Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2022 – 05:03 pm GMT

PDB ID	:	7NI3
Title	:	CRYSTAL STRUCTURE OF NATIVE HUMAN MYELOPEROXIDASE IN COMPLEX WITH CPD 3
Authors	:	Sjogren, T.; Inghardt, T.
Deposited on	:	2021-02-11
Resolution	:	2.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

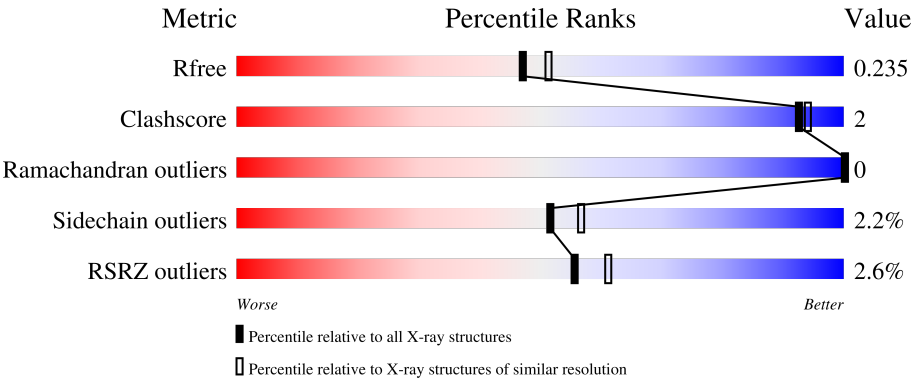
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	105	5% 92% 8%
1	B	105	2% 91% 7%
2	C	466	2% 92% 7%
2	D	466	3% 94% 5%
3	E	4	25% 75%

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Mol	Chain	Length	Quality of chain
3	F	4	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10213 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

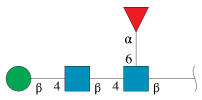
- Molecule 1 is a protein called Myeloperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			842	532	149	156	5			
1	B	103	Total	C	N	O	S	0	0	0
			832	526	147	154	5			

- Molecule 2 is a protein called Myeloperoxidase.

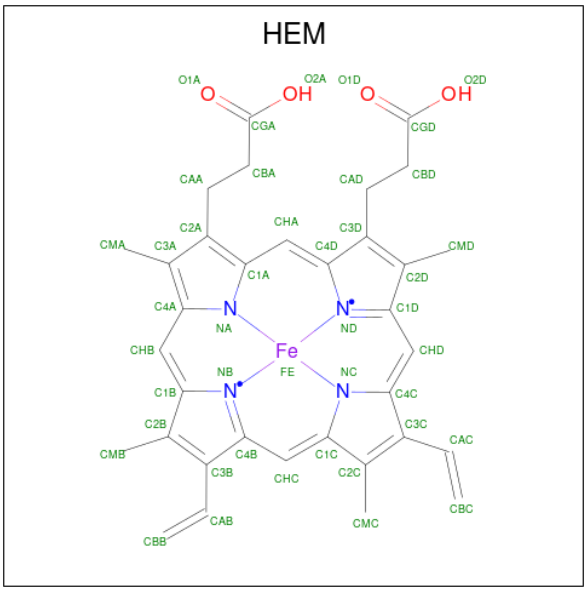
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	464	Total	C	N	O	S	0	0	0
			3720	2343	685	665	27			
2	D	464	Total	C	N	O	S	0	0	0
			3720	2343	685	665	27			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	0	0	0
			49	28	2	19			
3	F	4	Total	C	N	O	0	0	0
			49	28	2	19			

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

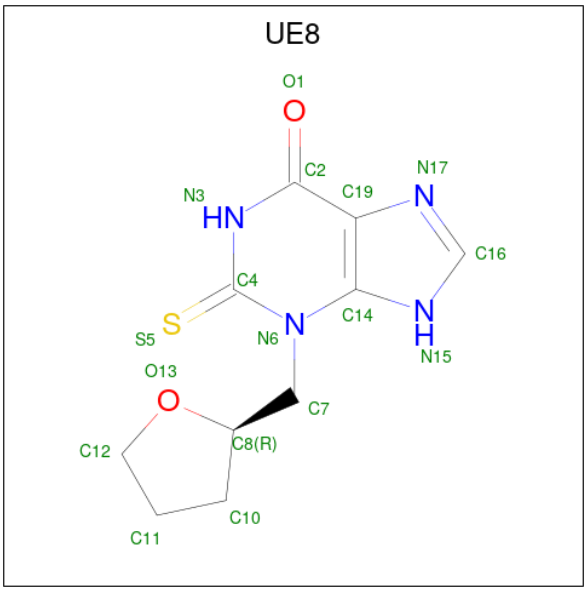


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	2	Total	Cl	0	0
			2	2		
5	C	2	Total	Cl	0	0
			2	2		

- Molecule 6 is 2-sulfanylidene-3-[(2R)-tetrahydro-2-furanylmethyl]-1,2,3,7-tetrahydro-6H-purin-6-one (three-letter code: UE8) (formula: $C_{10}H_{12}N_4O_2S$) (labeled as "Ligand of Interest" by depositor).

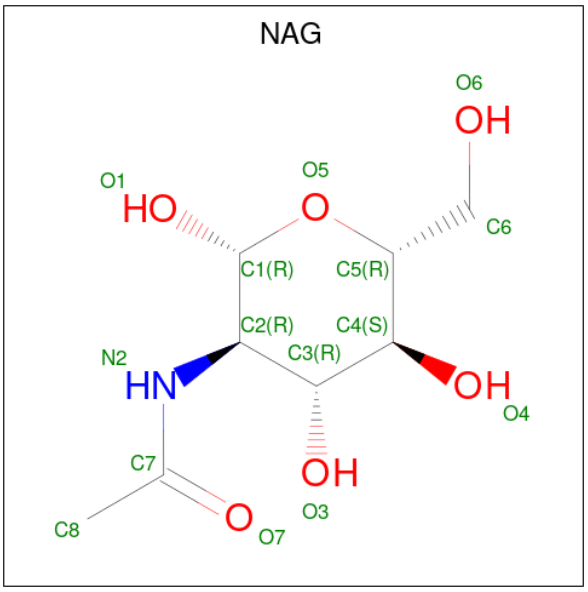


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	S	0	0
			17	10	4	2	1		
6	D	1	Total	C	N	O	S	0	0
			17	10	4	2	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

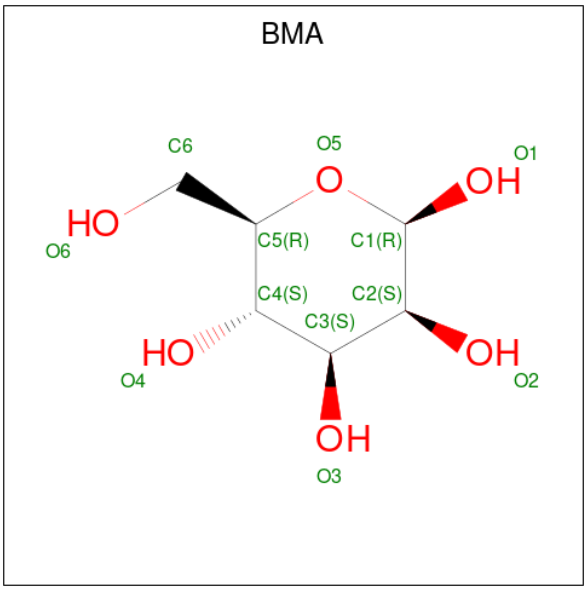
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Ca	0	0
			1	1		
7	D	1	Total	Ca	0	0
			1	1		

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



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

- Molecule 9 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 11 6 5	0	0
9	D	1	Total C O 11 6 5	0	0

- Molecule 10 is water.

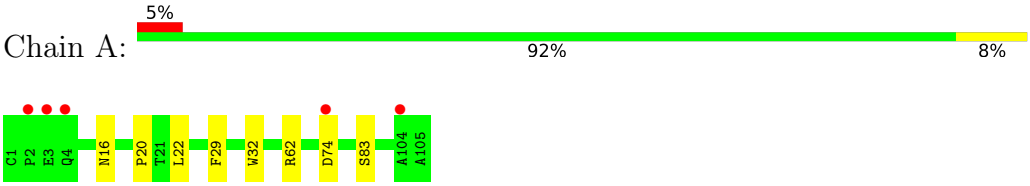
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	84	Total O 84 84	0	0
10	B	75	Total O 75 75	0	0
10	C	342	Total O 342 342	0	0
10	D	295	Total O 295 295	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

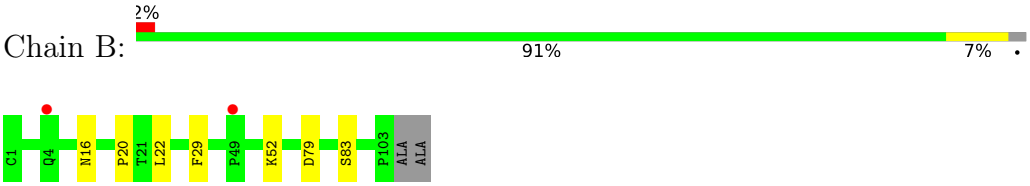
• Molecule 1: Myeloperoxidase

Chain A:



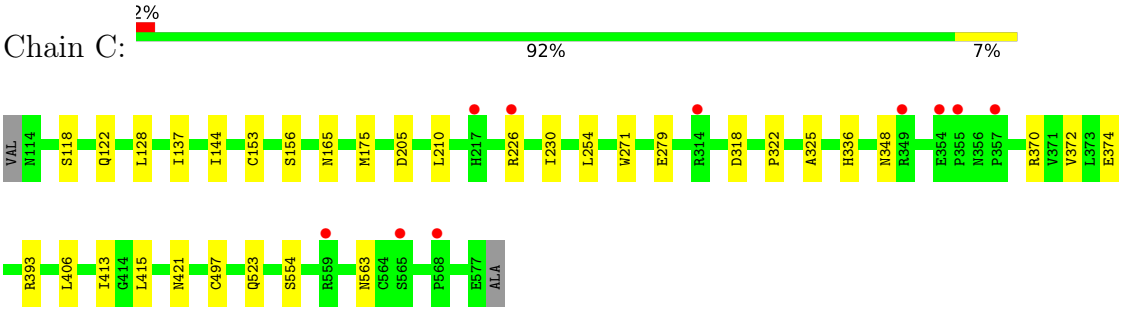
• Molecule 1: Myeloperoxidase

Chain B:



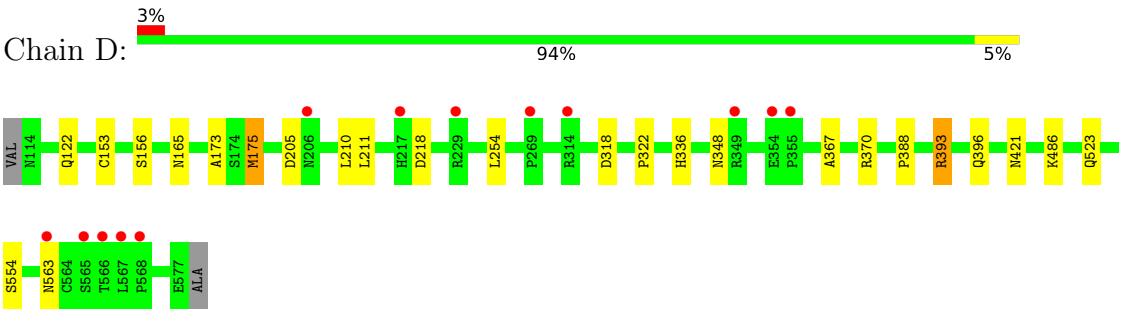
• Molecule 2: Myeloperoxidase

Chain C:



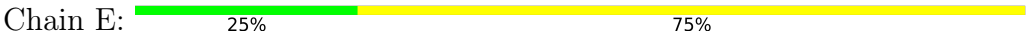
• Molecule 2: Myeloperoxidase

Chain D:



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

Chain E:



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

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.66Å 63.64Å 111.03Å 90.00° 97.15° 90.00°	Depositor
Resolution (Å)	30.61 – 2.10 30.61 – 2.10	Depositor EDS
% Data completeness (in resolution range)	75.0 (30.61-2.10) 75.0 (30.61-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.175 , 0.224 0.182 , 0.235	Depositor DCC
R_{free} test set	2737 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	12.2	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10213	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: UE8, BMA, CA, HEM, NAG, FUC, CSO, CL

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	0.51	0/867	0.70	0/1181
1	B	0.49	0/857	0.69	0/1167
2	C	0.51	0/3798	0.64	0/5151
2	D	0.50	0/3798	0.64	0/5151
All	All	0.51	0/9320	0.65	0/12650

There are no bond length outliers.

There are no bond angle outliers.

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	842	0	803	6	0
1	B	832	0	793	5	0
2	C	3720	0	3711	14	0
2	D	3720	0	3711	11	0
3	E	49	0	43	0	0
3	F	49	0	43	0	0
4	A	43	0	30	0	0
4	B	43	0	30	1	0
5	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	2	0	0	0	0
5	C	2	0	0	0	0
6	C	17	0	0	0	0
6	D	17	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	C	28	0	26	0	0
8	D	28	0	26	0	0
9	C	11	0	10	0	0
9	D	11	0	10	0	0
10	A	84	0	0	0	0
10	B	75	0	0	0	0
10	C	342	0	0	0	0
10	D	295	0	0	0	0
All	All	10213	0	9236	28	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 2.

All (28) 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)
2:D:336:HIS:HD1	2:D:421:ASN:HD21	1.22	0.85
2:C:336:HIS:HD1	2:C:421:ASN:HD21	1.21	0.83
2:C:137:ILE:HG12	2:C:413:ILE:HD11	1.90	0.53
1:A:83:SER:HB3	2:C:554:SER:O	2.09	0.52
4:B:202:HEM:HMC2	4:B:202:HEM:HBC2	1.92	0.49
1:B:83:SER:HB3	2:D:554:SER:O	2.12	0.49
1:A:22:LEU:HB3	2:C:322:PRO:HD2	1.95	0.49
1:B:22:LEU:HB3	2:D:322:PRO:HD2	1.95	0.49
2:D:205:ASP:HB2	2:D:210:LEU:HD21	1.96	0.48
1:B:79:ASP:O	2:D:388:PRO:HB3	2.13	0.48
1:B:29:PHE:CE1	2:D:165:ASN:HB2	2.50	0.47
2:D:367:ALA:HB1	2:D:370:ARG:HG3	1.97	0.46
1:A:62:ARG:HD3	2:C:144:ILE:HD11	1.98	0.45
2:D:153:CYS:SG	2:D:156:SER:HB2	2.57	0.44
1:A:16:ASN:O	1:A:20:PRO:HA	2.17	0.44
1:B:16:ASN:O	1:B:20:PRO:HA	2.18	0.44
1:A:29:PHE:CE1	2:C:165:ASN:HB2	2.53	0.43
2:C:370:ARG:O	2:C:374:GLU:HB2	2.18	0.43
2:C:230:ILE:HD12	2:C:372:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:153:CYS:SG	2:C:156:SER:HB2	2.59	0.42
2:D:211:LEU:HD23	2:D:254:LEU:HD13	2.00	0.42
2:C:271:TRP:CZ3	2:C:279:GLU:HG3	2.55	0.42
1:A:32:TRP:CE2	2:C:325:ALA:HB2	2.55	0.42
2:D:393:ARG:HB2	2:D:396:GLN:HB2	2.01	0.42
2:C:406:LEU:HB3	2:C:415:LEU:HB2	2.02	0.41
2:D:173:ALA:HA	2:D:175:MET:SD	2.60	0.41
2:C:128:LEU:HB2	2:C:144:ILE:HB	2.03	0.41
2:C:205:ASP:HB2	2:C:210:LEU:HD21	2.03	0.41

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	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
1	B	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
2	C	461/466 (99%)	450 (98%)	11 (2%)	0	100	100
2	D	461/466 (99%)	450 (98%)	11 (2%)	0	100	100
All	All	1126/1142 (99%)	1099 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	90/90 (100%)	89 (99%)	1 (1%)	73	79
1	B	90/90 (100%)	89 (99%)	1 (1%)	73	79
2	C	409/410 (100%)	398 (97%)	11 (3%)	44	48
2	D	409/410 (100%)	400 (98%)	9 (2%)	52	57
All	All	998/1000 (100%)	976 (98%)	22 (2%)	52	57

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ASP
1	B	52	LYS
2	C	118	SER
2	C	122	GLN
2	C	175	MET
2	C	226	ARG
2	C	254	LEU
2	C	318	ASP
2	C	348	ASN
2	C	393	ARG
2	C	497	CYS
2	C	523	GLN
2	C	563	ASN
2	D	122	GLN
2	D	175	MET
2	D	218	ASP
2	D	318	ASP
2	D	348	ASN
2	D	393	ARG
2	D	486	LYS
2	D	523	GLN
2	D	563	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	348	ASN
2	C	396	GLN
2	C	467	GLN
2	C	523	GLN
2	D	348	ASN

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Mol	Chain	Res	Type
2	D	467	GLN
2	D	523	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	$\#\|Z\| > 2$
2	CSO	C	150	2	3,6,7	0.76	0	0,6,8	-	-
2	CSO	D	150	2	3,6,7	0.83	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	C	150	2	-	0/1/5/7	-
2	CSO	D	150	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)

8 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	$\#\|Z\| > 2$
3	NAG	E	1	3,2	14,14,15	0.28	0	17,19,21	1.07	1 (5%)
3	NAG	E	2	3	14,14,15	0.29	0	17,19,21	1.12	2 (11%)
3	BMA	E	3	3	11,11,12	0.29	0	15,15,17	0.88	1 (6%)
3	FUC	E	4	3	10,10,11	0.48	0	14,14,16	0.62	0
3	NAG	F	1	3,2	14,14,15	0.39	0	17,19,21	0.94	1 (5%)
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.89	1 (5%)
3	BMA	F	3	3	11,11,12	0.37	0	15,15,17	0.74	0
3	FUC	F	4	3	10,10,11	0.52	0	14,14,16	0.61	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
3	NAG	E	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	FUC	E	4	3	-	-	0/1/1/1
3	NAG	F	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
3	FUC	F	4	3	-	-	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	2	NAG	C1-O5-C5	3.43	116.84	112.19
3	E	1	NAG	O5-C1-C2	-3.09	106.41	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	3	BMA	C1-O5-C5	3.07	116.35	112.19
3	F	1	NAG	O5-C1-C2	-2.72	106.99	111.29
3	F	2	NAG	C1-O5-C5	2.40	115.44	112.19
3	E	2	NAG	O5-C1-C2	2.35	115.01	111.29

There are no chirality outliers.

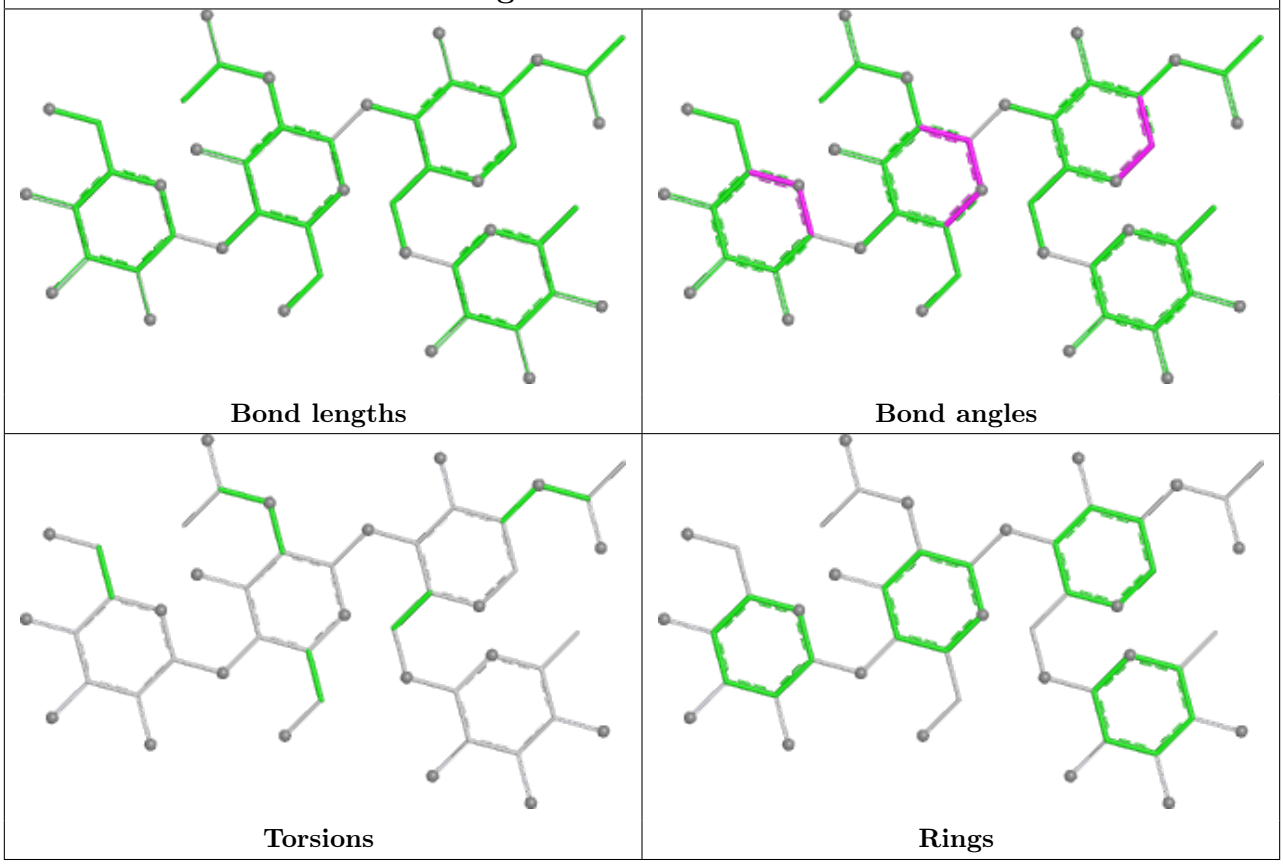
There are no torsion outliers.

There are no ring outliers.

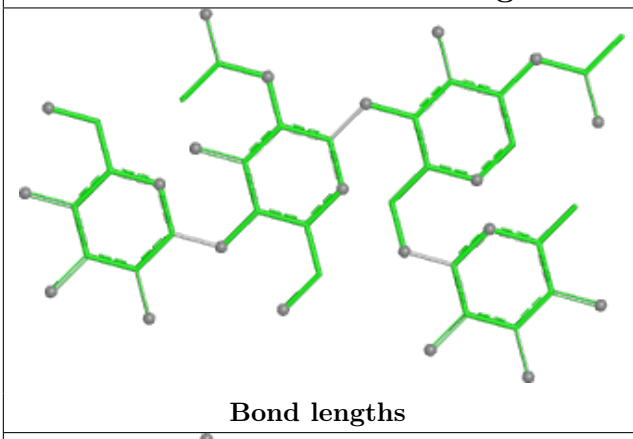
No monomer is involved in short contacts.

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

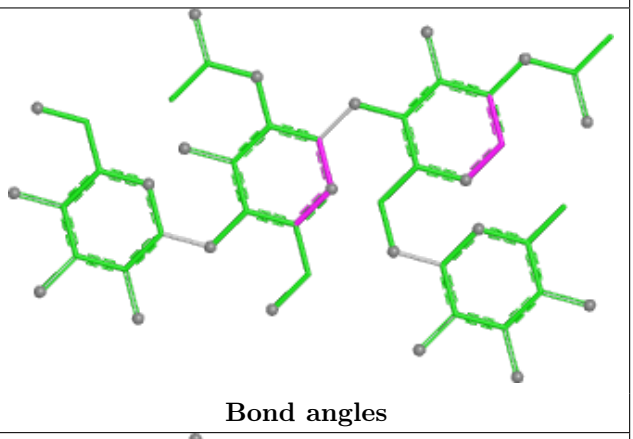
Oligosaccharide Chain E



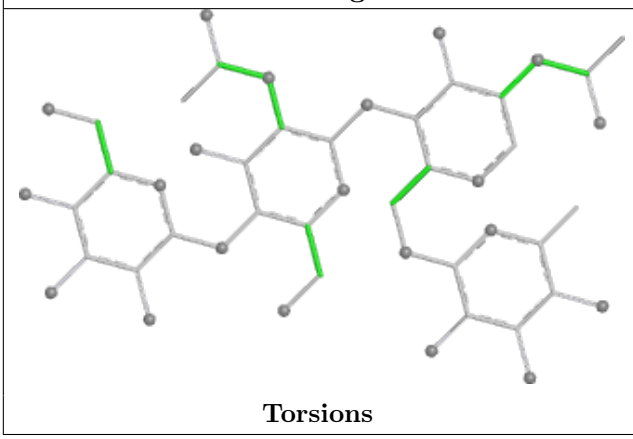
Oligosaccharide Chain F



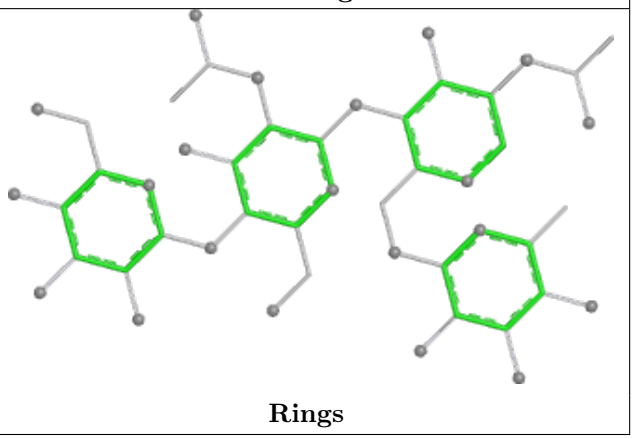
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 7 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
8	NAG	D	2203	2	14,14,15	0.31	0	17,19,21	0.78	1 (5%)
4	HEM	A	201	1,2,10	27,50,50	1.16	2 (7%)	17,82,82	2.23	7 (41%)
4	HEM	B	202	1,2	27,50,50	1.23	3 (11%)	17,82,82	2.43	6 (35%)
6	UE8	D	2201	-	12,19,19	1.73	2 (16%)	13,27,27	4.82	5 (38%)
6	UE8	C	602	-	12,19,19	1.66	2 (16%)	13,27,27	5.01	5 (38%)
8	NAG	D	2204	2	14,14,15	0.28	0	17,19,21	0.70	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	BMA	D	2202	-	11,11,12	0.36	0	15,15,17	0.85	1 (6%)
8	NAG	C	605	2	14,14,15	0.31	0	17,19,21	0.72	1 (5%)
9	BMA	C	607	-	11,11,12	0.36	0	15,15,17	0.94	2 (13%)
8	NAG	C	606	2	14,14,15	0.36	0	17,19,21	0.64	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
8	NAG	D	2203	2	-	0/6/23/26	0/1/1/1
4	HEM	A	201	1,2,10	-	0/6/54/54	-
4	HEM	B	202	1,2	-	0/6/54/54	-
6	UE8	D	2201	-	-	0/4/11/11	0/3/3/3
6	UE8	C	602	-	-	0/4/11/11	0/3/3/3
8	NAG	D	2204	2	-	0/6/23/26	0/1/1/1
9	BMA	D	2202	-	-	2/2/19/22	0/1/1/1
8	NAG	C	605	2	-	0/6/23/26	0/1/1/1
9	BMA	C	607	-	-	2/2/19/22	0/1/1/1
8	NAG	C	606	2	-	0/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	602	UE8	C2-N3	4.73	1.41	1.33
6	D	2201	UE8	C2-N3	4.72	1.41	1.33
4	B	202	HEM	C3D-C4D	3.10	1.49	1.42
6	D	2201	UE8	C7-N6	-2.98	1.45	1.48
4	B	202	HEM	C3C-CAC	2.61	1.53	1.47
6	C	602	UE8	C7-N6	-2.55	1.45	1.48
4	B	202	HEM	C4B-CHC	-2.50	1.34	1.41
4	A	201	HEM	CMB-C2B	2.44	1.57	1.51
4	A	201	HEM	C2A-C3A	-2.31	1.30	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	602	UE8	C2-N3-C4	13.78	130.02	115.93
6	D	2201	UE8	C2-N3-C4	13.16	129.39	115.93
6	C	602	UE8	C19-C2-N3	-9.76	110.08	123.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	2201	UE8	C19-C2-N3	-9.25	110.78	123.43
4	A	201	HEM	CBA-CAA-C2A	-5.28	102.74	112.49
4	B	202	HEM	CBD-CAD-C3D	-5.00	103.26	112.48
4	B	202	HEM	CAA-CBA-CGA	4.61	120.41	112.67
4	A	201	HEM	CAA-CBA-CGA	4.57	120.34	112.67
6	D	2201	UE8	C14-C19-N17	-4.24	104.98	109.40
6	C	602	UE8	C14-C19-N17	-4.20	105.02	109.40
6	C	602	UE8	C14-C19-C2	3.99	124.60	120.80
6	D	2201	UE8	C14-C19-C2	3.72	124.35	120.80
4	B	202	HEM	CBA-CAA-C2A	-3.62	105.81	112.49
4	B	202	HEM	CAD-CBD-CGD	3.33	118.26	112.67
4	A	201	HEM	CBD-CAD-C3D	-3.25	106.50	112.48
6	D	2201	UE8	C7-N6-C14	3.18	121.26	118.41
4	B	202	HEM	C2C-C3C-C4C	-2.97	104.83	106.90
8	C	605	NAG	C1-O5-C5	2.77	115.94	112.19
8	D	2203	NAG	C1-O5-C5	2.67	115.80	112.19
4	A	201	HEM	CMC-C2C-C3C	2.49	129.33	124.68
8	C	606	NAG	C1-O5-C5	2.40	115.45	112.19
4	A	201	HEM	CMB-C2B-C3B	2.34	129.05	124.68
9	C	607	BMA	C1-O5-C5	2.33	115.35	112.19
9	D	2202	BMA	C1-O5-C5	2.26	115.25	112.19
6	C	602	UE8	C7-N6-C14	2.23	120.40	118.41
8	D	2204	NAG	C1-O5-C5	2.20	115.17	112.19
4	A	201	HEM	CAD-CBD-CGD	2.18	116.32	112.67
9	C	607	BMA	C1-C2-C3	2.15	112.31	109.67
4	A	201	HEM	C2C-C3C-C4C	-2.09	105.44	106.90
4	B	202	HEM	CMB-C2B-C3B	2.07	128.55	124.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	607	BMA	C4-C5-C6-O6
9	D	2202	BMA	C4-C5-C6-O6
9	D	2202	BMA	O5-C5-C6-O6
9	C	607	BMA	O5-C5-C6-O6

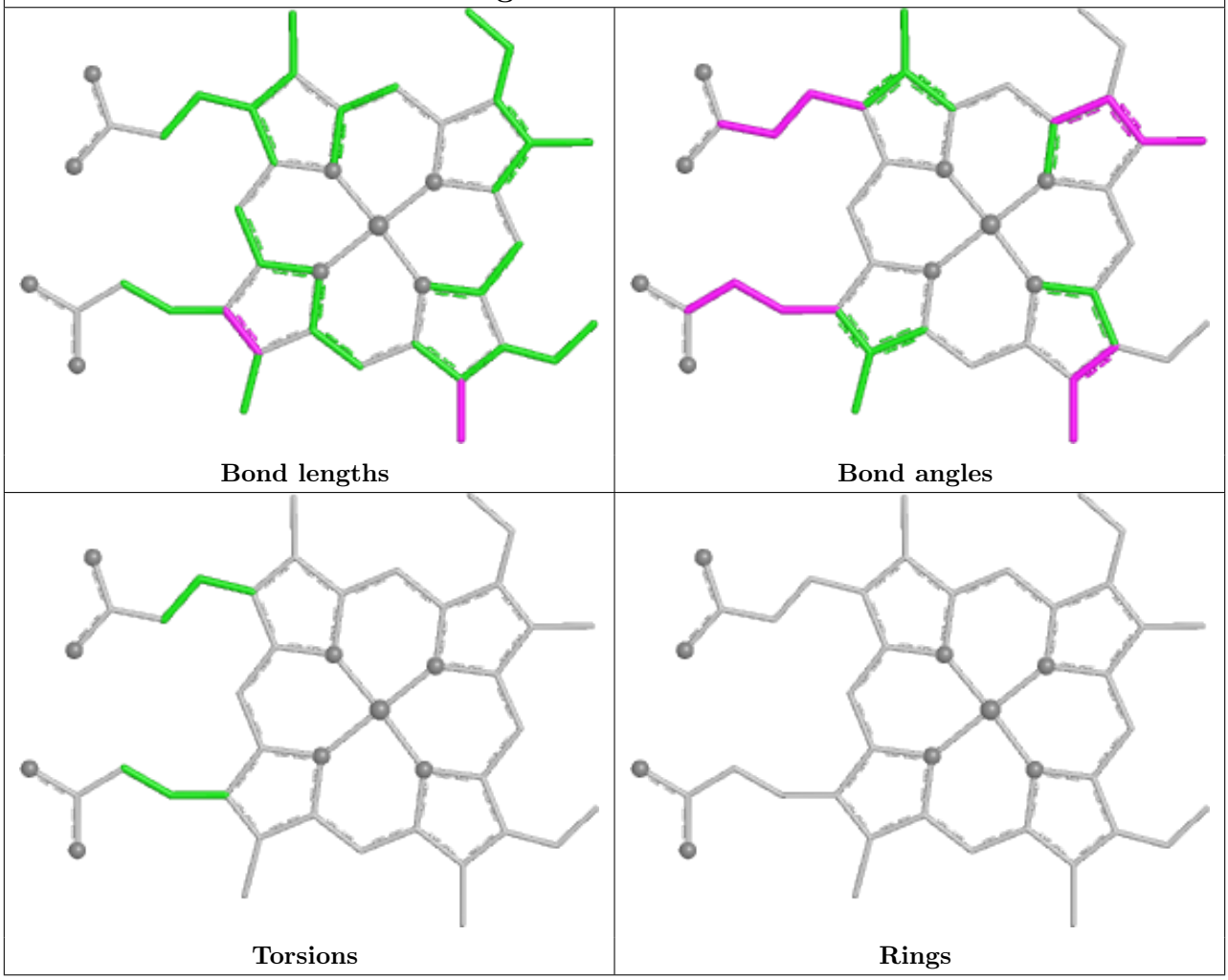
There are no ring outliers.

1 monomer is involved in 1 short contact:

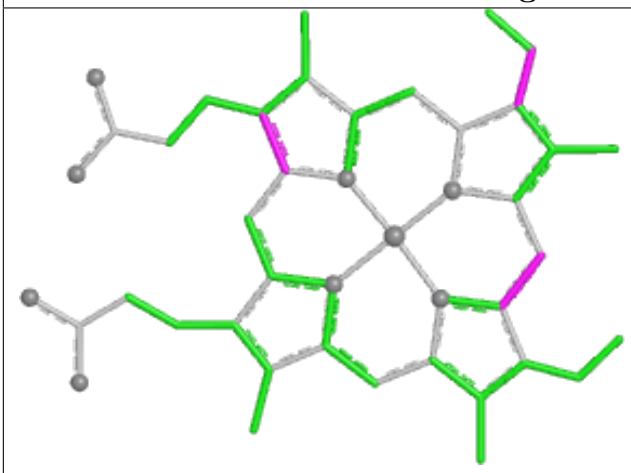
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	202	HEM	1	0

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

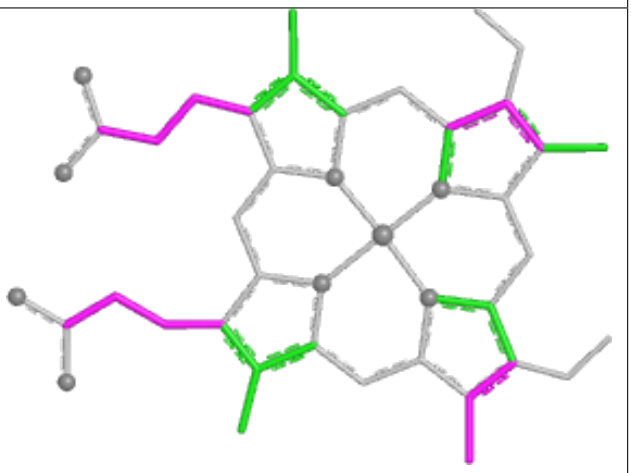
Ligand HEM A 201



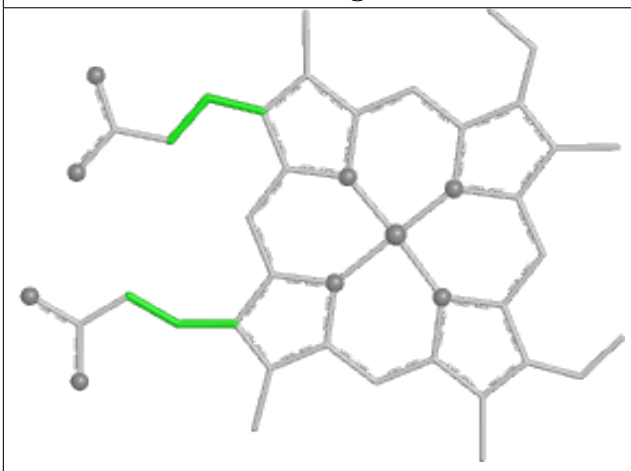
Ligand HEM B 202



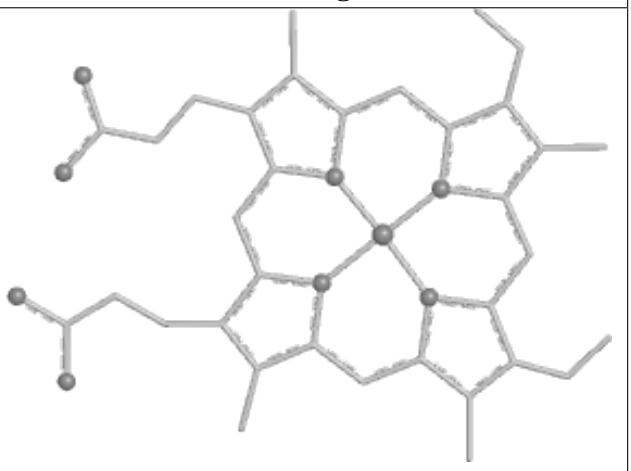
Bond lengths



Bond angles

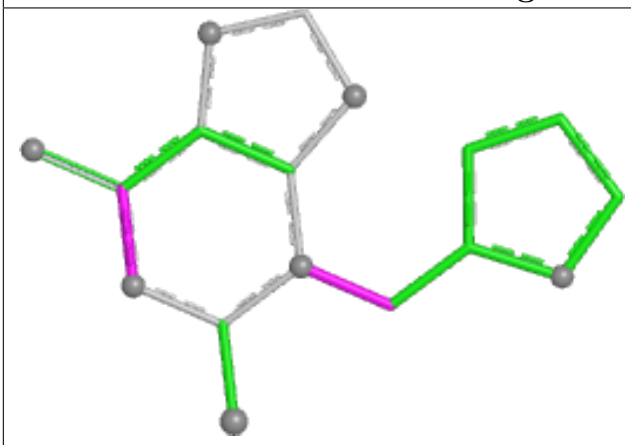


Torsions

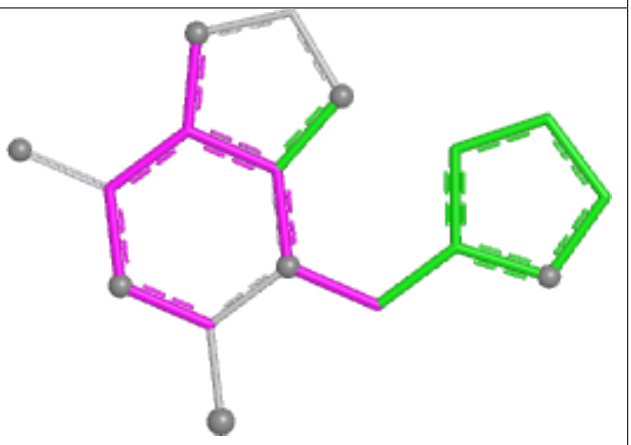


Rings

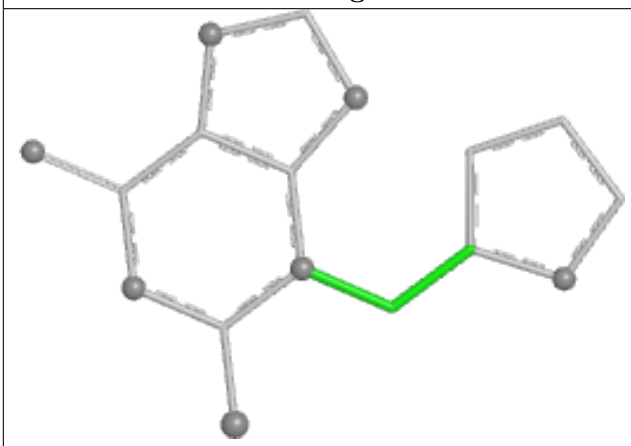
Ligand UE8 D 2201



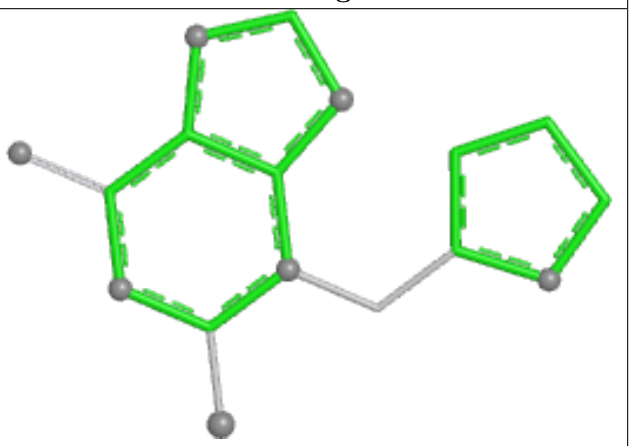
Bond lengths



Bond angles

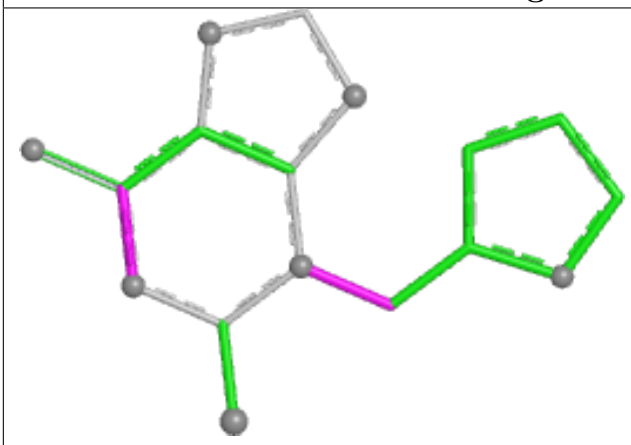


Torsions

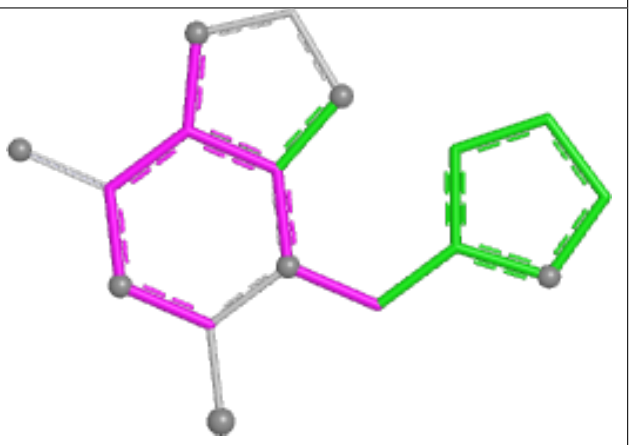


Rings

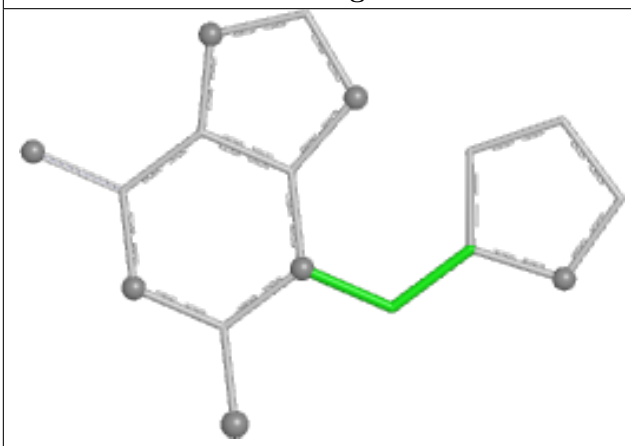
Ligand UE8 C 602



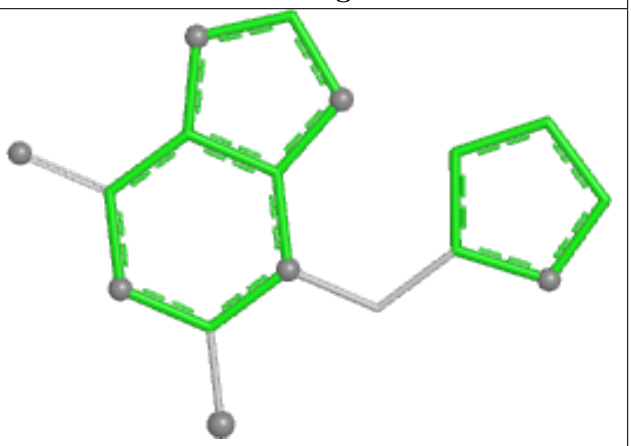
Bond lengths



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	105/105 (100%)	-0.03	5 (4%)	30	36	4, 10, 36, 57	0
1	B	103/105 (98%)	-0.10	2 (1%)	66	71	6, 13, 28, 44	0
2	C	463/466 (99%)	-0.08	10 (2%)	62	66	4, 13, 33, 52	0
2	D	463/466 (99%)	0.05	13 (2%)	53	59	5, 16, 35, 56	0
All	All	1134/1142 (99%)	-0.03	30 (2%)	56	61	4, 14, 35, 57	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	355	PRO	6.5
2	C	355	PRO	5.7
1	A	3	GLU	5.6
2	C	217	HIS	5.0
2	D	217	HIS	4.3
1	A	4	GLN	4.1
2	D	354	GLU	3.3
1	B	4	GLN	3.3
2	C	226	ARG	3.1
1	A	2	PRO	2.9
2	C	568	PRO	2.9
2	D	314	ARG	2.8
2	D	568	PRO	2.8
2	C	314	ARG	2.6
2	D	206	ASN	2.5
1	A	104	ALA	2.3
2	C	349	ARG	2.3
2	C	357	PRO	2.3
2	C	354	GLU	2.3
2	D	566	THR	2.2
2	C	559	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	563	ASN	2.2
2	C	565	SER	2.2
2	D	565	SER	2.1
2	D	567	LEU	2.1
2	D	229	ARG	2.1
2	D	269	PRO	2.1
2	D	349	ARG	2.0
1	A	74	ASP	2.0
1	B	49	PRO	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	D	150	7/8	0.95	0.10	13,15,25,26	0
2	CSO	C	150	7/8	0.98	0.07	6,12,15,15	0

6.3 Carbohydrates (i)

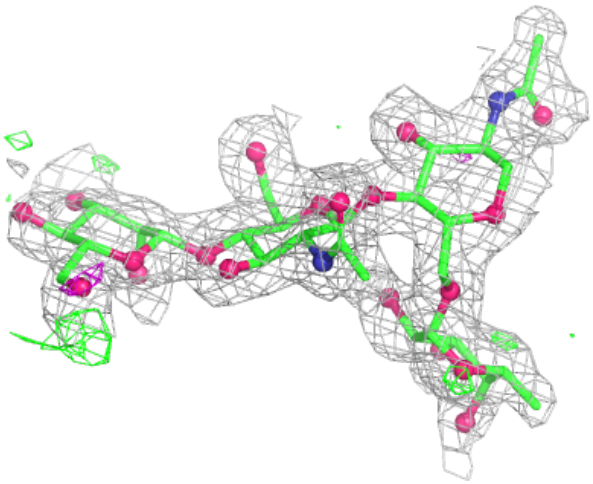
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

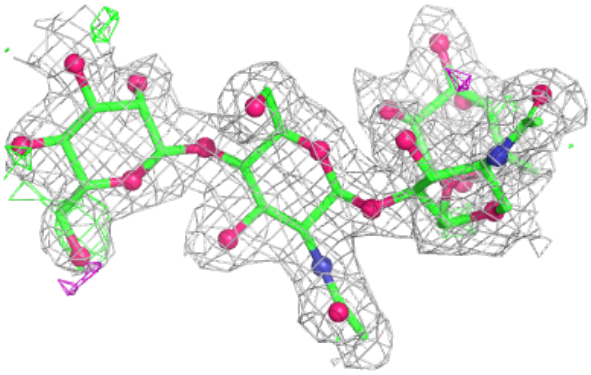
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FUC	F	4	10/11	0.75	0.30	35,38,41,45	0
3	BMA	F	3	11/12	0.82	0.19	28,35,36,36	0
3	BMA	E	3	11/12	0.87	0.18	31,35,38,40	0
3	FUC	E	4	10/11	0.90	0.18	22,27,28,30	0
3	NAG	F	1	14/15	0.93	0.14	14,18,21,28	0
3	NAG	F	2	14/15	0.96	0.11	10,16,19,25	0
3	NAG	E	1	14/15	0.98	0.08	6,10,22,24	0
3	NAG	E	2	14/15	0.98	0.09	9,10,14,23	0

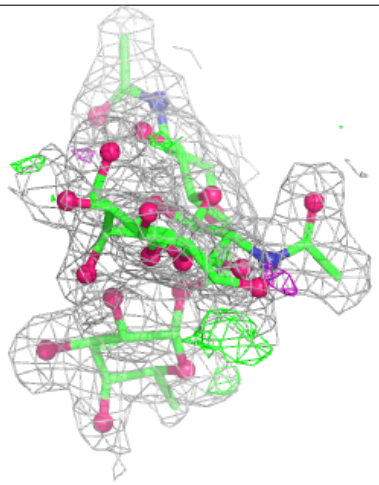
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain E:

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

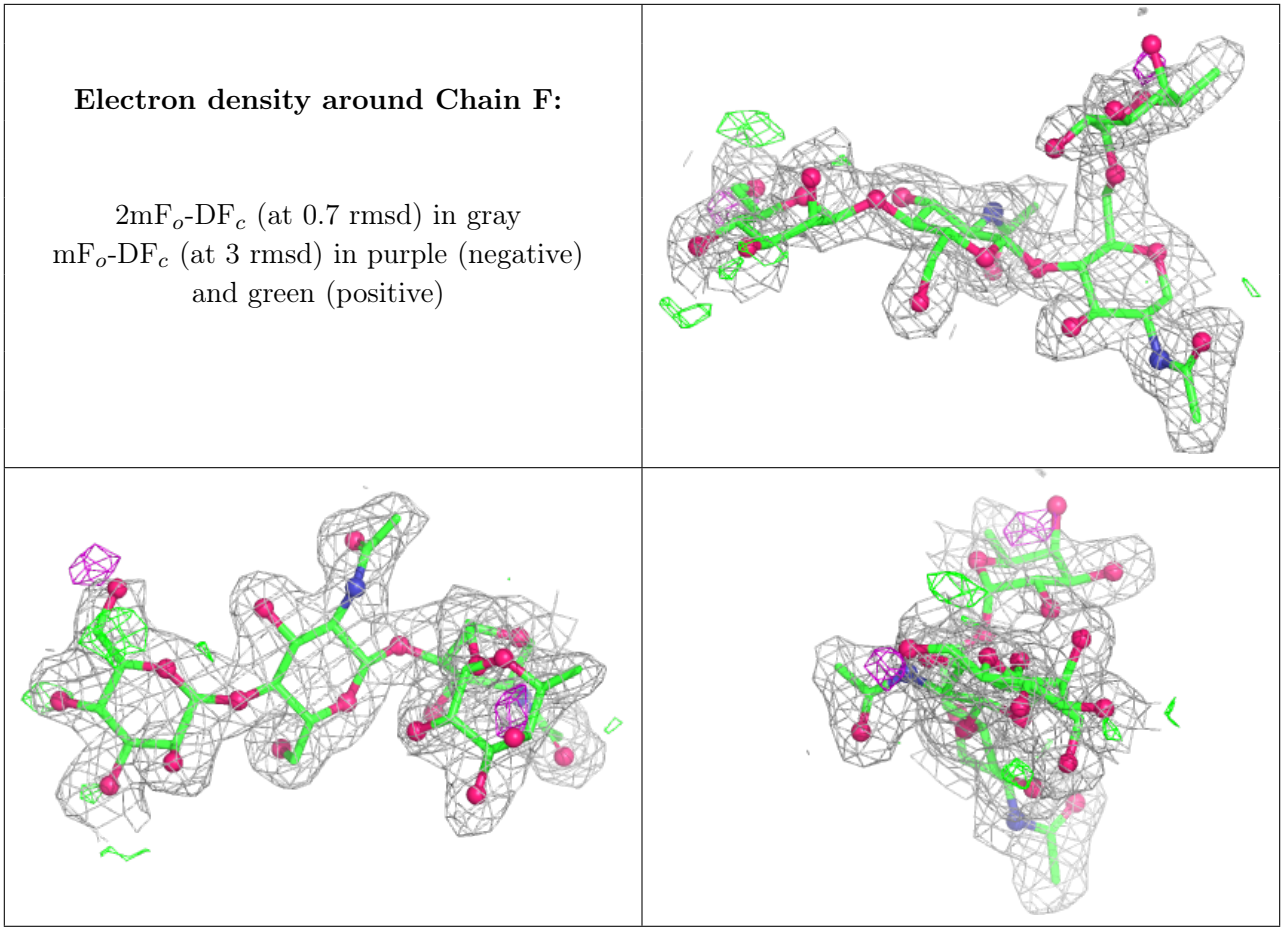






Electron density around Chain F:

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



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
9	BMA	D	2202	11/12	0.56	0.29	68,70,72,73	0
9	BMA	C	607	11/12	0.81	0.16	30,36,39,40	0
6	UE8	D	2201	17/17	0.83	0.20	30,40,50,50	0
8	NAG	D	2204	14/15	0.85	0.25	38,42,47,48	0
8	NAG	C	606	14/15	0.89	0.22	31,35,37,38	0
6	UE8	C	602	17/17	0.90	0.17	12,31,43,44	0
8	NAG	D	2203	14/15	0.92	0.15	13,22,27,29	0
8	NAG	C	605	14/15	0.94	0.18	18,23,27,28	0
5	CL	C	604	1/1	0.97	0.07	31,31,31,31	0
4	HEM	A	201	43/43	0.97	0.12	7,8,11,17	0
4	HEM	B	202	43/43	0.97	0.14	11,12,15,19	0
5	CL	A	202	1/1	0.99	0.05	23,23,23,23	0

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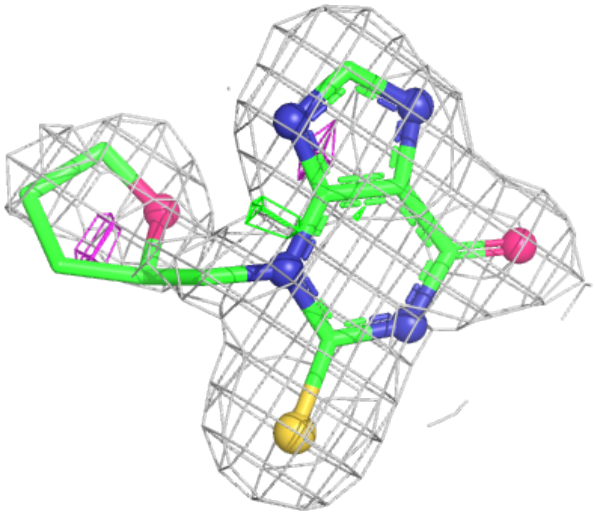
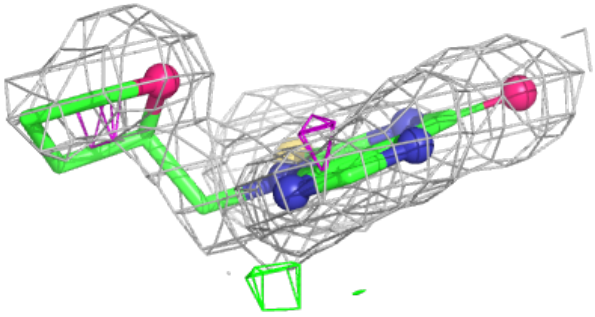
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	B	201	1/1	0.99	0.11	11,11,11,11	0
5	CL	B	203	1/1	0.99	0.04	25,25,25,25	0
5	CL	C	601	1/1	1.00	0.09	6,6,6,6	0
7	CA	C	603	1/1	1.00	0.08	3,3,3,3	0
7	CA	D	2205	1/1	1.00	0.14	3,3,3,3	1

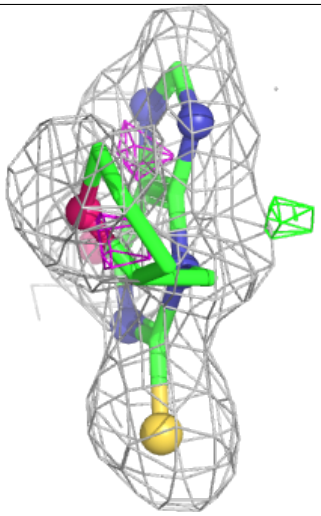
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UE8 D 2201:

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

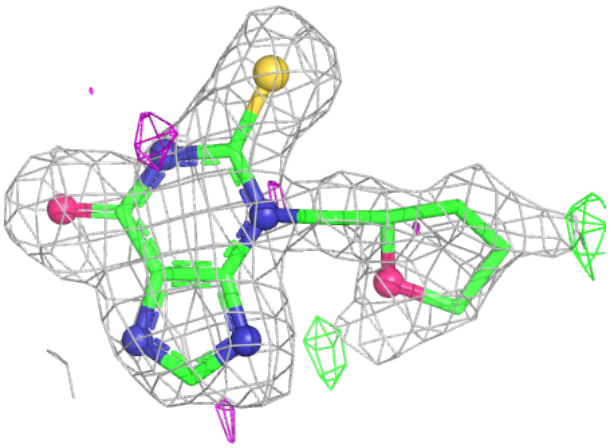


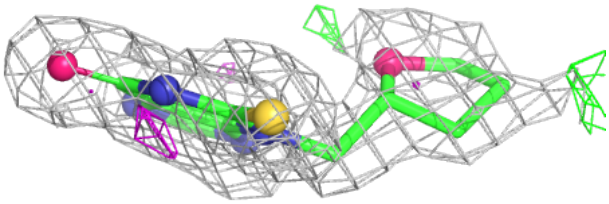


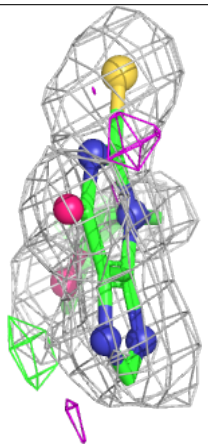


Electron density around UE8 C 602:

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

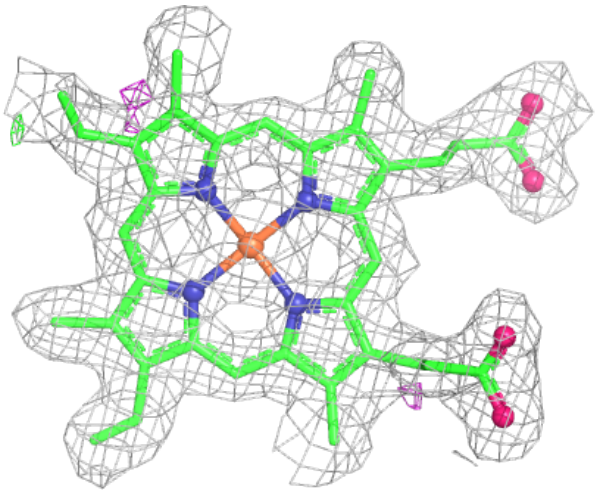


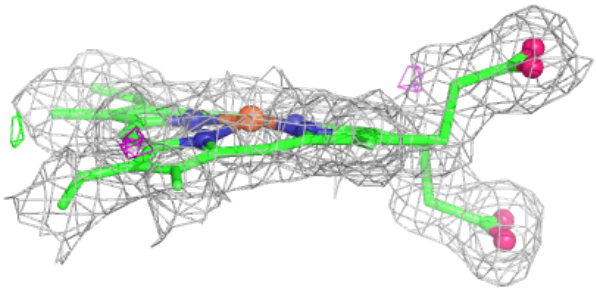


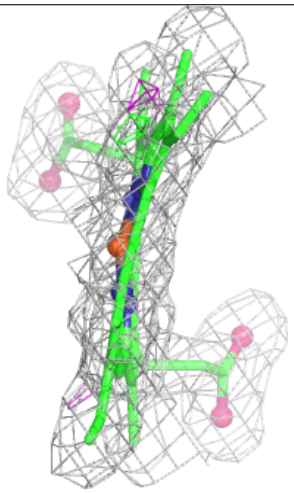


Electron density around HEM A 201:

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

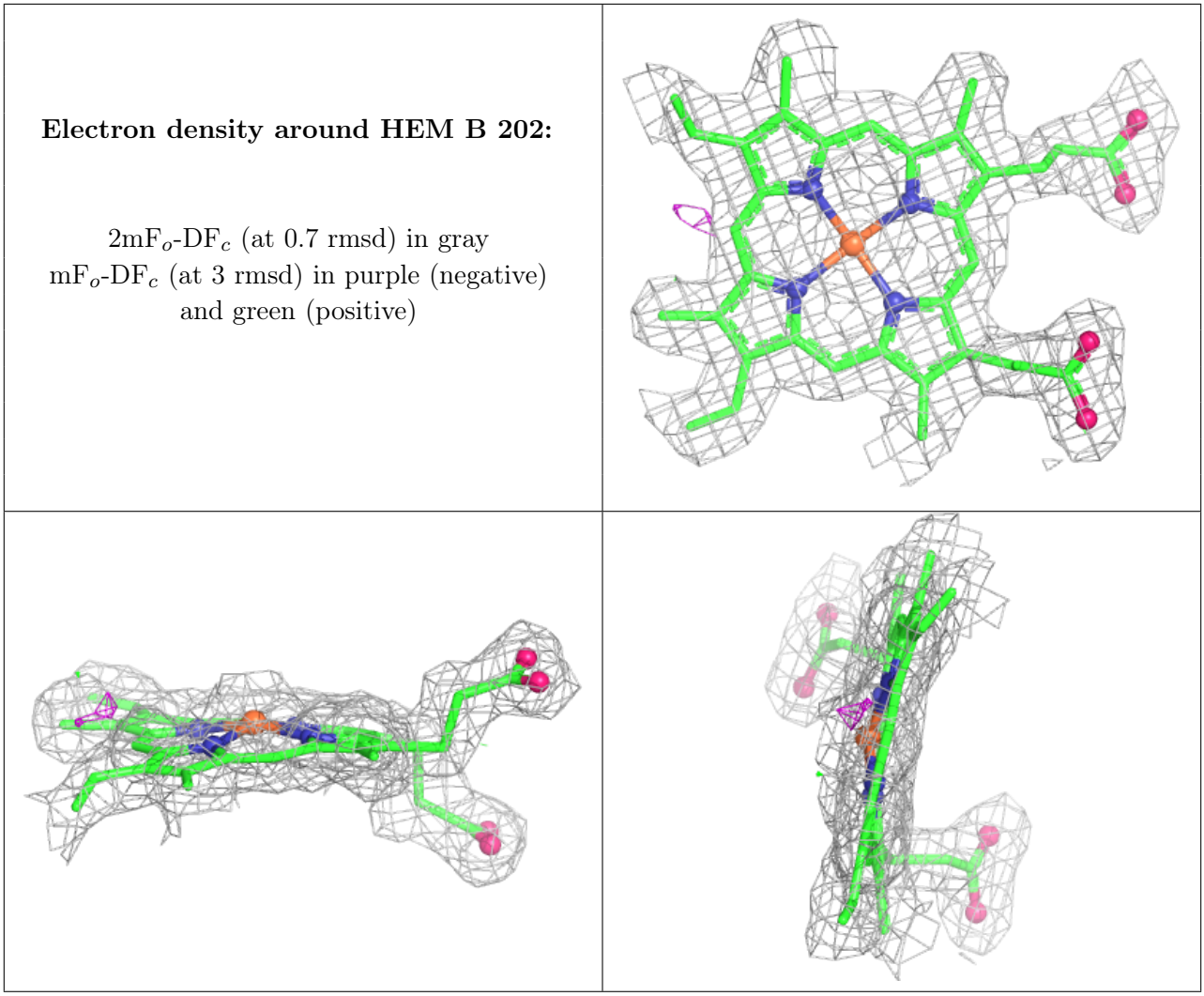






Electron density around HEM B 202:

$2mF_o$-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

There are no such residues in this entry.