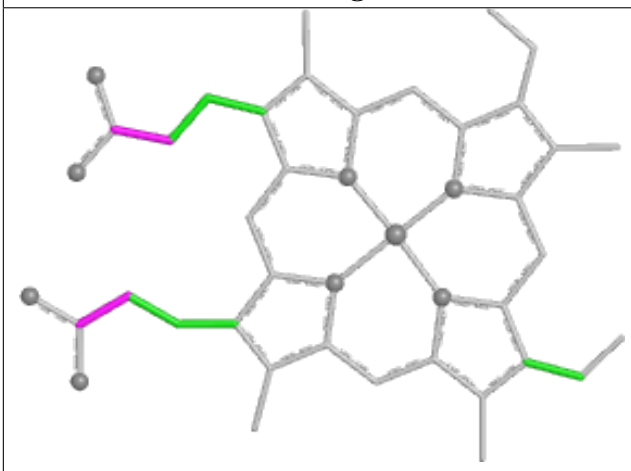
Ligand HEM D 805



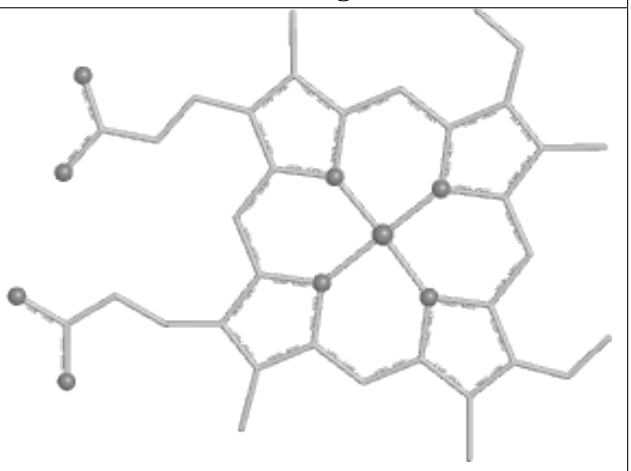
Bond lengths



Bond angles

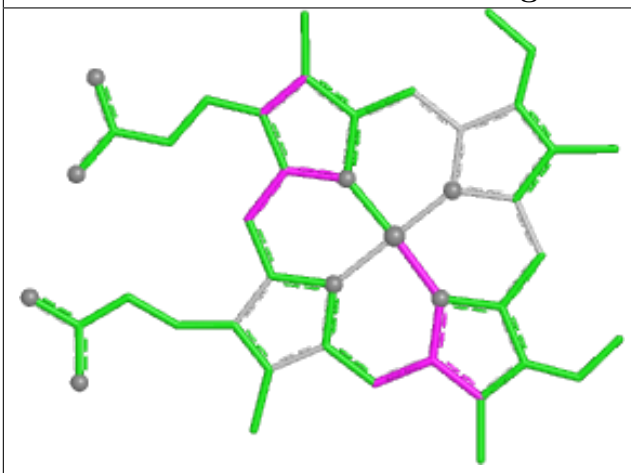


Torsions

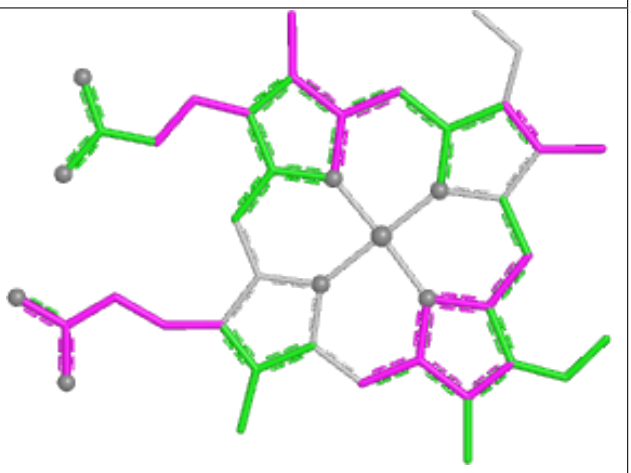


Rings

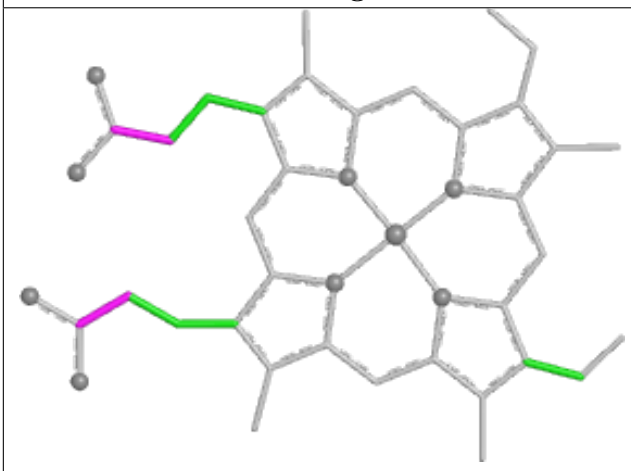
Ligand HEM F 805



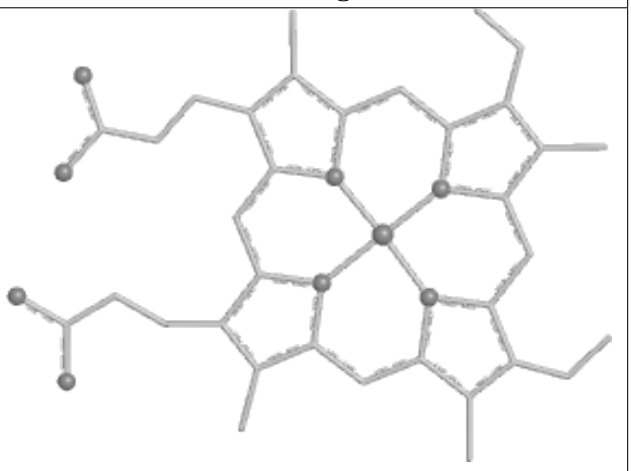
Bond lengths



Bond angles

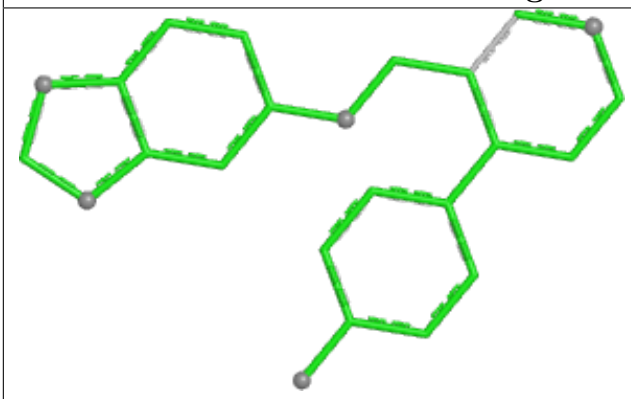


Torsions

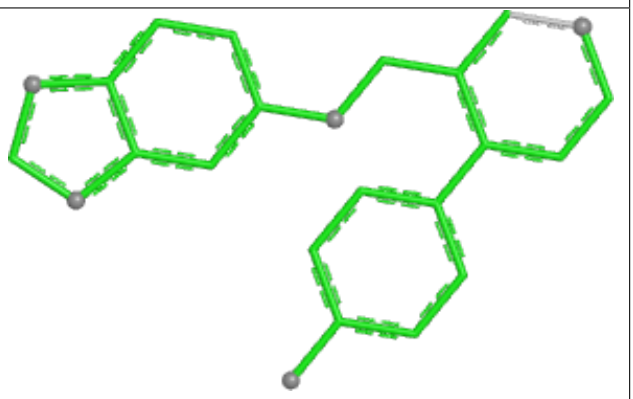


Rings

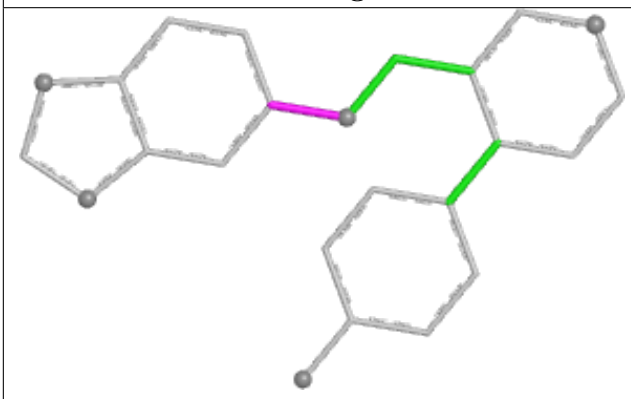
Ligand 8PR H 807



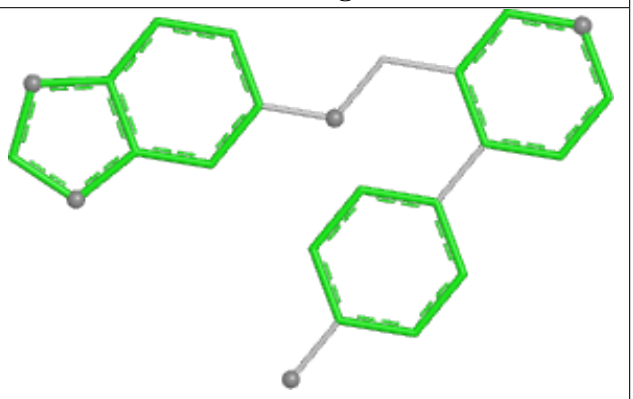
Bond lengths



Bond angles

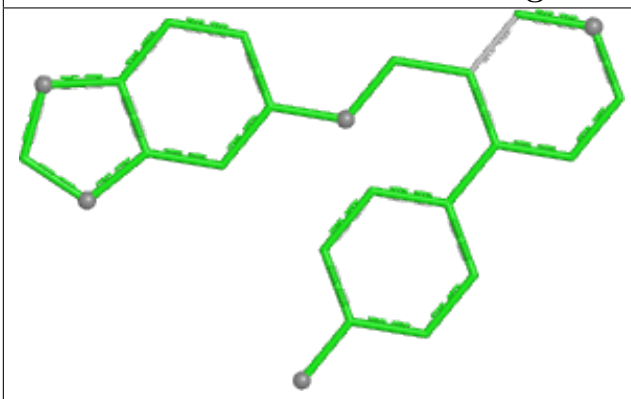


Torsions



Rings

Ligand 8PR A 807



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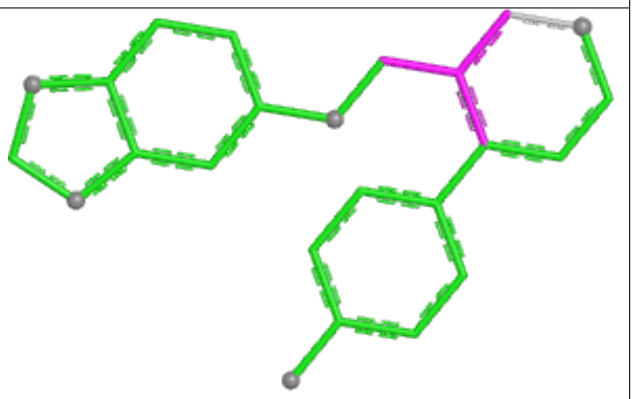

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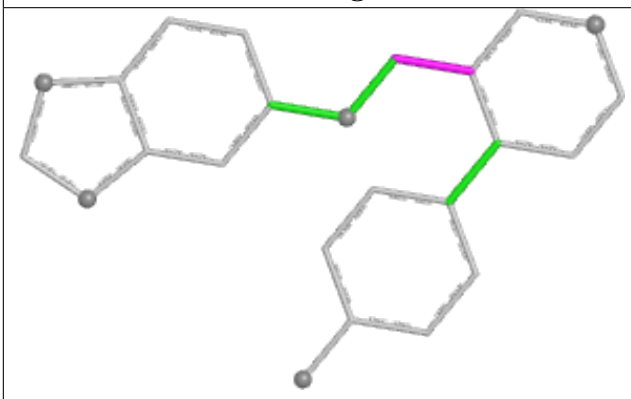

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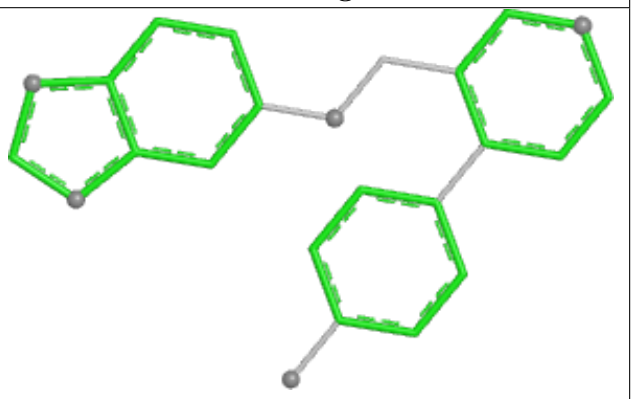
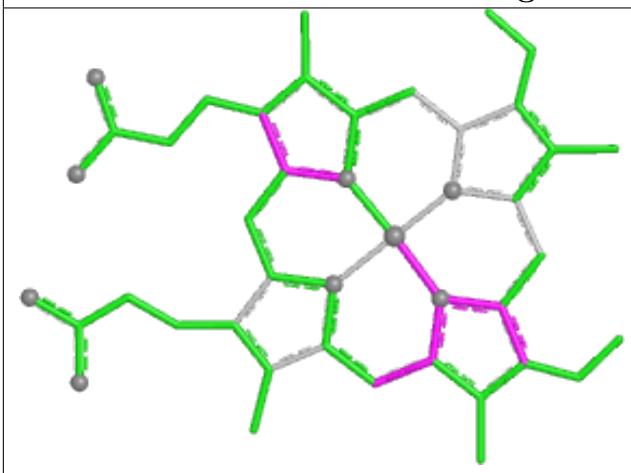


Rings

Ligand HEM H 805



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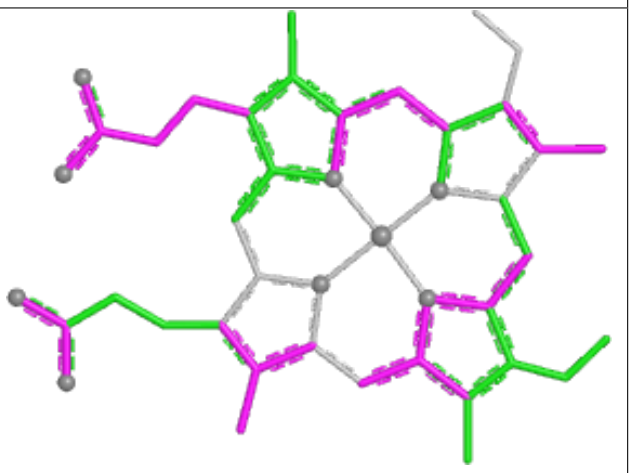

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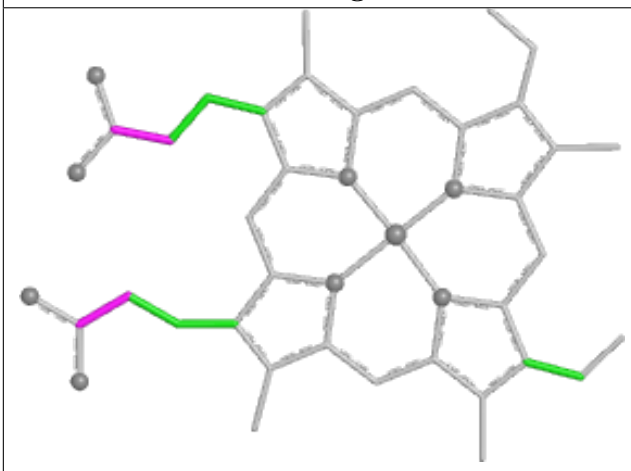

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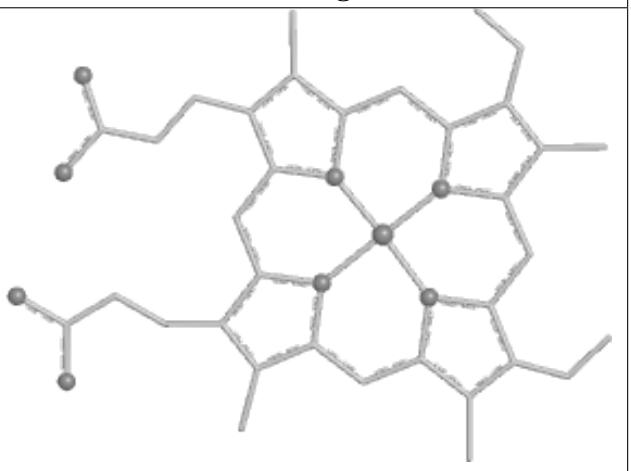
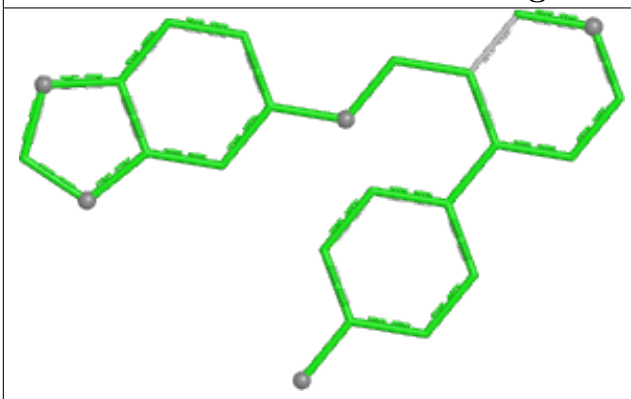


Rings

Ligand 8PR F 807



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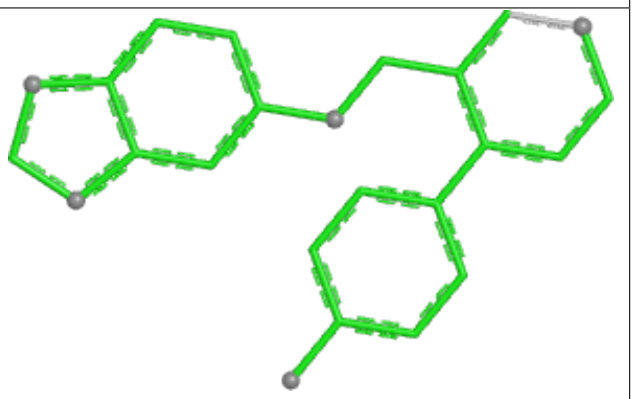

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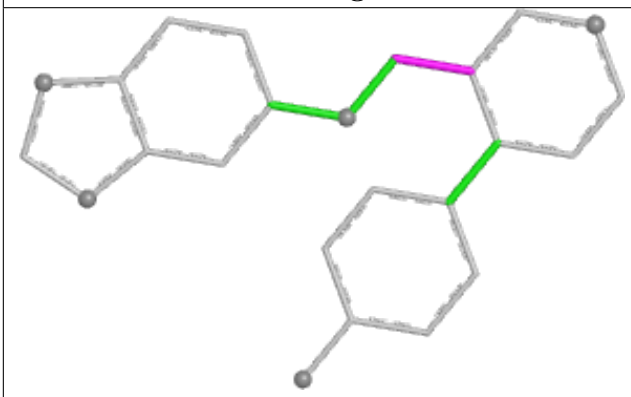

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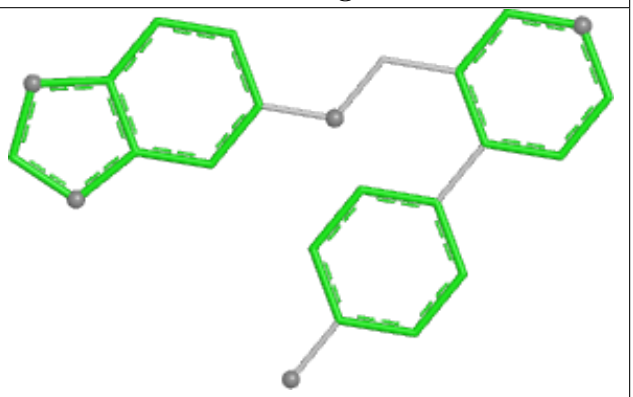
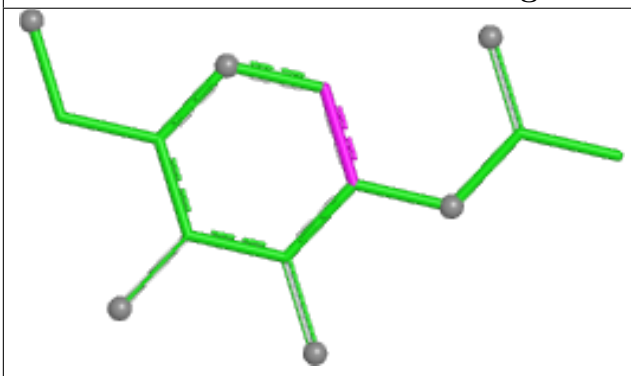


Rings

Ligand NAG C 804



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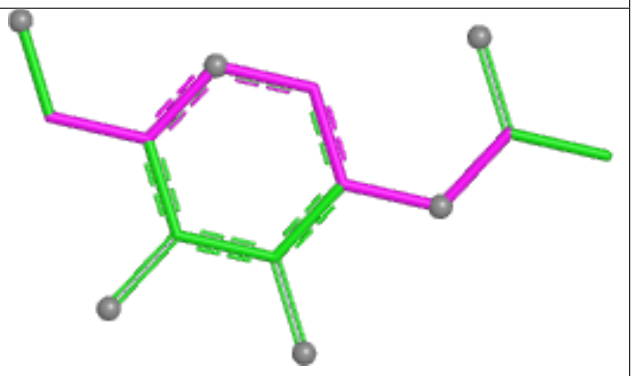

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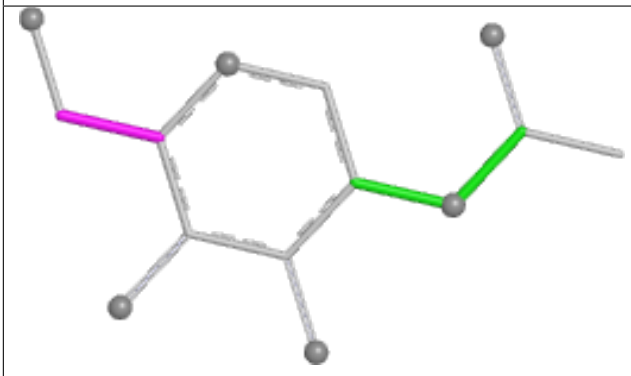
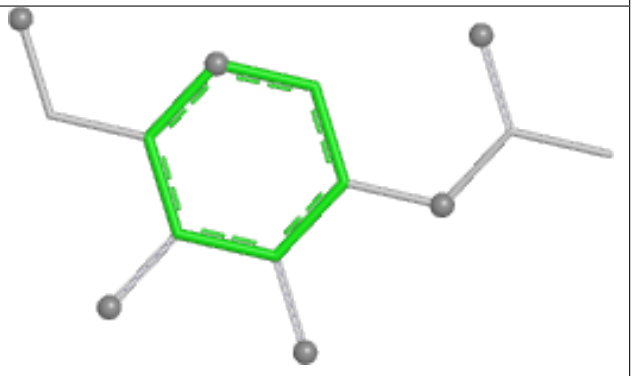
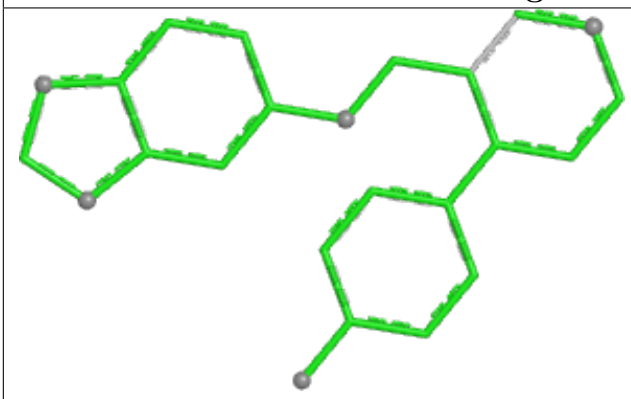


Torsions

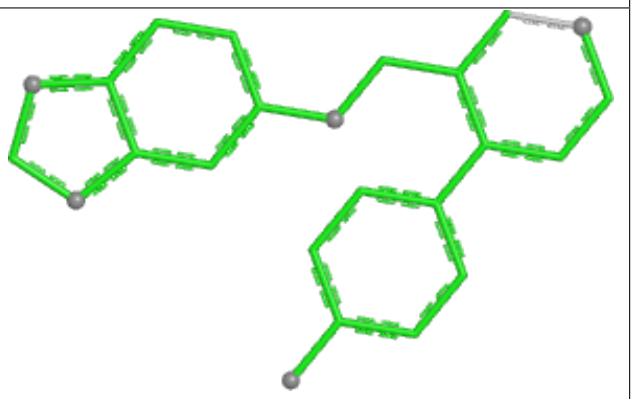


Rings

Ligand 8PR D 807



Bond lengths



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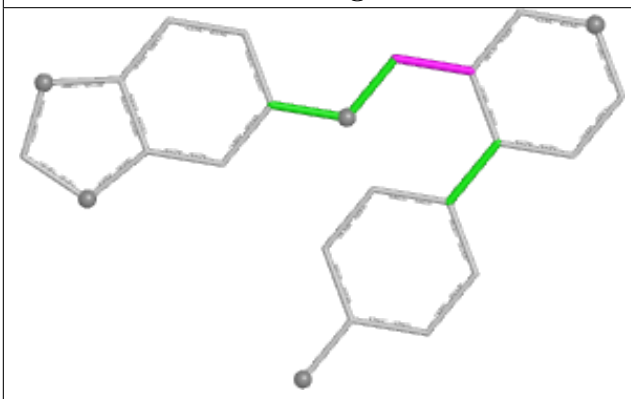

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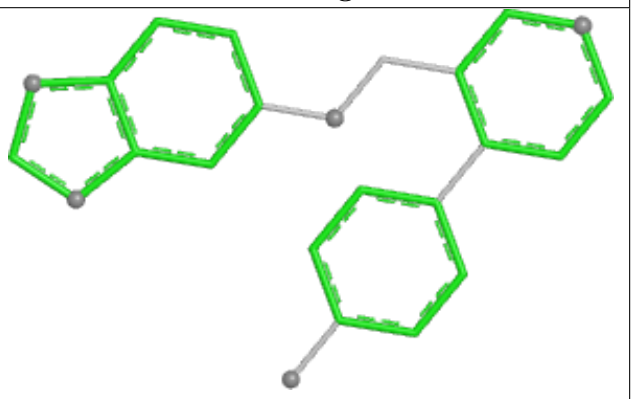
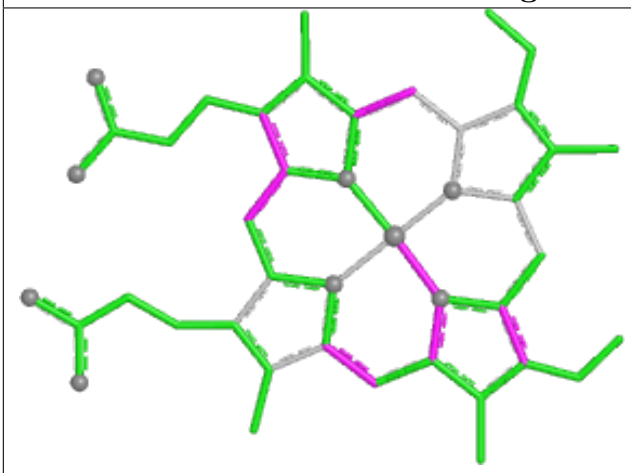


Rings

Ligand HEM E 805



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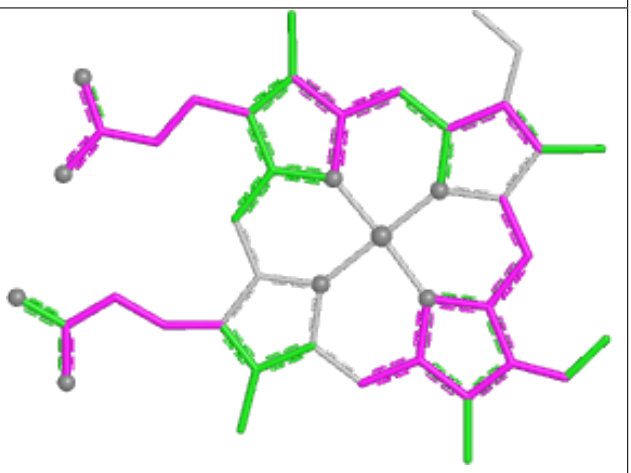

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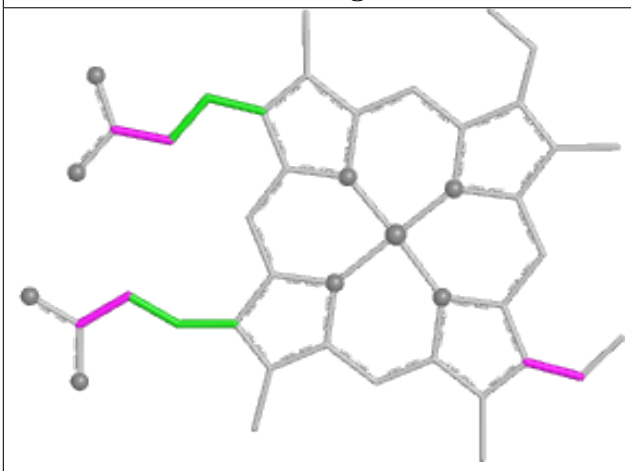

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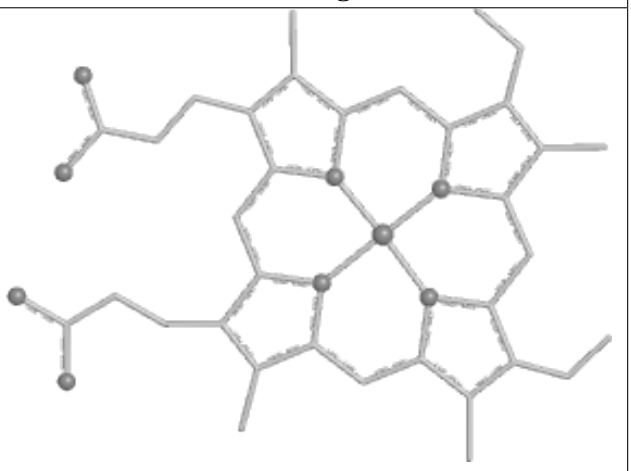
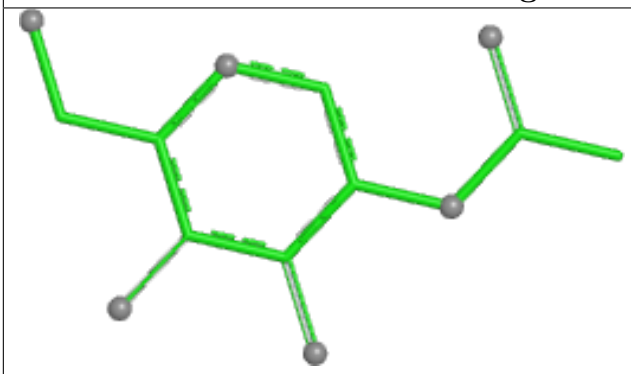


Rings

Ligand NAG D 804



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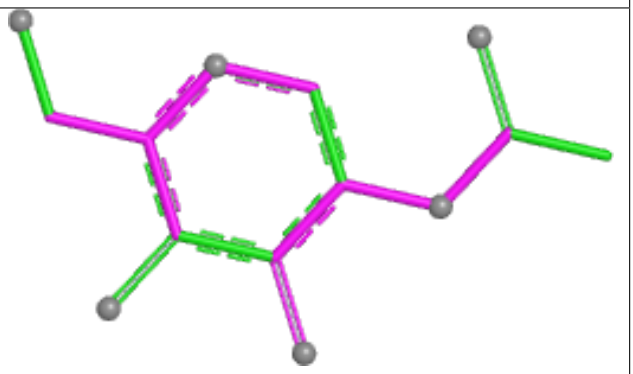

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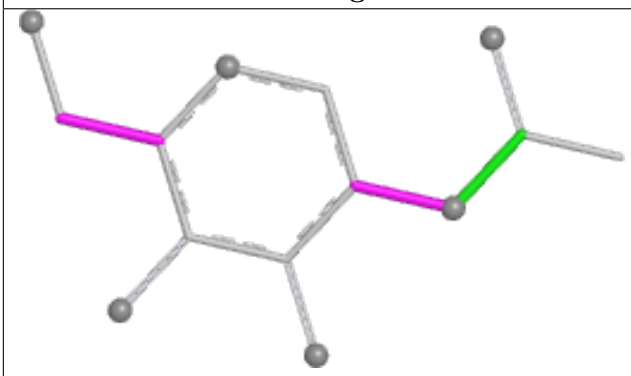

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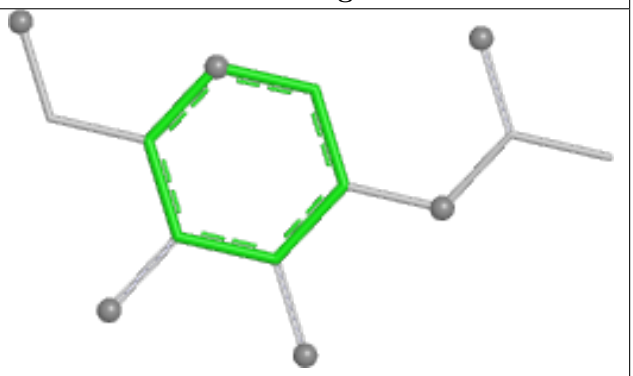
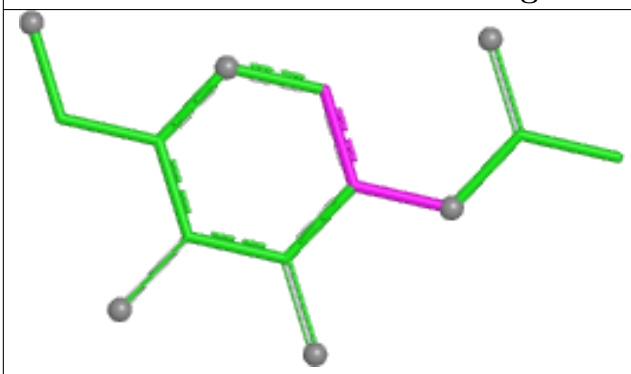


Rings

Ligand NAG B 805



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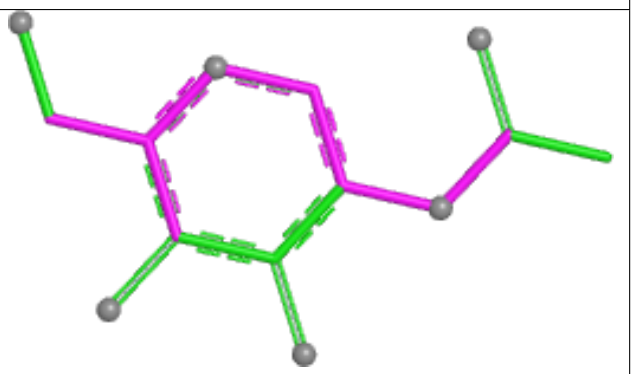

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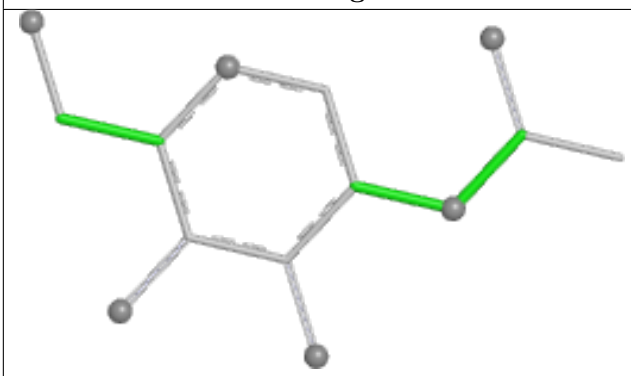

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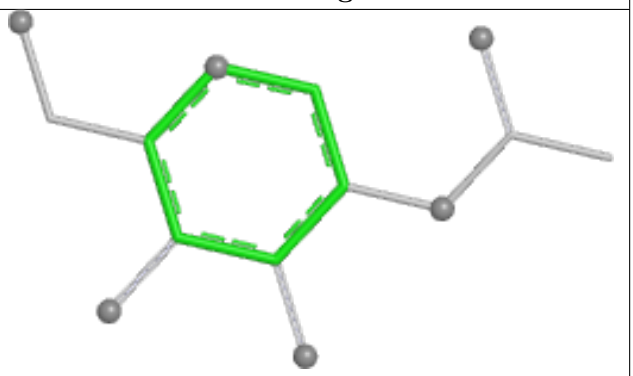
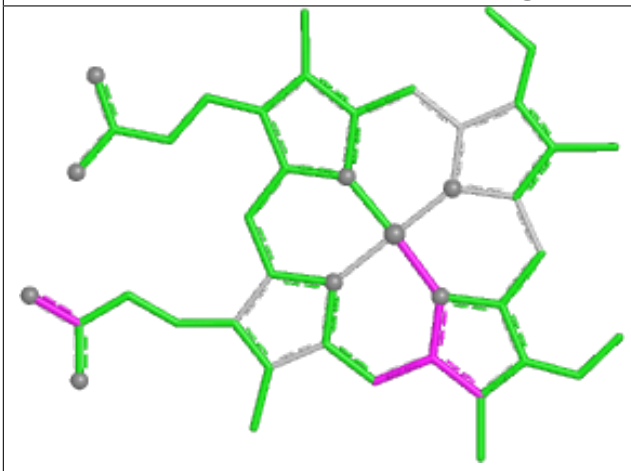


Rings

Ligand HEM C 806



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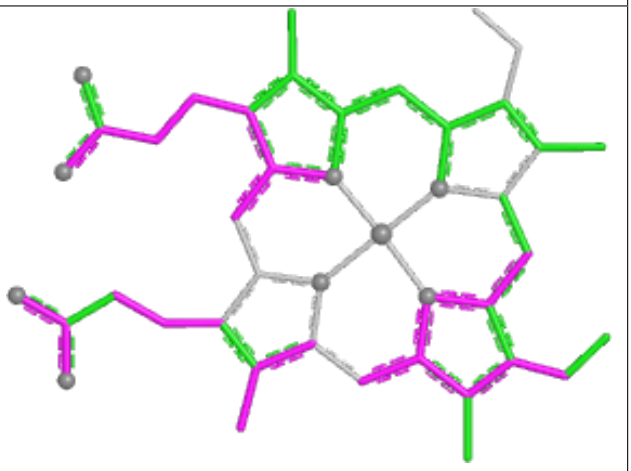

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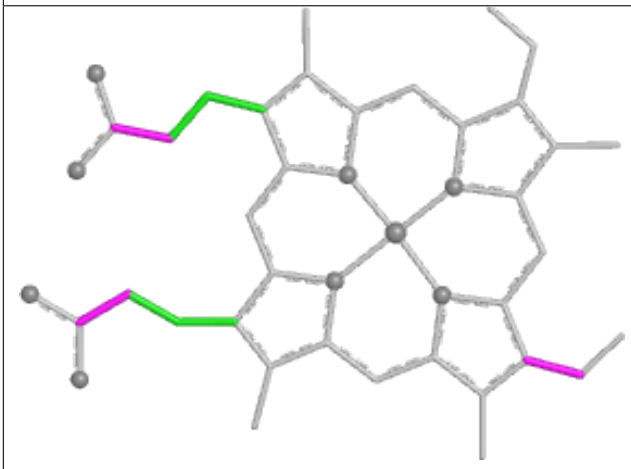

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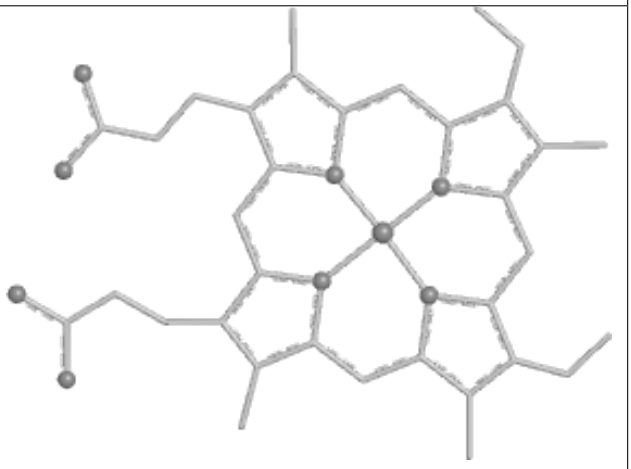
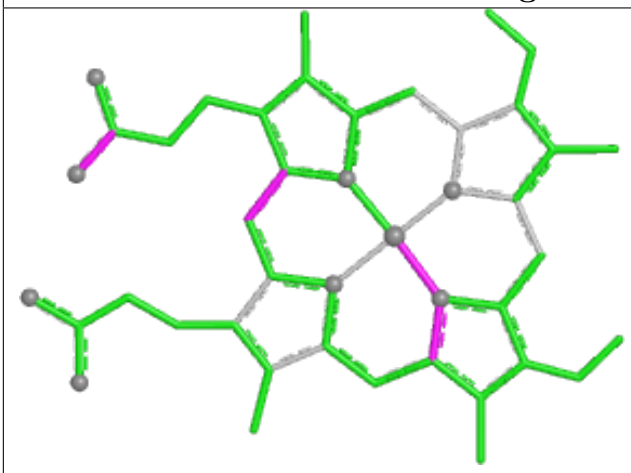


Rings

Ligand HEM B 807



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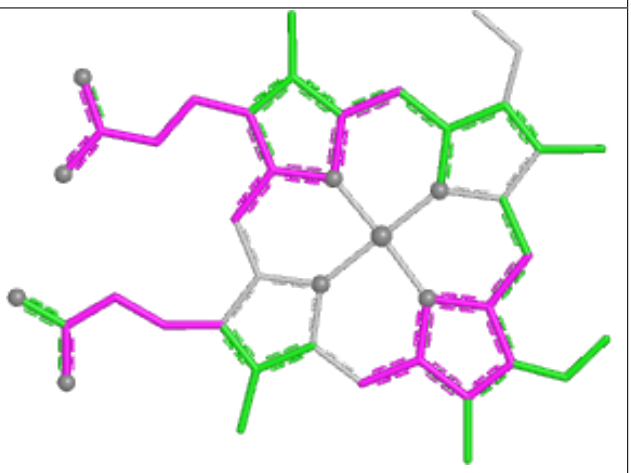
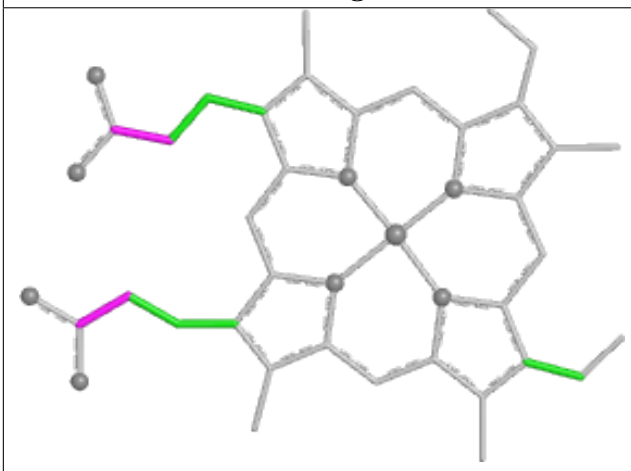


Bond angles



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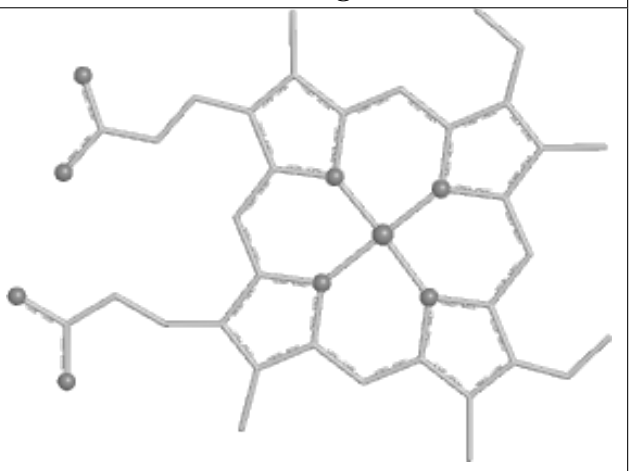
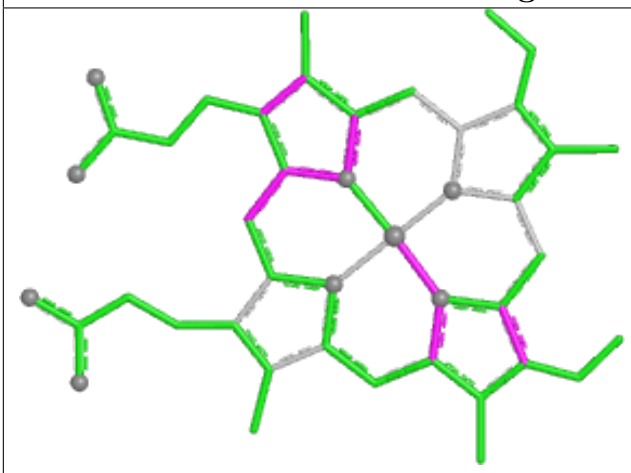


Rings

Ligand HEM A 805



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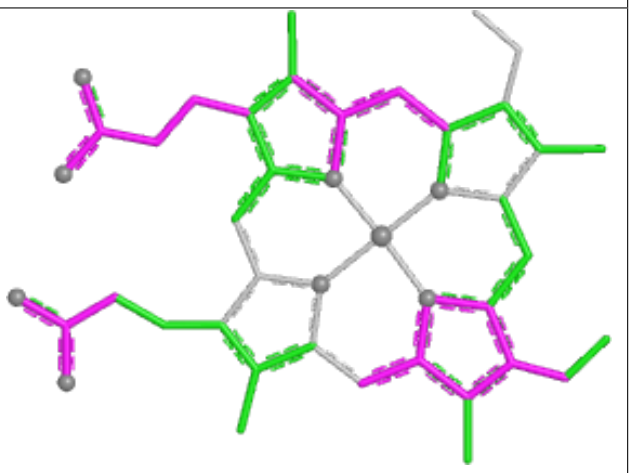

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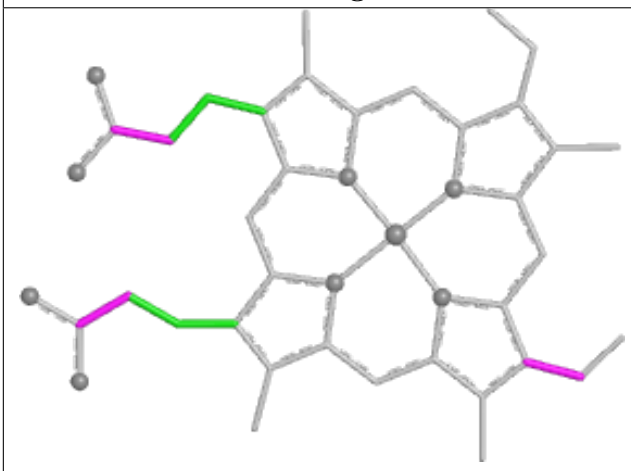

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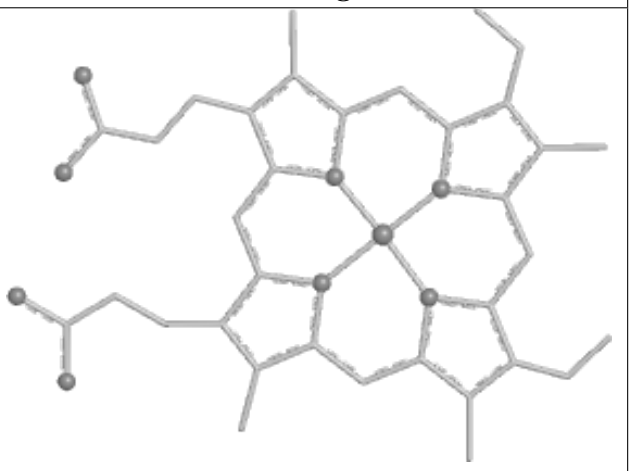
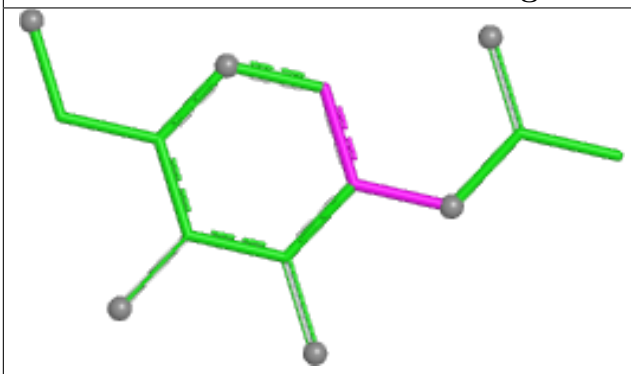
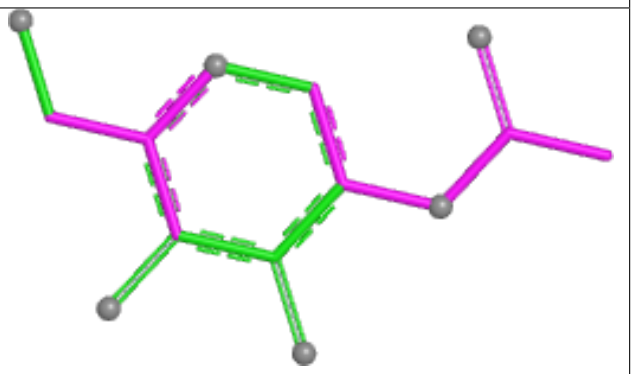
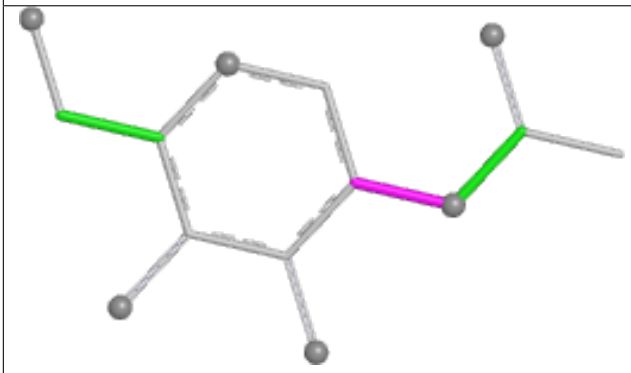
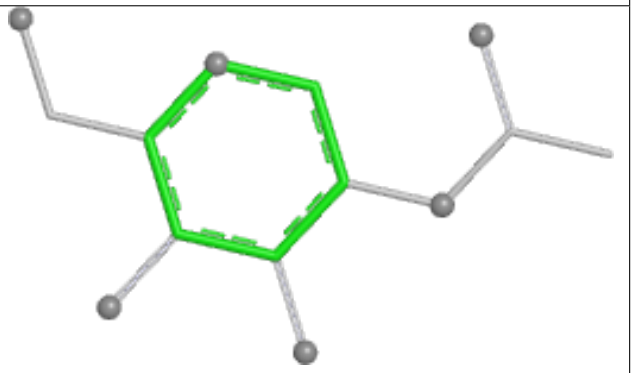


Rings

Ligand NAG B 806	
	
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	572/579 (98%)	-0.18	11 (1%)	66	62	33, 52, 83, 128	0
1	B	569/579 (98%)	-0.11	15 (2%)	56	50	34, 54, 85, 118	0
1	C	569/579 (98%)	-0.05	18 (3%)	47	40	36, 59, 91, 115	0
1	D	570/579 (98%)	-0.14	13 (2%)	60	54	36, 54, 84, 117	0
1	E	571/579 (98%)	-0.04	15 (2%)	56	50	37, 59, 93, 138	0
1	F	570/579 (98%)	-0.18	10 (1%)	68	64	38, 55, 86, 115	0
1	G	568/579 (98%)	-0.12	8 (1%)	75	71	34, 53, 84, 120	0
1	H	570/579 (98%)	-0.20	8 (1%)	75	71	35, 55, 85, 119	0
All	All	4559/4632 (98%)	-0.13	98 (2%)	63	58	33, 55, 87, 138	0

The worst 5 of 98 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	271	ALA	13.7
1	D	744	ALA	6.2
1	F	744	ALA	5.6
1	E	270	ALA	4.7
1	B	744	ALA	4.1

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

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
1	CSO	E	316	7/8	0.95	0.12	38,43,56,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSO	F	316	7/8	0.95	0.12	45,49,53,55	0
1	CSO	A	316	7/8	0.96	0.11	38,40,46,47	0
1	CSO	C	316	7/8	0.96	0.17	50,51,59,65	0
1	CSO	H	316	7/8	0.96	0.11	41,49,53,55	0
1	CSO	G	316	7/8	0.97	0.11	33,39,49,60	0
1	CSO	D	316	7/8	0.97	0.11	41,48,58,64	0
1	CSO	B	316	7/8	0.98	0.13	48,51,55,60	0

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
2	BMA	b	3	11/12	0.43	0.38	120,145,165,168	0
2	BMA	Y	3	11/12	0.64	0.34	101,144,163,169	0
8	BMA	X	3	11/12	0.67	0.27	111,137,163,164	0
2	BMA	e	3	11/12	0.69	0.35	92,132,143,150	0
5	NAG	d	2	14/15	0.70	0.65	85,106,116,118	14
5	NAG	d	1	14/15	0.70	0.54	86,113,123,125	14
4	MAN	K	6	11/12	0.71	0.22	84,108,121,125	0
8	MAN	X	4	11/12	0.71	0.49	110,139,148,169	0
3	NAG	c	5	14/15	0.75	0.35	60,70,75,79	14
2	NAG	b	2	14/15	0.75	0.38	77,119,139,159	0
2	NAG	Y	2	14/15	0.76	0.30	84,118,128,145	0
2	BMA	J	3	11/12	0.77	0.27	71,104,119,122	0
7	MAN	P	4	11/12	0.77	0.36	135,159,163,177	0
5	NAG	f	2	14/15	0.79	0.31	85,114,127,127	0
2	NAG	e	2	14/15	0.80	0.32	73,122,143,152	0
2	BMA	I	3	11/12	0.80	0.49	30,30,30,30	0
5	NAG	V	2	14/15	0.80	0.43	86,124,133,146	0
3	NAG	L	5	14/15	0.81	0.24	78,97,107,115	0
8	MAN	U	4	11/12	0.81	0.25	60,96,134,154	0
9	MAN	a	6	11/12	0.81	0.31	96,123,141,155	0
7	BMA	P	3	11/12	0.82	0.32	113,140,151,163	0
4	MAN	R	5	11/12	0.82	0.19	96,111,127,127	0
4	MAN	R	6	11/12	0.83	0.25	101,117,135,140	0
4	BMA	R	3	11/12	0.84	0.21	95,108,123,148	0
6	MAN	N	4	11/12	0.85	0.20	78,87,99,100	0
4	NAG	R	2	14/15	0.85	0.23	79,97,125,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	g	5	14/15	0.85	0.29	66,83,90,91	14
8	NAG	U	2	14/15	0.85	0.26	74,101,109,119	0
5	NAG	S	2	14/15	0.86	0.31	98,111,119,131	0
8	BMA	U	3	11/12	0.86	0.11	87,97,107,112	0
7	NAG	P	2	14/15	0.86	0.38	102,113,126,145	0
8	NAG	X	1	14/15	0.87	0.22	73,91,104,121	0
5	NAG	f	1	14/15	0.87	0.30	78,94,107,118	0
2	NAG	e	1	14/15	0.88	0.21	71,90,104,125	0
6	MAN	Q	5	11/12	0.88	0.20	52,64,76,81	0
4	MAN	R	4	11/12	0.88	0.16	75,93,98,122	0
9	MAN	a	4	11/12	0.88	0.14	86,91,99,100	0
5	NAG	M	2	14/15	0.88	0.40	78,114,126,148	0
7	NAG	P	1	14/15	0.89	0.27	90,95,105,112	0
3	MAN	L	6	11/12	0.89	0.20	76,90,97,109	0
2	NAG	I	2	14/15	0.90	0.46	30,30,30,30	0
5	NAG	O	2	14/15	0.90	0.31	84,115,128,129	0
6	BMA	Z	3	11/12	0.90	0.12	60,65,78,88	0
9	NAG	a	2	14/15	0.90	0.20	72,96,104,104	0
2	NAG	J	2	14/15	0.90	0.27	84,99,111,112	0
4	BMA	K	3	11/12	0.90	0.14	74,91,100,116	0
4	MAN	K	5	11/12	0.91	0.19	94,105,110,117	0
2	NAG	I	1	14/15	0.91	0.40	30,30,30,30	0
6	MAN	T	4	11/12	0.91	0.24	74,87,94,96	0
2	NAG	Y	1	14/15	0.91	0.22	74,85,95,113	0
8	NAG	X	2	14/15	0.91	0.26	80,118,142,155	0
4	MAN	K	4	11/12	0.92	0.13	66,82,89,89	0
6	MAN	N	5	11/12	0.92	0.12	30,30,30,30	0
5	NAG	S	1	14/15	0.92	0.21	69,76,88,104	0
5	NAG	V	1	14/15	0.92	0.21	76,98,104,106	0
6	MAN	W	4	11/12	0.92	0.18	83,98,104,120	0
6	FUC	Z	6	10/11	0.93	0.27	30,30,30,30	0
5	NAG	M	1	14/15	0.93	0.17	56,71,78,101	0
3	MAN	c	6	11/12	0.93	0.18	90,94,100,101	0
9	BMA	a	3	11/12	0.93	0.12	88,93,108,109	0
6	FUC	Q	6	10/11	0.93	0.16	54,62,65,66	0
6	MAN	Z	4	11/12	0.93	0.25	81,87,91,95	0
6	MAN	Q	4	11/12	0.94	0.19	71,88,93,95	0
2	NAG	b	1	14/15	0.94	0.26	71,85,92,102	0
2	NAG	J	1	14/15	0.94	0.17	62,67,74,86	0
5	NAG	O	1	14/15	0.94	0.21	78,92,108,108	0
6	MAN	T	5	11/12	0.94	0.14	55,60,66,66	0
6	NAG	W	1	14/15	0.94	0.15	41,52,65,65	0

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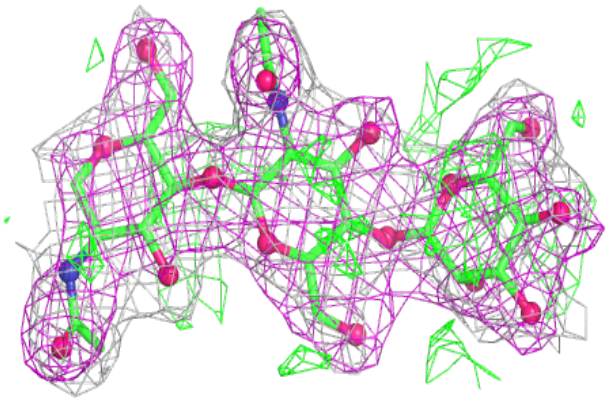
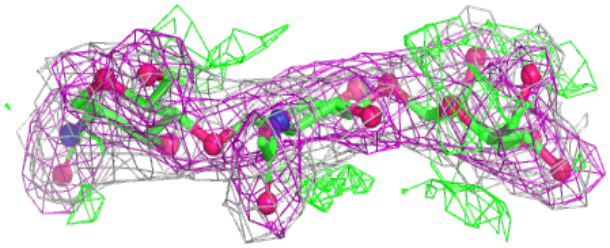
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	K	2	14/15	0.94	0.17	61,87,100,104	0
6	MAN	W	5	11/12	0.94	0.13	53,60,65,66	0
6	NAG	Z	1	14/15	0.94	0.12	45,52,64,70	0
6	NAG	Z	2	14/15	0.94	0.14	38,50,61,65	0
3	BMA	g	3	11/12	0.94	0.14	49,55,65,71	0
6	BMA	N	3	11/12	0.94	0.11	55,59,66,76	0
3	MAN	c	4	11/12	0.94	0.12	56,59,62,69	0
3	MAN	g	6	11/12	0.94	0.17	70,84,87,88	0
6	NAG	Q	1	14/15	0.95	0.13	45,52,58,64	0
6	NAG	Q	2	14/15	0.95	0.15	43,54,56,57	0
6	BMA	Q	3	11/12	0.95	0.09	50,55,61,65	0
4	NAG	R	1	14/15	0.95	0.15	59,77,84,89	0
9	NAG	a	1	14/15	0.95	0.16	55,69,80,89	0
3	BMA	L	3	11/12	0.95	0.09	56,60,69,83	0
3	FUC	c	7	10/11	0.95	0.11	56,63,65,66	0
6	BMA	T	3	11/12	0.95	0.09	57,64,69,81	0
9	MAN	a	5	11/12	0.95	0.13	67,74,80,80	0
6	FUC	N	6	10/11	0.95	0.11	61,64,67,72	0
6	MAN	Z	5	11/12	0.96	0.14	61,74,79,89	0
3	NAG	L	1	14/15	0.96	0.12	39,47,57,59	0
6	BMA	W	3	11/12	0.96	0.08	49,56,63,76	0
6	NAG	N	2	14/15	0.96	0.12	42,51,57,60	0
6	NAG	T	1	14/15	0.96	0.11	43,53,56,57	0
6	NAG	T	2	14/15	0.96	0.12	41,53,57,57	0
8	NAG	U	1	14/15	0.96	0.19	63,82,93,94	0
4	NAG	K	1	14/15	0.96	0.12	47,70,78,80	0
3	MAN	g	4	11/12	0.96	0.14	50,60,73,75	0
3	FUC	g	7	10/11	0.96	0.13	54,59,63,82	0
3	NAG	L	2	14/15	0.97	0.11	37,42,48,49	0
3	BMA	c	3	11/12	0.97	0.09	51,56,66,85	0
3	MAN	L	4	11/12	0.97	0.10	58,61,69,71	0
3	NAG	c	1	14/15	0.97	0.15	49,54,66,70	0
3	NAG	g	1	14/15	0.97	0.11	39,43,52,52	0
6	FUC	T	6	10/11	0.97	0.11	46,52,58,61	0
3	FUC	L	7	10/11	0.97	0.10	46,53,57,59	0
6	NAG	W	2	14/15	0.97	0.10	36,39,43,47	0
6	NAG	N	1	14/15	0.97	0.10	46,49,60,65	0
3	NAG	g	2	14/15	0.97	0.11	33,39,44,45	0
3	NAG	c	2	14/15	0.97	0.11	39,44,46,50	0
6	FUC	W	6	10/11	0.97	0.10	57,59,63,63	0

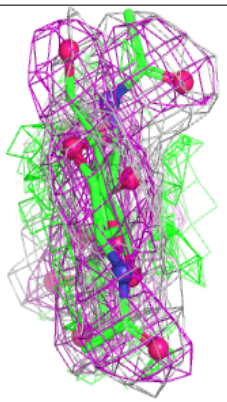
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

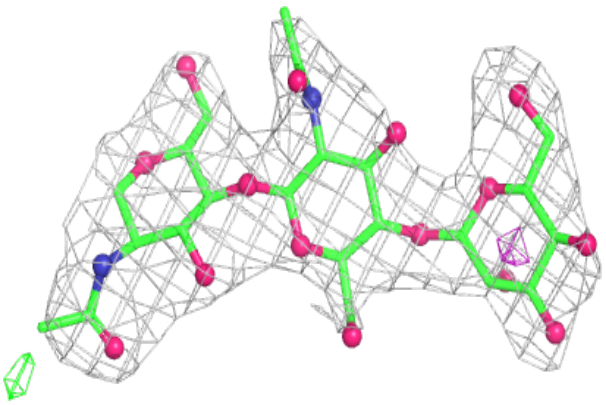


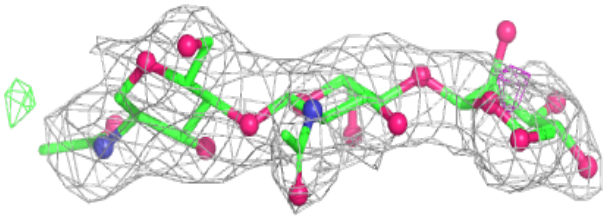


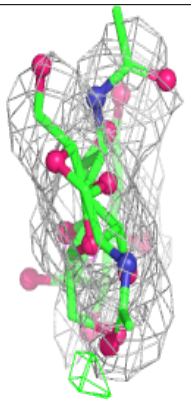


Electron density around Chain J:

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

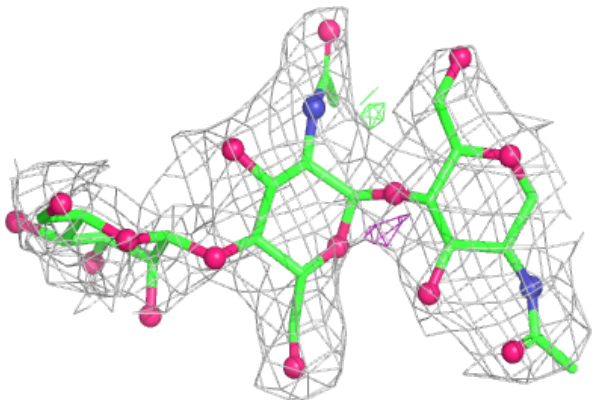


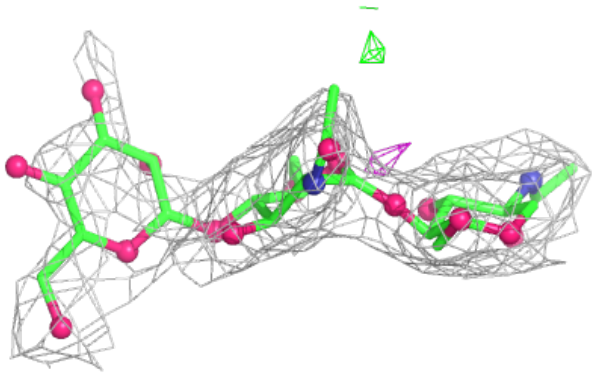


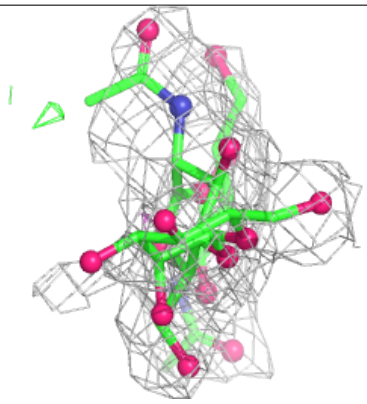


Electron density around Chain Y:

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

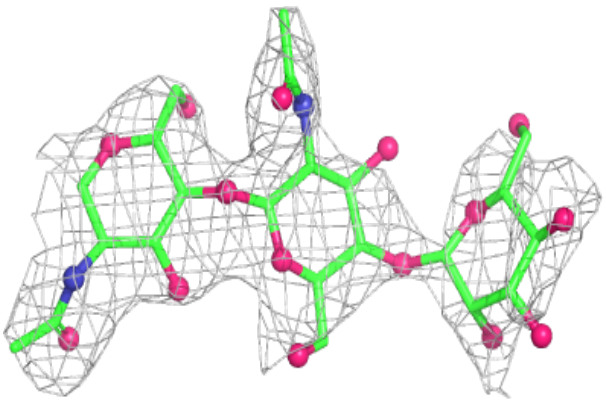


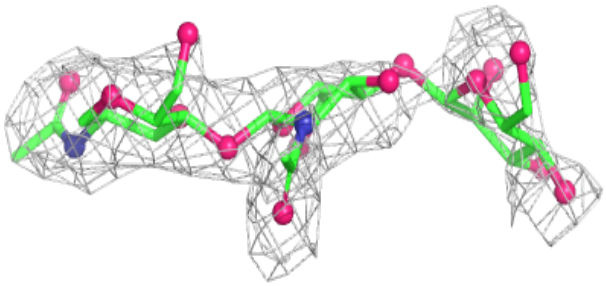


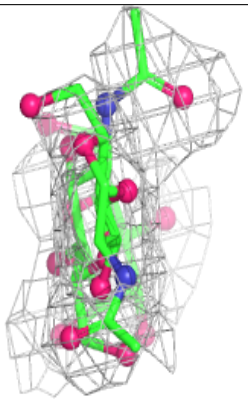


Electron density around Chain b:

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

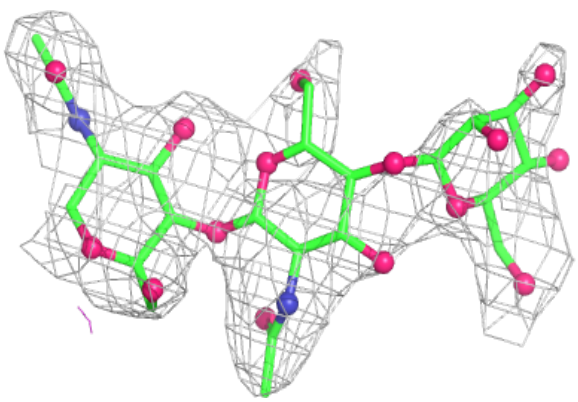


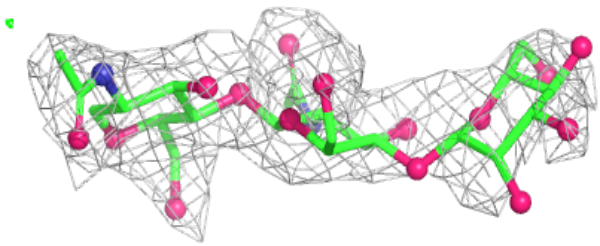


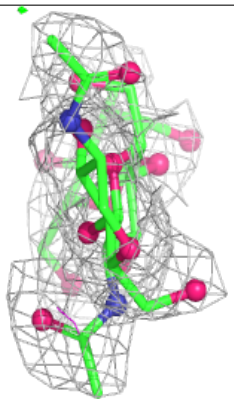


Electron density around Chain e:

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

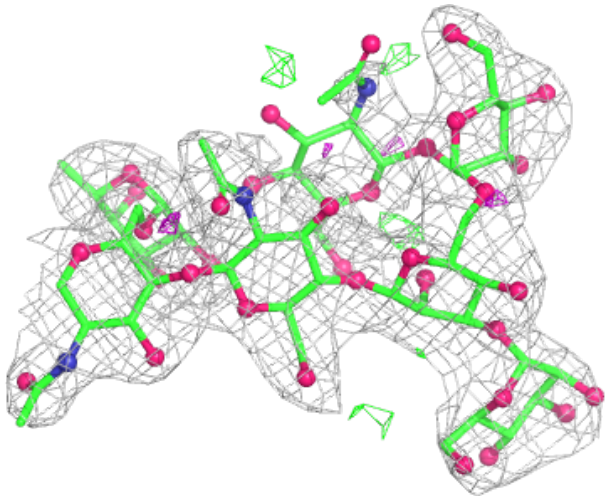


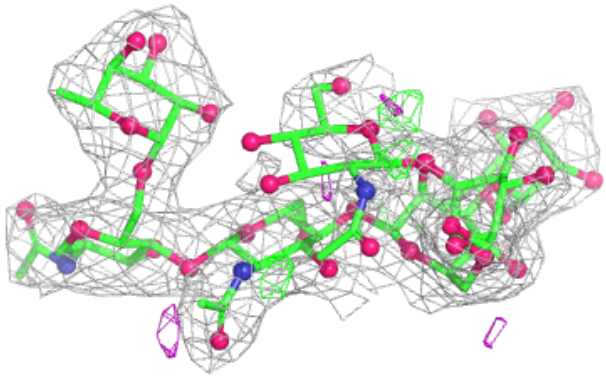


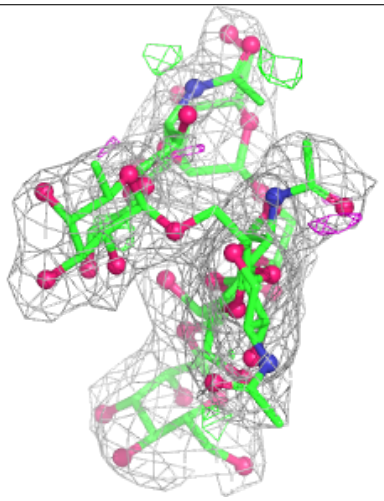


Electron density around Chain c:

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

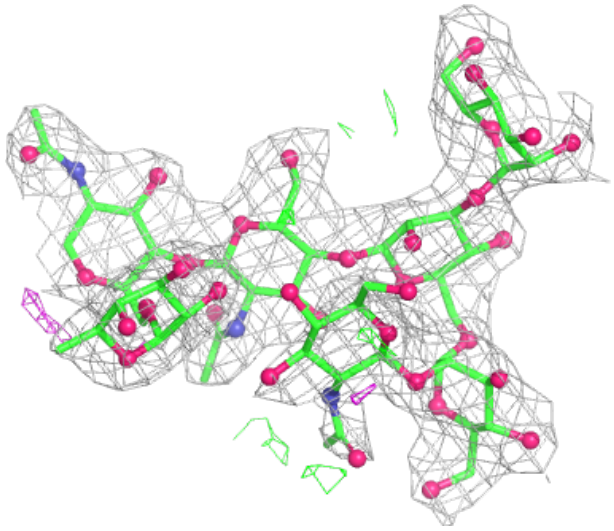


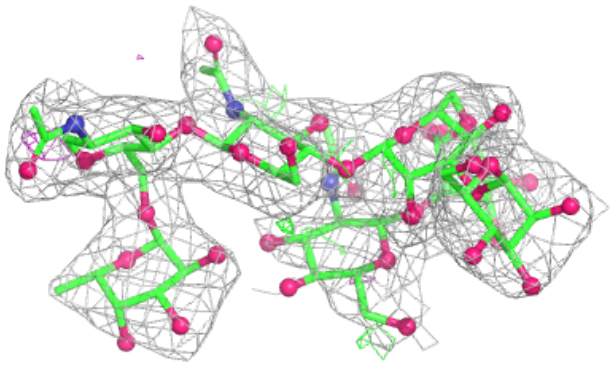


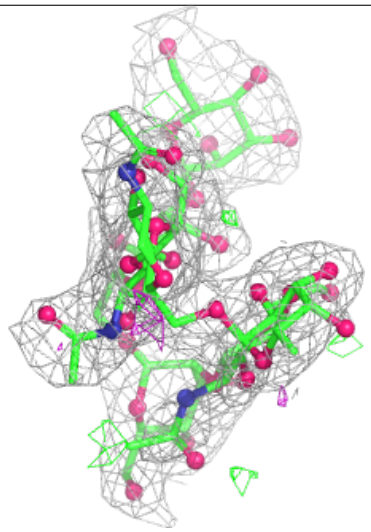


Electron density around Chain g:

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

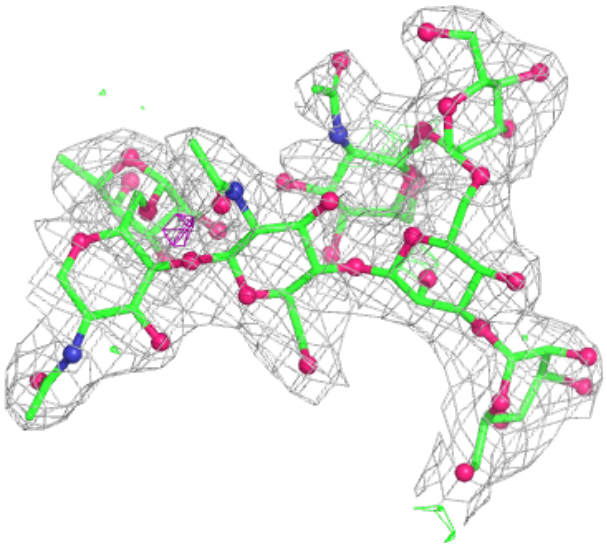


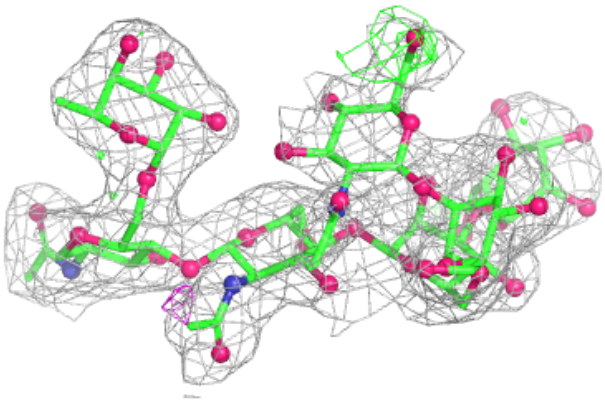


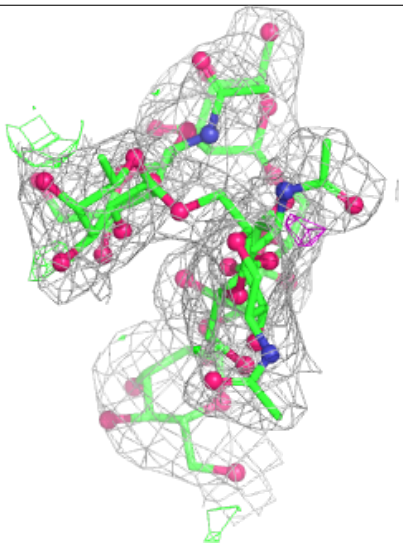


Electron density around Chain L:

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

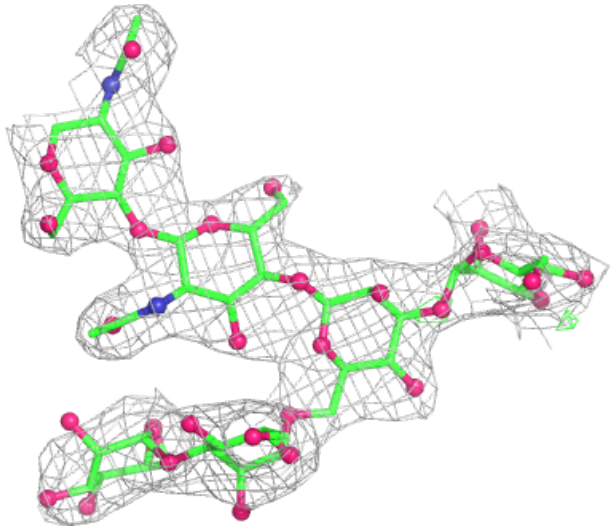


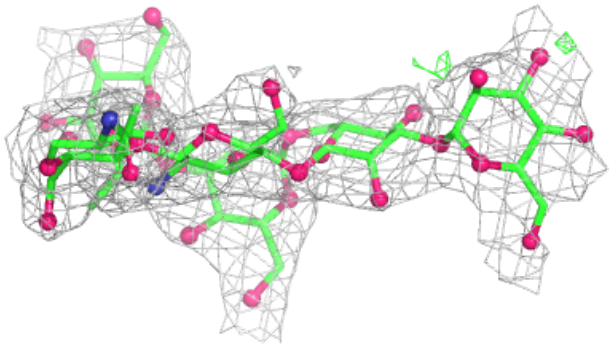


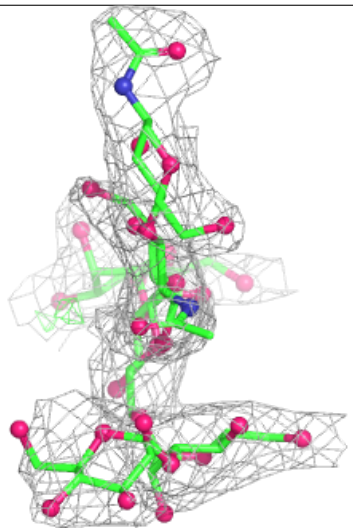


Electron density around Chain K:

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

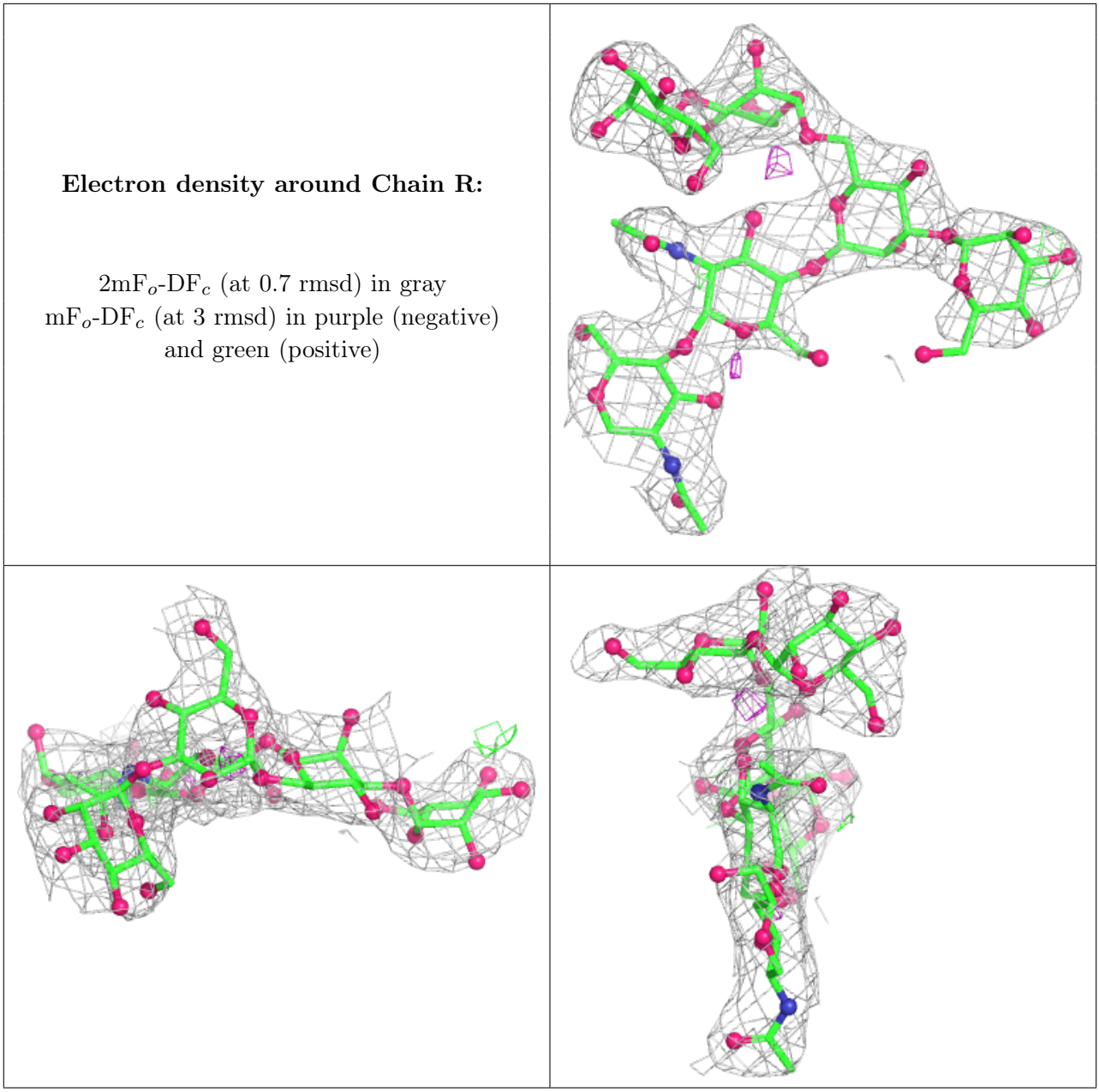






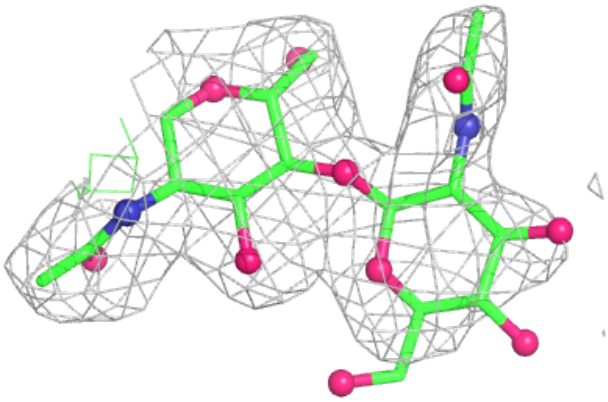
Electron density around Chain R:

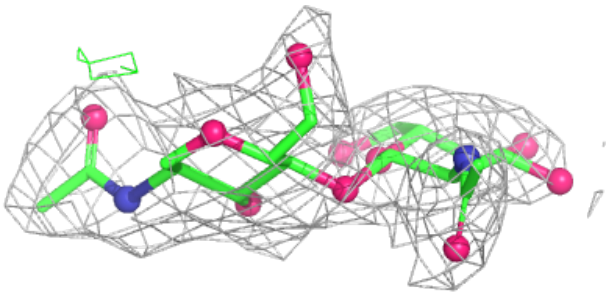
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

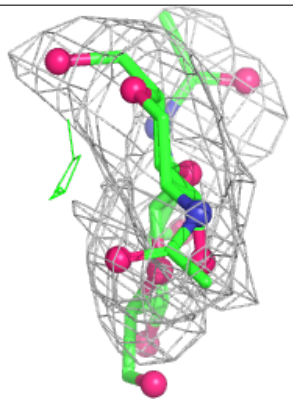


Electron density around Chain M:

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

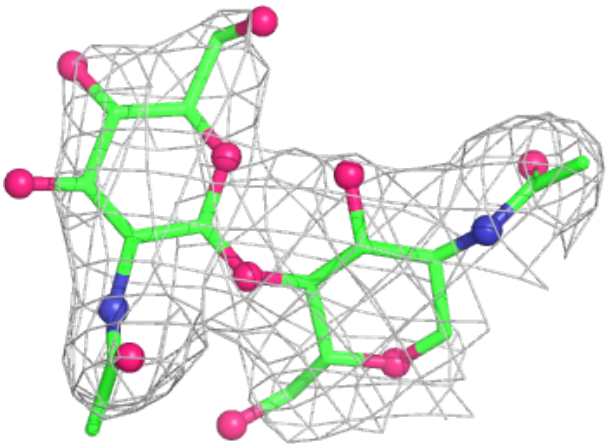


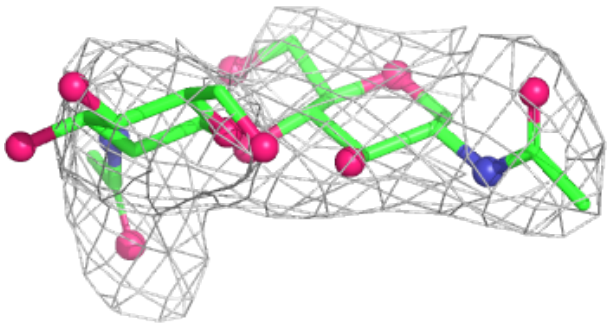


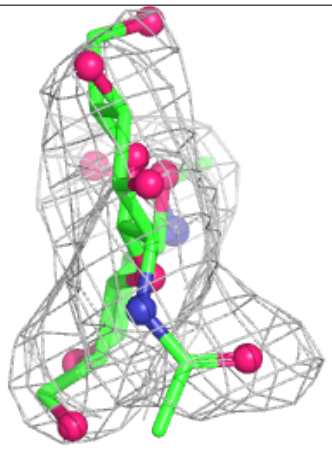


Electron density around Chain O:

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

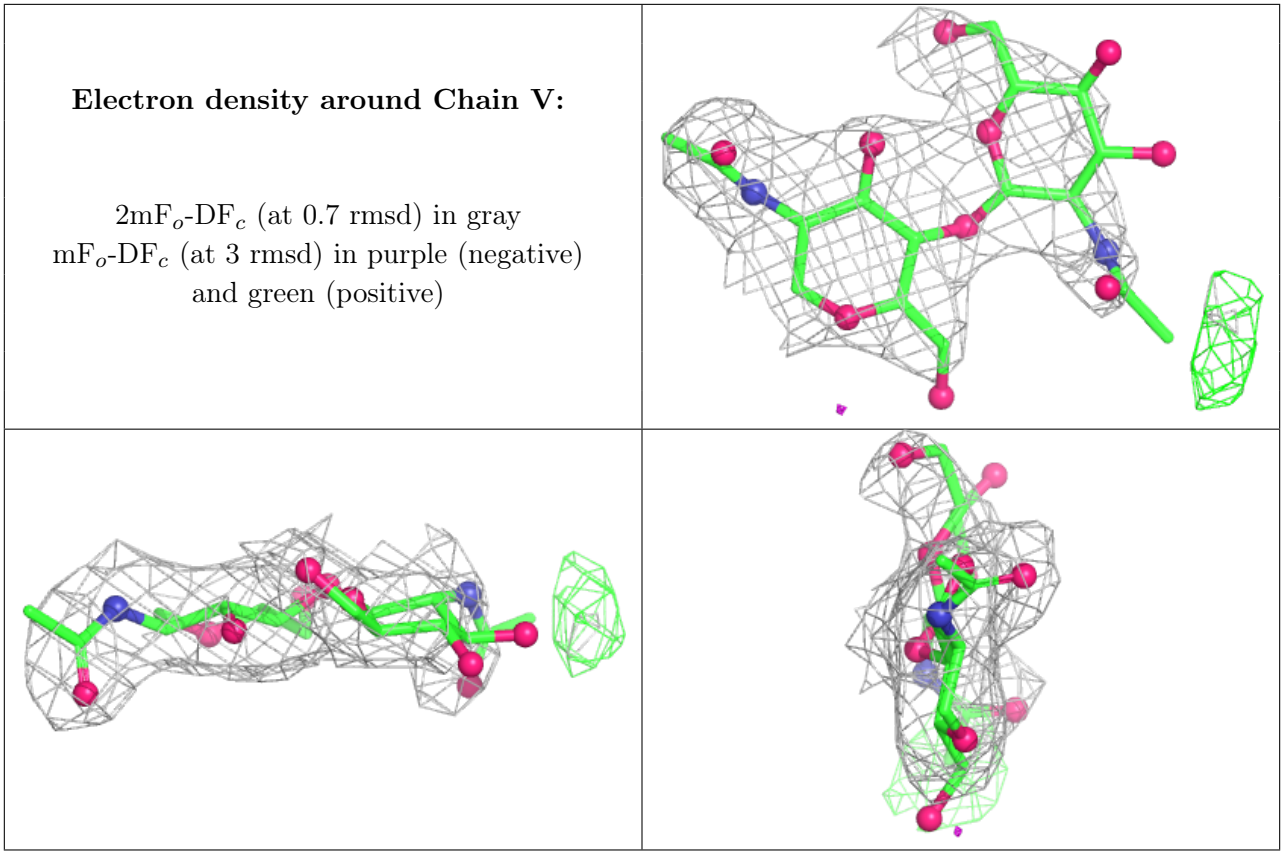






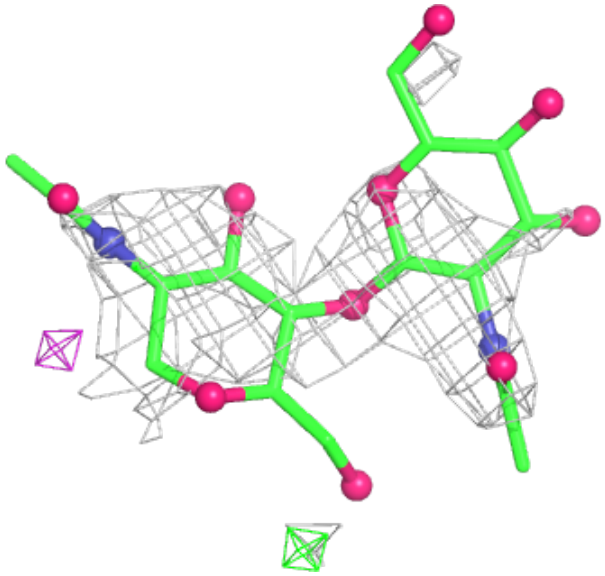
Electron density around Chain V:

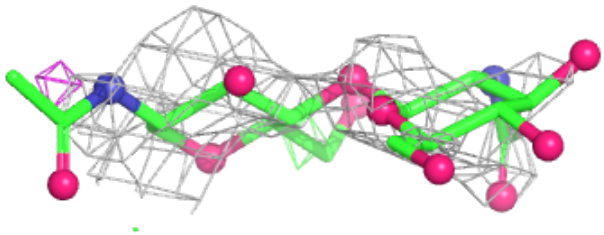
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

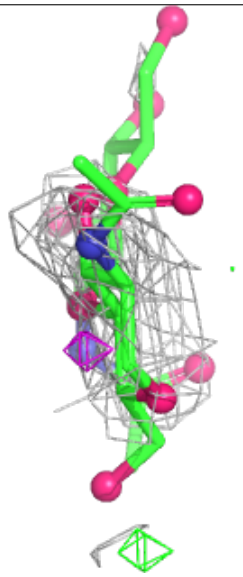


Electron density around Chain d:

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

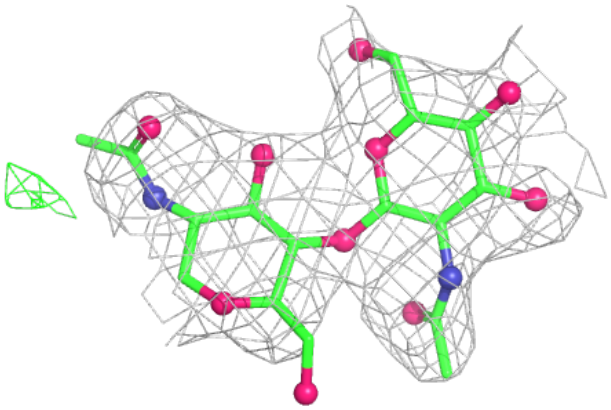


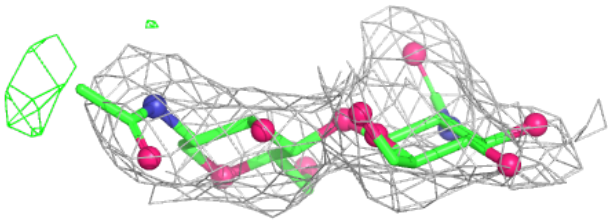


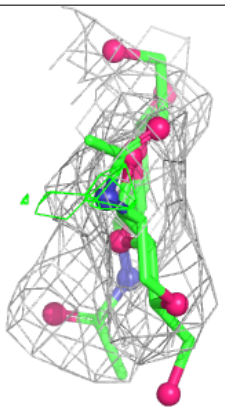


Electron density around Chain f:

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

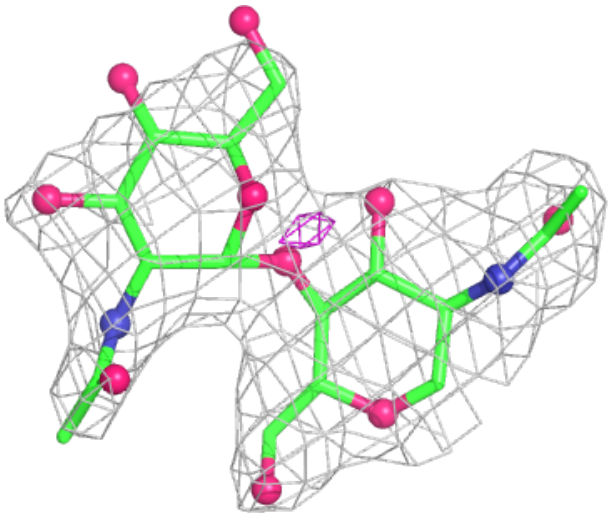


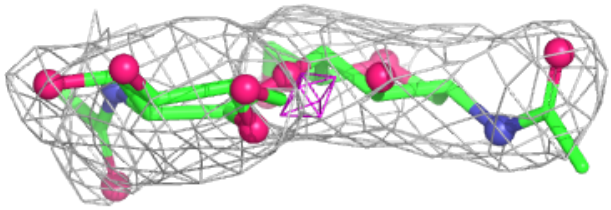


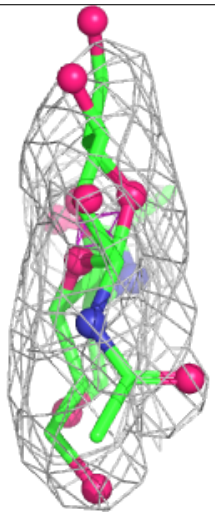


Electron density around Chain S:

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

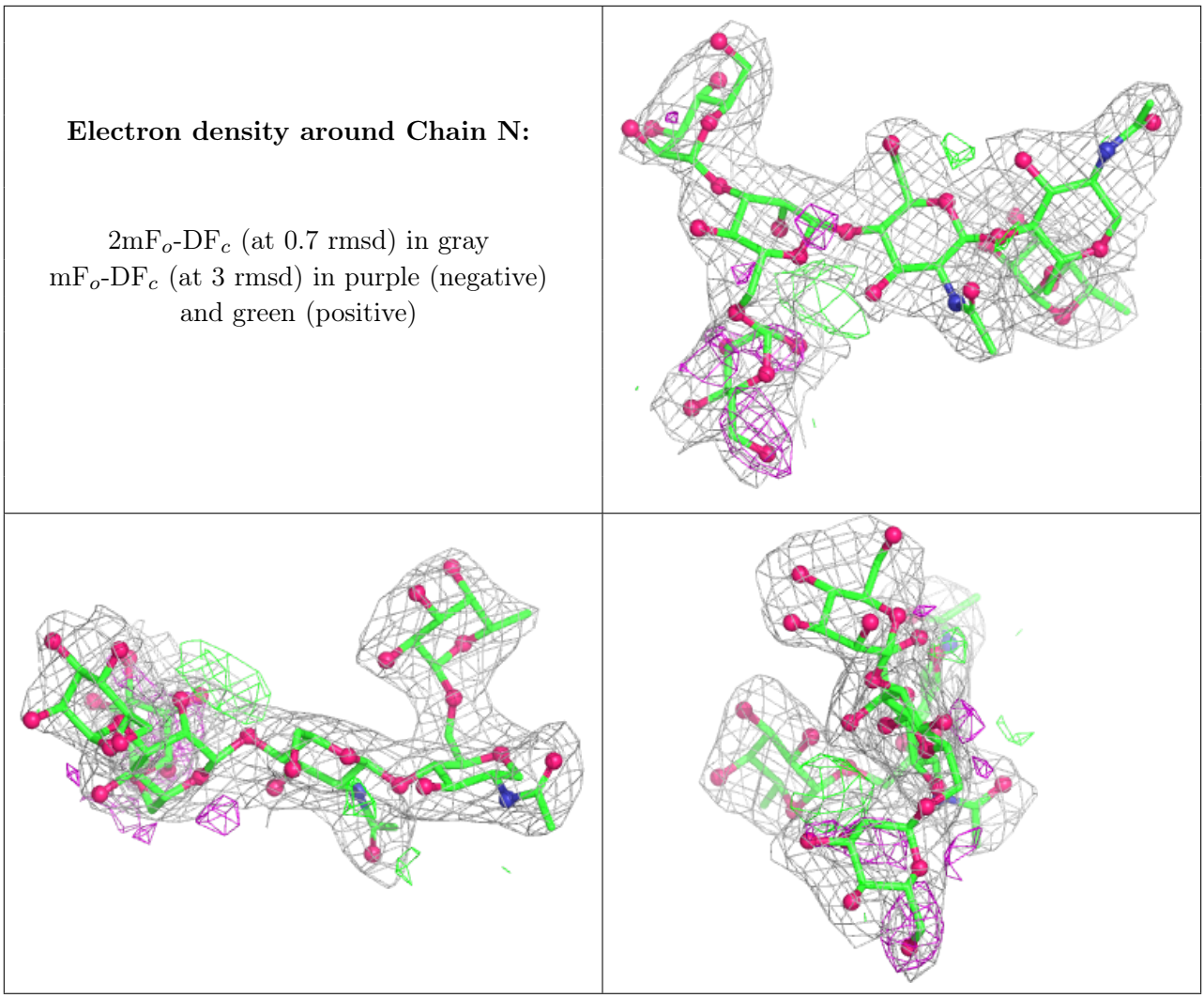






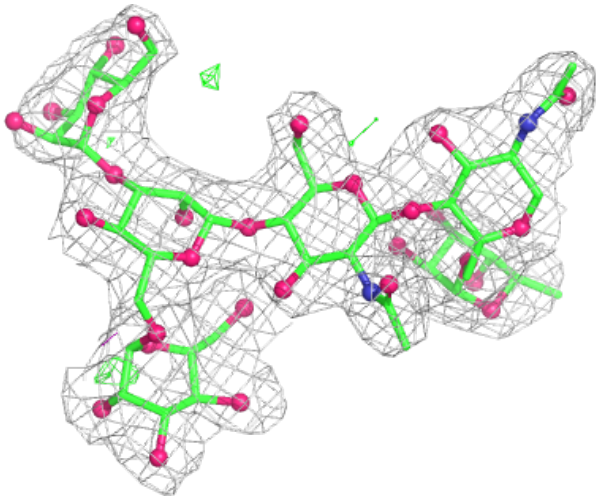
Electron density around Chain N:

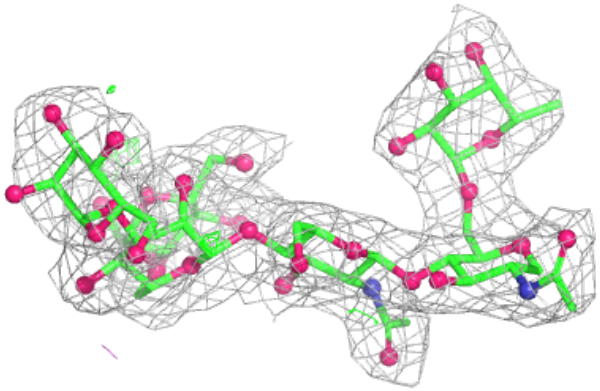
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain Q:

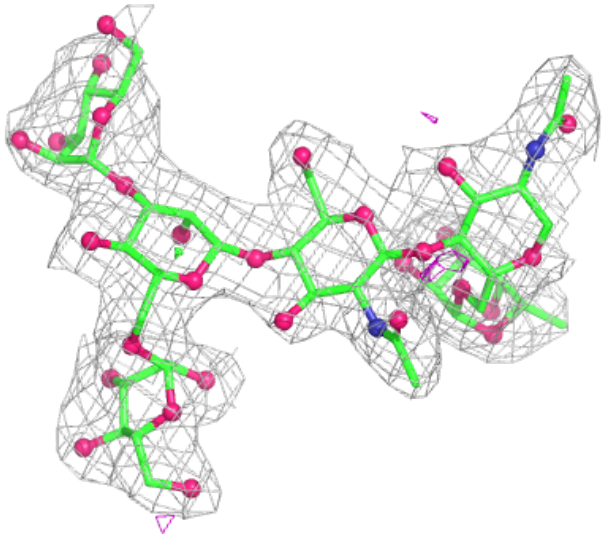
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

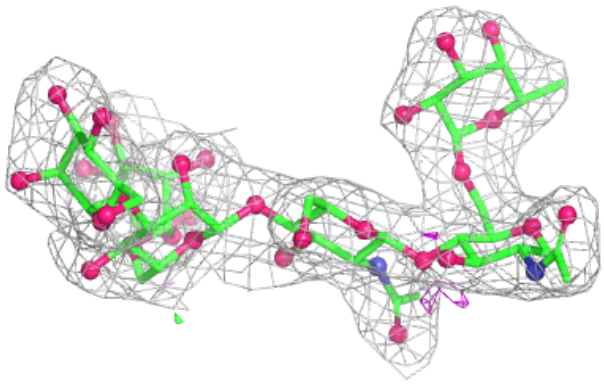


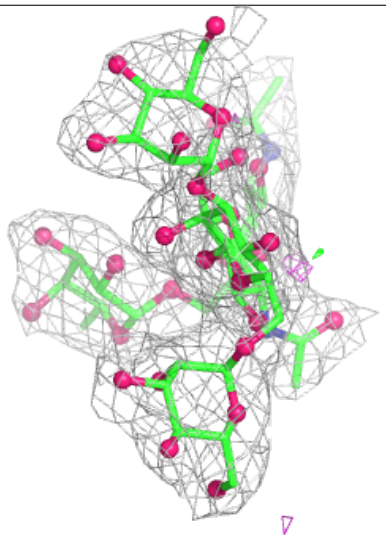


Electron density around Chain T:

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

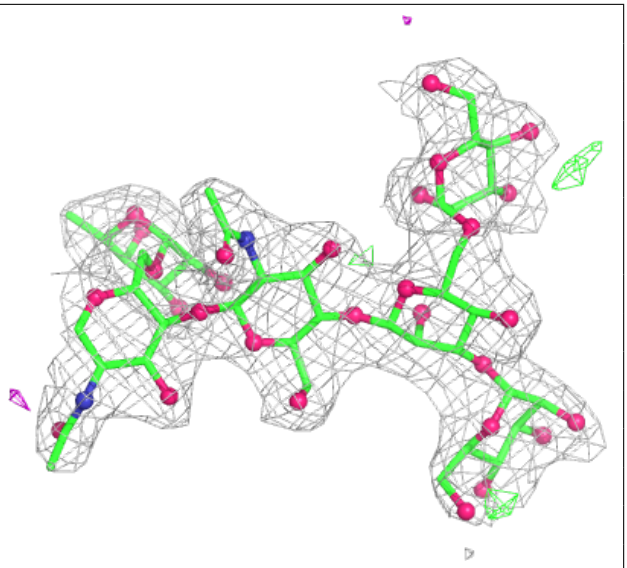


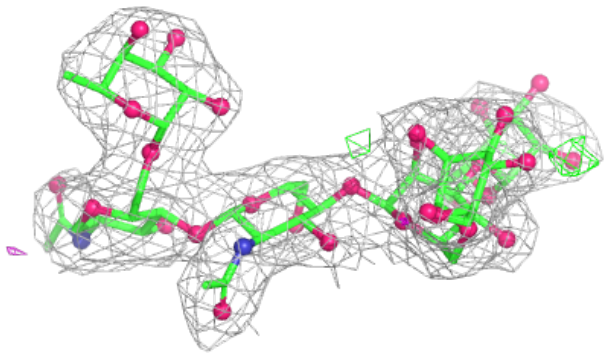


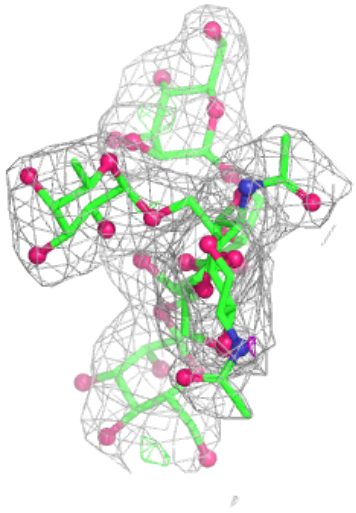


Electron density around Chain W:

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

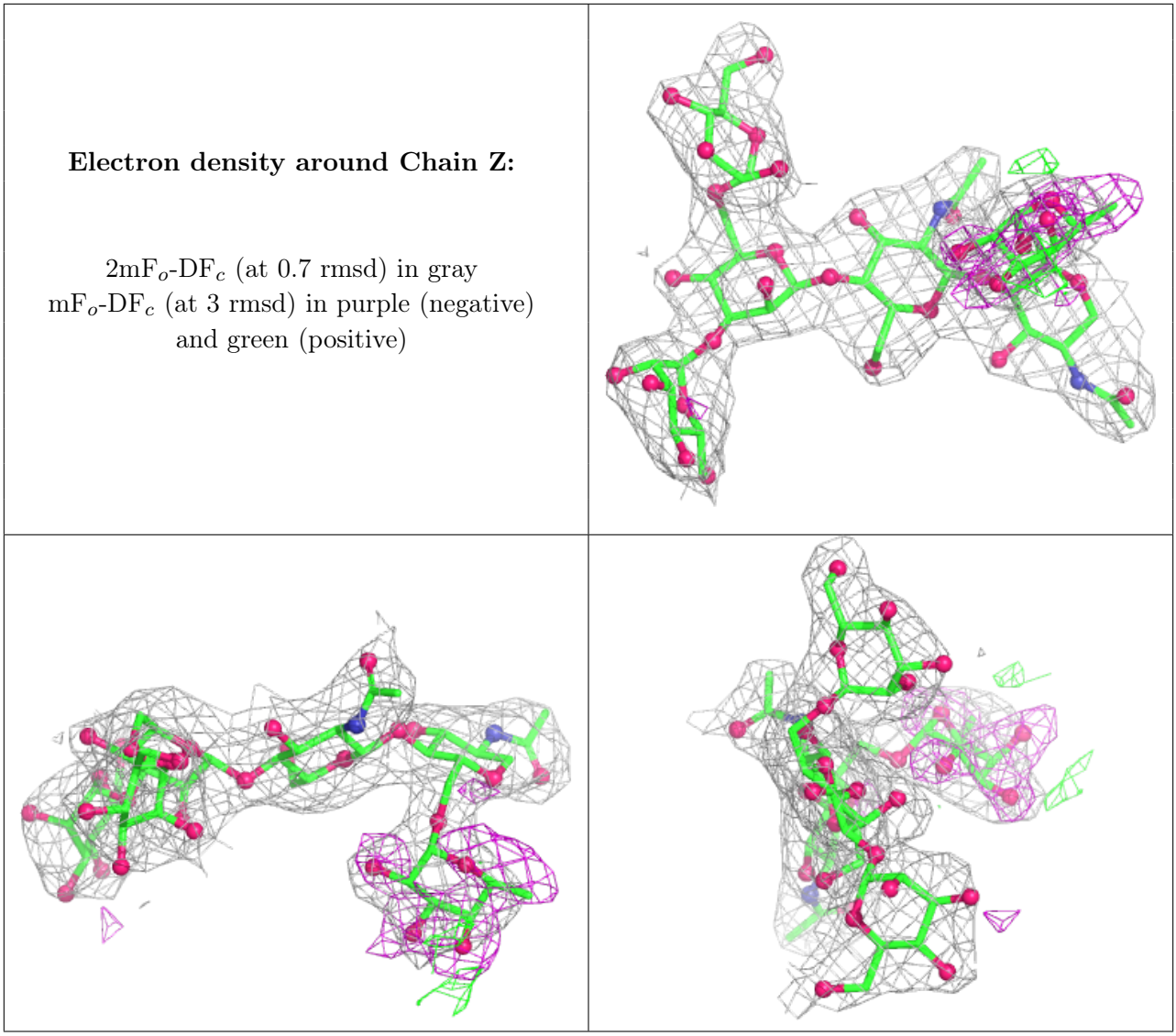






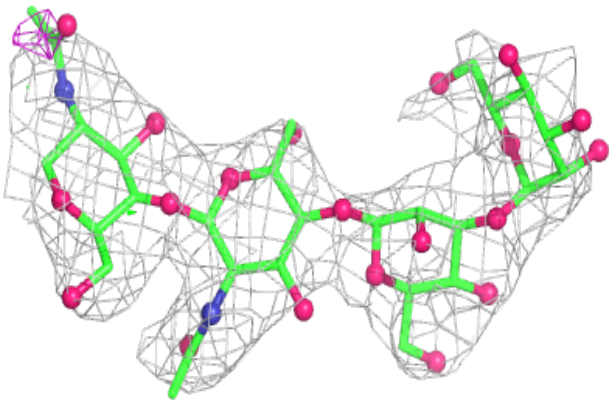
Electron density around Chain Z:

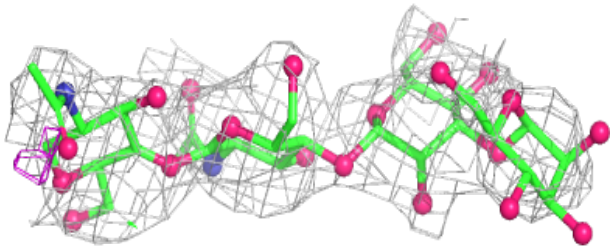
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

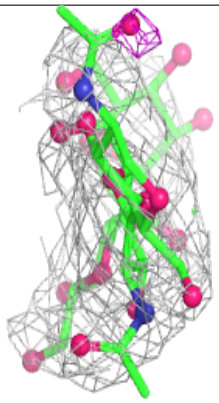


Electron density around Chain P:

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

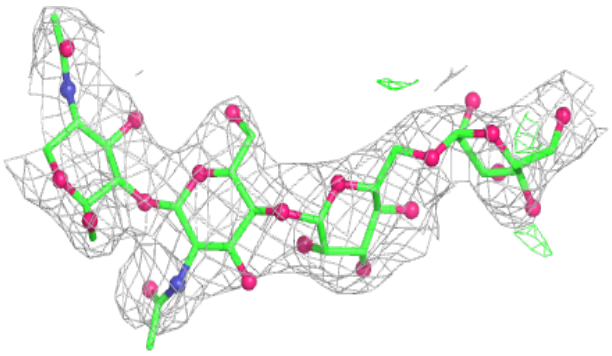


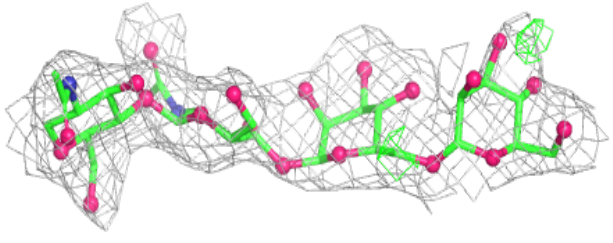


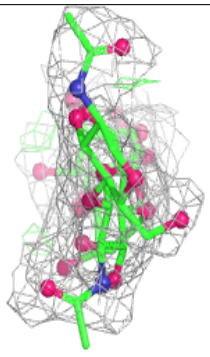


Electron density around Chain U:

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

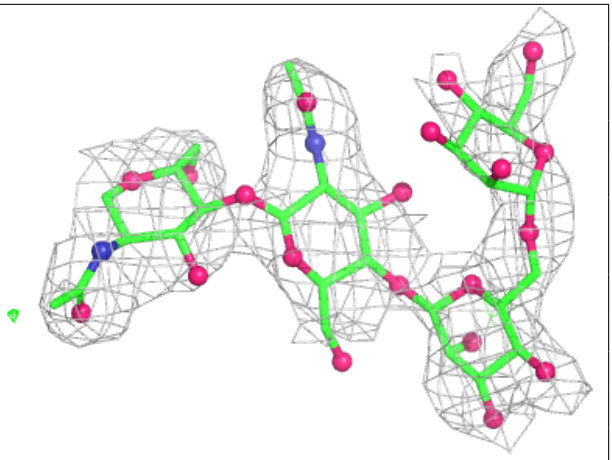


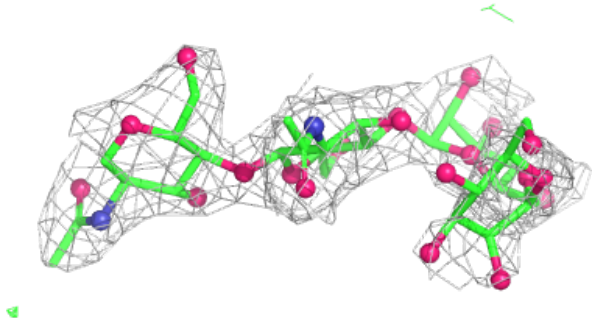


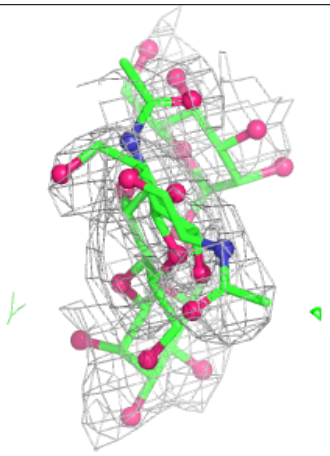


Electron density around Chain X:

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

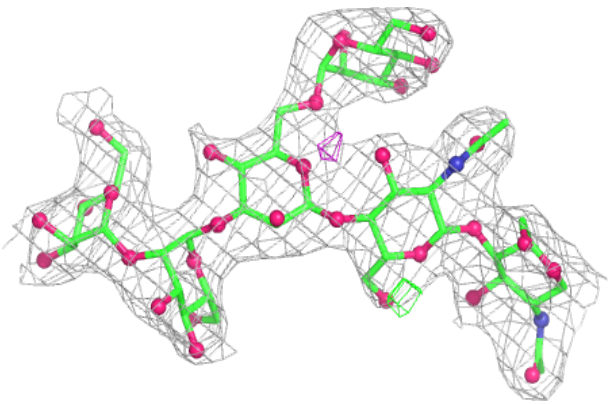


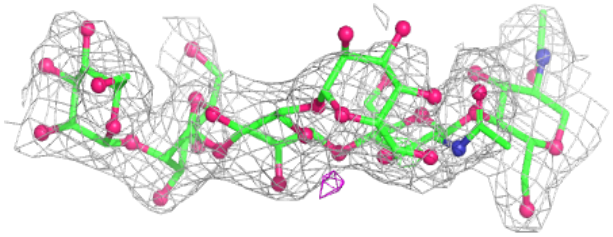


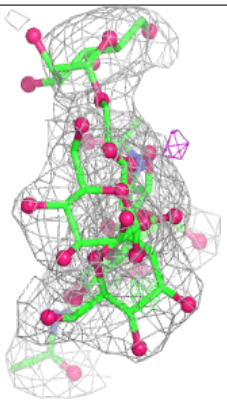


Electron density around Chain a:

$2mF_o$-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
16	NAG	B	805	14/15	0.56	0.63	95,143,152,153	0
15	PO4	H	810	5/5	0.65	0.45	118,137,162,163	0
10	CL	B	810	1/1	0.67	0.18	78,78,78,78	0
15	PO4	B	813	5/5	0.68	0.34	115,116,121,136	0
16	NAG	C	805	14/15	0.68	0.31	93,130,139,147	0
14	8PR	F	807	24/24	0.70	0.43	76,103,112,115	24
14	8PR	H	807	24/24	0.71	0.43	76,87,102,106	24
16	NAG	C	804	14/15	0.72	0.53	99,139,147,149	0
15	PO4	G	810	5/5	0.73	0.55	133,148,154,166	0
14	8PR	D	807	24/24	0.74	0.36	79,107,126,134	24
16	NAG	B	806	14/15	0.75	0.27	86,122,138,141	0
15	PO4	C	810	5/5	0.76	0.52	102,128,135,137	0
15	PO4	B	812	5/5	0.78	0.46	116,123,139,140	0
14	8PR	A	807	24/24	0.79	0.27	77,93,110,117	0
16	NAG	D	804	14/15	0.79	0.43	75,91,96,102	14
15	PO4	D	811	5/5	0.81	0.25	93,98,111,112	0
15	PO4	F	810	5/5	0.87	0.28	78,100,112,114	0
15	PO4	G	809	5/5	0.87	0.37	107,107,131,141	0
15	PO4	E	808	5/5	0.87	0.31	100,101,114,140	0
15	PO4	D	812	5/5	0.89	0.31	91,92,118,120	0
15	PO4	D	813	5/5	0.89	0.34	94,97,120,124	0
10	CL	E	802	1/1	0.89	0.14	85,85,85,85	0
10	CL	C	802	1/1	0.90	0.18	93,93,93,93	0
10	CL	F	808	1/1	0.90	0.09	68,68,68,68	0
10	CL	G	803	1/1	0.91	0.12	75,75,75,75	0
13	SCN	B	809	3/3	0.91	0.42	62,62,75,86	0
13	SCN	D	806	3/3	0.91	0.26	53,53,70,72	0
15	PO4	A	810	5/5	0.91	0.30	113,116,126,142	0
10	CL	A	803	1/1	0.91	0.09	51,51,51,51	0
13	SCN	G	807	3/3	0.92	0.32	50,50,56,65	0
15	PO4	C	811	5/5	0.92	0.26	97,102,115,115	0
10	CL	C	809	1/1	0.92	0.14	58,58,58,58	0
13	SCN	B	808	3/3	0.92	0.37	62,62,71,77	0
13	SCN	E	806	3/3	0.92	0.45	64,64,67,73	0
13	SCN	F	806	3/3	0.93	0.27	69,69,71,79	0
13	SCN	C	807	3/3	0.93	0.31	74,74,75,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	CL	B	811	1/1	0.94	0.09	60,60,60,60	0
15	PO4	H	809	5/5	0.94	0.38	91,94,111,128	0
10	CL	A	802	1/1	0.95	0.06	77,77,77,77	0
10	CL	C	808	1/1	0.95	0.14	69,69,69,69	0
10	CL	G	808	1/1	0.95	0.10	62,62,62,62	0
10	CL	H	802	1/1	0.95	0.08	61,61,61,61	0
10	CL	H	808	1/1	0.95	0.14	72,72,72,72	0
12	HEM	F	805	43/43	0.95	0.27	38,53,63,65	0
13	SCN	H	806	3/3	0.96	0.17	60,60,60,74	0
12	HEM	E	805	43/43	0.96	0.28	45,52,60,74	0
10	CL	E	807	1/1	0.96	0.12	65,65,65,65	0
12	HEM	H	805	43/43	0.96	0.26	41,52,59,75	0
13	SCN	A	806	3/3	0.96	0.28	76,76,77,83	0
10	CL	D	809	1/1	0.96	0.11	53,53,53,53	0
10	CL	E	803	1/1	0.96	0.18	62,62,62,62	0
11	CA	E	804	1/1	0.96	0.13	49,49,49,49	0
12	HEM	A	805	43/43	0.96	0.22	39,47,57,67	0
12	HEM	B	807	43/43	0.96	0.30	35,45,53,67	0
12	HEM	C	806	43/43	0.96	0.29	40,49,59,91	0
12	HEM	D	805	43/43	0.96	0.22	38,47,56,62	0
11	CA	A	804	1/1	0.97	0.15	41,41,41,41	0
10	CL	F	804	1/1	0.97	0.06	58,58,58,58	0
10	CL	D	810	1/1	0.97	0.13	54,54,54,54	0
10	CL	F	809	1/1	0.97	0.22	63,63,63,63	0
10	CL	G	801	1/1	0.97	0.11	54,54,54,54	0
10	CL	G	802	1/1	0.97	0.23	54,54,54,54	0
10	CL	A	808	1/1	0.97	0.06	62,62,62,62	0
10	CL	G	804	1/1	0.97	0.14	57,57,57,57	0
12	HEM	G	806	43/43	0.97	0.24	32,39,48,65	0
10	CL	D	802	1/1	0.97	0.07	56,56,56,56	0
10	CL	H	801	1/1	0.97	0.15	45,45,45,45	0
10	CL	A	809	1/1	0.97	0.12	51,51,51,51	0
10	CL	H	803	1/1	0.97	0.17	49,49,49,49	0
10	CL	F	802	1/1	0.97	0.12	49,49,49,49	0
10	CL	D	808	1/1	0.98	0.07	62,62,62,62	0
11	CA	C	803	1/1	0.98	0.14	54,54,54,54	0
11	CA	D	803	1/1	0.98	0.12	39,39,39,39	0
13	SCN	D	801	3/3	0.98	0.18	47,47,53,61	0
10	CL	B	802	1/1	0.98	0.11	54,54,54,54	0
11	CA	G	805	1/1	0.98	0.12	47,47,47,47	0
10	CL	B	803	1/1	0.98	0.11	51,51,51,51	1
10	CL	E	801	1/1	0.98	0.25	59,59,59,59	0

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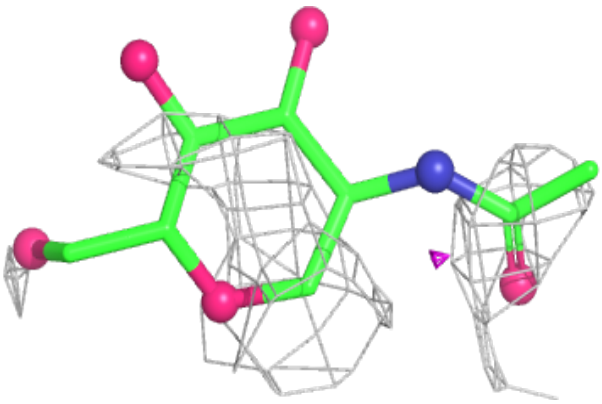
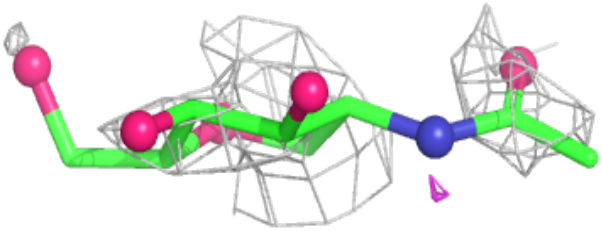
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	CA	H	804	1/1	0.99	0.18	40,40,40,40	0
11	CA	B	804	1/1	0.99	0.14	45,45,45,45	0
10	CL	B	801	1/1	0.99	0.20	50,50,50,50	0
10	CL	F	801	1/1	0.99	0.20	47,47,47,47	0
10	CL	C	801	1/1	0.99	0.24	50,50,50,50	0
11	CA	F	803	1/1	0.99	0.16	41,41,41,41	0
10	CL	A	801	1/1	0.99	0.20	43,43,43,43	0

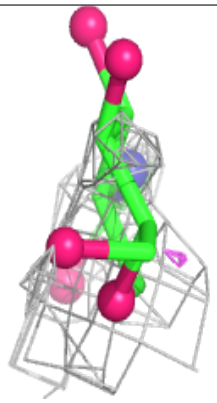
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around NAG B 805:

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

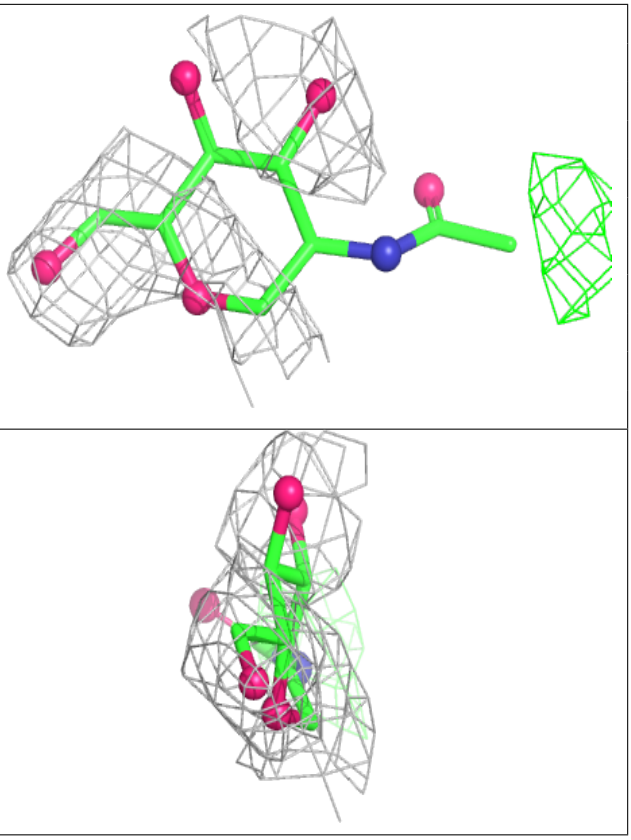


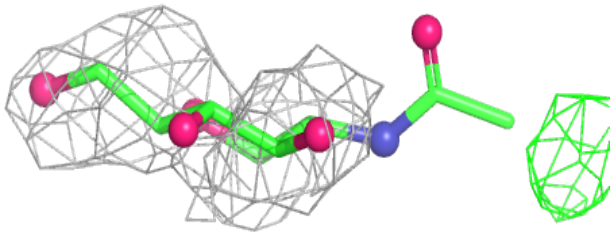




Electron density around NAG C 805:

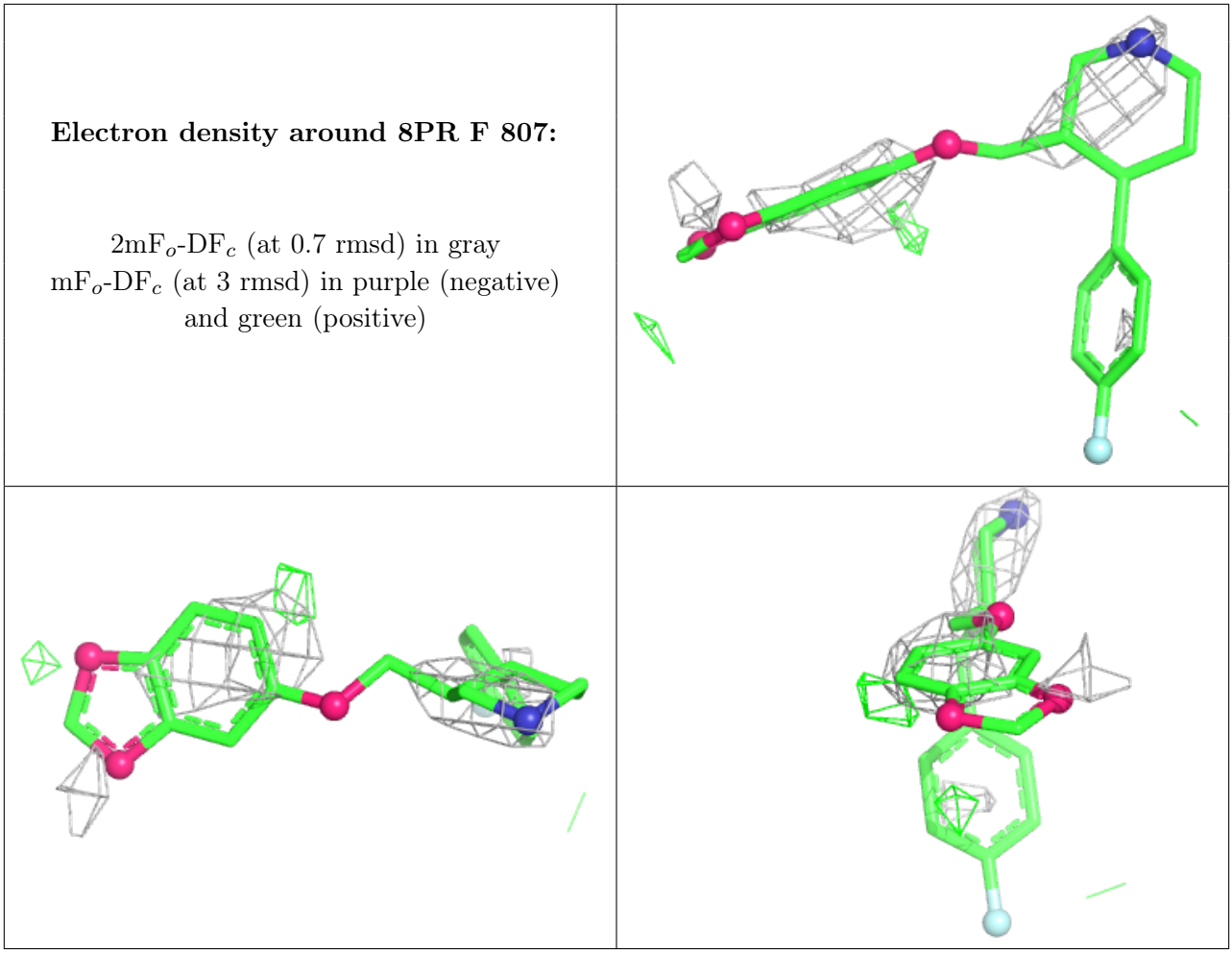
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





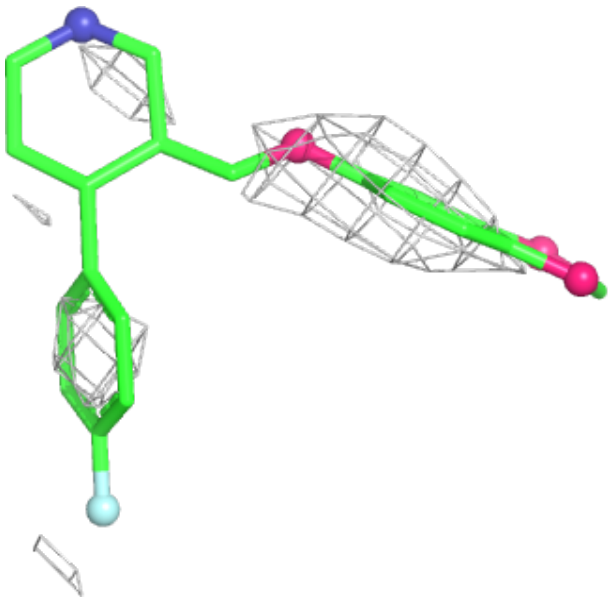
Electron density around 8PR F 807:

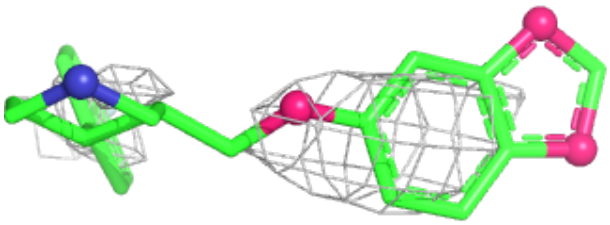
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

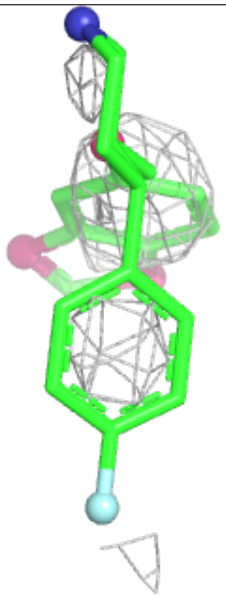


Electron density around 8PR H 807:

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

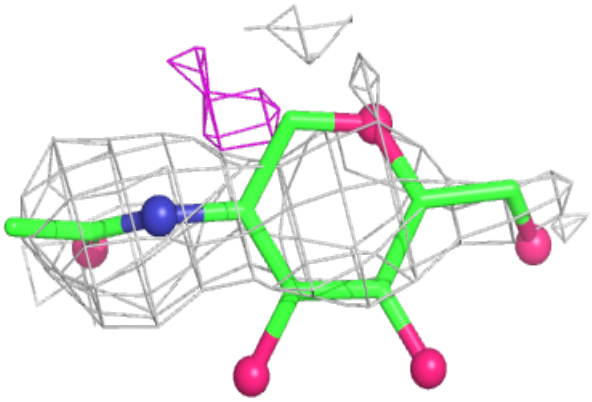


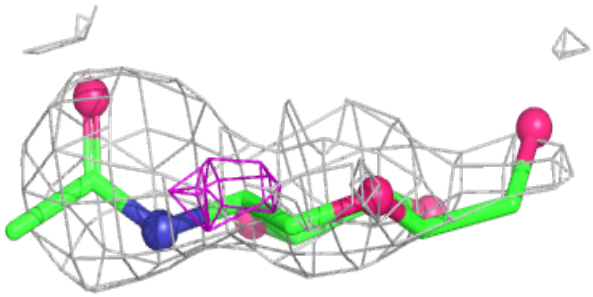


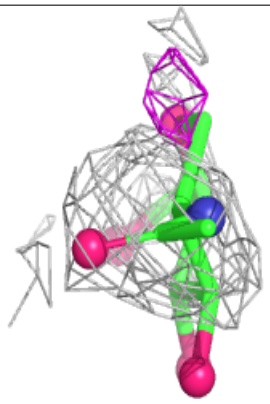


Electron density around NAG C 804:

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

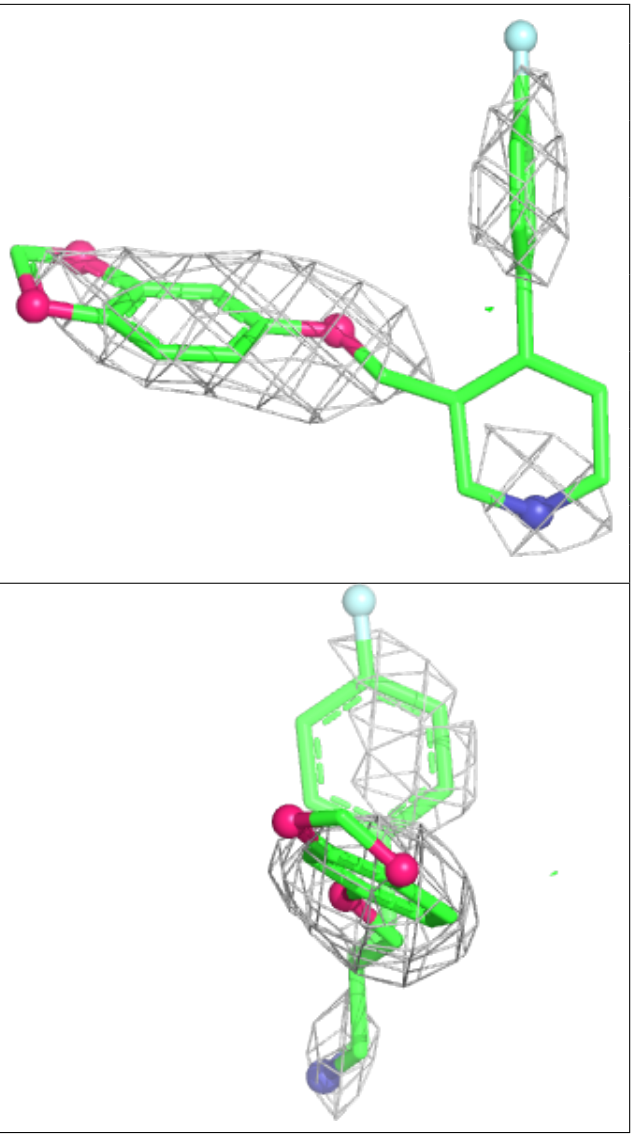






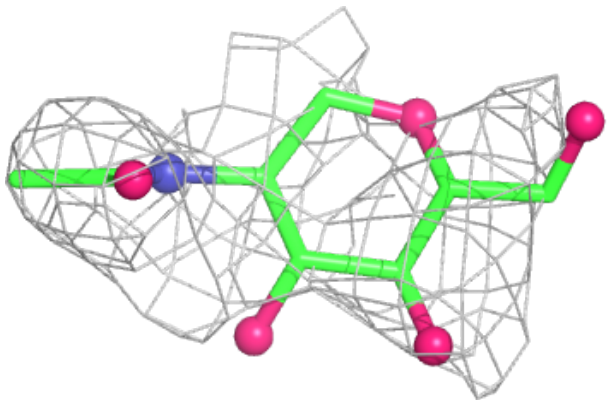
Electron density around 8PR D 807:

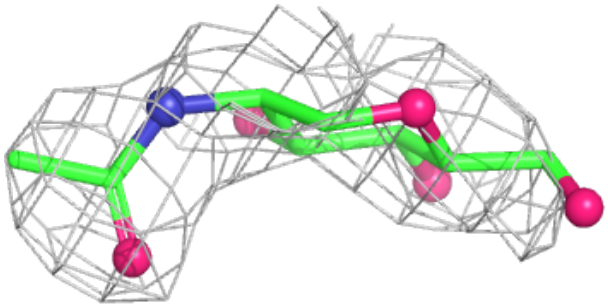
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

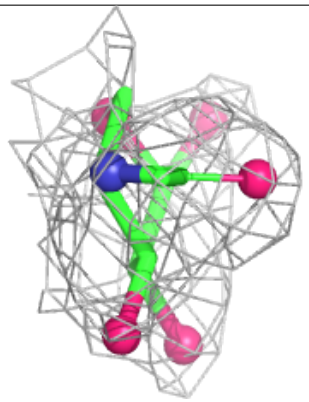


Electron density around NAG B 806:

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

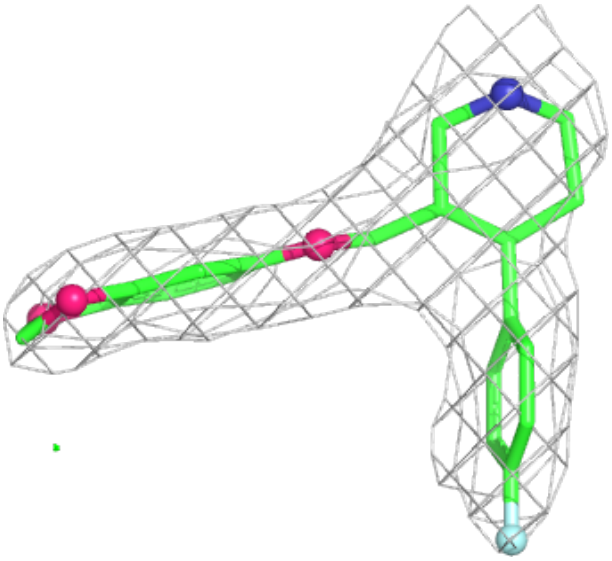


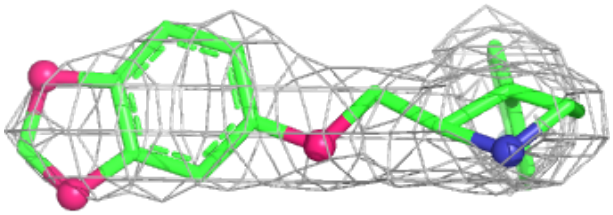


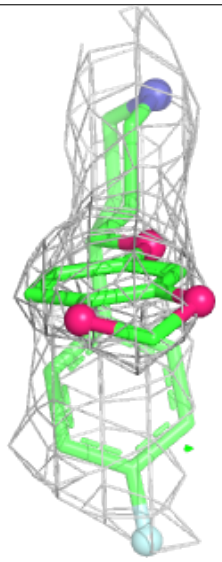


Electron density around 8PR A 807:

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

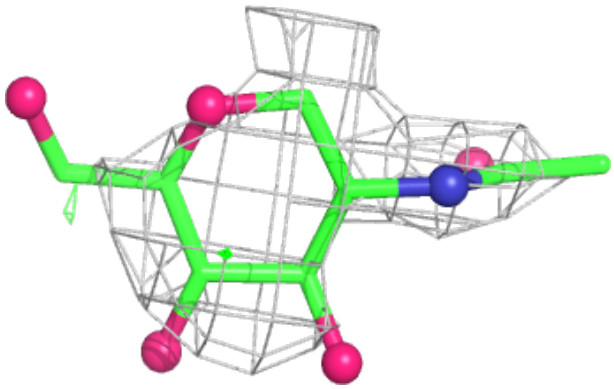


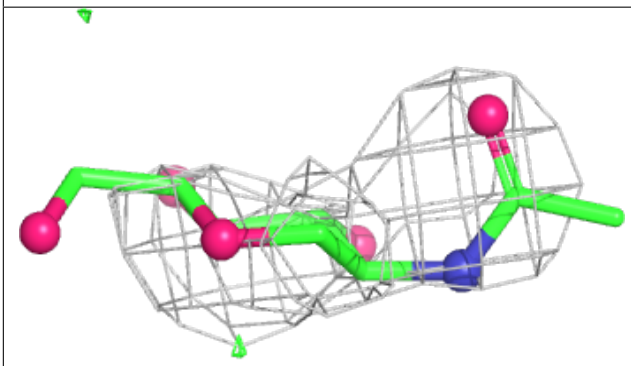


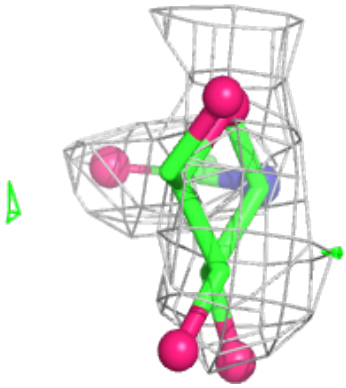


Electron density around NAG D 804:

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

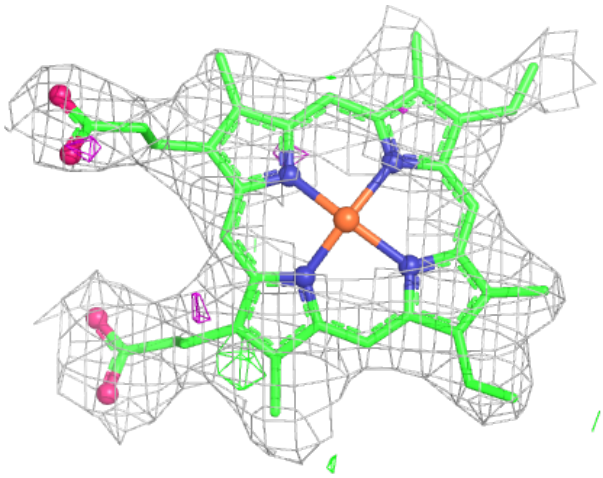


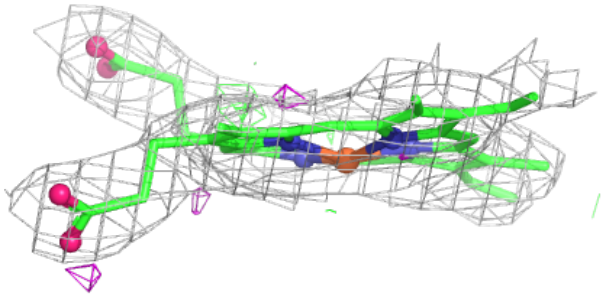


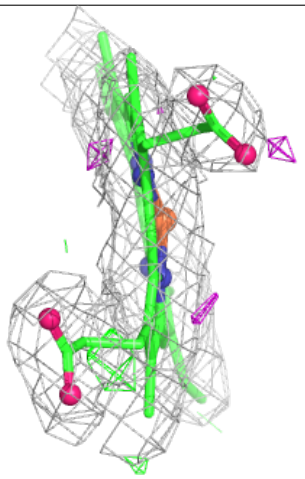


Electron density around HEM F 805:

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

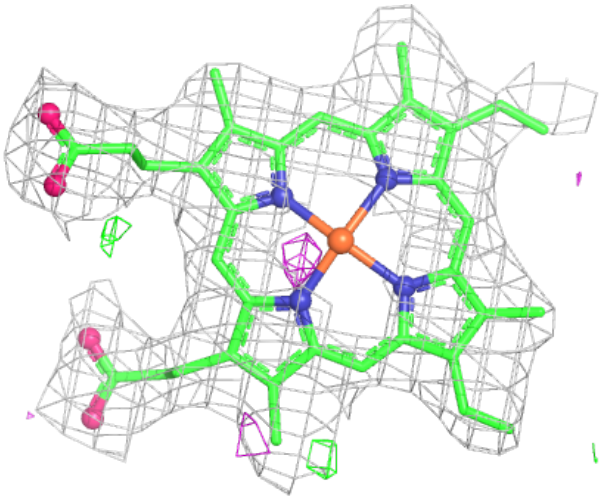


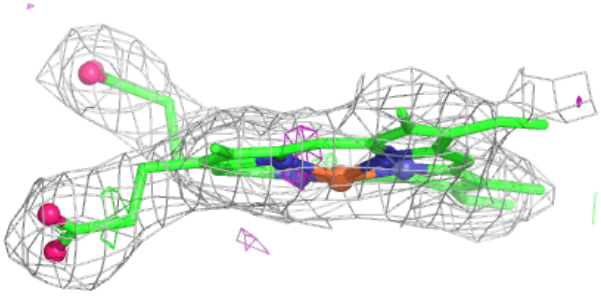




Electron density around HEM E 805:

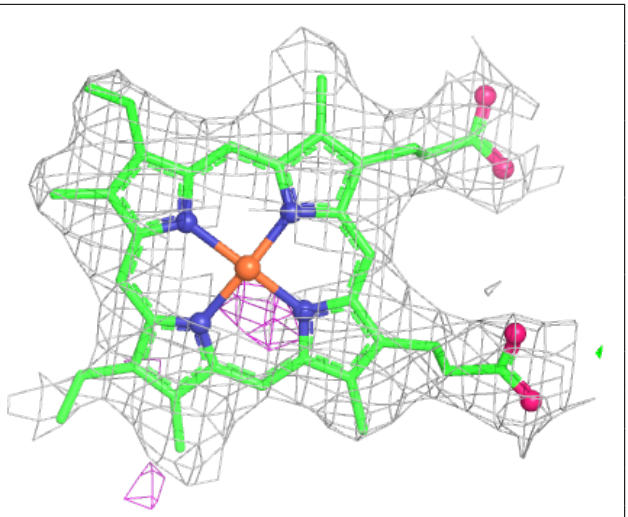
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

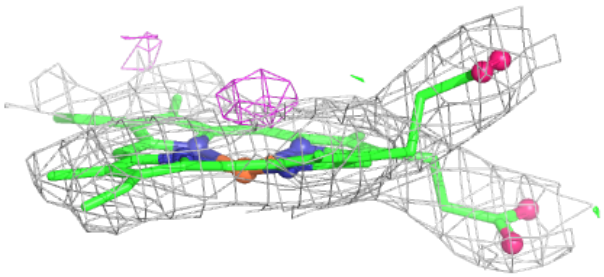


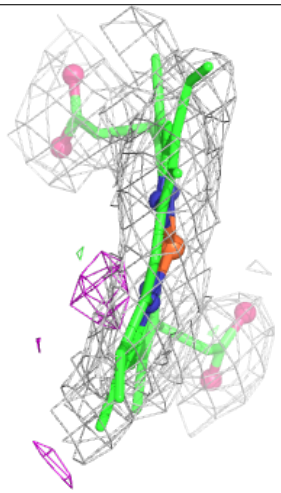


Electron density around HEM H 805:

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

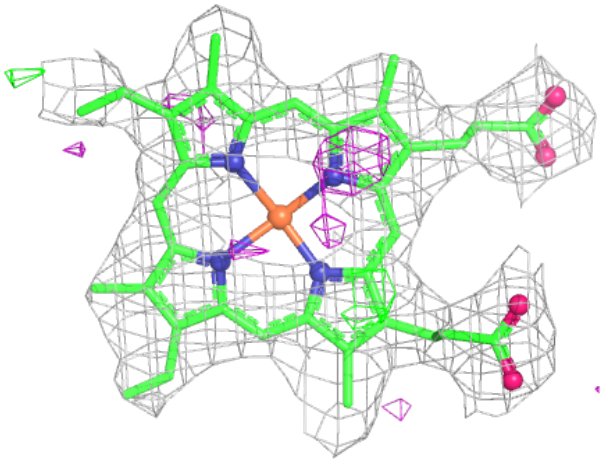


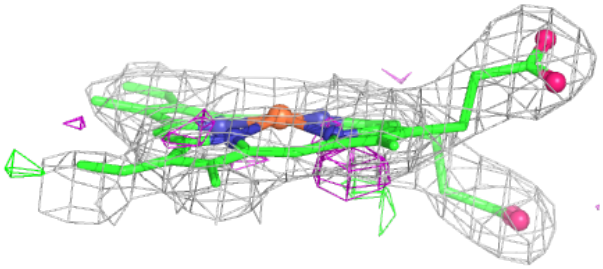


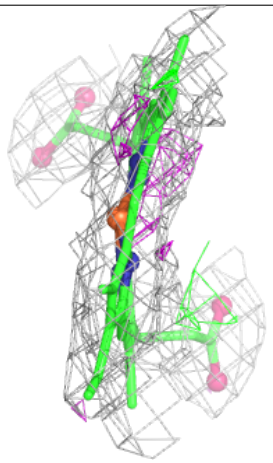


Electron density around HEM A 805:

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

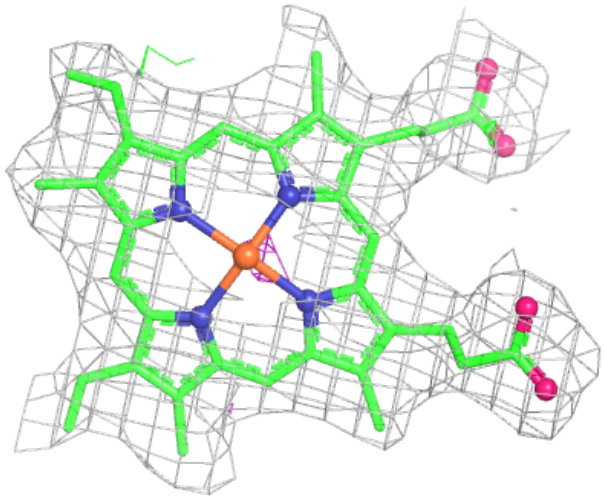


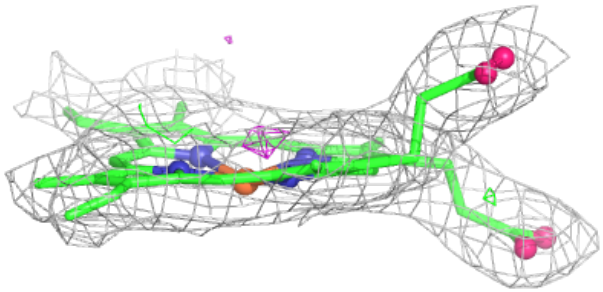


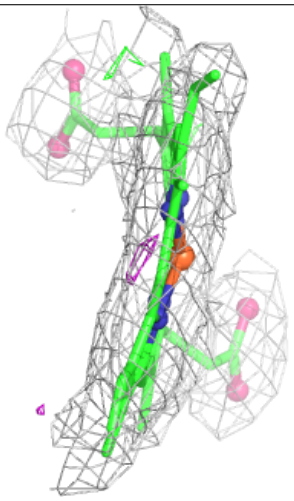


Electron density around HEM B 807:

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

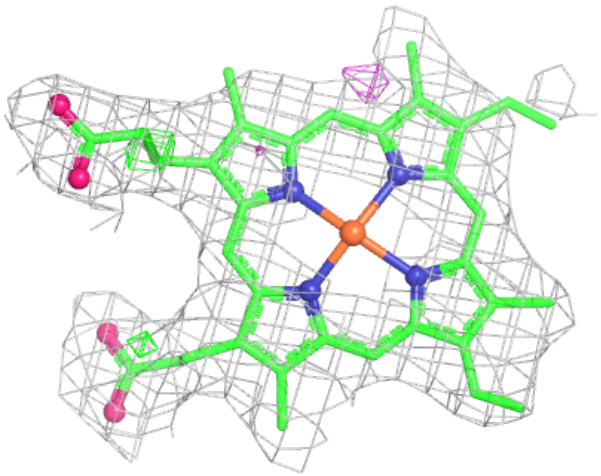


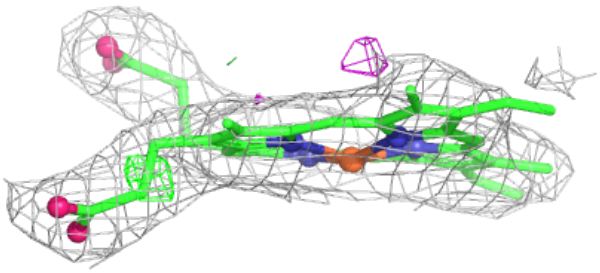




Electron density around HEM C 806:

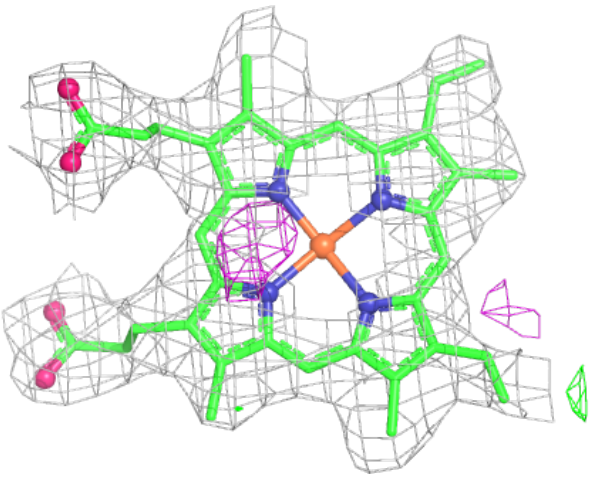
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

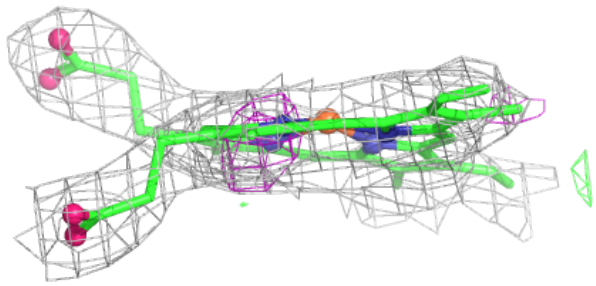


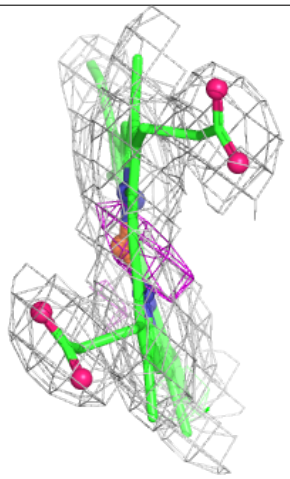


Electron density around HEM D 805:

$2mF_o$-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 G 806:

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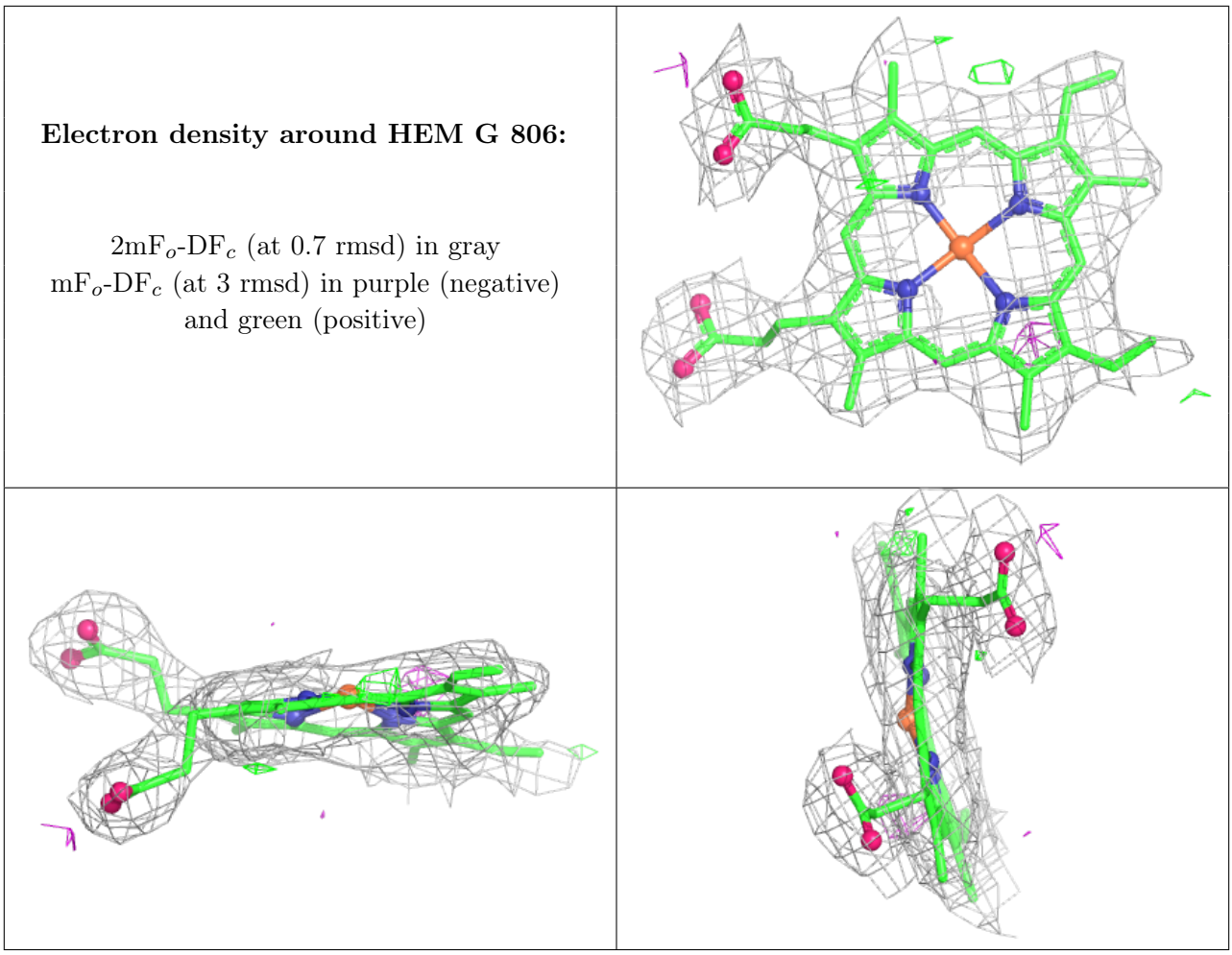
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.