wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 07:35 PM EDT

PDB ID	:	3N8F / pdb_00003n8f
Title	:	Crystal structure of the complex of goat lactoperoxidase with thiocyanate at 3.2 A resolution
Authors	:	Vikram, G.; Singh, A.K.; Singh, R.P.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on	:	2010-05-28
Resolution	:	3.25 Å(reported)

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

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

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

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

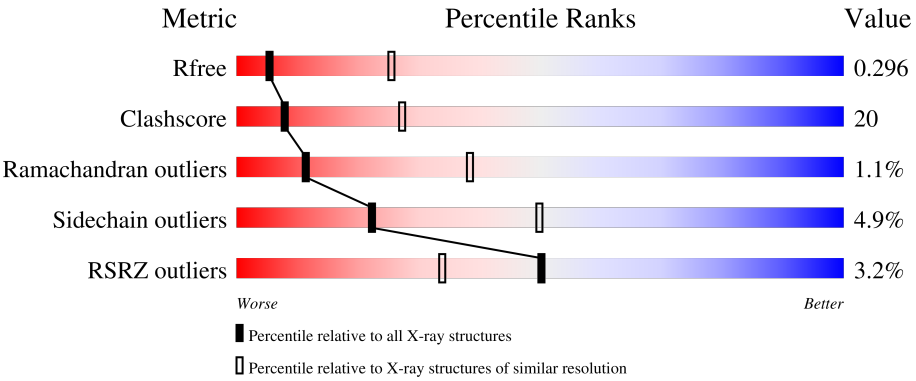
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.25 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	595	3%, 66%, 28%, 5% •
1	B	595	3%, 71%, 22%, 5% •
2	C	2	100%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	100%
2	G	2	100%
2	I	2	50% 50%
2	J	2	100%
3	D	3	100%
3	H	3	67% 33%

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
6	SCN	B	902	-	-	X	-
7	HEM	A	801	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10057 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4757	3021	844	865	1	26			
1	B	595	Total	C	N	O	P	S	0	0	0
			4757	3021	844	865	1	26			

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



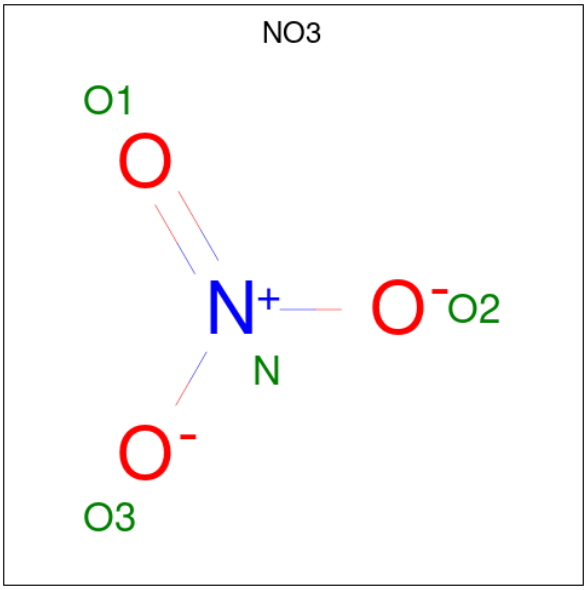
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 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
3	D	3	Total C N O 39 22 2 15	0	0	0
3	H	3	Total C N O 39 22 2 15	0	0	0

- Molecule 4 is NITRATE ION (CCD ID: NO3) (formula: NO_3).

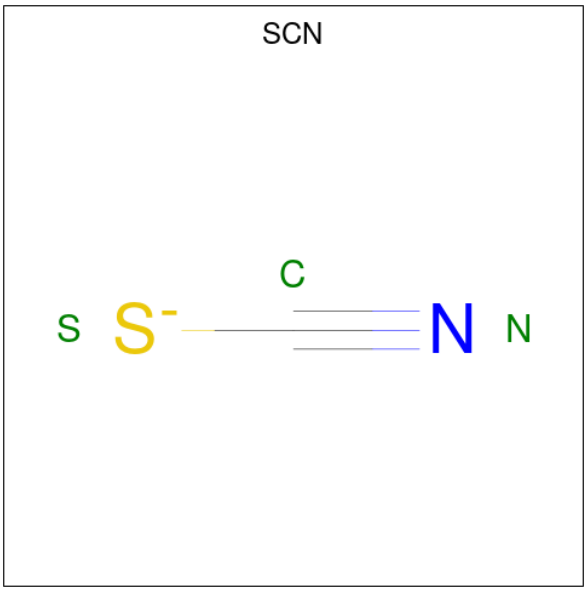


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total N O 4 1 3	0	0
4	A	1	Total N O 4 1 3	0	0
4	B	1	Total N O 4 1 3	0	0
4	B	1	Total N O 4 1 3	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

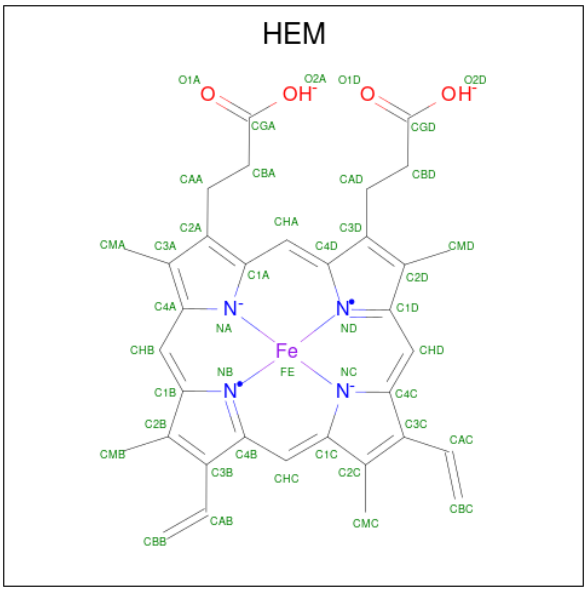
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N S 3 1 1 1	0	0
6	B	1	Total C N S 3 1 1 1	0	0

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



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

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

- Molecule 8 is water.

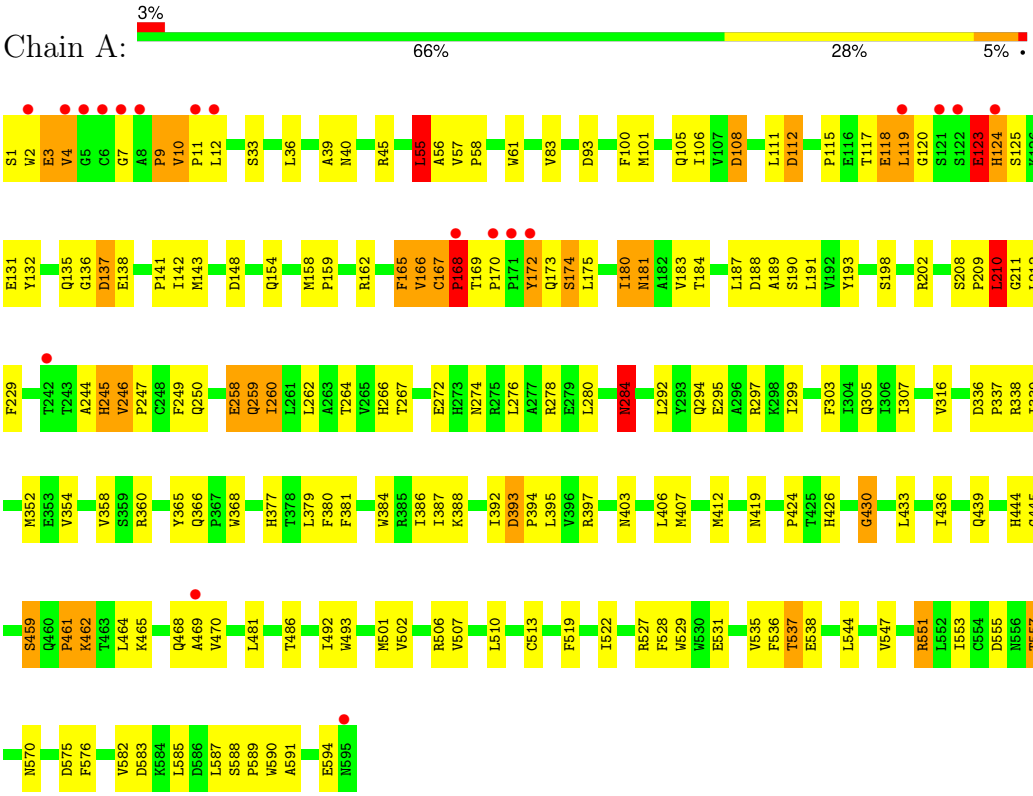
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	87	Total	O	0	0
			87	87		
8	B	100	Total	O	0	0
			100	100		

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.

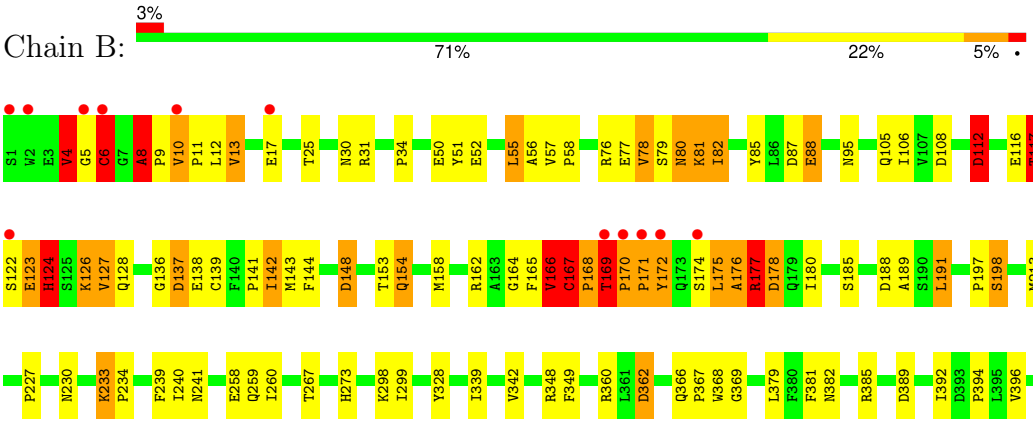
• Molecule 1: Lactoperoxidase

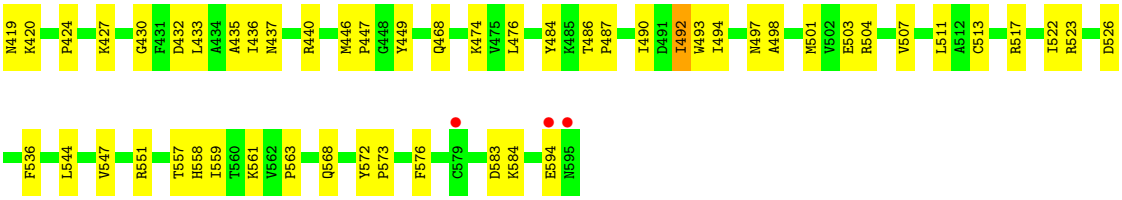
Chain A:



• Molecule 1: Lactoperoxidase

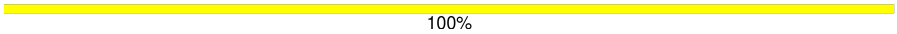
Chain B:





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

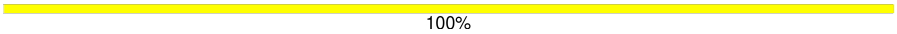
Chain C:





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

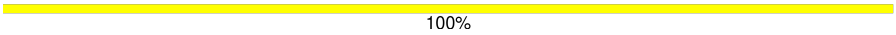
Chain E:





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

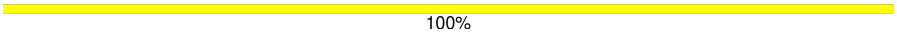
Chain F:





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

Chain G:





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

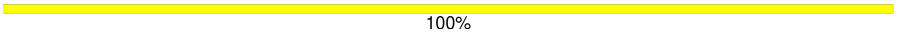
Chain I:





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

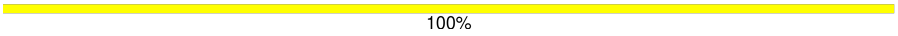
Chain J:





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

Chain D:





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

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.52Å 72.54Å 83.98Å 85.30° 84.06° 75.68°	Depositor
Resolution (Å)	24.98 – 3.25 24.98 – 3.25	Depositor EDS
% Data completeness (in resolution range)	94.6 (24.98-3.25) 94.6 (24.98-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 3.23Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.248 0.210 , 0.296	Depositor DCC
R_{free} test set	1011 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 71.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	10057	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NO3, SCN, BMA, NAG, HEM, CA, SEP

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	0.75	15/4875 (0.3%)	0.98	21/6621 (0.3%)
1	B	0.73	13/4875 (0.3%)	1.04	33/6621 (0.5%)
All	All	0.74	28/9750 (0.3%)	1.01	54/13242 (0.4%)

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	366	GLN	C-O	-7.55	1.16	1.24
1	B	176	ALA	CA-CB	-7.07	1.42	1.53
1	A	244	ALA	CA-CB	-6.95	1.43	1.53
1	A	137	ASP	CA-C	-6.41	1.47	1.53
1	A	10	VAL	CA-C	-6.35	1.46	1.52

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	168	PRO	CA-N-CD	-13.76	92.74	112.00
1	B	166	VAL	N-CA-C	12.80	127.39	113.43
1	B	4	VAL	N-CA-C	10.74	120.63	110.53
1	A	119	LEU	N-CA-C	-10.12	101.59	112.93
1	B	166	VAL	CA-C-N	-9.95	107.65	120.09

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4757	0	4644	185	0
1	B	4757	0	4644	192	0
2	C	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	I	28	0	25	2	0
2	J	28	0	25	0	0
3	D	39	0	34	0	0
3	H	39	0	34	1	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	3	0	0	1	0
6	B	3	0	0	3	0
7	A	43	0	30	22	0
7	B	43	0	30	18	0
8	A	87	0	0	1	0
8	B	100	0	0	3	0
All	All	10057	0	9566	383	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 383 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLU:OE2	7:B:821:HEM:CMB	1.63	1.46
1:B:108:ASP:OD2	7:B:821:HEM:CMD	1.65	1.45
1:A:258:GLU:OE2	7:A:801:HEM:CMB	1.67	1.39
1:B:170:PRO:CB	1:B:171:PRO:HD3	1.50	1.36
1:B:170:PRO:HB2	1:B:171:PRO:CD	1.46	1.36

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	592/595 (100%)	555 (94%)	30 (5%)	7 (1%)	10	36
1	B	592/595 (100%)	556 (94%)	30 (5%)	6 (1%)	12	40
All	All	1184/1190 (100%)	1111 (94%)	60 (5%)	13 (1%)	11	38

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	167	CYS
1	A	168	PRO
1	B	168	PRO
1	B	170	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	516/516 (100%)	492 (95%)	24 (5%)	23	51
1	B	516/516 (100%)	489 (95%)	27 (5%)	21	48
All	All	1032/1032 (100%)	981 (95%)	51 (5%)	22	50

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	79	SER

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Mol	Chain	Res	Type
1	B	121	SER
1	B	191	LEU
1	B	82	ILE
1	B	117	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	545	GLN
1	B	105	GLN
1	B	532	ASN
1	B	63	GLN
1	B	128	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	SEP	B	198	1	8,9,10	1.73	1 (12%)	7,12,14	1.26	1 (14%)
1	SEP	A	198	1	8,9,10	1.75	2 (25%)	7,12,14	1.57	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	B	198	1	-	1/6/8/10	-
1	SEP	A	198	1	-	2/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	3.89	1.62	1.50
1	B	198	SEP	P-O1P	3.89	1.62	1.50
1	A	198	SEP	P-O2P	2.01	1.62	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	198	SEP	OG-CB-CA	3.22	111.28	108.14
1	B	198	SEP	OG-CB-CA	2.17	110.26	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	198	SEP	CB-OG-P-O2P
1	A	198	SEP	CA-CB-OG-P
1	B	198	SEP	CA-CB-OG-P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	198	SEP	2	0

5.5 Carbohydrates (i)

18 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	C	1	2,1	14,14,15	1.10	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	C	2	2	14,14,15	1.42	4 (28%)	17,19,21	1.56	3 (17%)
3	NAG	D	1	3,1	14,14,15	0.74	0	17,19,21	0.78	1 (5%)
3	NAG	D	2	3	14,14,15	0.80	0	17,19,21	1.55	2 (11%)
3	BMA	D	3	3	11,11,12	1.06	1 (9%)	15,15,17	1.57	4 (26%)
2	NAG	E	1	2,1	14,14,15	0.56	0	17,19,21	1.28	2 (11%)
2	NAG	E	2	2	14,14,15	0.57	0	17,19,21	1.79	3 (17%)
2	NAG	F	1	2,1	14,14,15	0.57	0	17,19,21	1.17	1 (5%)
2	NAG	F	2	2	14,14,15	0.65	0	17,19,21	1.51	2 (11%)
2	NAG	G	1	2	14,14,15	1.10	1 (7%)	17,19,21	1.09	1 (5%)
2	NAG	G	2	2	14,14,15	1.41	4 (28%)	17,19,21	1.55	3 (17%)
3	NAG	H	1	3,1	14,14,15	0.73	0	17,19,21	0.78	1 (5%)
3	NAG	H	2	3	14,14,15	0.81	0	17,19,21	1.56	2 (11%)
3	BMA	H	3	3	11,11,12	1.05	1 (9%)	15,15,17	1.57	4 (26%)
2	NAG	I	1	2,1	14,14,15	0.45	0	17,19,21	1.46	2 (11%)
2	NAG	I	2	2	14,14,15	0.58	0	17,19,21	1.28	2 (11%)
2	NAG	J	1	2,1	14,14,15	0.61	0	17,19,21	1.49	2 (11%)
2	NAG	J	2	2	14,14,15	0.54	0	17,19,21	0.93	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
3	BMA	D	3	3	-	2/2/19/22	0/1/1/1
2	NAG	E	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
2	NAG	F	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	2	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1

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

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	NAG	C3-C2	2.94	1.58	1.52
2	C	2	NAG	C3-C2	2.91	1.58	1.52
3	H	3	BMA	C2-C3	2.71	1.56	1.52
3	D	3	BMA	C2-C3	2.70	1.56	1.52
2	G	2	NAG	C4-C3	2.35	1.58	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C1-O5-C5	5.33	119.33	112.19
3	H	2	NAG	C4-C3-C2	4.90	118.19	111.02
3	D	2	NAG	C4-C3-C2	4.86	118.14	111.02
2	C	2	NAG	C4-C3-C2	4.86	118.14	111.02
2	G	2	NAG	C4-C3-C2	4.83	118.09	111.02

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	J	1	NAG	O7-C7-N2-C2
2	J	2	NAG	O7-C7-N2-C2
2	F	2	NAG	O5-C5-C6-O6

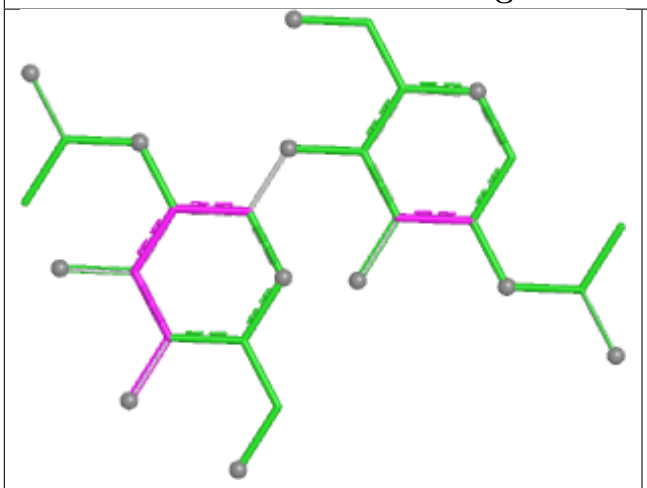
There are no ring outliers.

2 monomers are involved in 3 short contacts:

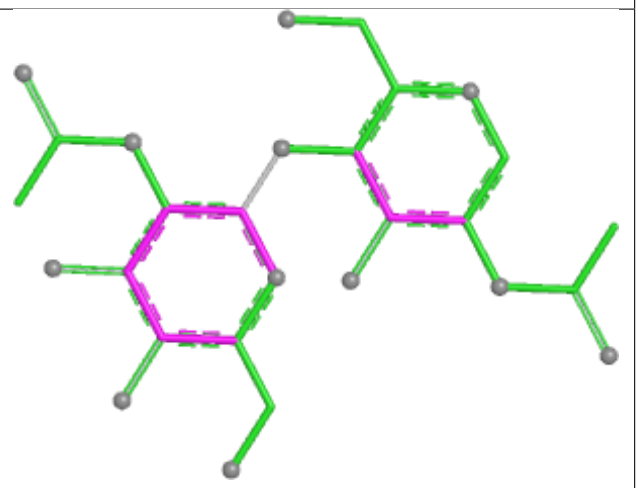
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1	NAG	2	0
3	H	1	NAG	1	0

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

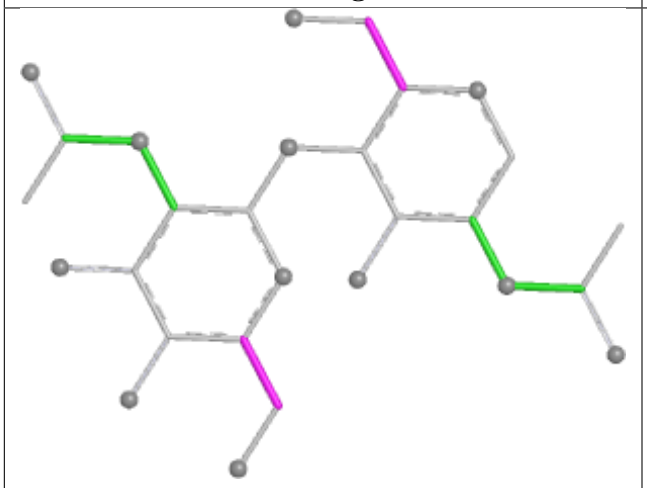
Oligosaccharide Chain C



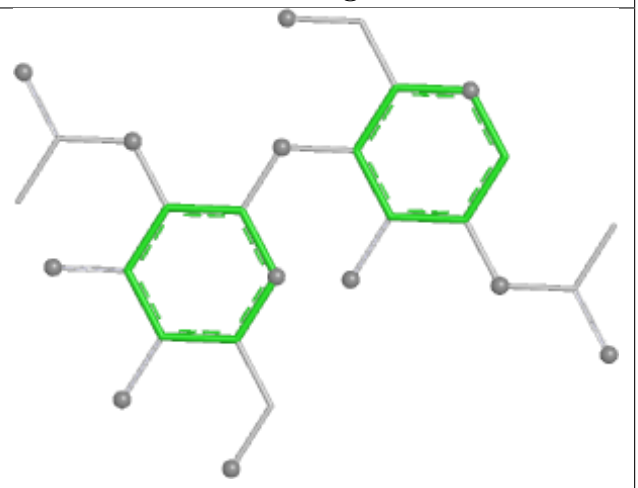
Bond lengths



Bond angles

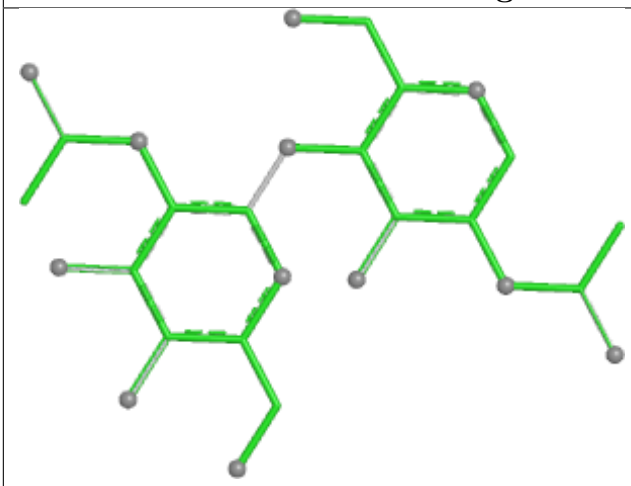


Torsions

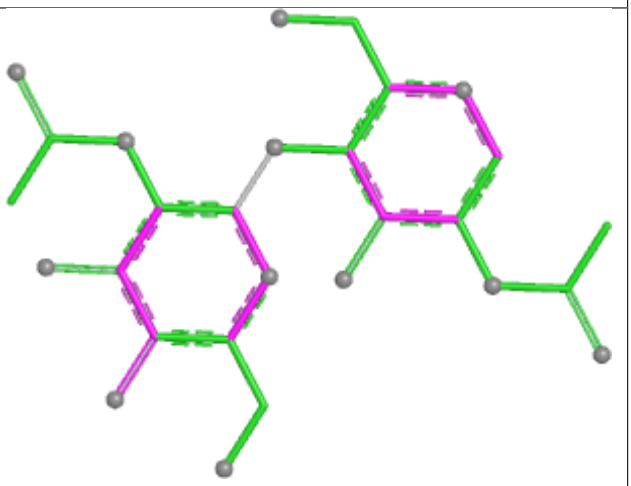


Rings

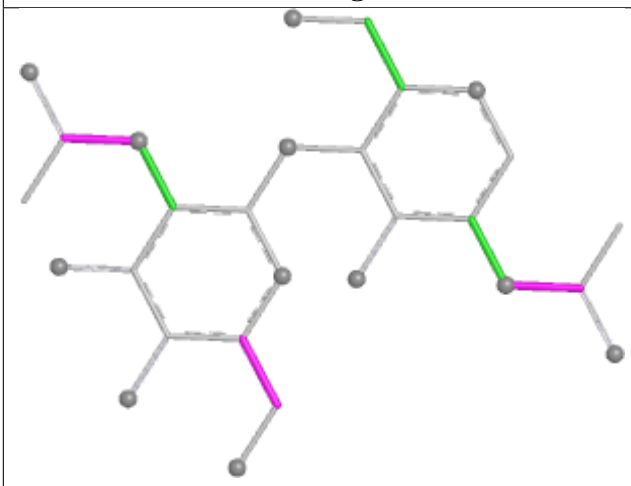
Oligosaccharide Chain E



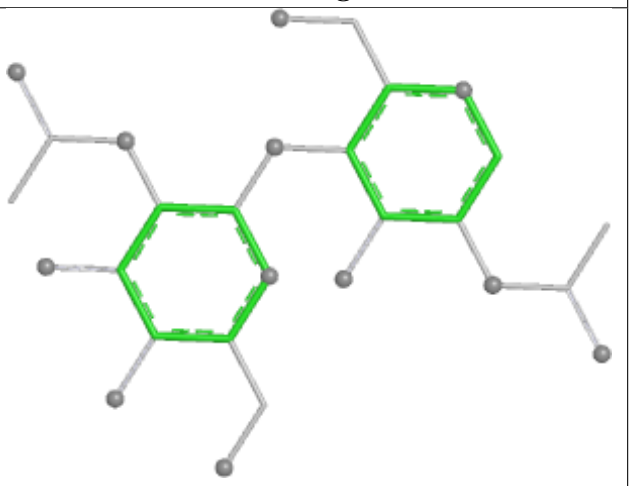
Bond lengths



Bond angles

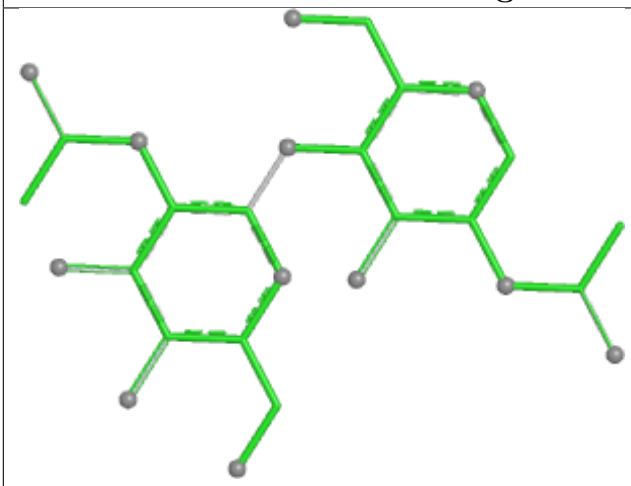


Torsions

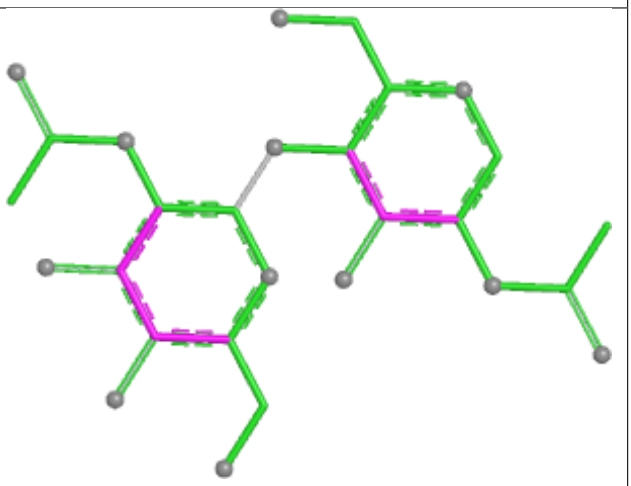


Rings

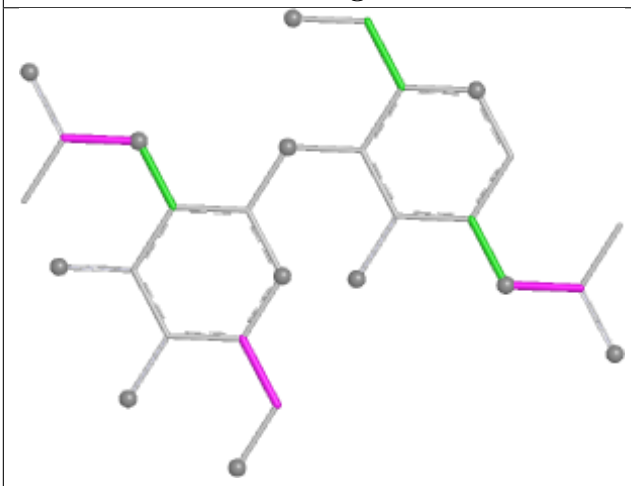
Oligosaccharide Chain F



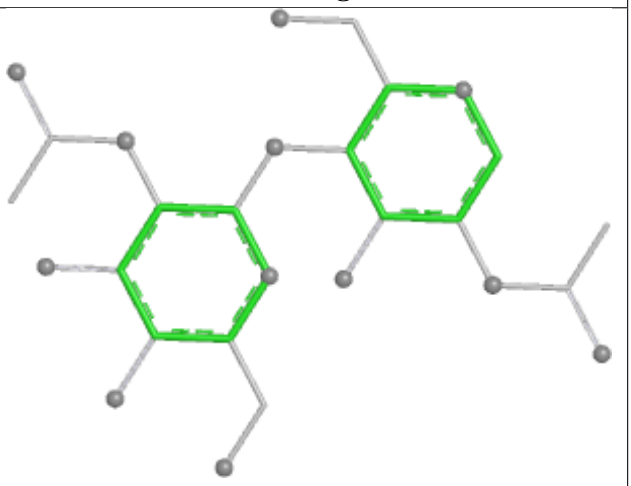
Bond lengths



Bond angles

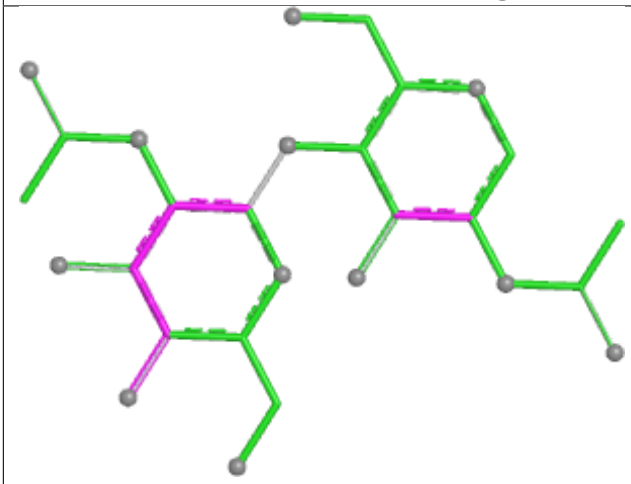


Torsions

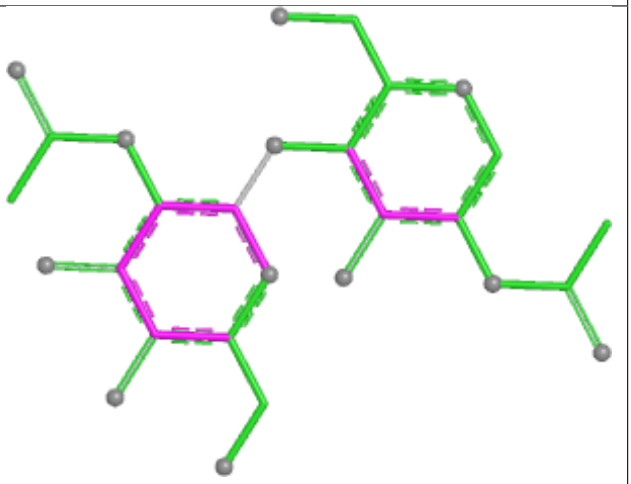


Rings

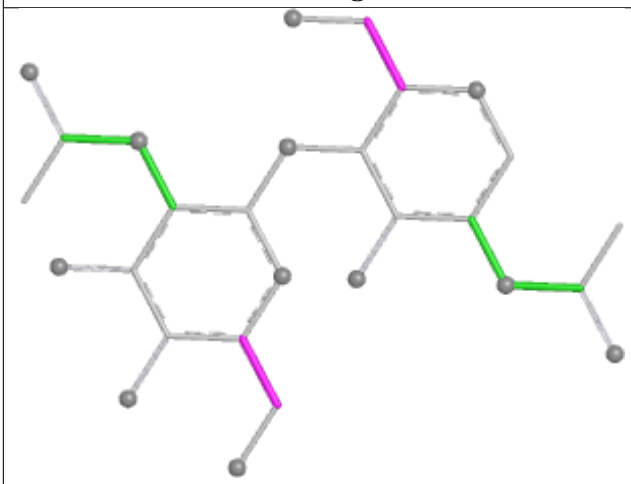
Oligosaccharide Chain G



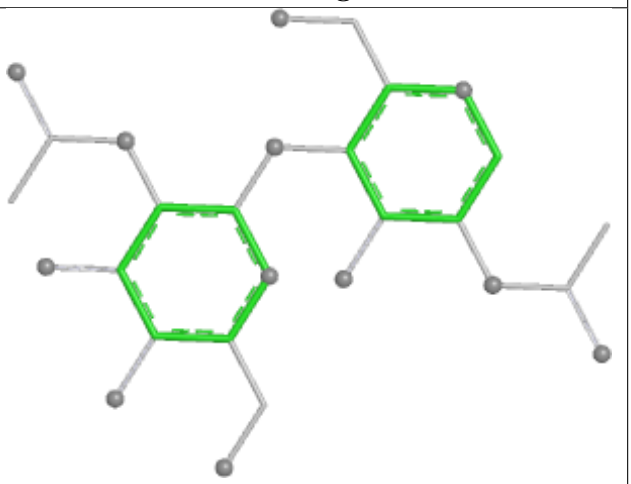
Bond lengths



Bond angles

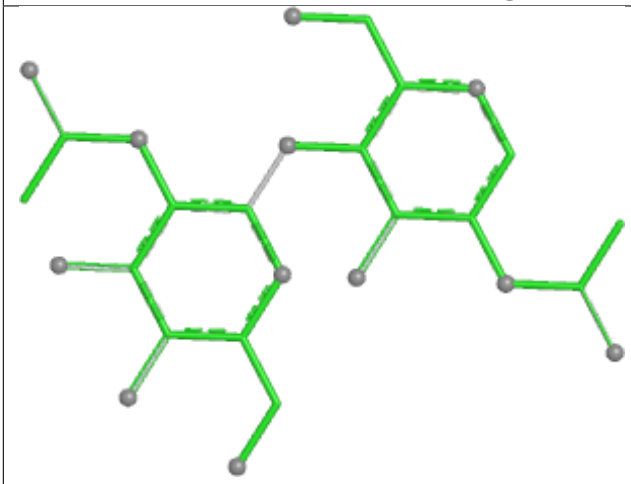


Torsions

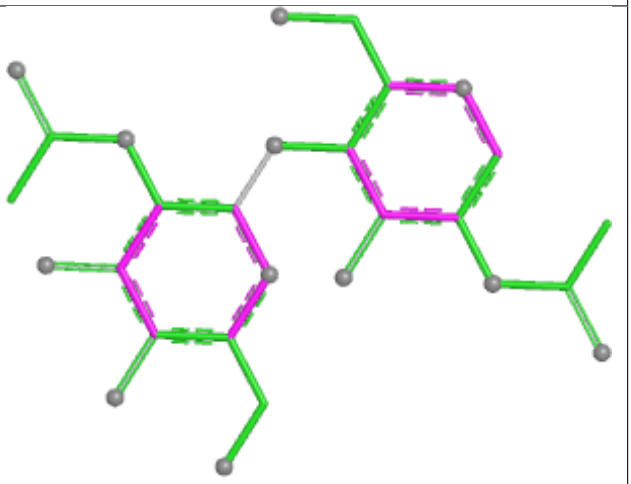


Rings

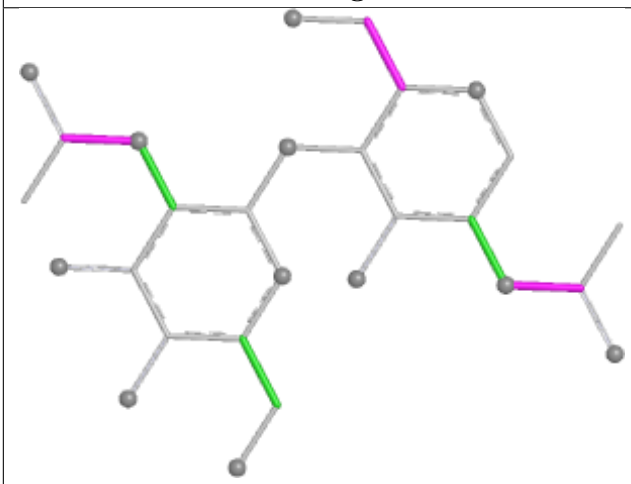
Oligosaccharide Chain I



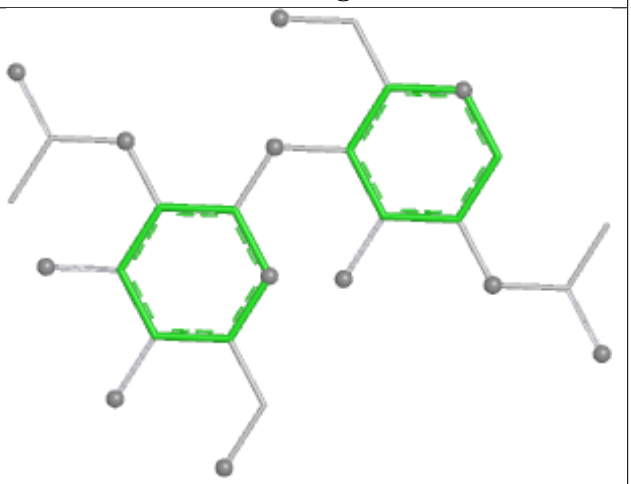
Bond lengths



Bond angles

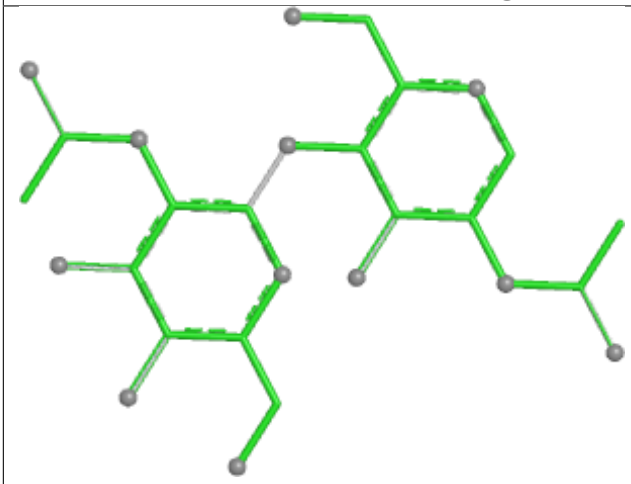


Torsions

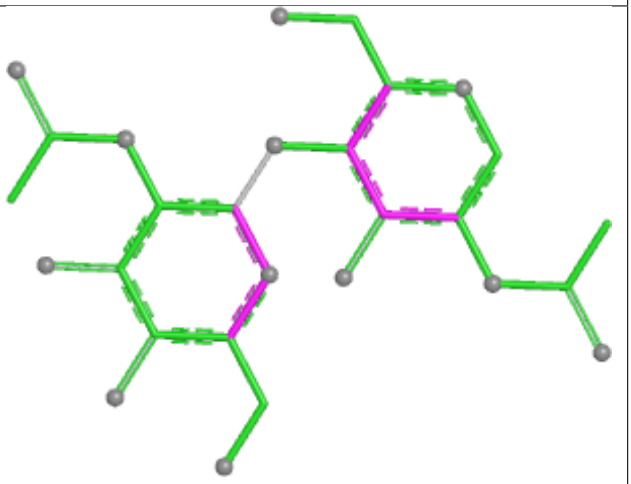


Rings

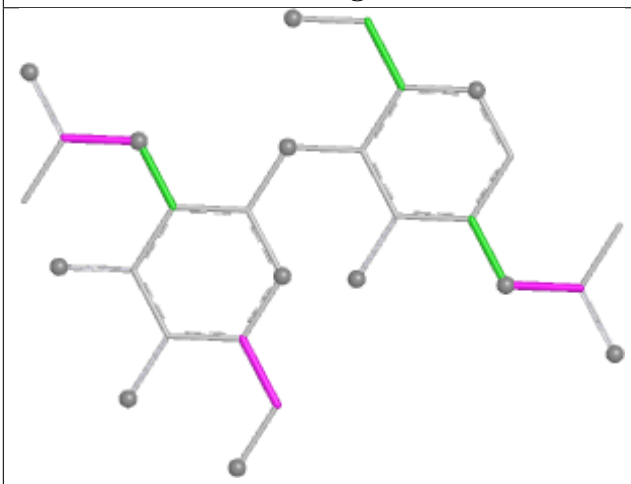
Oligosaccharide Chain J



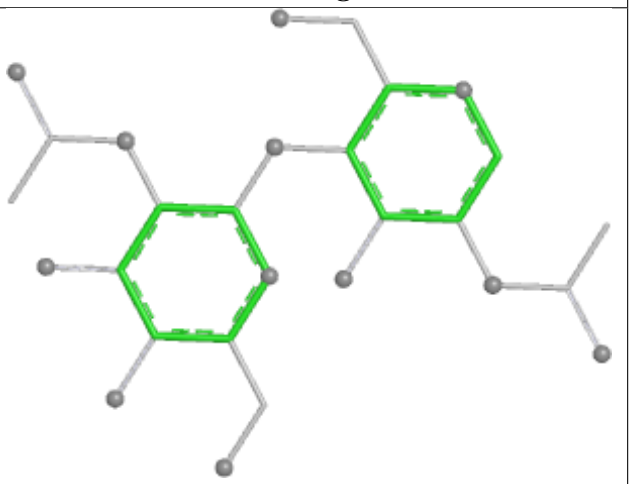
Bond lengths



Bond angles

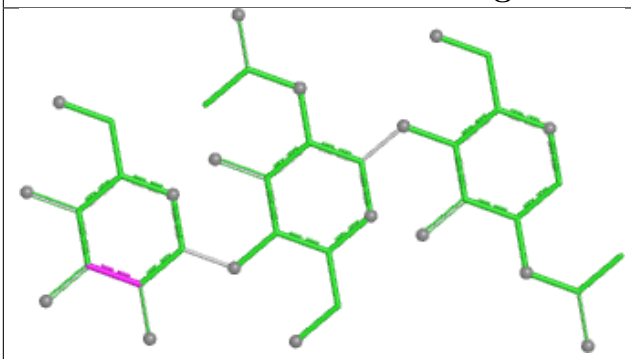


Torsions

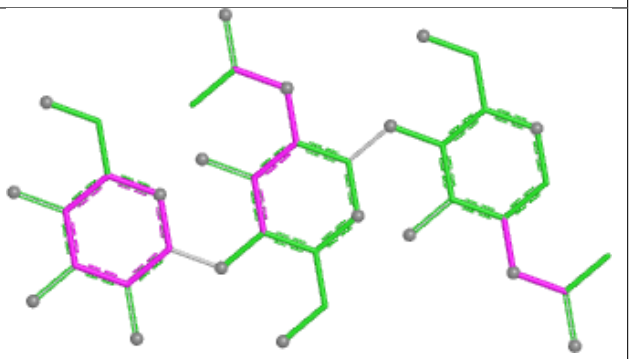


Rings

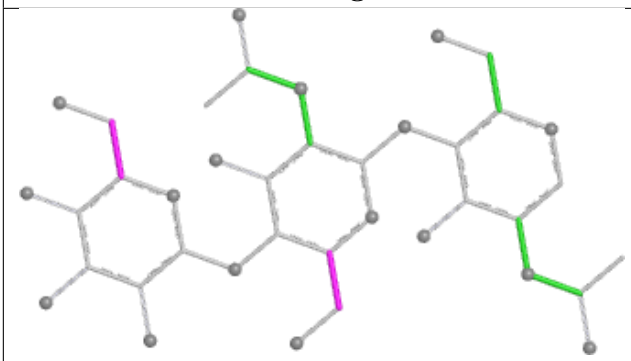
Oligosaccharide Chain D



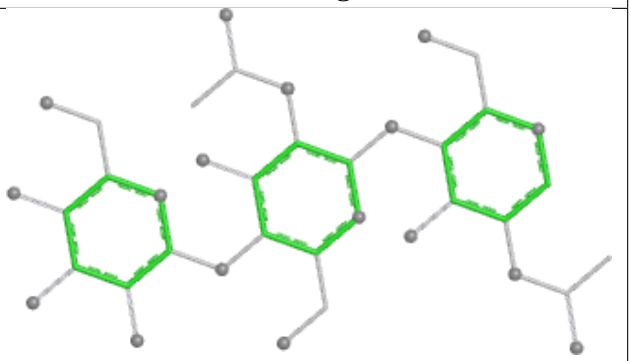
Bond lengths



Bond angles

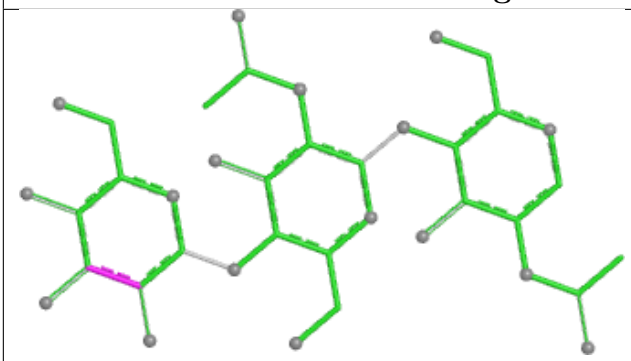


Torsions

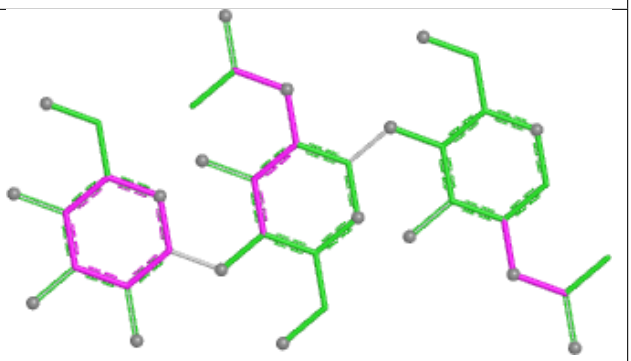


Rings

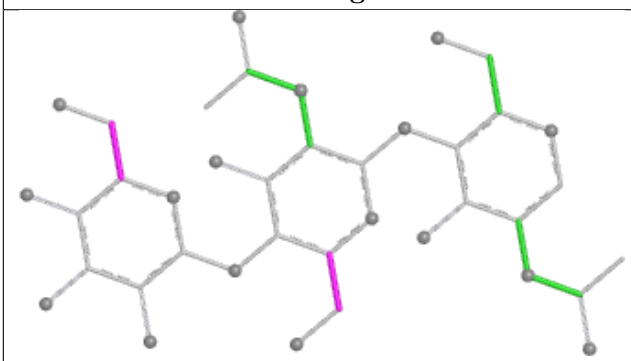
Oligosaccharide Chain H



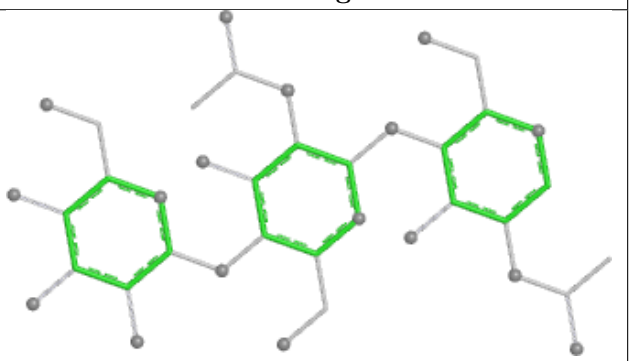
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
4	NO3	A	608	-	1,3,3	3.29	1 (100%)	0,3,3	-	-
4	NO3	A	607	-	1,3,3	3.39	1 (100%)	0,3,3	-	-
4	NO3	B	608	-	1,3,3	3.12	1 (100%)	0,3,3	-	-
7	HEM	B	821	1,8	50,50,50	1.94	10 (20%)	67,82,82	1.37	7 (10%)
7	HEM	A	801	1,8	50,50,50	1.96	10 (20%)	67,82,82	1.32	7 (10%)
6	SCN	A	901	-	1,2,2	3.58	1 (100%)	0,1,1	-	-
4	NO3	B	607	-	1,3,3	3.41	1 (100%)	0,3,3	-	-
6	SCN	B	902	-	1,2,2	3.14	1 (100%)	0,1,1	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEM	B	821	1,8	-	4/14/54/54	-
7	HEM	A	801	1,8	-	7/14/54/54	-

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	821	HEM	C3D-C2D	7.66	1.53	1.36
7	A	801	HEM	C3D-C2D	7.66	1.53	1.36
7	A	801	HEM	FE-NB	6.02	2.13	1.94
7	B	821	HEM	FE-ND	4.41	2.08	1.94
7	B	821	HEM	FE-NC	4.33	2.09	1.95

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	821	HEM	C4D-ND-C1D	5.76	112.03	105.21
7	A	801	HEM	C4D-ND-C1D	5.61	111.85	105.21
7	A	801	HEM	CMD-C2D-C1D	2.95	129.65	125.03
7	B	821	HEM	C3B-C2B-C1B	2.89	108.58	106.41
7	B	821	HEM	CMD-C2D-C1D	2.76	129.35	125.03

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	801	HEM	C1A-C2A-CAA-CBA
7	A	801	HEM	C3A-C2A-CAA-CBA
7	A	801	HEM	CAA-CBA-CGA-O2A
7	B	821	HEM	CAA-CBA-CGA-O2A
7	B	821	HEM	CAA-CBA-CGA-O1A

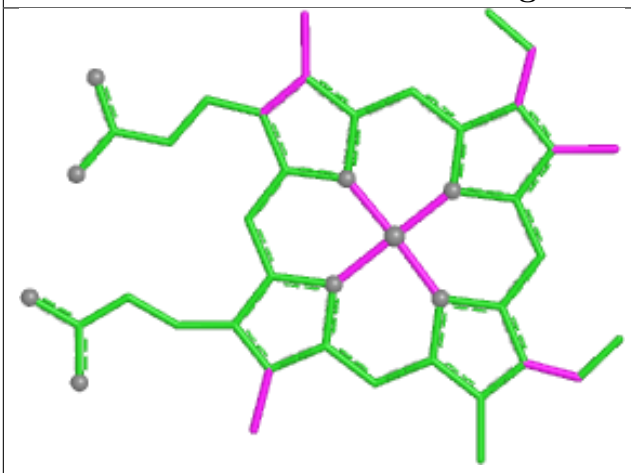
There are no ring outliers.

4 monomers are involved in 42 short contacts:

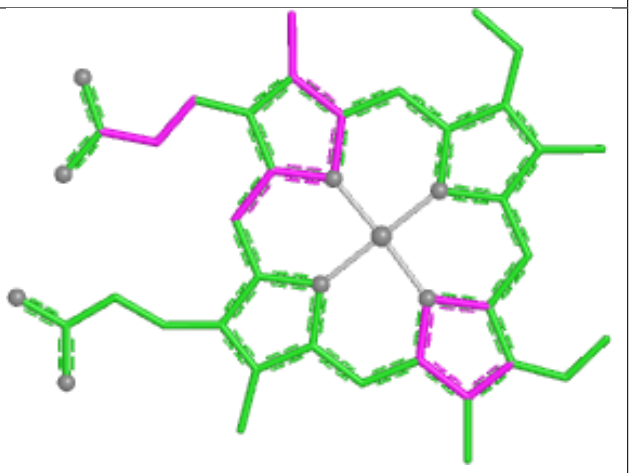
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	821	HEM	18	0
7	A	801	HEM	22	0
6	A	901	SCN	1	0
6	B	902	SCN	3	0

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

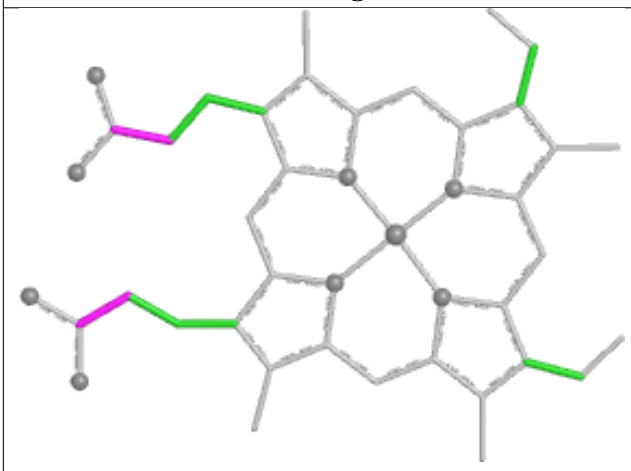
Ligand HEM B 821



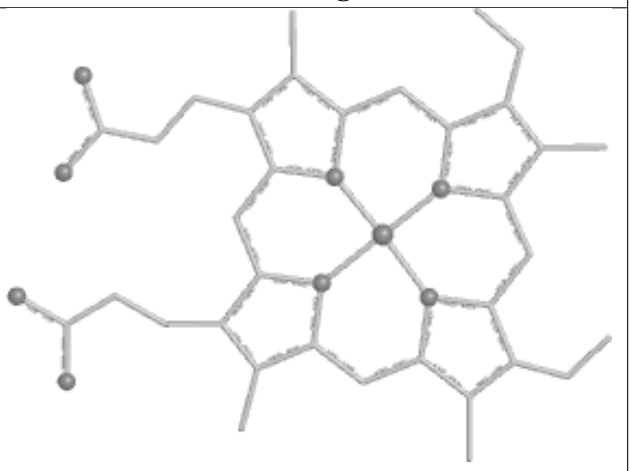
Bond lengths



Bond angles

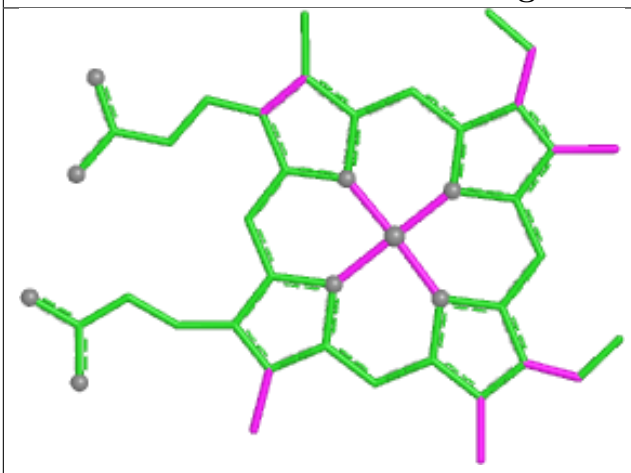


Torsions

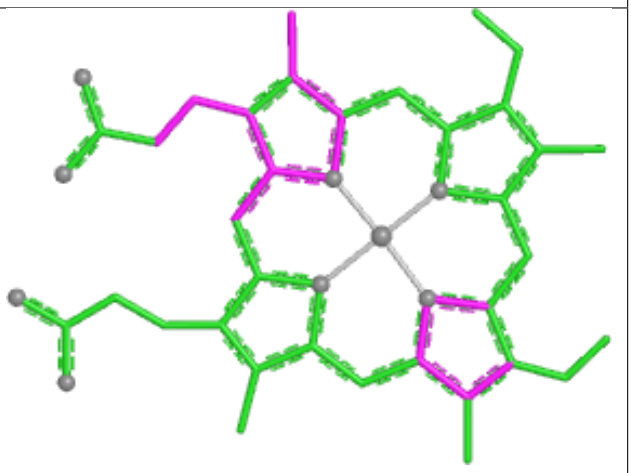


Rings

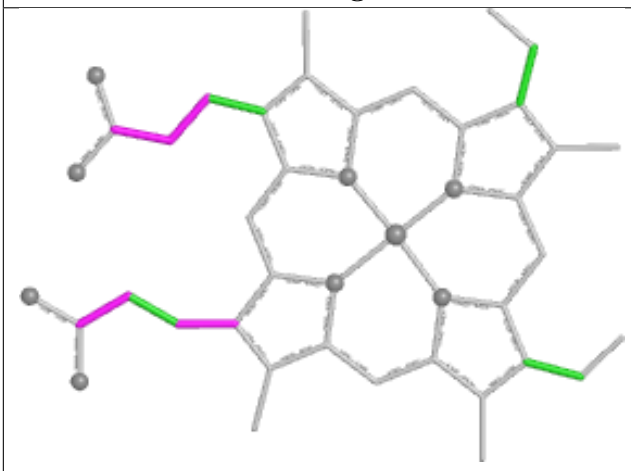
Ligand HEM A 801



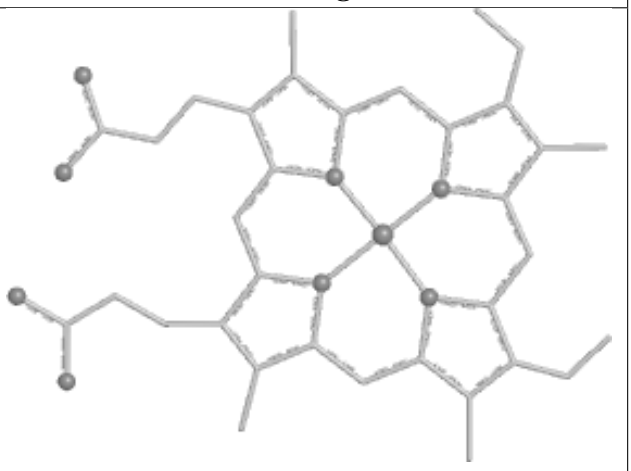
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	594/595 (99%)	0.13	19 (3%)	50	34	6, 21, 48, 75	0
1	B	594/595 (99%)	0.18	19 (3%)	50	34	4, 22, 46, 71	0
All	All	1188/1190 (99%)	0.16	38 (3%)	50	34	4, 22, 47, 75	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	VAL	5.6
1	B	6	CYS	4.9
1	A	122	SER	4.3
1	B	174	SER	4.1
1	A	124	HIS	3.6

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SEP	A	198	10/11	0.73	0.25	31,32,38,39	0
1	SEP	B	198	10/11	0.80	0.20	29,30,35,35	0

6.3 Carbohydrates

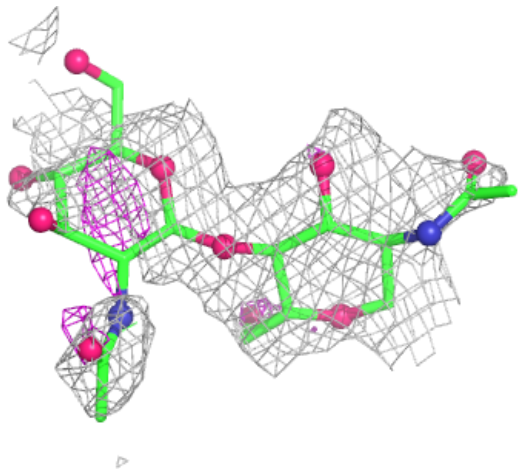
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

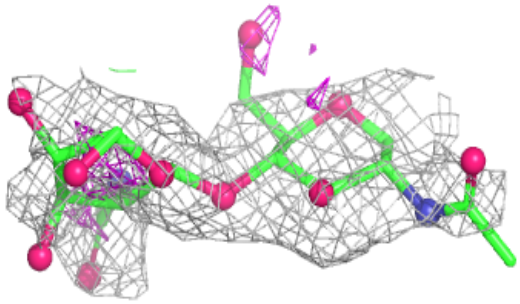
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BMA	D	3	11/12	0.39	0.28	36,38,39,39	0
2	NAG	C	2	14/15	0.48	0.17	35,39,39,39	0
2	NAG	F	2	14/15	0.49	0.18	52,52,53,53	0
2	NAG	F	1	14/15	0.49	0.17	44,47,48,50	0
2	NAG	G	2	14/15	0.52	0.16	35,39,39,39	0
2	NAG	E	2	14/15	0.53	0.19	49,52,53,54	0
2	NAG	G	1	14/15	0.56	0.17	30,31,38,39	0
2	NAG	J	2	14/15	0.63	0.15	49,51,51,51	0
3	NAG	H	2	14/15	0.63	0.16	30,37,39,39	0
3	BMA	H	3	11/12	0.63	0.17	36,38,39,39	0
2	NAG	I	2	14/15	0.64	0.17	50,53,54,56	0
2	NAG	J	1	14/15	0.67	0.14	37,40,43,46	0
2	NAG	C	1	14/15	0.69	0.14	30,31,38,39	0
3	NAG	D	2	14/15	0.76	0.14	30,37,39,39	0
3	NAG	H	1	14/15	0.80	0.17	30,35,39,39	0
2	NAG	I	1	14/15	0.86	0.13	38,40,42,46	0
3	NAG	D	1	14/15	0.88	0.14	30,35,39,39	0
2	NAG	E	1	14/15	0.88	0.11	38,40,42,46	0

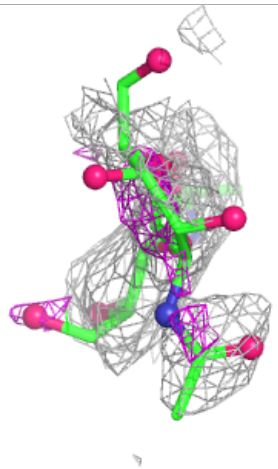
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

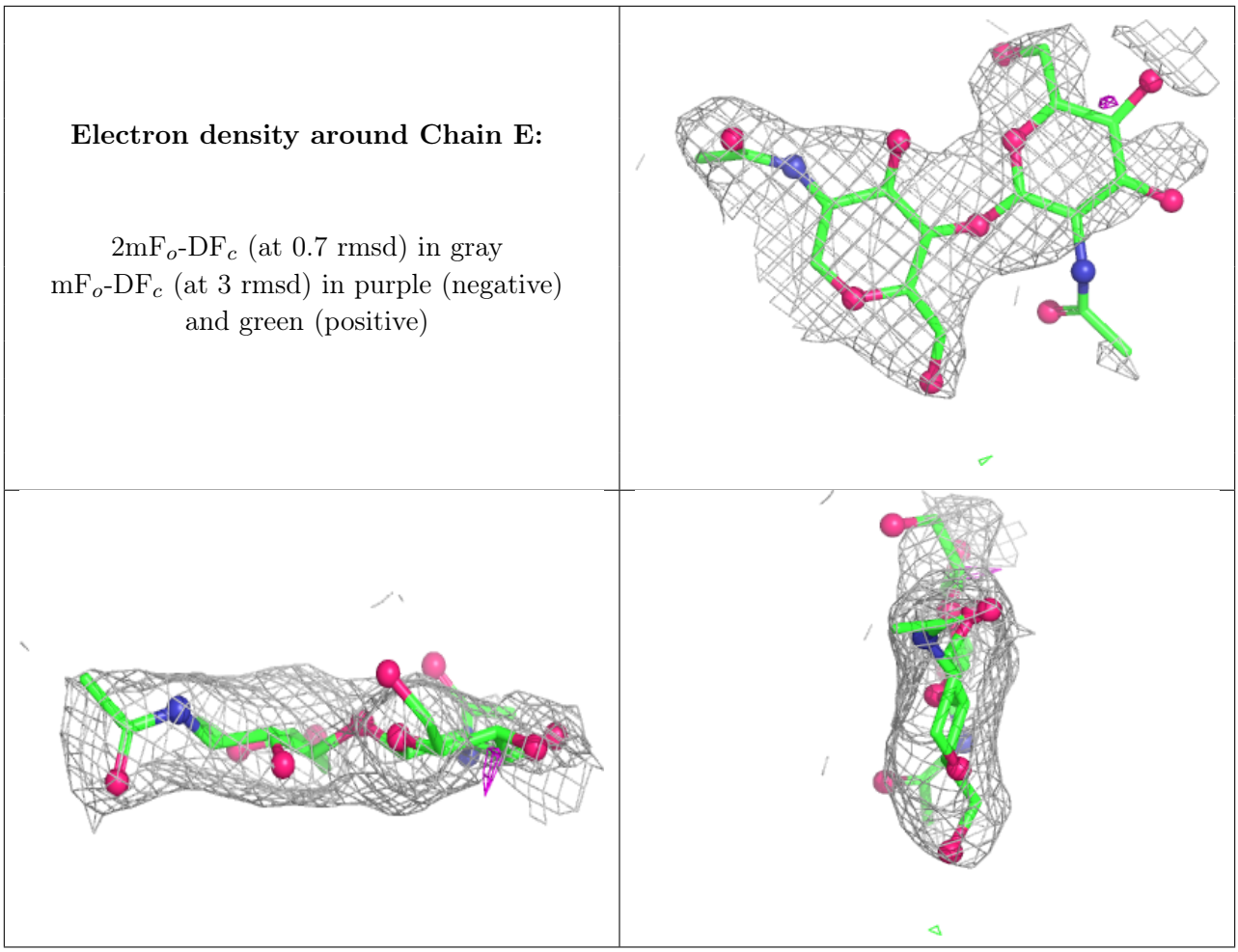






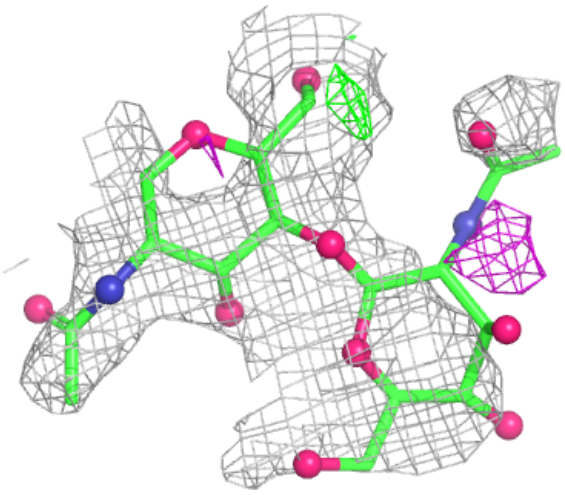
Electron density around Chain E:

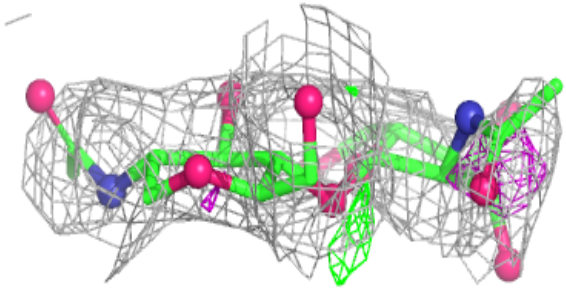
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

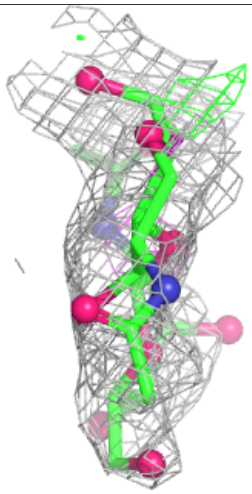


Electron density around Chain F:

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

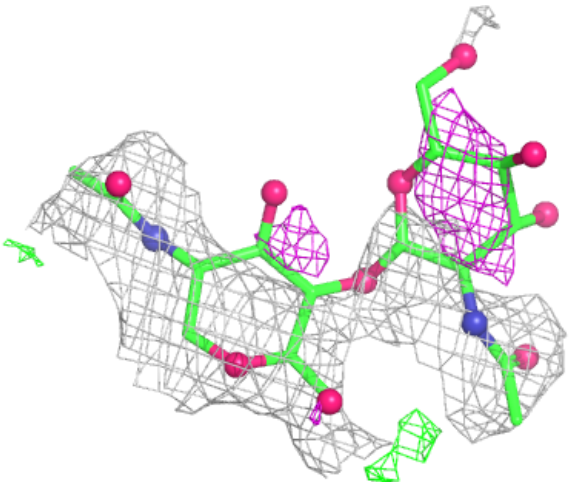


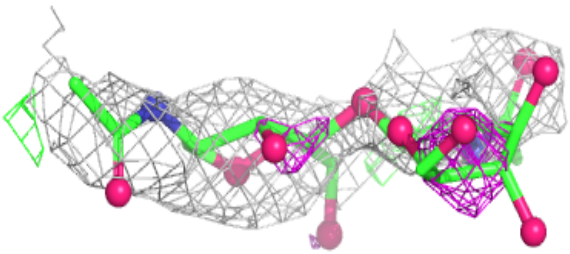


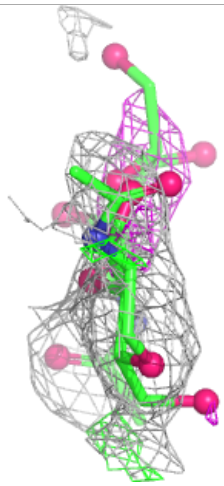


Electron density around Chain G:

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

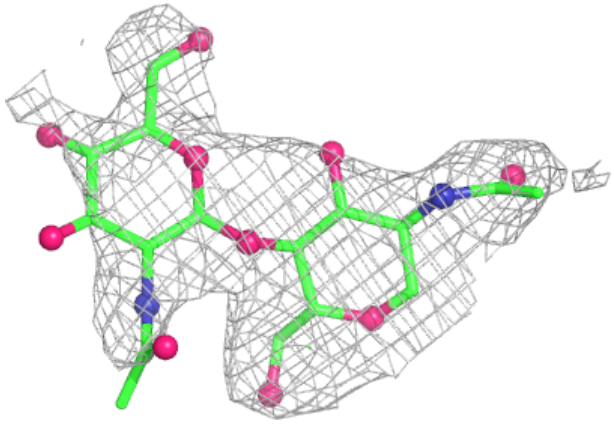


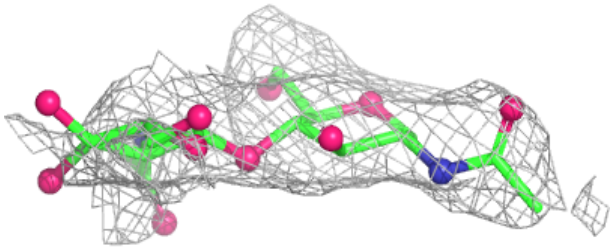


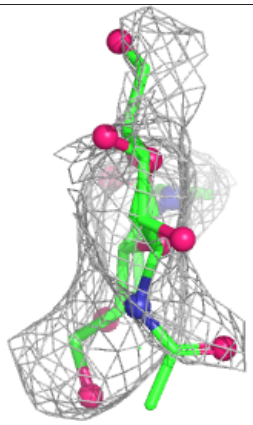


Electron density around Chain I:

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

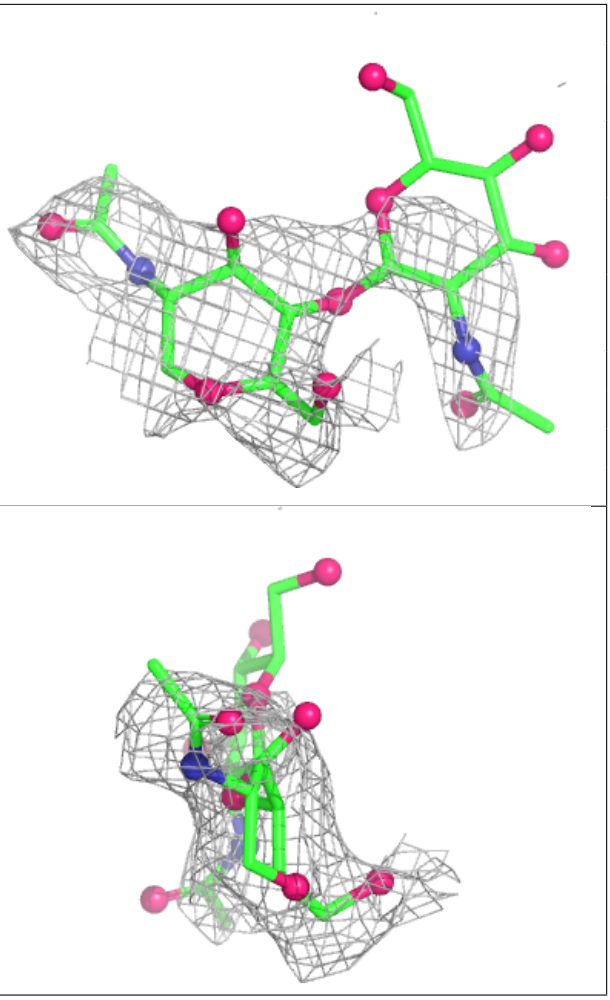


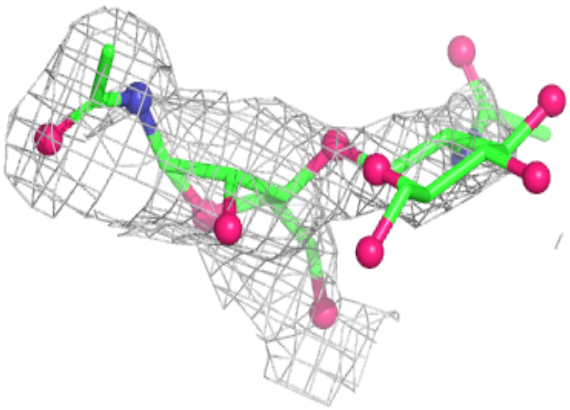




Electron density around Chain J:

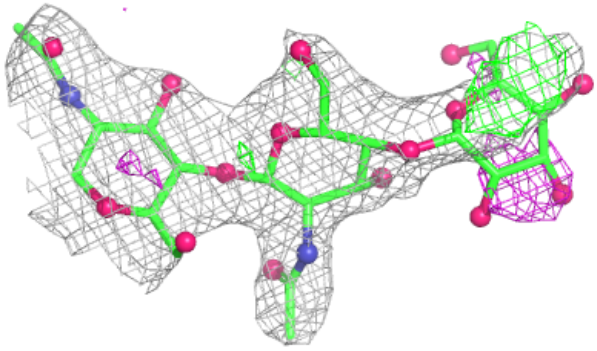
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

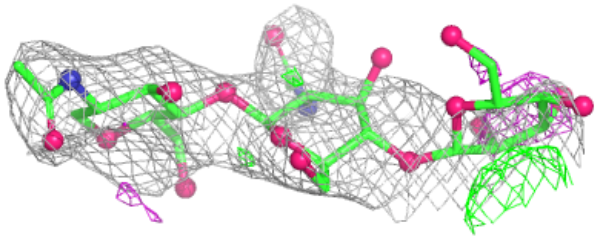


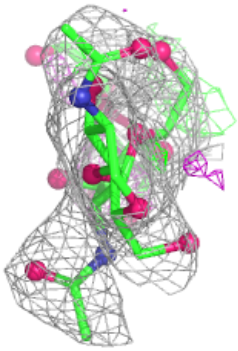


Electron density around Chain D:

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

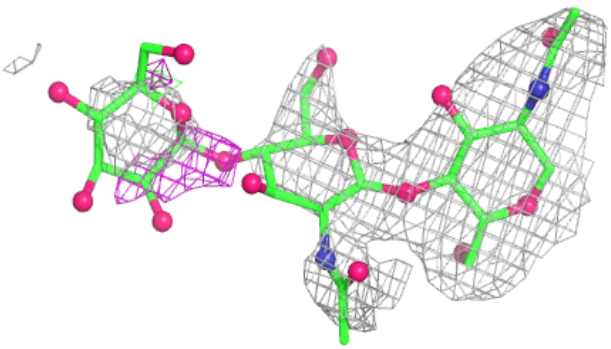


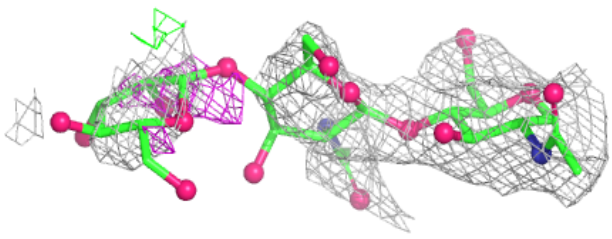


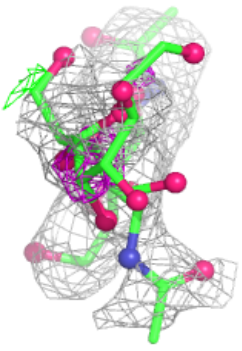


Electron density around Chain H:

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







6.4 Ligands (i)

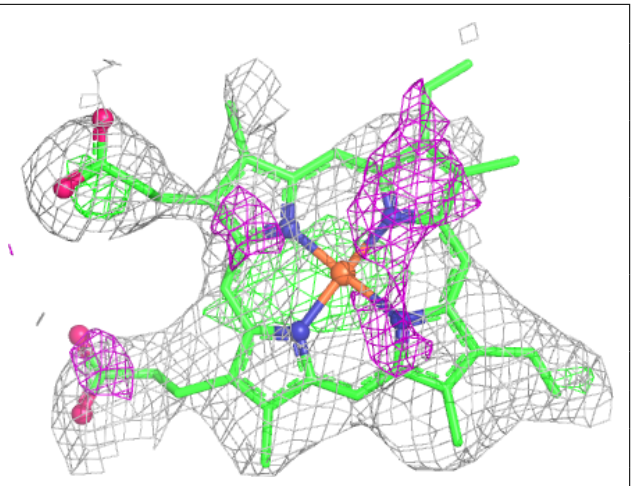
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

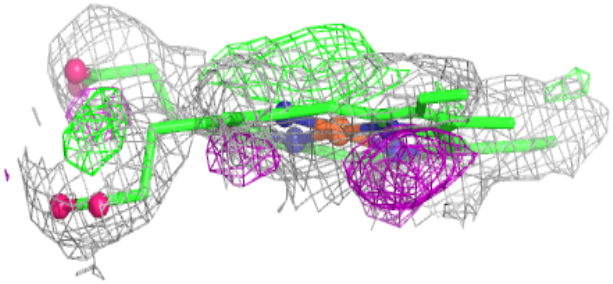
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SCN	A	901	3/3	0.82	0.12	26,26,26,26	0
6	SCN	B	902	3/3	0.82	0.19	23,23,23,24	0
7	HEM	A	801	43/43	0.82	0.20	22,24,26,27	0
7	HEM	B	821	43/43	0.82	0.21	15,18,18,19	0
4	NO3	A	607	4/4	0.91	0.15	69,69,69,69	0
4	NO3	B	607	4/4	0.91	0.17	44,44,44,44	0
4	NO3	B	608	4/4	0.92	0.12	11,11,11,11	0
5	CA	A	704	1/1	0.95	0.06	28,28,28,28	0
4	NO3	A	608	4/4	0.96	0.11	25,25,26,26	0
5	CA	B	724	1/1	0.98	0.07	21,21,21,21	0

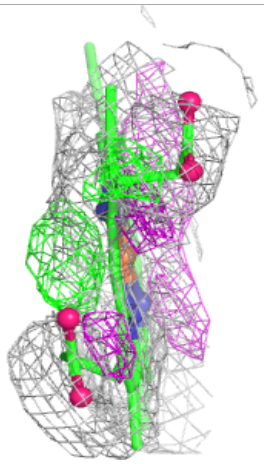
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM A 801:

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

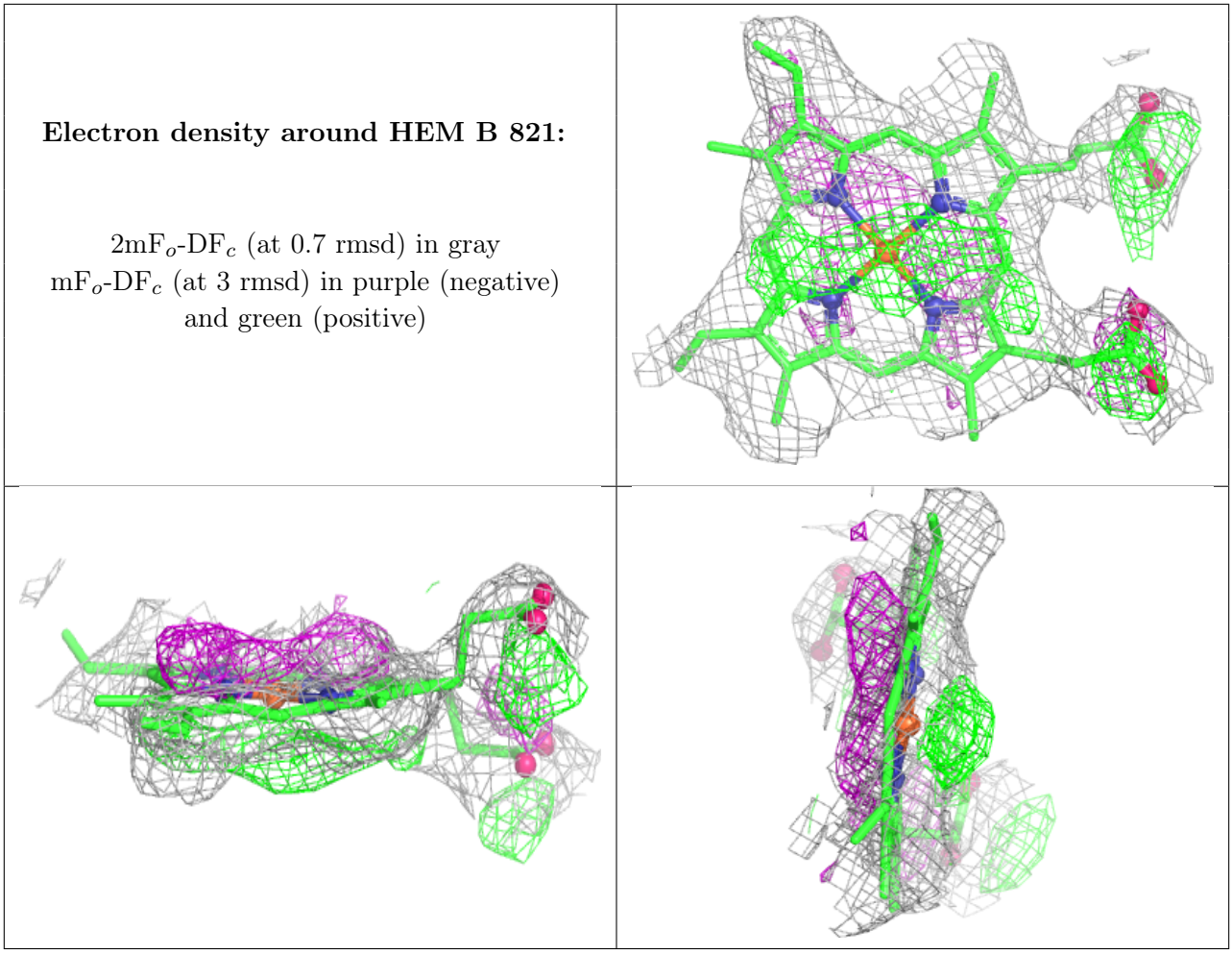






Electron density around HEM B 821:

$2mF_o$-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.