



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:38 PM BST

PDB ID : 1IW1
Title : Crystal structure of a heme oxygenase (HmuO) from *Corynebacterium diphtheriae* complexed with heme in the ferrous 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 : 1.50 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

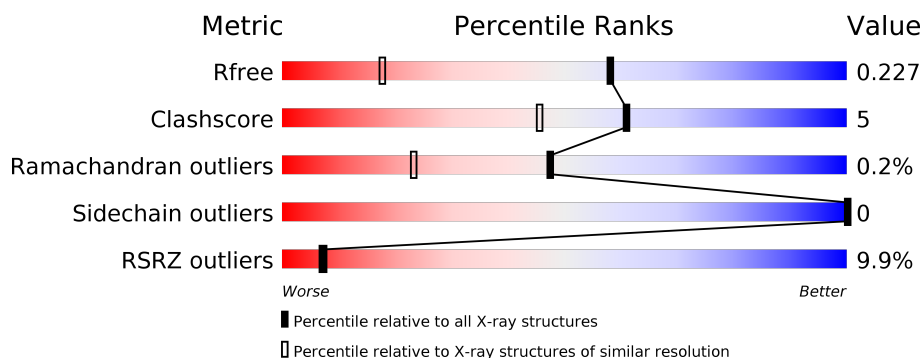
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 on 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	<div> <div>3%</div> <div>91%</div> <div>8%</div> </div>
1	B	215	<div> <div>5%</div> <div>90%</div> <div>7%</div> </div>
1	C	215	<div> <div>20%</div> <div>84%</div> <div>13%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition [i](#)

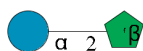
There are 5 unique types of molecules in this entry. The entry contains 5791 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

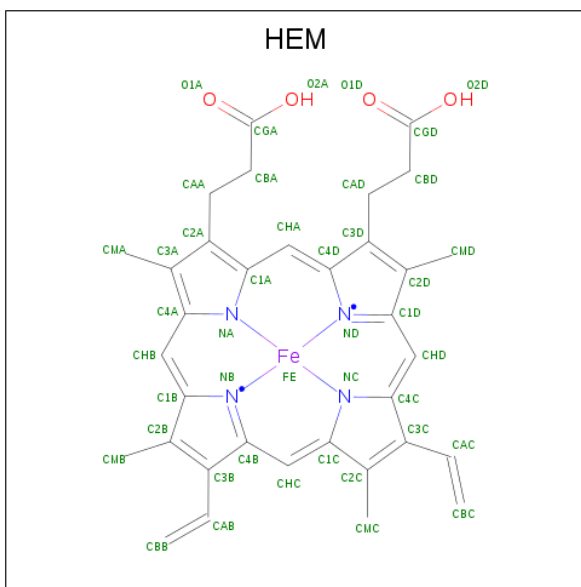
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1683	1060	298	322	3			
1	B	209	Total	C	N	O	S	0	0	0
			1665	1050	295	317	3			
1	C	208	Total	C	N	O	S	0	0	0
			1657	1045	294	315	3			

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



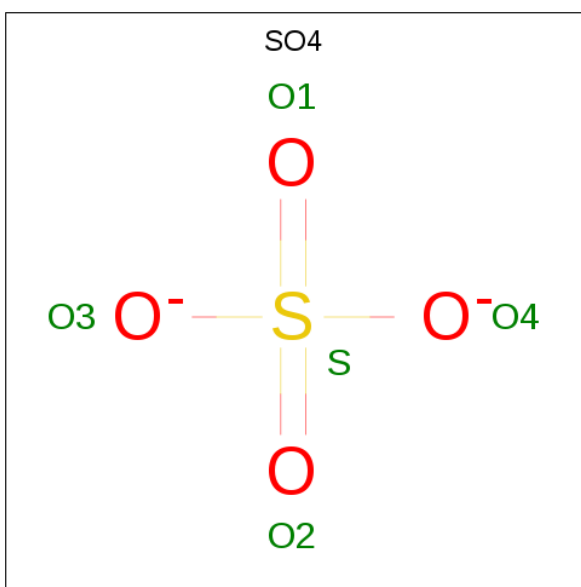
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	D	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
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 (three-letter code: SO4) (formula: O_4S).



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

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

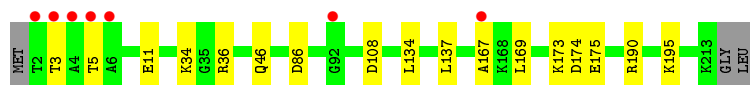
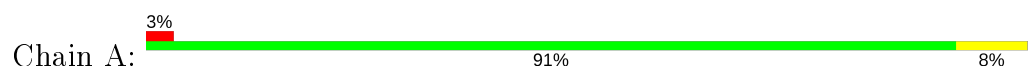
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	240	Total	O	0	0
			240	240		
5	B	199	Total	O	0	0
			199	199		
5	C	145	Total	O	0	0
			145	145		

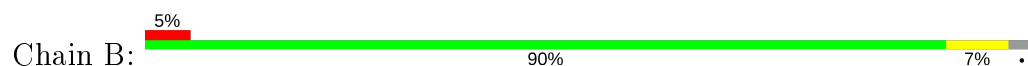
3 Residue-property plots [i](#)

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.

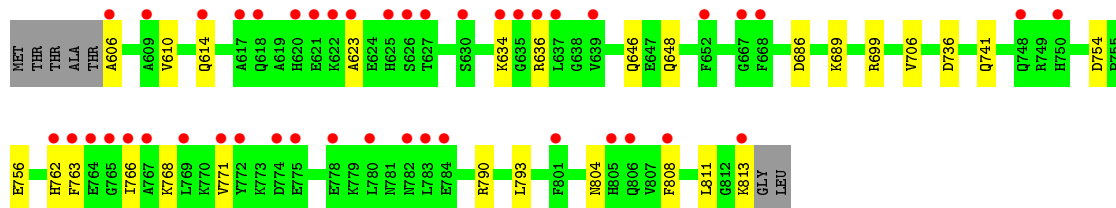
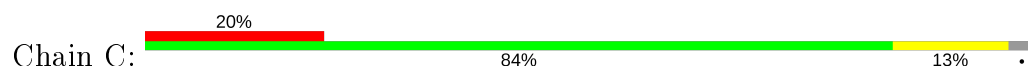
- Molecule 1: Heme oxygenase



- 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	53.87Å 62.84Å 107.21Å 90.00° 101.02° 90.00°	Depositor
Resolution (Å)	12.00 – 1.50 43.99 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.9 (12.00-1.50) 98.5 (43.99-1.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.177 , 0.202 0.209 , 0.227	Depositor DCC
R_{free} test set	5586 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5791	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 5.11% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, GLC, SO4, 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	0.60	0/1715	0.81	3/2318 (0.1%)
1	B	0.62	0/1697	0.79	2/2290 (0.1%)
1	C	0.58	0/1689	0.72	2/2281 (0.1%)
All	All	0.60	0/5101	0.78	7/6889 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	686	ASP	CB-CG-OD2	7.34	124.91	118.30
1	A	86	ASP	CB-CG-OD2	6.50	124.16	118.30
1	B	474	ASP	CB-CG-OD2	6.34	124.00	118.30
1	C	736	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	436	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	108	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	174	ASP	CB-CG-OD2	5.50	123.25	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1683	0	1642	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1665	0	1625	13	0
1	C	1657	0	1616	24	0
2	D	23	0	21	0	0
3	A	43	0	30	0	0
3	B	43	0	30	0	0
3	C	43	0	30	1	0
4	A	25	0	0	0	0
4	B	25	0	0	0	0
5	A	240	0	0	2	0
5	B	199	0	0	8	0
5	C	145	0	0	5	0
All	All	5791	0	4994	46	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 5.

All (46) 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:395:GLU:N	5:B:2108:HOH:O	2.17	0.77
1:C:762:HIS:CE1	5:C:2161:HOH:O	2.39	0.76
1:A:3:THR:OG1	1:A:5:THR:HG22	1.91	0.71
1:A:137:LEU:HD22	1:A:169:LEU:HD11	1.78	0.65
1:A:175:GLU:OE1	5:A:1232:HOH:O	2.15	0.64
1:C:610:VAL:HG23	5:C:2077:HOH:O	2.07	0.55
1:C:689:LYS:HD2	1:C:756:GLU:O	2.07	0.54
1:B:394:SER:HB2	1:B:397:ARG:NH1	2.23	0.54
1:C:634:LYS:HD2	5:C:2140:HOH:O	2.07	0.54
1:C:610:VAL:HG12	1:C:614:GLN:HE21	1.75	0.52
1:A:195:LYS:HG3	5:A:1066:HOH:O	2.10	0.51
1:C:610:VAL:CG1	1:C:614:GLN:HE21	2.24	0.50
1:B:358:GLN:NE2	5:B:2191:HOH:O	2.45	0.50
1:C:768:LYS:HD2	1:C:771:VAL:HG21	1.93	0.50
1:B:490:ARG:HD2	5:B:2053:HOH:O	2.12	0.49
1:C:646:GLN:HA	1:C:646:GLN:NE2	2.28	0.48
1:C:804:ASN:O	1:C:808:PHE:HD1	1.97	0.47
1:C:623:ALA:HB1	3:C:903:HEM:CBB	2.44	0.47
1:C:646:GLN:HA	1:C:646:GLN:HE21	1.82	0.45
1:C:689:LYS:HD3	1:C:756:GLU:HG3	1.99	0.44
1:C:636:ARG:HG3	5:C:2152:HOH:O	2.18	0.44
1:C:763:PHE:HB3	1:C:766:ILE:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ASP:CG	5:B:2091:HOH:O	2.56	0.43
1:C:610:VAL:HG12	1:C:614:GLN:NE2	2.33	0.43
1:B:493:LEU:HD23	1:B:493:LEU:C	2.38	0.43
1:B:498:THR:HG23	5:B:2166:HOH:O	2.18	0.43
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.83	0.43
1:B:502:VAL:HG23	5:B:2197:HOH:O	2.17	0.43
1:A:11:GLU:OE2	1:A:190:ARG:NH2	2.52	0.43
1:A:34:LYS:HG3	1:A:36:ARG:HG3	2.01	0.43
1:A:46:GLN:HA	1:A:46:GLN:NE2	2.33	0.43
1:C:754:ASP:OD1	1:C:756:GLU:HG2	2.19	0.43
1:C:811:LEU:C	1:C:813:LYS:H	2.21	0.43
1:C:768:LYS:HB2	1:C:771:VAL:HB	2.01	0.42
1:C:699:ARG:HB3	5:C:2116:HOH:O	2.20	0.42
1:C:606:ALA:O	1:C:790:ARG:NH2	2.53	0.42
1:B:346:GLN:NE2	1:B:346:GLN:HA	2.35	0.42
1:C:648:GLN:HB3	1:C:706:VAL:HG21	2.02	0.42
1:C:768:LYS:NZ	1:C:771:VAL:HG11	2.35	0.41
1:B:381:GLU:HG2	5:B:2103:HOH:O	2.20	0.41
1:B:336:ARG:HG2	1:B:336:ARG:HH11	1.86	0.41
1:B:434:LEU:HA	1:B:434:LEU:HD12	1.88	0.41
1:A:134:LEU:HD11	1:A:173:LYS:HG2	2.02	0.40
1:C:741:GLN:CD	1:C:741:GLN:H	2.25	0.40
1:B:503:PHE:HA	5:B:2064:HOH:O	2.22	0.40
1:C:793:LEU:C	1:C:793:LEU:HD23	2.42	0.40

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	210/215 (98%)	204 (97%)	5 (2%)	1 (0%)	29 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	207/215 (96%)	203 (98%)	4 (2%)	0	100	100
1	C	206/215 (96%)	200 (97%)	6 (3%)	0	100	100
All	All	623/645 (97%)	607 (97%)	15 (2%)	1 (0%)	47	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ALA

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	173/175 (99%)	173 (100%)	0	100	100
1	B	171/175 (98%)	171 (100%)	0	100	100
1	C	170/175 (97%)	170 (100%)	0	100	100
All	All	514/525 (98%)	514 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	B	325	HIS
1	B	346	GLN
1	B	358	GLN
1	B	506	GLN
1	C	614	GLN
1	C	618	GLN
1	C	646	GLN

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	0.54	0	15,15,17	0.99	0
2	FRU	D	2	2	11,12,12	0.81	1 (9%)	10,18,18	0.79	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	-	0/5/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	FRU	O2-C2	2.13	1.44	1.40

There are no bond angle outliers.

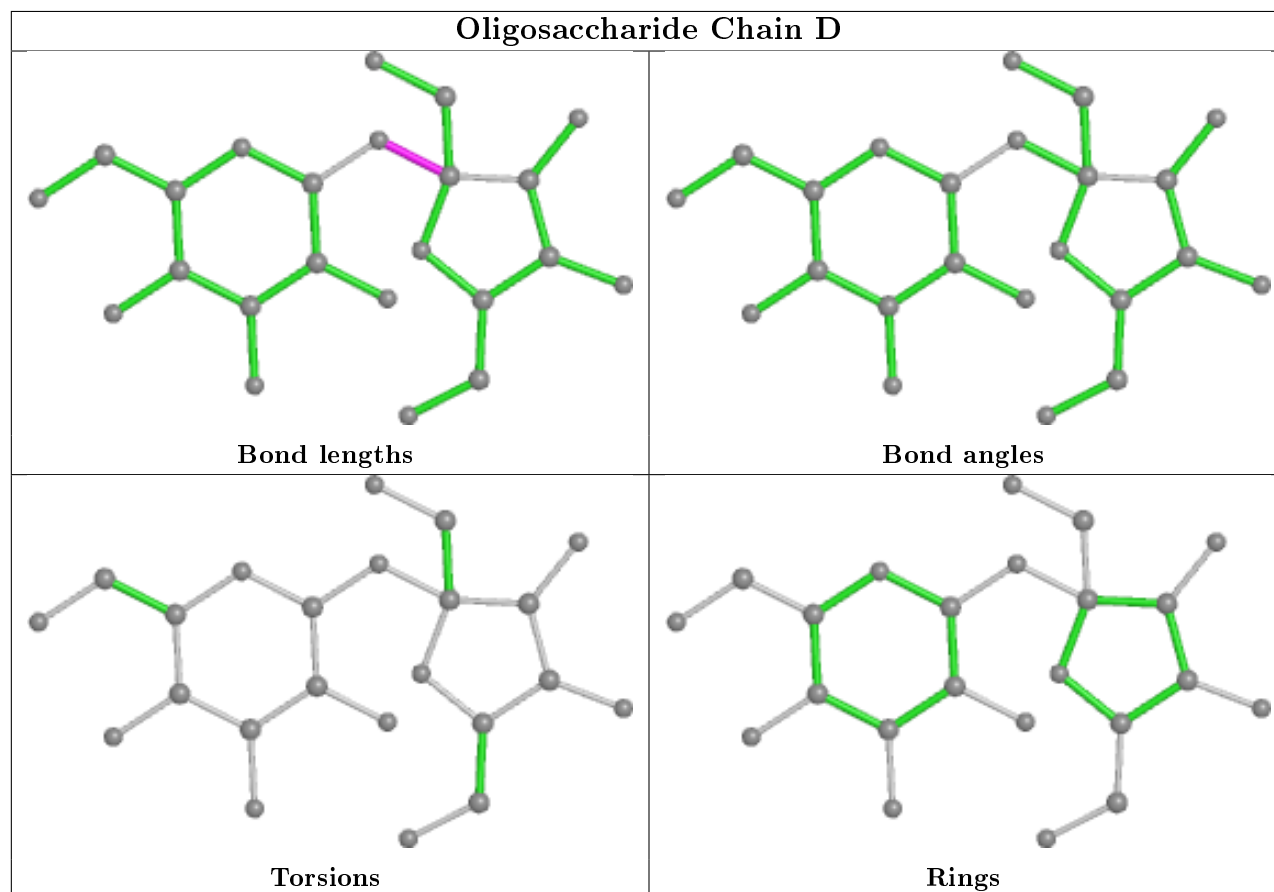
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

13 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	$\# Z > 2$
3	HEM	C	903	1	27,50,50	2.95	12 (44%)	17,82,82	3.92	9 (52%)
4	SO4	B	911	-	4,4,4	0.14	0	6,6,6	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	907	-	4,4,4	0.05	0	6,6,6	0.20	0
4	SO4	B	906	-	4,4,4	0.09	0	6,6,6	0.20	0
4	SO4	A	909	-	4,4,4	0.15	0	6,6,6	0.07	0
4	SO4	A	914	-	4,4,4	0.13	0	6,6,6	0.25	0
3	HEM	A	901	1	27,50,50	2.44	9 (33%)	17,82,82	4.10	7 (41%)
4	SO4	B	910	-	4,4,4	0.12	0	6,6,6	0.21	0
4	SO4	A	908	-	4,4,4	0.16	0	6,6,6	0.26	0
4	SO4	A	905	-	4,4,4	0.15	0	6,6,6	0.53	0
4	SO4	B	913	-	4,4,4	0.14	0	6,6,6	0.41	0
3	HEM	B	902	1	27,50,50	3.59	13 (48%)	17,82,82	8.91	14 (82%)
4	SO4	B	912	-	4,4,4	0.07	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	-	1/6/54/54	-
3	HEM	A	901	1	-	0/6/54/54	-
3	HEM	B	902	1	-	0/6/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	HEM	C3B-C2B	-8.82	1.28	1.40
3	C	903	HEM	C3B-C2B	-8.58	1.28	1.40
3	C	903	HEM	C3C-C2C	-8.17	1.29	1.40
3	B	902	HEM	C4A-NA	7.92	1.52	1.36
3	B	902	HEM	C3C-C2C	-7.02	1.30	1.40
3	B	902	HEM	C1D-ND	6.82	1.50	1.36
3	B	902	HEM	C1C-C2C	5.81	1.55	1.42
3	B	902	HEM	C3C-CAC	5.18	1.58	1.47
3	B	902	HEM	CMD-C2D	5.08	1.62	1.51
3	B	902	HEM	CAA-C2A	-4.67	1.45	1.52
3	B	902	HEM	CMA-C3A	4.17	1.60	1.51
3	C	903	HEM	CMA-C3A	4.12	1.60	1.51
3	A	901	HEM	CAD-C3D	-3.94	1.45	1.52
3	A	901	HEM	C3C-CAC	3.52	1.55	1.47
3	B	902	HEM	C4A-CHB	-3.46	1.31	1.41
3	B	902	HEM	C1A-NA	-3.34	1.29	1.36
3	B	902	HEM	C4D-C3D	3.22	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	HEM	C3C-C2C	-3.20	1.35	1.40
3	A	901	HEM	C4A-NA	3.00	1.42	1.36
3	C	903	HEM	C3C-CAC	2.95	1.53	1.47
3	C	903	HEM	C3D-C2D	2.82	1.46	1.37
3	B	902	HEM	C1B-C2B	-2.73	1.36	1.42
3	C	903	HEM	C1D-CHD	-2.68	1.33	1.41
3	C	903	HEM	CMD-C2D	2.64	1.57	1.51
3	C	903	HEM	CMC-C2C	2.50	1.57	1.51
3	B	902	HEM	C1D-CHD	-2.38	1.34	1.41
3	A	901	HEM	C1D-ND	2.34	1.41	1.36
3	A	901	HEM	CBB-CAB	2.33	1.44	1.29
3	A	901	HEM	C1D-CHD	-2.31	1.34	1.41
3	C	903	HEM	CMB-C2B	2.20	1.56	1.51
3	A	901	HEM	CAA-C2A	-2.16	1.48	1.52
3	C	903	HEM	C4D-C3D	2.14	1.47	1.42
3	C	903	HEM	C1A-CHA	-2.01	1.35	1.41
3	C	903	HEM	C4B-NB	2.01	1.40	1.36

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	HEM	C1D-C2D-C3D	21.66	122.07	107.00
3	B	902	HEM	C4A-C3A-C2A	20.53	121.28	107.00
3	B	902	HEM	C4C-C3C-C2C	12.06	115.32	106.90
3	C	903	HEM	C1D-C2D-C3D	11.18	114.78	107.00
3	A	901	HEM	C1D-C2D-C3D	10.78	114.49	107.00
3	B	902	HEM	C3B-C4B-NB	10.53	122.82	109.21
3	B	902	HEM	CMA-C3A-C4A	-8.86	114.85	128.46
3	A	901	HEM	C4C-C3C-C2C	6.53	111.46	106.90
3	B	902	HEM	CMD-C2D-C3D	-6.43	112.81	124.94
3	A	901	HEM	CMA-C3A-C4A	-5.98	119.27	128.46
3	A	901	HEM	CMD-C2D-C1D	-5.68	119.73	128.46
3	A	901	HEM	C4A-C3A-C2A	5.60	110.89	107.00
3	C	903	HEM	C4C-C3C-C2C	5.41	110.67	106.90
3	C	903	HEM	CMD-C2D-C1D	-5.32	120.29	128.46
3	B	902	HEM	CAD-C3D-C2D	4.84	141.14	127.25
3	C	903	HEM	C4A-C3A-C2A	4.54	110.16	107.00
3	B	902	HEM	CAA-CBA-CGA	-4.44	105.22	112.67
3	C	903	HEM	CMA-C3A-C4A	-3.77	122.67	128.46
3	A	901	HEM	C3C-C4C-NC	-3.53	104.28	110.94
3	C	903	HEM	C3C-C4C-NC	-3.46	104.40	110.94
3	C	903	HEM	CBD-CAD-C3D	-3.30	106.39	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	HEM	CAD-CBD-CGD	-3.15	107.39	112.67
3	C	903	HEM	CMC-C2C-C3C	2.93	130.16	124.68
3	B	902	HEM	CBD-CAD-C3D	-2.69	107.53	112.48
3	A	901	HEM	CMA-C3A-C2A	2.56	129.77	124.94
3	B	902	HEM	C3C-C4C-NC	-2.30	106.59	110.94
3	B	902	HEM	CMB-C2B-C3B	2.25	128.88	124.68
3	B	902	HEM	CMD-C2D-C1D	-2.18	125.12	128.46
3	C	903	HEM	C3B-C4B-NB	-2.06	106.55	109.21
3	B	902	HEM	CMC-C2C-C3C	2.04	128.49	124.68

There are no chirality outliers.

All (1) torsion outliers are listed below:

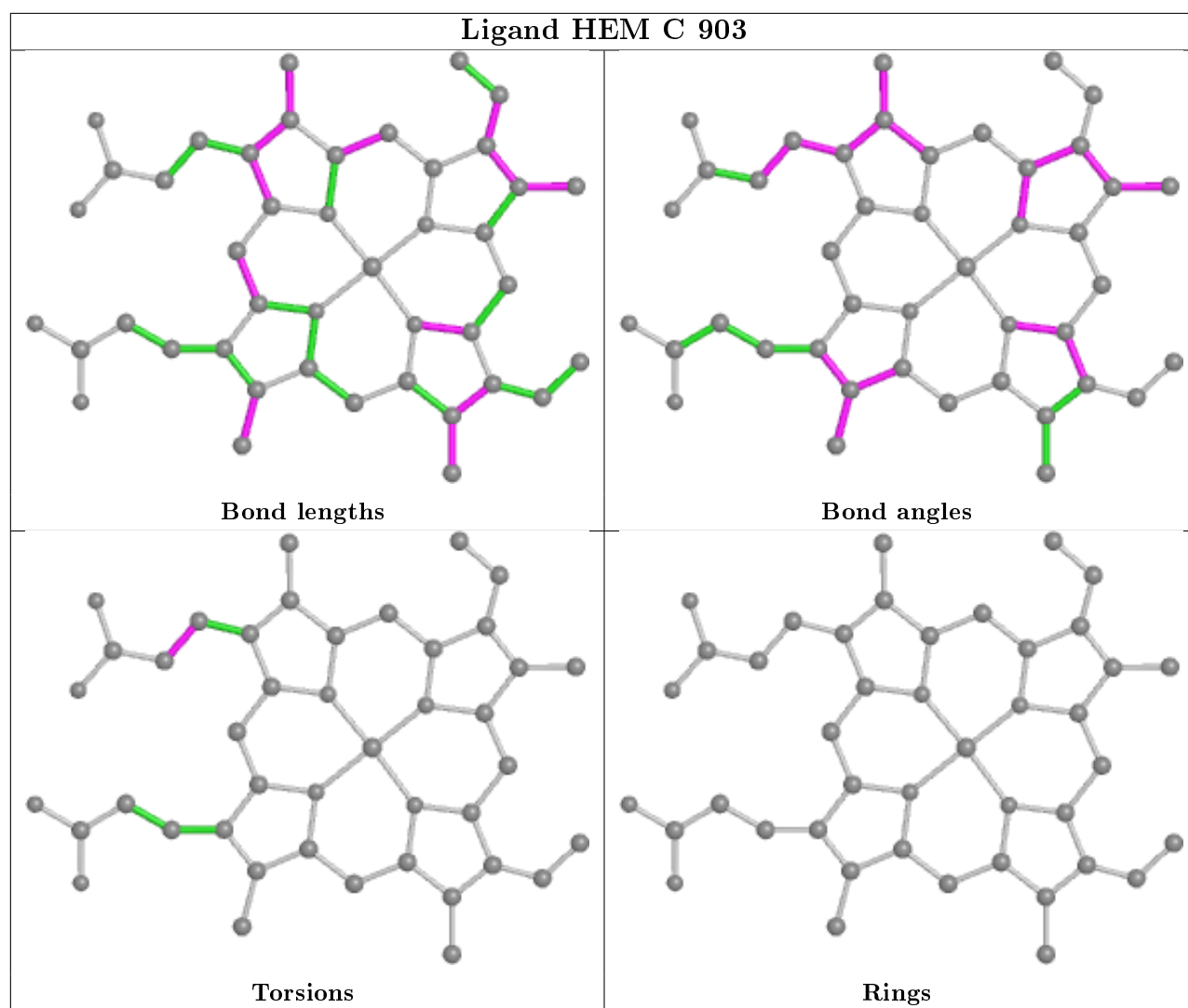
Mol	Chain	Res	Type	Atoms
3	C	903	HEM	C3D-CAD-CBD-CGD

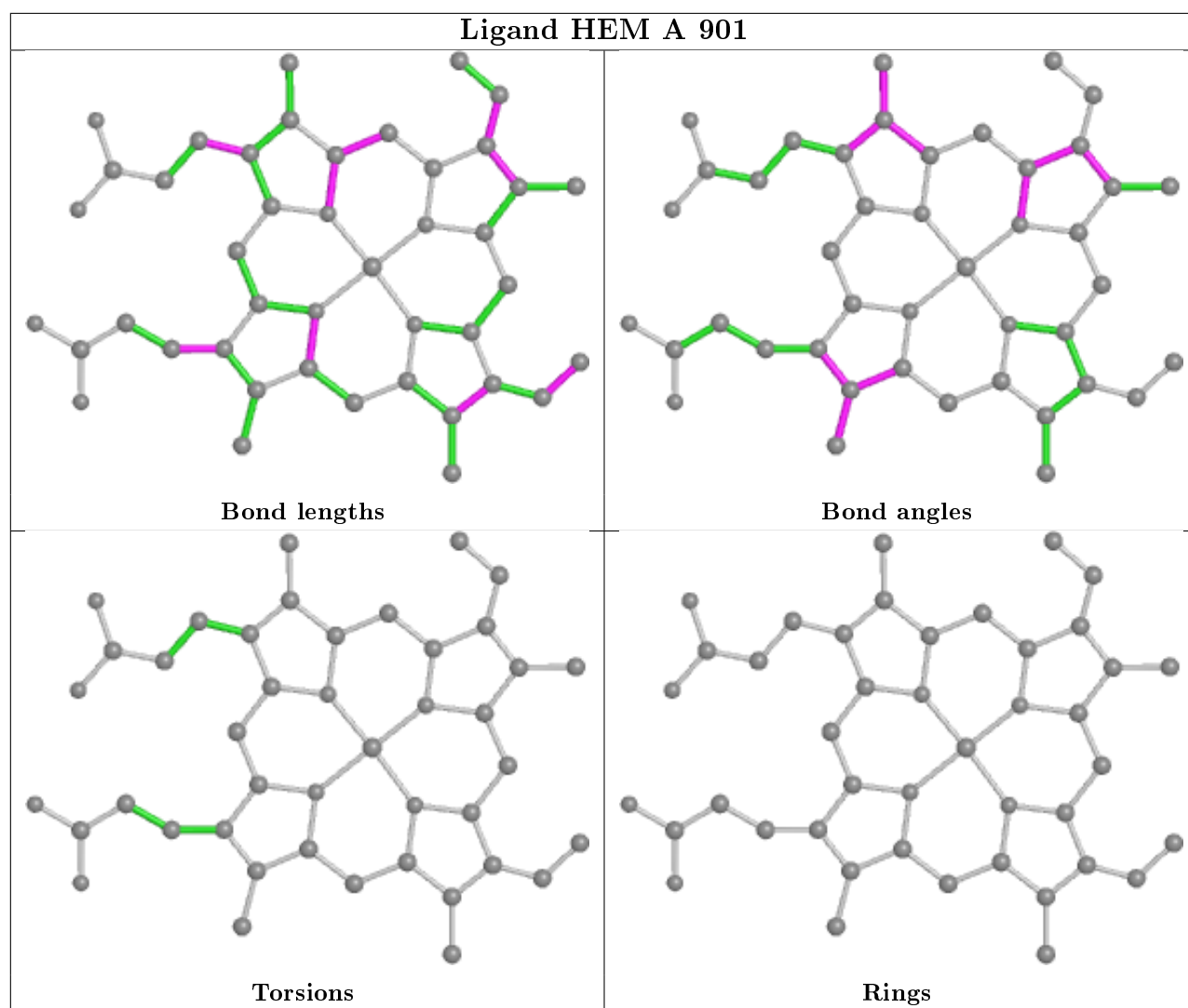
There are no ring outliers.

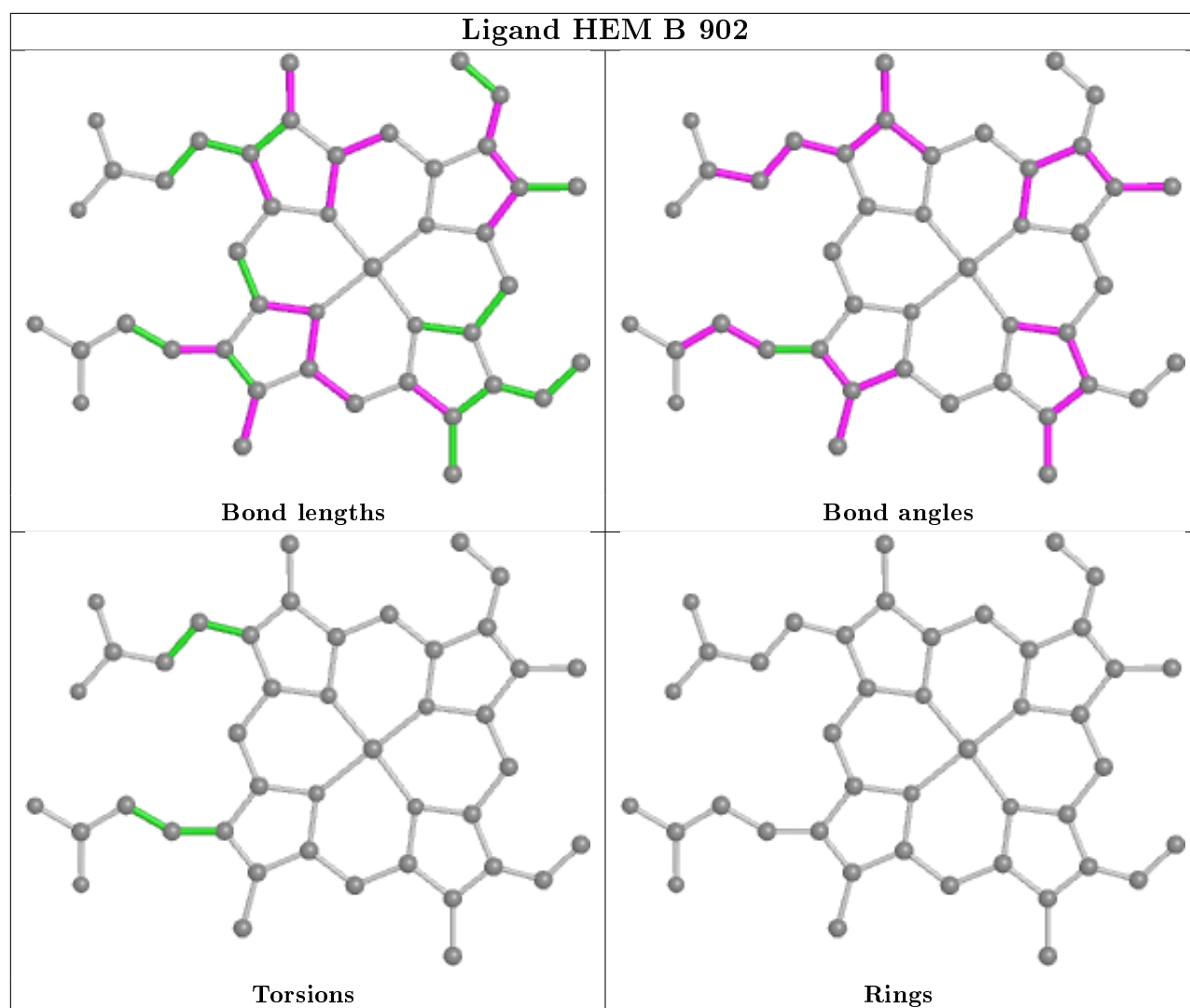
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	903	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.







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, 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	212/215 (98%)	0.50	7 (3%) 46 51	8, 13, 25, 39	1 (0%)
1	B	209/215 (97%)	0.68	11 (5%) 26 29	8, 15, 28, 32	0
1	C	208/215 (96%)	1.46	44 (21%) 0 0	11, 20, 36, 43	0
All	All	629/645 (97%)	0.88	62 (9%) 7 7	8, 16, 31, 43	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	765	GLY	7.2
1	C	771	VAL	6.7
1	A	4	ALA	6.0
1	C	767	ALA	5.9
1	A	3	THR	5.9
1	A	5	THR	5.5
1	C	606	ALA	5.0
1	C	636	ARG	4.9
1	A	2	THR	4.7
1	C	621	GLU	3.8
1	B	484	GLU	3.7
1	C	618	GLN	3.7
1	C	813	LYS	3.6
1	C	808	PHE	3.5
1	B	483	LEU	3.4
1	C	617	ALA	3.3
1	C	764	GLU	3.2
1	C	634	LYS	3.2
1	C	635	GLY	3.2
1	C	769	LEU	3.1
1	A	167	ALA	3.1
1	C	630	SER	3.1
1	B	392	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	806	GLN	3.0
1	C	620	HIS	3.0
1	C	622	LYS	3.0
1	C	772	TYR	3.0
1	C	625	HIS	3.0
1	C	626	SER	2.9
1	C	783	LEU	2.9
1	C	623	ALA	2.8
1	C	667	GLY	2.8
1	C	784	GLU	2.7
1	C	609	ALA	2.7
1	C	805	HIS	2.7
1	B	393	SER	2.7
1	C	762	HIS	2.6
1	C	614	GLN	2.6
1	C	652	PHE	2.5
1	A	92	GLY	2.5
1	C	639	VAL	2.5
1	C	766	ILE	2.5
1	C	750	HIS	2.5
1	C	627	THR	2.4
1	C	774	ASP	2.3
1	B	456	GLU	2.3
1	B	515	LEU	2.3
1	B	474	ASP	2.3
1	C	778	GLU	2.3
1	A	6	ALA	2.3
1	C	748	GLN	2.3
1	B	383	LEU	2.3
1	C	637	LEU	2.2
1	C	780	LEU	2.2
1	C	801	PHE	2.2
1	B	384	ALA	2.1
1	B	512	GLY	2.1
1	C	775	GLU	2.1
1	C	668	PHE	2.1
1	B	387	LEU	2.1
1	C	763	PHE	2.0
1	C	782	ASN	2.0

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

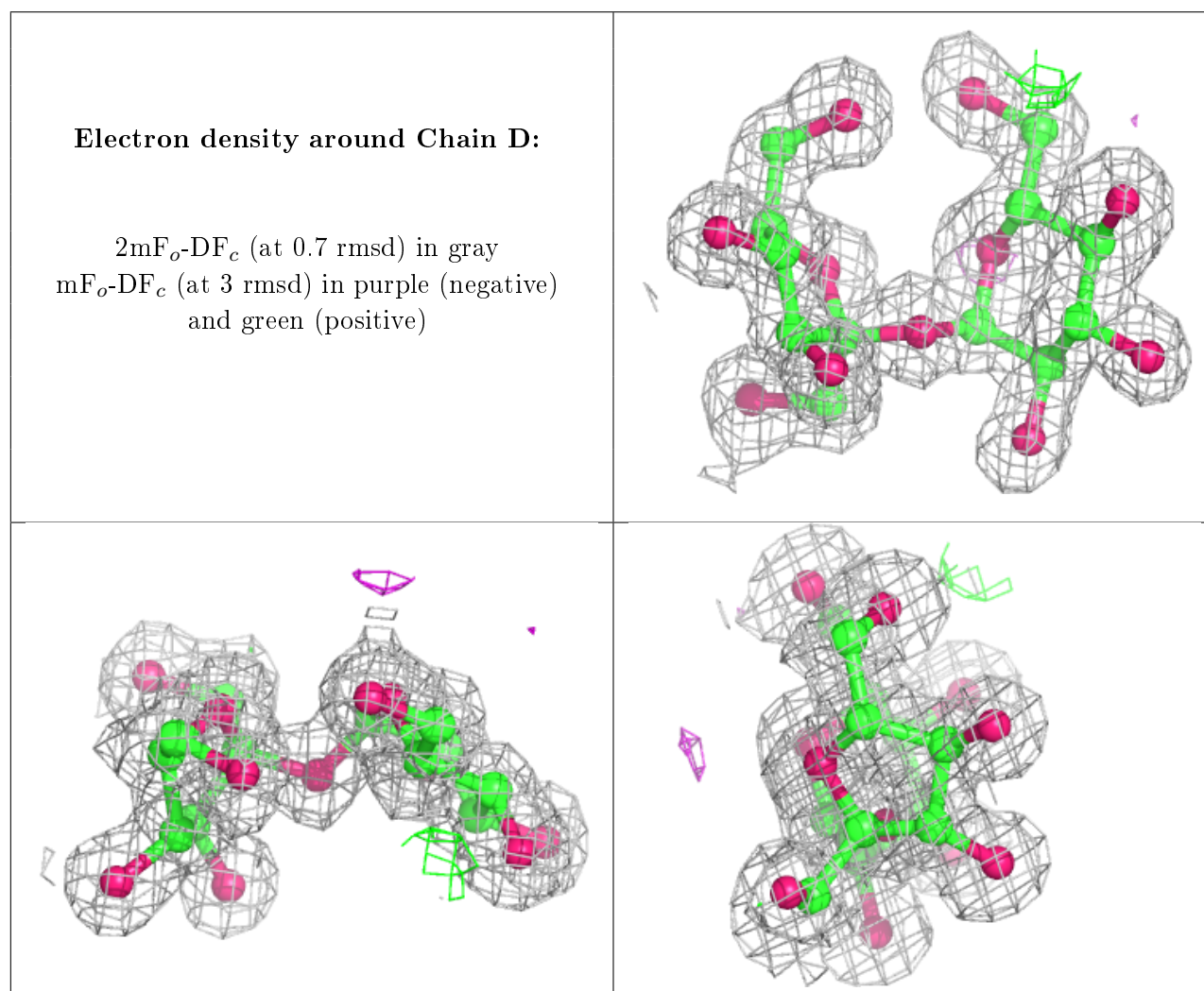
There are no non-standard protein/DNA/RNA residues in this entry.

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(\AA^2)	Q<0.9
2	FRU	D	2	12/12	0.93	0.11	9,11,12,13	11
2	GLC	D	1	11/12	0.96	0.09	10,11,13,14	7

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

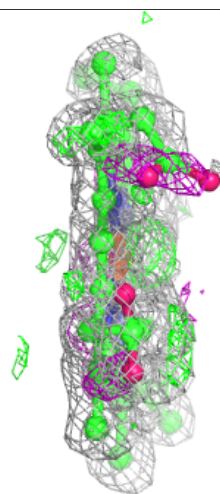
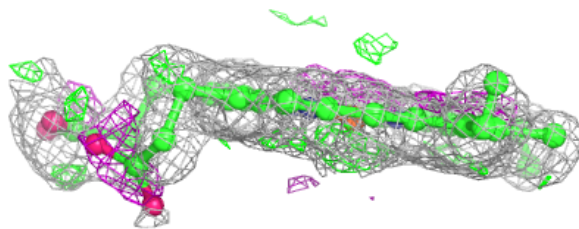
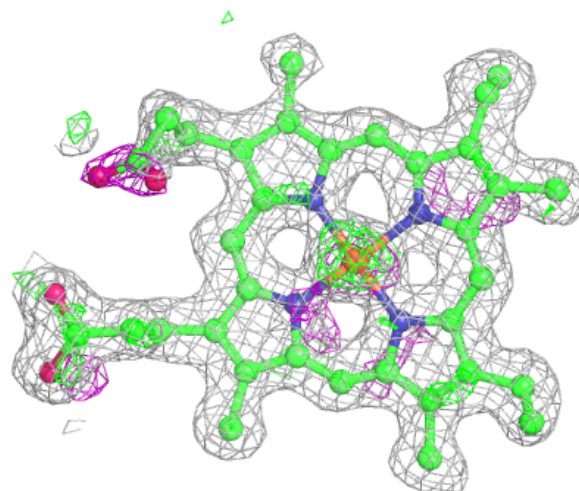
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	912	5/5	0.67	0.17	39,39,39,40	5
4	SO4	A	909	5/5	0.72	0.17	32,32,33,33	5
4	SO4	A	914	5/5	0.81	0.17	29,32,34,35	3
4	SO4	A	905	5/5	0.86	0.14	22,23,24,24	4
4	SO4	A	907	5/5	0.91	0.17	21,21,22,23	5
3	HEM	C	903	43/43	0.92	0.15	15,20,33,41	0
4	SO4	B	906	5/5	0.93	0.15	27,28,28,29	2
3	HEM	B	902	43/43	0.94	0.13	11,17,32,40	0
4	SO4	A	908	5/5	0.94	0.10	24,24,25,25	4
4	SO4	B	911	5/5	0.95	0.20	22,22,22,23	5
4	SO4	B	913	5/5	0.97	0.08	24,24,26,26	5
4	SO4	B	910	5/5	0.98	0.10	29,29,30,31	5
3	HEM	A	901	43/43	0.98	0.10	6,10,15,22	0

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

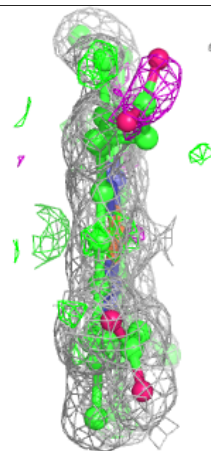
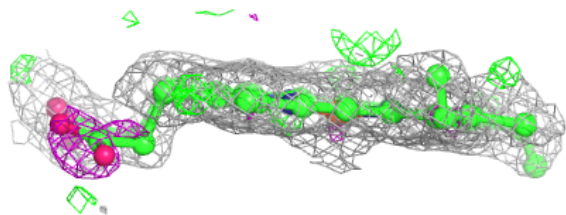
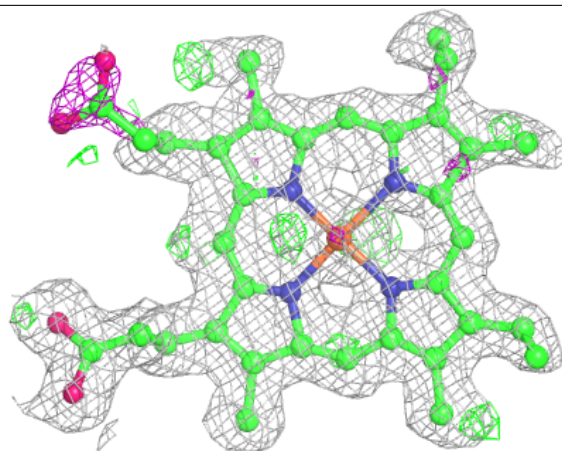
Electron density around HEM C 903:

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



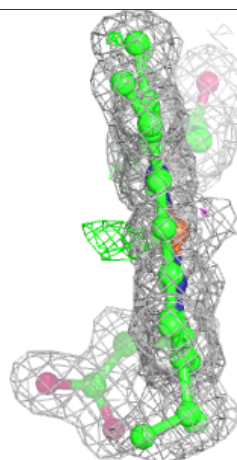
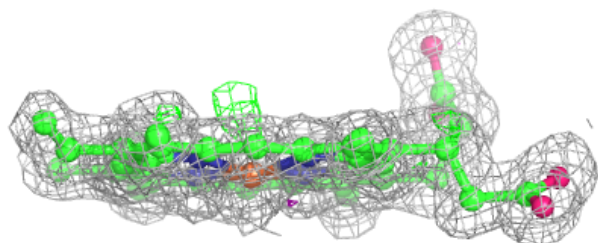
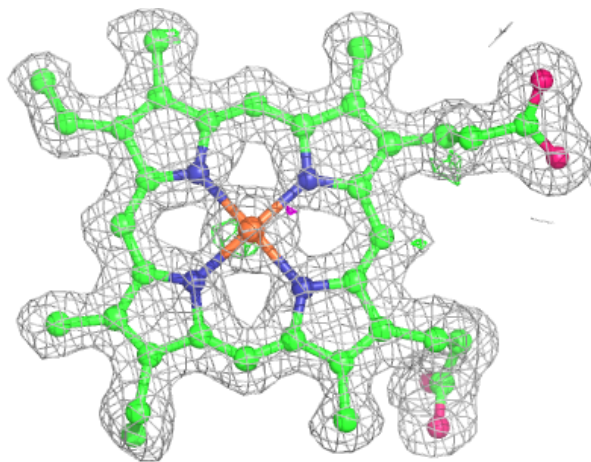
Electron density around HEM B 902:

$2mF_o-DF_c$ (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:

$2mF_o-DF_c$ (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.