



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 02:53 AM BST

PDB ID : 3I8R
Title : Crystal structure of the heme oxygenase from *Corynebacterium diphtheriae* (HmuO) in complex with heme binding dithiothreitol (DTT)
Authors : Matsui, T.; Unno, M.; Ikeda-Saito, M.
Deposited on : 2009-07-10
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

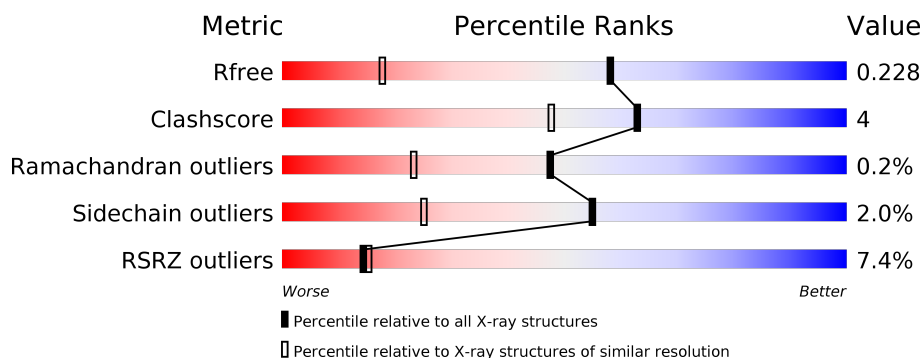
1 Overall quality at a glance

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>10%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>.</div> </div> </div>
1	B	215	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>.</div> </div> </div>
1	C	215	<div> <div>10%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

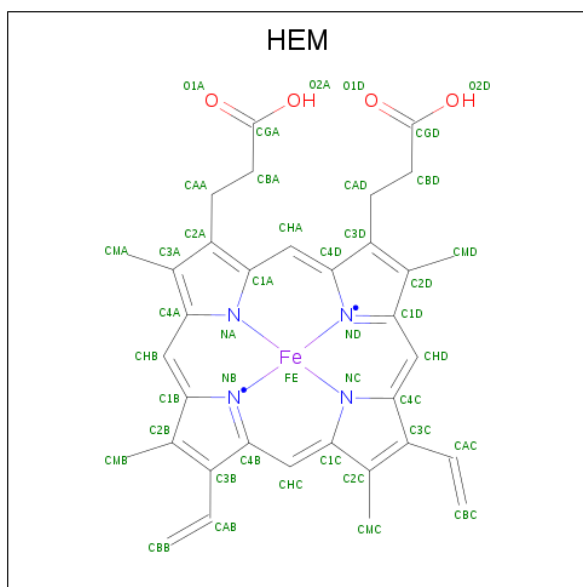
There are 5 unique types of molecules in this entry. The entry contains 5643 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

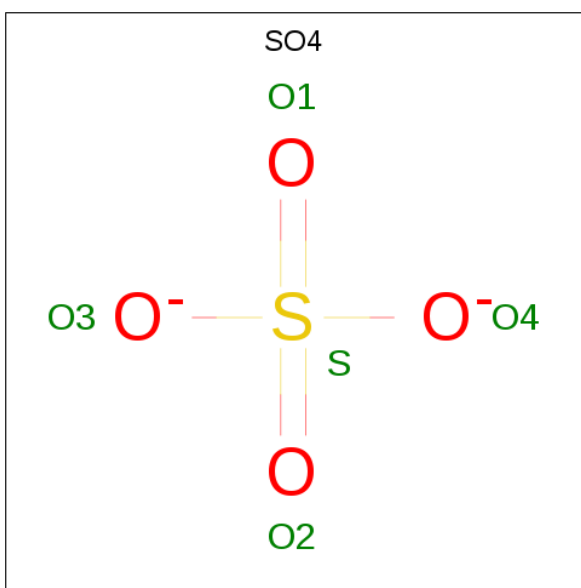
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	1	0
			1656	1043	296	314	3			
1	B	209	Total	C	N	O	S	0	0	0
			1665	1050	295	317	3			
1	C	207	Total	C	N	O	S	0	0	0
			1640	1034	290	313	3			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



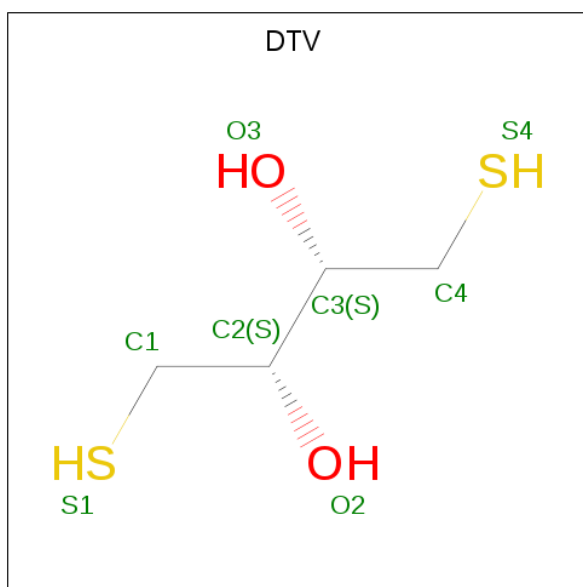
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is (2S,3S)-1,4-DIMERCAPTOBUTANE-2,3-DIOL (three-letter code: DTV) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		
4	B	1	Total	C	O	S	0	0
			8	4	2	2		
4	C	1	Total	C	O	S	0	0
			8	4	2	2		

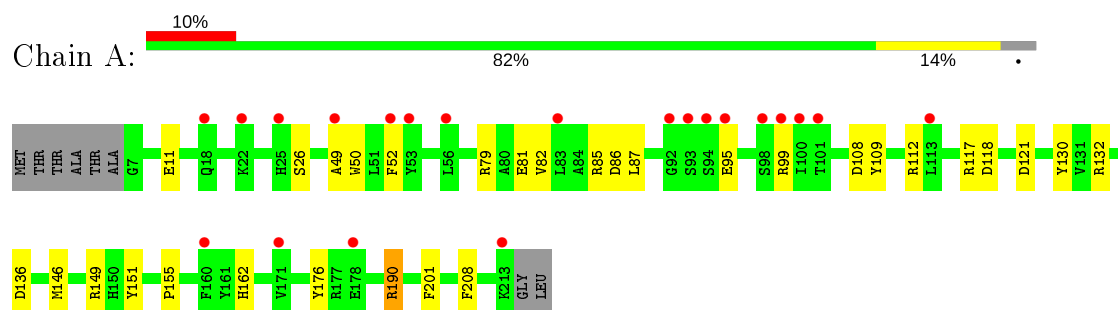
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total	O	0	0
			163	163		
5	B	195	Total	O	0	0
			195	195		
5	C	126	Total	O	0	0
			126	126		

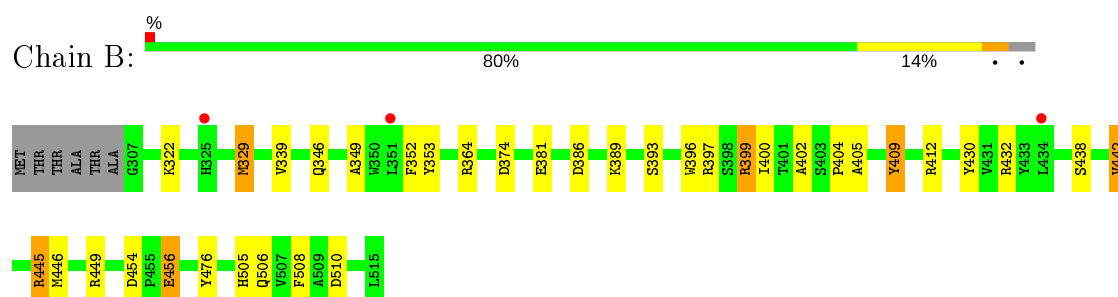
3 Residue-property plots [i](#)

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.

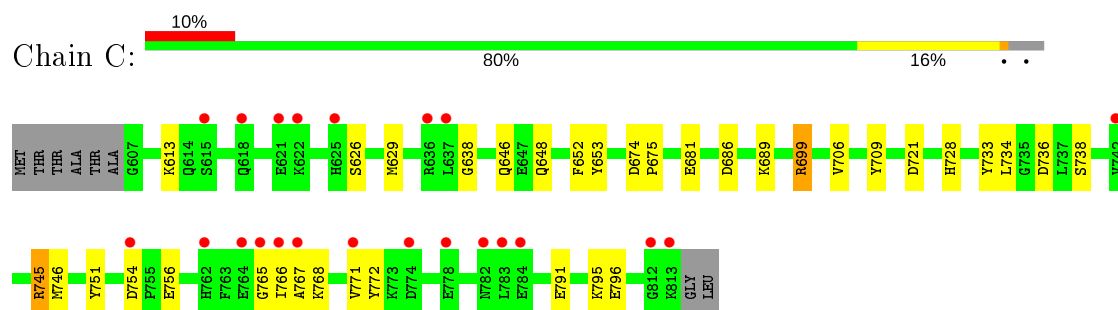
• Molecule 1: Heme oxygenase



• Molecule 1: Heme oxygenase



• Molecule 1: Heme oxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.12 Å 62.56 Å 108.00 Å 90.00° 100.67° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 30.80 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-1.50) 98.0 (30.80-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.50 Å)	Xtriage
Refinement program	CNS, REFMAC 5.1.24	Depositor
R, R_{free}	0.194 , 0.224 0.200 , 0.228	Depositor DCC
R_{free} test set	11109 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 48.8	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	5643	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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, SO4, DTV

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	1.44	7/1695 (0.4%)	1.44	23/2288 (1.0%)
1	B	1.50	14/1697 (0.8%)	1.44	17/2290 (0.7%)
1	C	1.38	6/1672 (0.4%)	1.26	11/2261 (0.5%)
All	All	1.44	27/5064 (0.5%)	1.38	51/6839 (0.7%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	681	GLU	CD-OE2	7.39	1.33	1.25
1	B	432	ARG	CZ-NH2	7.15	1.42	1.33
1	C	681	GLU	CG-CD	7.05	1.62	1.51
1	B	456	GLU	CG-CD	7.05	1.62	1.51
1	A	95	GLU	CB-CG	6.92	1.65	1.52
1	A	201	PHE	CE2-CZ	6.66	1.50	1.37
1	A	49	ALA	CA-CB	6.48	1.66	1.52
1	A	130	TYR	CD2-CE2	6.27	1.48	1.39
1	B	442	VAL	CB-CG1	-6.19	1.39	1.52
1	B	381	GLU	CD-OE1	6.15	1.32	1.25
1	B	339	VAL	CB-CG1	-5.80	1.40	1.52
1	C	681	GLU	CB-CG	5.76	1.63	1.52
1	B	438	SER	CA-CB	5.69	1.61	1.52
1	B	409	TYR	CE2-CZ	-5.58	1.31	1.38
1	C	772	TYR	CD2-CE2	5.57	1.47	1.39
1	B	402	ALA	C-O	5.49	1.33	1.23
1	A	201	PHE	CE1-CZ	5.46	1.47	1.37
1	C	653	TYR	CD2-CE2	5.39	1.47	1.39
1	B	438	SER	CB-OG	-5.26	1.35	1.42
1	B	397	ARG	CZ-NH1	-5.24	1.26	1.33
1	A	50	TRP	CE3-CZ3	5.20	1.47	1.38
1	B	456	GLU	CD-OE2	5.20	1.31	1.25
1	B	381	GLU	CG-CD	5.14	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	733	TYR	CE1-CZ	5.07	1.45	1.38
1	A	50	TRP	CD1-NE1	5.06	1.46	1.38
1	B	349	ALA	CA-CB	5.04	1.63	1.52
1	B	329	MET	CG-SD	-5.00	1.68	1.81

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	409	TYR	CB-CG-CD2	-10.54	114.67	121.00
1	A	109	TYR	CB-CG-CD1	9.70	126.82	121.00
1	A	109	TYR	CB-CG-CD2	-9.18	115.49	121.00
1	B	352	PHE	CB-CG-CD2	-9.10	114.43	120.80
1	B	409	TYR	CB-CG-CD1	8.62	126.17	121.00
1	A	99	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	510	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	A	130	TYR	CZ-CE2-CD2	-7.98	112.62	119.80
1	A	112[A]	ARG	NE-CZ-NH2	7.93	124.26	120.30
1	A	112[B]	ARG	NE-CZ-NH2	7.93	124.26	120.30
1	A	112[A]	ARG	NE-CZ-NH1	-7.76	116.42	120.30
1	A	112[B]	ARG	NE-CZ-NH1	-7.76	116.42	120.30
1	B	445	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	A	121	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	A	99	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	136	ASP	CB-CG-OD1	-7.39	111.65	118.30
1	A	79	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	108	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	C	699	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	B	445	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	A	117	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	C	699	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	A	87	LEU	CB-CG-CD1	-6.63	99.72	111.00
1	B	386	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	132	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	364	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	C	686	ASP	CB-CG-OD2	6.38	124.05	118.30
1	B	449	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	C	652	PHE	CB-CG-CD2	-6.31	116.38	120.80
1	C	709	TYR	CB-CG-CD1	6.27	124.76	121.00
1	C	754	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	86	ASP	CB-CG-OD2	6.07	123.76	118.30
1	B	374	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	B	430	TYR	CZ-CE2-CD2	-5.79	114.59	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	674	ASP	CB-CG-OD1	5.76	123.49	118.30
1	C	736	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	412	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	C	721	ASP	CB-CG-OD1	-5.39	113.44	118.30
1	B	432	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	52	PHE	CG-CD1-CE1	-5.32	114.95	120.80
1	B	353	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	A	190	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	C	736	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	A	176	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	B	430	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	A	208	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	B	508	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	C	613	LYS	CD-CE-NZ	-5.08	100.02	111.70
1	A	151	TYR	CB-CG-CD2	5.08	124.05	121.00
1	B	476	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	A	109	TYR	CD1-CE1-CZ	-5.04	115.27	119.80

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	1656	0	1612	8	0
1	B	1665	0	1625	16	0
1	C	1640	0	1583	17	0
2	A	43	0	30	0	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
3	A	10	0	0	0	0
3	B	20	0	0	0	0
3	C	15	0	0	0	0
4	A	8	0	6	0	0
4	B	8	0	9	0	0
4	C	8	0	9	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	163	0	0	1	0
5	B	195	0	0	2	0
5	C	126	0	0	0	0
All	All	5643	0	4934	43	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 4.

All (43) 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:454:ASP:HB3	1:B:456:GLU:OE2	1.77	0.84
1:C:745:ARG:HG3	1:C:746:MET:CE	2.12	0.80
1:C:768:LYS:CB	1:C:771:VAL:HG12	2.17	0.75
1:C:745:ARG:HG3	1:C:746:MET:HE2	1.74	0.70
1:C:728:HIS:HE1	1:C:796:GLU:OE2	1.76	0.69
1:A:11:GLU:OE2	1:A:190:ARG:NH2	2.27	0.68
1:C:738:SER:HB3	2:C:903:HEM:HAD1	1.74	0.67
1:B:322:LYS:HG2	1:B:505:HIS:HE1	1.62	0.64
1:C:745:ARG:HG3	1:C:746:MET:HE1	1.79	0.64
1:A:118:ASP:OD2	1:B:445:ARG:NH1	2.31	0.63
1:A:149:ARG:HB2	5:A:377:HOH:O	1.99	0.63
1:C:689:LYS:HD2	1:C:756:GLU:O	1.99	0.62
1:C:791:GLU:OE2	1:C:795:LYS:HE3	1.98	0.61
1:C:745:ARG:CG	1:C:746:MET:CE	2.79	0.61
1:B:405:ALA:HB2	1:B:506:GLN:HG3	1.85	0.58
1:B:389:LYS:HD2	1:B:456:GLU:O	2.03	0.57
1:C:745:ARG:CG	1:C:746:MET:HE2	2.35	0.57
2:B:902:HEM:HHD	2:B:902:HEM:HBC2	1.87	0.55
1:B:322:LYS:HG2	1:B:505:HIS:CE1	2.41	0.55
2:C:903:HEM:C1C	4:C:2003:DTV:H4C2	2.44	0.53
1:A:155:PRO:O	1:A:162:HIS:HE1	1.92	0.52
1:B:322:LYS:HE3	1:B:505:HIS:CE1	2.47	0.49
1:B:456:GLU:H	1:B:456:GLU:CD	2.17	0.48
1:B:506:GLN:CG	5:B:545:HOH:O	2.63	0.47
2:B:902:HEM:HHD	2:B:902:HEM:CBC	2.44	0.46
1:A:82:VAL:HG22	1:A:85:ARG:NH2	2.29	0.46
1:B:346:GLN:NE2	1:B:346:GLN:HA	2.31	0.46
1:B:400:ILE:HD13	1:B:400:ILE:HG21	1.46	0.46
1:A:155:PRO:O	1:A:162:HIS:CE1	2.68	0.46
1:C:648:GLN:HB3	1:C:706:VAL:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:VAL:HG22	1:B:446:MET:HE2	1.98	0.45
1:B:506:GLN:HG2	5:B:545:HOH:O	2.16	0.45
1:A:82:VAL:HG22	1:A:85:ARG:HH22	1.82	0.45
1:C:765:GLY:O	1:C:767:ALA:N	2.51	0.44
1:B:442:VAL:HG22	1:B:446:MET:CE	2.49	0.43
1:A:146:MET:HA	1:A:146:MET:CE	2.50	0.42
1:C:626:SER:HB3	1:C:629:MET:HB2	2.02	0.42
1:B:396:TRP:HA	1:B:399:ARG:HG3	2.02	0.42
1:C:638:GLY:HA2	1:C:751:TYR:CD2	2.54	0.41
1:B:346:GLN:HA	1:B:346:GLN:HE21	1.84	0.41
1:C:734:LEU:HA	1:C:734:LEU:HD12	1.93	0.41
1:C:768:LYS:CB	1:C:771:VAL:CG1	2.95	0.40
1:C:646:GLN:NE2	1:C:646:GLN:HA	2.36	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	206/215 (96%)	201 (98%)	5 (2%)	0	100	100
1	B	207/215 (96%)	203 (98%)	4 (2%)	0	100	100
1	C	205/215 (95%)	200 (98%)	4 (2%)	1 (0%)	29	9
All	All	618/645 (96%)	604 (98%)	13 (2%)	1 (0%)	47	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	766	ILE

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	171/175 (98%)	169 (99%)	2 (1%)	71	48
1	B	171/175 (98%)	166 (97%)	5 (3%)	42	13
1	C	167/175 (95%)	164 (98%)	3 (2%)	59	30
All	All	509/525 (97%)	499 (98%)	10 (2%)	55	25

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	81	GLU
1	B	329	MET
1	B	393	SER
1	B	399	ARG
1	B	404	PRO
1	B	409	TYR
1	C	675	PRO
1	C	699	ARG
1	C	745	ARG

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

Mol	Chain	Res	Type
1	A	78	ASN
1	A	182	ASN
1	B	346	GLN
1	B	378	ASN
1	C	646	GLN
1	C	678	ASN
1	C	728	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 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$
2	HEM	A	901	1,4	27,50,50	2.06	9 (33%)	17,82,82	4.10	10 (58%)
3	SO4	B	1002	-	4,4,4	0.39	0	6,6,6	0.40	0
3	SO4	B	1008	-	4,4,4	0.70	0	6,6,6	0.76	0
2	HEM	B	902	1,4	27,50,50	2.39	11 (40%)	17,82,82	3.82	9 (52%)
3	SO4	C	1010	-	4,4,4	0.54	0	6,6,6	0.56	0
4	DTV	A	2001	2	7,7,7	1.87	1 (14%)	4,8,8	4.57	2 (50%)
3	SO4	C	1011	-	4,4,4	0.13	0	6,6,6	0.17	0
2	HEM	C	903	1,4	27,50,50	2.37	12 (44%)	17,82,82	2.45	6 (35%)
4	DTV	B	2002	2	7,7,7	1.16	0	4,8,8	1.71	1 (25%)
3	SO4	A	1005	-	4,4,4	0.11	0	6,6,6	0.32	0
3	SO4	B	1003	-	4,4,4	0.26	0	6,6,6	0.86	0
3	SO4	B	1004	-	4,4,4	0.32	0	6,6,6	0.89	0
3	SO4	A	1001	-	4,4,4	0.40	0	6,6,6	0.64	0
4	DTV	C	2003	2	7,7,7	1.26	1 (14%)	4,8,8	1.65	1 (25%)
3	SO4	C	1009	-	4,4,4	0.27	0	6,6,6	0.73	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	HEM	A	901	1,4	-	0/6/54/54	-
2	HEM	B	902	1,4	-	0/6/54/54	-
4	DTV	A	2001	2	-	6/8/8/8	-
2	HEM	C	903	1,4	-	0/6/54/54	-
4	DTV	B	2002	2	-	0/8/8/8	-
4	DTV	C	2003	2	-	1/8/8/8	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	HEM	C3B-C2B	-6.40	1.31	1.40
2	A	901	HEM	C3C-C2C	-5.57	1.32	1.40
2	C	903	HEM	C3B-C2B	-5.00	1.33	1.40
2	A	901	HEM	C3D-C2D	4.35	1.50	1.37
2	C	903	HEM	C3C-CAC	4.30	1.56	1.47
4	A	2001	DTV	O3-C3	-4.06	1.34	1.43
2	B	902	HEM	C4A-NA	3.94	1.44	1.36
2	B	902	HEM	C3C-C2C	-3.91	1.34	1.40
2	C	903	HEM	C3C-C2C	-3.79	1.35	1.40
2	B	902	HEM	C3C-CAC	3.78	1.55	1.47
2	C	903	HEM	CMA-C3A	3.78	1.59	1.51
2	B	902	HEM	C3D-C2D	3.65	1.48	1.37
2	C	903	HEM	C4A-NA	3.63	1.43	1.36
2	C	903	HEM	C1D-ND	3.41	1.43	1.36
2	B	902	HEM	C1D-ND	3.36	1.43	1.36
2	A	901	HEM	C3B-CAB	3.00	1.54	1.47
2	C	903	HEM	C3D-C2D	2.93	1.46	1.37
2	B	902	HEM	CMD-C2D	2.88	1.57	1.51
4	C	2003	DTV	C4-C3	2.82	1.59	1.51
2	A	901	HEM	C1D-ND	2.72	1.41	1.36
2	A	901	HEM	C3C-CAC	2.72	1.53	1.47
2	C	903	HEM	C1B-C2B	-2.72	1.36	1.42
2	C	903	HEM	C3B-CAB	2.52	1.53	1.47
2	A	901	HEM	C4A-NA	2.51	1.41	1.36
2	C	903	HEM	CMB-C2B	2.36	1.57	1.51
2	B	902	HEM	C1C-C2C	2.29	1.47	1.42
2	C	903	HEM	CMD-C2D	2.27	1.56	1.51
2	A	901	HEM	C1C-C2C	2.26	1.47	1.42
2	A	901	HEM	CAD-C3D	2.25	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	903	HEM	C4D-C3D	2.18	1.47	1.42
2	A	901	HEM	CMB-C2B	2.14	1.56	1.51
2	B	902	HEM	CMA-C3A	2.10	1.56	1.51
2	B	902	HEM	CMC-C2C	-2.08	1.46	1.51
2	B	902	HEM	C1D-CHD	-2.05	1.35	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	HEM	C4A-C3A-C2A	9.64	113.70	107.00
2	B	902	HEM	CMA-C3A-C4A	-8.51	115.38	128.46
2	A	901	HEM	CAD-CBD-CGD	8.12	126.30	112.67
2	A	901	HEM	C4C-C3C-C2C	8.09	112.55	106.90
2	A	901	HEM	CBD-CAD-C3D	-6.69	100.16	112.48
4	A	2001	DTV	C3-C4-S4	-6.65	95.13	114.47
2	C	903	HEM	C1D-C2D-C3D	6.39	111.44	107.00
2	A	901	HEM	C4A-C3A-C2A	6.25	111.34	107.00
4	A	2001	DTV	C2-C1-S1	-5.73	97.80	114.47
2	A	901	HEM	CMA-C3A-C4A	-4.74	121.18	128.46
2	B	902	HEM	CAA-CBA-CGA	-4.60	104.95	112.67
2	C	903	HEM	C4A-C3A-C2A	4.53	110.15	107.00
2	B	902	HEM	C1D-C2D-C3D	4.13	109.87	107.00
2	A	901	HEM	CMD-C2D-C1D	-3.24	123.48	128.46
2	B	902	HEM	CBD-CAD-C3D	-3.21	106.57	112.48
2	A	901	HEM	C1D-C2D-C3D	3.19	109.22	107.00
2	B	902	HEM	CMA-C3A-C2A	3.13	130.84	124.94
2	C	903	HEM	CMA-C3A-C4A	-3.08	123.73	128.46
4	B	2002	DTV	O3-C3-C2	-3.05	103.47	109.72
2	C	903	HEM	CAA-CBA-CGA	-2.91	107.80	112.67
2	A	901	HEM	CBA-CAA-C2A	-2.77	107.38	112.49
4	C	2003	DTV	C2-C1-S1	-2.75	106.48	114.47
2	A	901	HEM	C3C-C4C-NC	-2.70	105.85	110.94
2	C	903	HEM	CMD-C2D-C1D	-2.52	124.59	128.46
2	C	903	HEM	CAD-CBD-CGD	-2.51	108.46	112.67
2	B	902	HEM	CMB-C2B-C3B	2.47	129.30	124.68
2	B	902	HEM	CAD-CBD-CGD	-2.25	108.90	112.67
2	B	902	HEM	CBA-CAA-C2A	-2.18	108.46	112.49
2	A	901	HEM	CAA-CBA-CGA	-2.09	109.17	112.67

There are no chirality outliers.

All (7) torsion outliers are listed below:

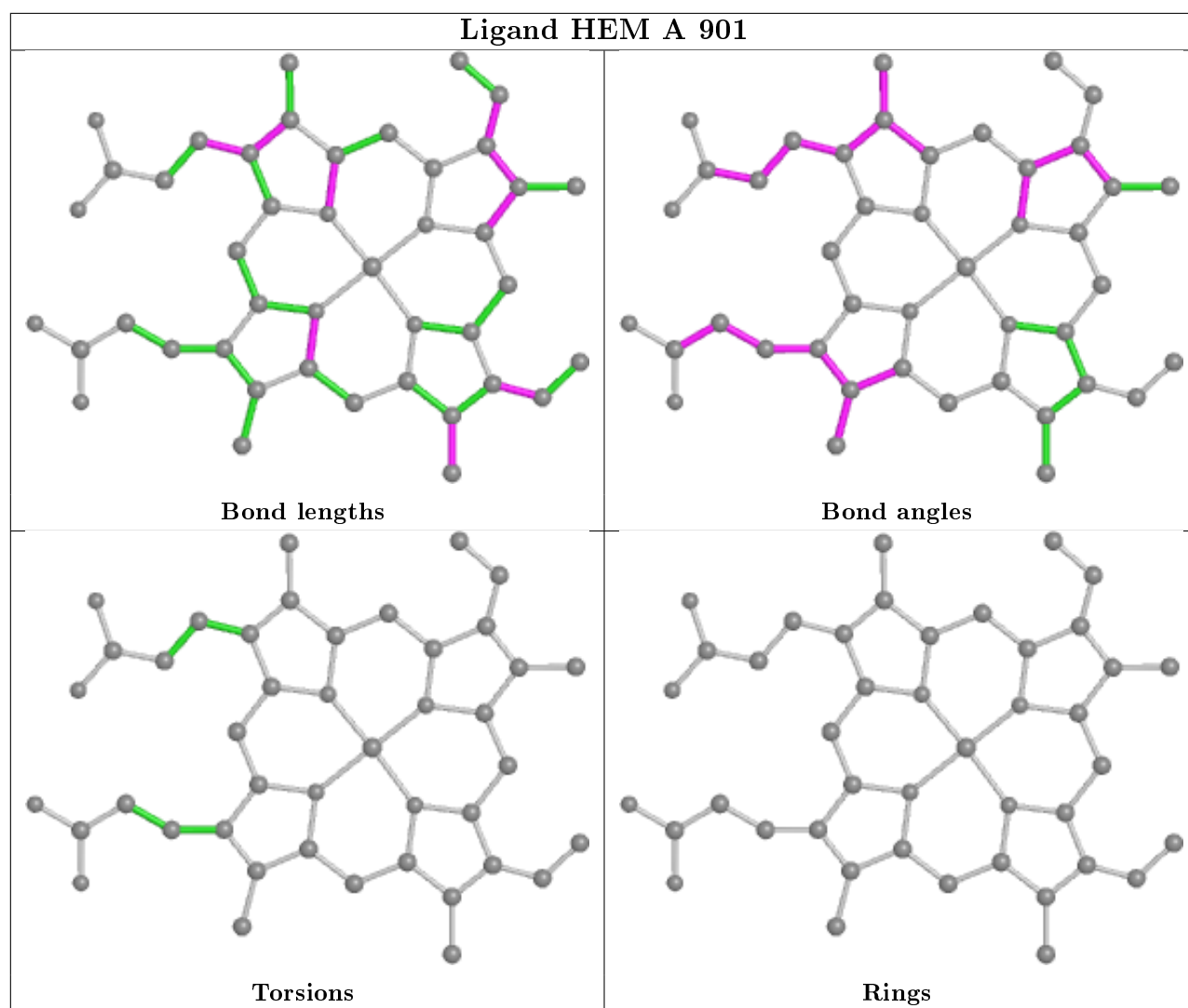
Mol	Chain	Res	Type	Atoms
4	A	2001	DTV	S1-C1-C2-O2
4	A	2001	DTV	S1-C1-C2-C3
4	A	2001	DTV	C1-C2-C3-C4
4	A	2001	DTV	O2-C2-C3-O3
4	A	2001	DTV	C2-C3-C4-S4
4	A	2001	DTV	O3-C3-C4-S4
4	C	2003	DTV	C1-C2-C3-C4

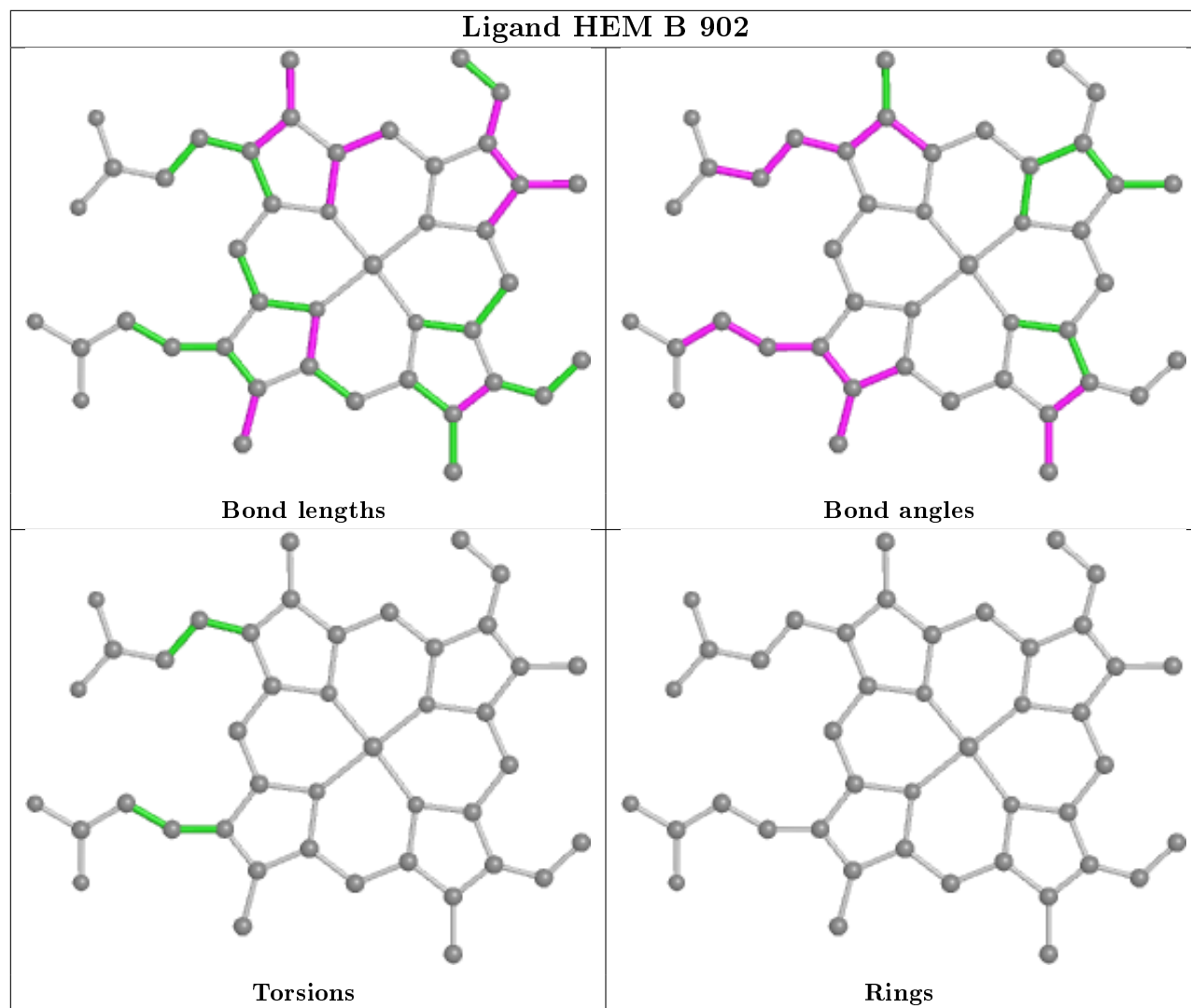
There are no ring outliers.

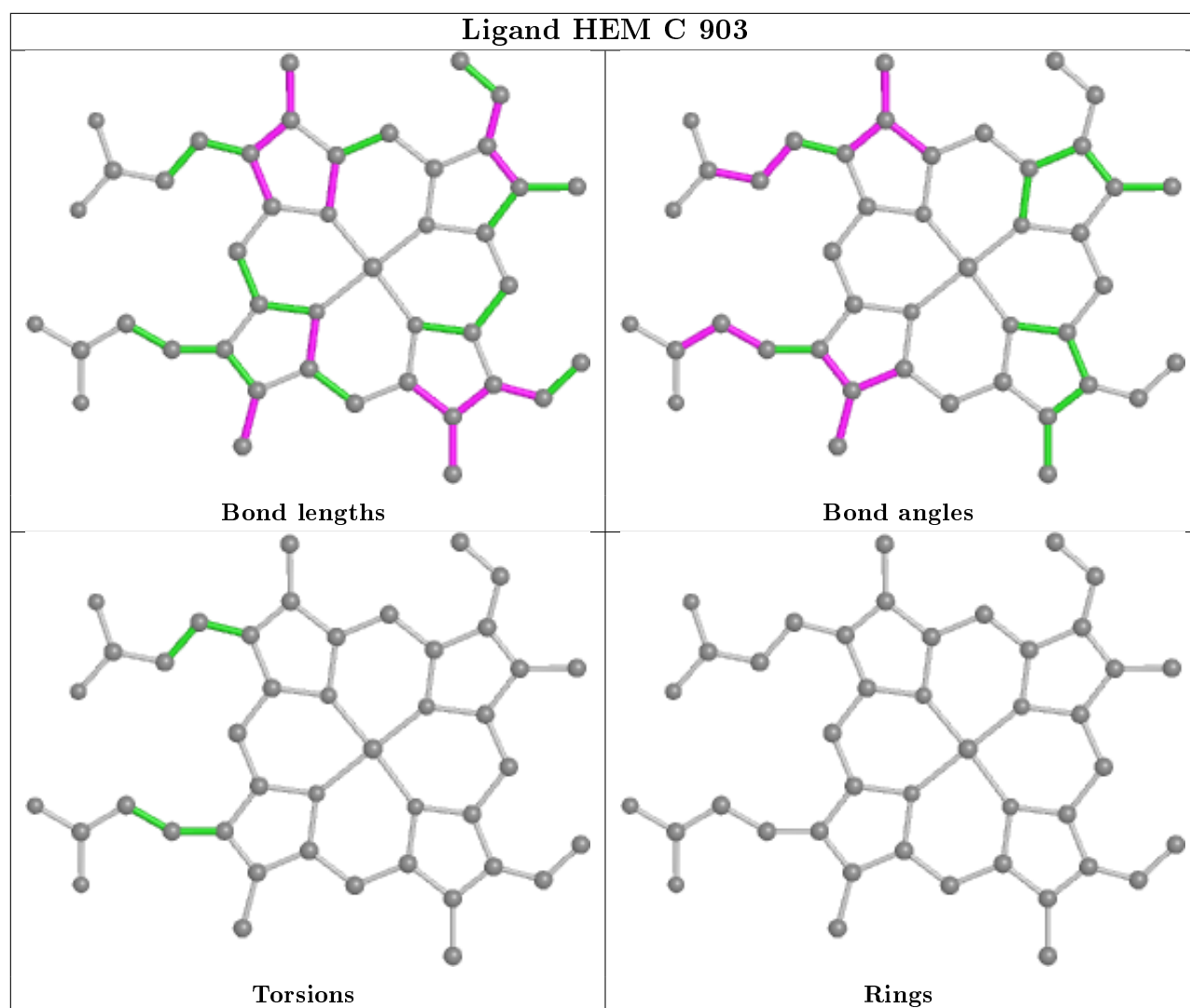
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	902	HEM	2	0
2	C	903	HEM	2	0
4	C	2003	DTV	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	207/215 (96%)	0.55	21 (10%) 7 7	13, 22, 36, 42	0
1	B	209/215 (97%)	0.08	3 (1%) 75 79	12, 21, 33, 42	0
1	C	207/215 (96%)	0.74	22 (10%) 6 6	16, 26, 42, 54	0
All	All	623/645 (96%)	0.46	46 (7%) 14 15	12, 23, 37, 54	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	767	ALA	9.1
1	C	765	GLY	5.8
1	C	771	VAL	5.3
1	C	636	ARG	4.0
1	C	764	GLU	3.9
1	C	637	LEU	3.6
1	A	93	SER	3.5
1	C	766	ILE	3.5
1	A	52	PHE	3.4
1	C	618	GLN	3.3
1	C	625	HIS	3.1
1	A	94	SER	3.0
1	A	98	SER	3.0
1	C	622	LYS	2.9
1	C	812	GLY	2.8
1	A	101	THR	2.7
1	C	784	GLU	2.7
1	C	742	VAL	2.6
1	B	325	HIS	2.6
1	C	774	ASP	2.6
1	A	213	LYS	2.5
1	A	25	HIS	2.5
1	A	53	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	783	LEU	2.4
1	A	95	GLU	2.4
1	A	49	ALA	2.3
1	C	621	GLU	2.3
1	A	100	ILE	2.3
1	A	56	LEU	2.3
1	C	762	HIS	2.3
1	A	171	VAL	2.3
1	A	160	PHE	2.3
1	A	92	GLY	2.3
1	C	778	GLU	2.2
1	A	22	LYS	2.2
1	B	351	LEU	2.2
1	A	99	ARG	2.2
1	C	782	ASN	2.2
1	A	83	LEU	2.2
1	C	754	ASP	2.1
1	B	434	LEU	2.1
1	A	178	GLU	2.1
1	C	615	SER	2.0
1	C	813	LYS	2.0
1	A	113	LEU	2.0
1	A	18	GLN	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](#)

There are no monosaccharides in this entry.

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.

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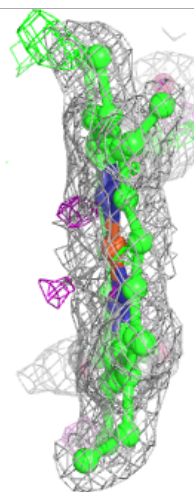
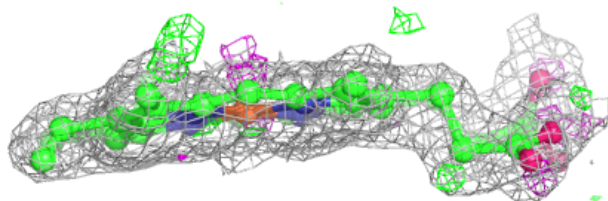
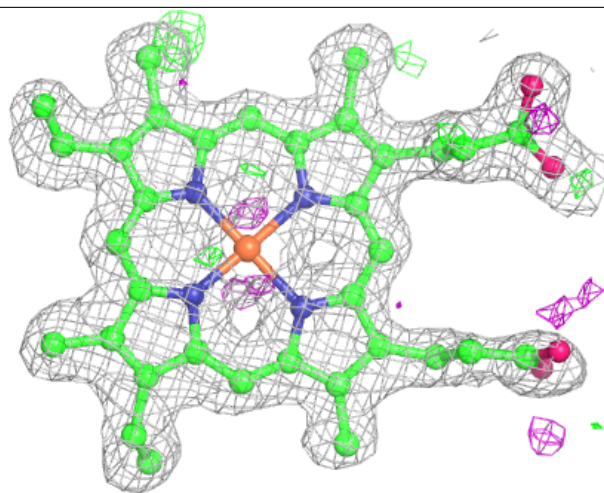
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	1005	5/5	0.62	0.29	108,109,109,109	0
3	SO4	C	1010	5/5	0.79	0.29	55,58,61,62	0
3	SO4	C	1009	5/5	0.89	0.20	56,58,60,60	0
3	SO4	B	1008	5/5	0.91	0.20	35,35,44,46	0
3	SO4	B	1004	5/5	0.94	0.15	41,44,47,51	0
3	SO4	C	1011	5/5	0.94	0.28	95,96,97,97	0
4	DTV	A	2001	8/8	0.96	0.14	20,30,32,32	0
3	SO4	B	1002	5/5	0.96	0.28	45,49,51,52	0
3	SO4	A	1001	5/5	0.96	0.17	43,43,46,51	0
4	DTV	C	2003	8/8	0.96	0.10	27,30,39,45	0
2	HEM	C	903	43/43	0.96	0.11	18,26,39,50	0
2	HEM	B	902	43/43	0.97	0.10	14,19,30,51	0
2	HEM	A	901	43/43	0.97	0.10	16,22,33,39	0
4	DTV	B	2002	8/8	0.98	0.08	18,21,24,28	0
3	SO4	B	1003	5/5	0.98	0.08	35,37,41,42	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.

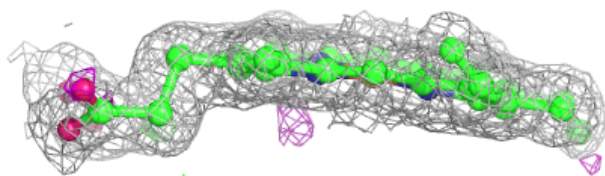
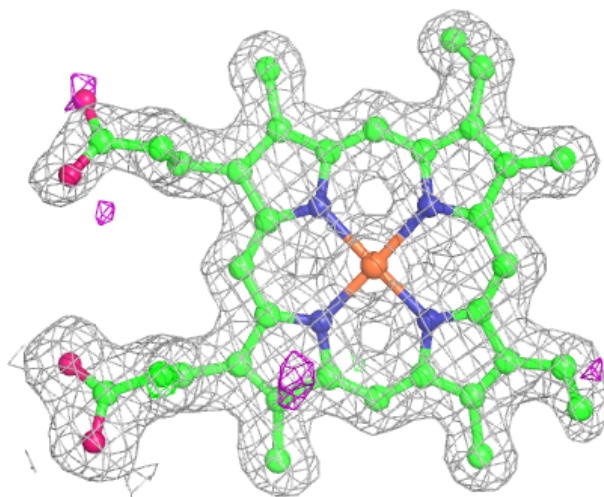
Electron density around HEM C 903:

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



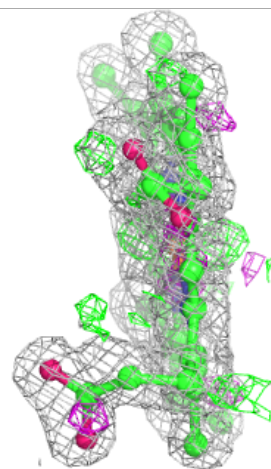
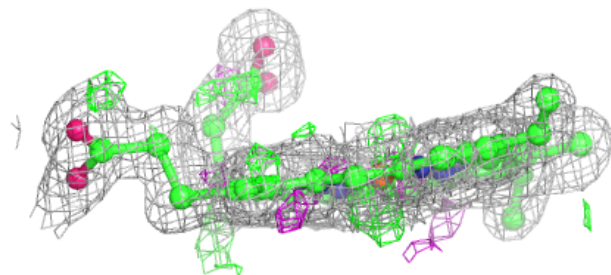
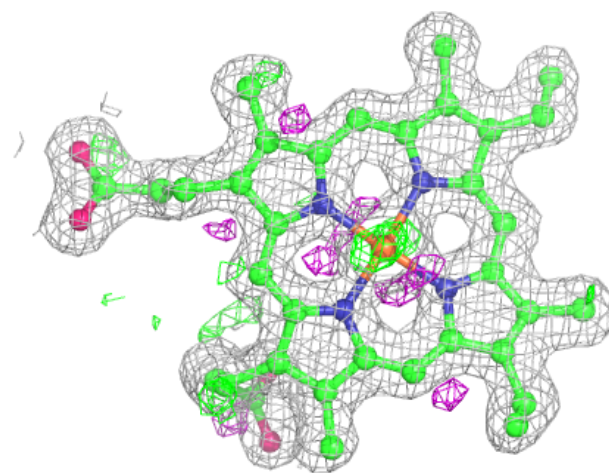
Electron density around HEM B 902:

$2mF_o-DF_c$ (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.