



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 06:22 PM UTC

PDB ID : 1IW0 / pdb_00001iw0
Title : Crystal structure of a heme oxygenase (HmuO) from *Corynebacterium diphtheriae* complexed with heme in the ferric state
Authors : Hirotsu, S.; Unno, M.; Chu, G.C.; Lee, D.S.; Park, S.Y.; Shiro, Y.; Ikeda-Saito, M.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-04-04
Resolution : 1.40 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	:	4-5-2 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

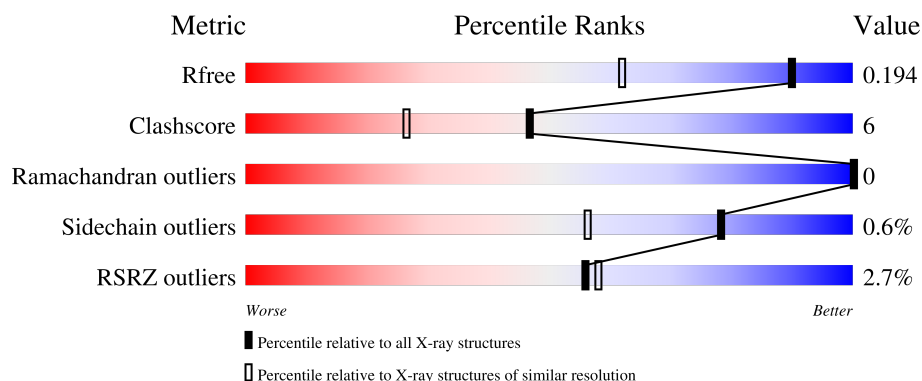
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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 $\leq 5\%$. 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	215	
1	B	215	
1	C	215	
2	D	2	

2 Entry composition

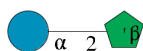
There are 5 unique types of molecules in this entry. The entry contains 5838 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Heme oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1652	1042	293	314	3			
1	B	209	Total	C	N	O	S	0	5	0
			1678	1058	297	320	3			
1	C	207	Total	C	N	O	S	0	5	0
			1666	1051	293	319	3			

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.



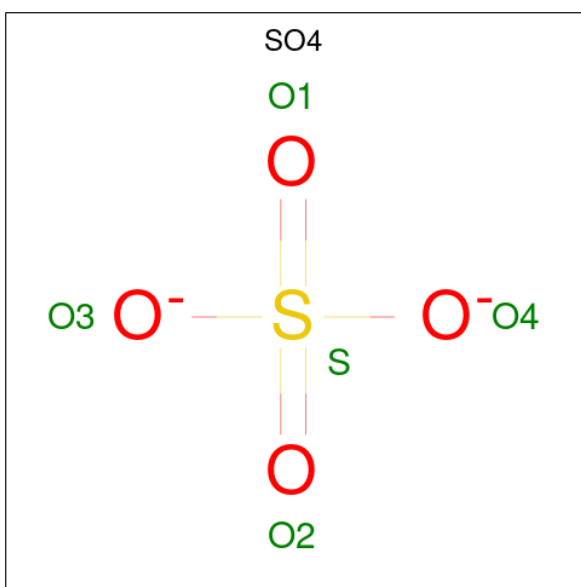
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 46	C 35	Fe 1	N 4	O 6	0	1
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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

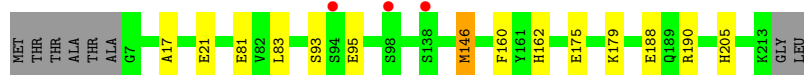
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total	O	0	2
			205	205		
5	B	239	Total	O	0	0
			239	239		
5	C	213	Total	O	0	0
			213	213		

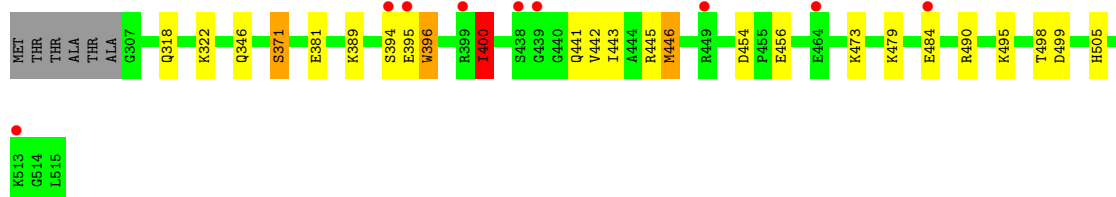
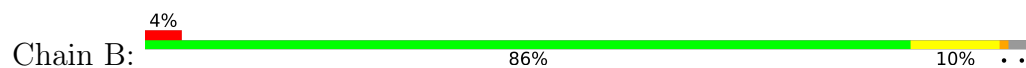
3 Residue-property plots [i](#)

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.

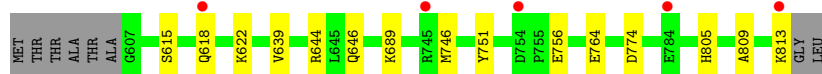
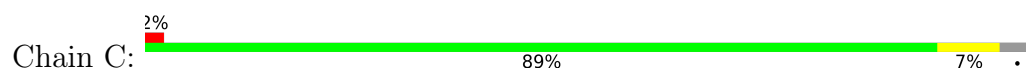
- Molecule 1: Heme oxygenase



- Molecule 1: Heme oxygenase



- Molecule 1: Heme oxygenase



- Molecule 2: beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.56Å 62.84Å 107.66Å 90.00° 100.86° 90.00°	Depositor
Resolution (Å)	12.00 – 1.40 12.00 – 1.40	Depositor EDS
% Data completeness (in resolution range)	90.1 (12.00-1.40) 89.9 (12.00-1.40)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.165 , 0.192 0.167 , 0.194	Depositor DCC
R_{free} test set	14659 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	13.5	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.51 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5838	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: GLC, SO4, HEM, FRU

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	0.70	1/1684 (0.1%)	0.87	1/2274 (0.0%)
1	B	0.76	1/1728 (0.1%)	0.92	3/2333 (0.1%)
1	C	0.75	1/1723 (0.1%)	0.88	0/2327
All	All	0.74	3/5135 (0.1%)	0.89	4/6934 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	746	MET	SD-CE	-11.71	1.50	1.79
1	A	146	MET	SD-CE	-7.52	1.60	1.79
1	B	446	MET	SD-CE	-7.51	1.60	1.79

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	396	TRP	N-CA-C	-7.38	103.24	111.28
1	A	162	HIS	N-CA-C	5.91	119.68	112.23
1	B	400[A]	ILE	N-CA-C	5.56	116.11	110.05
1	B	400[B]	ILE	N-CA-C	5.56	116.11	110.05

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	1652	0	1611	11	0
1	B	1678	0	1632	25	1
1	C	1666	0	1620	21	0
2	D	23	0	21	0	0
3	A	46	0	4	1	0
3	B	43	0	30	0	0
3	C	43	0	30	0	0
4	B	15	0	0	2	0
4	C	15	0	0	0	0
5	A	205	0	0	6	1
5	B	239	0	0	7	0
5	C	213	0	0	9	0
All	All	5838	0	4948	58	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 6.

All (58) 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:441:GLN:HB2	5:B:1575:HOH:O	1.45	1.14
1:C:689:LYS:HD3	1:C:756:GLU:HG3	1.42	0.99
1:A:205:HIS:ND1	5:A:1406:HOH:O	2.02	0.92
1:B:395:GLU:HA	5:B:1475:HOH:O	1.70	0.91
1:A:179:LYS:HE3	5:A:1400:HOH:O	1.71	0.89
1:C:644:ARG:NH1	5:C:1373:HOH:O	2.05	0.88
1:B:442:VAL:HG12	1:B:446:MET:HE2	1.53	0.87
1:C:774:ASP:HB3	5:C:1384:HOH:O	1.81	0.79
1:B:454:ASP:HB3	1:B:456:GLU:OE1	1.86	0.75
1:C:774:ASP:CB	5:C:1384:HOH:O	2.39	0.71
1:B:396:TRP:O	1:B:400[A]:ILE:HD12	1.92	0.70
1:C:639[A]:VAL:HG23	1:C:751:TYR:HB3	1.74	0.70
1:B:394:SER:O	1:B:395:GLU:HB3	1.96	0.65
1:A:190:ARG:NH1	5:A:1262:HOH:O	2.28	0.65
1:C:689:LYS:HD2	1:C:756:GLU:O	1.97	0.65
1:C:618:GLN:NE2	1:C:618:GLN:H	1.99	0.60
1:C:644:ARG:NH1	5:C:1246:HOH:O	2.34	0.60
1:A:146:MET:HA	1:A:146:MET:HE2	1.84	0.59
1:A:175:GLU:HB3	5:A:1400:HOH:O	2.03	0.59
1:C:774:ASP:CG	5:C:1384:HOH:O	2.45	0.58
1:B:495:LYS:HG2	5:B:1551:HOH:O	2.04	0.57
3:A:901[A]:HEM:O1D	5:A:1377:HOH:O	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ILE:HA	1:B:446:MET:HE3	1.85	0.57
1:C:615[A]:SER:OG	5:C:1079:HOH:O	2.12	0.56
1:B:394:SER:C	1:B:396:TRP:H	2.13	0.56
1:C:764:GLU:OE2	5:C:1260:HOH:O	2.18	0.56
1:B:381:GLU:HG2	5:B:1481:HOH:O	2.05	0.55
1:B:490:ARG:NH1	5:B:1632:HOH:O	2.34	0.55
1:C:809:ALA:O	1:C:813:LYS:HE2	2.07	0.55
1:C:764:GLU:HG2	5:C:1050:HOH:O	2.10	0.52
1:B:394:SER:C	1:B:396:TRP:N	2.68	0.52
1:A:188:GLU:OE2	5:A:1256:HOH:O	2.18	0.51
1:B:394:SER:O	1:B:395:GLU:CB	2.52	0.51
1:B:445:ARG:NE	5:B:1171:HOH:O	2.33	0.51
1:B:442:VAL:HG12	1:B:446:MET:CE	2.35	0.50
1:C:646:GLN:NE2	1:C:646:GLN:HA	2.27	0.49
1:B:495:LYS:CE	1:B:499:ASP:OD2	2.62	0.48
1:C:618:GLN:H	1:C:618:GLN:CD	2.21	0.48
1:A:81:GLU:H	1:A:81:GLU:CD	2.23	0.47
1:C:689:LYS:HD3	1:C:756:GLU:CG	2.30	0.47
1:B:505:HIS:HE1	4:B:907:SO4:O1	1.98	0.47
1:A:93:SER:OG	1:A:95:GLU:HG2	2.16	0.46
1:C:646:GLN:HA	1:C:646:GLN:HE21	1.81	0.46
1:B:318:GLN:NE2	5:B:1569:HOH:O	2.49	0.46
1:C:813:LYS:HG3	5:C:1313:HOH:O	2.16	0.45
1:B:346:GLN:NE2	1:B:346:GLN:HA	2.32	0.45
1:B:389:LYS:NZ	1:B:456:GLU:HB3	2.32	0.44
1:B:389:LYS:HD2	1:B:456:GLU:O	2.18	0.44
1:C:622:LYS:HD3	1:C:805:HIS:CE1	2.53	0.43
1:B:456:GLU:H	1:B:456:GLU:CD	2.26	0.43
1:C:689:LYS:CD	1:C:756:GLU:O	2.67	0.42
1:A:83:LEU:HG	1:A:160:PHE:HD1	1.86	0.41
1:A:146:MET:HE2	1:A:146:MET:CA	2.50	0.41
1:B:371[A]:SER:OG	1:B:479:LYS:HE2	2.21	0.40
1:A:17:ALA:O	1:A:21:GLU:HG3	2.21	0.40
1:C:809:ALA:C	1:C:813:LYS:HE2	2.46	0.40
1:B:318:GLN:O	1:B:322:LYS:HG2	2.21	0.40
1:B:473:LYS:HE3	4:B:906:SO4:O3	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)
1:B:484:GLU:OE2	5:A:1250:HOH:O[1_455]	2.13	0.07

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	205/215 (95%)	200 (98%)	5 (2%)	0	100	100
1	B	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
1	C	210/215 (98%)	207 (99%)	3 (1%)	0	100	100
All	All	627/645 (97%)	612 (98%)	15 (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	170/175 (97%)	170 (100%)	0	100	100
1	B	175/175 (100%)	170 (97%)	5 (3%)	37	9
1	C	175/175 (100%)	175 (100%)	0	100	100
All	All	520/525 (99%)	515 (99%)	5 (1%)	78	40

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	371[A]	SER
1	B	371[B]	SER
1	B	400[A]	ILE
1	B	400[B]	ILE
1	B	498	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	182	ASN
1	B	325	HIS
1	B	346	GLN
1	B	378	ASN
1	B	441	GLN
1	B	448	GLN
1	B	462	HIS
1	B	505	HIS
1	C	618	GLN
1	C	678	ASN
1	C	748	GLN
1	C	750	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

2 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	GLC	D	1	2	11,11,12	0.34	0	15,15,17	0.73	0
2	FRU	D	2	2	11,12,12	0.50	0	10,18,18	0.53	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
2	GLC	D	1	2	-	0/2/19/22	0/1/1/1
2	FRU	D	2	2	-	2/5/24/24	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

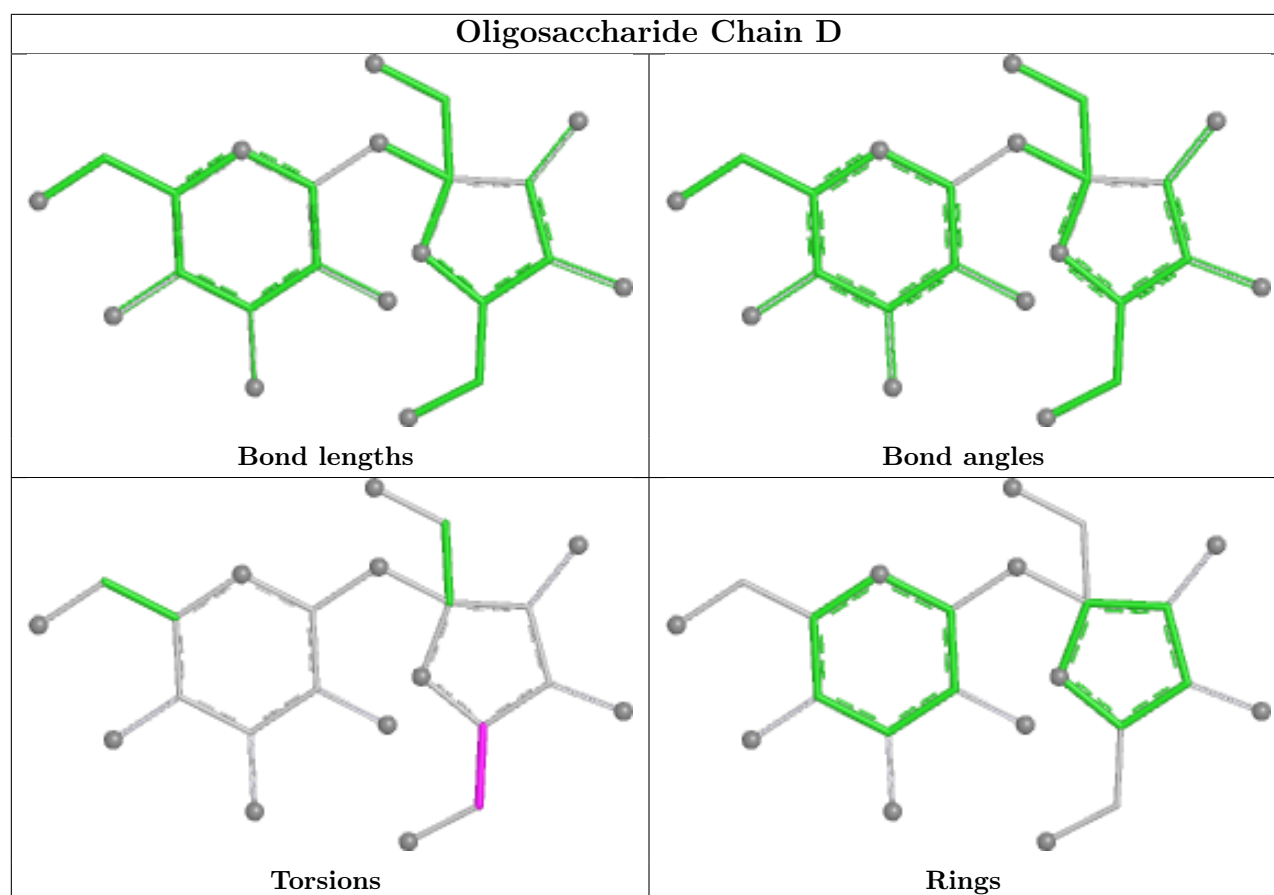
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2	FRU	O5-C5-C6-O6
2	D	2	FRU	C4-C5-C6-O6

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.



5.6 Ligand geometry [i](#)

10 ligands 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	SO4	B	906	-	4,4,4	0.31	0	6,6,6	0.27	0
4	SO4	C	905	-	4,4,4	0.24	0	6,6,6	0.30	0
3	HEM	B	902	1,5	50,50,50	1.94	14 (28%)	67,82,82	3.32	36 (53%)
3	HEM	C	903	1,5	50,50,50	1.67	16 (32%)	67,82,82	2.60	33 (49%)
4	SO4	C	909	-	4,4,4	0.23	0	6,6,6	0.35	0
4	SO4	B	907	-	4,4,4	0.29	0	6,6,6	0.27	0
3	HEM	A	901[A]	-	50,50,50	2.28	16 (32%)	67,82,82	3.49	39 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	908	-	4,4,4	0.29	0	6,6,6	0.38	0
3	HEM	A	901[B]	-	50,50,50	2.23	15 (30%)	67,82,82	3.37	38 (56%)
4	SO4	C	910	-	4,4,4	0.36	0	6,6,6	0.26	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	HEM	C	903	1,5	-	4/14/54/54	-
3	HEM	B	902	1,5	-	6/14/54/54	-
3	HEM	A	901[A]	-	-	9/14/54/54	-
3	HEM	A	901[B]	-	-	8/14/54/54	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901[A]	HEM	C1C-NC	-6.42	1.27	1.39
3	A	901[B]	HEM	C1C-NC	-6.42	1.27	1.39
3	A	901[A]	HEM	C3D-C2D	5.82	1.49	1.36
3	A	901[B]	HEM	C3D-C2D	5.82	1.49	1.36
3	A	901[A]	HEM	C4B-NB	-4.92	1.29	1.38
3	A	901[B]	HEM	C4B-NB	-4.92	1.29	1.38
3	A	901[A]	HEM	C4D-C3D	4.70	1.53	1.45
3	A	901[B]	HEM	C4D-C3D	4.70	1.53	1.45
3	B	902	HEM	C4D-ND	-4.66	1.32	1.40
3	B	902	HEM	FE-NC	4.29	2.09	1.95
3	C	903	HEM	C3B-C2B	-4.19	1.28	1.37
3	A	901[A]	HEM	CBD-CGD	-3.99	1.41	1.50
3	B	902	HEM	FE-ND	3.88	2.06	1.94
3	B	902	HEM	C3C-C2C	-3.72	1.29	1.37
3	A	901[A]	HEM	C3C-C2C	-3.33	1.30	1.37
3	A	901[B]	HEM	C3C-C2C	-3.33	1.30	1.37
3	C	903	HEM	C1A-NA	-3.30	1.33	1.39
3	B	902	HEM	CMD-C2D	3.29	1.57	1.50
3	B	902	HEM	C1D-C2D	-3.29	1.37	1.44
3	B	902	HEM	CAC-C3C	3.17	1.55	1.47
3	A	901[A]	HEM	FE-NB	2.98	2.04	1.94
3	A	901[B]	HEM	FE-NB	2.98	2.04	1.94
3	A	901[A]	HEM	C3C-C4C	-2.97	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901[B]	HEM	C3C-C4C	-2.97	1.40	1.46
3	A	901[A]	HEM	O2D-CGD	-2.93	1.21	1.30
3	A	901[B]	HEM	O2D-CGD	-2.85	1.21	1.30
3	B	902	HEM	CHD-C4C	-2.79	1.32	1.38
3	C	903	HEM	FE-NC	2.69	2.04	1.95
3	A	901[A]	HEM	CMD-C2D	2.62	1.56	1.50
3	A	901[B]	HEM	CMD-C2D	2.62	1.56	1.50
3	C	903	HEM	C4D-ND	-2.60	1.35	1.40
3	B	902	HEM	O2D-CGD	-2.59	1.22	1.30
3	C	903	HEM	CHD-C4C	-2.58	1.33	1.38
3	B	902	HEM	C1B-NB	-2.48	1.35	1.40
3	A	901[A]	HEM	CHD-C4C	-2.47	1.33	1.38
3	A	901[B]	HEM	CHD-C4C	-2.47	1.33	1.38
3	B	902	HEM	CHD-C1D	-2.41	1.33	1.39
3	B	902	HEM	C3C-C4C	-2.39	1.41	1.46
3	A	901[A]	HEM	FE-ND	2.39	2.02	1.94
3	A	901[B]	HEM	FE-ND	2.39	2.02	1.94
3	C	903	HEM	CMC-C2C	2.39	1.55	1.50
3	A	901[A]	HEM	C1A-NA	-2.37	1.35	1.39
3	A	901[B]	HEM	C1A-NA	-2.37	1.35	1.39
3	C	903	HEM	C3D-C2D	2.33	1.41	1.36
3	B	902	HEM	C1A-C2A	2.33	1.49	1.44
3	A	901[A]	HEM	CAB-C3B	2.30	1.53	1.47
3	A	901[B]	HEM	CAB-C3B	2.30	1.53	1.47
3	B	902	HEM	C4B-NB	-2.27	1.34	1.38
3	C	903	HEM	CBD-CGD	2.25	1.55	1.50
3	C	903	HEM	O1A-CGA	2.24	1.29	1.22
3	C	903	HEM	CAC-C3C	2.24	1.53	1.47
3	C	903	HEM	FE-ND	2.23	2.01	1.94
3	C	903	HEM	C1B-C2B	-2.22	1.40	1.44
3	A	901[A]	HEM	C4A-C3A	2.15	1.48	1.43
3	A	901[B]	HEM	C4A-C3A	2.15	1.48	1.43
3	C	903	HEM	FE-NB	2.14	2.01	1.94
3	C	903	HEM	CHB-C1B	-2.07	1.34	1.38
3	C	903	HEM	C4B-NB	-2.06	1.34	1.38
3	C	903	HEM	C3C-C2C	-2.05	1.33	1.37
3	A	901[A]	HEM	FE-NA	2.03	2.01	1.95
3	A	901[B]	HEM	FE-NA	2.03	2.01	1.95

All (146) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	HEM	C4C-C3C-C2C	8.70	114.36	106.81
3	A	901[A]	HEM	CAD-C3D-C4D	7.70	138.12	124.70
3	A	901[B]	HEM	CAD-C3D-C4D	7.70	138.12	124.70
3	A	901[A]	HEM	CAD-CBD-CGD	7.07	132.43	113.67
3	A	901[A]	HEM	C4A-C3A-C2A	6.96	114.79	106.82
3	A	901[B]	HEM	C4A-C3A-C2A	6.96	114.79	106.82
3	A	901[A]	HEM	C2A-C1A-NA	6.94	117.85	110.15
3	A	901[B]	HEM	C2A-C1A-NA	6.94	117.85	110.15
3	A	901[A]	HEM	CHA-C4D-ND	6.83	132.81	124.37
3	A	901[B]	HEM	CHA-C4D-ND	6.83	132.81	124.37
3	A	901[A]	HEM	CHC-C4B-NB	6.80	131.75	124.42
3	A	901[B]	HEM	CHC-C4B-NB	6.80	131.75	124.42
3	A	901[A]	HEM	O1D-CGD-CBD	6.41	143.41	123.09
3	B	902	HEM	CHC-C1C-NC	6.27	131.28	124.45
3	B	902	HEM	C1D-C2D-C3D	6.25	113.56	106.98
3	B	902	HEM	CHD-C4C-C3C	6.17	135.62	125.21
3	C	903	HEM	CHD-C4C-C3C	6.16	135.60	125.21
3	B	902	HEM	C4D-ND-C1D	6.16	112.50	105.21
3	B	902	HEM	C4A-C3A-C2A	5.94	113.62	106.82
3	A	901[A]	HEM	C4D-ND-C1D	5.88	112.17	105.21
3	A	901[B]	HEM	C4D-ND-C1D	5.88	112.17	105.21
3	A	901[A]	HEM	CMA-C3A-C4A	-5.85	116.51	125.42
3	A	901[B]	HEM	CMA-C3A-C4A	-5.85	116.51	125.42
3	C	903	HEM	C1D-C2D-C3D	5.83	113.11	106.98
3	B	902	HEM	CHA-C4D-ND	5.80	131.54	124.37
3	B	902	HEM	C2D-C1D-ND	-5.57	103.46	109.90
3	B	902	HEM	CHD-C1D-C2D	5.36	133.50	125.03
3	B	902	HEM	CHC-C4B-NB	5.30	130.12	124.42
3	A	901[B]	HEM	O2D-CGD-CBD	-5.23	97.48	114.00
3	C	903	HEM	CHC-C1C-NC	5.12	130.02	124.45
3	A	901[A]	HEM	C1A-C2A-C3A	-4.90	99.29	106.87
3	A	901[B]	HEM	C1A-C2A-C3A	-4.90	99.29	106.87
3	B	902	HEM	C3B-C4B-NB	4.89	112.98	109.47
3	C	903	HEM	C3B-C2B-C1B	4.85	110.05	106.41
3	A	901[A]	HEM	C1B-NB-C4B	4.76	110.85	105.21
3	A	901[B]	HEM	C1B-NB-C4B	4.76	110.85	105.21
3	A	901[A]	HEM	CAA-C2A-C1A	4.74	134.19	124.94
3	A	901[B]	HEM	CAA-C2A-C1A	4.74	134.19	124.94
3	A	901[B]	HEM	O1D-CGD-CBD	4.71	138.04	123.09
3	B	902	HEM	CMA-C3A-C4A	-4.69	118.28	125.42
3	B	902	HEM	C2B-C1B-NB	4.67	115.20	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	903	HEM	CHD-C4C-NC	-4.48	119.58	124.45
3	C	903	HEM	CMA-C3A-C4A	-4.42	118.68	125.42
3	B	902	HEM	CHB-C1B-NB	-4.36	118.97	124.37
3	C	903	HEM	C4D-C3D-C2D	-4.36	100.55	106.89
3	A	901[A]	HEM	C1D-C2D-C3D	4.35	111.56	106.98
3	A	901[B]	HEM	C1D-C2D-C3D	4.35	111.56	106.98
3	A	901[A]	HEM	C4C-C3C-C2C	4.27	110.52	106.81
3	A	901[B]	HEM	C4C-C3C-C2C	4.27	110.52	106.81
3	A	901[A]	HEM	CAD-C3D-C2D	-4.24	119.93	127.87
3	A	901[B]	HEM	CAD-C3D-C2D	-4.24	119.93	127.87
3	A	901[A]	HEM	CHA-C1A-C2A	-4.23	116.04	125.30
3	A	901[B]	HEM	CHA-C1A-C2A	-4.23	116.04	125.30
3	A	901[A]	HEM	C3A-C4A-NA	-4.20	103.41	110.14
3	A	901[B]	HEM	C3A-C4A-NA	-4.20	103.41	110.14
3	B	902	HEM	CMD-C2D-C1D	-4.18	118.50	125.03
3	C	903	HEM	C2D-C1D-ND	-4.18	105.07	109.90
3	B	902	HEM	CHC-C4B-C3B	-4.13	116.82	125.07
3	C	903	HEM	C4C-C3C-C2C	4.12	110.38	106.81
3	B	902	HEM	C3B-C2B-C1B	-4.06	103.36	106.41
3	A	901[A]	HEM	CAC-C3C-C2C	-4.01	115.39	128.43
3	A	901[B]	HEM	CAC-C3C-C2C	-4.01	115.39	128.43
3	B	902	HEM	C1A-C2A-C3A	-3.98	100.70	106.87
3	A	901[B]	HEM	CAD-CBD-CGD	3.95	124.14	113.67
3	C	903	HEM	O2D-CGD-CBD	3.92	126.39	114.00
3	B	902	HEM	C4C-NC-C1C	3.89	112.16	105.82
3	A	901[A]	HEM	CAC-C3C-C4C	3.88	134.09	124.82
3	A	901[B]	HEM	CAC-C3C-C4C	3.88	134.09	124.82
3	C	903	HEM	C4D-ND-C1D	3.81	109.72	105.21
3	C	903	HEM	CBD-CAD-C3D	-3.77	102.11	112.53
3	A	901[A]	HEM	O2D-CGD-O1D	-3.72	113.76	123.33
3	C	903	HEM	CHC-C4B-NB	3.62	128.32	124.42
3	B	902	HEM	C4C-CHD-C1D	3.60	133.67	126.02
3	A	901[A]	HEM	CHA-C4D-C3D	-3.58	118.63	125.23
3	A	901[B]	HEM	CHA-C4D-C3D	-3.58	118.63	125.23
3	A	901[A]	HEM	C2D-C1D-ND	-3.56	105.79	109.90
3	A	901[B]	HEM	C2D-C1D-ND	-3.56	105.79	109.90
3	B	902	HEM	CBC-CAC-C3C	-3.55	109.78	127.53
3	A	901[A]	HEM	O2D-CGD-CBD	-3.54	102.83	114.00
3	A	901[A]	HEM	CMB-C2B-C1B	-3.54	119.51	125.03
3	A	901[B]	HEM	CMB-C2B-C1B	-3.54	119.51	125.03
3	A	901[A]	HEM	C2B-C1B-NB	-3.44	105.88	109.84
3	A	901[B]	HEM	C2B-C1B-NB	-3.44	105.88	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	HEM	C2A-C1A-NA	3.44	113.97	110.15
3	C	903	HEM	O2D-CGD-O1D	-3.40	114.60	123.33
3	A	901[A]	HEM	C4D-C3D-C2D	-3.39	101.95	106.89
3	A	901[B]	HEM	C4D-C3D-C2D	-3.39	101.95	106.89
3	C	903	HEM	CBC-CAC-C3C	-3.38	110.61	127.53
3	C	903	HEM	CHA-C1A-C2A	-3.35	117.97	125.30
3	B	902	HEM	C4D-C3D-C2D	-3.27	102.13	106.89
3	C	903	HEM	CHA-C4D-ND	3.19	128.31	124.37
3	B	902	HEM	CAD-C3D-C4D	3.17	130.23	124.70
3	A	901[A]	HEM	CBC-CAC-C3C	-3.16	111.73	127.53
3	A	901[B]	HEM	CBC-CAC-C3C	-3.16	111.73	127.53
3	B	902	HEM	O2D-CGD-CBD	3.12	123.84	114.00
3	A	901[A]	HEM	CHD-C4C-NC	3.10	127.83	124.45
3	A	901[B]	HEM	CHD-C4C-NC	3.10	127.83	124.45
3	B	902	HEM	C1B-NB-C4B	-3.09	101.55	105.21
3	A	901[A]	HEM	CHC-C1C-NC	3.09	127.82	124.45
3	A	901[B]	HEM	CHC-C1C-NC	3.09	127.82	124.45
3	A	901[A]	HEM	C3C-C2C-C1C	-3.05	104.16	107.05
3	A	901[B]	HEM	C3C-C2C-C1C	-3.05	104.16	107.05
3	B	902	HEM	CAA-CBA-CGA	-3.03	105.63	113.67
3	C	903	HEM	CMA-C3A-C2A	3.00	131.98	125.62
3	B	902	HEM	C3A-C4A-NA	-2.98	105.37	110.14
3	C	903	HEM	C2A-C1A-NA	2.92	113.39	110.15
3	B	902	HEM	CAA-C2A-C1A	2.80	130.40	124.94
3	B	902	HEM	CHA-C4D-C3D	-2.78	120.11	125.23
3	A	901[A]	HEM	C1A-CHA-C4D	-2.77	119.73	126.25
3	A	901[B]	HEM	C1A-CHA-C4D	-2.77	119.73	126.25
3	C	903	HEM	CHA-C4D-C3D	-2.76	120.14	125.23
3	A	901[A]	HEM	CHC-C4B-C3B	-2.72	119.64	125.07
3	A	901[B]	HEM	CHC-C4B-C3B	-2.72	119.64	125.07
3	A	901[A]	HEM	CBD-CAD-C3D	-2.72	105.02	112.53
3	A	901[B]	HEM	CBD-CAD-C3D	-2.72	105.02	112.53
3	B	902	HEM	C1C-CHC-C4B	-2.67	120.34	126.02
3	C	903	HEM	CHA-C1A-NA	2.60	128.58	123.86
3	C	903	HEM	C2B-C1B-NB	-2.59	106.86	109.84
3	C	903	HEM	CAA-C2A-C1A	2.57	129.95	124.94
3	B	902	HEM	O2A-CGA-O1A	-2.55	116.78	123.33
3	B	902	HEM	CHA-C1A-C2A	-2.54	119.74	125.30
3	A	901[A]	HEM	CHD-C1D-C2D	2.51	128.99	125.03
3	A	901[B]	HEM	CHD-C1D-C2D	2.51	128.99	125.03
3	C	903	HEM	CAD-C3D-C4D	2.45	128.96	124.70
3	C	903	HEM	CMC-C2C-C1C	2.42	129.00	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	903	HEM	CMB-C2B-C1B	-2.39	121.30	125.03
3	A	901[A]	HEM	C3B-C2B-C1B	2.38	108.20	106.41
3	A	901[B]	HEM	C3B-C2B-C1B	2.38	108.20	106.41
3	A	901[A]	HEM	O1A-CGA-CBA	-2.28	115.85	123.09
3	A	901[B]	HEM	O1A-CGA-CBA	-2.28	115.85	123.09
3	C	903	HEM	CAA-CBA-CGA	-2.27	107.63	113.67
3	C	903	HEM	CMC-C2C-C3C	-2.24	123.00	128.43
3	A	901[A]	HEM	CAA-CBA-CGA	-2.24	107.72	113.67
3	A	901[B]	HEM	CAA-CBA-CGA	-2.24	107.72	113.67
3	B	902	HEM	O2D-CGD-O1D	-2.24	117.58	123.33
3	C	903	HEM	C4A-C3A-C2A	2.17	109.30	106.82
3	A	901[A]	HEM	O2A-CGA-CBA	2.10	120.62	114.00
3	A	901[B]	HEM	O2A-CGA-CBA	2.10	120.62	114.00
3	C	903	HEM	CAD-CBD-CGD	2.09	119.20	113.67
3	C	903	HEM	CHD-C1D-C2D	2.08	128.31	125.03
3	A	901[A]	HEM	CHC-C1C-C2C	-2.07	121.19	125.49
3	A	901[B]	HEM	CHC-C1C-C2C	-2.07	121.19	125.49
3	B	902	HEM	C3C-C2C-C1C	-2.05	105.10	107.05
3	C	903	HEM	CHC-C1C-C2C	-2.05	121.23	125.49
3	C	903	HEM	CHD-C1D-ND	2.03	126.61	124.42
3	B	902	HEM	CHD-C4C-NC	-2.01	122.26	124.45

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901[A]	HEM	C3D-CAD-CBD-CGD
3	A	901[A]	HEM	C2B-C3B-CAB-CBB
3	A	901[A]	HEM	C2C-C3C-CAC-CBC
3	A	901[B]	HEM	C2B-C3B-CAB-CBB
3	A	901[B]	HEM	C2C-C3C-CAC-CBC
3	B	902	HEM	C2C-C3C-CAC-CBC
3	C	903	HEM	C2C-C3C-CAC-CBC
3	A	901[A]	HEM	C4C-C3C-CAC-CBC
3	A	901[B]	HEM	C4C-C3C-CAC-CBC
3	B	902	HEM	C4C-C3C-CAC-CBC
3	C	903	HEM	C4C-C3C-CAC-CBC
3	B	902	HEM	CAA-CBA-CGA-O1A
3	C	903	HEM	CAA-CBA-CGA-O1A
3	A	901[A]	HEM	CAA-CBA-CGA-O1A
3	A	901[B]	HEM	CAA-CBA-CGA-O1A
3	A	901[A]	HEM	CAD-CBD-CGD-O2D

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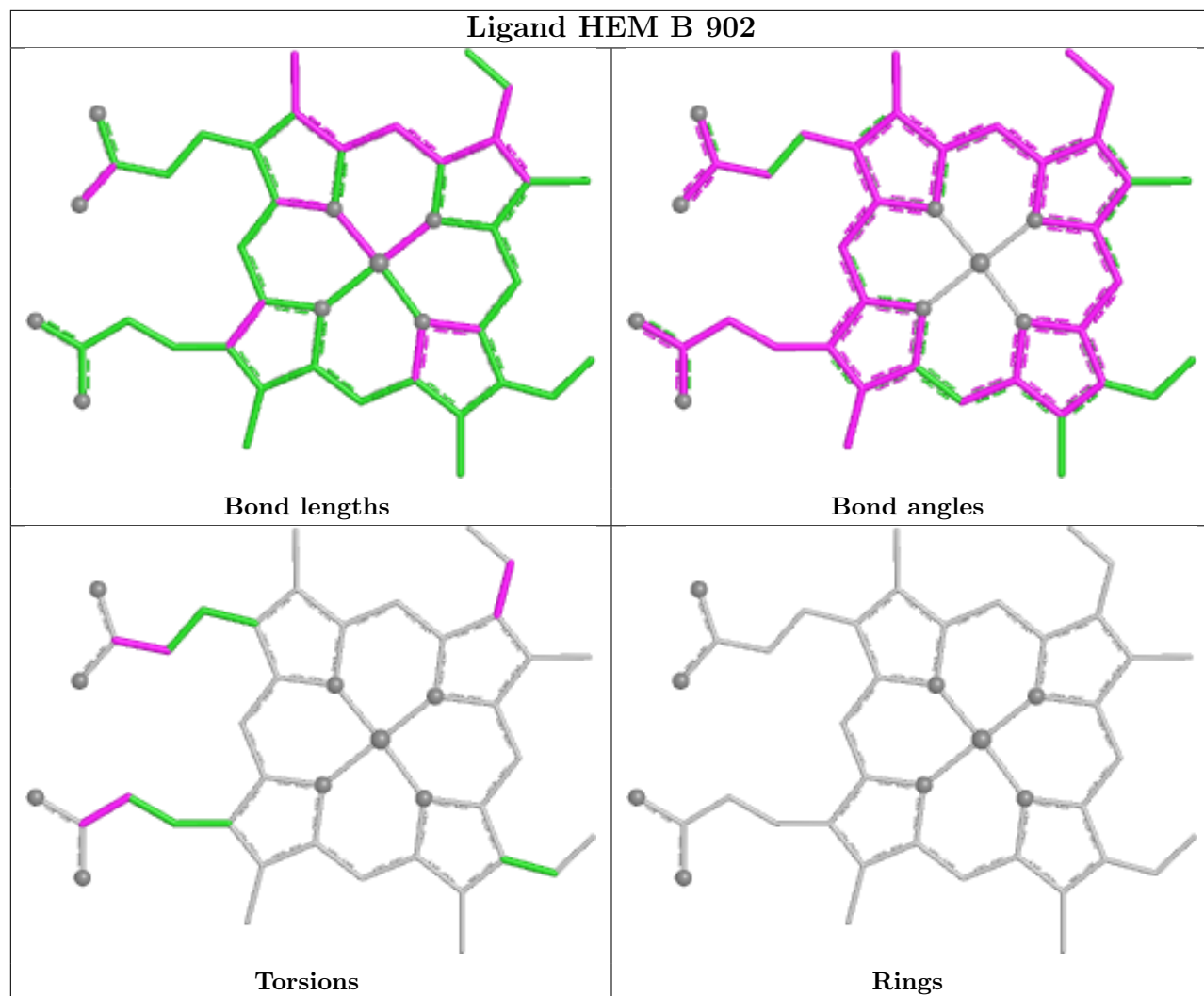
Mol	Chain	Res	Type	Atoms
3	C	903	HEM	CAA-CBA-CGA-O2A
3	A	901[A]	HEM	CAA-CBA-CGA-O2A
3	A	901[B]	HEM	CAA-CBA-CGA-O2A
3	A	901[A]	HEM	CAD-CBD-CGD-O1D
3	B	902	HEM	CAA-CBA-CGA-O2A
3	A	901[B]	HEM	CAD-CBD-CGD-O2D
3	B	902	HEM	CAD-CBD-CGD-O2D
3	A	901[B]	HEM	CAD-CBD-CGD-O1D
3	A	901[A]	HEM	C4B-C3B-CAB-CBB
3	A	901[B]	HEM	C4B-C3B-CAB-CBB
3	B	902	HEM	CAD-CBD-CGD-O1D

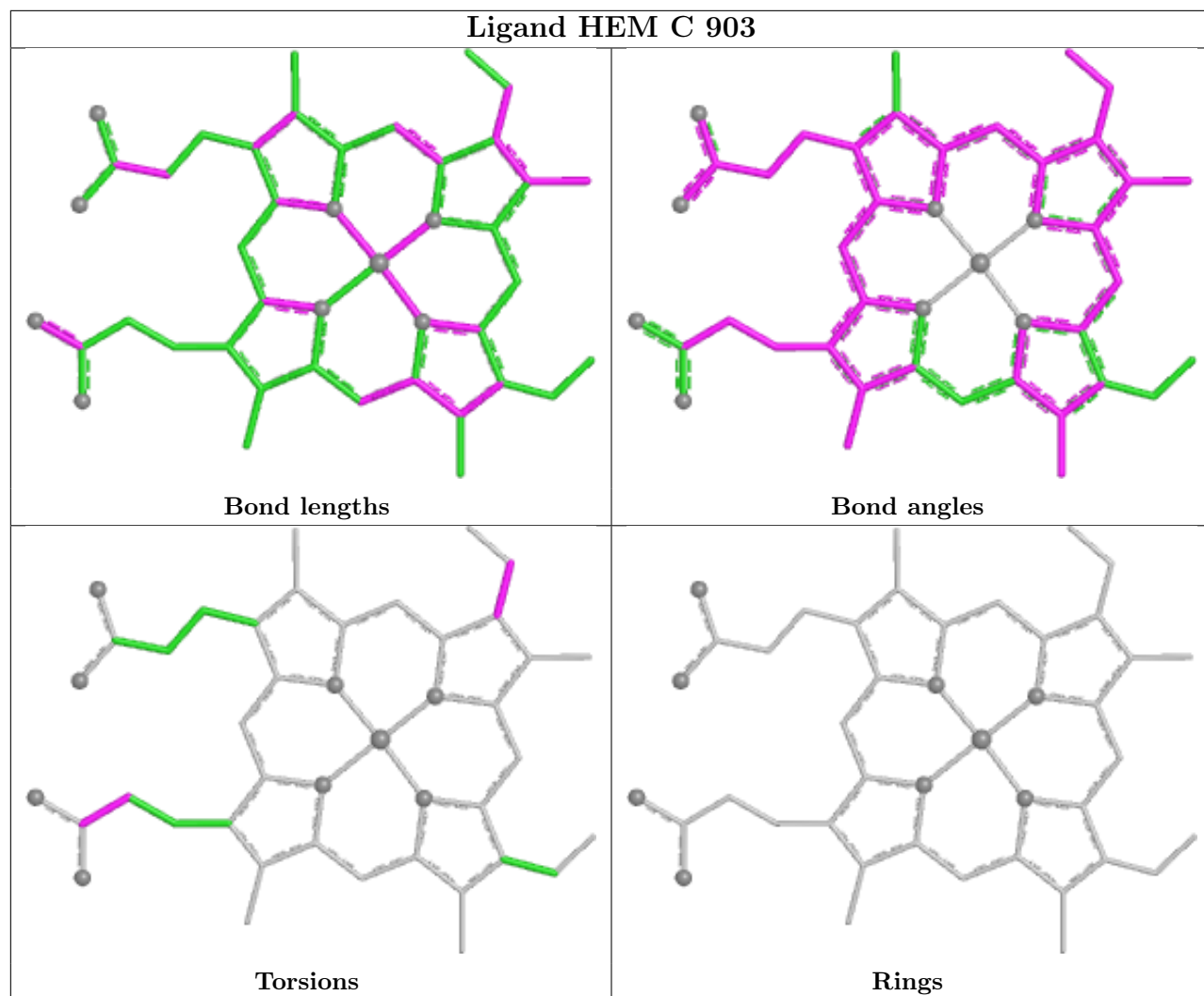
There are no ring outliers.

3 monomers are involved in 3 short contacts:

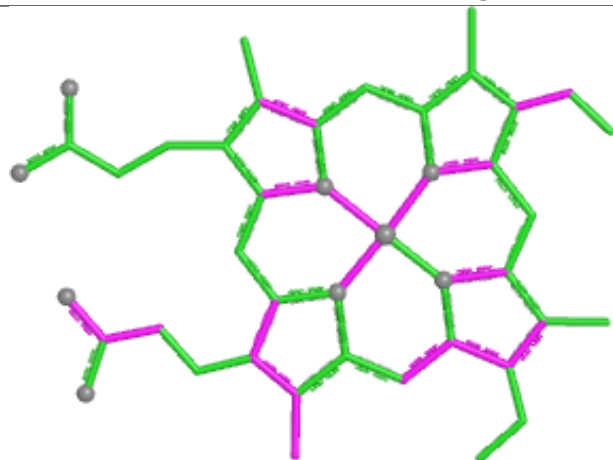
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	906	SO4	1	0
4	B	907	SO4	1	0
3	A	901[A]	HEM	1	0

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 than 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.

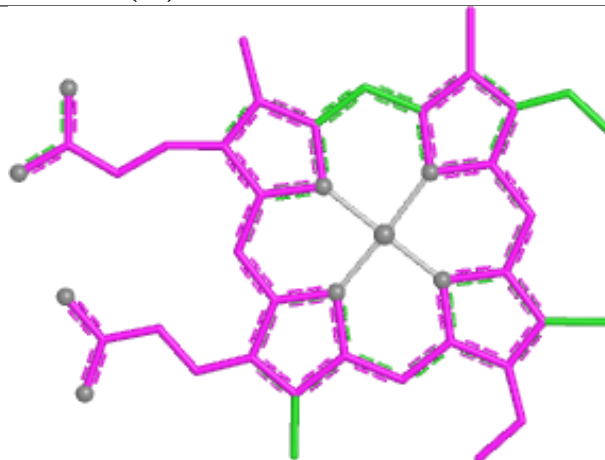




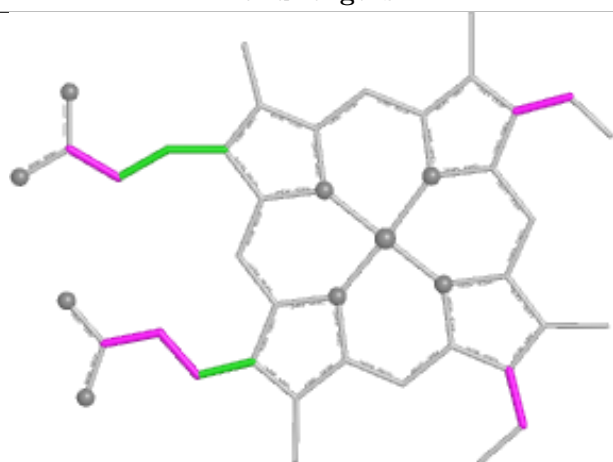
Ligand HEM A 901 (A)



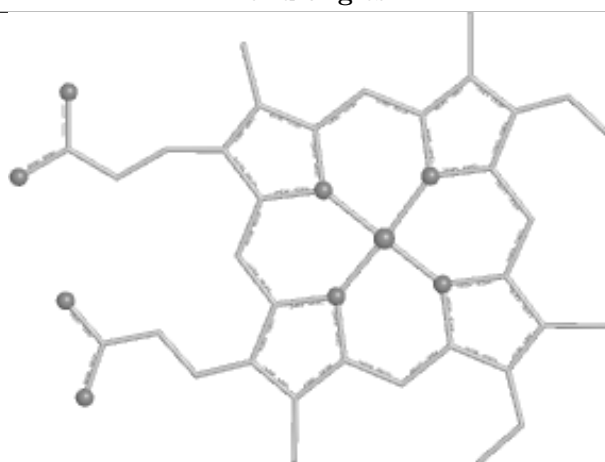
Bond lengths



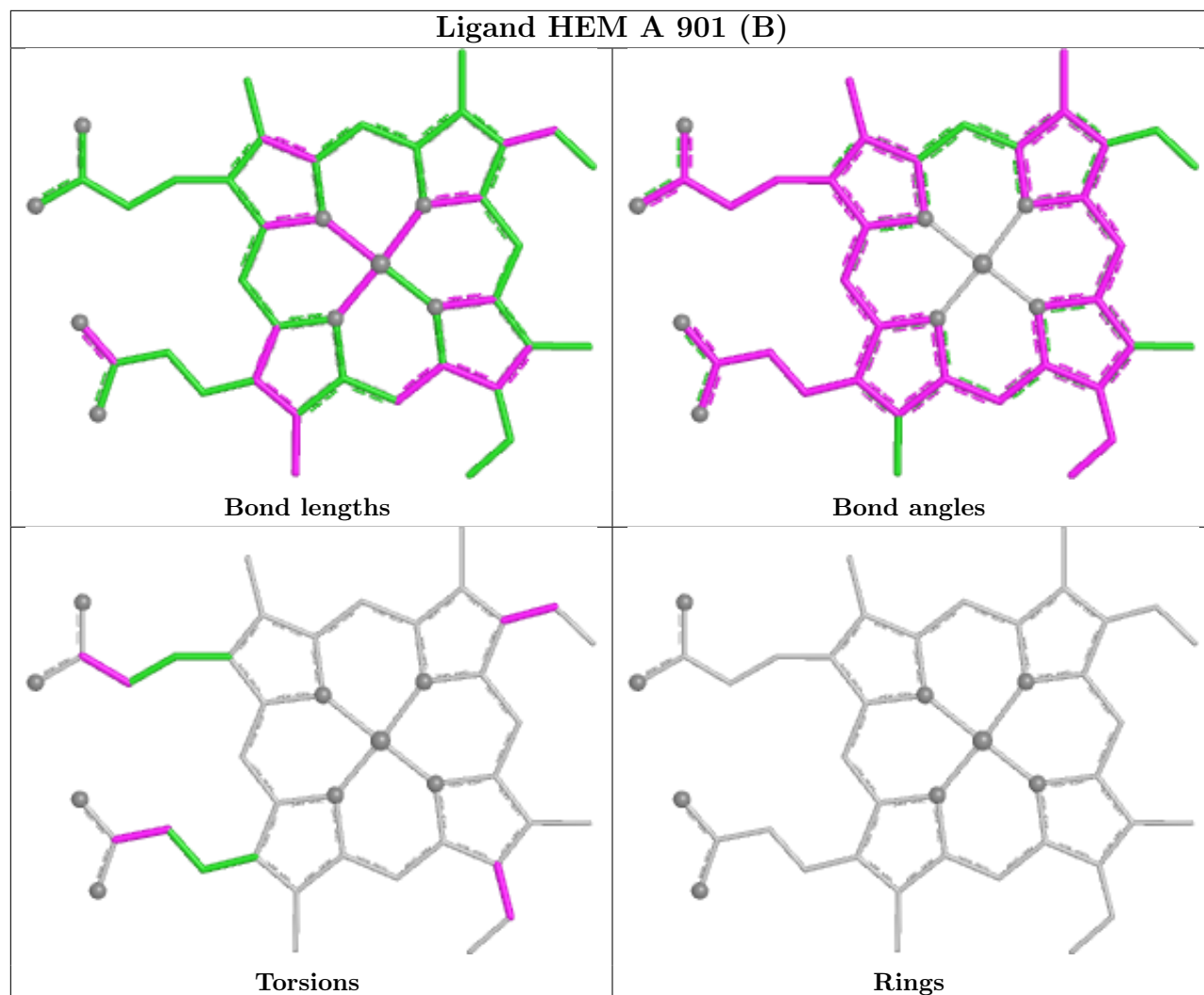
Bond angles



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	207/215 (96%)	0.04	3 (1%) 73 76	11, 18, 30, 39	0
1	B	209/215 (97%)	-0.07	9 (4%) 40 41	8, 15, 26, 31	5 (2%)
1	C	207/215 (96%)	-0.01	5 (2%) 59 62	9, 16, 26, 35	5 (2%)
All	All	623/645 (96%)	-0.02	17 (2%) 56 58	8, 17, 28, 39	10 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	394	SER	4.2
1	B	484	GLU	4.0
1	B	439[A]	GLY	3.4
1	A	98	SER	3.0
1	A	94	SER	2.9
1	B	399	ARG	2.8
1	B	395	GLU	2.7
1	C	618	GLN	2.6
1	B	438[A]	SER	2.6
1	B	449	ARG	2.5
1	C	784	GLU	2.4
1	B	513	LYS	2.4
1	C	754	ASP	2.3
1	C	745	ARG	2.1
1	C	813	LYS	2.1
1	B	464	GLU	2.1
1	A	138	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

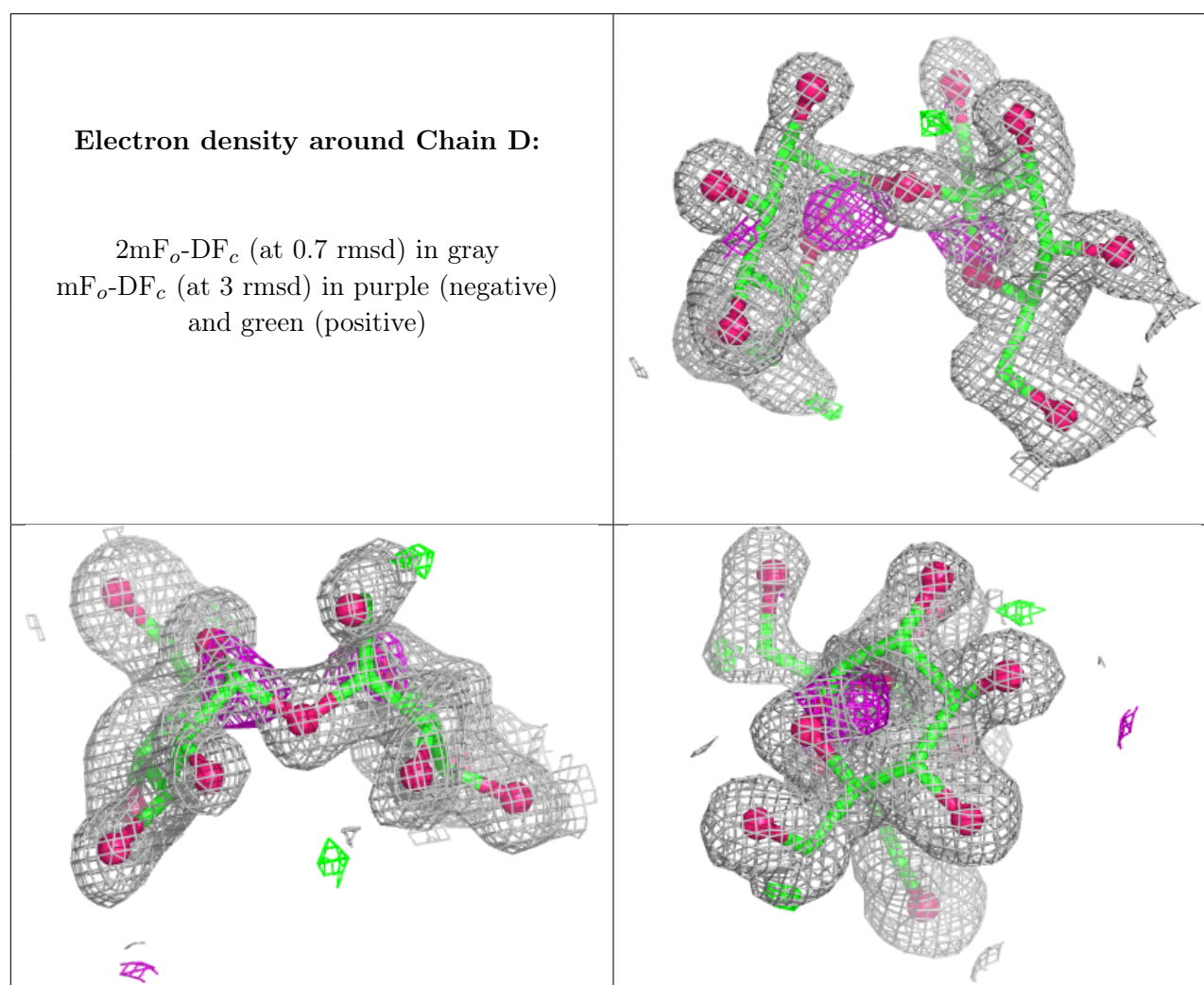
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FRU	D	2	12/12	0.85	0.09	25,27,30,30	0
2	GLC	D	1	11/12	0.92	0.08	21,22,24,26	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.



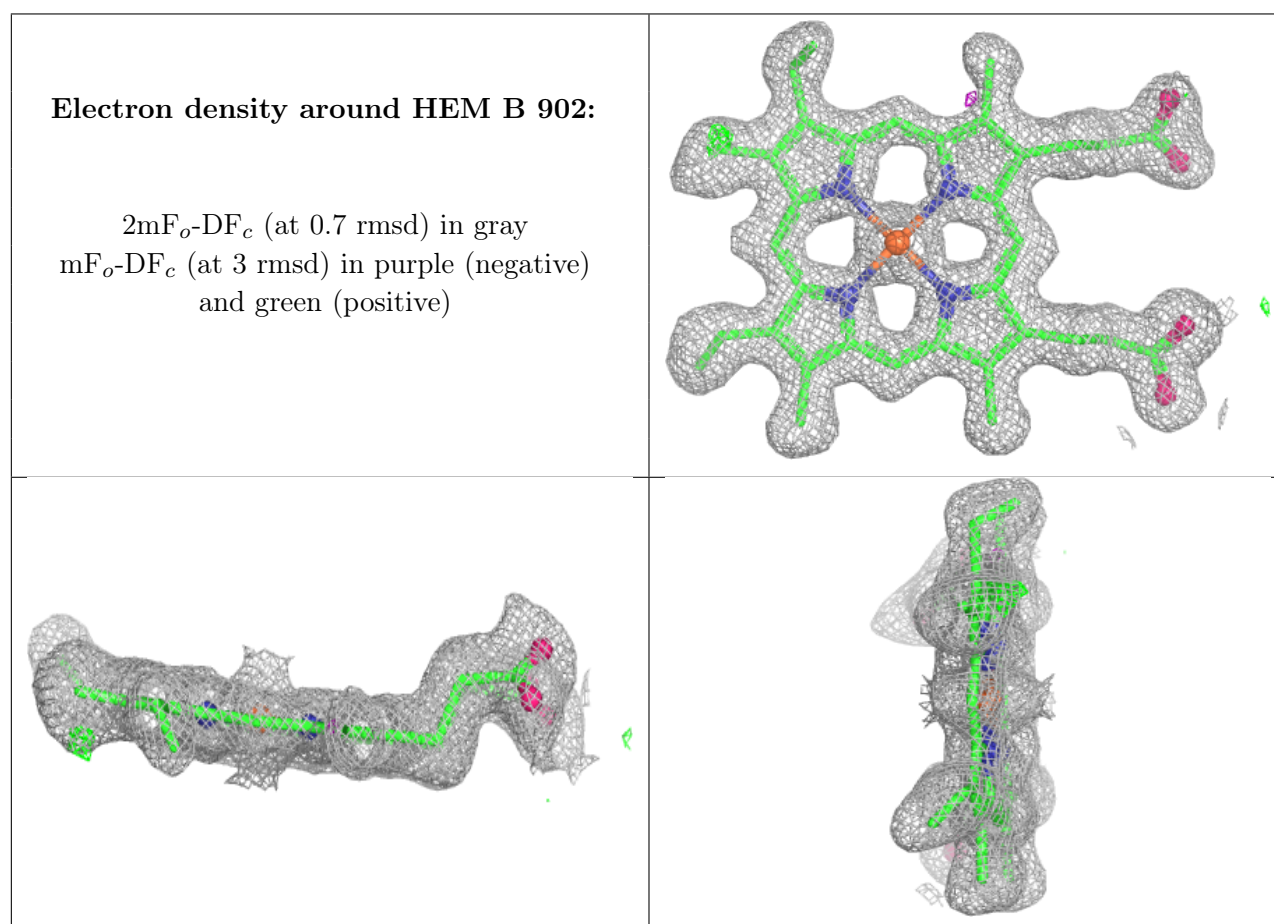
6.4 Ligands [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

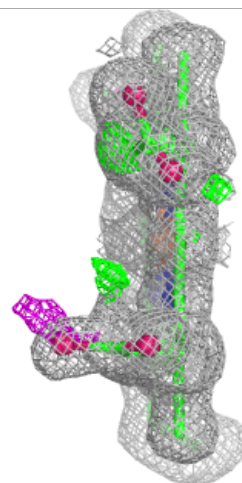
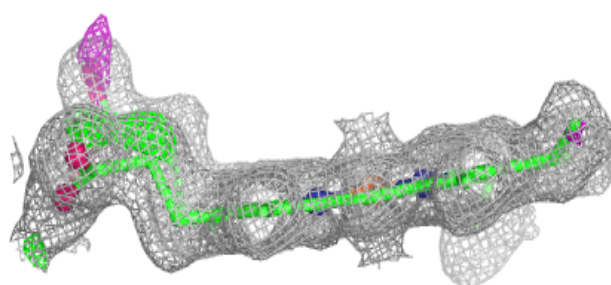
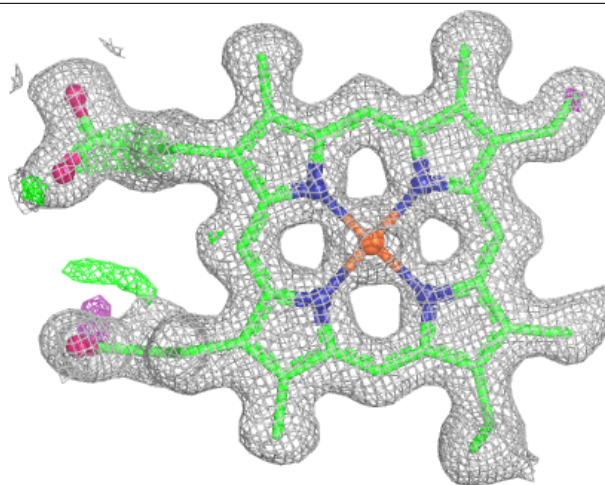
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	C	910	5/5	0.82	0.25	13,13,14,15	5
4	SO4	B	908	5/5	0.85	0.11	36,36,37,37	0
4	SO4	C	909	5/5	0.88	0.14	14,16,16,17	5
4	SO4	B	907	5/5	0.90	0.11	34,34,35,37	0
4	SO4	B	906	5/5	0.94	0.08	32,32,33,33	0
4	SO4	C	905	5/5	0.95	0.10	18,18,19,21	5
3	HEM	B	902	43/43	0.98	0.06	9,13,21,28	0
3	HEM	C	903	43/43	0.98	0.05	10,12,19,25	0
3	HEM	A	901[A]	43/43	0.98	0.07	11,17,27,31	3
3	HEM	A	901[B]	43/43	0.98	0.07	11,17,28,31	3

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.



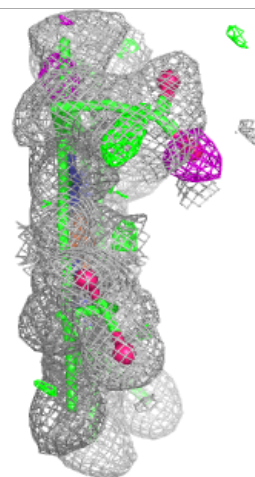
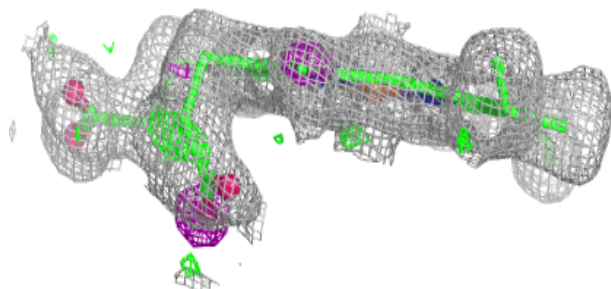
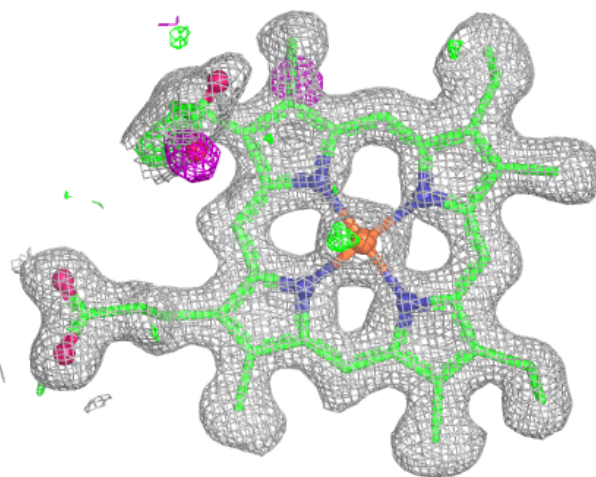
Electron density around HEM C 903:

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



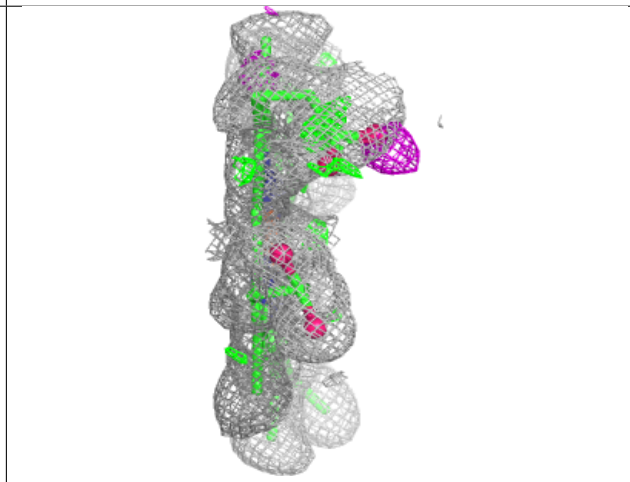
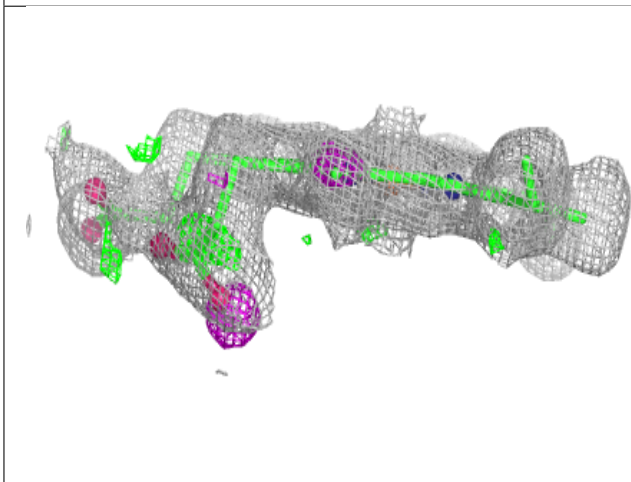
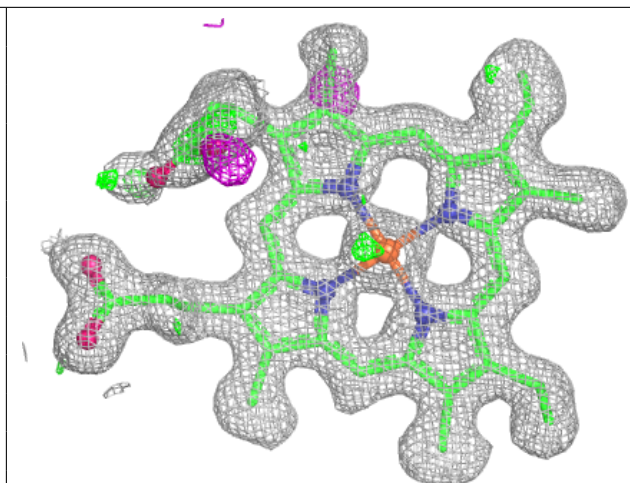
Electron density around HEM A 901 (A):

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



Electron density around HEM A 901 (B):

$2mF_o-DF_c$ (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.