Full wwPDB X-ray Structure Validation Report ⓘ

Dec 1, 2022 – 03:46 pm GMT

PDB ID	:	7Z53
Title	:	Structure of native leukocyte myeloperoxidase in complex with a truncated version (SPIN truncated) of the Staphyloccal Peroxidase Inhibitor SPIN from Staphylococcus aureus
Authors	:	Pfanzagl, V.; Brito, J.A.
Deposited on	:	2022-03-07
Resolution	:	2.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

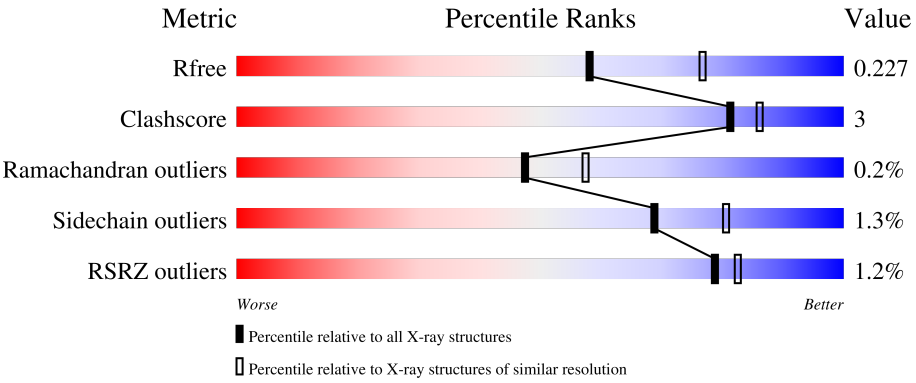
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	106	93% 6%
1	C	106	94% 6%
1	G	106	95% 5%
1	I	106	90% 9%

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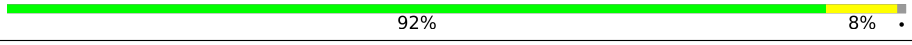
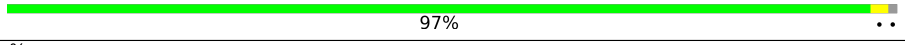
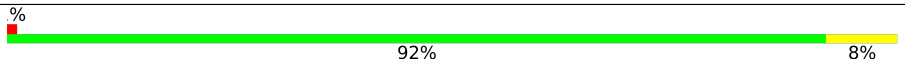
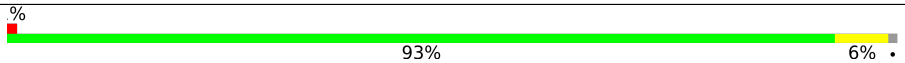
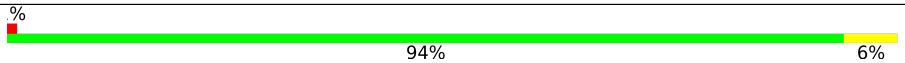
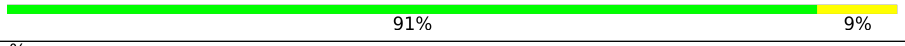
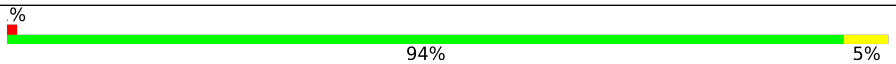
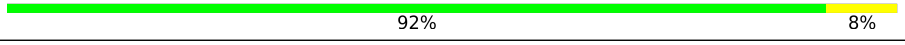
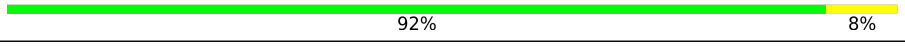
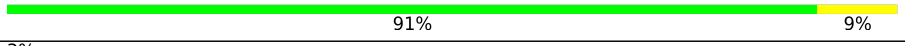
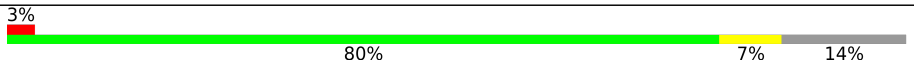
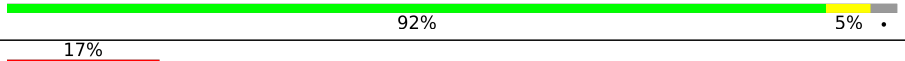
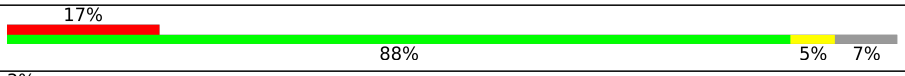
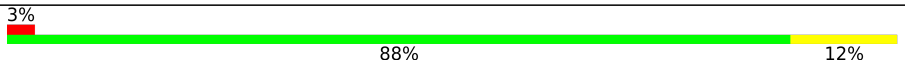
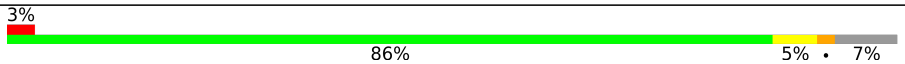
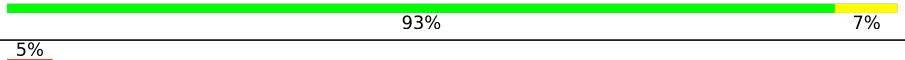
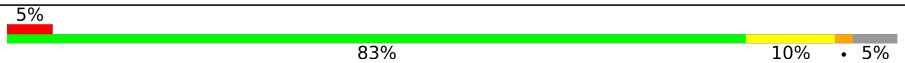
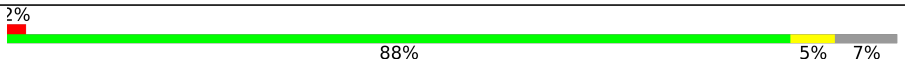
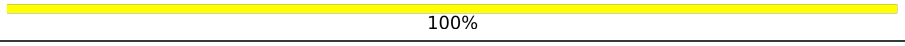
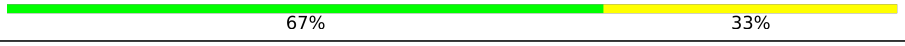
Mol	Chain	Length	Quality of chain
1	M	106	
1	O	106	
1	S	106	
1	U	106	
2	B	466	
2	D	466	
2	H	466	
2	J	466	
2	N	466	
2	P	466	
2	T	466	
2	V	466	
3	E	59	
3	F	59	
3	K	59	
3	L	59	
3	Q	59	
3	R	59	
3	W	59	
3	X	59	
4	Y	3	
4	f	3	
4	l	3	
4	o	3	
4	r	3	

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Mol	Chain	Length	Quality of chain
5	Z	4	100%
6	a	6	33% 67%
6	c	6	17% 83%
6	e	6	33% 67%
6	h	6	50% 50%
6	k	6	17% 83%
6	n	6	33% 67%
6	q	6	17% 83%
6	t	6	17% 83%
7	b	2	50% 50%
7	d	2	50% 50%
7	g	2	50% 50%
7	m	2	100%
7	p	2	50% 50%
7	s	2	100%
8	i	4	50% 50%
9	j	5	20% 80%

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
15	ACT	D	1004	-	-	X	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 83733 atoms, of which 40937 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 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	105	Total	C	H	N	O	S	0	0	0
			1643	532	800	149	157	5			
1	C	106	Total	C	H	N	O	S	0	0	0
			1657	536	807	150	159	5			
1	G	106	Total	C	H	N	O	S	0	0	0
			1657	536	807	150	159	5			
1	I	105	Total	C	H	N	O	S	0	0	0
			1643	532	800	149	157	5			
1	M	105	Total	C	H	N	O	S	0	0	0
			1643	532	800	149	157	5			
1	O	105	Total	C	H	N	O	S	0	0	0
			1643	532	800	149	157	5			
1	S	106	Total	C	H	N	O	S	0	0	0
			1657	536	807	150	159	5			
1	U	105	Total	C	H	N	O	S	0	0	0
			1643	532	800	149	157	5			

- Molecule 2 is a protein called Myeloperoxidase heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	465	Total	C	H	N	O	S	0	0	0
			7448	2348	3721	686	666	27			
2	D	465	Total	C	H	N	O	S	0	0	0
			7446	2348	3719	686	666	27			
2	H	466	Total	C	H	N	O	S	0	0	0
			7458	2351	3726	687	667	27			
2	J	465	Total	C	H	N	O	S	0	0	0
			7447	2348	3720	686	666	27			
2	N	465	Total	C	H	N	O	S	0	0	0
			7447	2348	3720	686	666	27			
2	P	465	Total	C	H	N	O	S	0	0	0
			7445	2348	3718	686	666	27			

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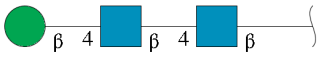
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	T	465	Total	C	H	N	O	S	0	0	0
			7447	2348	3720	686	666	27			
2	V	466	Total	C	H	N	O	S	0	0	0
			7457	2351	3725	687	667	27			

- Molecule 3 is a protein called Myeloperoxidase inhibitor SPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	51	Total	C	H	N	O	0	0	0
			814	261	400	70	83			
3	F	57	Total	C	H	N	O	0	0	0
			916	295	449	79	93			
3	K	55	Total	C	H	N	O	0	0	0
			873	278	432	75	88			
3	L	59	Total	C	H	N	O	0	0	0
			941	303	462	81	95			
3	Q	55	Total	C	H	N	O	0	0	0
			873	278	432	75	88			
3	R	59	Total	C	H	N	O	0	0	0
			942	303	463	81	95			
3	W	56	Total	C	H	N	O	0	0	0
			894	287	441	76	90			
3	X	55	Total	C	H	N	O	0	0	0
			873	278	432	75	88			

- Molecule 4 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
4	Y	3	Total	C	H	N	O	0	0	0
			73	22	34	2	15			
4	f	3	Total	C	H	N	O	0	0	0
			73	22	34	2	15			
4	l	3	Total	C	H	N	O	0	0	0
			73	22	34	2	15			
4	o	3	Total	C	H	N	O	0	0	0
			73	22	34	2	15			

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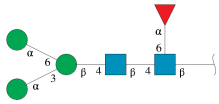
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	r	3	Total	C	H	N	O	0	0	0
			73	22	34	2	15			

- Molecule 5 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
5	Z	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			

- 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	a	6	Total	C	H	N	O	0	0	0
			132	40	61	2	29			
6	c	6	Total	C	H	N	O	0	0	0
			132	40	61	2	29			
6	e	6	Total	C	H	N	O	0	0	0
			132	40	61	2	29			
6	h	6	Total	C	H	N	O	0	0	0
			132	40	61	2	29			
6	k	6	Total	C	H	N	O	0	0	0
			132	40	61	2	29			
6	n	6	Total	C	H	N	O	0	0	0
			132	40	61	2	29			
6	q	6	Total	C	H	N	O	0	0	0
			132	40	61	2	29			
6	t	6	Total	C	H	N	O	0	0	0
			132	40	61	2	29			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

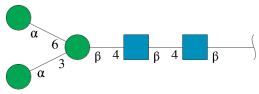
cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	b	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
7	d	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
7	g	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
7	m	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
7	p	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
7	s	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 8 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
8	i	4	Total	C	H	N	O	0	0	0
			93	28	43	2	20			

- Molecule 9 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.

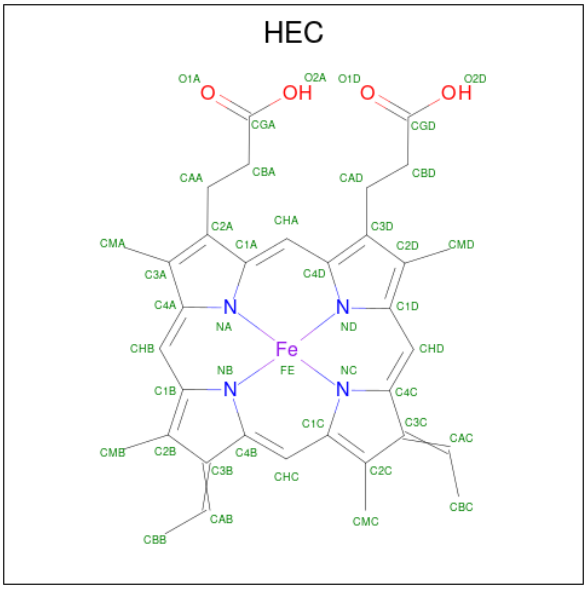


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	j	5	Total	C	H	N	O	0	0	0
			113	34	52	2	25			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total Cl 1 1	0	0
10	C	1	Total Cl 1 1	0	0
10	G	1	Total Cl 1 1	0	0
10	I	1	Total Cl 1 1	0	0
10	M	1	Total Cl 1 1	0	0
10	O	1	Total Cl 1 1	0	0
10	S	1	Total Cl 1 1	0	0
10	U	1	Total Cl 1 1	0	0

- Molecule 11 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C Fe H N O 71 34 1 28 4 4	0	0
11	C	1	Total C Fe H N O 71 34 1 28 4 4	0	0

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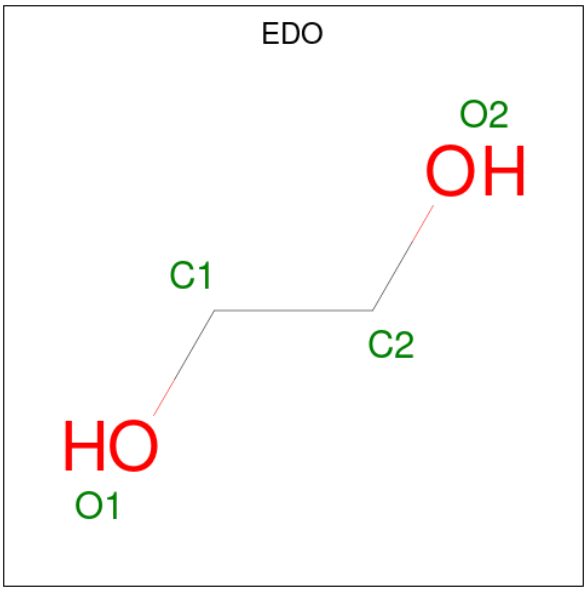
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	G	1	Total	C	Fe	H	N	O	0	0
			72	34	1	29	4	4		
11	I	1	Total	C	Fe	H	N	O	0	0
			72	34	1	29	4	4		
11	M	1	Total	C	Fe	H	N	O	0	0
			72	34	1	29	4	4		
11	O	1	Total	C	Fe	H	N	O	0	0
			72	34	1	29	4	4		
11	S	1	Total	C	Fe	H	N	O	0	0
			72	34	1	29	4	4		
11	U	1	Total	C	Fe	H	N	O	0	0
			71	34	1	28	4	4		

- Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca).

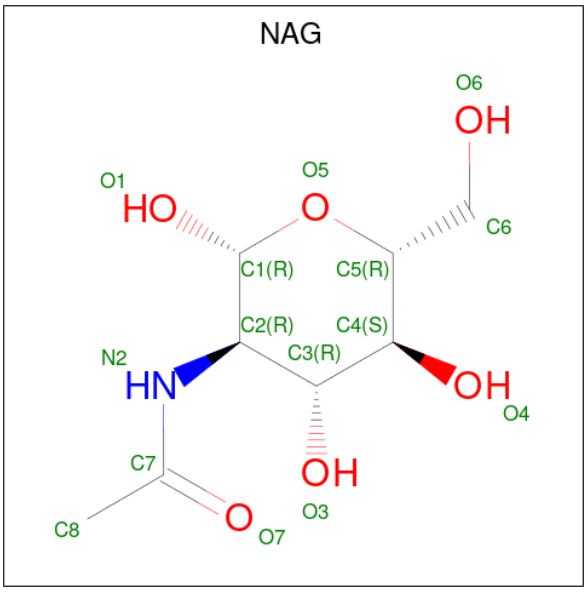
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	B	1	Total	Ca	0	0
			1	1		
12	D	1	Total	Ca	0	0
			1	1		
12	H	1	Total	Ca	0	0
			1	1		
12	J	1	Total	Ca	0	0
			1	1		
12	N	1	Total	Ca	0	0
			1	1		
12	P	1	Total	Ca	0	0
			1	1		
12	T	1	Total	Ca	0	0
			1	1		
12	V	1	Total	Ca	0	0
			1	1		

- Molecule 13 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
14	D	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

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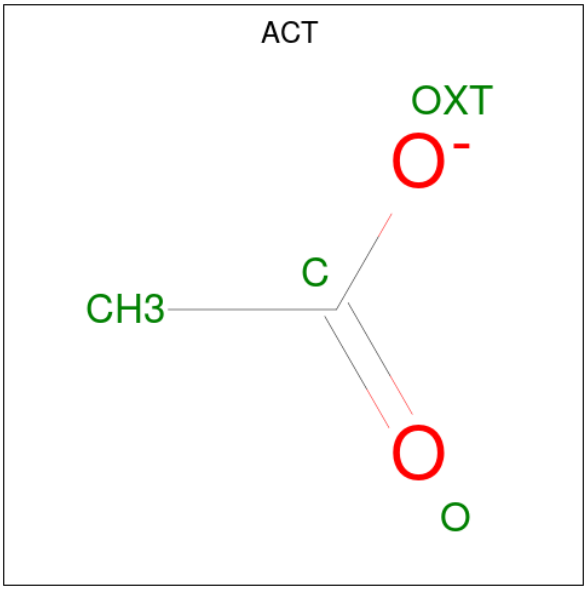
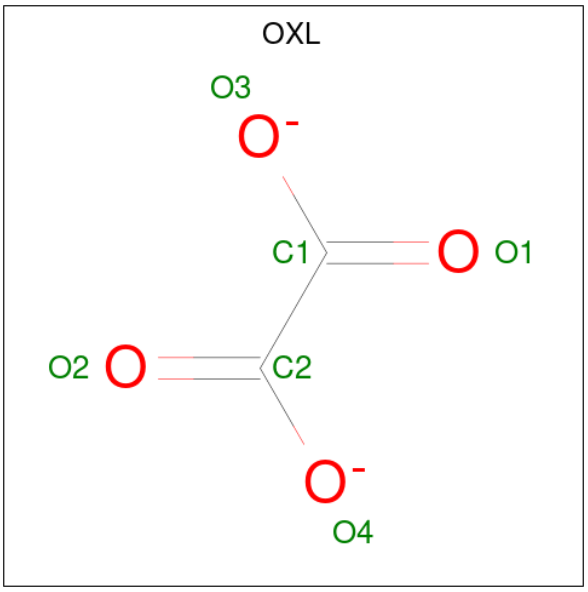
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	H	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
14	P	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 15 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	D	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 16 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	P	1	Total C O 6 2 4	0	0

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	36	Total O 36 36	0	0
17	B	109	Total O 109 109	0	0
17	C	27	Total O 27 27	0	0
17	D	73	Total O 73 73	0	0
17	E	1	Total O 1 1	0	0
17	F	3	Total O 3 3	0	0
17	G	17	Total O 17 17	0	0
17	H	57	Total O 57 57	0	0
17	I	23	Total O 23 23	0	0
17	J	83	Total O 83 83	0	0
17	L	8	Total O 8 8	0	0

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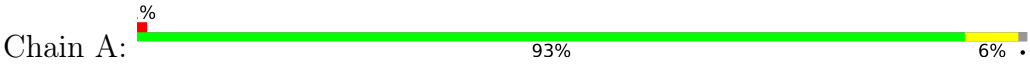
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	M	36	Total O 36 36	0	0
17	N	115	Total O 115 115	0	0
17	O	35	Total O 35 35	0	0
17	P	95	Total O 95 95	0	0
17	Q	2	Total O 2 2	0	0
17	R	2	Total O 2 2	0	0
17	S	33	Total O 33 33	0	0
17	T	127	Total O 127 127	0	0
17	U	43	Total O 43 43	0	0
17	V	138	Total O 138 138	0	0
17	W	1	Total O 1 1	0	0
17	X	4	Total O 4 4	0	0

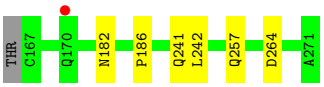
3 Residue-property plots (i)

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 light chain

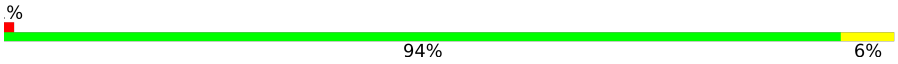
Chain A:

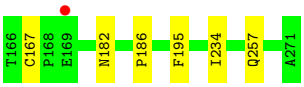




• Molecule 1: Myeloperoxidase light chain

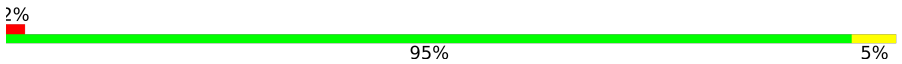
Chain C:

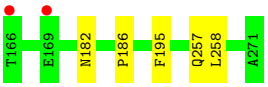




• Molecule 1: Myeloperoxidase light chain

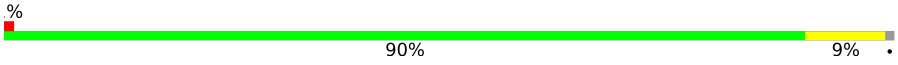
Chain G:

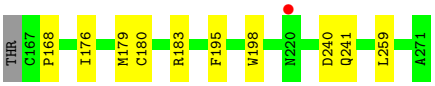




• Molecule 1: Myeloperoxidase light chain

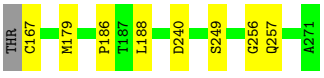
Chain I:





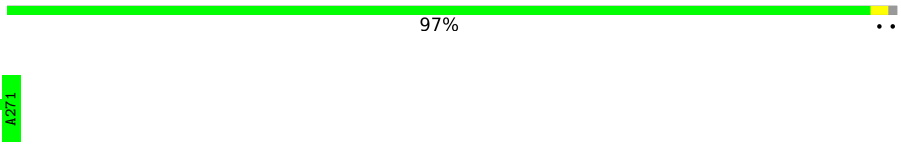
• Molecule 1: Myeloperoxidase light chain

Chain M:



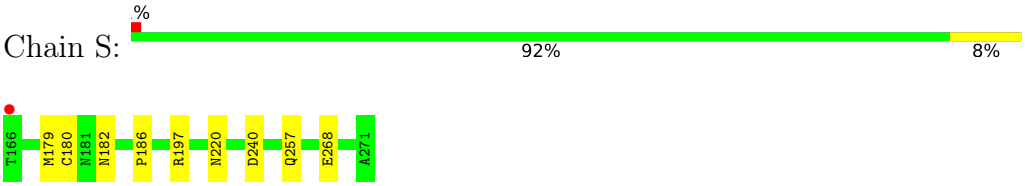
• Molecule 1: Myeloperoxidase light chain

Chain O:



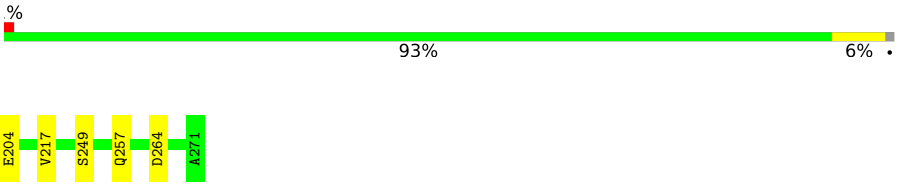
• Molecule 1: Myeloperoxidase light chain

Chain S:



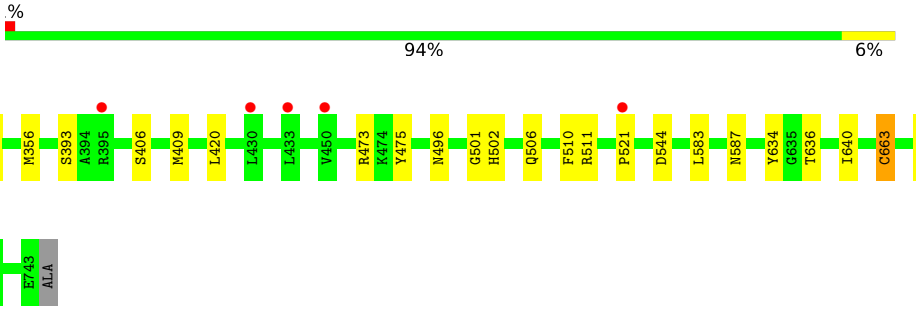
• Molecule 1: Myeloperoxidase light chain

Chain U:



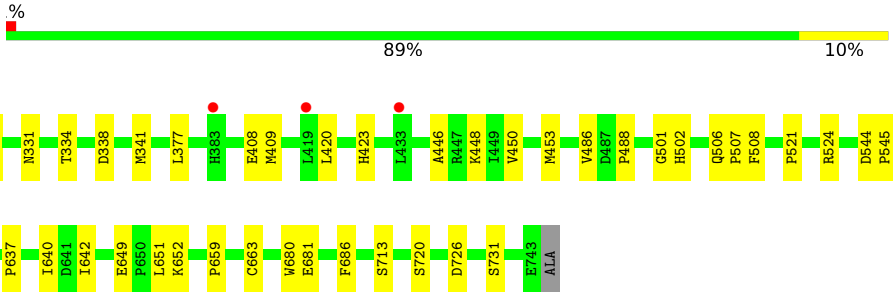
• Molecule 2: Myeloperoxidase heavy chain

Chain B:



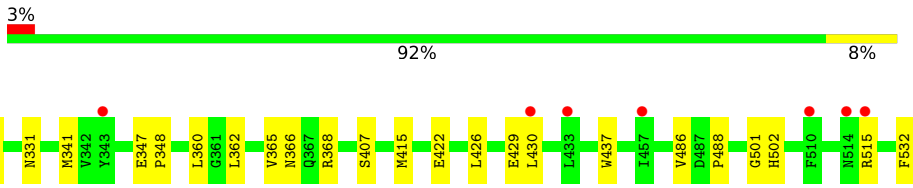
• Molecule 2: Myeloperoxidase heavy chain

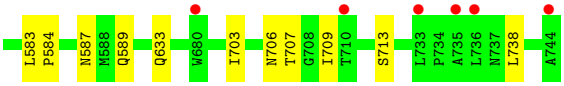
Chain D:



• Molecule 2: Myeloperoxidase heavy chain

Chain H:



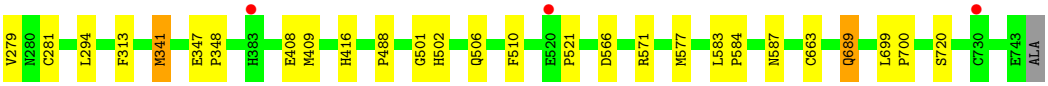


• Molecule 2: Myeloperoxidase heavy chain

Chain J:

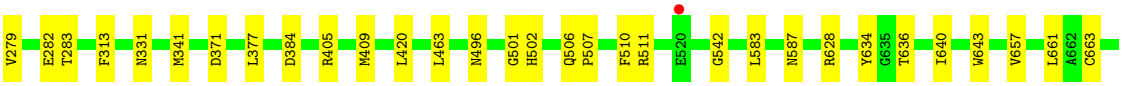
• Molecule 2: Myeloperoxidase heavy chain

Chain N:



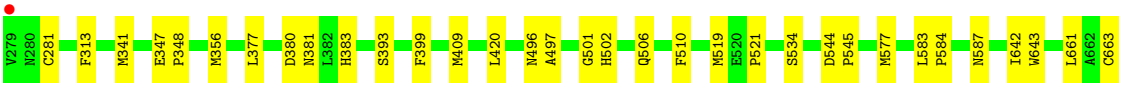
• Molecule 2: Myeloperoxidase heavy chain

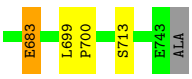
Chain P:



• Molecule 2: Myeloperoxidase heavy chain

Chain T:



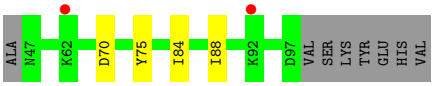


• Molecule 2: Myeloperoxidase heavy chain

Chain V:

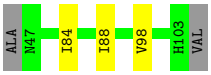
• Molecule 3: Myeloperoxidase inhibitor SPIN

Chain E:



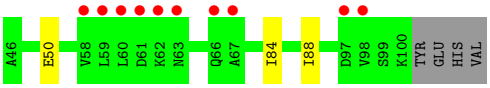
• Molecule 3: Myeloperoxidase inhibitor SPIN

Chain F:



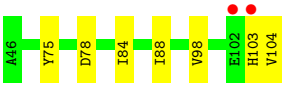
• Molecule 3: Myeloperoxidase inhibitor SPIN

Chain K:



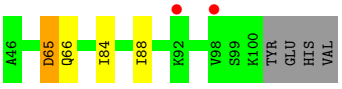
• Molecule 3: Myeloperoxidase inhibitor SPIN

Chain L:



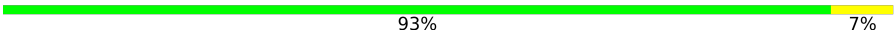
• Molecule 3: Myeloperoxidase inhibitor SPIN

Chain Q:



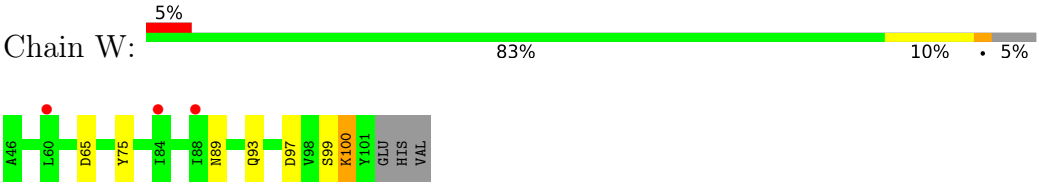
• Molecule 3: Myeloperoxidase inhibitor SPIN

Chain R:



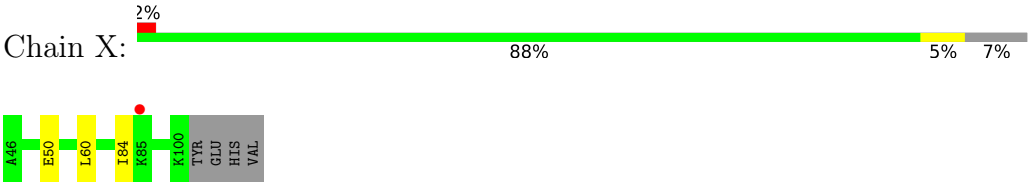
• Molecule 3: Myeloperoxidase inhibitor SPIN

Chain W:



• Molecule 3: Myeloperoxidase inhibitor SPIN

Chain X:

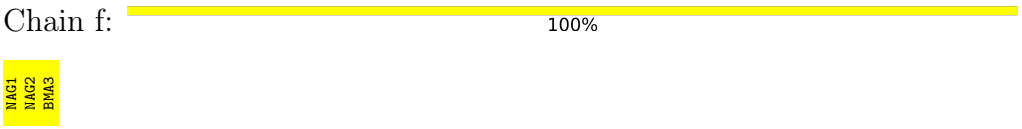


• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

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

Chain f:



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

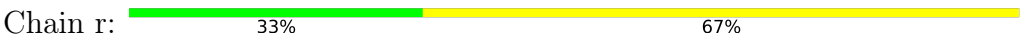
Chain l:

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

Chain o:

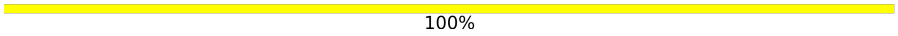
• Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:



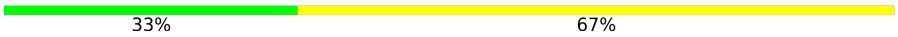
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



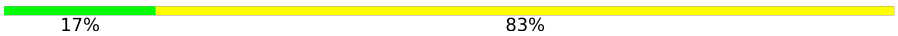
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

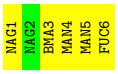
Chain a:



• 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

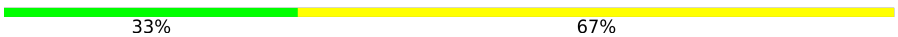
Chain c:

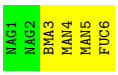




• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

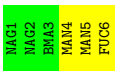
Chain e:





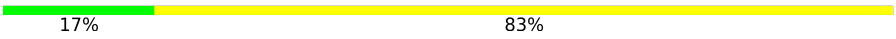
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



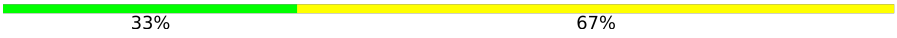
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

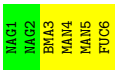
Chain k:



• 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

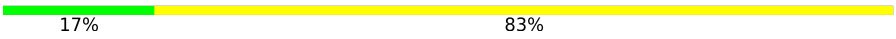
Chain n:





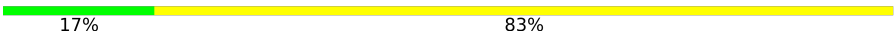
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

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 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:

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

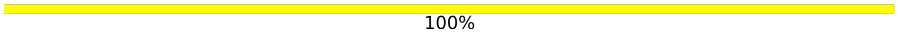
Chain d:

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

Chain g:

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

Chain m:

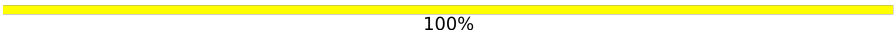


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:

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

Chain s:



• Molecule 8: 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 i:

• Molecule 9: 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 j:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	257.02Å 157.20Å 166.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.19 – 2.28 166.56 – 2.28	Depositor EDS
% Data completeness (in resolution range)	79.2 (76.19-2.28) 73.7 (166.56-2.28)	Depositor EDS
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.20rc4_4425	Depositor
R, R_{free}	0.174 , 0.229 0.174 , 0.227	Depositor DCC
R_{free} test set	12022 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	83733	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0943e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: MAN, OXL, NAG, FUC, CL, EDO, CA, CSO, BMA, HEC, ACT

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	0.73	0/868	0.84	0/1181
1	C	0.62	0/875	0.79	0/1191
1	G	0.64	0/875	0.79	0/1191
1	I	0.61	0/868	0.83	0/1181
1	M	0.71	0/868	0.81	0/1181
1	O	0.67	0/868	0.81	0/1181
1	S	0.69	0/875	0.79	0/1191
1	U	0.72	0/868	0.82	0/1181
2	B	0.64	0/3805	0.77	0/5161
2	D	0.57	0/3805	0.73	0/5161
2	H	0.59	0/3810	0.74	0/5168
2	J	0.62	0/3805	0.76	0/5161
2	N	0.64	2/3805 (0.1%)	0.76	0/5161
2	P	0.62	0/3805	0.76	0/5161
2	T	0.64	0/3805	0.78	0/5161
2	V	0.65	0/3810	0.78	1/5168 (0.0%)
3	E	0.57	0/420	0.68	0/563
3	F	0.59	0/475	0.64	0/637
3	K	0.51	0/447	0.60	0/599
3	L	0.60	0/487	0.71	0/654
3	Q	0.54	0/447	0.64	0/599
3	R	0.61	0/487	0.70	0/654
3	W	0.54	0/460	0.69	0/617
3	X	0.57	0/447	0.63	0/599
All	All	0.63	2/41085 (0.0%)	0.76	1/55702 (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
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	566	ASP	CB-CG	5.41	1.63	1.51
2	N	408	GLU	CG-CD	5.38	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V	527	LEU	CB-CG-CD1	-5.06	102.40	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	715	ASN	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	843	800	800	4	0
1	C	850	807	807	5	0
1	G	850	807	807	4	0
1	I	843	800	800	7	0
1	M	843	800	800	5	0
1	O	843	800	800	2	0
1	S	850	807	807	5	0
1	U	843	800	800	5	0
2	B	3727	3721	3720	13	0
2	D	3727	3719	3717	25	0
2	H	3732	3726	3726	24	0
2	J	3727	3720	3719	21	0
2	N	3727	3720	3720	13	1
2	P	3727	3718	3719	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	T	3727	3720	3720	16	1
2	V	3732	3725	3724	22	0
3	E	414	400	400	2	0
3	F	467	449	449	3	0
3	K	441	432	432	2	0
3	L	479	462	463	4	0
3	Q	441	432	432	2	0
3	R	479	463	463	3	0
3	W	453	441	441	4	0
3	X	441	432	432	2	0
4	Y	39	34	34	0	0
4	f	39	34	34	0	0
4	l	39	34	34	0	0
4	o	39	34	34	0	0
4	r	39	34	34	0	0
5	Z	50	43	43	0	0
6	a	71	61	61	0	0
6	c	71	61	61	0	0
6	e	71	61	61	0	0
6	h	71	61	61	0	0
6	k	71	61	61	0	0
6	n	71	61	61	0	0
6	q	71	61	61	0	0
6	t	71	61	61	0	0
7	b	28	25	25	0	0
7	d	28	25	25	0	0
7	g	28	25	25	0	0
7	m	28	25	25	0	0
7	p	28	25	25	0	0
7	s	28	25	25	0	0
8	i	50	43	43	0	0
9	j	61	52	52	0	0
10	A	1	0	0	0	0
10	C	1	0	0	0	0
10	G	1	0	0	0	0
10	I	1	0	0	0	0
10	M	1	0	0	0	0
10	O	1	0	0	0	0
10	S	1	0	0	0	0
10	U	1	0	0	0	0
11	A	43	28	29	5	0
11	C	43	28	29	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	G	43	29	30	4	0
11	I	43	29	30	3	0
11	M	43	29	30	5	0
11	O	43	29	30	3	0
11	S	43	29	30	4	0
11	U	43	28	29	7	0
12	B	1	0	0	0	0
12	D	1	0	0	0	0
12	H	1	0	0	0	0
12	J	1	0	0	0	0
12	N	1	0	0	0	0
12	P	1	0	0	0	0
12	T	1	0	0	0	0
12	V	1	0	0	0	0
13	B	4	6	6	0	0
14	D	28	26	26	0	0
14	H	14	13	13	0	0
14	P	14	13	13	0	0
15	D	4	3	3	2	0
16	P	6	0	0	0	0
17	A	36	0	0	0	0
17	B	109	0	0	1	0
17	C	27	0	0	0	0
17	D	73	0	0	0	0
17	E	1	0	0	0	0
17	F	3	0	0	0	0
17	G	17	0	0	0	0
17	H	57	0	0	1	0
17	I	23	0	0	0	0
17	J	83	0	0	0	0
17	L	8	0	0	1	0
17	M	36	0	0	0	0
17	N	115	0	0	0	0
17	O	35	0	0	0	0
17	P	95	0	0	0	0
17	Q	2	0	0	0	0
17	R	2	0	0	0	0
17	S	33	0	0	1	0
17	T	127	0	0	1	0
17	U	43	0	0	0	0
17	V	138	0	0	1	0
17	W	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	X	4	0	0	0	0
All	All	42796	40937	40942	210	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (210) 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)
11:U:302:HEC:CMB	2:V:408:GLU:OE2	1.65	1.40
2:B:406:SER:OG	17:B:1101:HOH:O	1.59	1.21
11:S:302:HEC:HBC2	2:T:501:GLY:HA3	1.45	0.99
11:A:3002:HEC:HBC2	2:B:501:GLY:HA3	1.53	0.91
11:U:302:HEC:HBC2	2:V:501:GLY:HA3	1.53	0.90
11:C:302:HEC:HBC2	2:D:501:GLY:HA3	1.52	0.88
11:G:302:HEC:HBC2	2:H:501:GLY:HA3	1.56	0.87
11:O:302:HEC:HBC2	2:P:501:GLY:HA3	1.57	0.87
11:M:302:HEC:HBC2	2:N:501:GLY:HA3	1.62	0.81
11:I:302:HEC:HBC2	2:J:501:GLY:HA3	1.62	0.81
2:H:703:ILE:O	2:H:707:THR:HG22	1.82	0.80
11:U:302:HEC:C2B	2:V:408:GLU:OE2	2.34	0.76
2:V:502:HIS:HD1	2:V:587:ASN:HD21	1.36	0.73
3:Q:65:ASP:OD1	3:Q:66:GLN:N	2.28	0.66
2:J:450:VAL:HA	2:J:453:MET:HE2	1.78	0.66
2:P:502:HIS:HD1	2:P:587:ASN:HD21	1.44	0.66
2:T:502:HIS:HD1	2:T:587:ASN:HD21	1.44	0.65
2:H:502:HIS:HD1	2:H:587:ASN:HD21	1.46	0.63
2:V:448:LYS:NZ	17:V:902:HOH:O	2.31	0.63
2:N:502:HIS:HD1	2:N:587:ASN:HD21	1.48	0.62
2:B:502:HIS:HD1	2:B:587:ASN:HD21	1.48	0.61
3:F:98:VAL:HG12	3:F:98:VAL:O	1.99	0.61
2:J:335:SER:HB2	2:J:490:ILE:HG12	1.81	0.61
2:H:707:THR:HG23	2:H:709:ILE:H	1.65	0.61
1:C:257:GLN:OE1	11:C:302:HEC:HBB3	2.01	0.61
3:W:89:ASN:O	3:W:93:GLN:HG2	2.01	0.61
2:P:506:GLN:HG3	2:P:507:PRO:HD2	1.82	0.60
2:J:502:HIS:HD1	2:J:587:ASN:HD21	1.49	0.59
1:U:257:GLN:OE1	11:U:302:HEC:HBB3	2.02	0.59
3:F:98:VAL:O	3:F:98:VAL:CG1	2.51	0.58
2:T:506:GLN:HG2	2:T:510:PHE:HE1	1.69	0.57
2:H:633:GLN:OE1	17:H:1101:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:502:HIS:HD1	2:D:587:ASN:HD21	1.54	0.56
11:S:302:HEC:HMC1	11:S:302:HEC:HBC3	1.87	0.56
2:P:725:ARG:NH1	2:P:726:ASP:OD1	2.40	0.55
1:S:257:GLN:OE1	11:S:302:HEC:HBB3	2.06	0.55
2:V:377:LEU:HD23	2:V:420:LEU:HD13	1.89	0.55
1:S:268:GLU:OE2	17:S:401:HOH:O	2.19	0.54
2:J:279:VAL:HG12	2:J:280:ASN:N	2.23	0.54
3:W:99:SER:O	3:W:100:LYS:HB2	2.07	0.54
1:A:182:ASN:O	1:A:186:PRO:HA	2.08	0.53
2:J:582:ASP:OD1	2:J:584:PRO:HD2	2.08	0.53
2:P:506:GLN:HG2	2:P:510:PHE:HE1	1.73	0.53
2:P:282:GLU:HG2	2:P:283:THR:HG23	1.89	0.53
2:P:687:SER:OG	2:P:690:GLN:HG3	2.08	0.53
1:M:256:GLY:HA3	11:M:302:HEC:HBC3	1.89	0.53
1:M:257:GLN:OE1	11:M:302:HEC:HBB3	2.09	0.53
2:H:360:LEU:HB3	2:H:362:LEU:HD13	1.90	0.53
11:G:302:HEC:HMC1	11:G:302:HEC:HBC3	1.90	0.52
11:S:302:HEC:HMC1	11:S:302:HEC:CBC	2.39	0.52
2:N:506:GLN:HG2	2:N:510:PHE:HE1	1.73	0.52
3:E:84:ILE:O	3:E:88:ILE:HG12	2.09	0.52
2:B:506:GLN:HG2	2:B:510:PHE:HE1	1.75	0.51
3:R:98:VAL:O	3:R:98:VAL:CG1	2.58	0.51
2:H:429:GLU:CD	2:H:738:LEU:HD23	2.32	0.51
11:I:302:HEC:CBC	11:I:302:HEC:HMC1	2.41	0.51
3:K:84:ILE:O	3:K:88:ILE:HG12	2.11	0.50
3:R:98:VAL:O	3:R:98:VAL:HG12	2.10	0.50
3:L:98:VAL:HG12	3:L:98:VAL:O	2.10	0.50
11:O:302:HEC:HBC3	11:O:302:HEC:HMC1	1.93	0.50
3:L:103:HIS:O	3:L:104:VAL:HB	2.12	0.50
2:D:450:VAL:HA	2:D:453:MET:HE2	1.94	0.50
2:H:583:LEU:HB3	2:H:584:PRO:HD3	1.94	0.50
2:H:430:LEU:HD12	2:H:437:TRP:CZ3	2.48	0.49
2:B:720:SER:HB3	2:B:726:ASP:HB3	1.94	0.49
11:I:302:HEC:HMC1	11:I:302:HEC:HBC3	1.93	0.49
2:H:536:ARG:NH1	2:H:540:GLU:OE1	2.46	0.49
2:J:351:ARG:HD2	17:L:202:HOH:O	2.12	0.49
2:J:356:MET:HG3	3:L:75:TYR:CD1	2.47	0.49
2:V:368:ARG:HD3	3:X:50:GLU:OE2	2.13	0.49
1:S:182:ASN:O	1:S:186:PRO:HA	2.13	0.49
1:I:240:ASP:OD1	1:I:241:GLN:HG3	2.13	0.48
2:T:506:GLN:HG2	2:T:510:PHE:CE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:738:LEU:HD22	2:H:738:LEU:N	2.28	0.48
2:D:652:LYS:NZ	15:D:1004:ACT:H2	2.27	0.48
2:V:673:ARG:HG3	2:V:679:TRP:CE2	2.48	0.48
1:S:197:ARG:HD2	17:T:1213:HOH:O	2.14	0.48
11:U:302:HEC:HBB2	2:V:408:GLU:OE1	2.14	0.48
2:H:422:GLU:OE1	2:H:706:ASN:ND2	2.41	0.48
2:H:360:LEU:CB	2:H:362:LEU:HD13	2.43	0.48
2:N:294:LEU:HD12	2:N:294:LEU:N	2.28	0.48
2:N:583:LEU:HB3	2:N:584:PRO:HD3	1.96	0.48
3:W:99:SER:O	3:W:100:LYS:CB	2.62	0.48
11:A:3002:HEC:HMC1	11:A:3002:HEC:HBC3	1.95	0.48
2:J:377:LEU:HD23	2:J:420:LEU:HD13	1.96	0.48
1:I:168:PRO:O	1:I:183:ARG:NH1	2.48	0.47
2:J:544:ASP:OD1	2:J:707:THR:HB	2.13	0.47
1:G:257:GLN:HB2	11:G:302:HEC:HMC3	1.97	0.47
2:H:294:LEU:HG	2:H:589:GLN:HG3	1.95	0.47
2:V:657:VAL:HB	2:V:661:LEU:HB2	1.96	0.47
2:H:407:SER:O	2:H:532:PHE:HA	2.15	0.47
2:J:347:GLU:N	2:J:348:PRO:CD	2.78	0.46
2:P:502:HIS:CE1	2:P:583:LEU:HD21	2.51	0.46
2:V:506:GLN:HG2	2:V:510:PHE:HE1	1.80	0.46
11:C:302:HEC:HBB2	2:D:408:GLU:OE1	2.15	0.46
1:M:249:SER:HB3	2:N:720:SER:O	2.15	0.46
11:A:3002:HEC:HMC1	11:A:3002:HEC:CBC	2.45	0.46
2:B:281:CYS:HB2	2:B:313:PHE:CZ	2.49	0.46
2:D:377:LEU:HD23	2:D:420:LEU:HD13	1.97	0.46
1:O:261:HIS:HA	2:P:405:ARG:NH2	2.31	0.46
2:D:423:HIS:CE1	2:D:446:ALA:HB3	2.51	0.46
2:D:506:GLN:HG3	2:D:507:PRO:HD2	1.97	0.46
2:H:486:VAL:O	2:H:488:PRO:HD3	2.16	0.46
3:X:60:LEU:HD21	3:X:84:ILE:HG21	1.96	0.46
2:H:365:VAL:HG12	2:H:366:ASN:O	2.16	0.46
1:C:195:PHE:CE1	2:D:331:ASN:HB2	2.51	0.46
11:C:302:HEC:HBC3	11:C:302:HEC:HMC1	1.96	0.46
1:C:234:ILE:HD13	2:D:630:LEU:HD23	1.98	0.46
2:P:720:SER:HB3	2:P:726:ASP:HB3	1.97	0.46
2:H:368:ARG:HD3	3:K:50:GLU:OE2	2.16	0.45
2:D:448:LYS:HG2	2:D:686:PHE:CZ	2.52	0.45
2:H:426:LEU:O	2:H:430:LEU:HD23	2.17	0.45
2:T:377:LEU:HD23	2:T:420:LEU:HD13	1.98	0.45
2:J:572:LEU:HD22	2:J:583:LEU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:544:ASP:OD1	2:B:707:THR:HB	2.17	0.44
3:Q:84:ILE:O	3:Q:88:ILE:HG12	2.17	0.44
2:D:720:SER:HB3	2:D:726:ASP:HB3	1.98	0.44
3:F:84:ILE:O	3:F:88:ILE:HG12	2.17	0.44
2:T:699:LEU:N	2:T:700:PRO:CD	2.81	0.44
2:D:599:TYR:CZ	2:D:603:ARG:HD3	2.52	0.44
1:M:167:CYS:SG	1:M:186:PRO:HB3	2.57	0.44
2:D:651:LEU:N	2:D:651:LEU:CD1	2.81	0.44
2:T:642:ILE:HG23	2:T:643:TRP:N	2.32	0.44
1:A:257:GLN:OE1	11:A:3002:HEC:HBB3	2.18	0.44
2:J:279:VAL:HG12	2:J:280:ASN:H	1.83	0.44
2:J:410:PRO:HD3	2:J:530:VAL:O	2.18	0.44
2:V:520:GLU:N	2:V:521:PRO:HD2	2.33	0.44
1:I:198:TRP:CE2	2:J:491:ALA:HB2	2.52	0.44
2:B:356:MET:HG3	3:E:75:TYR:CD1	2.52	0.44
2:D:602:TRP:CD1	2:D:642:ILE:HD13	2.53	0.44
2:V:670:ARG:NH1	2:V:674:ASP:OD2	2.51	0.44
2:P:506:GLN:HG2	2:P:510:PHE:CE1	2.53	0.44
11:U:302:HEC:HMC1	11:U:302:HEC:HBC3	2.00	0.44
1:C:182:ASN:O	1:C:186:PRO:HA	2.18	0.43
2:D:486:VAL:O	2:D:488:PRO:HD3	2.18	0.43
2:N:699:LEU:N	2:N:700:PRO:CD	2.81	0.43
3:L:84:ILE:O	3:L:88:ILE:HG12	2.17	0.43
2:B:420:LEU:HD23	2:B:420:LEU:C	2.39	0.43
1:C:167:CYS:SG	1:C:186:PRO:HB3	2.58	0.43
2:V:475:TYR:O	2:V:670:ARG:HD2	2.18	0.43
11:G:302:HEC:HBA1	11:G:302:HEC:HMA2	2.01	0.43
2:V:463:LEU:N	2:V:464:PRO:CD	2.82	0.43
2:D:281:CYS:HB2	2:D:313:PHE:CZ	2.54	0.43
2:D:551:MET:HE2	2:D:713:SER:H	1.83	0.43
2:D:680:TRP:CE2	2:D:681:GLU:HG3	2.53	0.43
2:J:680:TRP:CE2	2:J:681:GLU:HG3	2.54	0.43
2:P:377:LEU:HD23	2:P:420:LEU:HD13	2.01	0.43
1:U:171:ASP:OD1	1:U:171:ASP:N	2.52	0.43
2:V:365:VAL:HG12	2:V:420:LEU:HD21	2.00	0.43
1:I:259:LEU:HD21	2:J:669:PHE:CZ	2.54	0.43
2:D:637:PRO:HA	2:D:640:ILE:HD12	2.01	0.42
2:T:583:LEU:HB3	2:T:584:PRO:HD3	1.99	0.42
2:V:450:VAL:HA	2:V:453:MET:HE2	2.00	0.42
1:M:188:LEU:HB3	2:N:488:PRO:HD2	2.01	0.42
2:P:688:MET:O	2:P:692:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:179:MET:O	1:S:180:CYS:HB2	2.18	0.42
2:H:294:LEU:N	2:H:294:LEU:HD12	2.35	0.42
2:J:531:PHE:O	2:J:532:PHE:HB2	2.19	0.42
2:N:281:CYS:HB2	2:N:313:PHE:CZ	2.54	0.42
2:T:496:ASN:OD1	2:T:643:TRP:HB2	2.20	0.42
2:V:280:ASN:OD1	2:V:282:GLU:HG2	2.19	0.42
2:V:410:PRO:HD3	2:V:530:VAL:O	2.20	0.42
2:T:356:MET:HG3	3:W:75:TYR:CD1	2.55	0.42
2:B:475:TYR:OH	2:B:663:CYS:HB2	2.19	0.42
11:M:302:HEC:HMC1	11:M:302:HEC:CBC	2.49	0.42
1:U:204:GLU:HG3	1:U:217:VAL:HG11	2.01	0.42
1:A:264:ASP:OD2	11:A:3002:HEC:O2D	2.38	0.42
2:H:347:GLU:N	2:H:348:PRO:CD	2.83	0.42
2:P:371:ASP:OD1	2:P:542:GLY:HA3	2.20	0.42
2:T:281:CYS:HB2	2:T:313:PHE:CZ	2.55	0.42
2:P:657:VAL:HB	2:P:661:LEU:HB2	2.02	0.41
2:T:399:PHE:CE2	2:T:534:SER:HB2	2.55	0.41
2:P:496:ASN:OD1	2:P:643:TRP:HB2	2.19	0.41
2:D:544:ASP:HB2	2:D:545:PRO:HD3	2.01	0.41
1:G:195:PHE:CE1	2:H:331:ASN:HB2	2.55	0.41
2:B:634:TYR:CD2	2:B:640:ILE:HG12	2.55	0.41
2:D:334:THR:OG1	2:D:338:ASP:OD2	2.37	0.41
2:J:701:ARG:HD3	2:J:734:PRO:O	2.21	0.41
11:O:302:HEC:HMC1	11:O:302:HEC:CBC	2.50	0.41
2:P:279:VAL:HG12	2:P:313:PHE:HE2	1.86	0.41
2:P:463:LEU:HD23	2:P:463:LEU:HA	1.85	0.41
11:M:302:HEC:HAC	11:M:302:HEC:HHD	1.92	0.41
2:P:634:TYR:CD2	2:P:640:ILE:HG12	2.56	0.41
2:B:473:ARG:HD3	2:V:383:HIS:O	2.20	0.41
2:D:649:GLU:OE1	2:D:659:PRO:HD2	2.20	0.41
1:O:195:PHE:CE1	2:P:331:ASN:HB2	2.56	0.41
2:T:380:ASP:OD1	2:T:381:ASN:N	2.52	0.41
1:A:241:GLN:O	1:A:242:LEU:C	2.58	0.41
1:G:182:ASN:O	1:G:186:PRO:HA	2.21	0.41
1:G:258:LEU:HD22	2:H:415:MET:HB3	2.03	0.41
2:J:583:LEU:HB3	2:J:584:PRO:HD3	2.03	0.41
2:N:689:GLN:H	2:N:689:GLN:CD	2.23	0.41
2:T:544:ASP:HB2	2:T:545:PRO:HD3	2.02	0.41
2:D:652:LYS:HZ2	15:D:1004:ACT:H2	1.85	0.41
1:I:179:MET:O	1:I:180:CYS:HB2	2.19	0.40
2:N:347:GLU:N	2:N:348:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:C:302:HEC:HMC1	11:C:302:HEC:CBC	2.52	0.40
2:D:508:PHE:CE2	2:D:524:ARG:NH2	2.89	0.40
3:R:52:GLU:OE2	3:R:75:TYR:OH	2.31	0.40
2:T:497:ALA:HB1	2:T:661:LEU:HD22	2.03	0.40
2:B:502:HIS:CE1	2:B:583:LEU:HD21	2.56	0.40
2:H:281:CYS:HB2	2:H:313:PHE:CZ	2.56	0.40
2:N:506:GLN:HG2	2:N:510:PHE:CE1	2.55	0.40
2:V:347:GLU:N	2:V:348:PRO:CD	2.84	0.40
1:I:176:ILE:HD13	1:I:176:ILE:HA	1.98	0.40
1:I:195:PHE:CE1	2:J:331:ASN:HB2	2.56	0.40
2:T:347:GLU:N	2:T:348:PRO:CD	2.84	0.40
1:U:264:ASP:OD2	11:U:302:HEC:O2D	2.39	0.40
2:N:341:MET:HB2	2:N:416:HIS:CE1	2.56	0.40
1:U:249:SER:HB3	2:V:720:SER:O	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:571:ARG:HH21	2:T:683:GLU:OE2[4_447]	1.54	0.06

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	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
1	C	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
1	G	104/106 (98%)	100 (96%)	4 (4%)	0	100	100
1	I	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
1	M	103/106 (97%)	101 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	103/106 (97%)	100 (97%)	3 (3%)	0	100	100
1	S	104/106 (98%)	99 (95%)	5 (5%)	0	100	100
1	U	103/106 (97%)	98 (95%)	5 (5%)	0	100	100
2	B	462/466 (99%)	445 (96%)	16 (4%)	1 (0%)	47	57
2	D	462/466 (99%)	443 (96%)	17 (4%)	2 (0%)	34	40
2	H	463/466 (99%)	445 (96%)	18 (4%)	0	100	100
2	J	462/466 (99%)	447 (97%)	13 (3%)	2 (0%)	34	40
2	N	462/466 (99%)	447 (97%)	14 (3%)	1 (0%)	47	57
2	P	462/466 (99%)	445 (96%)	17 (4%)	0	100	100
2	T	462/466 (99%)	449 (97%)	12 (3%)	1 (0%)	47	57
2	V	463/466 (99%)	448 (97%)	15 (3%)	0	100	100
3	E	49/59 (83%)	47 (96%)	2 (4%)	0	100	100
3	F	55/59 (93%)	54 (98%)	1 (2%)	0	100	100
3	K	53/59 (90%)	52 (98%)	1 (2%)	0	100	100
3	L	57/59 (97%)	53 (93%)	3 (5%)	1 (2%)	8	7
3	Q	53/59 (90%)	50 (94%)	2 (4%)	1 (2%)	8	6
3	R	57/59 (97%)	57 (100%)	0	0	100	100
3	W	54/59 (92%)	50 (93%)	2 (4%)	2 (4%)	3	1
3	X	53/59 (90%)	52 (98%)	1 (2%)	0	100	100
All	All	4956/5048 (98%)	4779 (96%)	166 (3%)	11 (0%)	47	57

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	W	100	LYS
2	B	521	PRO
2	D	521	PRO
2	N	521	PRO
2	T	521	PRO
3	L	78	ASP
3	Q	65	ASP
2	D	731	SER
3	W	65	ASP
2	J	477	PRO
2	J	522	ASN

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	90/91 (99%)	90 (100%)	0	100	100
1	C	91/91 (100%)	91 (100%)	0	100	100
1	G	91/91 (100%)	91 (100%)	0	100	100
1	I	90/91 (99%)	90 (100%)	0	100	100
1	M	90/91 (99%)	88 (98%)	2 (2%)	52	66
1	O	90/91 (99%)	90 (100%)	0	100	100
1	S	91/91 (100%)	89 (98%)	2 (2%)	52	66
1	U	90/91 (99%)	90 (100%)	0	100	100
2	B	410/410 (100%)	402 (98%)	8 (2%)	55	70
2	D	410/410 (100%)	406 (99%)	4 (1%)	76	86
2	H	410/410 (100%)	407 (99%)	3 (1%)	84	91
2	J	410/410 (100%)	402 (98%)	8 (2%)	55	70
2	N	410/410 (100%)	404 (98%)	6 (2%)	65	77
2	P	410/410 (100%)	403 (98%)	7 (2%)	60	74
2	T	410/410 (100%)	401 (98%)	9 (2%)	52	66
2	V	410/410 (100%)	403 (98%)	7 (2%)	60	74
3	E	45/52 (86%)	44 (98%)	1 (2%)	52	66
3	F	51/52 (98%)	51 (100%)	0	100	100
3	K	48/52 (92%)	48 (100%)	0	100	100
3	L	52/52 (100%)	52 (100%)	0	100	100
3	Q	48/52 (92%)	48 (100%)	0	100	100
3	R	52/52 (100%)	51 (98%)	1 (2%)	57	71
3	W	49/52 (94%)	48 (98%)	1 (2%)	55	70
3	X	48/52 (92%)	48 (100%)	0	100	100
All	All	4396/4424 (99%)	4337 (99%)	59 (1%)	69	80

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	341	MET
2	B	393	SER
2	B	409	MET
2	B	496	ASN
2	B	511	ARG
2	B	636	THR
2	B	663	CYS
2	B	713	SER
2	D	283	THR
2	D	341	MET
2	D	409	MET
2	D	663	CYS
3	E	70	ASP
2	H	341	MET
2	H	515	ARG
2	H	713	SER
2	J	341	MET
2	J	408	GLU
2	J	409	MET
2	J	484	ASP
2	J	514	ASN
2	J	577	MET
2	J	663	CYS
2	J	713	SER
1	M	179	MET
1	M	240	ASP
2	N	279	VAL
2	N	341	MET
2	N	409	MET
2	N	577	MET
2	N	663	CYS
2	N	689	GLN
2	P	341	MET
2	P	384	ASP
2	P	409	MET
2	P	511	ARG
2	P	628	ARG
2	P	636	THR
2	P	663	CYS
3	R	101	TYR
1	S	220	ASN
1	S	240	ASP
2	T	341	MET

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Mol	Chain	Res	Type
2	T	383	HIS
2	T	393	SER
2	T	409	MET
2	T	519	MET
2	T	577	MET
2	T	663	CYS
2	T	683	GLU
2	T	713	SER
2	V	341	MET
2	V	409	MET
2	V	484	ASP
2	V	519	MET
2	V	663	CYS
2	V	683	GLU
2	V	713	SER
3	W	97	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	71	ASN
2	H	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	$\#\|Z\| > 2$
2	CSO	N	316	2	3,6,7	0.62	0	0,6,8	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CSO	H	316	2	3,6,7	0.50	0	0,6,8	-	-
2	CSO	B	316	2	3,6,7	0.63	0	0,6,8	-	-
2	CSO	P	316	2	3,6,7	0.24	0	0,6,8	-	-
2	CSO	T	316	2	3,6,7	0.53	0	0,6,8	-	-
2	CSO	J	316	2	3,6,7	0.63	0	0,6,8	-	-
2	CSO	V	316	2	3,6,7	0.70	0	0,6,8	-	-
2	CSO	D	316	2	3,6,7	0.48	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
2	CSO	N	316	2	-	0/1/5/7	-
2	CSO	H	316	2	-	0/1/5/7	-
2	CSO	B	316	2	-	0/1/5/7	-
2	CSO	P	316	2	-	0/1/5/7	-
2	CSO	T	316	2	-	0/1/5/7	-
2	CSO	J	316	2	-	0/1/5/7	-
2	CSO	V	316	2	-	0/1/5/7	-
2	CSO	D	316	2	-	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.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

88 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	$\#\|Z\| > 2$
4	NAG	Y	1	4,2	14,14,15	0.31	0	17,19,21	0.87	0
4	NAG	Y	2	4	14,14,15	0.95	1 (7%)	17,19,21	0.67	0
4	BMA	Y	3	4	11,11,12	2.27	6 (54%)	15,15,17	0.92	0
5	NAG	Z	1	2,5	14,14,15	0.88	1 (7%)	17,19,21	0.84	1 (5%)
5	NAG	Z	2	5	14,14,15	0.90	1 (7%)	17,19,21	1.10	2 (11%)
5	BMA	Z	3	5	11,11,12	1.27	1 (9%)	15,15,17	1.27	1 (6%)
5	MAN	Z	4	5	11,11,12	2.31	6 (54%)	15,15,17	1.33	2 (13%)
6	NAG	a	1	2,6	14,14,15	0.40	0	17,19,21	0.78	0
6	NAG	a	2	6	14,14,15	0.49	0	17,19,21	0.78	0
6	BMA	a	3	6	11,11,12	1.47	2 (18%)	15,15,17	1.17	1 (6%)
6	MAN	a	4	6	11,11,12	2.28	5 (45%)	15,15,17	1.92	3 (20%)
6	MAN	a	5	6	11,11,12	1.44	2 (18%)	15,15,17	0.71	0
6	FUC	a	6	6	10,10,11	1.38	2 (20%)	14,14,16	1.58	3 (21%)
7	NAG	b	1	2,7	14,14,15	0.29	0	17,19,21	0.62	0
7	NAG	b	2	7	14,14,15	1.52	2 (14%)	17,19,21	0.70	0
6	NAG	c	1	2,6	14,14,15	0.89	1 (7%)	17,19,21	1.10	1 (5%)
6	NAG	c	2	6	14,14,15	0.51	0	17,19,21	0.57	0
6	BMA	c	3	6	11,11,12	1.12	2 (18%)	15,15,17	1.37	2 (13%)
6	MAN	c	4	6	11,11,12	0.99	1 (9%)	15,15,17	1.56	2 (13%)
6	MAN	c	5	6	11,11,12	1.34	1 (9%)	15,15,17	1.17	0
6	FUC	c	6	6	10,10,11	1.16	0	14,14,16	1.16	1 (7%)
7	NAG	d	1	2,7	14,14,15	0.24	0	17,19,21	1.01	1 (5%)
7	NAG	d	2	7	14,14,15	0.44	0	17,19,21	0.58	0
6	NAG	e	1	2,6	14,14,15	0.42	0	17,19,21	0.86	0
6	NAG	e	2	6	14,14,15	0.42	0	17,19,21	0.37	0
6	BMA	e	3	6	11,11,12	1.42	2 (18%)	15,15,17	1.00	1 (6%)
6	MAN	e	4	6	11,11,12	1.85	4 (36%)	15,15,17	1.34	2 (13%)
6	MAN	e	5	6	11,11,12	1.35	1 (9%)	15,15,17	1.10	1 (6%)
6	FUC	e	6	6	10,10,11	0.92	0	14,14,16	1.11	1 (7%)
4	NAG	f	1	4,2	14,14,15	0.75	1 (7%)	17,19,21	0.89	1 (5%)
4	NAG	f	2	4	14,14,15	0.38	0	17,19,21	0.91	1 (5%)
4	BMA	f	3	4	11,11,12	2.31	5 (45%)	15,15,17	1.17	1 (6%)
7	NAG	g	1	2,7	14,14,15	0.29	0	17,19,21	1.01	1 (5%)
7	NAG	g	2	7	14,14,15	0.42	0	17,19,21	0.75	0
6	NAG	h	1	2,6	14,14,15	0.48	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	h	2	6	14,14,15	0.40	0	17,19,21	0.56	0
6	BMA	h	3	6	11,11,12	0.89	0	15,15,17	0.86	0
6	MAN	h	4	6	11,11,12	1.14	0	15,15,17	1.02	1 (6%)
6	MAN	h	5	6	11,11,12	1.59	2 (18%)	15,15,17	0.97	1 (6%)
6	FUC	h	6	6	10,10,11	1.54	3 (30%)	14,14,16	1.43	2 (14%)
8	NAG	i	1	2,8	14,14,15	0.53	0	17,19,21	0.74	0
8	NAG	i	2	8	14,14,15	0.54	0	17,19,21	0.46	0
8	BMA	i	3	8	11,11,12	2.07	2 (18%)	15,15,17	1.21	2 (13%)
8	MAN	i	4	8	11,11,12	1.94	5 (45%)	15,15,17	1.48	3 (20%)
9	NAG	j	1	2,9	14,14,15	1.00	1 (7%)	17,19,21	0.87	0
9	NAG	j	2	9	14,14,15	0.47	0	17,19,21	0.60	0
9	BMA	j	3	9	11,11,12	1.02	0	15,15,17	1.43	2 (13%)
9	MAN	j	4	9	11,11,12	2.71	7 (63%)	15,15,17	1.48	3 (20%)
9	MAN	j	5	9	11,11,12	2.29	5 (45%)	15,15,17	0.93	0
6	NAG	k	1	2,6	14,14,15	0.30	0	17,19,21	0.85	1 (5%)
6	NAG	k	2	6	14,14,15	0.49	0	17,19,21	0.74	0
6	BMA	k	3	6	11,11,12	1.28	1 (9%)	15,15,17	1.36	2 (13%)
6	MAN	k	4	6	11,11,12	1.82	2 (18%)	15,15,17	1.60	4 (26%)
6	MAN	k	5	6	11,11,12	1.07	0	15,15,17	1.53	3 (20%)
6	FUC	k	6	6	10,10,11	1.63	3 (30%)	14,14,16	1.24	1 (7%)
4	NAG	l	1	4,2	14,14,15	0.41	0	17,19,21	0.41	0
4	NAG	l	2	4	14,14,15	0.64	0	17,19,21	0.59	0
4	BMA	l	3	4	11,11,12	1.78	6 (54%)	15,15,17	1.29	2 (13%)
7	NAG	m	1	2,7	14,14,15	0.71	1 (7%)	17,19,21	0.63	0
7	NAG	m	2	7	14,14,15	0.70	1 (7%)	17,19,21	0.92	1 (5%)
6	NAG	n	1	2,6	14,14,15	0.34	0	17,19,21	0.74	0
6	NAG	n	2	6	14,14,15	0.52	0	17,19,21	0.62	0
6	BMA	n	3	6	11,11,12	1.35	1 (9%)	15,15,17	1.49	2 (13%)
6	MAN	n	4	6	11,11,12	1.51	2 (18%)	15,15,17	1.16	1 (6%)
6	MAN	n	5	6	11,11,12	1.50	1 (9%)	15,15,17	1.09	1 (6%)
6	FUC	n	6	6	10,10,11	0.91	0	14,14,16	1.16	1 (7%)
4	NAG	o	1	4,2	14,14,15	0.74	1 (7%)	17,19,21	0.57	0
4	NAG	o	2	4	14,14,15	0.27	0	17,19,21	0.61	0
4	BMA	o	3	4	11,11,12	2.19	4 (36%)	15,15,17	1.84	5 (33%)
7	NAG	p	1	2,7	14,14,15	0.32	0	17,19,21	1.06	2 (11%)
7	NAG	p	2	7	14,14,15	0.52	0	17,19,21	0.67	0
6	NAG	q	1	2,6	14,14,15	0.67	0	17,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	q	2	6	14,14,15	0.66	1 (7%)	17,19,21	0.73	0
6	BMA	q	3	6	11,11,12	1.03	1 (9%)	15,15,17	0.94	0
6	MAN	q	4	6	11,11,12	2.38	4 (36%)	15,15,17	1.55	2 (13%)
6	MAN	q	5	6	11,11,12	1.88	3 (27%)	15,15,17	0.88	0
6	FUC	q	6	6	10,10,11	0.87	0	14,14,16	1.30	2 (14%)
4	NAG	r	1	4,2	14,14,15	0.64	0	17,19,21	1.00	2 (11%)
4	NAG	r	2	4	14,14,15	0.50	0	17,19,21	0.63	0
4	BMA	r	3	4	11,11,12	2.04	6 (54%)	15,15,17	1.40	2 (13%)
7	NAG	s	1	2,7	14,14,15	0.70	1 (7%)	17,19,21	0.99	1 (5%)
7	NAG	s	2	7	14,14,15	0.63	0	17,19,21	1.46	1 (5%)
6	NAG	t	1	2,6	14,14,15	0.49	0	17,19,21	0.95	1 (5%)
6	NAG	t	2	6	14,14,15	0.66	0	17,19,21	0.63	0
6	BMA	t	3	6	11,11,12	1.40	1 (9%)	15,15,17	1.02	1 (6%)
6	MAN	t	4	6	11,11,12	1.37	1 (9%)	15,15,17	1.40	2 (13%)
6	MAN	t	5	6	11,11,12	1.56	1 (9%)	15,15,17	0.72	0
6	FUC	t	6	6	10,10,11	1.35	2 (20%)	14,14,16	1.19	1 (7%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	c	2	6	-	0/6/23/26	0/1/1/1
6	BMA	c	3	6	-	0/2/19/22	0/1/1/1
6	MAN	c	4	6	-	0/2/19/22	0/1/1/1
6	MAN	c	5	6	-	0/2/19/22	0/1/1/1
6	FUC	c	6	6	-	-	0/1/1/1
7	NAG	d	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	d	2	7	-	0/6/23/26	0/1/1/1
6	NAG	e	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	e	2	6	-	0/6/23/26	0/1/1/1
6	BMA	e	3	6	-	0/2/19/22	0/1/1/1
6	MAN	e	4	6	-	0/2/19/22	0/1/1/1
6	MAN	e	5	6	-	0/2/19/22	0/1/1/1
6	FUC	e	6	6	-	-	0/1/1/1
4	NAG	f	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	f	2	4	-	0/6/23/26	0/1/1/1
4	BMA	f	3	4	-	0/2/19/22	0/1/1/1
7	NAG	g	1	2,7	-	3/6/23/26	0/1/1/1
7	NAG	g	2	7	-	2/6/23/26	0/1/1/1
6	NAG	h	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	h	2	6	-	0/6/23/26	0/1/1/1
6	BMA	h	3	6	-	0/2/19/22	0/1/1/1
6	MAN	h	4	6	-	2/2/19/22	0/1/1/1
6	MAN	h	5	6	-	0/2/19/22	0/1/1/1
6	FUC	h	6	6	-	-	0/1/1/1
8	NAG	i	1	2,8	-	1/6/23/26	0/1/1/1
8	NAG	i	2	8	-	2/6/23/26	0/1/1/1
8	BMA	i	3	8	-	0/2/19/22	0/1/1/1
8	MAN	i	4	8	-	0/2/19/22	1/1/1/1
9	NAG	j	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	j	2	9	-	0/6/23/26	0/1/1/1
9	BMA	j	3	9	-	2/2/19/22	0/1/1/1
9	MAN	j	4	9	-	1/2/19/22	1/1/1/1
9	MAN	j	5	9	-	1/2/19/22	0/1/1/1
6	NAG	k	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	k	2	6	-	0/6/23/26	0/1/1/1
6	BMA	k	3	6	-	0/2/19/22	0/1/1/1
6	MAN	k	4	6	-	1/2/19/22	0/1/1/1
6	MAN	k	5	6	-	0/2/19/22	0/1/1/1
6	FUC	k	6	6	-	-	0/1/1/1
4	NAG	l	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	l	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	l	3	4	-	1/2/19/22	0/1/1/1
7	NAG	m	1	2,7	-	2/6/23/26	0/1/1/1
7	NAG	m	2	7	-	0/6/23/26	0/1/1/1
6	NAG	n	1	2,6	-	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	-	2/2/19/22	1/1/1/1
6	MAN	n	5	6	-	0/2/19/22	0/1/1/1
6	FUC	n	6	6	-	-	0/1/1/1
4	NAG	o	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	o	2	4	-	1/6/23/26	0/1/1/1
4	BMA	o	3	4	-	2/2/19/22	0/1/1/1
7	NAG	p	1	2,7	-	3/6/23/26	0/1/1/1
7	NAG	p	2	7	-	2/6/23/26	0/1/1/1
6	NAG	q	1	2,6	-	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	-	0/2/19/22	0/1/1/1
6	MAN	q	4	6	-	0/2/19/22	0/1/1/1
6	MAN	q	5	6	-	0/2/19/22	0/1/1/1
6	FUC	q	6	6	-	-	0/1/1/1
4	NAG	r	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	r	2	4	-	0/6/23/26	0/1/1/1
4	BMA	r	3	4	-	0/2/19/22	0/1/1/1
7	NAG	s	1	2,7	-	3/6/23/26	0/1/1/1
7	NAG	s	2	7	-	2/6/23/26	0/1/1/1
6	NAG	t	1	2,6	-	0/6/23/26	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	-	1/2/19/22	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

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	q	4	MAN	C2-C3	4.89	1.59	1.52
4	Y	3	BMA	C2-C3	4.63	1.59	1.52
4	f	3	BMA	C2-C3	4.60	1.59	1.52
8	i	3	BMA	C2-C3	4.59	1.59	1.52
9	j	5	MAN	C2-C3	4.55	1.59	1.52
6	h	5	MAN	O5-C1	-4.35	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	o	3	BMA	C1-C2	4.33	1.62	1.52
6	n	5	MAN	O5-C1	-4.22	1.37	1.43
6	k	4	MAN	C1-C2	4.17	1.61	1.52
9	j	4	MAN	O5-C5	4.11	1.51	1.43
7	b	2	NAG	O5-C1	4.04	1.50	1.43
6	n	3	BMA	O5-C5	3.84	1.51	1.43
9	j	4	MAN	C1-C2	3.82	1.60	1.52
6	c	5	MAN	O5-C1	-3.78	1.37	1.43
7	b	2	NAG	C1-C2	3.78	1.58	1.52
6	q	4	MAN	O5-C5	3.77	1.51	1.43
6	a	4	MAN	O5-C5	3.72	1.51	1.43
6	a	4	MAN	C4-C5	3.69	1.60	1.53
9	j	1	NAG	O5-C1	-3.58	1.38	1.43
6	q	5	MAN	O2-C2	3.53	1.50	1.43
5	Z	4	MAN	O5-C5	3.51	1.50	1.43
4	Y	2	NAG	O5-C1	-3.40	1.38	1.43
4	f	3	BMA	C4-C5	3.39	1.60	1.53
6	q	4	MAN	C4-C5	3.37	1.60	1.53
5	Z	4	MAN	C4-C5	3.30	1.60	1.53
4	o	3	BMA	O5-C5	3.26	1.50	1.43
6	t	5	MAN	O5-C1	-3.22	1.38	1.43
8	i	4	MAN	O5-C5	3.19	1.49	1.43
6	k	4	MAN	C4-C5	3.19	1.59	1.53
9	j	5	MAN	C1-C2	3.12	1.59	1.52
5	Z	1	NAG	O5-C1	-3.11	1.38	1.43
9	j	4	MAN	C4-C5	3.11	1.59	1.53
6	t	3	BMA	O5-C5	3.10	1.49	1.43
6	e	4	MAN	C4-C3	3.08	1.60	1.52
4	o	3	BMA	C4-C5	3.08	1.59	1.53
5	Z	2	NAG	O5-C1	3.07	1.48	1.43
6	a	3	BMA	O5-C5	3.05	1.49	1.43
4	r	3	BMA	C4-C5	3.05	1.59	1.53
4	f	3	BMA	O5-C5	3.00	1.49	1.43
6	k	6	FUC	O5-C5	2.99	1.50	1.43
9	j	4	MAN	O4-C4	2.99	1.50	1.43
6	e	4	MAN	C1-C2	2.99	1.59	1.52
6	e	5	MAN	O4-C4	2.95	1.49	1.43
8	i	4	MAN	C2-C3	2.95	1.56	1.52
6	a	4	MAN	C1-C2	2.93	1.58	1.52
6	a	4	MAN	O2-C2	2.90	1.49	1.43
6	e	3	BMA	O5-C5	2.89	1.49	1.43
5	Z	4	MAN	C4-C3	2.88	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	a	4	MAN	C6-C5	2.87	1.61	1.51
5	Z	4	MAN	C2-C3	2.86	1.56	1.52
5	Z	4	MAN	O3-C3	2.81	1.49	1.43
9	j	4	MAN	C4-C3	2.81	1.59	1.52
6	t	6	FUC	O5-C1	-2.79	1.39	1.43
6	a	3	BMA	C2-C3	2.79	1.56	1.52
4	f	3	BMA	O3-C3	2.76	1.49	1.43
6	q	5	MAN	C4-C3	2.74	1.59	1.52
9	j	4	MAN	O5-C1	2.72	1.48	1.43
6	q	5	MAN	O5-C5	2.70	1.48	1.43
6	n	4	MAN	O5-C5	2.66	1.48	1.43
9	j	5	MAN	C4-C3	2.66	1.59	1.52
4	r	3	BMA	C2-C3	2.66	1.56	1.52
4	Y	3	BMA	C1-C2	2.65	1.58	1.52
6	e	4	MAN	O2-C2	2.64	1.48	1.43
6	h	6	FUC	O5-C5	2.64	1.49	1.43
6	c	1	NAG	O5-C1	-2.63	1.39	1.43
9	j	5	MAN	O5-C5	2.63	1.48	1.43
4	l	3	BMA	C1-C2	2.61	1.58	1.52
4	o	1	NAG	O5-C1	-2.58	1.39	1.43
8	i	3	BMA	C4-C3	2.56	1.58	1.52
4	Y	3	BMA	C4-C3	2.55	1.58	1.52
9	j	4	MAN	C2-C3	2.54	1.56	1.52
6	c	3	BMA	O2-C2	-2.51	1.38	1.43
4	r	3	BMA	O3-C3	2.50	1.48	1.43
7	s	1	NAG	O5-C1	2.48	1.47	1.43
7	m	1	NAG	O5-C1	-2.48	1.39	1.43
6	h	6	FUC	C4-C5	2.46	1.58	1.52
6	t	4	MAN	C4-C3	2.46	1.58	1.52
6	a	6	FUC	C1-C2	2.45	1.57	1.52
4	l	3	BMA	C4-C3	2.44	1.58	1.52
5	Z	3	BMA	C6-C5	2.44	1.60	1.51
4	r	3	BMA	C1-C2	2.43	1.57	1.52
6	q	4	MAN	O2-C2	2.43	1.48	1.43
4	r	3	BMA	C6-C5	2.42	1.60	1.51
4	Y	3	BMA	O5-C1	2.41	1.47	1.43
4	Y	3	BMA	O5-C5	2.37	1.48	1.43
8	i	4	MAN	O2-C2	2.32	1.48	1.43
6	c	3	BMA	O5-C5	2.30	1.48	1.43
4	l	3	BMA	O4-C4	2.30	1.48	1.43
6	e	3	BMA	C2-C3	2.29	1.55	1.52
4	o	3	BMA	O3-C3	2.29	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	k	3	BMA	O3-C3	-2.29	1.37	1.43
6	c	4	MAN	C1-C2	2.28	1.57	1.52
6	a	5	MAN	O2-C2	2.27	1.48	1.43
4	l	3	BMA	C2-C3	2.24	1.55	1.52
5	Z	4	MAN	C1-C2	2.23	1.57	1.52
9	j	5	MAN	C4-C5	2.23	1.57	1.53
6	n	4	MAN	O6-C6	2.23	1.51	1.42
4	f	1	NAG	O5-C1	2.23	1.47	1.43
4	r	3	BMA	C4-C3	2.21	1.58	1.52
4	l	3	BMA	C4-C5	2.20	1.57	1.53
6	k	6	FUC	O5-C1	-2.19	1.40	1.43
6	t	6	FUC	C4-C5	-2.18	1.47	1.52
6	a	6	FUC	O5-C5	2.18	1.48	1.43
7	m	2	NAG	O5-C1	2.17	1.47	1.43
6	h	6	FUC	C1-C2	2.15	1.57	1.52
6	q	3	BMA	O5-C1	-2.08	1.40	1.43
6	a	5	MAN	O5-C1	-2.08	1.40	1.43
6	q	2	NAG	O5-C1	-2.08	1.40	1.43
4	f	3	BMA	C4-C3	2.07	1.57	1.52
6	e	4	MAN	O5-C5	2.05	1.47	1.43
8	i	4	MAN	C4-C3	2.04	1.57	1.52
6	h	5	MAN	C1-C2	-2.04	1.47	1.52
4	Y	3	BMA	O2-C2	2.03	1.47	1.43
8	i	4	MAN	C4-C5	2.03	1.57	1.53
6	k	6	FUC	O2-C2	2.02	1.47	1.43
4	l	3	BMA	O5-C5	2.00	1.47	1.43

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	s	2	NAG	C1-O5-C5	4.96	118.91	112.19
6	a	4	MAN	C1-O5-C5	4.94	118.89	112.19
8	i	4	MAN	C1-O5-C5	4.30	118.02	112.19
6	c	3	BMA	O2-C2-C3	-4.28	101.57	110.14
6	q	4	MAN	O5-C1-C2	-4.18	104.32	110.77
6	t	4	MAN	C1-O5-C5	3.70	117.20	112.19
4	o	3	BMA	O2-C2-C3	-3.67	102.78	110.14
5	Z	3	BMA	O5-C5-C6	3.62	112.88	107.20
6	n	3	BMA	O5-C5-C6	3.42	112.56	107.20
6	k	5	MAN	C1-C2-C3	-3.37	105.52	109.67
6	k	6	FUC	O2-C2-C1	3.36	116.03	109.15
6	n	3	BMA	O5-C1-C2	-3.35	105.59	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	a	6	FUC	C1-C2-C3	3.35	113.78	109.67
4	r	3	BMA	C1-O5-C5	3.35	116.73	112.19
4	o	3	BMA	C1-C2-C3	3.28	113.70	109.67
6	h	6	FUC	C1-C2-C3	3.28	113.70	109.67
6	t	3	BMA	O2-C2-C3	-3.25	103.64	110.14
6	q	6	FUC	O2-C2-C1	3.17	115.64	109.15
6	c	4	MAN	C1-O5-C5	3.15	116.46	112.19
6	a	4	MAN	O5-C1-C2	3.09	115.55	110.77
6	k	5	MAN	C1-O5-C5	3.09	116.37	112.19
7	d	1	NAG	C1-O5-C5	3.07	116.35	112.19
4	o	3	BMA	O5-C1-C2	3.05	115.47	110.77
6	n	6	FUC	O2-C2-C1	3.05	115.39	109.15
6	n	4	MAN	C1-O5-C5	3.03	116.29	112.19
6	e	6	FUC	O2-C2-C1	3.00	115.28	109.15
6	e	4	MAN	C1-O5-C5	2.97	116.22	112.19
9	j	3	BMA	C2-C3-C4	2.96	116.02	110.89
6	e	5	MAN	C1-O5-C5	2.87	116.08	112.19
8	i	3	BMA	C2-C3-C4	2.83	115.79	110.89
9	j	4	MAN	O2-C2-C1	2.83	114.93	109.15
5	Z	2	NAG	C1-O5-C5	2.77	115.95	112.19
9	j	4	MAN	O5-C5-C6	2.73	111.49	107.20
5	Z	4	MAN	C1-O5-C5	2.72	115.88	112.19
6	k	3	BMA	O5-C1-C2	-2.72	106.58	110.77
6	t	6	FUC	C2-C3-C4	-2.66	106.28	110.89
6	t	1	NAG	C1-O5-C5	2.65	115.79	112.19
4	o	3	BMA	C1-O5-C5	2.65	115.78	112.19
7	p	1	NAG	C4-C3-C2	-2.64	107.15	111.02
4	f	3	BMA	O3-C3-C2	2.61	114.99	109.99
6	c	3	BMA	C1-C2-C3	2.61	112.87	109.67
4	f	2	NAG	C1-O5-C5	2.61	115.72	112.19
7	m	2	NAG	C1-O5-C5	2.61	115.72	112.19
5	Z	2	NAG	C4-C3-C2	-2.54	107.30	111.02
8	i	4	MAN	O5-C1-C2	2.53	114.68	110.77
4	r	1	NAG	C1-O5-C5	2.50	115.57	112.19
6	a	6	FUC	O2-C2-C1	2.49	114.24	109.15
7	s	1	NAG	C1-C2-N2	2.49	114.74	110.49
6	c	6	FUC	O2-C2-C1	2.46	114.18	109.15
6	h	6	FUC	O2-C2-C1	2.44	114.15	109.15
4	r	3	BMA	O3-C3-C2	2.44	114.67	109.99
5	Z	4	MAN	O2-C2-C3	-2.44	105.25	110.14
4	o	3	BMA	O2-C2-C1	2.43	114.13	109.15
6	k	3	BMA	O3-C3-C4	-2.42	104.76	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	k	4	MAN	O4-C4-C3	-2.41	104.77	110.35
6	a	6	FUC	O2-C2-C3	-2.40	105.33	110.14
6	k	1	NAG	C1-O5-C5	2.39	115.43	112.19
6	e	3	BMA	C2-C3-C4	2.37	114.99	110.89
8	i	3	BMA	C3-C4-C5	2.34	114.42	110.24
6	k	4	MAN	O2-C2-C1	2.33	113.92	109.15
4	f	1	NAG	O3-C3-C2	-2.29	104.72	109.47
4	l	3	BMA	O2-C2-C3	-2.28	105.57	110.14
6	e	4	MAN	O2-C2-C1	2.26	113.78	109.15
9	j	3	BMA	C3-C4-C5	2.26	114.27	110.24
6	t	4	MAN	C1-C2-C3	-2.26	106.89	109.67
8	i	4	MAN	O3-C3-C2	2.24	114.28	109.99
6	c	4	MAN	O2-C2-C3	-2.23	105.68	110.14
6	a	3	BMA	O5-C5-C6	2.22	110.68	107.20
6	a	4	MAN	O4-C4-C3	-2.20	105.26	110.35
4	l	3	BMA	O5-C1-C2	2.20	114.16	110.77
6	h	5	MAN	O2-C2-C3	-2.17	105.80	110.14
6	h	4	MAN	C1-C2-C3	-2.16	107.01	109.67
6	k	4	MAN	O2-C2-C3	-2.15	105.84	110.14
7	p	1	NAG	C1-C2-N2	2.14	114.15	110.49
7	g	1	NAG	C4-C3-C2	-2.14	107.88	111.02
9	j	4	MAN	C1-O5-C5	2.13	115.08	112.19
6	n	5	MAN	O5-C1-C2	-2.12	107.49	110.77
5	Z	1	NAG	O4-C4-C5	-2.11	104.07	109.30
6	c	1	NAG	O3-C3-C2	2.11	113.82	109.47
6	k	4	MAN	C2-C3-C4	-2.10	107.26	110.89
6	q	6	FUC	C2-C3-C4	-2.07	107.31	110.89
6	q	4	MAN	C6-C5-C4	2.06	117.83	113.00
6	k	5	MAN	O6-C6-C5	-2.04	104.28	111.29
4	r	1	NAG	O4-C4-C3	-2.02	105.67	110.35

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	p	1	NAG	C1-C2-N2-C7
5	Z	3	BMA	O5-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
7	m	1	NAG	C4-C5-C6-O6
4	o	3	BMA	O5-C5-C6-O6
5	Z	3	BMA	C4-C5-C6-O6
7	g	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
7	s	1	NAG	C1-C2-N2-C7
6	a	4	MAN	C4-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
6	a	4	MAN	O5-C5-C6-O6
9	j	3	BMA	O5-C5-C6-O6
6	n	4	MAN	O5-C5-C6-O6
7	s	1	NAG	C4-C5-C6-O6
7	m	1	NAG	O5-C5-C6-O6
9	j	3	BMA	C4-C5-C6-O6
7	b	1	NAG	C4-C5-C6-O6
7	s	2	NAG	O5-C5-C6-O6
4	o	3	BMA	C4-C5-C6-O6
7	s	1	NAG	O5-C5-C6-O6
4	l	3	BMA	O5-C5-C6-O6
6	k	4	MAN	O5-C5-C6-O6
7	b	1	NAG	O5-C5-C6-O6
7	p	1	NAG	C4-C5-C6-O6
9	j	5	MAN	O5-C5-C6-O6
6	n	4	MAN	C4-C5-C6-O6
6	t	4	MAN	O5-C5-C6-O6
7	p	2	NAG	C4-C5-C6-O6
8	i	2	NAG	C4-C5-C6-O6
9	j	4	MAN	C4-C5-C6-O6
7	g	2	NAG	C4-C5-C6-O6
6	h	4	MAN	C4-C5-C6-O6
7	p	2	NAG	O5-C5-C6-O6
8	i	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	C3-C2-N2-C7
8	i	1	NAG	C4-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	o	2	NAG	C4-C5-C6-O6
6	h	4	MAN	O5-C5-C6-O6
7	p	1	NAG	O5-C5-C6-O6
7	s	2	NAG	C4-C5-C6-O6

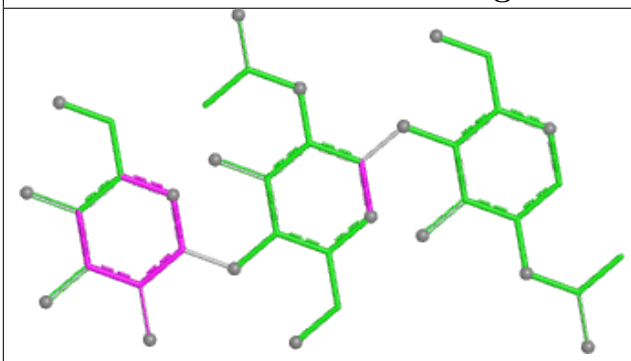
All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	j	4	MAN	C1-C2-C3-C4-C5-O5
8	i	4	MAN	C1-C2-C3-C4-C5-O5
6	n	4	MAN	C1-C2-C3-C4-C5-O5

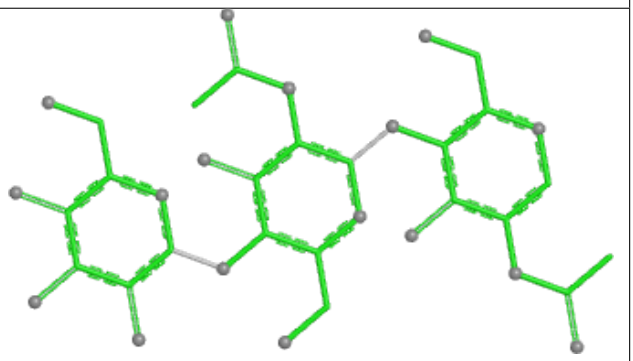
No monomer is involved in short contacts.

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

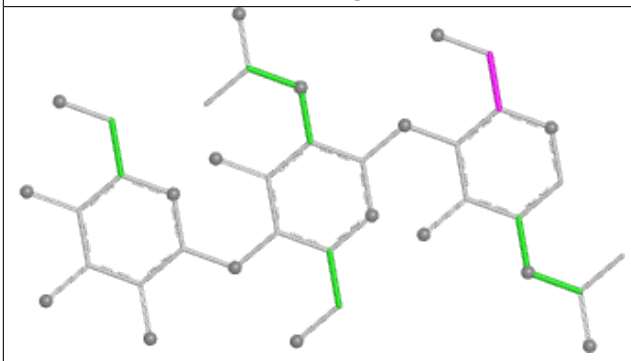
Oligosaccharide Chain Y



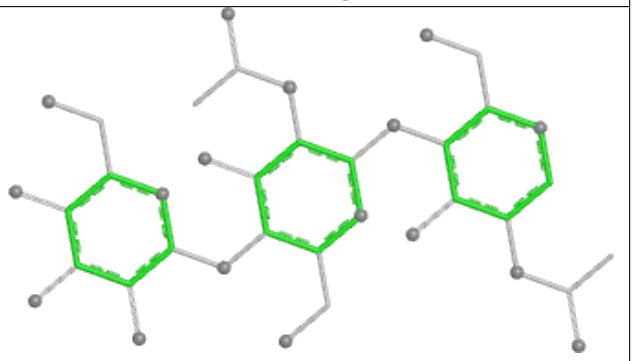
Bond lengths



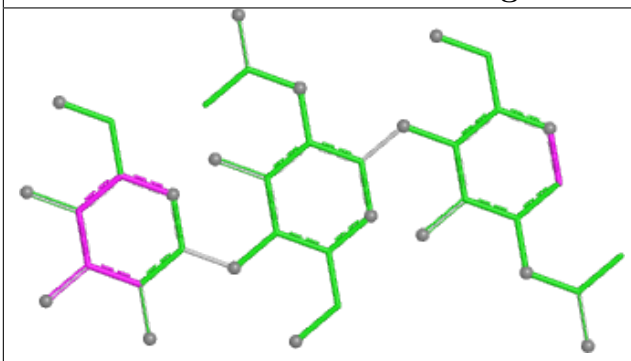
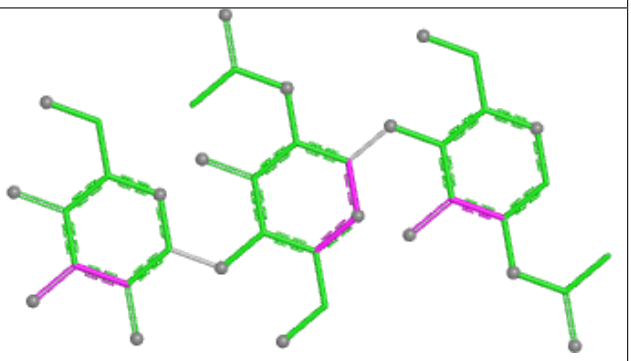
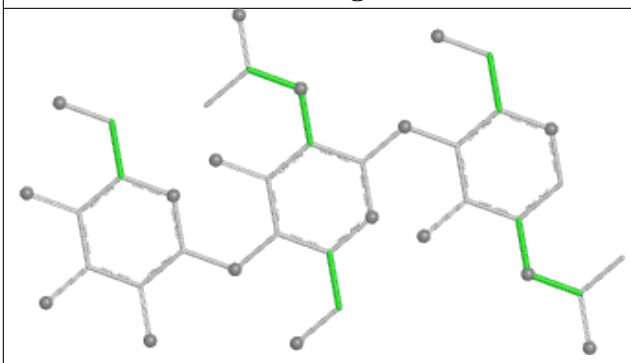
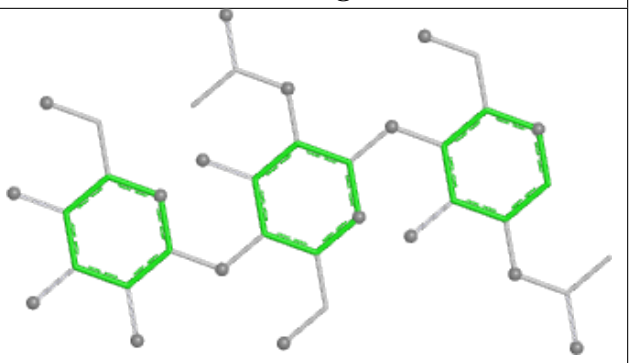
Bond angles

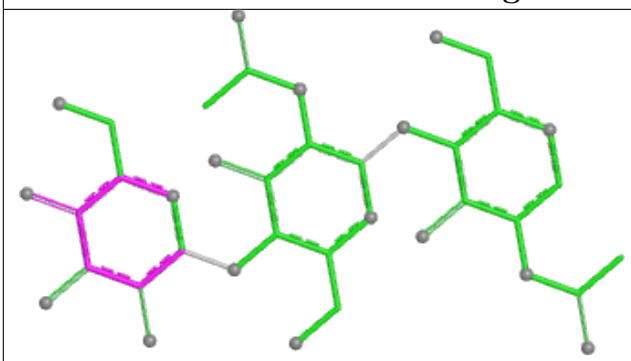
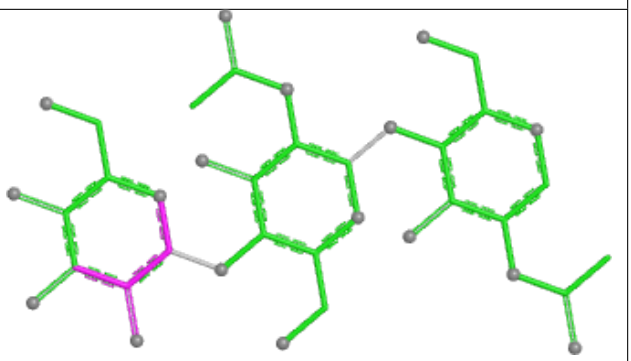
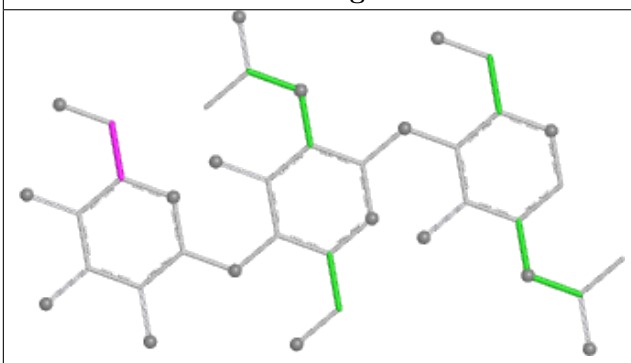
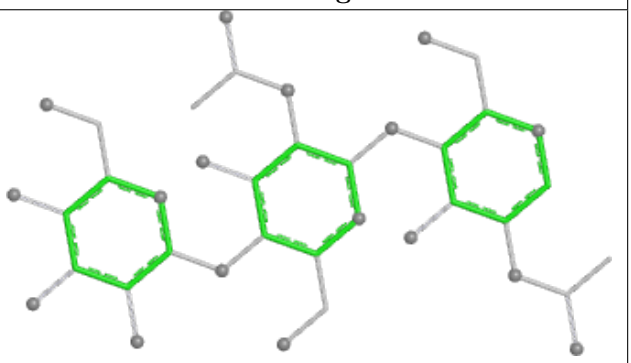


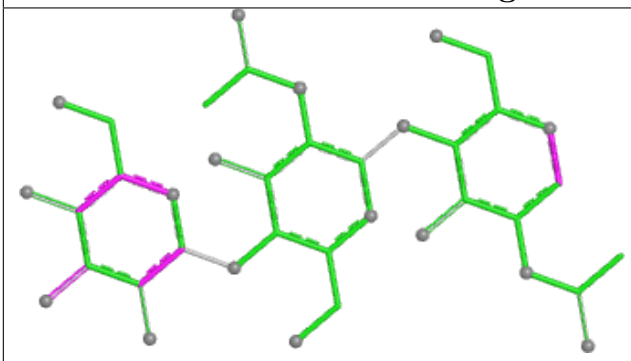
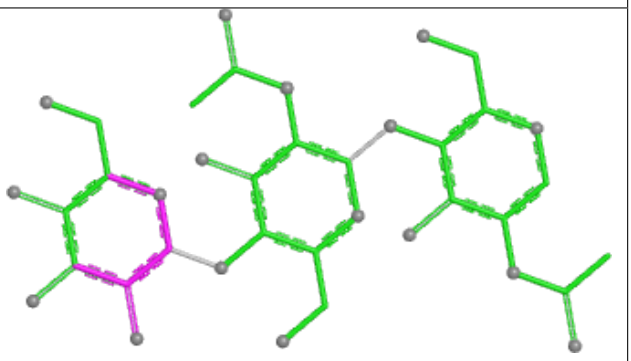
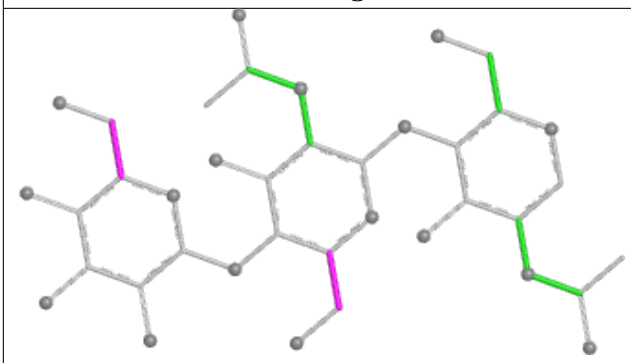
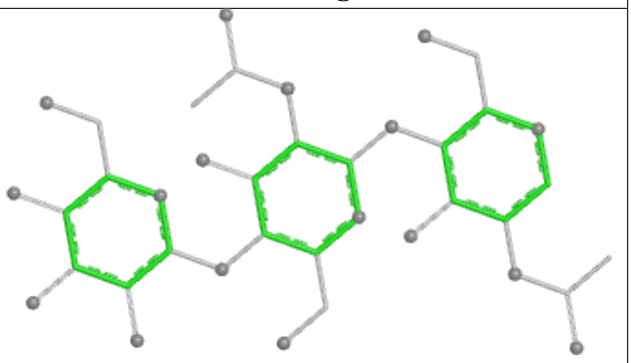
Torsions

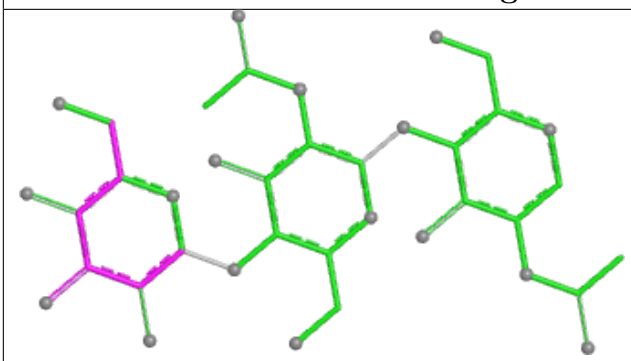
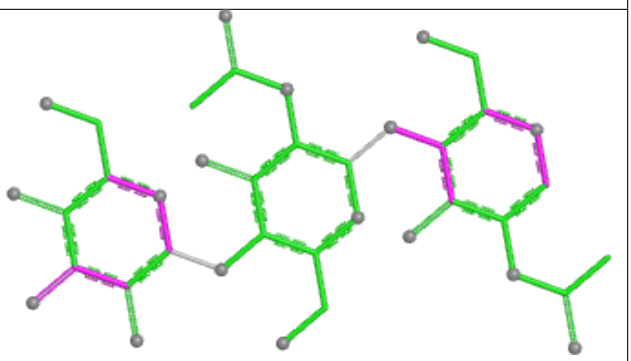
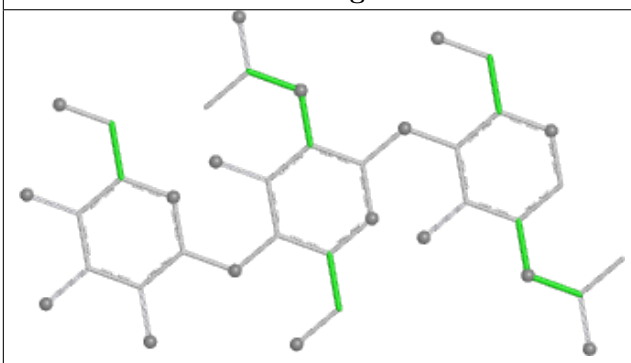
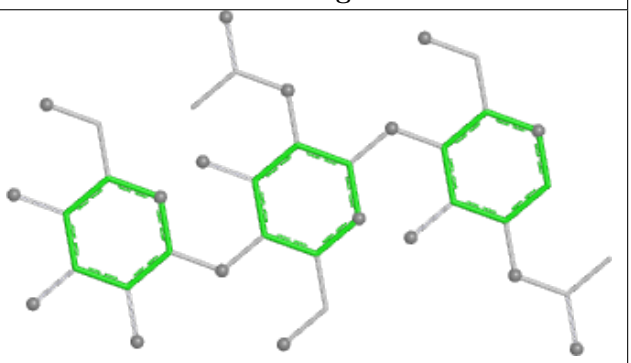


Rings

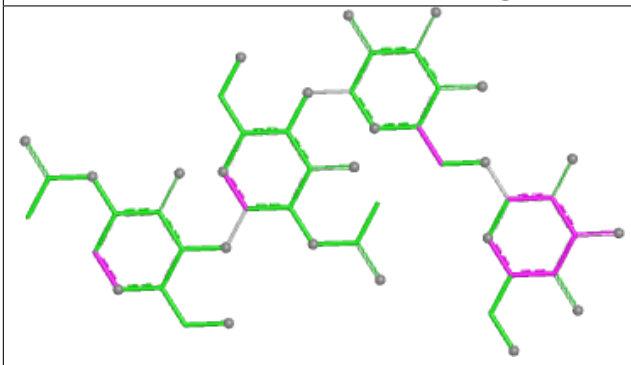
Oligosaccharide Chain f	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain l	
 Bond lengths	 Bond angles
 Torsions	 Rings

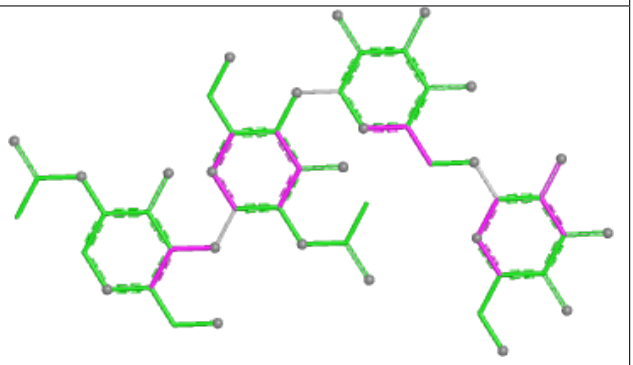
Oligosaccharide Chain o	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain r	
 Bond lengths	 Bond angles
 Torsions	 Rings

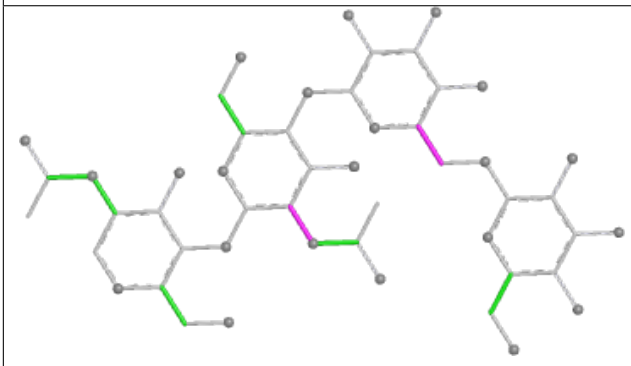
Oligosaccharide Chain Z



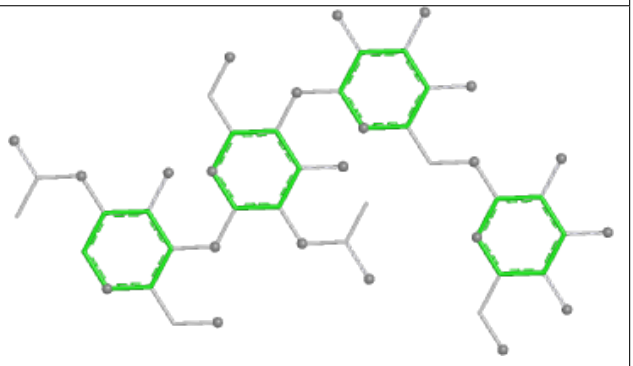
Bond lengths



Bond angles

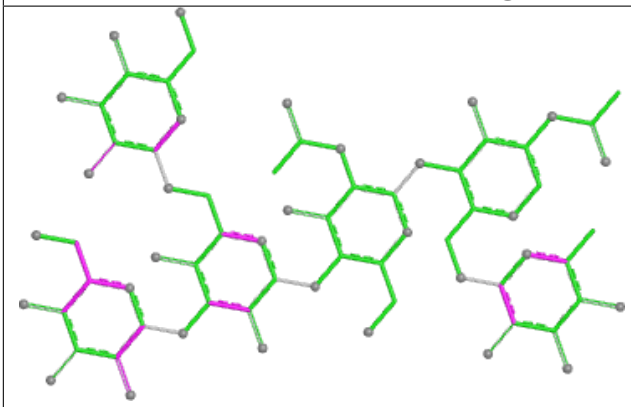


Torsions



Rings

Oligosaccharide Chain a



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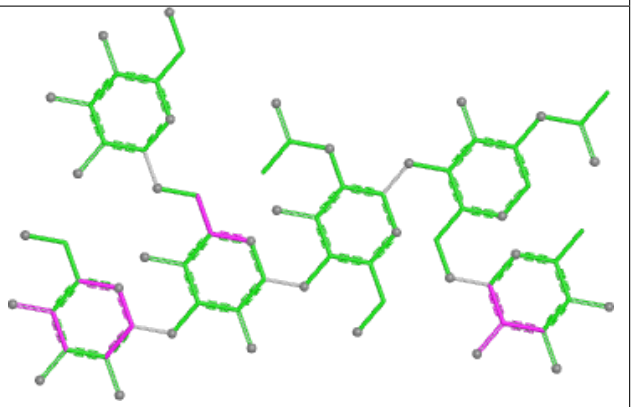

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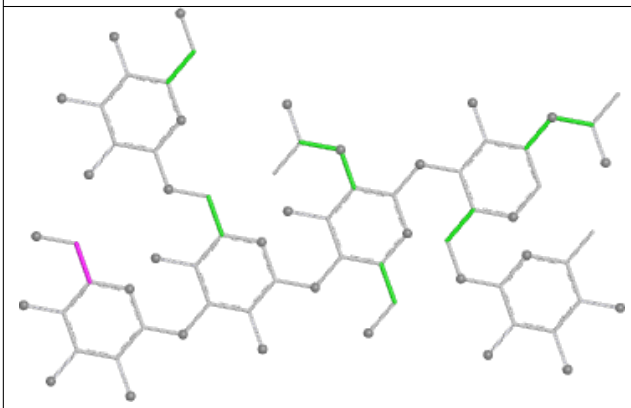

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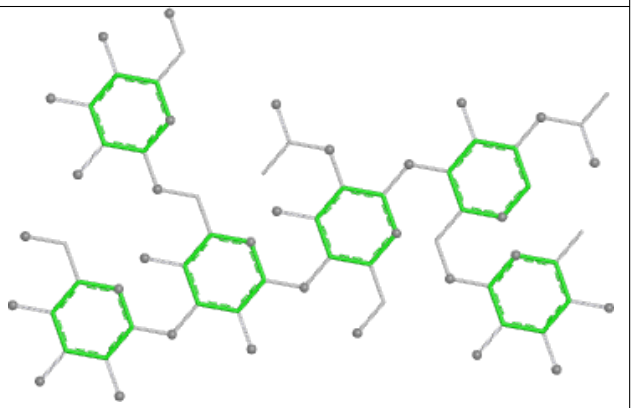
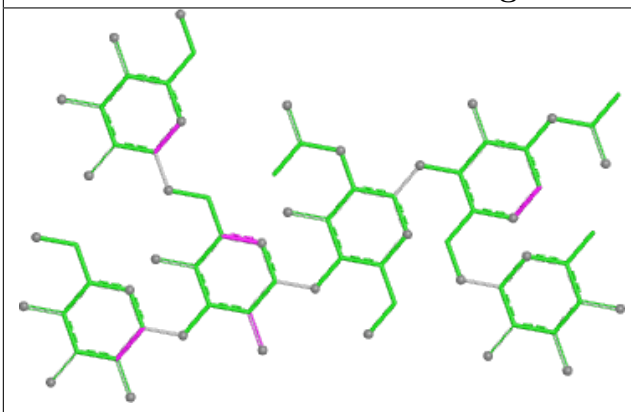


Rings

Oligosaccharide Chain c



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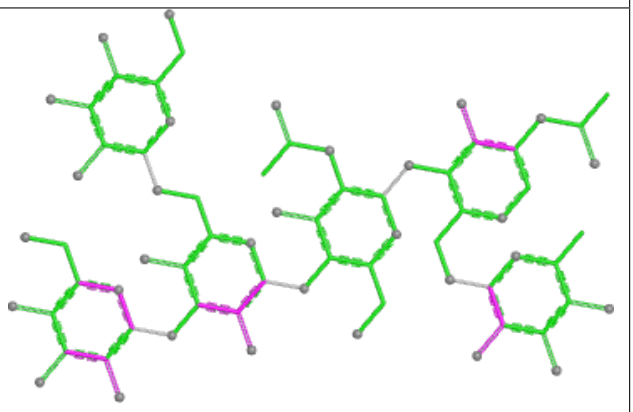

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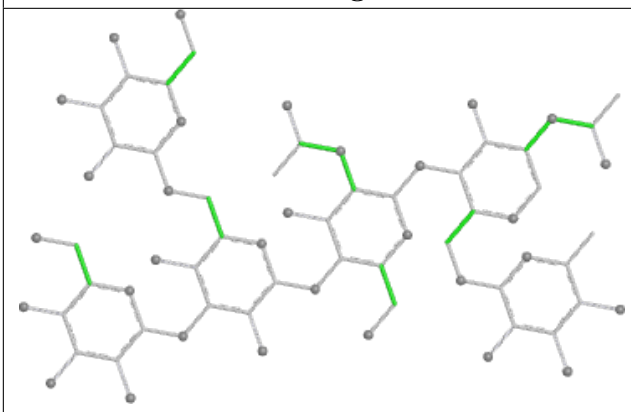

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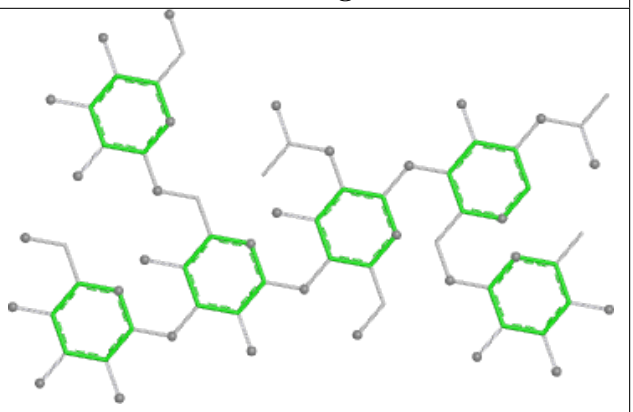
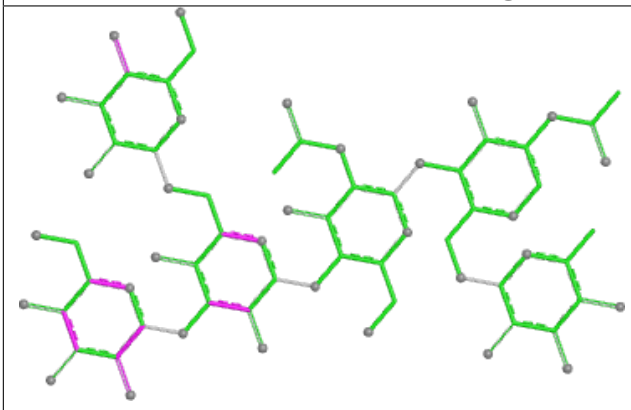


Rings

Oligosaccharide Chain e



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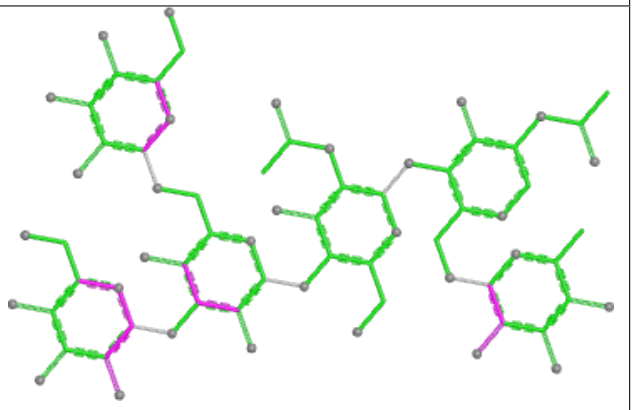

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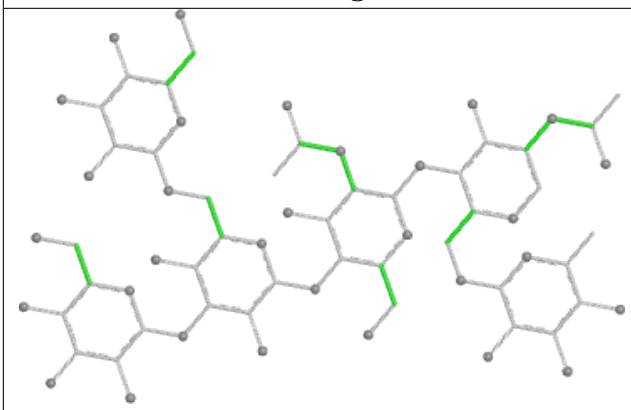

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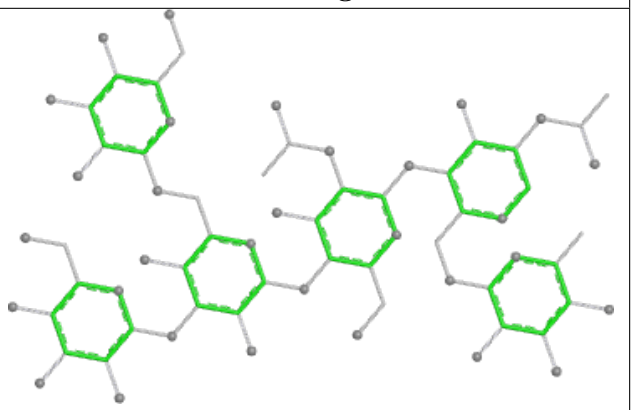
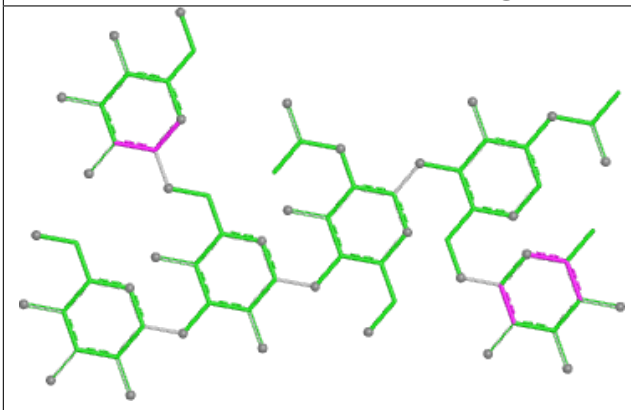


Rings

Oligosaccharide Chain h



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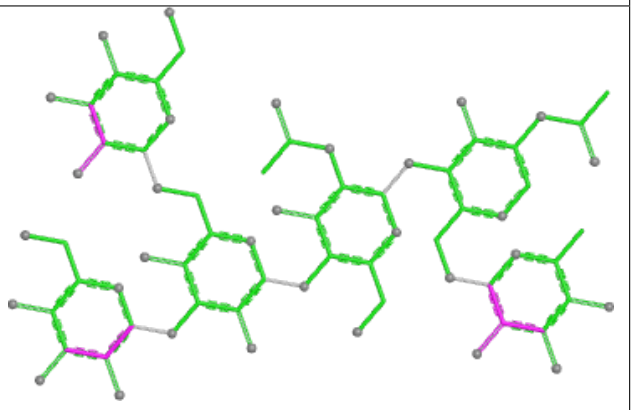

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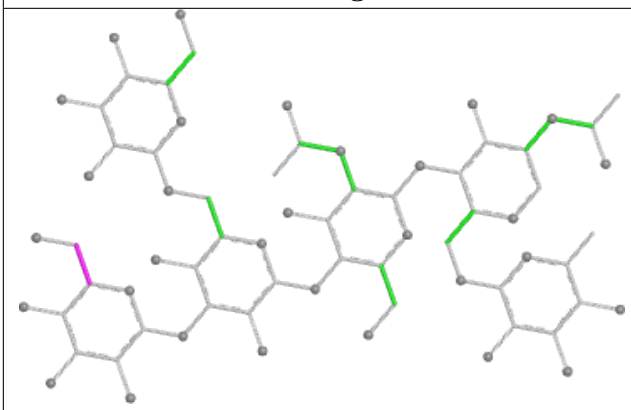

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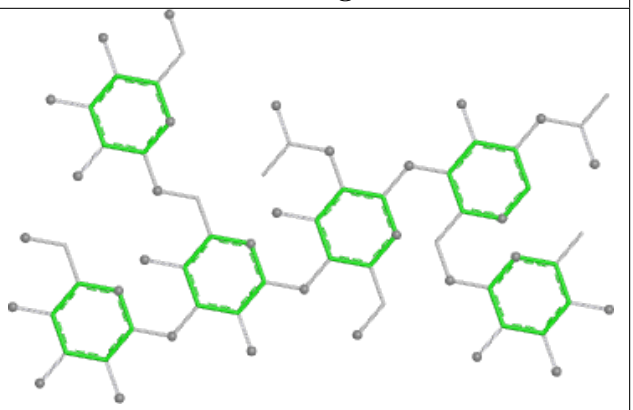
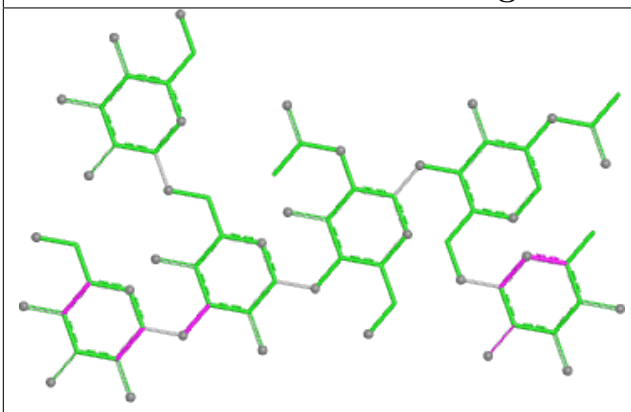


Rings

Oligosaccharide Chain k



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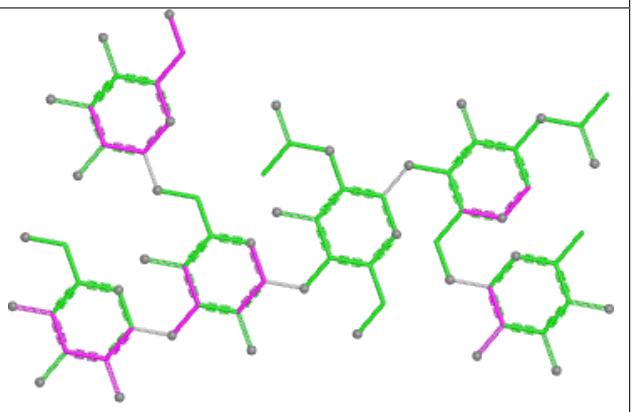
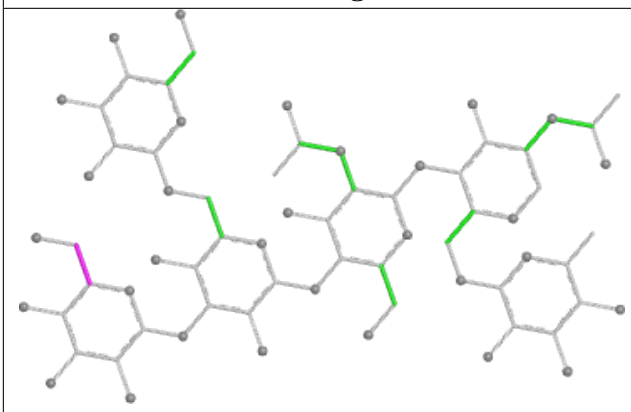


Bond angles



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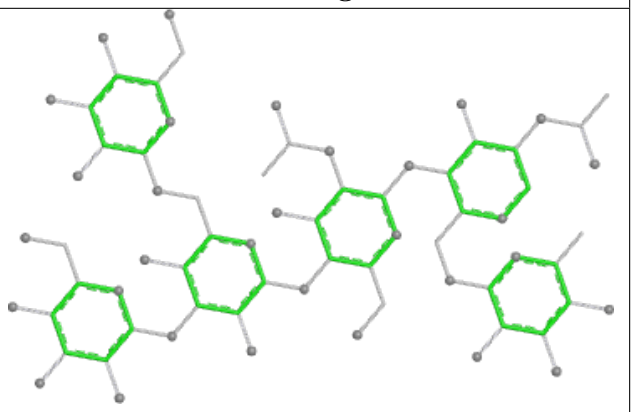
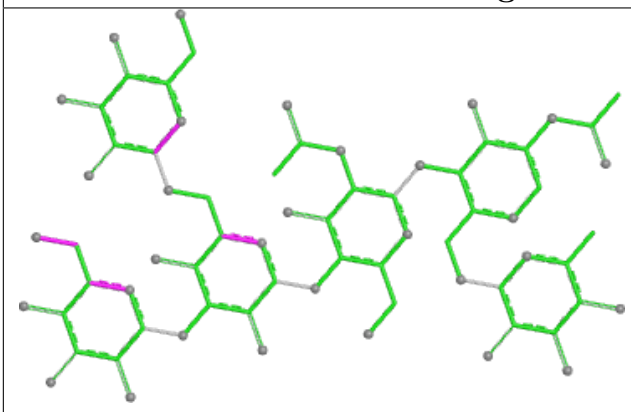
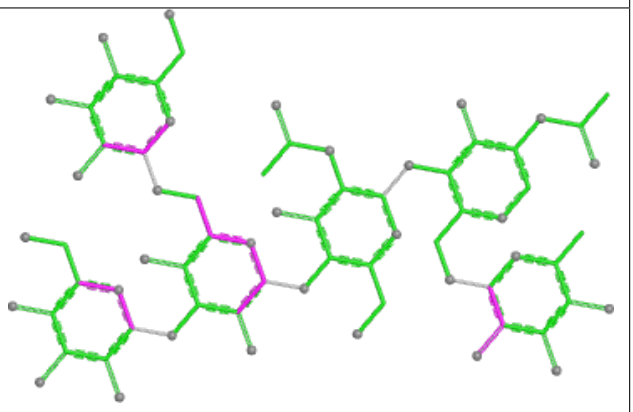
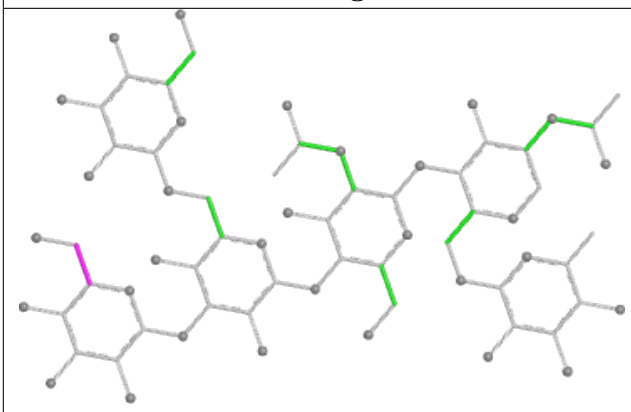
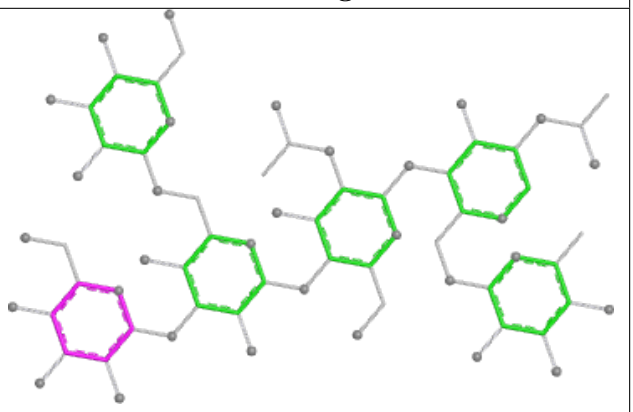
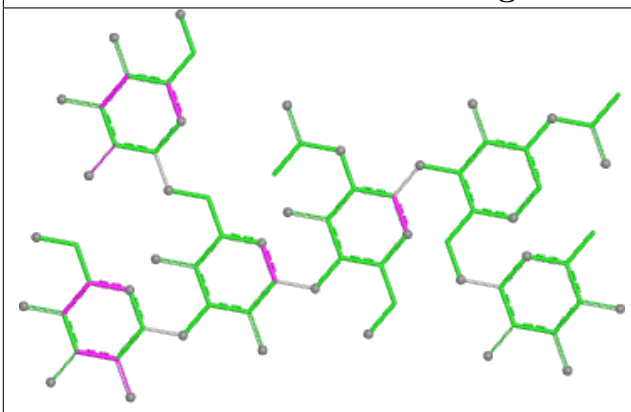


Rings

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

Oligosaccharide Chain q



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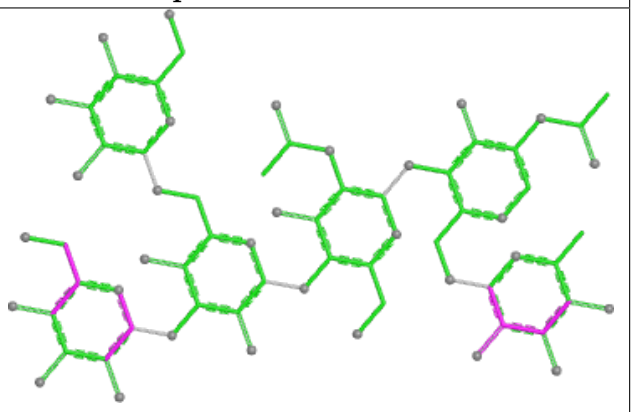
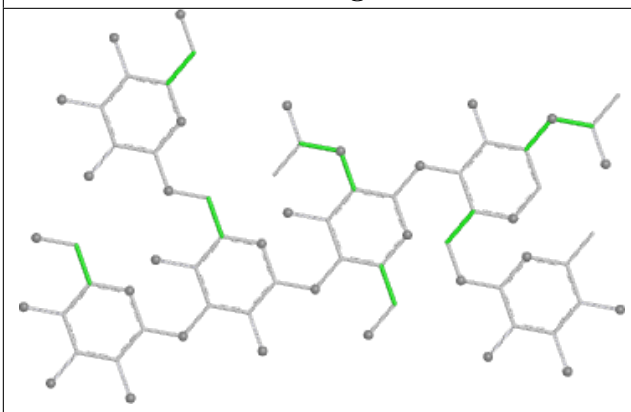


Bond angles



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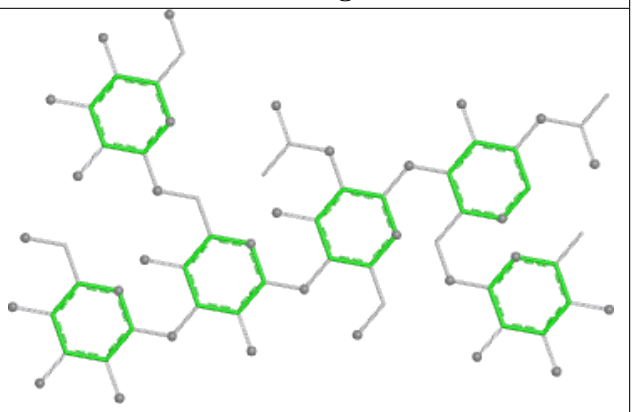
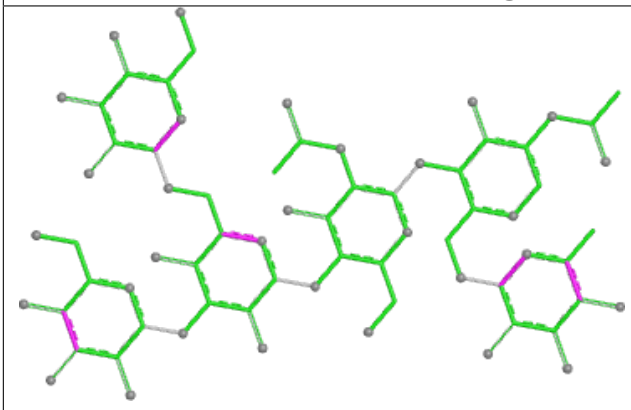


Rings

Oligosaccharide Chain t



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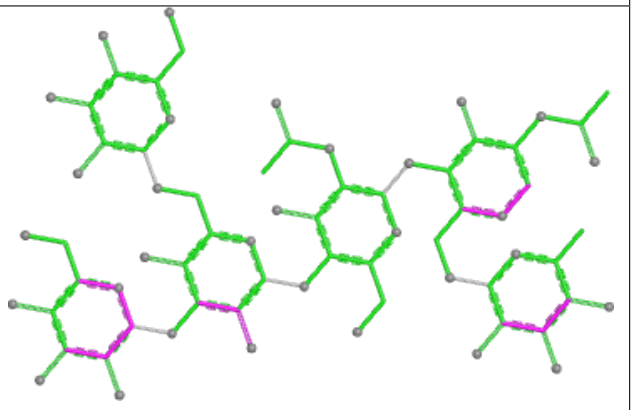
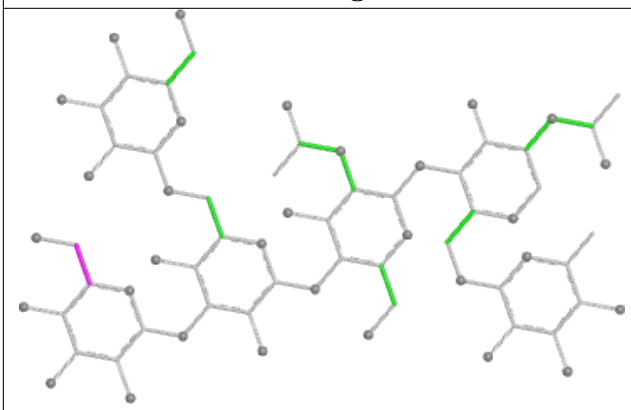


Bond angles



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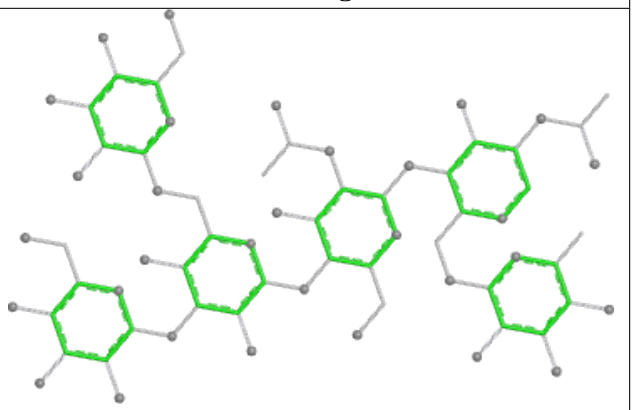
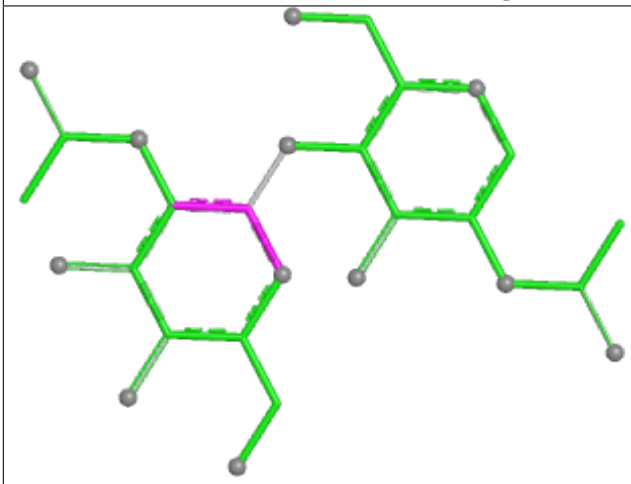


Rings

Oligosaccharide Chain b



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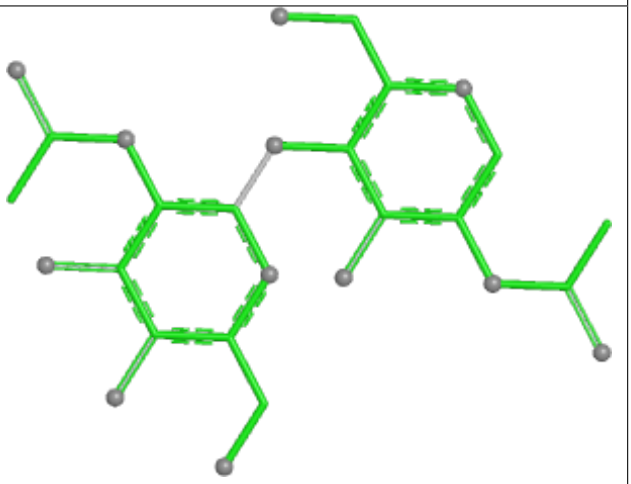
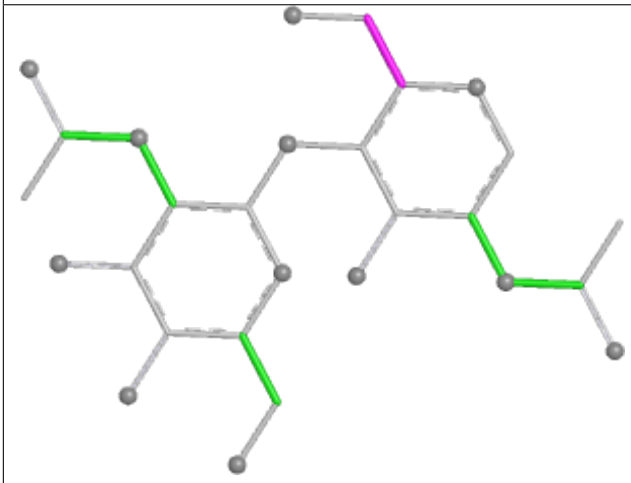


Bond angles



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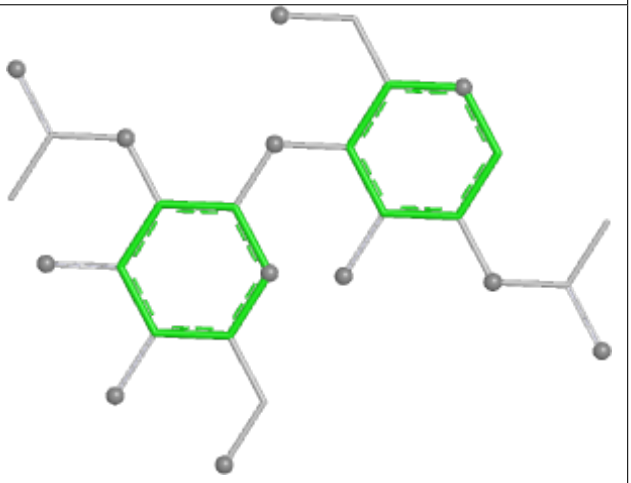
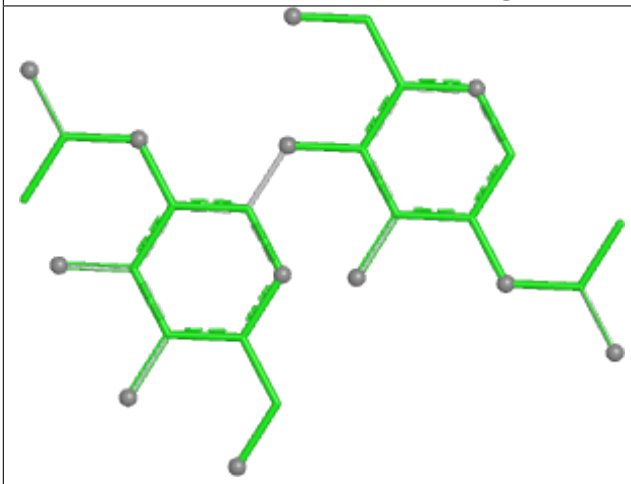


Rings

Oligosaccharide Chain d



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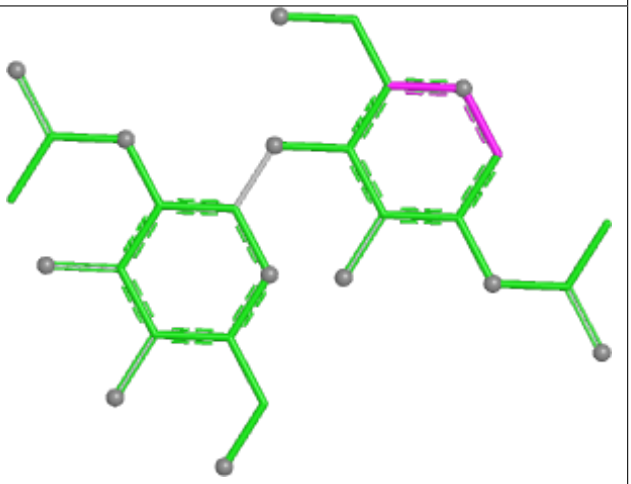
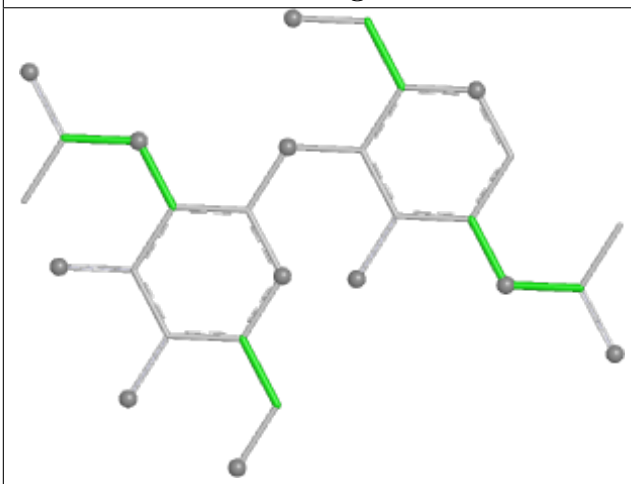


Bond angles



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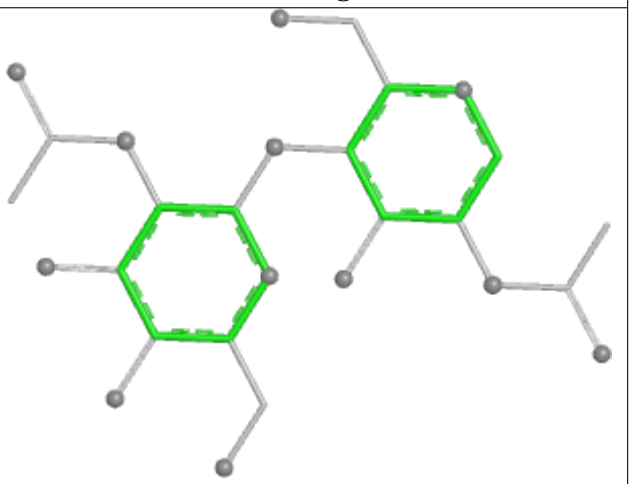
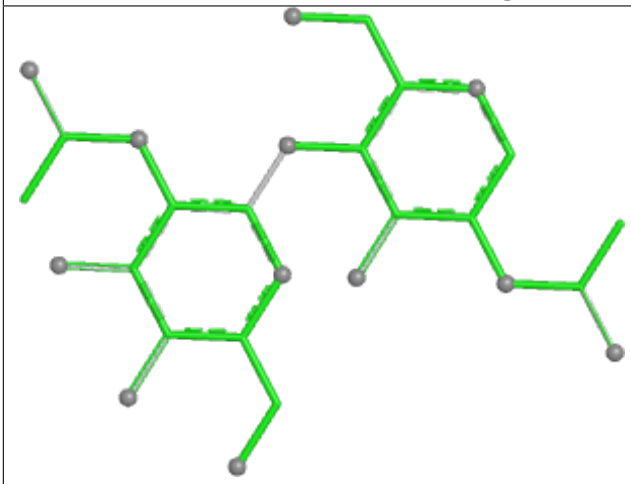


Rings

Oligosaccharide Chain g



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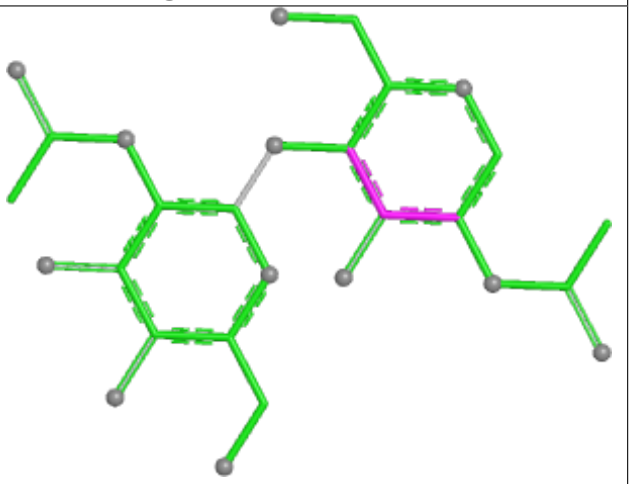
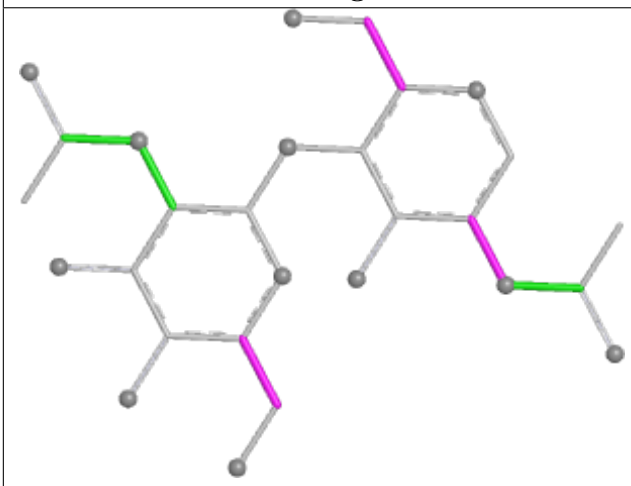
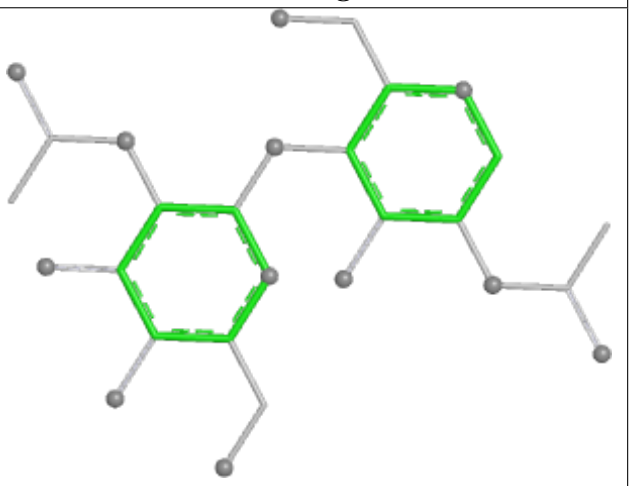


Bond angles

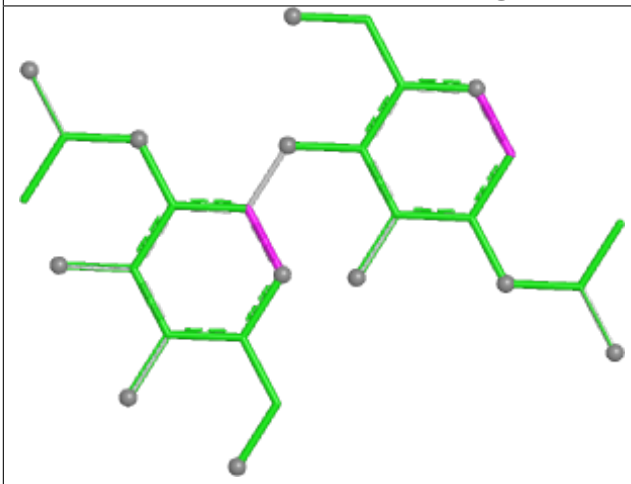


Torsions



Rings

Oligosaccharide Chain m



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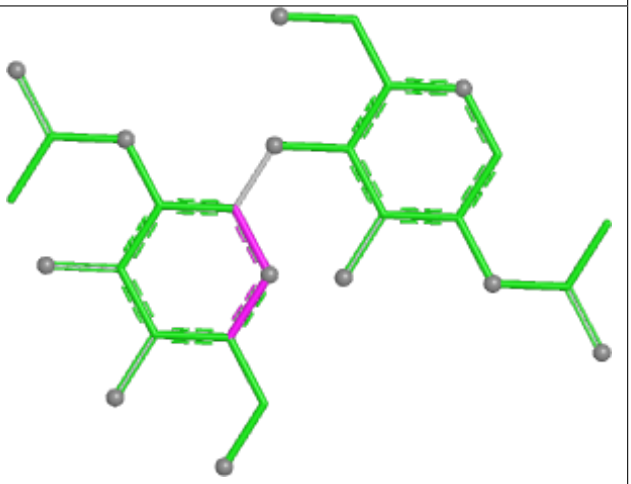
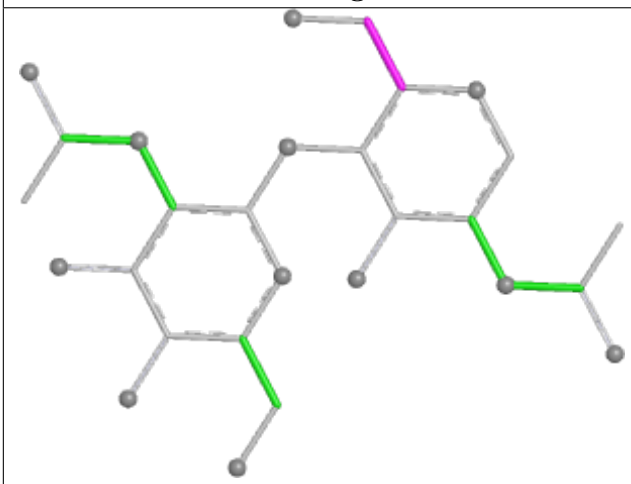


Bond angles



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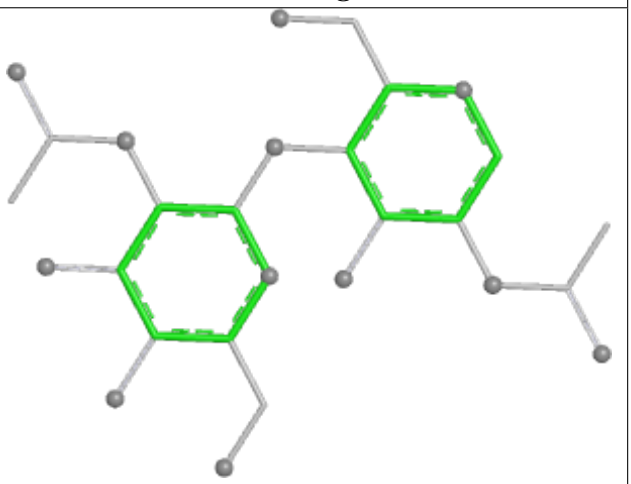
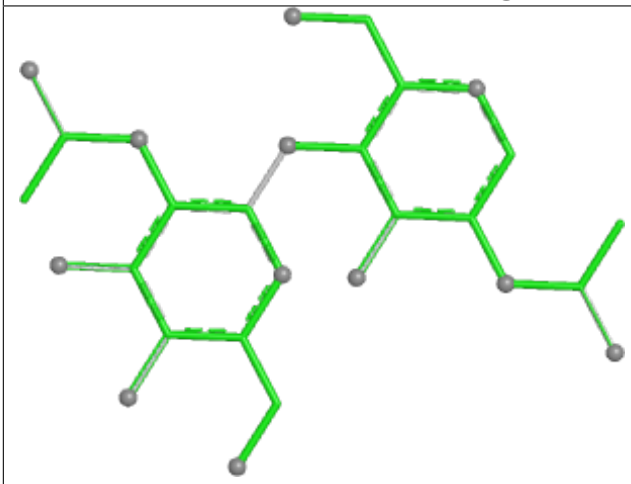
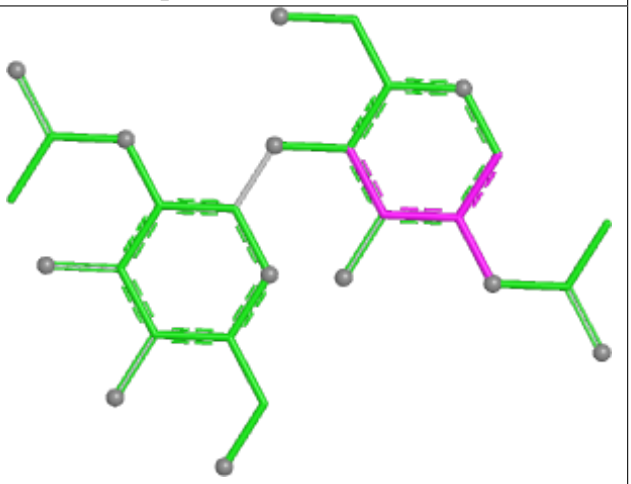


Rings

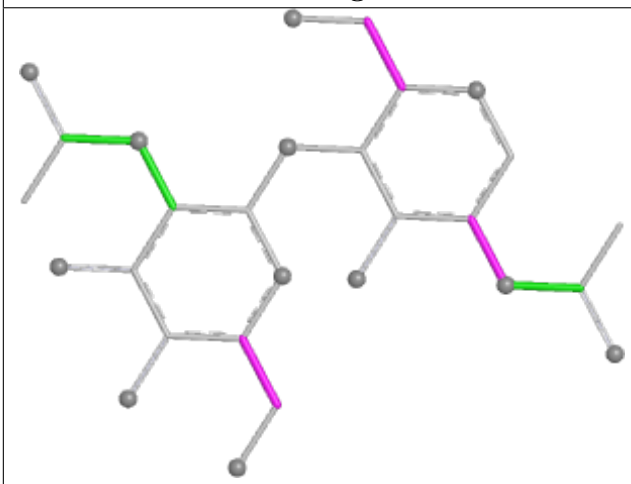
Oligosaccharide Chain p



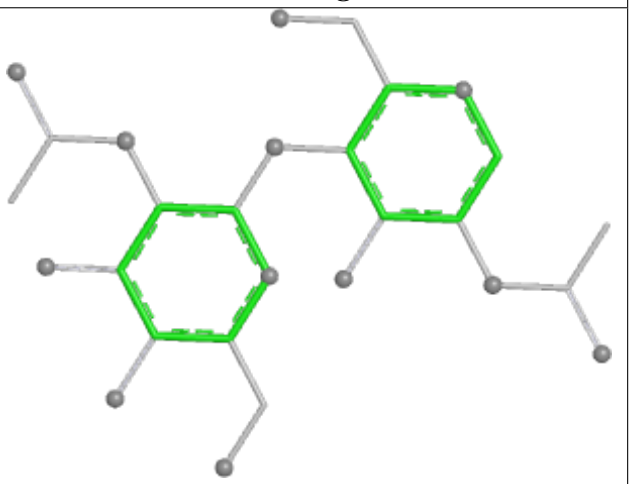
Bond lengths



Bond angles

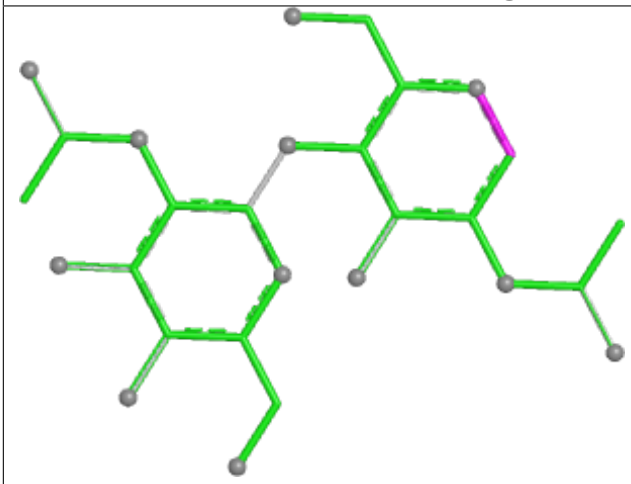


Torsions



Rings

Oligosaccharide Chain s



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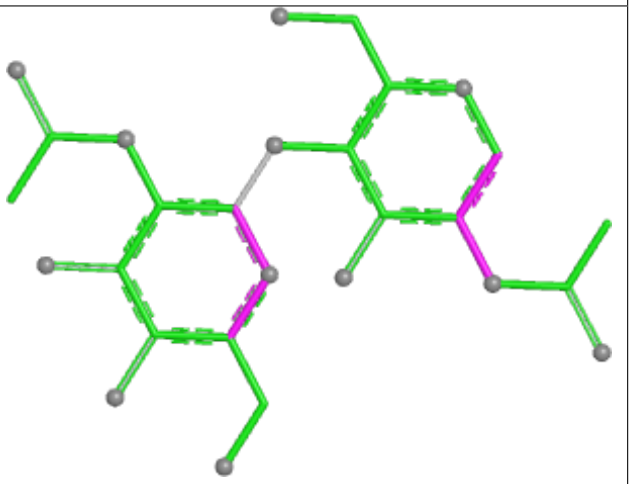
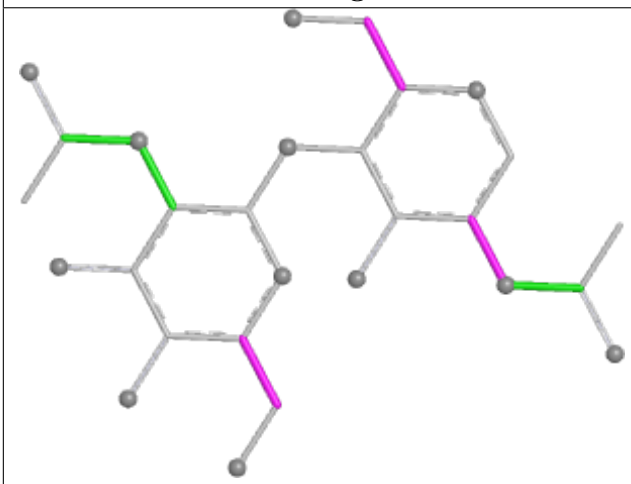
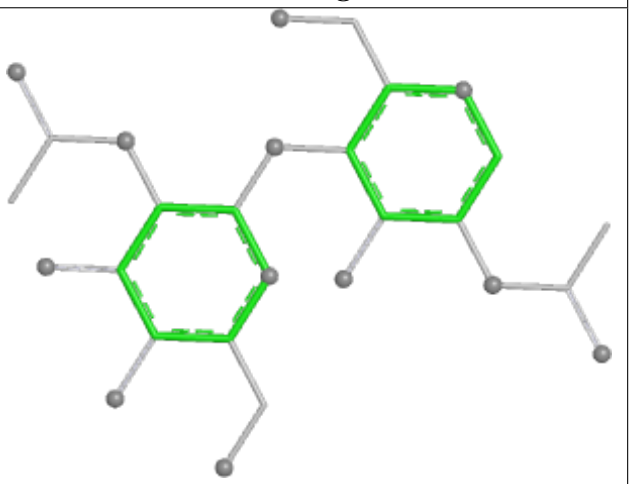


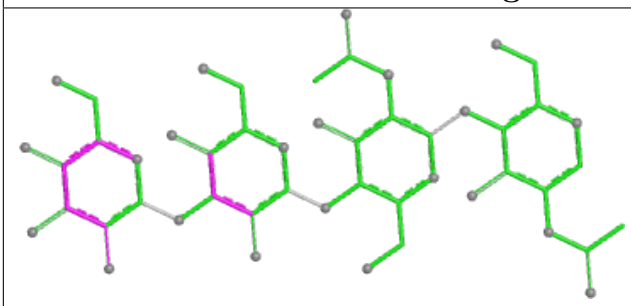
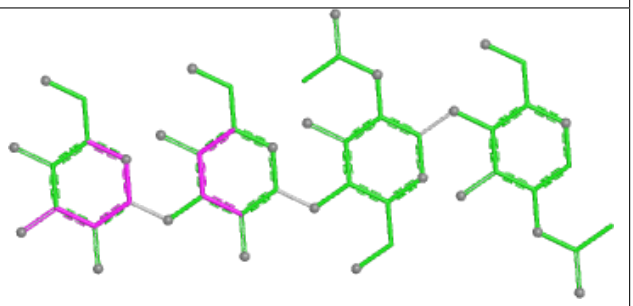
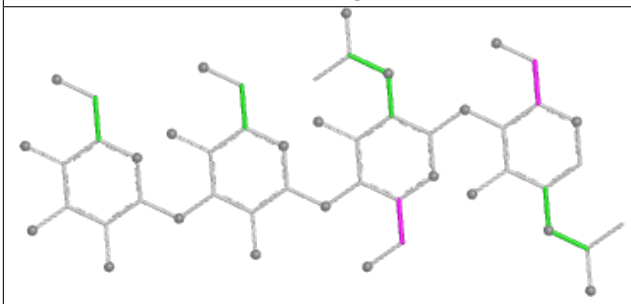
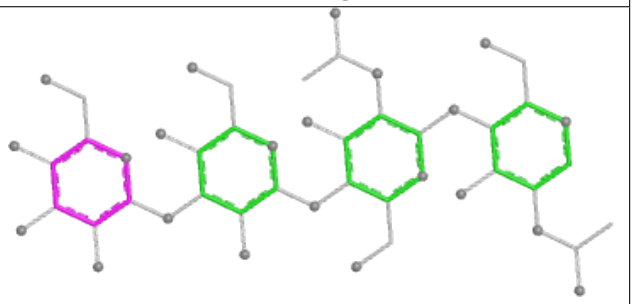
Bond angles

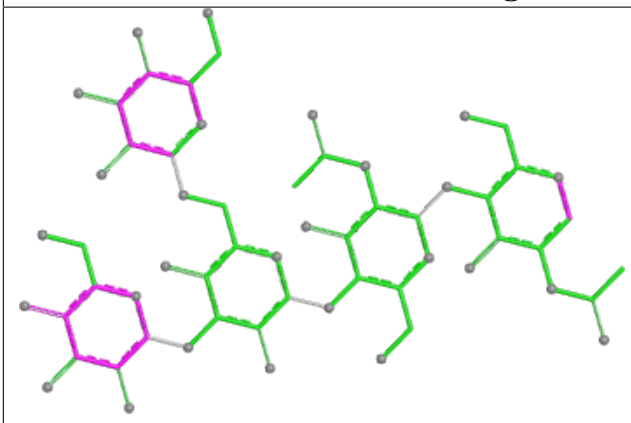
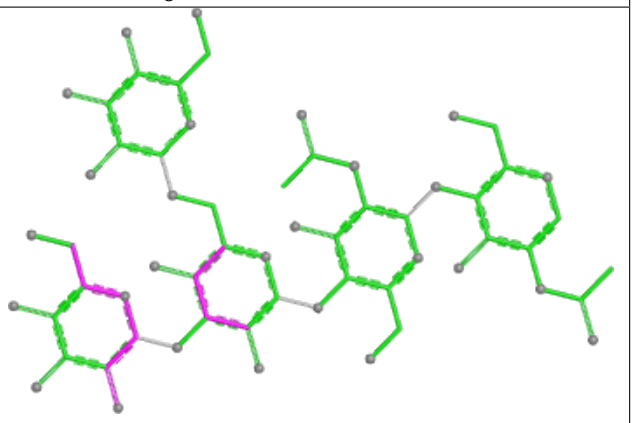
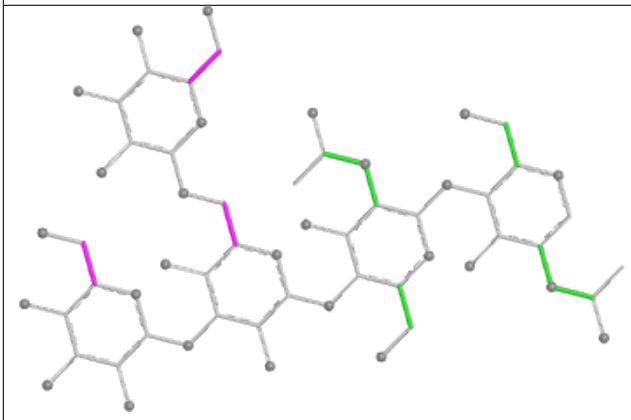
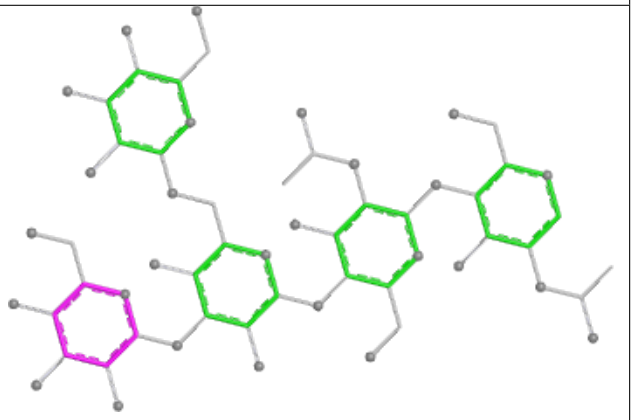


Torsions



Rings

Oligosaccharide Chain i	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain j	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 16 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	HEC	S	302	2,1	32,50,50	2.31	4 (12%)	24,82,82	1.45	3 (12%)
11	HEC	C	302	2,17,1	32,50,50	2.09	3 (9%)	24,82,82	1.69	5 (20%)
11	HEC	O	302	2,1	32,50,50	2.36	4 (12%)	24,82,82	1.50	5 (20%)
15	ACT	D	1004	-	3,3,3	1.28	0	3,3,3	1.59	0
11	HEC	I	302	2,1	32,50,50	2.44	7 (21%)	24,82,82	1.63	3 (12%)
14	NAG	H	1002	2	14,14,15	0.51	0	17,19,21	0.69	0
16	OXL	P	1003	-	5,5,5	2.31	2 (40%)	6,6,6	1.26	1 (16%)
11	HEC	U	302	2,1	32,50,50	2.33	5 (15%)	24,82,82	1.89	5 (20%)
14	NAG	P	1002	2	14,14,15	1.14	2 (14%)	17,19,21	0.54	0
13	EDO	B	1002	-	3,3,3	0.76	0	2,2,2	0.23	0
11	HEC	G	302	2,1	32,50,50	2.21	5 (15%)	24,82,82	1.58	6 (25%)
11	HEC	A	3002	2,1	32,50,50	2.53	5 (15%)	24,82,82	1.34	3 (12%)
14	NAG	D	1003	2	14,14,15	0.42	0	17,19,21	0.42	0
11	HEC	M	302	2,1	32,50,50	2.15	5 (15%)	24,82,82	1.40	4 (16%)
14	NAG	D	1002	2	14,14,15	0.61	0	17,19,21	0.66	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HEC	S	302	2,1	-	4/10/54/54	-
11	HEC	C	302	2,17,1	-	4/10/54/54	-
11	HEC	O	302	2,1	-	4/10/54/54	-
11	HEC	I	302	2,1	-	4/10/54/54	-
14	NAG	H	1002	2	-	1/6/23/26	0/1/1/1
16	OXL	P	1003	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HEC	U	302	2,1	-	4/10/54/54	-
14	NAG	P	1002	2	-	0/6/23/26	0/1/1/1
13	EDO	B	1002	-	-	0/1/1/1	-
11	HEC	G	302	2,1	-	4/10/54/54	-
11	HEC	A	3002	2,1	-	4/10/54/54	-
14	NAG	D	1003	2	-	0/6/23/26	0/1/1/1
11	HEC	M	302	2,1	-	4/10/54/54	-
14	NAG	D	1002	2	-	0/6/23/26	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	3002	HEC	C2B-C3B	-9.37	1.31	1.40
11	O	302	HEC	C2B-C3B	-7.98	1.32	1.40
11	U	302	HEC	C2B-C3B	-7.91	1.32	1.40
11	I	302	HEC	C2B-C3B	-7.83	1.32	1.40
11	C	302	HEC	C2B-C3B	-7.66	1.32	1.40
11	S	302	HEC	C2B-C3B	-7.62	1.32	1.40
11	S	302	HEC	C3C-C2C	-7.50	1.32	1.40
11	O	302	HEC	C3C-C2C	-7.43	1.33	1.40
11	M	302	HEC	C2B-C3B	-7.39	1.33	1.40
11	U	302	HEC	C3C-C2C	-7.30	1.33	1.40
11	I	302	HEC	C3C-C2C	-7.29	1.33	1.40
11	A	3002	HEC	C3C-C2C	-6.88	1.33	1.40
11	G	302	HEC	C3C-C2C	-6.68	1.33	1.40
11	G	302	HEC	C2B-C3B	-6.66	1.33	1.40
11	M	302	HEC	C3C-C2C	-5.68	1.34	1.40
11	C	302	HEC	C3C-C2C	-4.94	1.35	1.40
11	C	302	HEC	C3D-C2D	4.66	1.51	1.37
11	S	302	HEC	C3D-C2D	4.56	1.51	1.37
11	I	302	HEC	C3D-C2D	4.55	1.51	1.37
11	O	302	HEC	C3D-C2D	4.48	1.51	1.37
11	U	302	HEC	C3D-C2D	4.45	1.50	1.37
11	M	302	HEC	C3D-C2D	4.39	1.50	1.37
16	P	1003	OXL	O2-C2	4.27	1.34	1.22
11	A	3002	HEC	C3D-C2D	4.21	1.50	1.37
11	G	302	HEC	C3D-C2D	4.06	1.49	1.37
14	P	1002	NAG	O5-C1	3.00	1.48	1.43
11	G	302	HEC	CAD-C3D	2.70	1.56	1.52
14	P	1002	NAG	C1-C2	2.65	1.56	1.52
11	A	3002	HEC	CMA-C3A	2.56	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	302	HEC	C3C-C4C	2.52	1.47	1.43
11	A	3002	HEC	CAA-C2A	2.49	1.56	1.52
11	I	302	HEC	O2A-CGA	-2.31	1.23	1.30
16	P	1003	OXL	O4-C2	-2.30	1.23	1.30
11	I	302	HEC	C4D-CHA	-2.28	1.34	1.41
11	O	302	HEC	C4D-CHA	-2.19	1.34	1.41
11	G	302	HEC	CAA-C2A	2.16	1.56	1.52
11	U	302	HEC	C3C-C4C	2.10	1.46	1.43
11	M	302	HEC	O2A-CGA	-2.09	1.23	1.30
11	U	302	HEC	C1C-CHC	-2.09	1.35	1.41
11	I	302	HEC	CAD-C3D	2.08	1.55	1.52
11	M	302	HEC	C1B-NB	2.05	1.40	1.36
11	S	302	HEC	C4D-ND	2.01	1.40	1.36

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	U	302	HEC	CMC-C2C-C1C	-6.26	118.84	128.46
11	I	302	HEC	CBA-CAA-C2A	-4.78	104.56	112.60
11	C	302	HEC	CMC-C2C-C1C	-4.53	121.50	128.46
11	I	302	HEC	CMC-C2C-C1C	-4.17	122.05	128.46
11	G	302	HEC	CMC-C2C-C1C	-3.74	122.71	128.46
11	U	302	HEC	CBD-CAD-C3D	-3.57	106.52	112.62
11	O	302	HEC	CMC-C2C-C1C	-3.09	123.72	128.46
11	S	302	HEC	CBD-CAD-C3D	-3.08	107.36	112.62
11	A	3002	HEC	CMC-C2C-C1C	-2.99	123.87	128.46
11	I	302	HEC	CBD-CAD-C3D	-2.86	107.74	112.62
11	C	302	HEC	CBD-CAD-C3D	-2.80	107.84	112.62
11	C	302	HEC	CBA-CAA-C2A	-2.80	107.89	112.60
11	M	302	HEC	CBD-CAD-C3D	-2.77	107.90	112.62
11	G	302	HEC	CBD-CAD-C3D	-2.75	107.92	112.62
11	A	3002	HEC	CBD-CAD-C3D	-2.68	108.04	112.62
11	U	302	HEC	CBA-CAA-C2A	-2.65	108.14	112.60
16	P	1003	OXL	O4-C2-C1	2.44	120.42	113.16
11	S	302	HEC	O1A-CGA-CBA	-2.36	115.49	123.08
11	G	302	HEC	CBA-CAA-C2A	-2.34	108.65	112.60
11	G	302	HEC	CMC-C2C-C3C	2.32	128.55	125.82
11	M	302	HEC	CMB-C2B-C1B	-2.28	124.96	128.46
11	O	302	HEC	C1D-C2D-C3D	-2.27	105.41	107.00
11	S	302	HEC	O2A-CGA-CBA	2.23	121.21	114.03
11	A	3002	HEC	CMC-C2C-C3C	2.22	128.43	125.82
11	G	302	HEC	O2A-CGA-CBA	2.22	121.15	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	O	302	HEC	O2D-CGD-CBD	2.21	121.14	114.03
11	U	302	HEC	CAA-CBA-CGA	-2.12	107.81	113.76
11	M	302	HEC	CMC-C2C-C1C	-2.09	125.25	128.46
11	M	302	HEC	CBA-CAA-C2A	-2.08	109.11	112.60
11	C	302	HEC	O2A-CGA-CBA	2.05	120.61	114.03
11	O	302	HEC	CAD-CBD-CGD	-2.02	108.09	113.76
11	O	302	HEC	O1A-CGA-CBA	-2.02	116.60	123.08
11	C	302	HEC	CMA-C3A-C2A	2.02	128.74	124.94
11	G	302	HEC	O1A-CGA-CBA	-2.01	116.61	123.08
11	U	302	HEC	O2D-CGD-CBD	2.00	120.46	114.03

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	S	302	HEC	CAD-CBD-CGD-O2D
11	C	302	HEC	CAD-CBD-CGD-O1D
11	M	302	HEC	CAA-CBA-CGA-O1A
11	U	302	HEC	CAD-CBD-CGD-O1D
11	I	302	HEC	CAD-CBD-CGD-O2D
11	C	302	HEC	CAD-CBD-CGD-O2D
11	G	302	HEC	CAA-CBA-CGA-O1A
11	O	302	HEC	CAD-CBD-CGD-O2D
11	U	302	HEC	CAD-CBD-CGD-O2D
11	M	302	HEC	CAD-CBD-CGD-O1D
11	S	302	HEC	CAD-CBD-CGD-O1D
11	M	302	HEC	CAA-CBA-CGA-O2A
11	M	302	HEC	CAD-CBD-CGD-O2D
11	G	302	HEC	CAD-CBD-CGD-O2D
11	A	3002	HEC	CAA-CBA-CGA-O1A
11	G	302	HEC	CAA-CBA-CGA-O2A
11	A	3002	HEC	CAA-CBA-CGA-O2A
11	A	3002	HEC	CAD-CBD-CGD-O2D
11	I	302	HEC	CAD-CBD-CGD-O1D
11	O	302	HEC	CAD-CBD-CGD-O1D
11	A	3002	HEC	CAD-CBD-CGD-O1D
11	I	302	HEC	CAA-CBA-CGA-O1A
11	G	302	HEC	CAD-CBD-CGD-O1D
11	I	302	HEC	CAA-CBA-CGA-O2A
11	O	302	HEC	CAA-CBA-CGA-O2A
11	U	302	HEC	CAA-CBA-CGA-O2A
11	C	302	HEC	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
11	O	302	HEC	CAA-CBA-CGA-O1A
11	S	302	HEC	CAA-CBA-CGA-O2A
11	C	302	HEC	CAA-CBA-CGA-O1A
11	S	302	HEC	CAA-CBA-CGA-O1A
11	U	302	HEC	CAA-CBA-CGA-O1A
14	H	1002	NAG	C3-C2-N2-C7
16	P	1003	OXL	O3-C1-C2-O4

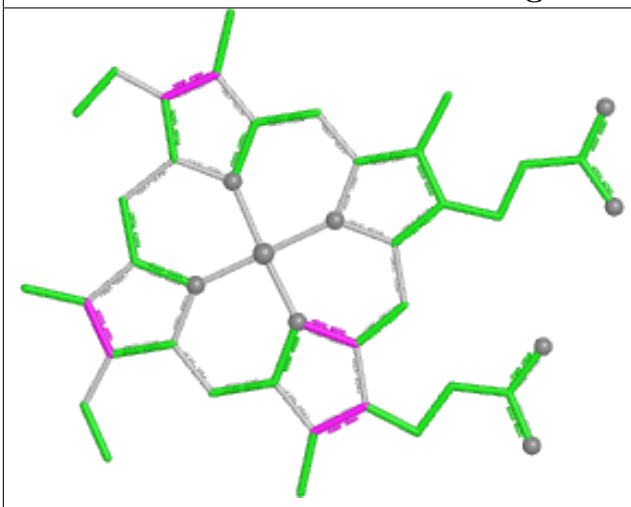
There are no ring outliers.

9 monomers are involved in 38 short contacts:

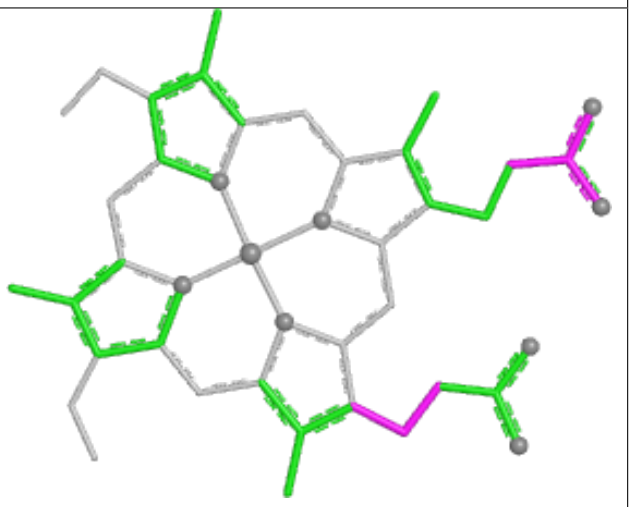
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	S	302	HEC	4	0
11	C	302	HEC	5	0
11	O	302	HEC	3	0
15	D	1004	ACT	2	0
11	I	302	HEC	3	0
11	U	302	HEC	7	0
11	G	302	HEC	4	0
11	A	3002	HEC	5	0
11	M	302	HEC	5	0

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

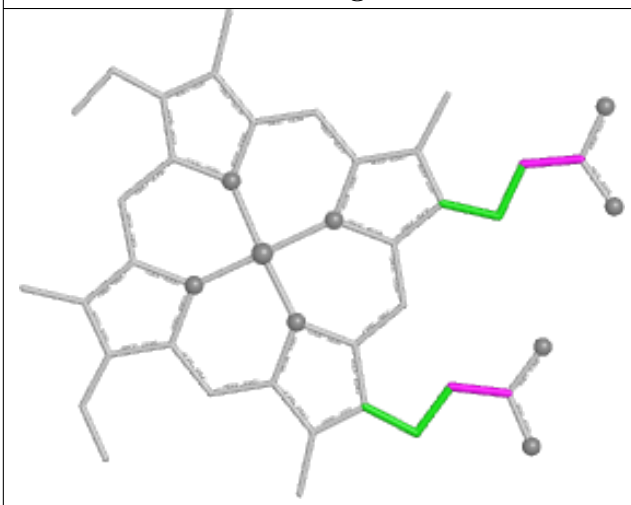
Ligand HEC S 302



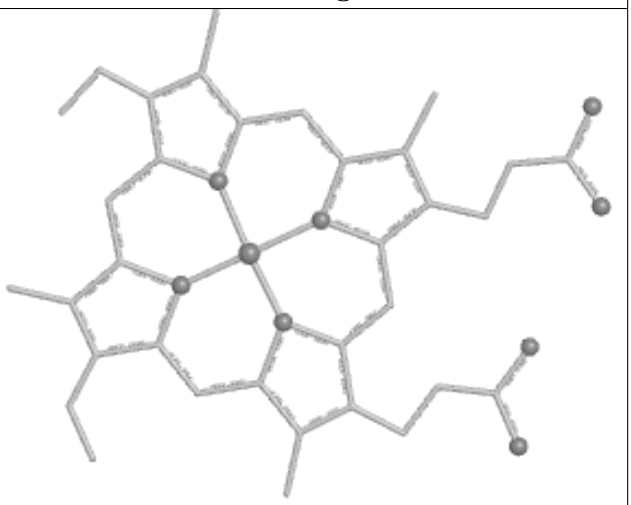
Bond lengths



Bond angles

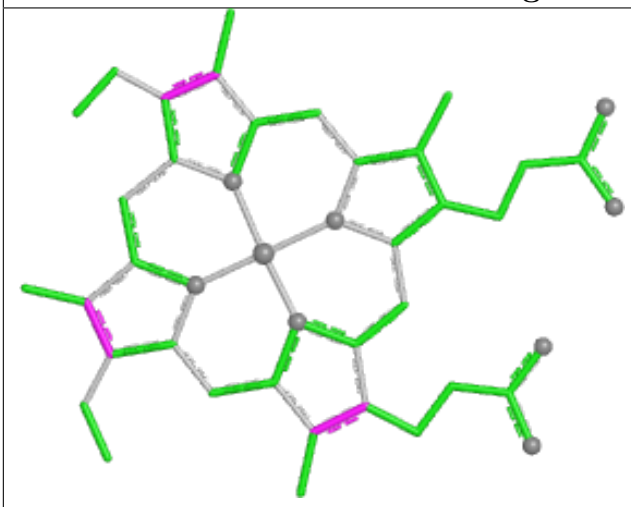


Torsions

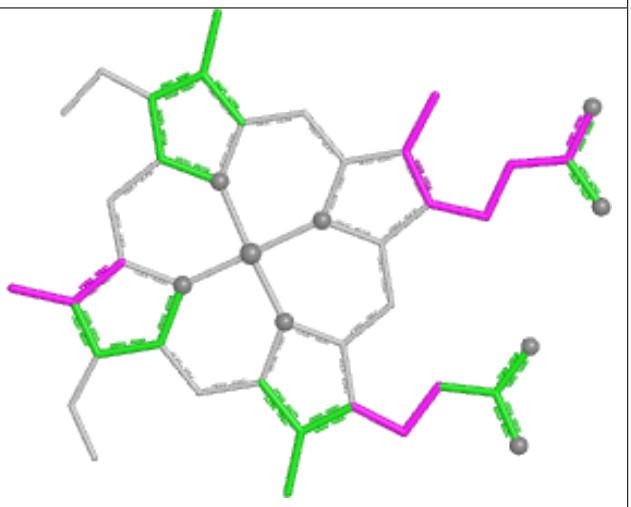


Rings

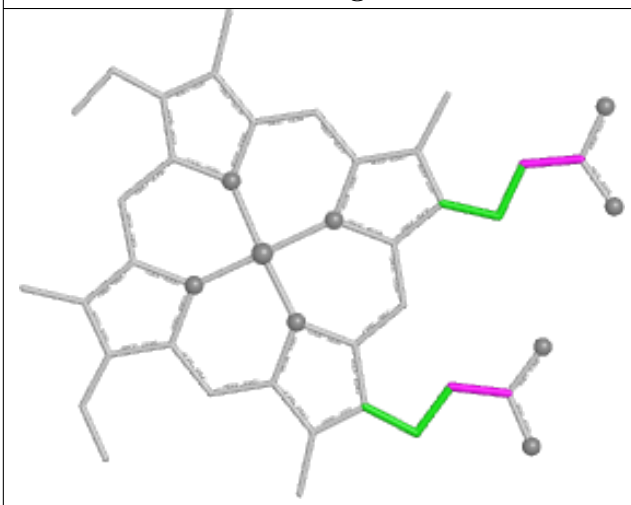
Ligand HEC C 302



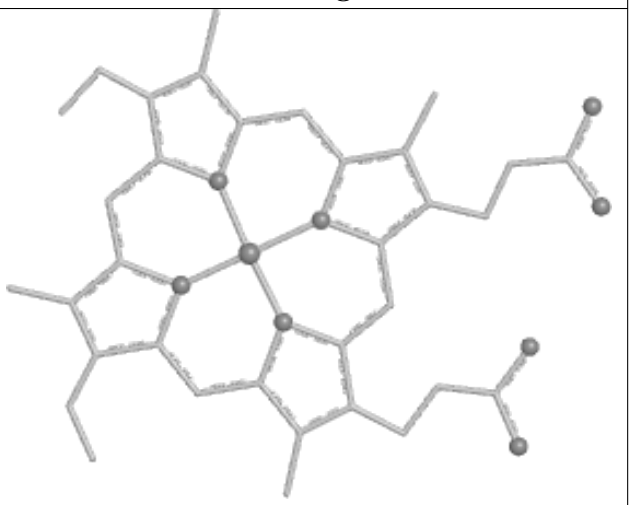
Bond lengths



Bond angles

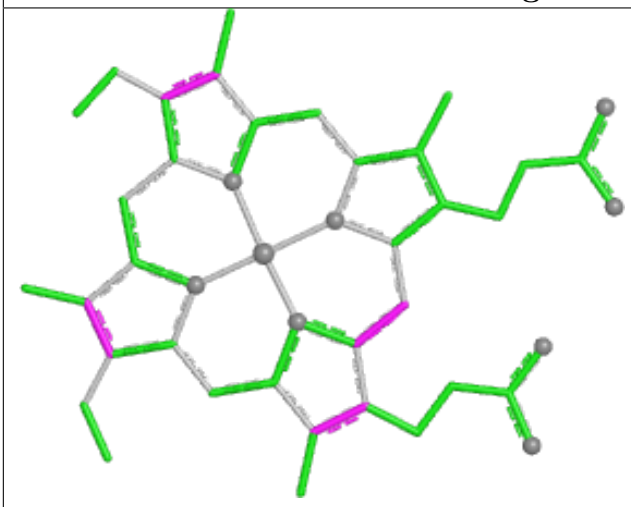


Torsions

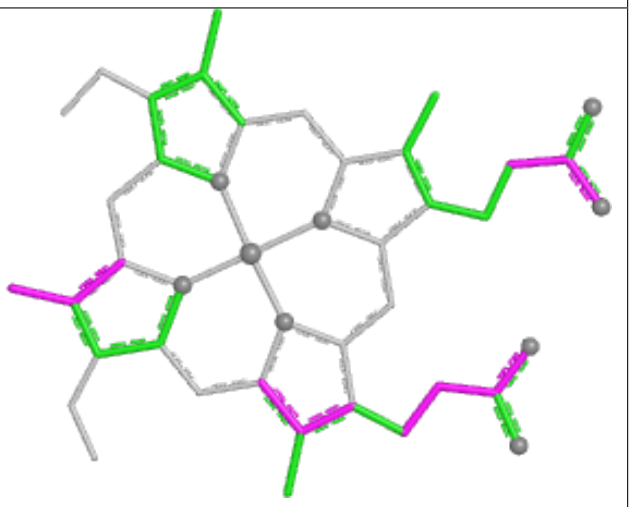


Rings

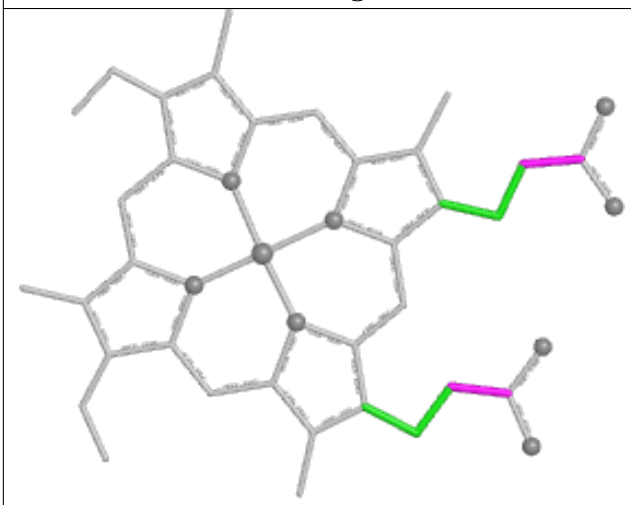
Ligand HEC O 302



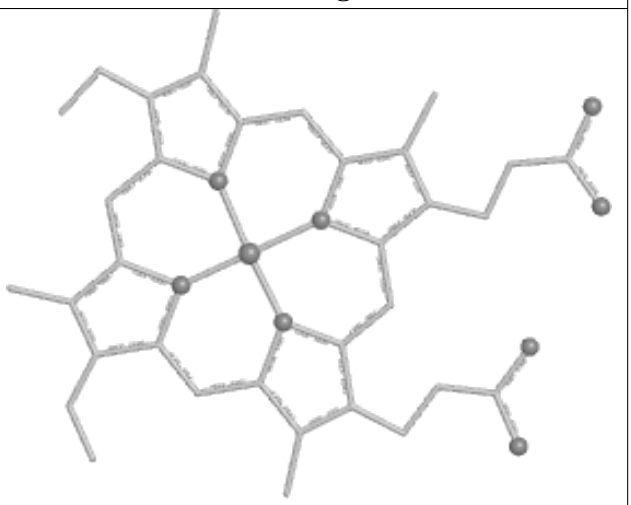
Bond lengths



Bond angles

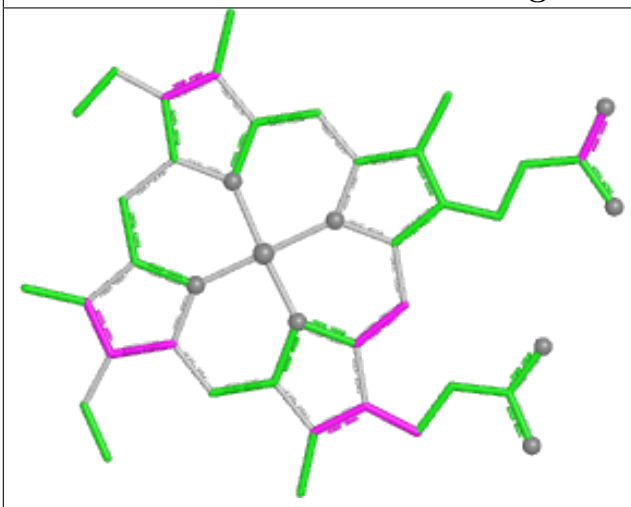


Torsions

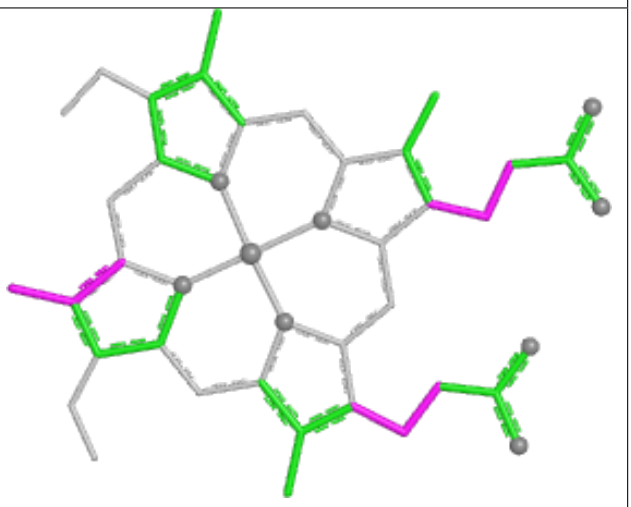


Rings

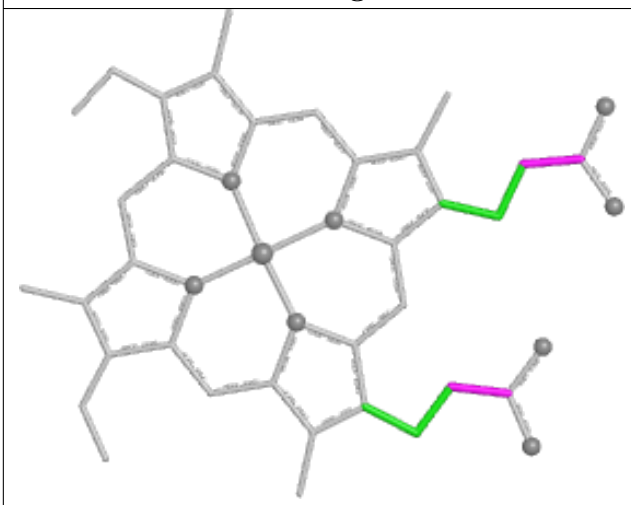
Ligand HEC I 302



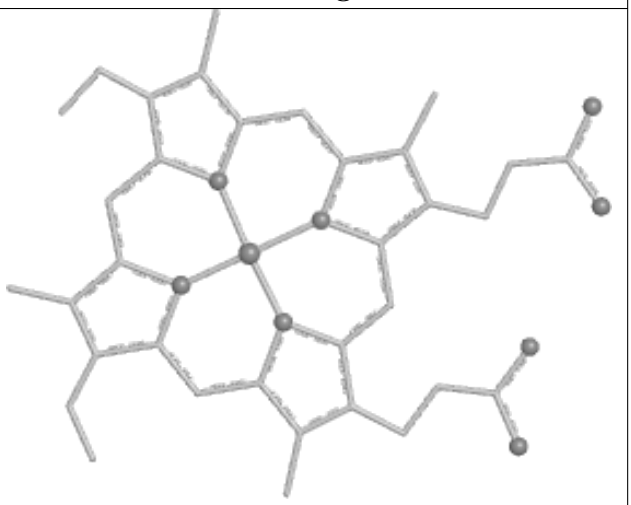
Bond lengths



Bond angles

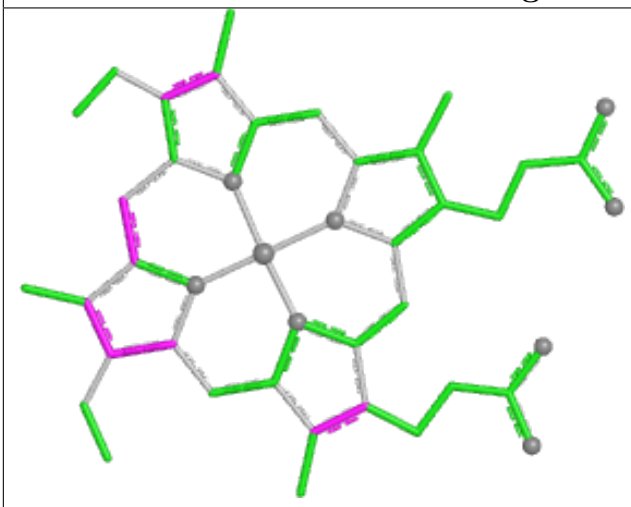


Torsions

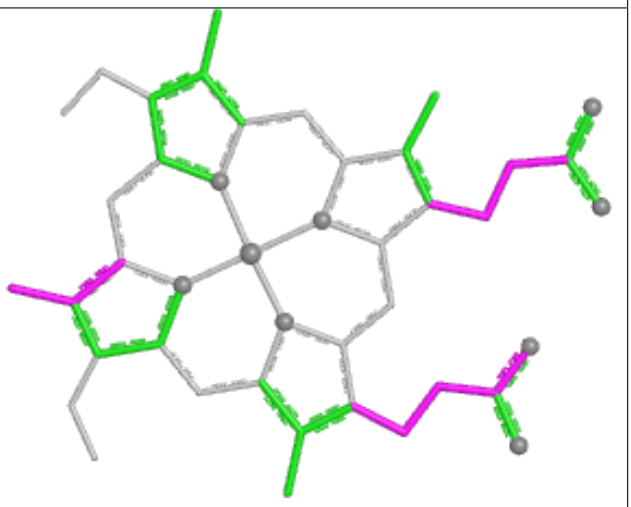


Rings

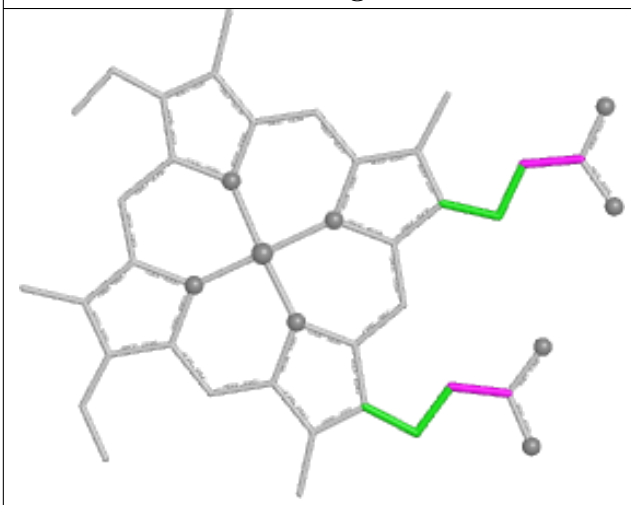
Ligand HEC U 302



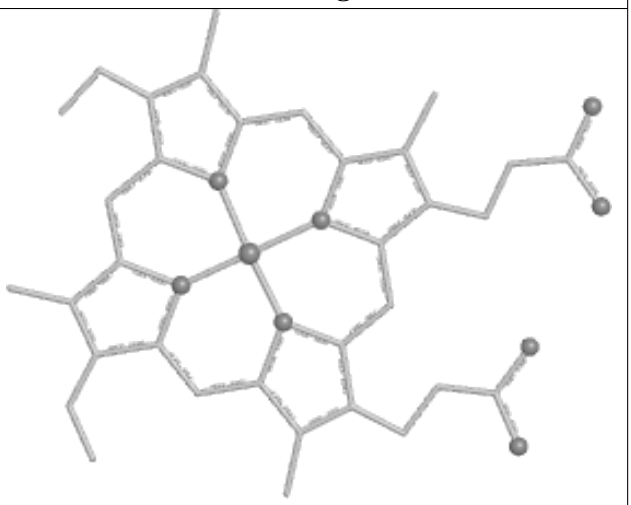
Bond lengths



Bond angles

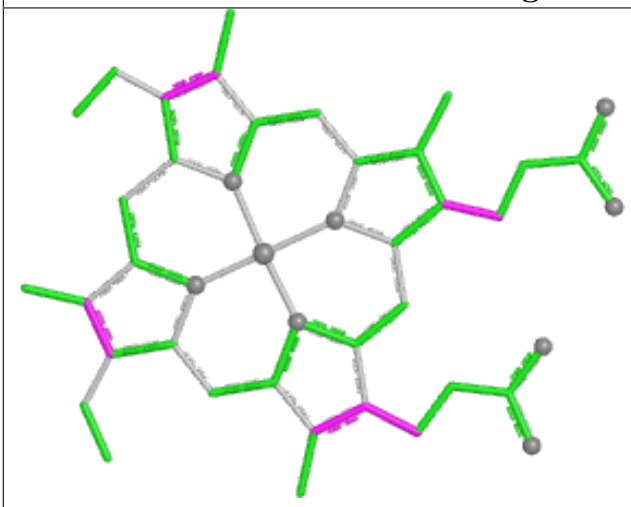


Torsions

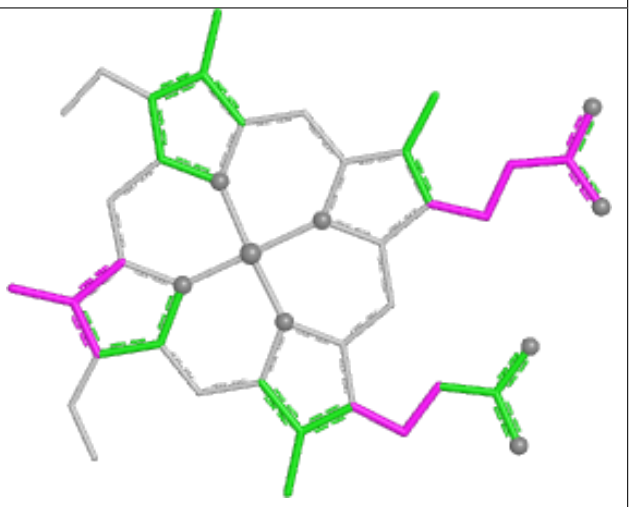


Rings

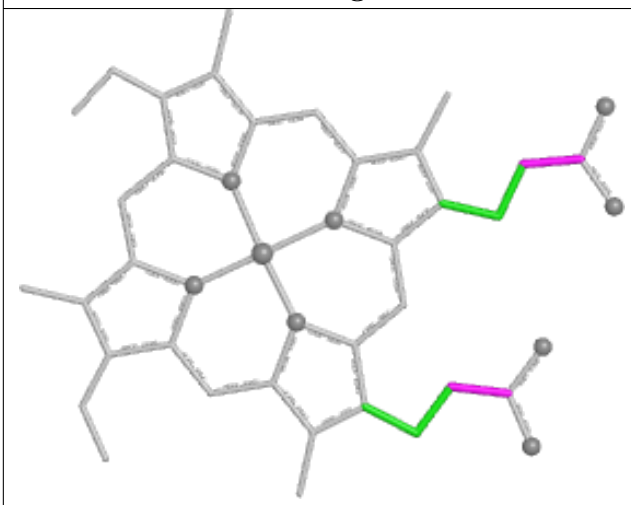
Ligand HEC G 302



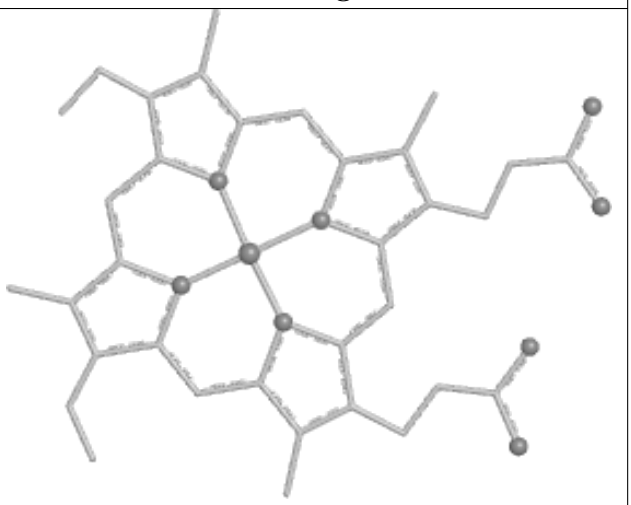
Bond lengths



Bond angles

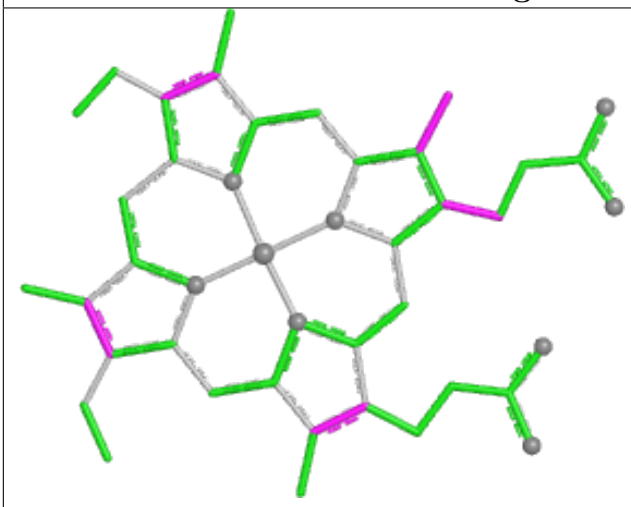


Torsions

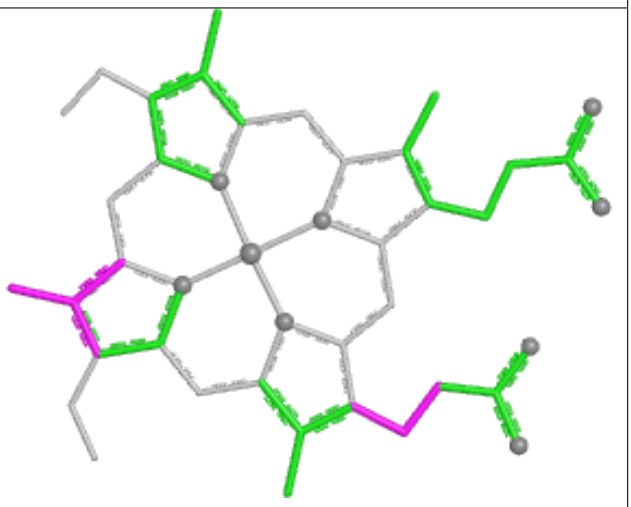


Rings

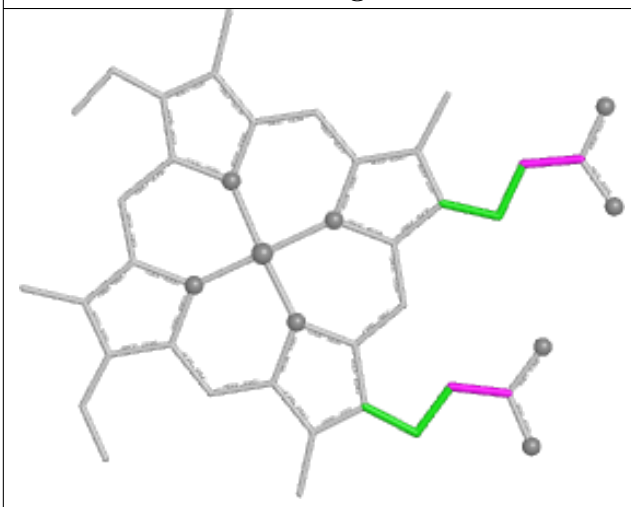
Ligand HEC A 3002



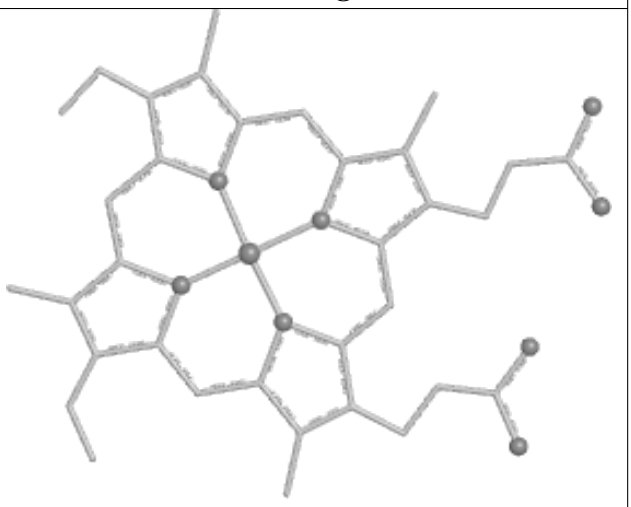
Bond lengths



Bond angles

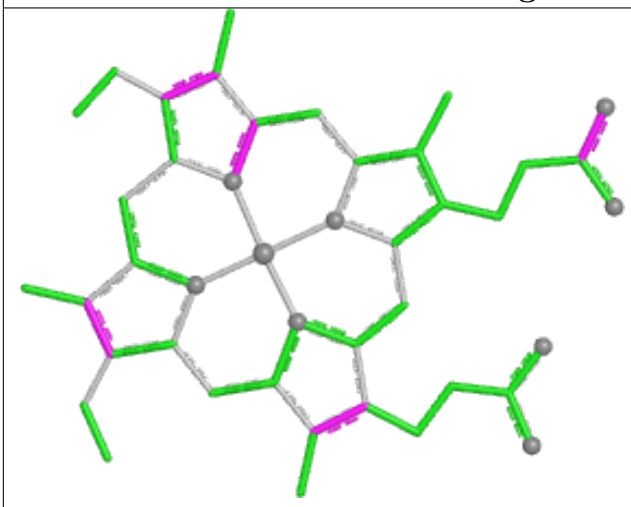


Torsions

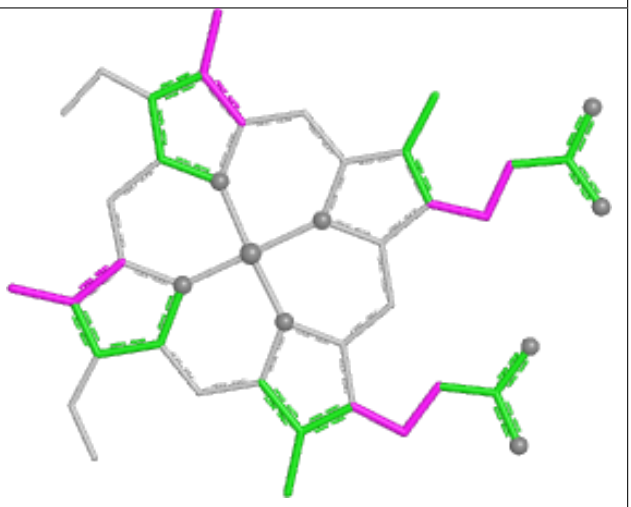


Rings

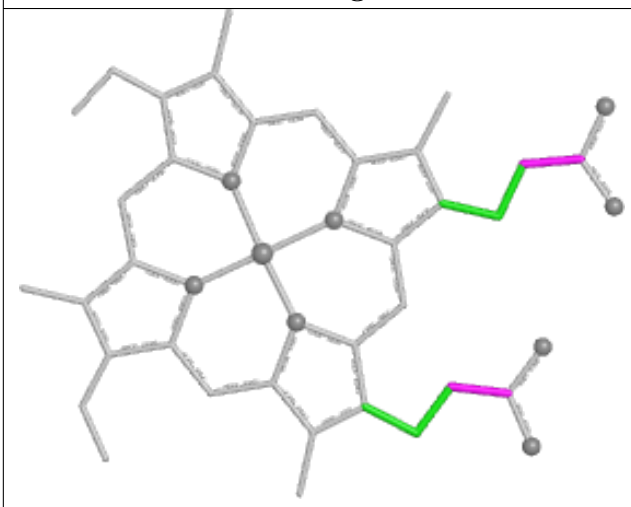
Ligand HEC M 302



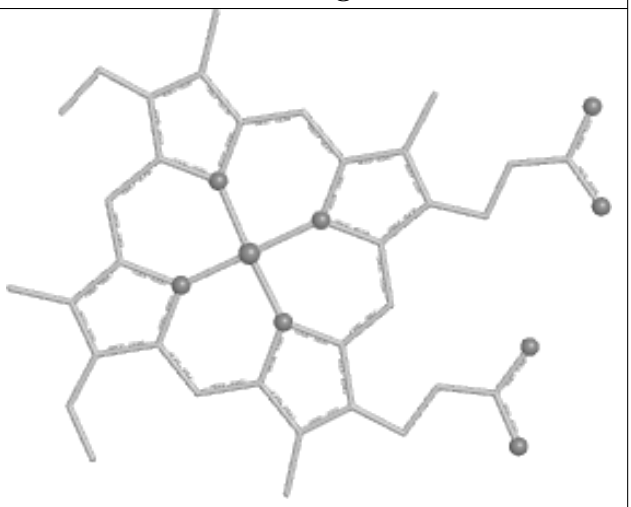
Bond lengths



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	105/106 (99%)	-0.14	1 (0%) 82 86	21, 30, 57, 95	0
1	C	106/106 (100%)	-0.05	1 (0%) 84 87	24, 37, 69, 96	0
1	G	106/106 (100%)	0.03	2 (1%) 66 72	24, 37, 73, 114	0
1	I	105/106 (99%)	-0.04	1 (0%) 82 86	24, 39, 58, 73	0
1	M	105/106 (99%)	-0.11	0 100 100	20, 29, 59, 87	0
1	O	105/106 (99%)	-0.06	0 100 100	21, 31, 57, 81	0
1	S	106/106 (100%)	-0.08	1 (0%) 84 87	20, 30, 54, 82	0
1	U	105/106 (99%)	-0.09	1 (0%) 82 86	19, 27, 59, 79	0
2	B	464/466 (99%)	-0.01	6 (1%) 77 81	18, 35, 58, 87	0
2	D	464/466 (99%)	0.04	5 (1%) 80 84	23, 44, 70, 101	0
2	H	465/466 (99%)	0.15	14 (3%) 50 56	24, 46, 72, 100	0
2	J	464/466 (99%)	-0.06	1 (0%) 95 96	24, 38, 60, 94	0
2	N	464/466 (99%)	-0.05	3 (0%) 89 91	19, 33, 55, 90	0
2	P	464/466 (99%)	-0.07	1 (0%) 95 96	21, 36, 59, 104	0
2	T	464/466 (99%)	-0.11	1 (0%) 95 96	21, 34, 53, 95	0
2	V	465/466 (99%)	-0.09	2 (0%) 92 94	18, 32, 53, 87	0
3	E	51/59 (86%)	0.45	2 (3%) 39 44	44, 65, 94, 102	0
3	F	57/59 (96%)	0.16	0 100 100	46, 54, 75, 82	0
3	K	55/59 (93%)	1.04	10 (18%) 1 1	58, 79, 103, 125	0
3	L	59/59 (100%)	0.14	2 (3%) 45 50	29, 52, 81, 104	0
3	Q	55/59 (93%)	0.28	2 (3%) 42 48	37, 58, 84, 95	0
3	R	59/59 (100%)	0.14	0 100 100	35, 50, 72, 84	0
3	W	56/59 (94%)	0.32	3 (5%) 25 31	35, 59, 80, 84	0
3	X	55/59 (93%)	0.19	1 (1%) 68 74	32, 55, 76, 87	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
All	All	5004/5048 (99%)	0.00	60 (1%) 79 82	18, 37, 69, 125	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	63	ASN	6.7
3	K	62	LYS	5.9
1	G	169	GLU	5.7
2	H	735	ALA	5.1
3	L	102	GLU	4.9
1	G	166	THR	4.3
3	W	84	ILE	3.9
3	E	92	LYS	3.3
2	P	520	GLU	3.2
2	B	433	LEU	3.2
2	D	383	HIS	3.1
3	K	60	LEU	3.1
2	H	514	ASN	3.1
3	K	67	ALA	3.0
2	T	279	VAL	3.0
3	K	61	ASP	3.0
2	D	433	LEU	2.9
2	N	520	GLU	2.9
2	H	430	LEU	2.9
2	D	280	ASN	2.9
2	B	450	VAL	2.9
2	V	733	LEU	2.8
3	K	59	LEU	2.8
2	H	744	ALA	2.6
1	U	169	GLU	2.6
3	Q	98	VAL	2.5
2	H	279	VAL	2.5
1	A	170	GLN	2.5
2	N	730	CYS	2.5
2	H	433	LEU	2.5
3	L	103	HIS	2.4
1	C	169	GLU	2.4
2	N	383	HIS	2.4
2	H	736	LEU	2.4
2	H	733	LEU	2.4
3	K	58	VAL	2.4
2	D	282	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	680	TRP	2.3
3	K	66	GLN	2.3
3	K	98	VAL	2.3
3	Q	92	LYS	2.3
2	H	457	ILE	2.3
2	D	419	LEU	2.2
2	B	738	LEU	2.2
3	K	97	ASP	2.2
2	H	515	ARG	2.2
2	H	510	PHE	2.2
2	J	383	HIS	2.2
2	B	521	PRO	2.1
2	V	279	VAL	2.1
1	S	166	THR	2.1
3	X	85	LYS	2.1
2	B	430	LEU	2.1
3	W	60	LEU	2.1
3	W	88	ILE	2.1
2	B	395	ARG	2.0
2	H	710	THR	2.0
2	H	343	TYR	2.0
3	E	62	LYS	2.0
1	I	220	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	CSO	B	316	7/8	0.96	0.11	26,32,43,52	0
2	CSO	D	316	7/8	0.96	0.13	30,36,47,57	0
2	CSO	J	316	7/8	0.96	0.09	32,39,49,54	0
2	CSO	P	316	7/8	0.97	0.11	22,30,40,46	0
2	CSO	T	316	7/8	0.97	0.14	22,27,38,39	0
2	CSO	H	316	7/8	0.98	0.11	31,38,46,46	0
2	CSO	N	316	7/8	0.98	0.12	20,26,41,49	0
2	CSO	V	316	7/8	0.98	0.10	21,26,32,39	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, 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
9	MAN	j	4	11/12	0.59	0.21	68,81,96,98	0
4	BMA	Y	3	11/12	0.61	0.16	66,74,86,89	0
4	BMA	o	3	11/12	0.68	0.19	62,72,86,88	0
8	BMA	i	3	11/12	0.70	0.13	62,74,89,89	0
4	BMA	r	3	11/12	0.72	0.16	57,68,83,91	0
4	BMA	l	3	11/12	0.73	0.14	69,79,92,98	0
7	NAG	s	2	14/15	0.73	0.18	54,70,84,92	0
7	NAG	m	2	14/15	0.75	0.27	61,78,99,105	0
8	MAN	i	4	11/12	0.78	0.15	63,76,89,96	0
7	NAG	b	2	14/15	0.78	0.15	52,75,90,92	0
7	NAG	p	2	14/15	0.81	0.18	57,72,89,91	0
6	MAN	k	4	11/12	0.81	0.15	53,67,81,88	0
6	MAN	q	4	11/12	0.81	0.15	46,66,78,94	0
4	BMA	f	3	11/12	0.81	0.15	58,69,80,88	0
4	NAG	f	2	14/15	0.81	0.22	48,63,78,79	0
5	MAN	Z	4	11/12	0.82	0.20	64,76,90,91	0
4	NAG	l	2	14/15	0.83	0.15	44,60,73,77	0
4	NAG	o	2	14/15	0.83	0.38	43,66,80,82	0
7	NAG	g	2	14/15	0.83	0.17	50,69,87,91	0
5	BMA	Z	3	11/12	0.84	0.12	58,68,82,84	0
4	NAG	Y	2	14/15	0.85	0.13	46,62,80,87	0
6	MAN	a	4	11/12	0.85	0.19	51,65,78,94	0
7	NAG	d	2	14/15	0.86	0.17	49,67,85,90	0
9	MAN	j	5	11/12	0.86	0.24	66,76,91,94	0
9	BMA	j	3	11/12	0.87	0.12	63,72,87,87	0
7	NAG	d	1	14/15	0.87	0.16	54,66,78,84	0
6	MAN	t	4	11/12	0.87	0.14	50,61,73,78	0
6	MAN	e	4	11/12	0.88	0.18	56,65,77,78	0
8	NAG	i	2	14/15	0.89	0.13	50,65,77,79	0
7	NAG	p	1	14/15	0.89	0.13	43,58,70,73	0
6	MAN	t	5	11/12	0.90	0.11	34,42,51,55	0
7	NAG	b	1	14/15	0.90	0.18	52,62,68,80	0
4	NAG	r	2	14/15	0.90	0.12	50,62,72,78	0
6	MAN	k	5	11/12	0.90	0.13	30,40,50,57	0
6	MAN	h	4	11/12	0.91	0.10	50,59,70,74	0
6	MAN	n	4	11/12	0.92	0.13	45,59,71,72	0
6	MAN	q	5	11/12	0.93	0.11	29,39,46,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	g	1	14/15	0.93	0.14	46,58,63,73	0
9	NAG	j	2	14/15	0.93	0.13	49,61,70,83	0
7	NAG	s	1	14/15	0.93	0.12	43,57,67,70	0
6	MAN	h	5	11/12	0.93	0.16	33,45,54,55	0
6	BMA	k	3	11/12	0.93	0.12	31,39,48,51	0
6	MAN	c	4	11/12	0.94	0.12	48,57,68,76	0
6	FUC	h	6	10/11	0.94	0.11	34,48,61,63	0
6	MAN	c	5	11/12	0.94	0.11	29,35,43,44	0
7	NAG	m	1	14/15	0.94	0.12	42,63,71,77	0
5	NAG	Z	2	14/15	0.94	0.14	46,55,64,69	0
6	MAN	e	5	11/12	0.94	0.13	35,43,51,54	0
4	NAG	Y	1	14/15	0.94	0.12	42,50,59,60	0
6	MAN	n	5	11/12	0.94	0.09	31,38,46,47	0
4	NAG	r	1	14/15	0.95	0.12	29,40,51,59	0
6	MAN	a	5	11/12	0.95	0.11	29,36,45,49	0
6	FUC	k	6	10/11	0.95	0.11	28,38,46,49	0
6	BMA	t	3	11/12	0.95	0.12	32,38,46,51	0
6	NAG	e	1	14/15	0.95	0.11	33,40,46,52	0
6	FUC	e	6	10/11	0.96	0.13	39,46,55,55	0
5	NAG	Z	1	14/15	0.96	0.14	33,43,55,70	0
6	FUC	c	6	10/11	0.96	0.12	28,37,48,55	0
6	FUC	n	6	10/11	0.96	0.12	33,44,51,62	0
6	BMA	q	3	11/12	0.96	0.09	29,36,48,48	0
4	NAG	l	1	14/15	0.96	0.12	34,44,53,55	0
9	NAG	j	1	14/15	0.96	0.14	38,48,57,63	0
6	NAG	e	2	14/15	0.96	0.13	29,39,48,53	0
6	FUC	q	6	10/11	0.96	0.10	36,47,59,61	0
6	FUC	a	6	10/11	0.96	0.12	31,40,48,53	0
6	BMA	a	3	11/12	0.96	0.11	29,35,49,49	0
6	BMA	e	3	11/12	0.97	0.09	34,40,48,49	0
6	NAG	t	1	14/15	0.97	0.12	24,32,40,43	0
6	NAG	n	1	14/15	0.97	0.12	22,28,34,41	0
6	BMA	n	3	11/12	0.97	0.11	26,33,44,45	0
6	BMA	c	3	11/12	0.97	0.10	27,33,40,41	0
6	FUC	t	6	10/11	0.97	0.10	37,48,59,65	0
4	NAG	o	1	14/15	0.97	0.12	34,41,47,49	0
6	NAG	k	2	14/15	0.97	0.14	19,28,33,35	0
6	NAG	q	1	14/15	0.97	0.14	22,28,36,43	0
6	NAG	q	2	14/15	0.97	0.13	21,27,32,32	0
4	NAG	f	1	14/15	0.97	0.13	29,39,48,51	0
6	NAG	h	1	14/15	0.97	0.12	26,31,39,40	0
6	BMA	h	3	11/12	0.97	0.09	32,40,48,54	0

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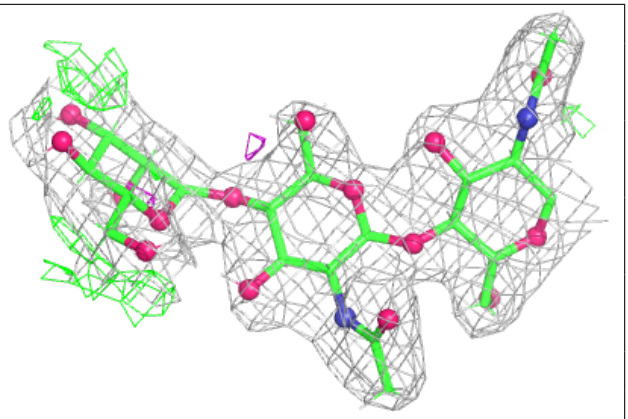
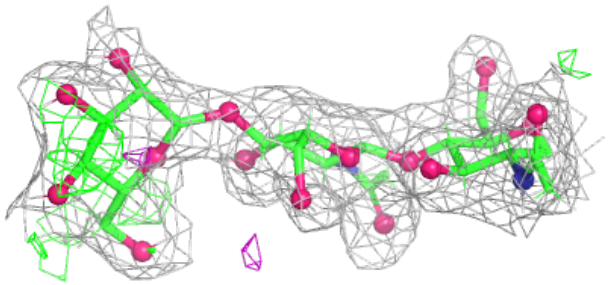
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	i	1	14/15	0.98	0.14	26,42,52,69	0
6	NAG	c	1	14/15	0.98	0.12	21,27,33,36	0
6	NAG	k	1	14/15	0.98	0.11	24,30,35,38	0
6	NAG	n	2	14/15	0.98	0.13	17,23,29,31	0
6	NAG	h	2	14/15	0.98	0.11	24,29,36,39	0
6	NAG	c	2	14/15	0.98	0.13	18,23,28,33	0
6	NAG	a	1	14/15	0.98	0.12	23,29,38,38	0
6	NAG	a	2	14/15	0.98	0.13	20,28,33,37	0
6	NAG	t	2	14/15	0.98	0.13	24,32,38,43	0

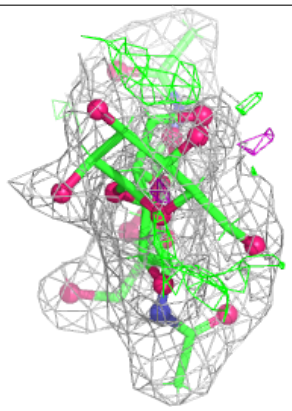
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain Y:

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

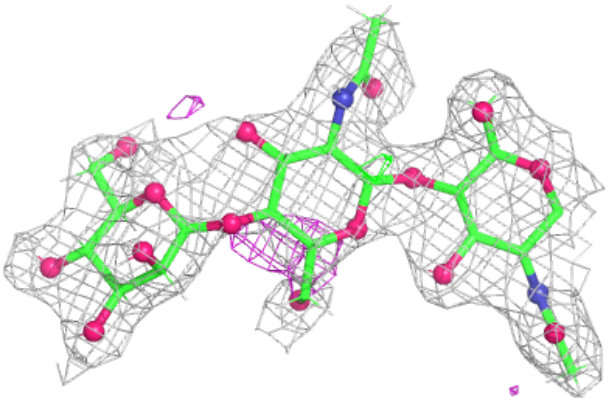


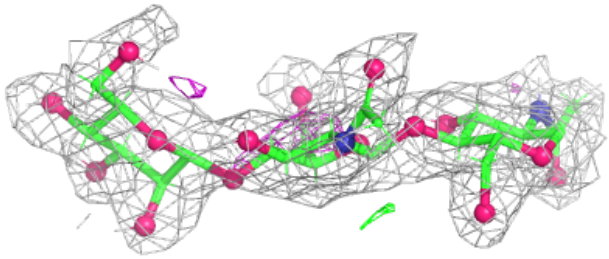


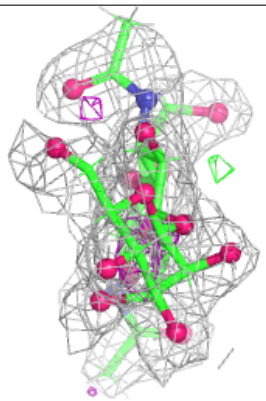


Electron density around Chain f:

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

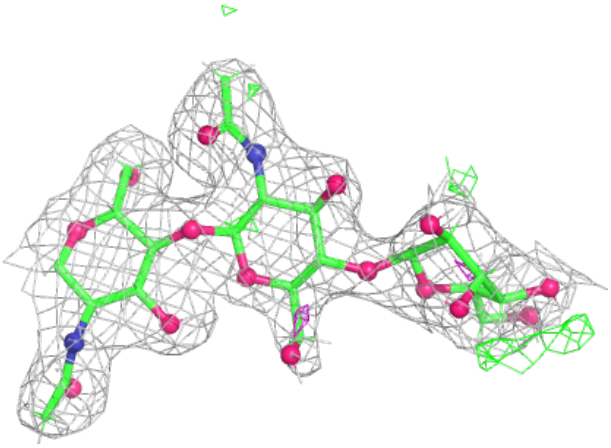


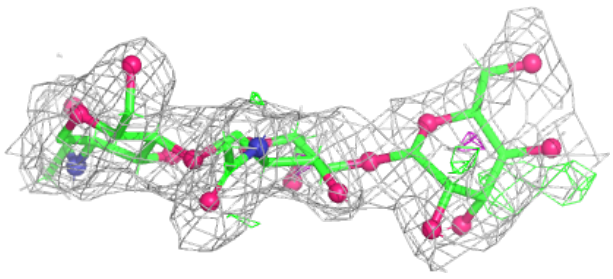


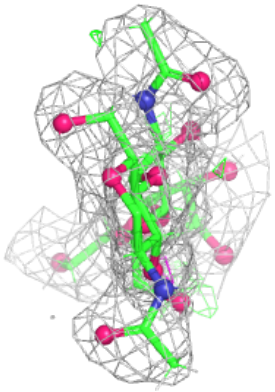


Electron density around Chain l:

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

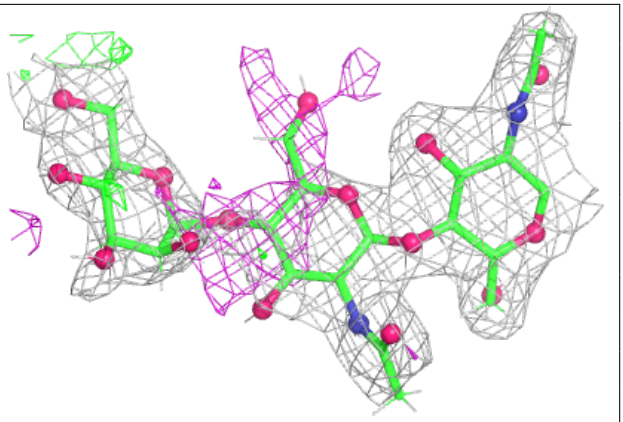


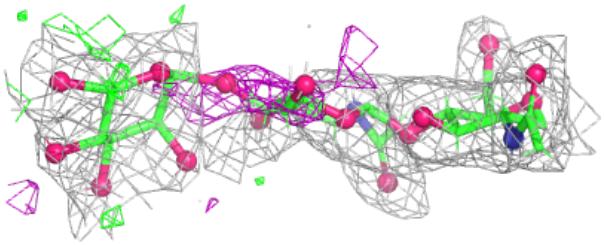


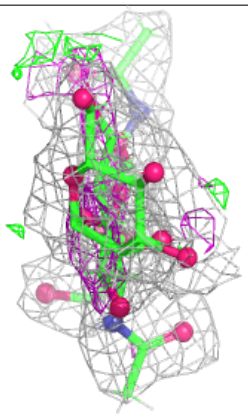


Electron density around Chain o:

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

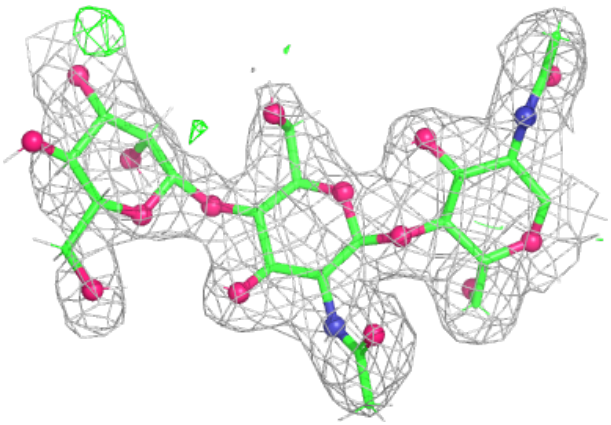


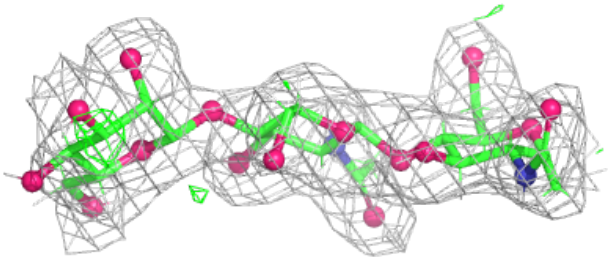


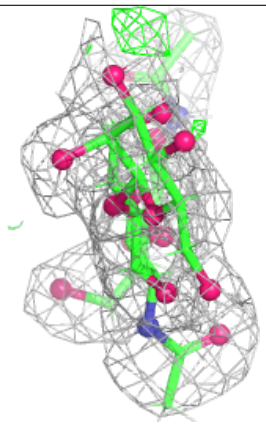


Electron density around Chain r:

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

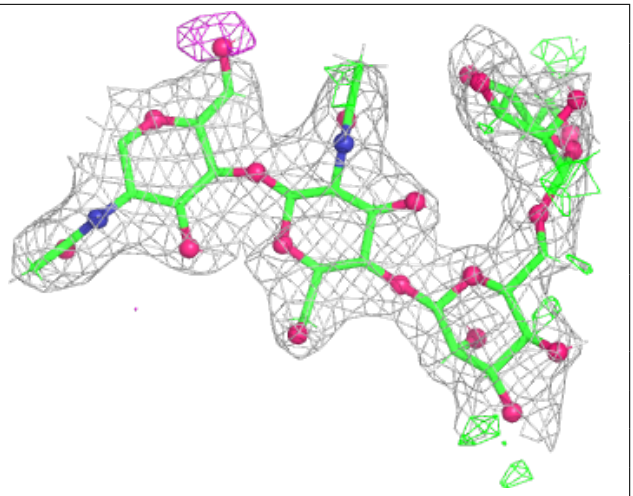


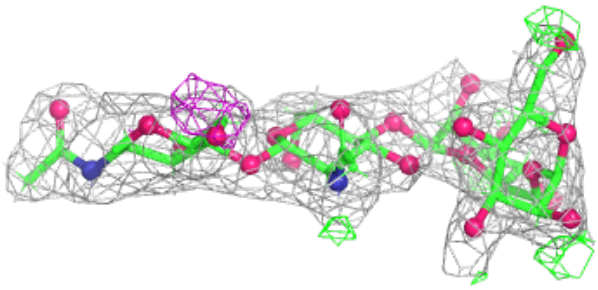


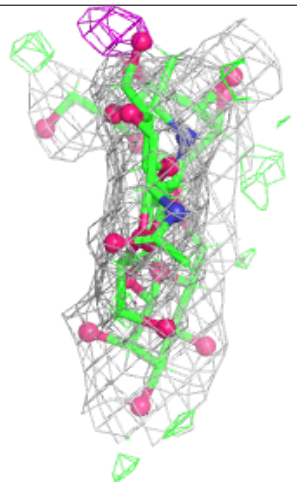


Electron density around Chain Z:

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

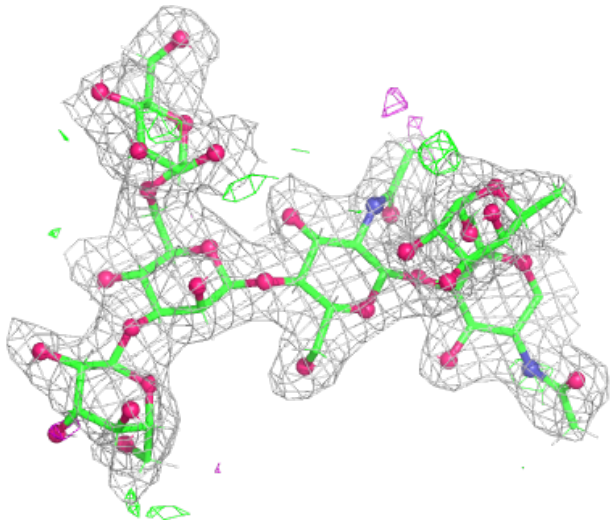


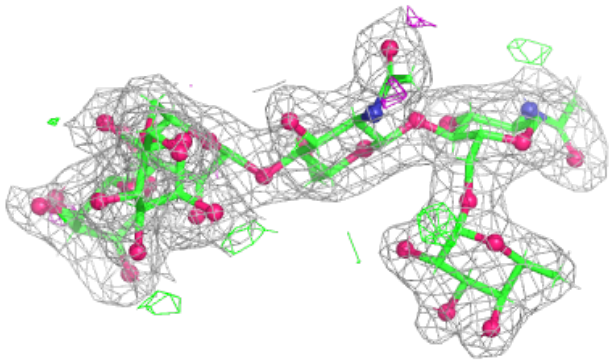


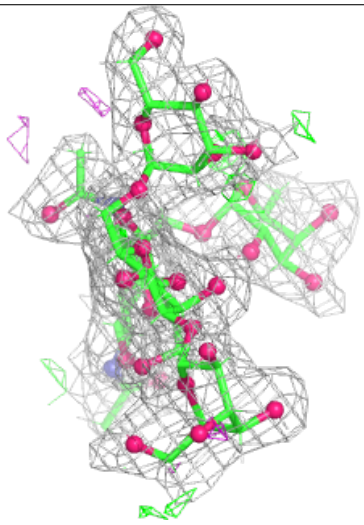


Electron density around Chain a:

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

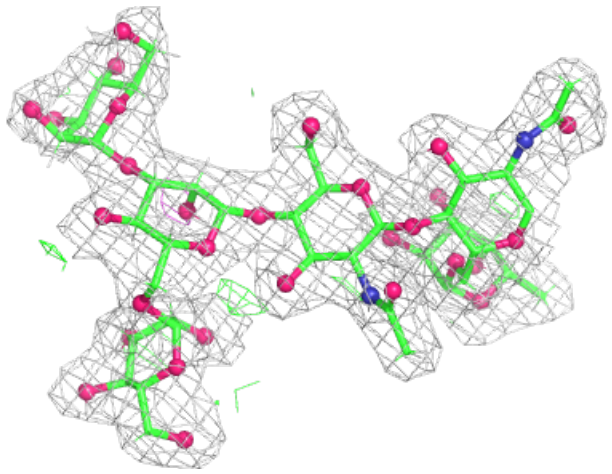


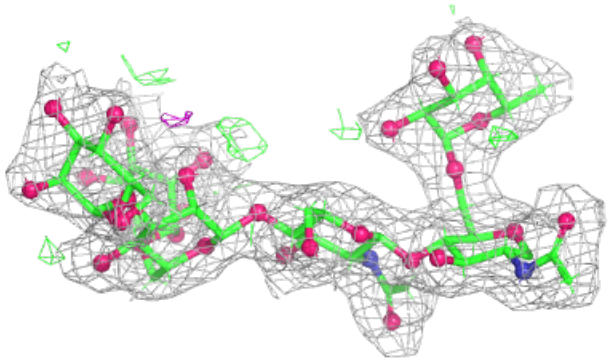


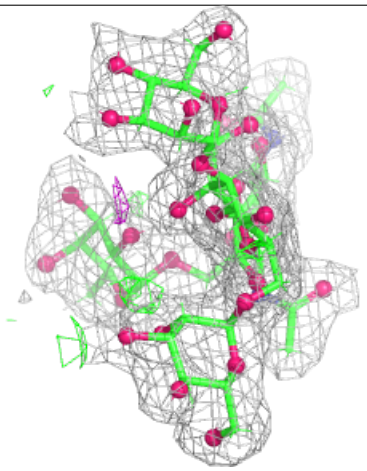


Electron density around Chain c:

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

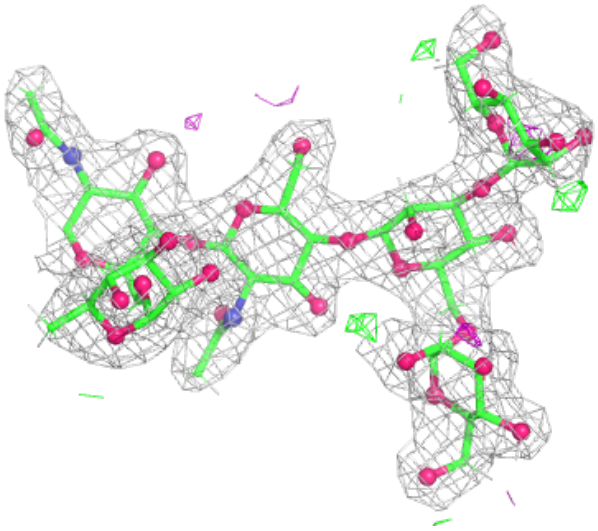


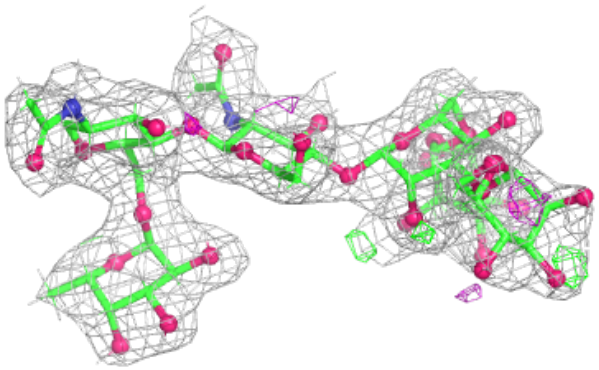


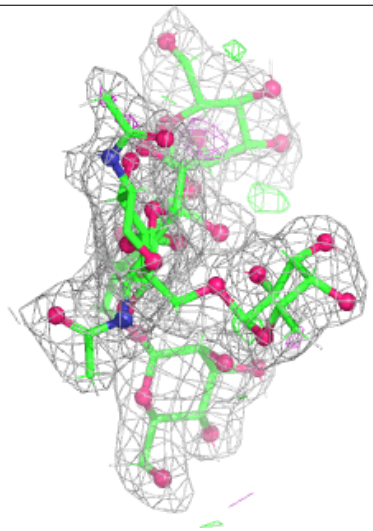


Electron density around Chain e:

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

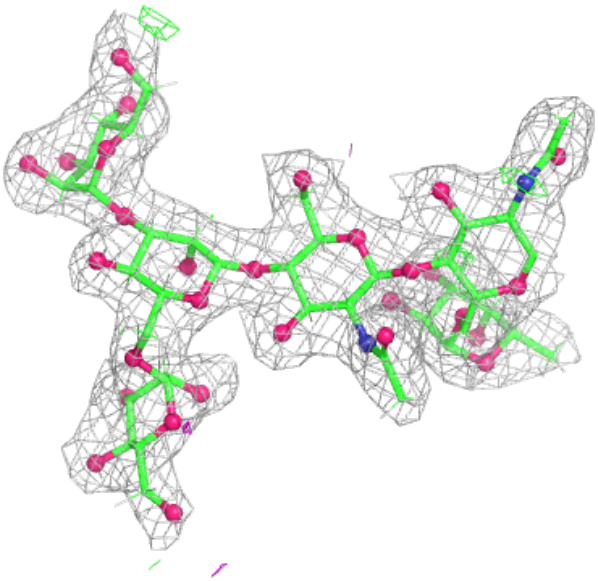


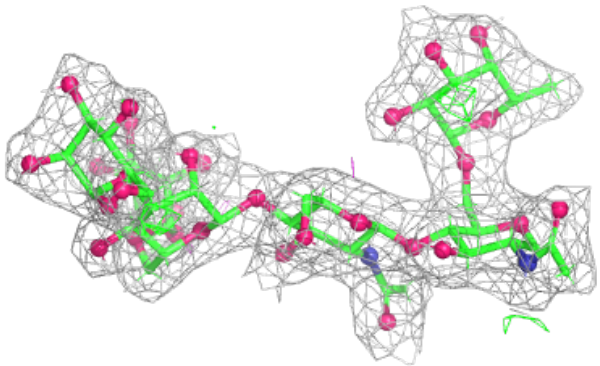


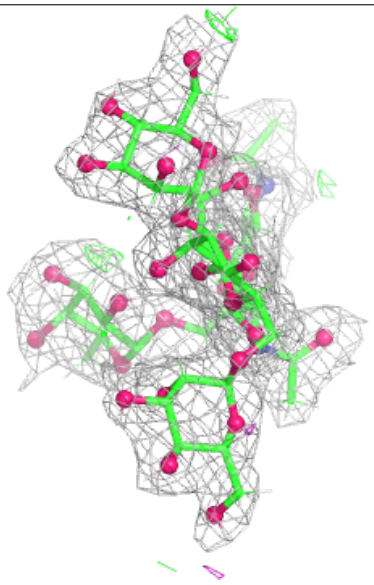


Electron density around Chain h:

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

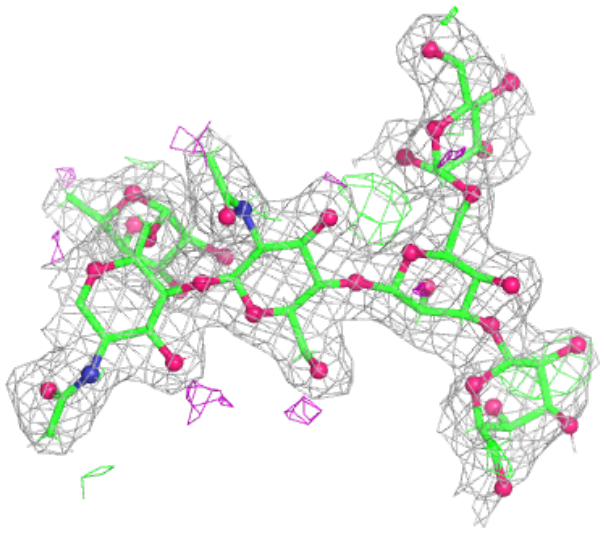


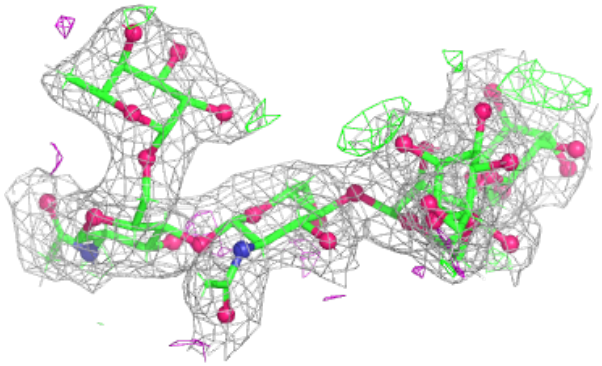


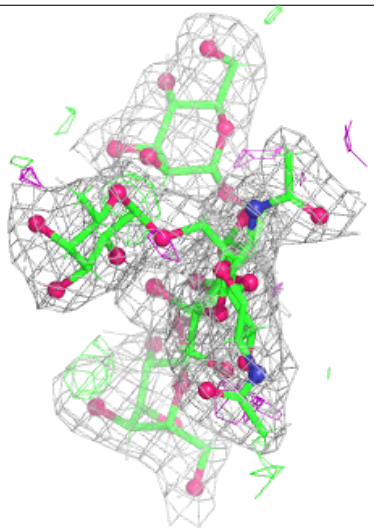


Electron density around Chain k:

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

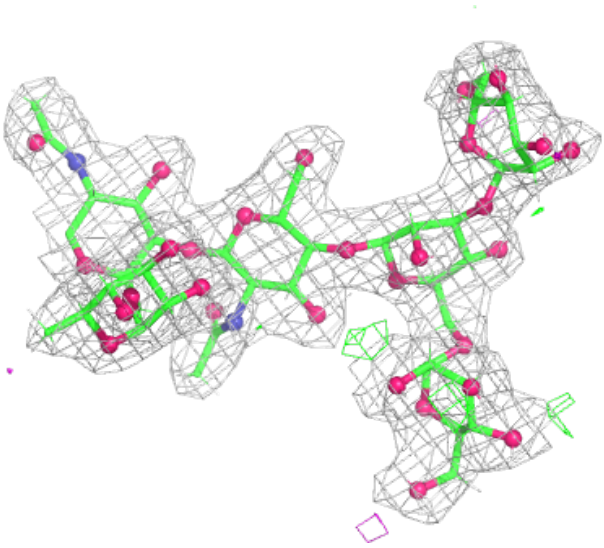


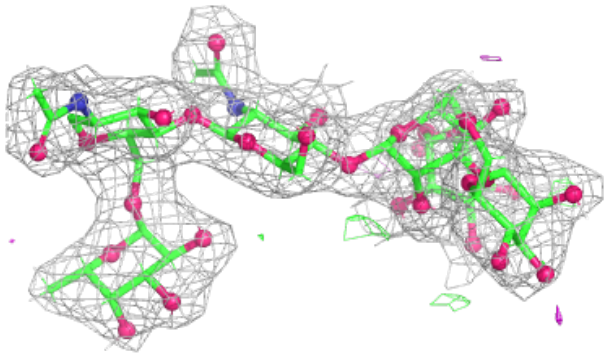


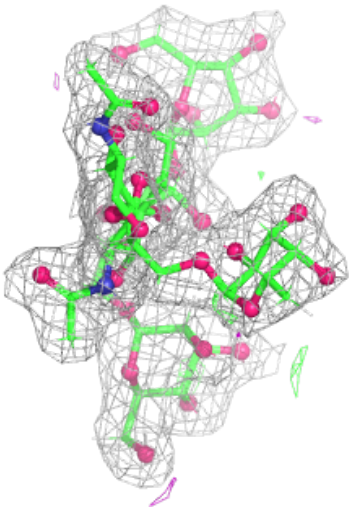


Electron density around Chain n:

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

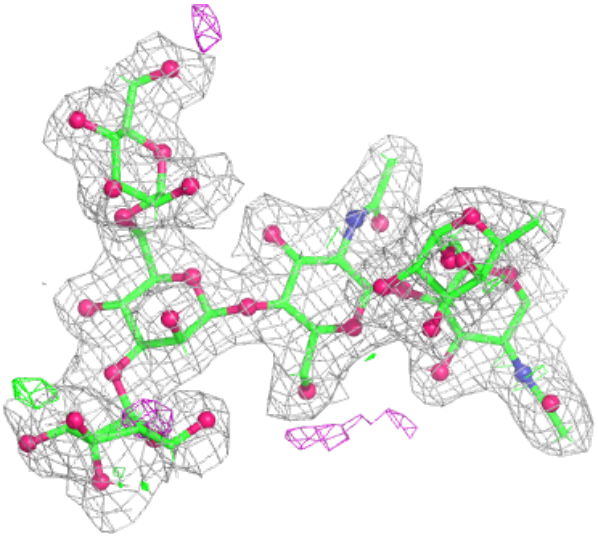


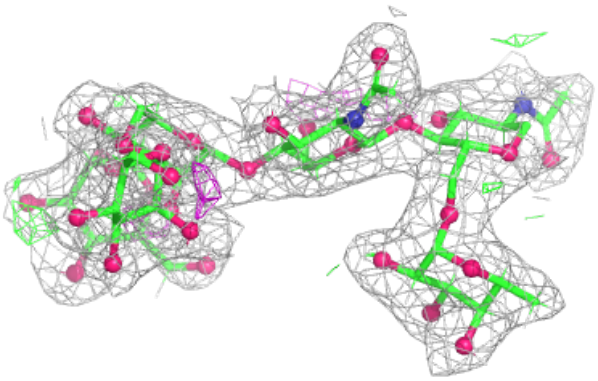


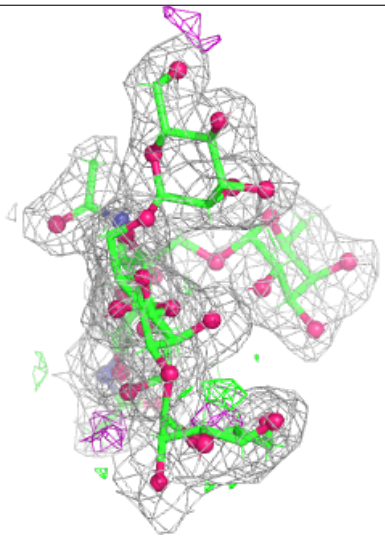


Electron density around Chain q:

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

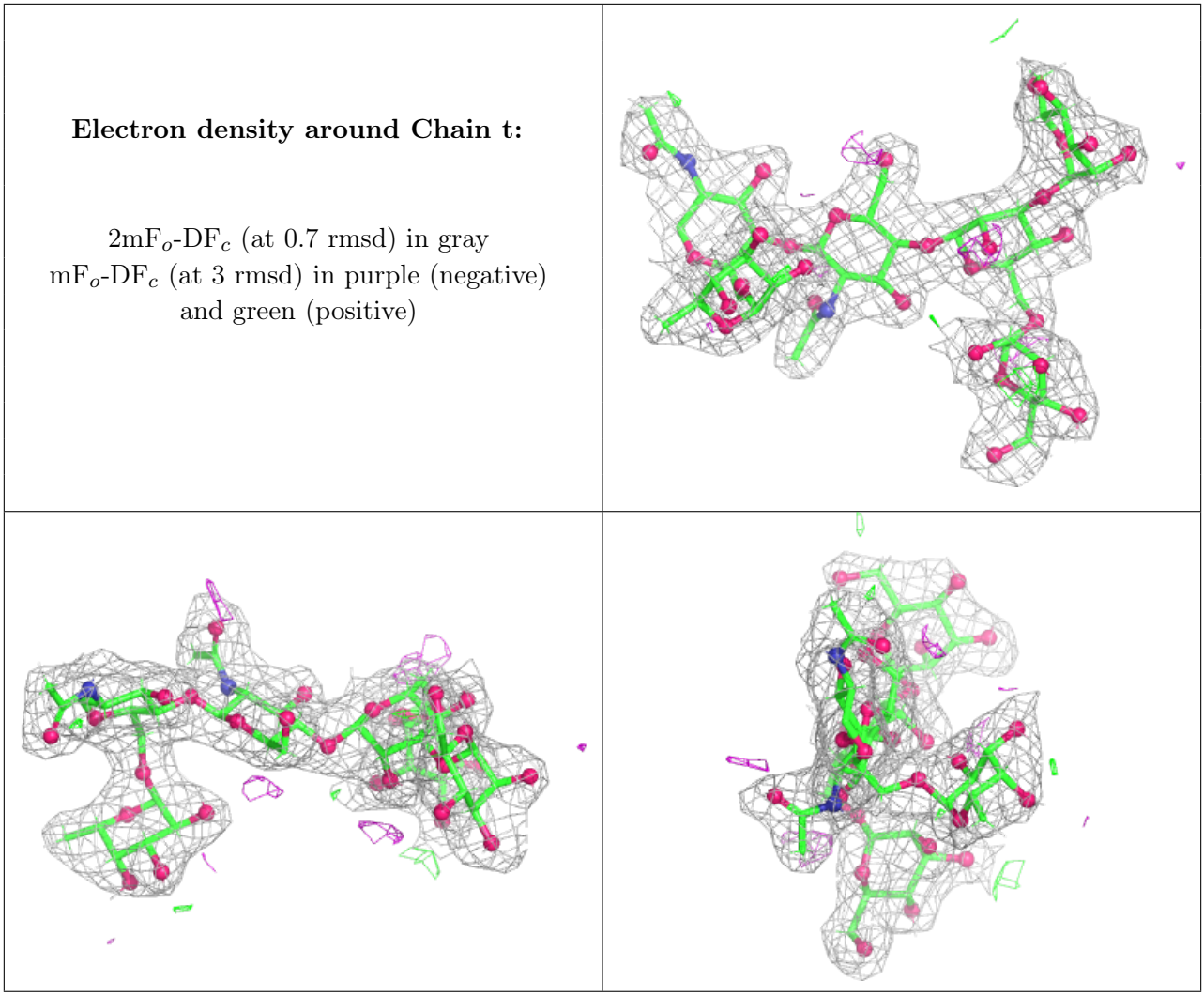






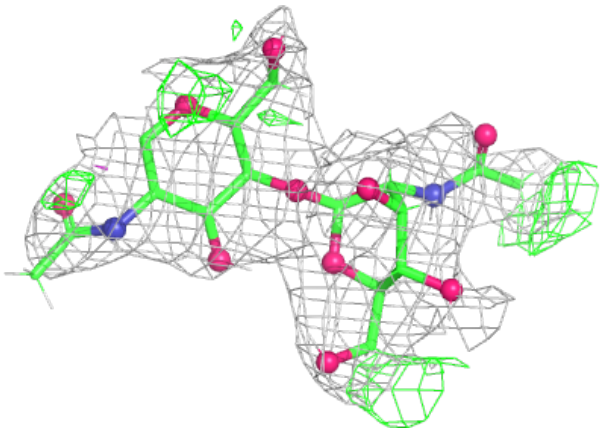
Electron density around Chain t:

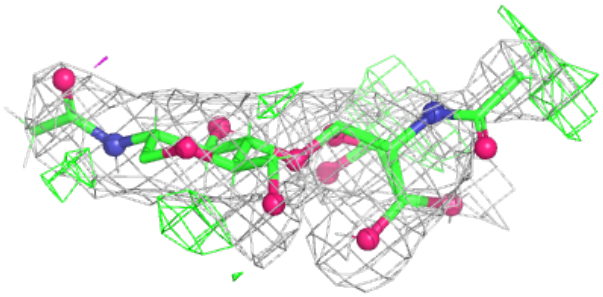
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

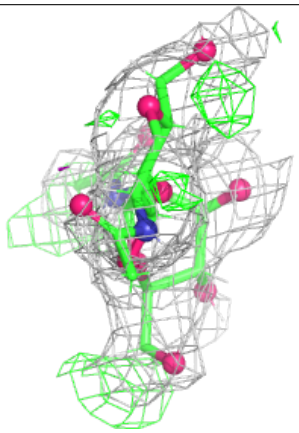


Electron density around Chain b:

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

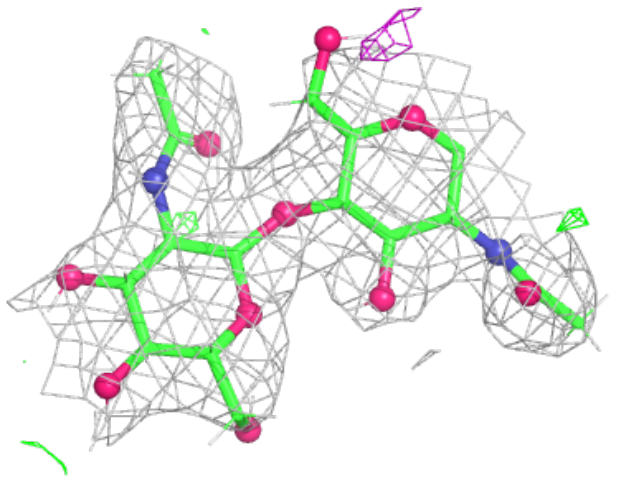


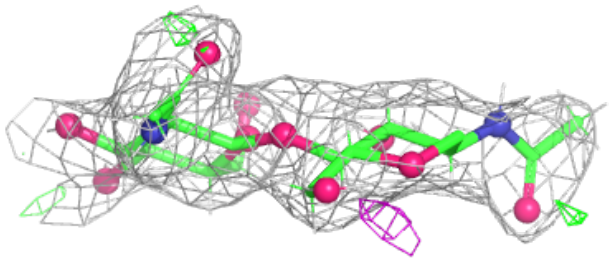


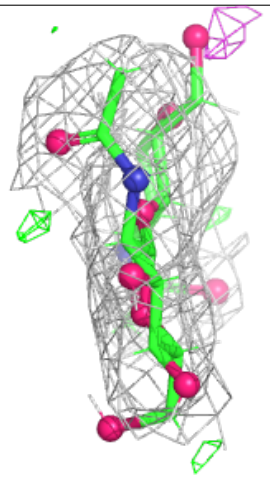


Electron density around Chain d:

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

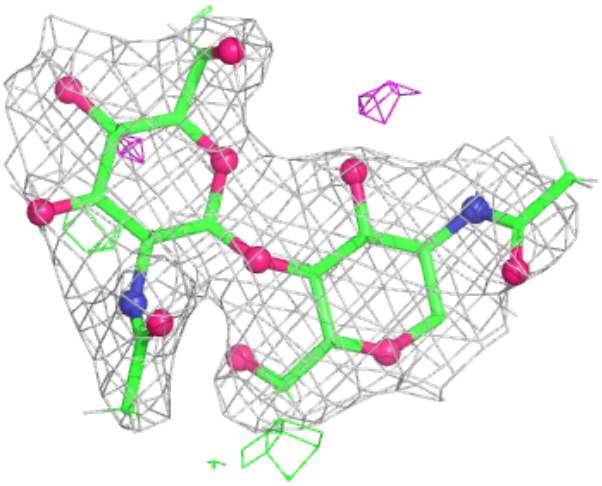


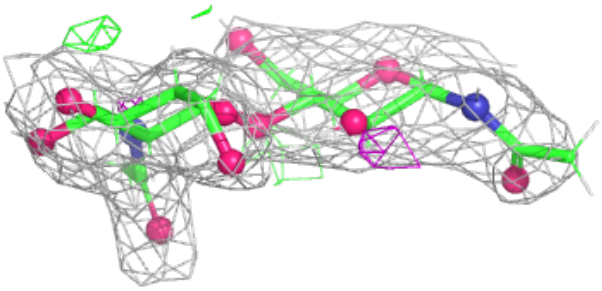


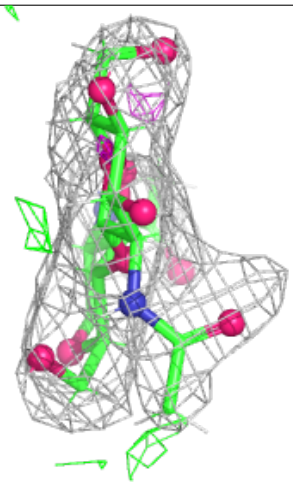


Electron density around Chain g:

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

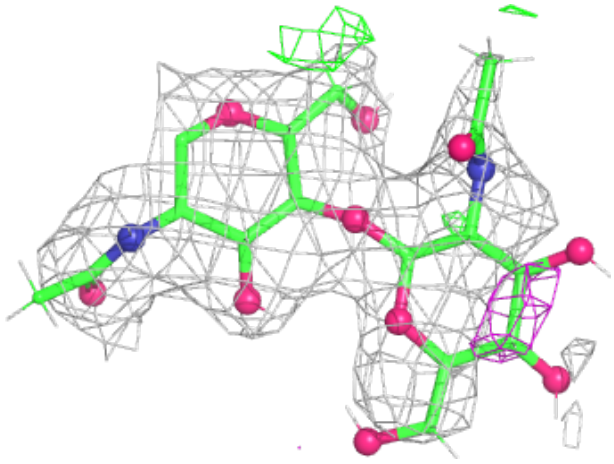


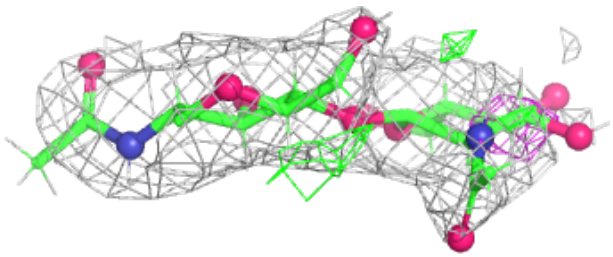


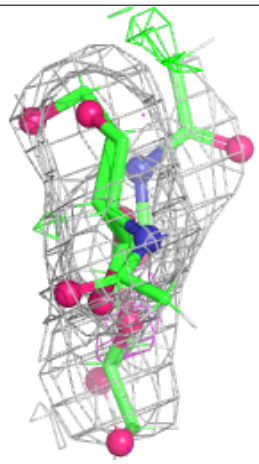


Electron density around Chain m:

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

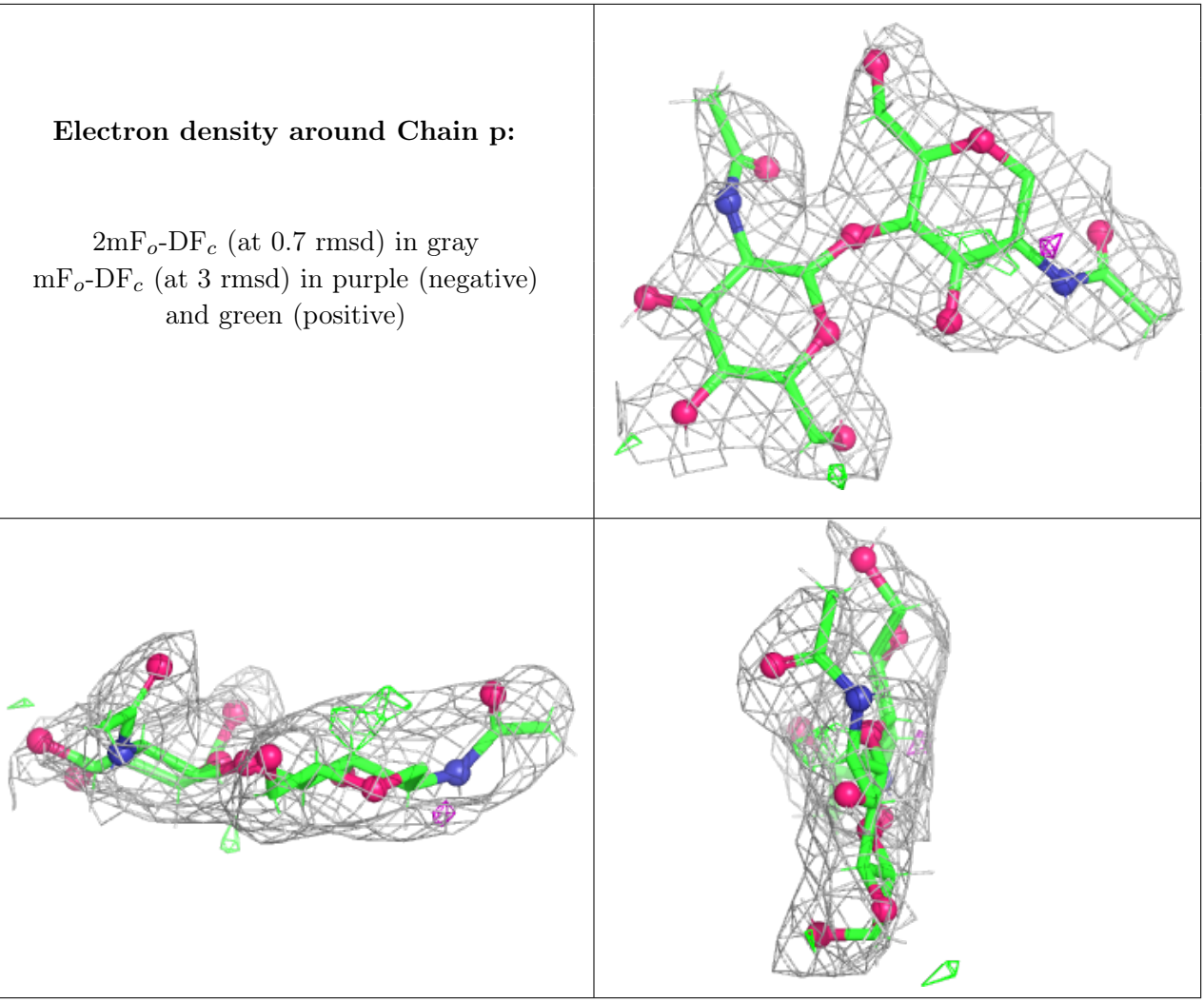






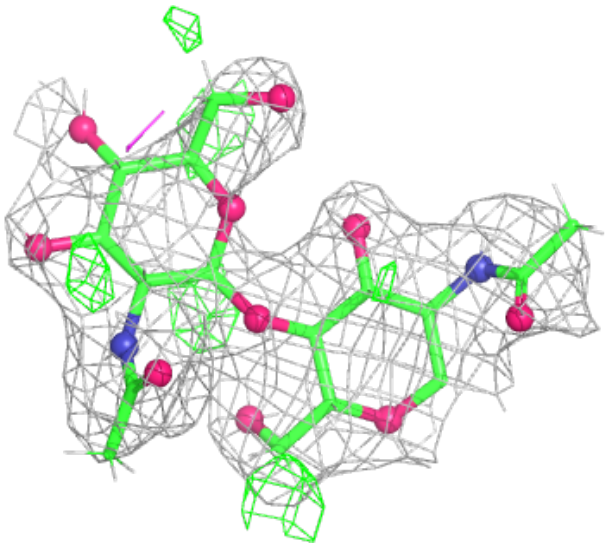
Electron density around Chain p:

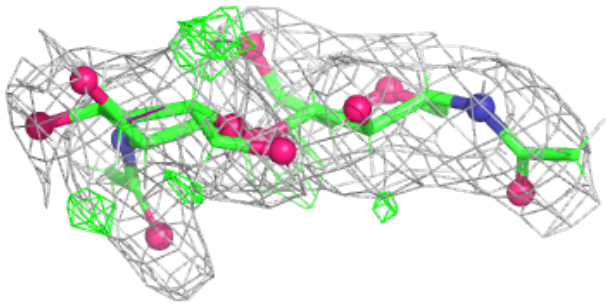
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

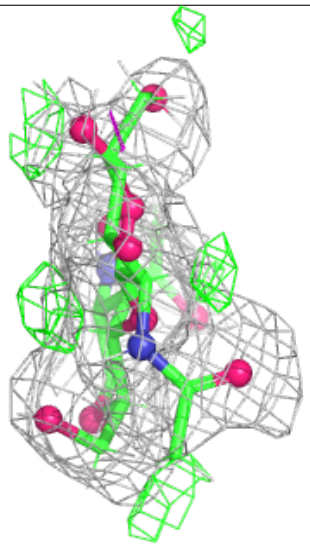


Electron density around Chain s:

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

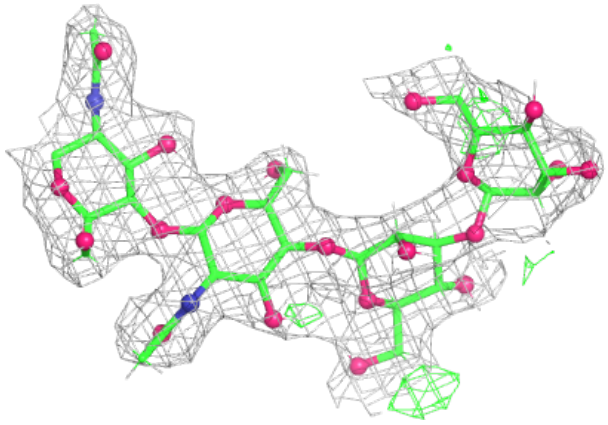


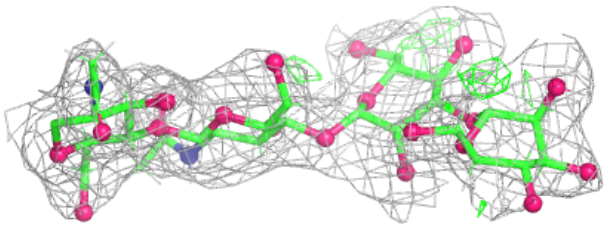


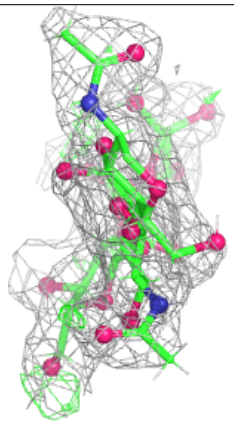


Electron density around Chain i:

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

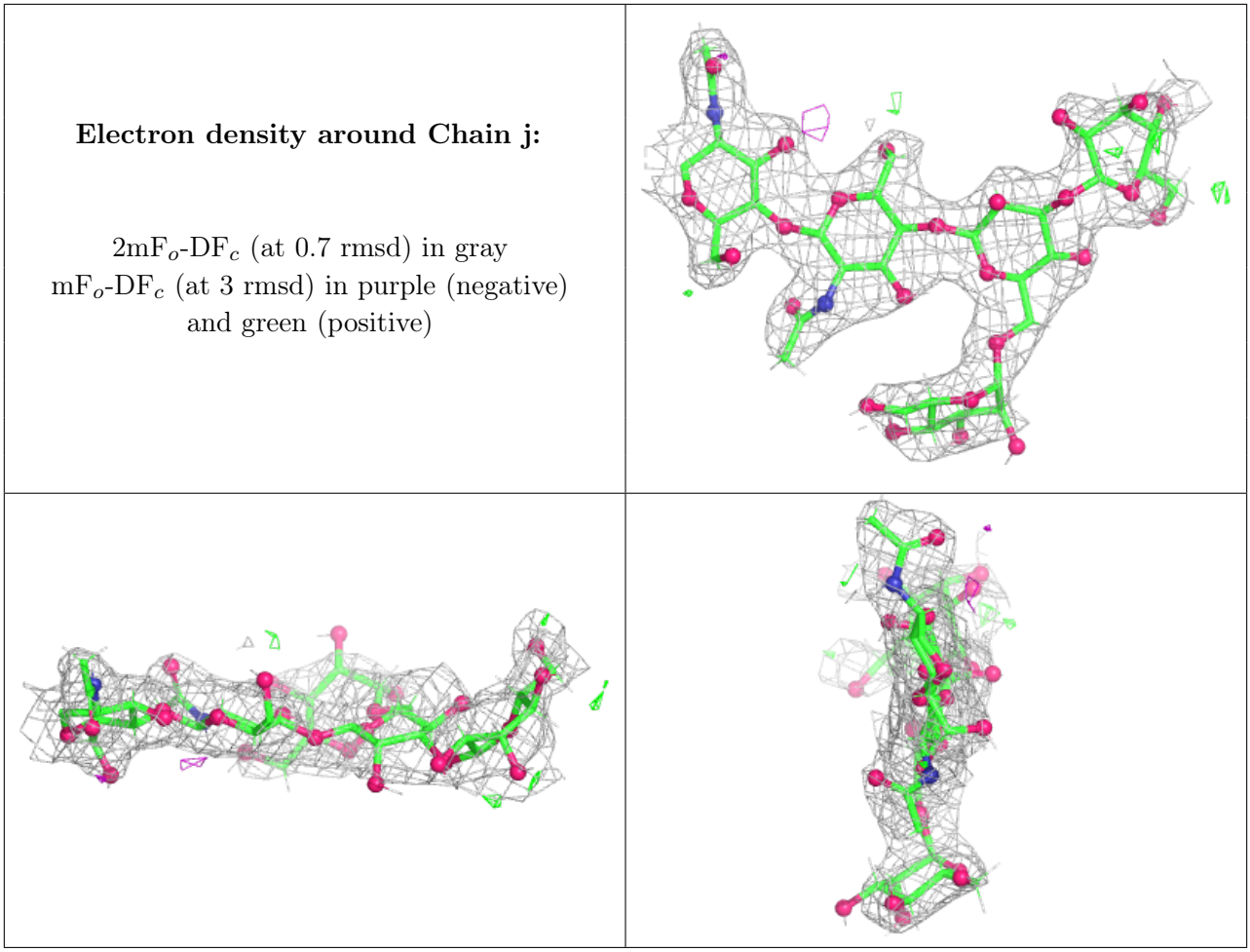






Electron density around Chain j:

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



6.4 Ligands

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
14	NAG	P	1002	14/15	0.59	0.23	59,82,99,106	0
16	OXL	P	1003	6/6	0.77	0.21	51,62,64,70	0
14	NAG	D	1003	14/15	0.79	0.22	62,78,94,98	0
14	NAG	H	1002	14/15	0.87	0.12	49,64,80,84	0
15	ACT	D	1004	4/4	0.88	0.11	44,50,63,63	0
14	NAG	D	1002	14/15	0.90	0.14	41,51,63,66	0
13	EDO	B	1002	4/4	0.91	0.13	37,45,54,54	0
11	HEC	A	3002	43/43	0.98	0.14	16,26,39,55	0
11	HEC	C	302	43/43	0.98	0.14	24,33,48,60	0
11	HEC	G	302	43/43	0.98	0.15	18,36,50,65	0
11	HEC	I	302	43/43	0.98	0.15	22,32,47,64	0

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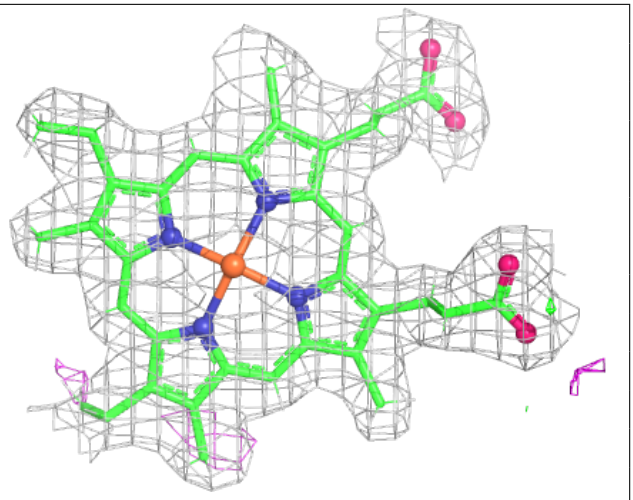
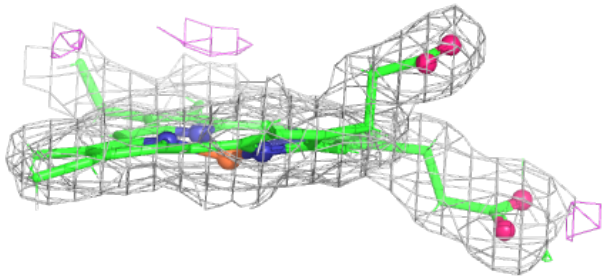
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	HEC	M	302	43/43	0.98	0.14	16,24,32,49	0
11	HEC	S	302	43/43	0.98	0.13	23,32,43,55	0
11	HEC	U	302	43/43	0.98	0.15	18,25,36,46	0
12	CA	B	1001	1/1	0.99	0.17	29,29,29,29	0
12	CA	H	1001	1/1	0.99	0.13	39,39,39,39	0
12	CA	J	1001	1/1	0.99	0.15	26,26,26,26	0
12	CA	N	1001	1/1	0.99	0.15	25,25,25,25	0
12	CA	P	1001	1/1	0.99	0.13	26,26,26,26	0
12	CA	T	1001	1/1	0.99	0.12	25,25,25,25	0
12	CA	V	802	1/1	0.99	0.12	23,23,23,23	0
10	CL	I	301	1/1	0.99	0.12	25,25,25,25	0
10	CL	M	301	1/1	0.99	0.18	20,20,20,20	0
10	CL	O	301	1/1	0.99	0.16	20,20,20,20	0
10	CL	S	301	1/1	0.99	0.13	23,23,23,23	0
11	HEC	O	302	43/43	0.99	0.14	20,27,46,56	0
10	CL	U	301	1/1	0.99	0.16	23,23,23,23	0
10	CL	G	301	1/1	0.99	0.14	25,25,25,25	0
10	CL	A	3001	1/1	1.00	0.17	20,20,20,20	0
12	CA	D	1001	1/1	1.00	0.12	31,31,31,31	0
10	CL	C	301	1/1	1.00	0.15	22,22,22,22	0

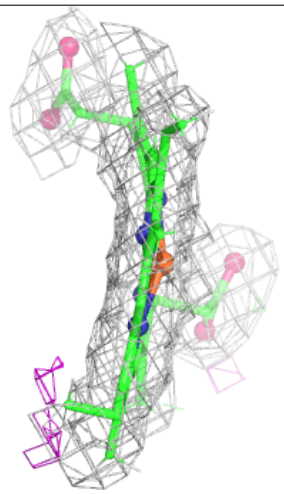
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC A 3002:

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

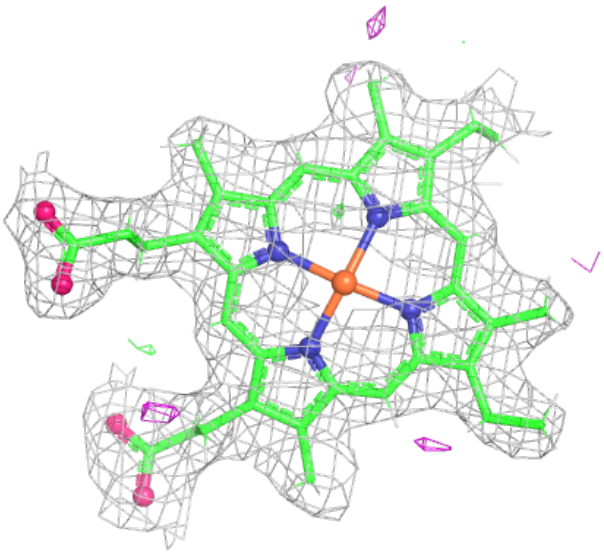


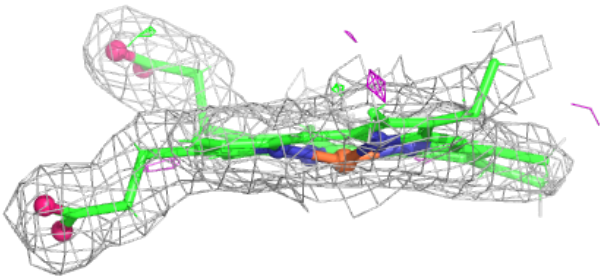


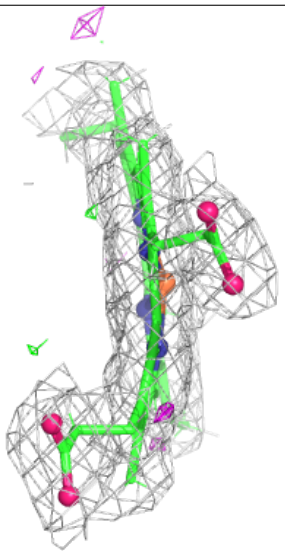


Electron density around HEC C 302:

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

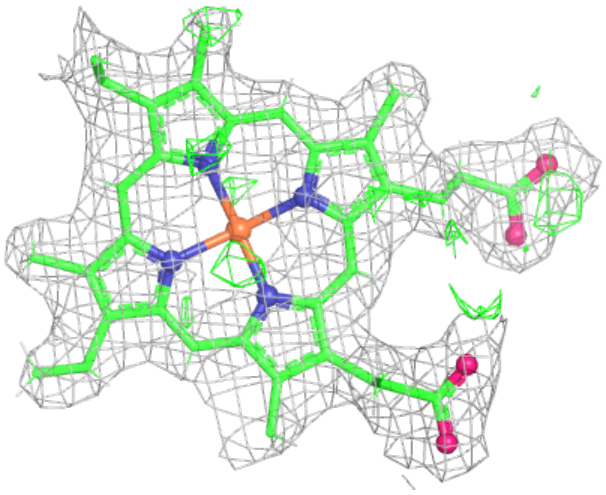


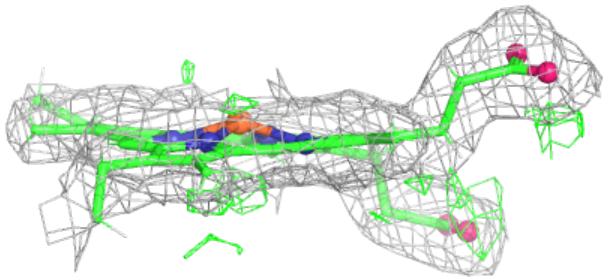


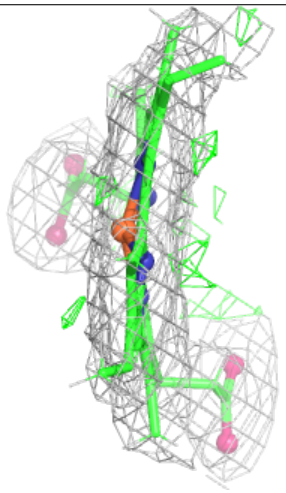


Electron density around HEC G 302:

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

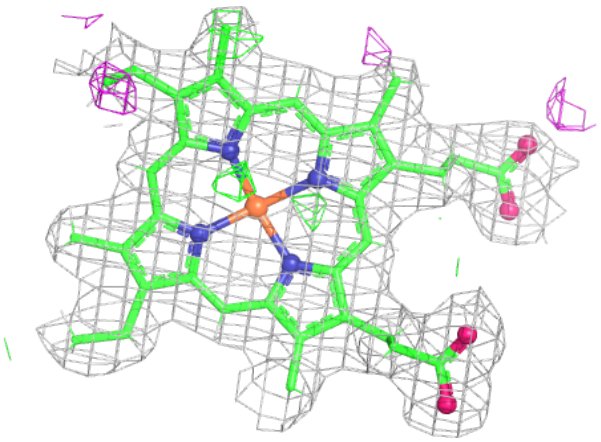


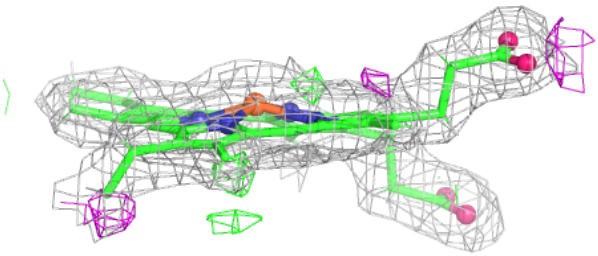


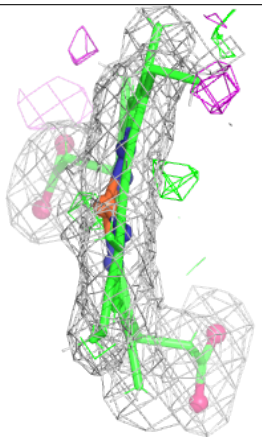


Electron density around HEC I 302:

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

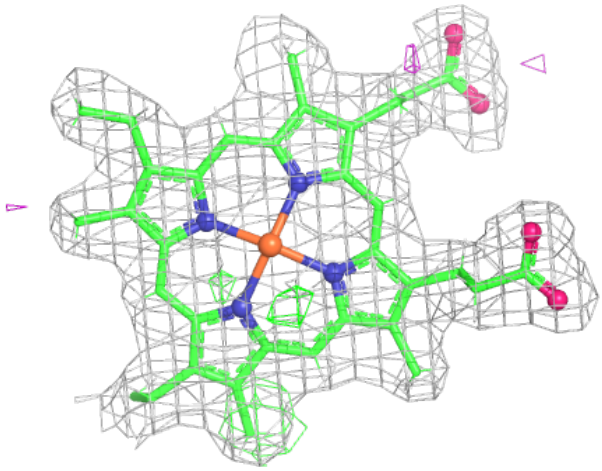


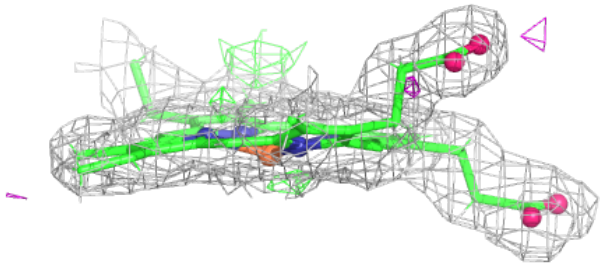


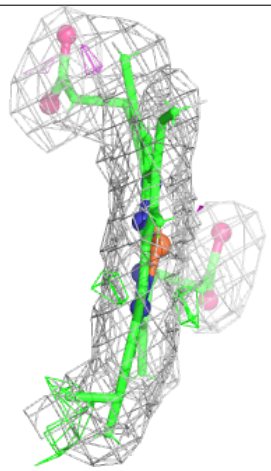


Electron density around HEC M 302:

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

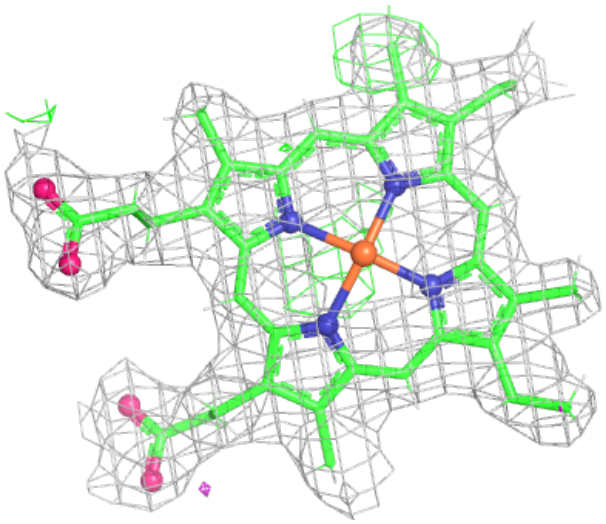


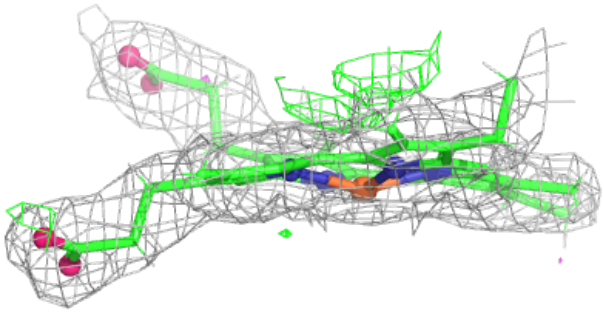


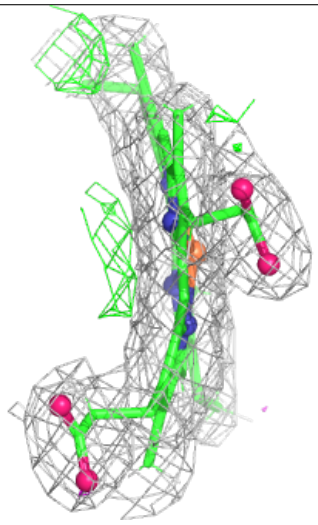


Electron density around HEC S 302:

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

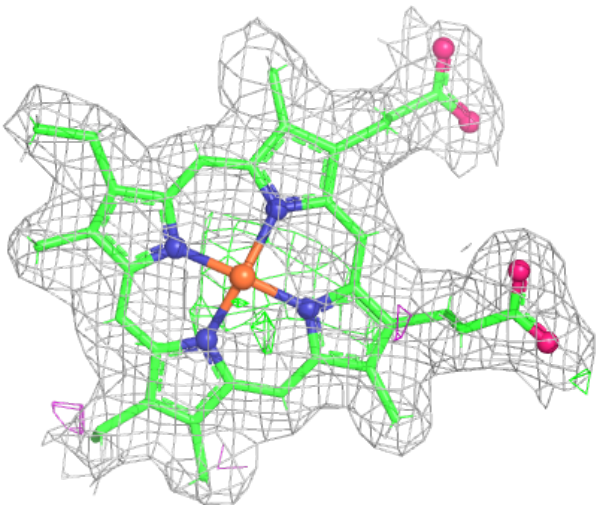


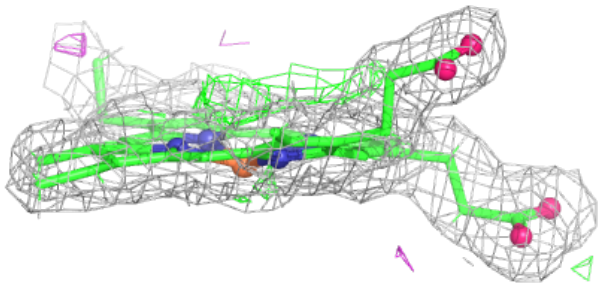


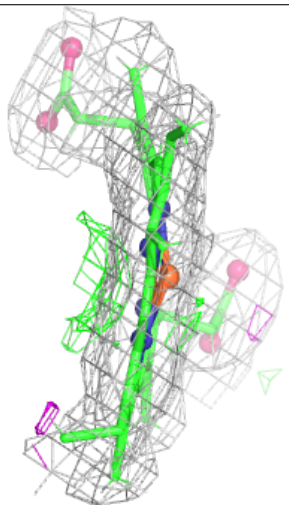


Electron density around HEC U 302:

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

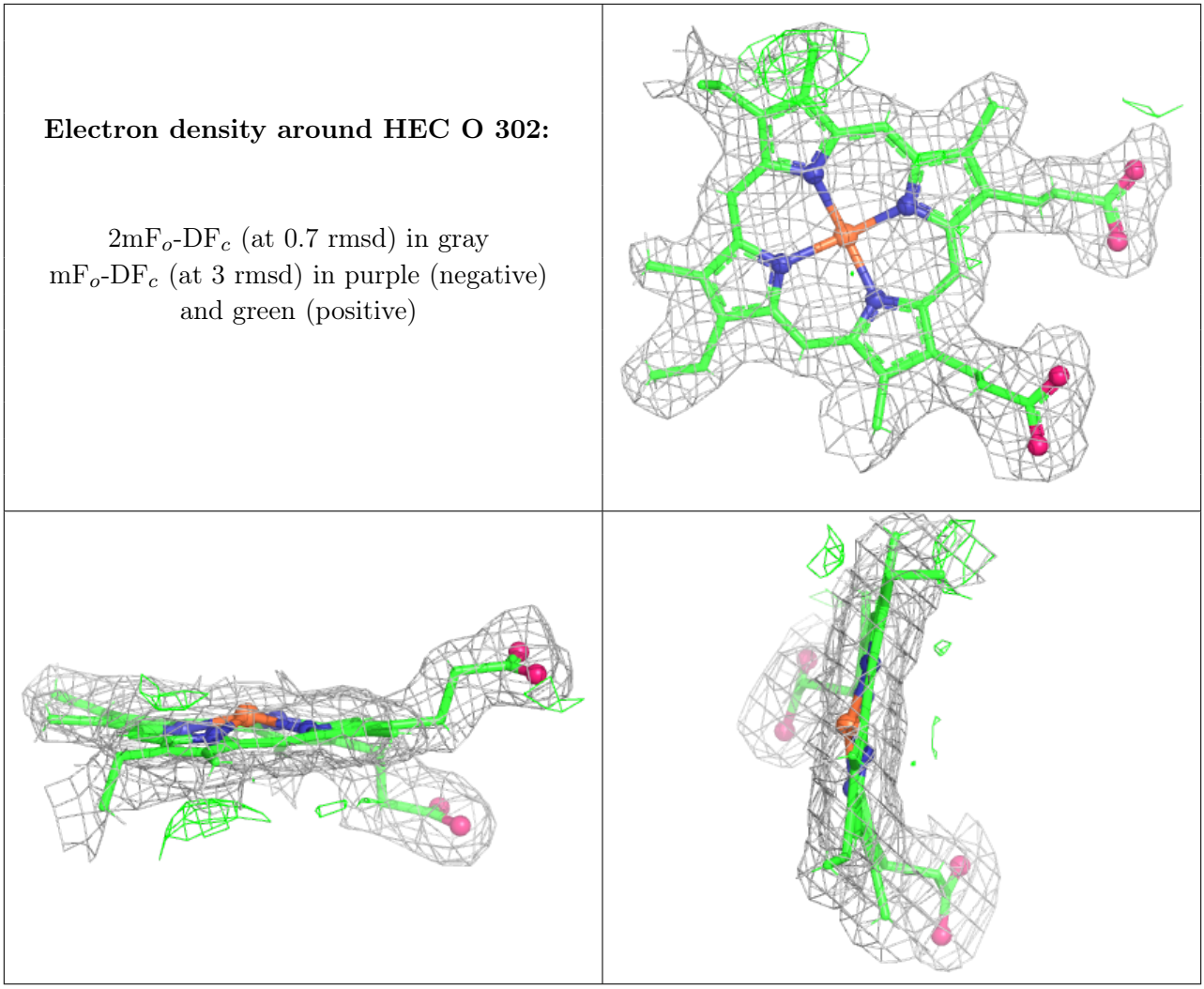






Electron density around HEC O 302:

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



6.5 Other polymers (i)

There are no such residues in this entry.