



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:56 AM UTC

PDB ID : 1V8X / pdb_00001v8x
Title : Crystal Structure of the Dioxygen-bound Heme Oxygenase from *Corynebacterium diphtheriae*
Authors : Unno, M.; Matsui, T.; Chu, G.C.; Couture, M.; Yoshida, T.; Rousseau, D.L.; Olson, J.S.; Ikeda-Saito, M.
Deposited on : 2004-01-15
Resolution : 1.85 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

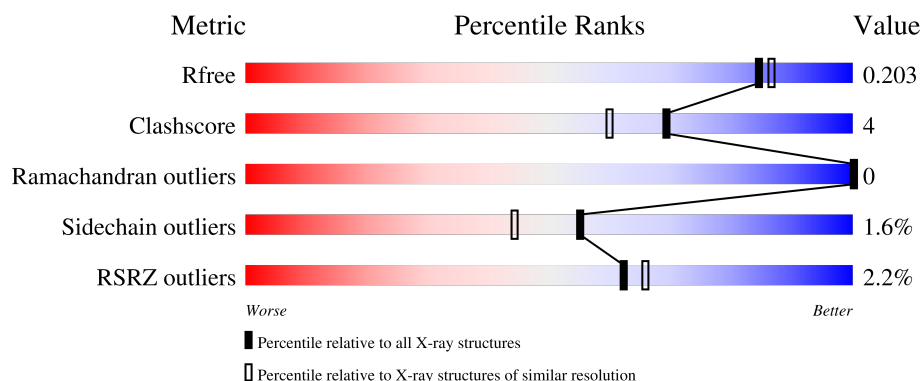
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

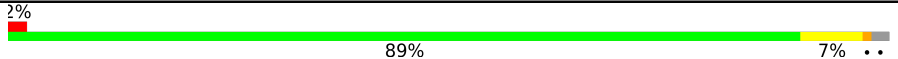
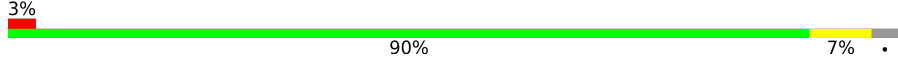
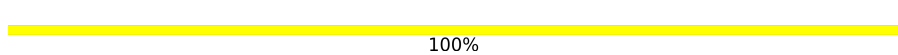
The reported resolution of this entry is 1.85 Å.

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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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 6 unique types of molecules in this entry. The entry contains 5679 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.

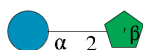
- Molecule 1 is a protein called Heme oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	1	0
			1674	1054	299	318	3			
1	B	209	Total	C	N	O	S	0	3	0
			1676	1054	298	321	3			
1	C	208	Total	C	N	O	S	0	1	0
			1662	1048	294	317	3			

There are 15 discrepancies between the modelled and reference sequences:

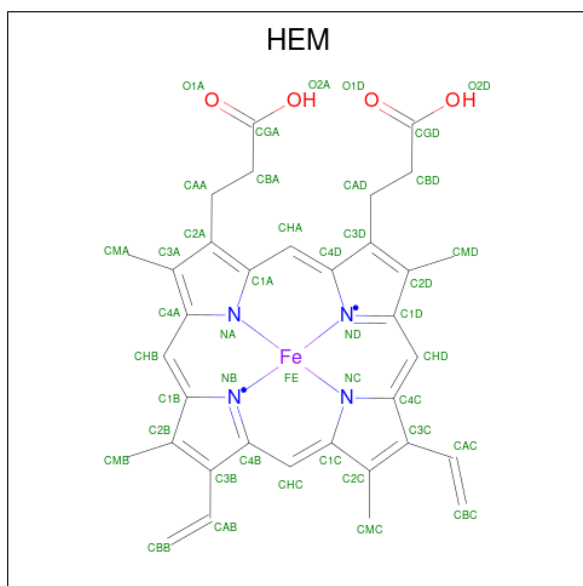
Chain	Residue	Modelled	Actual	Comment	Reference
A	34	LYS	GLU	SEE REMARK 999	UNP P71119
A	60	VAL	ALA	SEE REMARK 999	UNP P71119
A	92	GLY	ASP	SEE REMARK 999	UNP P71119
A	93	SER	GLY	SEE REMARK 999	UNP P71119
A	192	HIS	ASN	SEE REMARK 999	UNP P71119
B	334	LYS	GLU	SEE REMARK 999	UNP P71119
B	360	VAL	ALA	SEE REMARK 999	UNP P71119
B	392	GLY	ASP	SEE REMARK 999	UNP P71119
B	393	SER	GLY	SEE REMARK 999	UNP P71119
B	492	HIS	ASN	SEE REMARK 999	UNP P71119
C	634	LYS	GLU	SEE REMARK 999	UNP P71119
C	660	VAL	ALA	SEE REMARK 999	UNP P71119
C	692	GLY	ASP	SEE REMARK 999	UNP P71119
C	693	SER	GLY	SEE REMARK 999	UNP P71119
C	792	HIS	ASN	SEE REMARK 999	UNP P71119

- 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: $C_{34}H_{32}FeN_4O_4$).



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 (CCD ID: SO4) (formula: O_4S).



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	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		
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		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

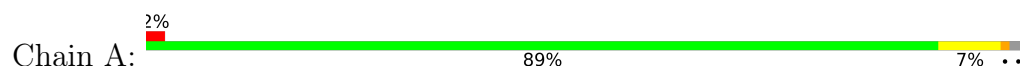
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	152	Total O 152 152	0	0
6	B	164	Total O 164 164	0	0
6	C	133	Total O 133 133	0	0

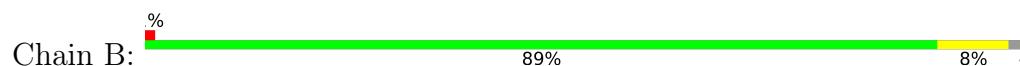
3 Residue-property plots [i](#)

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: 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	54.00Å 62.97Å 107.49Å 90.00° 100.96° 90.00°	Depositor
Resolution (Å)	40.00 – 1.85 40.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-1.85) 99.9 (40.00-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.153 , 0.193 0.166 , 0.203	Depositor DCC
R_{free} test set	6150 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.7	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	0.96	EDS
Total number of atoms	5679	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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: HEM, OXY, SO4, GLC, 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	1.14	3/1711 (0.2%)	1.04	1/2310 (0.0%)
1	B	1.18	3/1725 (0.2%)	1.10	1/2328 (0.0%)
1	C	1.12	1/1698 (0.1%)	1.07	1/2293 (0.0%)
All	All	1.15	7/5134 (0.1%)	1.07	3/6931 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	MET	SD-CE	-7.57	1.60	1.79
1	A	29	MET	SD-CE	-7.13	1.61	1.79
1	B	391	ASN	CA-C	6.56	1.61	1.52
1	A	19	ALA	CA-CB	-5.93	1.43	1.53
1	B	447	MET	SD-CE	-5.46	1.65	1.79
1	B	391	ASN	CA-CB	5.33	1.62	1.53
1	C	697	ARG	C-O	-5.03	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	740	GLY	N-CA-C	5.77	119.65	112.73
1	B	442	VAL	CB-CA-C	-5.61	104.72	112.24
1	A	169	LEU	N-CA-C	5.16	118.04	111.69

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	1674	0	1635	10	1
1	B	1676	0	1628	11	1
1	C	1662	0	1618	12	0
2	D	23	0	21	0	0
3	A	43	0	30	3	0
3	B	43	0	30	0	0
3	C	43	0	30	0	0
4	A	15	0	0	1	0
4	B	20	0	0	0	0
4	C	25	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
6	A	152	0	0	2	0
6	B	164	0	0	5	0
6	C	133	0	0	4	0
All	All	5679	0	4992	36	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 4.

All (36) 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)
4:A:2003:SO4:O3	6:A:5149:HOH:O	1.97	0.81
3:A:901:HEM:HBC2	3:A:901:HEM:HHD	1.67	0.77
1:A:168:LYS:HD2	1:A:168:LYS:H	1.61	0.63
1:B:307:GLY:N	6:B:5163:HOH:O	2.31	0.63
1:A:118:ASP:OD2	1:B:445[A]:ARG:NH2	2.32	0.61
1:B:358:GLN:NE2	6:B:5141:HOH:O	2.35	0.58
1:C:767:ALA:HA	6:C:272:HOH:O	2.02	0.58
1:C:695:GLU:HG3	6:C:438:HOH:O	2.04	0.57
1:C:646:GLN:HE21	1:C:646:GLN:HA	1.70	0.57
1:C:646:GLN:HA	1:C:646:GLN:NE2	2.20	0.55
1:B:448:GLN:HG2	1:B:453:VAL:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:LYS:CE	6:B:5080:HOH:O	2.56	0.54
1:B:510:ASP:HA	1:B:513:LYS:HE2	1.90	0.54
1:C:812:GLY:O	1:C:813:LYS:HB2	2.10	0.52
1:A:34:LYS:HG3	1:A:36:ARG:HG3	1.92	0.50
1:B:389:LYS:HE2	6:B:5080:HOH:O	2.11	0.50
1:C:689:LYS:HD2	1:C:756:GLU:O	2.14	0.48
1:B:389:LYS:HE3	6:B:5080:HOH:O	2.14	0.47
1:A:155:PRO:O	1:A:162:HIS:HE1	1.99	0.46
1:A:11:GLU:O	1:A:15:SER:HB2	2.16	0.45
1:A:168:LYS:H	1:A:168:LYS:CD	2.21	0.44
1:B:346:GLN:NE2	1:B:346:GLN:HA	2.33	0.44
1:A:146:MET:HA	1:A:146:MET:HE2	1.99	0.44
1:A:178:GLU:HG3	6:A:5142:HOH:O	2.17	0.44
1:B:505:HIS:O	1:B:505:HIS:HD2	2.01	0.43
1:C:689:LYS:HE3	6:C:362:HOH:O	2.18	0.43
1:A:46:GLN:NE2	1:A:46:GLN:HA	2.32	0.43
1:C:778[B]:GLU:HG3	1:C:782:ASN:ND2	2.34	0.42
1:C:689:LYS:CE	6:C:362:HOH:O	2.67	0.42
3:A:901:HEM:HBC2	3:A:901:HEM:CHD	2.37	0.42
1:A:112[B]:ARG:NH1	1:A:199:ASP:OD2	2.50	0.42
1:B:389:LYS:HD2	1:B:456:GLU:O	2.20	0.42
1:C:812:GLY:O	1:C:813:LYS:CB	2.68	0.42
1:C:725:LEU:C	1:C:725:LEU:HD13	2.44	0.41
1:C:646:GLN:HE21	1:C:646:GLN:CA	2.33	0.41
3:A:901:HEM:CMB	3:A:901:HEM:HBB2	2.51	0.41

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:A:167:ALA:O	1:B:449:ARG:NH2[2_645]	2.18	0.02

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	209/215 (97%)	203 (97%)	6 (3%)	0	100	100
1	B	210/215 (98%)	206 (98%)	4 (2%)	0	100	100
1	C	207/215 (96%)	203 (98%)	4 (2%)	0	100	100
All	All	626/645 (97%)	612 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	172/175 (98%)	170 (99%)	2 (1%)	63	55
1	B	174/175 (99%)	171 (98%)	3 (2%)	53	42
1	C	171/175 (98%)	168 (98%)	3 (2%)	51	40
All	All	517/525 (98%)	509 (98%)	8 (2%)	55	47

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	168	LYS
1	B	395	GLU
1	B	464	GLU
1	B	498	THR
1	C	769	LEU
1	C	784	GLU
1	C	798	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	B	346	GLN
1	B	358	GLN
1	C	646	GLN
1	C	762	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	1.03	0	15,15,17	1.37	3 (20%)
2	FRU	D	2	2	11,12,12	1.19	1 (9%)	10,18,18	1.44	1 (10%)

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	-	1/5/24/24	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	3.57	1.46	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	FRU	O1-C1-C2	-3.96	102.92	111.67
2	D	1	GLC	O3-C3-C2	3.45	117.10	110.05
2	D	1	GLC	C2-C3-C4	-2.54	106.40	110.86
2	D	1	GLC	O4-C4-C3	-2.15	105.31	110.38

There are no chirality outliers.

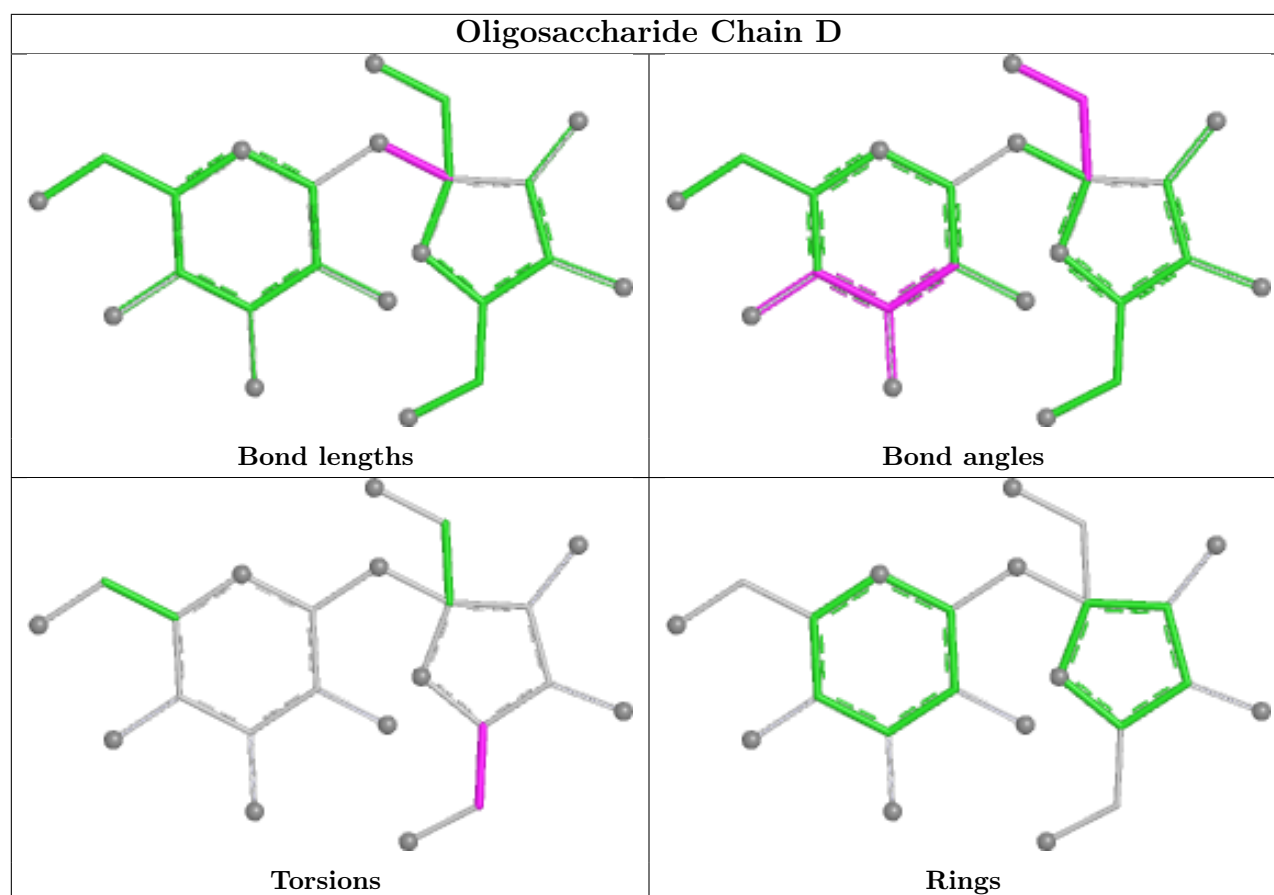
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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](#)

18 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	A	2007	-	4,4,4	0.19	0	6,6,6	0.39	0
4	SO4	B	2008	-	4,4,4	0.31	0	6,6,6	0.49	0
4	SO4	B	2001	-	4,4,4	0.40	0	6,6,6	0.58	0
5	OXY	B	5002	3	1,1,1	0.16	0	-		
4	SO4	A	2003	-	4,4,4	0.47	0	6,6,6	0.65	0
3	HEM	B	902	5,1	50,50,50	1.74	9 (18%)	67,82,82	1.96	17 (25%)
3	HEM	A	901	5,1	50,50,50	1.65	7 (14%)	67,82,82	1.61	15 (22%)
4	SO4	B	2009	-	4,4,4	0.32	0	6,6,6	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OXY	A	5001	3	1,1,1	0.06	0	-		
5	OXY	C	5003	3	1,1,1	0.26	0	-		
4	SO4	C	2002	-	4,4,4	0.37	0	6,6,6	0.34	0
3	HEM	C	903	5,1	50,50,50	1.81	8 (16%)	67,82,82	1.79	18 (26%)
4	SO4	B	2006	-	4,4,4	0.68	0	6,6,6	0.48	0
4	SO4	C	2005	-	4,4,4	0.35	0	6,6,6	0.62	0
4	SO4	C	2004	-	4,4,4	0.25	0	6,6,6	0.24	0
4	SO4	C	2012	-	4,4,4	0.29	0	6,6,6	0.30	0
4	SO4	C	2010	-	4,4,4	0.30	0	6,6,6	0.26	0
4	SO4	A	2011	-	4,4,4	0.21	0	6,6,6	0.85	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	B	902	5,1	-	5/14/54/54	-
3	HEM	A	901	5,1	-	2/14/54/54	-
3	HEM	C	903	5,1	-	6/14/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	903	HEM	C3D-C2D	6.96	1.51	1.36
3	A	901	HEM	C3D-C2D	6.78	1.51	1.36
3	B	902	HEM	C3D-C2D	6.49	1.50	1.36
3	B	902	HEM	FE-NC	5.33	2.12	1.95
3	C	903	HEM	FE-NC	5.04	2.11	1.95
3	A	901	HEM	FE-NB	3.84	2.06	1.94
3	C	903	HEM	FE-NB	3.41	2.05	1.94
3	A	901	HEM	FE-NC	3.21	2.05	1.95
3	B	902	HEM	FE-NA	3.10	2.05	1.95
3	C	903	HEM	FE-ND	3.05	2.04	1.94
3	C	903	HEM	CAB-C3B	2.88	1.55	1.47
3	A	901	HEM	FE-ND	2.72	2.03	1.94
3	C	903	HEM	FE-NA	2.70	2.04	1.95
3	C	903	HEM	CMC-C2C	2.67	1.56	1.50
3	A	901	HEM	FE-NA	2.52	2.03	1.95
3	C	903	HEM	C3B-C2B	-2.46	1.32	1.37
3	B	902	HEM	CAC-C3C	2.31	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	902	HEM	FE-NB	2.31	2.02	1.94
3	B	902	HEM	C3C-C2C	-2.27	1.32	1.37
3	B	902	HEM	C1B-NB	-2.23	1.36	1.40
3	B	902	HEM	CMD-C2D	2.22	1.55	1.50
3	B	902	HEM	CAB-C3B	2.13	1.53	1.47
3	A	901	HEM	C3C-C2C	-2.11	1.32	1.37
3	A	901	HEM	C4B-NB	-2.11	1.34	1.38

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	903	HEM	C4D-ND-C1D	5.98	112.29	105.21
3	B	902	HEM	C4D-ND-C1D	5.82	112.11	105.21
3	C	903	HEM	CHD-C1D-ND	5.57	130.42	124.42
3	B	902	HEM	CHD-C1D-ND	5.25	130.07	124.42
3	B	902	HEM	CHC-C4B-NB	4.61	129.38	124.42
3	A	901	HEM	C4C-C3C-C2C	3.94	110.23	106.81
3	B	902	HEM	C3B-C4B-NB	-3.67	106.83	109.47
3	A	901	HEM	CHA-C4D-ND	3.48	128.67	124.37
3	A	901	HEM	C4D-ND-C1D	3.45	109.29	105.21
3	B	902	HEM	C1B-NB-C4B	3.44	109.28	105.21
3	B	902	HEM	CHD-C4C-C3C	3.38	130.91	125.21
3	B	902	HEM	CHD-C4C-NC	-3.38	120.78	124.45
3	C	903	HEM	C3B-C2B-C1B	3.37	108.94	106.41
3	C	903	HEM	CBD-CAD-C3D	-3.18	103.74	112.53
3	A	901	HEM	C1B-NB-C4B	3.17	108.96	105.21
3	B	902	HEM	CHA-C4D-ND	3.14	128.25	124.37
3	C	903	HEM	CHB-C4A-NA	3.11	129.50	123.86
3	B	902	HEM	C3B-C2B-C1B	3.10	108.74	106.41
3	A	901	HEM	C4A-C3A-C2A	3.02	110.27	106.82
3	C	903	HEM	C2D-C1D-ND	-2.82	106.64	109.90
3	C	903	HEM	CHC-C4B-NB	2.81	127.44	124.42
3	B	902	HEM	CAA-CBA-CGA	-2.80	106.24	113.67
3	C	903	HEM	C3B-C4B-NB	-2.70	107.53	109.47
3	C	903	HEM	C4C-C3C-C2C	2.66	109.12	106.81
3	A	901	HEM	CMD-C2D-C1D	2.53	128.99	125.03
3	A	901	HEM	CHA-C4D-C3D	-2.53	120.57	125.23
3	A	901	HEM	CMC-C2C-C3C	-2.51	122.36	128.43
3	C	903	HEM	C1B-NB-C4B	2.47	108.13	105.21
3	A	901	HEM	CAD-C3D-C4D	2.45	128.97	124.70
3	C	903	HEM	C2A-C1A-NA	-2.43	107.46	110.15
3	B	902	HEM	CAD-C3D-C4D	2.42	128.91	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	902	HEM	C2B-C1B-NB	-2.41	107.07	109.84
3	C	903	HEM	CHA-C4D-ND	2.39	127.33	124.37
3	A	901	HEM	C3C-C2C-C1C	-2.37	104.81	107.05
3	C	903	HEM	CBC-CAC-C3C	-2.36	115.76	127.53
3	B	902	HEM	CMA-C3A-C4A	-2.30	121.92	125.42
3	A	901	HEM	C4D-C3D-C2D	-2.27	103.58	106.89
3	B	902	HEM	CBD-CAD-C3D	-2.26	106.27	112.53
3	C	903	HEM	C2B-C1B-NB	-2.26	107.24	109.84
3	A	901	HEM	CHC-C4B-NB	2.26	126.85	124.42
3	C	903	HEM	C3A-C4A-NA	-2.23	106.56	110.14
3	B	902	HEM	CBC-CAC-C3C	-2.19	116.57	127.53
3	A	901	HEM	O2D-CGD-CBD	2.16	120.82	114.00
3	A	901	HEM	CAC-C3C-C2C	-2.14	121.47	128.43
3	C	903	HEM	CAA-CBA-CGA	-2.12	108.03	113.67
3	B	902	HEM	CHD-C1D-C2D	-2.09	121.73	125.03
3	C	903	HEM	O1D-CGD-CBD	-2.07	116.52	123.09
3	A	901	HEM	CMA-C3A-C4A	-2.06	122.29	125.42
3	B	902	HEM	CHB-C1B-NB	2.05	126.91	124.37
3	C	903	HEM	CHD-C4C-C3C	2.04	128.64	125.21

There are no chirality outliers.

All (13) torsion outliers are listed below:

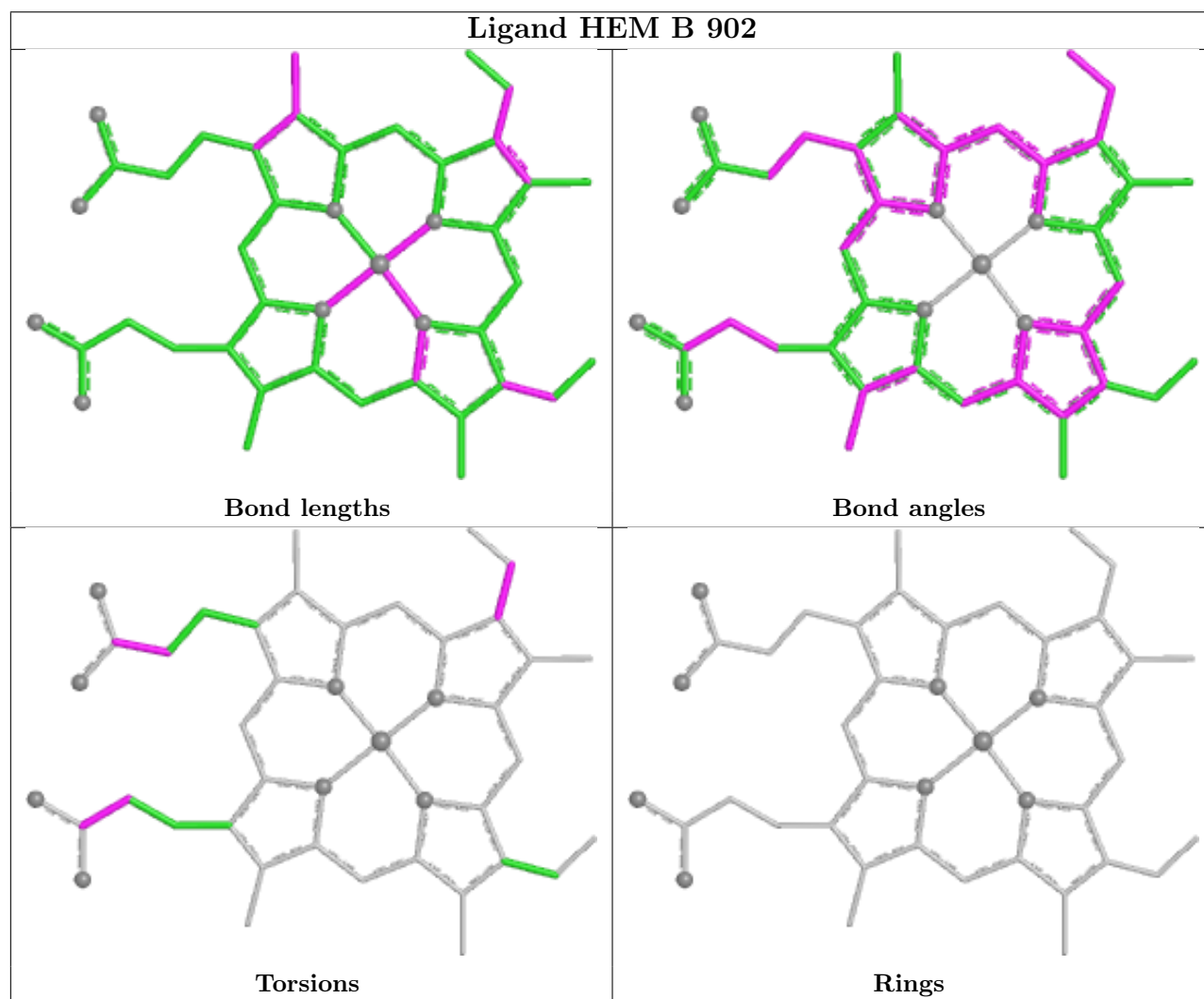
Mol	Chain	Res	Type	Atoms
3	B	902	HEM	C2C-C3C-CAC-CBC
3	C	903	HEM	C2C-C3C-CAC-CBC
3	B	902	HEM	CAD-CBD-CGD-O2D
3	C	903	HEM	C4C-C3C-CAC-CBC
3	B	902	HEM	CAD-CBD-CGD-O1D
3	A	901	HEM	CAA-CBA-CGA-O2A
3	B	902	HEM	CAA-CBA-CGA-O1A
3	A	901	HEM	CAA-CBA-CGA-O1A
3	B	902	HEM	CAA-CBA-CGA-O2A
3	C	903	HEM	CAA-CBA-CGA-O1A
3	C	903	HEM	CAA-CBA-CGA-O2A
3	C	903	HEM	C2B-C3B-CAB-CBB
3	C	903	HEM	C4B-C3B-CAB-CBB

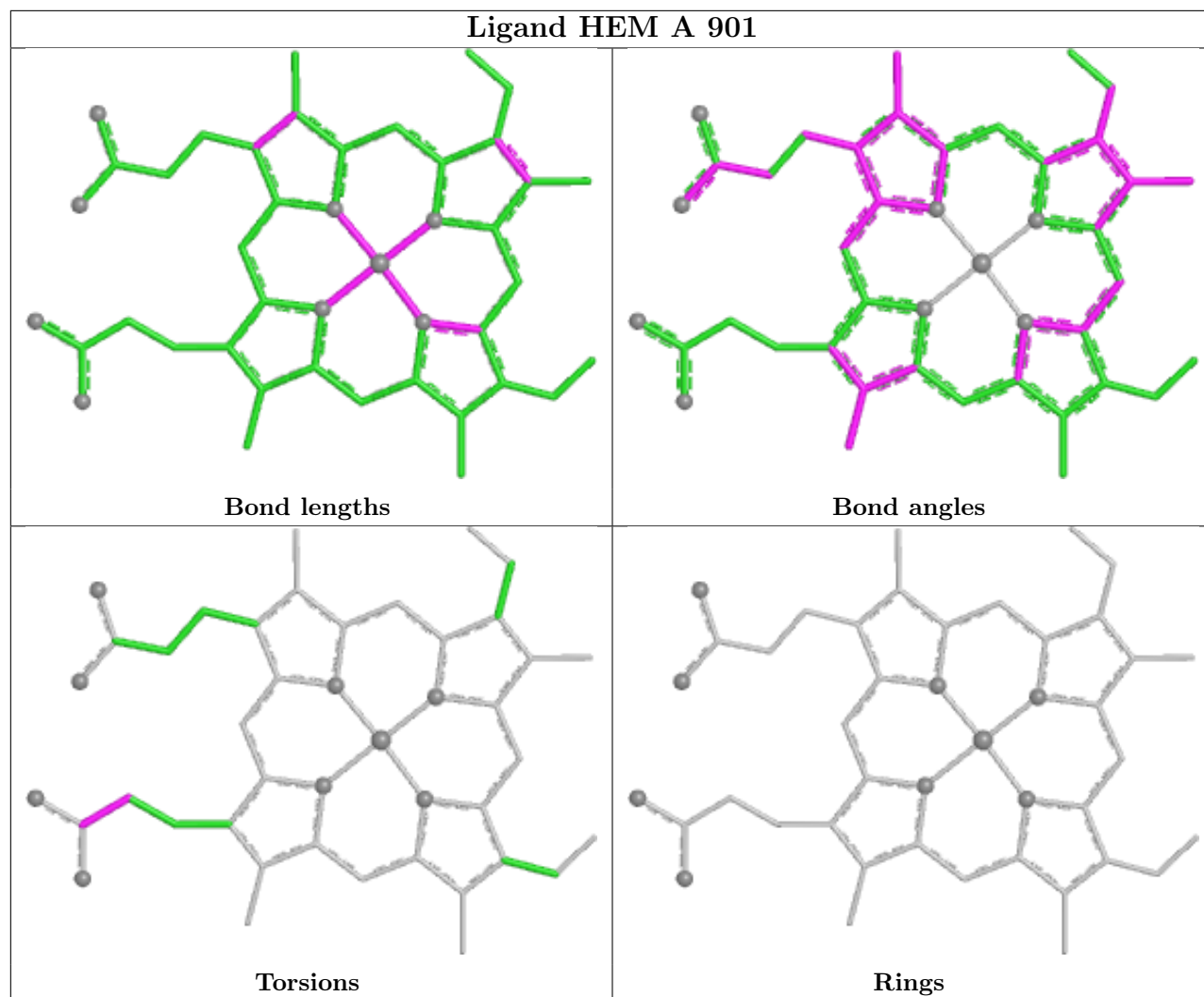
There are no ring outliers.

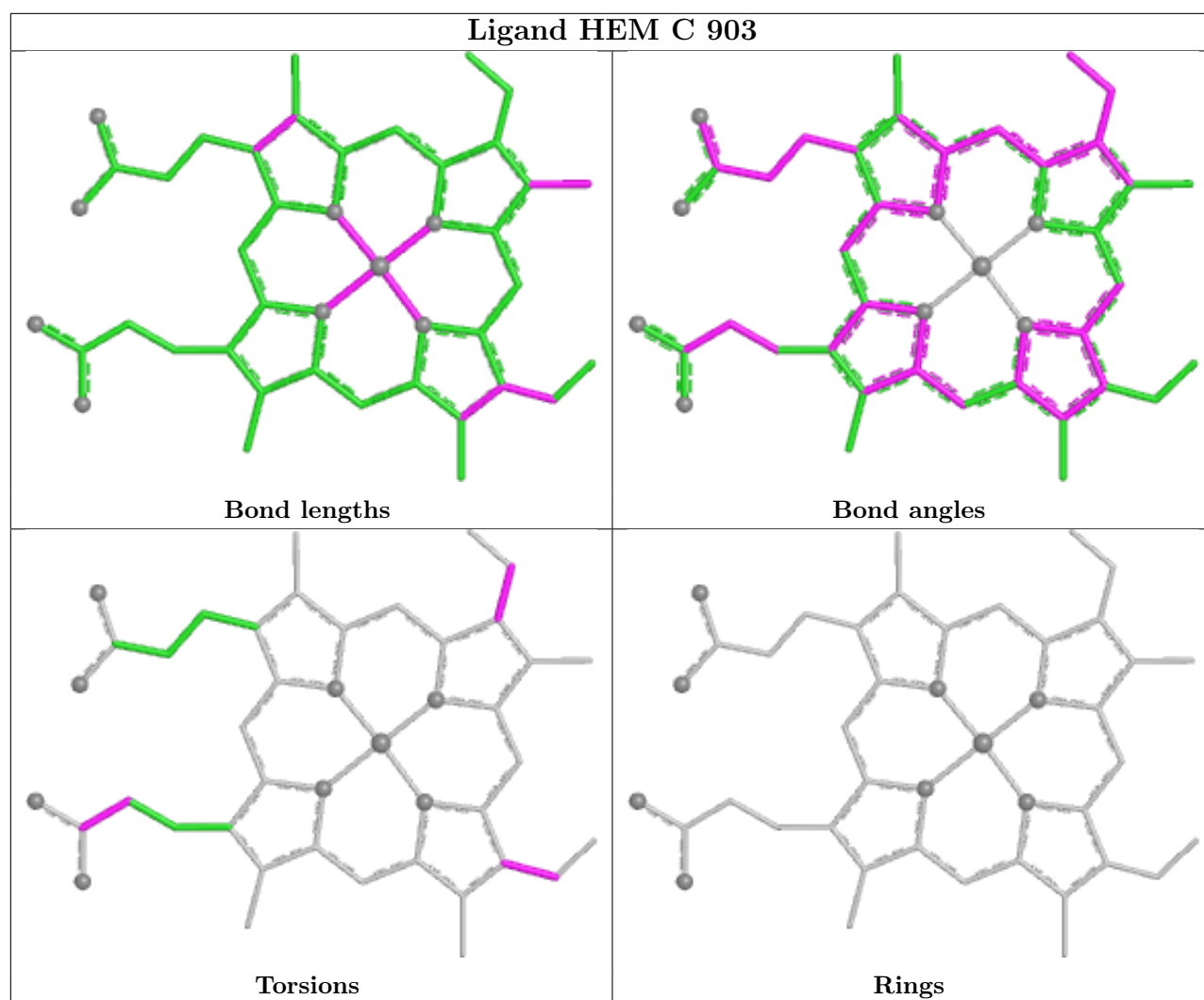
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2003	SO4	1	0
3	A	901	HEM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	210/215 (97%)	-0.15	5 (2%) 59 63	11, 20, 35, 48	1 (0%)
1	B	209/215 (97%)	-0.14	2 (0%) 79 83	10, 19, 35, 40	4 (1%)
1	C	208/215 (96%)	0.03	7 (3%) 48 52	12, 22, 40, 49	1 (0%)
All	All	627/645 (97%)	-0.09	14 (2%) 62 66	10, 20, 36, 49	6 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	767	ALA	5.1
1	C	606	ALA	5.0
1	A	214	GLY	3.3
1	A	21	GLU	3.0
1	C	765	GLY	2.9
1	B	392	GLY	2.6
1	A	167	ALA	2.5
1	C	762	HIS	2.5
1	B	399	ARG	2.3
1	C	699	ARG	2.3
1	C	813	LYS	2.3
1	A	188	GLU	2.2
1	A	169	LEU	2.2
1	C	805	HIS	2.0

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

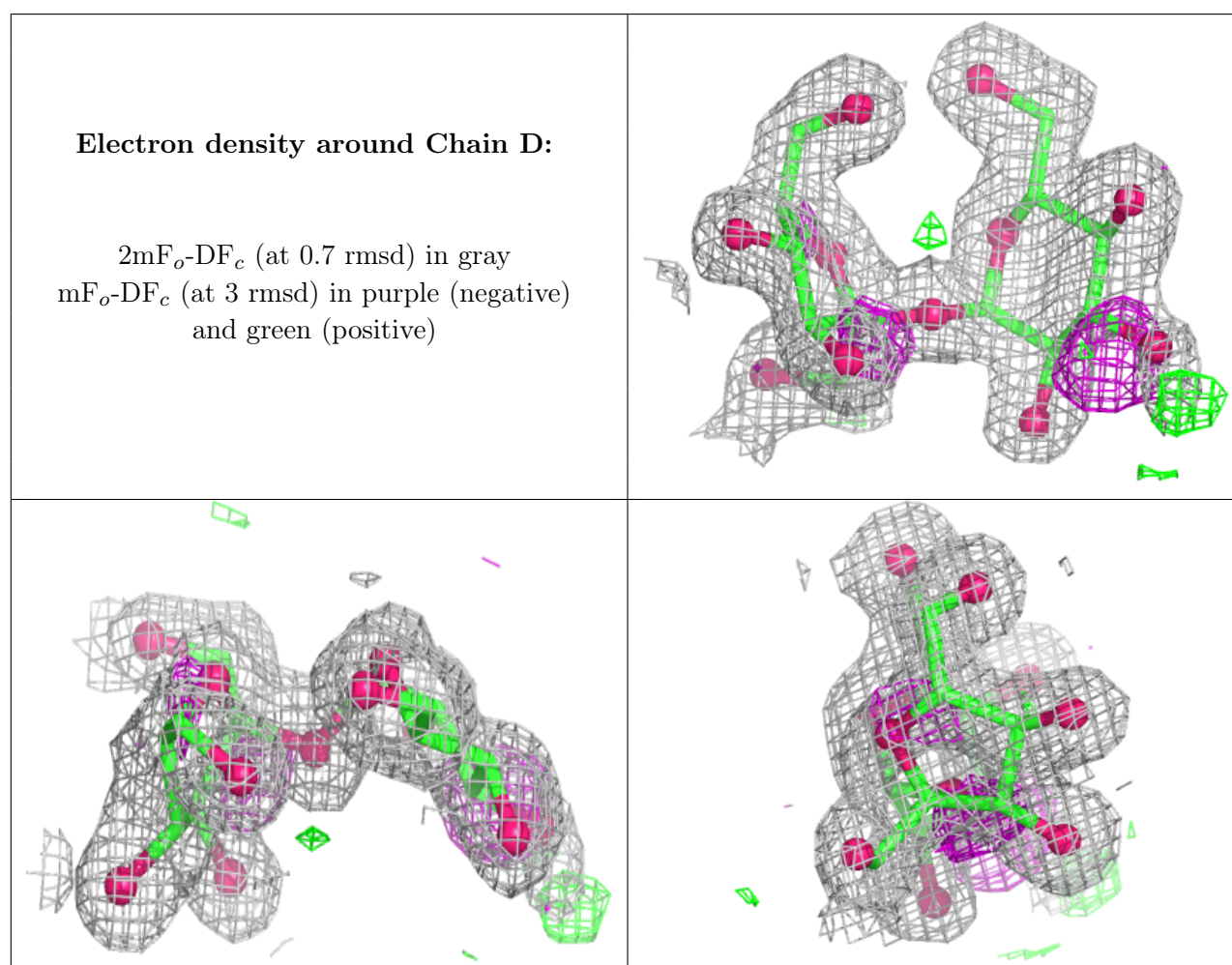
There are no non-standard protein/DNA/RNA residues in this entry.

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($\text{\AA}^2$)	Q<0.9
2	GLC	D	1	11/12	0.90	0.10	21,26,31,35	0
2	FRU	D	2	12/12	0.91	0.09	24,27,30,30	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,

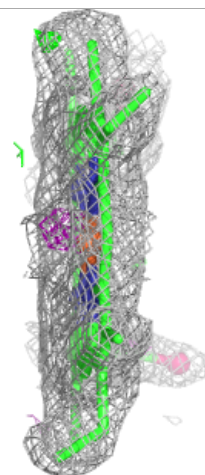
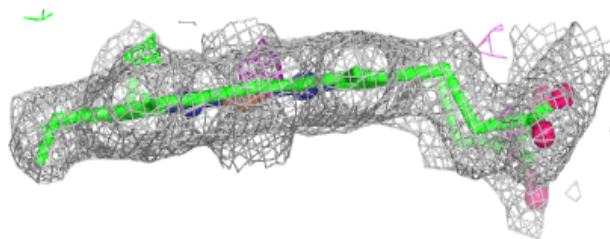
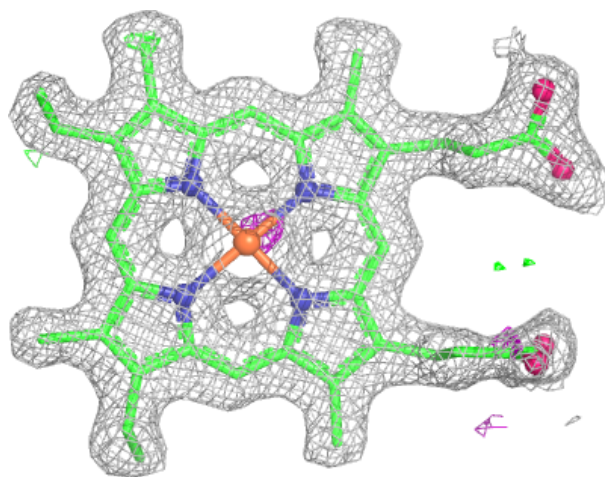
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	C	2010	5/5	0.47	0.22	92,93,94,94	0
4	SO4	C	2012	5/5	0.66	0.19	80,81,82,83	0
4	SO4	A	2003	5/5	0.71	0.17	55,56,59,60	0
4	SO4	A	2011	5/5	0.74	0.20	68,71,72,73	0
4	SO4	C	2004	5/5	0.74	0.13	74,75,76,76	0
4	SO4	C	2005	5/5	0.79	0.14	45,51,52,53	0
4	SO4	B	2009	5/5	0.83	0.12	52,52,53,56	0
4	SO4	B	2008	5/5	0.85	0.13	56,58,60,61	0
4	SO4	C	2002	5/5	0.85	0.12	45,45,50,50	0
4	SO4	B	2006	5/5	0.88	0.20	28,34,44,45	0
4	SO4	A	2007	5/5	0.89	0.11	52,53,57,58	0
4	SO4	B	2001	5/5	0.91	0.13	39,39,42,43	0
5	OXY	A	5001	2/2	0.96	0.17	31,31,31,31	0
5	OXY	B	5002	2/2	0.97	0.20	26,26,26,32	0
5	OXY	C	5003	2/2	0.97	0.17	33,33,33,33	0
3	HEM	C	903	43/43	0.98	0.07	17,22,36,48	0
3	HEM	B	902	43/43	0.98	0.07	15,22,43,57	0
3	HEM	A	901	43/43	0.99	0.06	10,16,23,31	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.

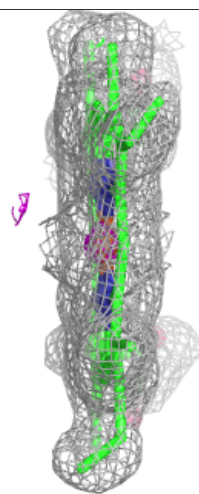
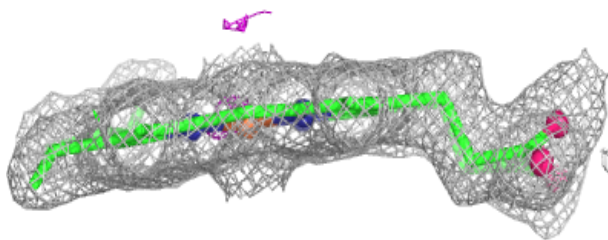
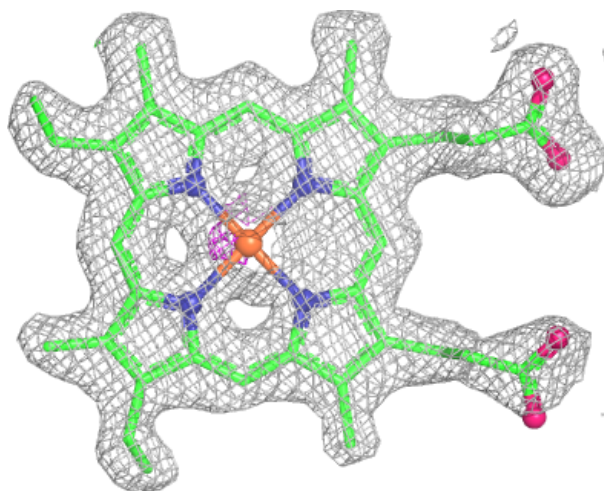
Electron density around HEM C 903:

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



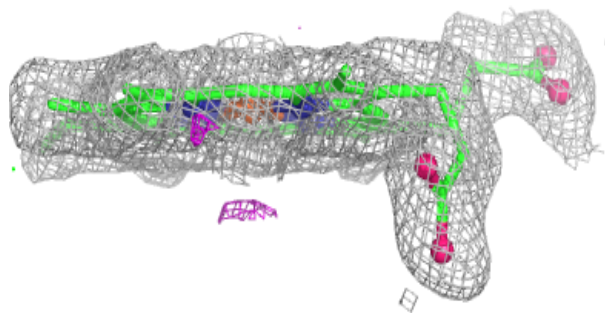
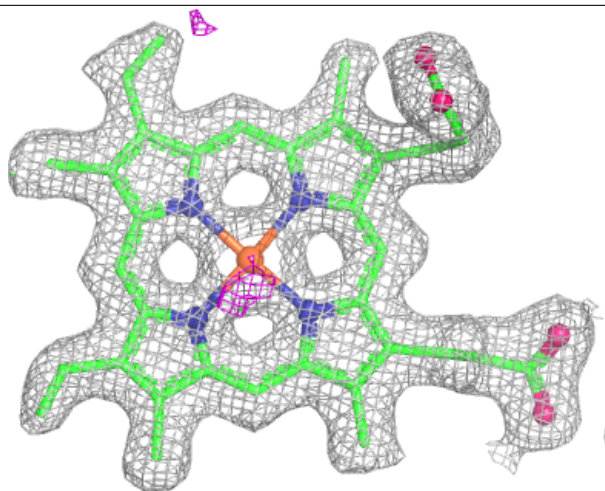
Electron density around HEM B 902:

$2mF_o-DF_c$ (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.