



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:02 AM UTC

PDB ID : 3I8R / pdb_00003i8r
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 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

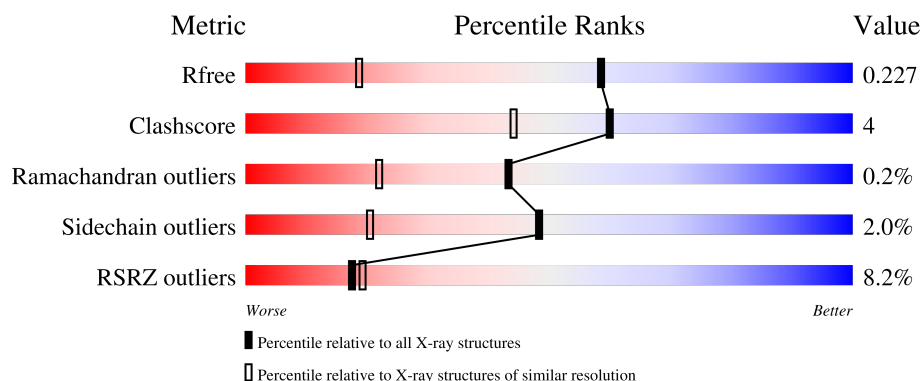
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 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	6% 77% 20% .
1	B	215	3% 78% 18% ..
1	C	215	15% 75% 20% ..

2 Entry composition [i](#)

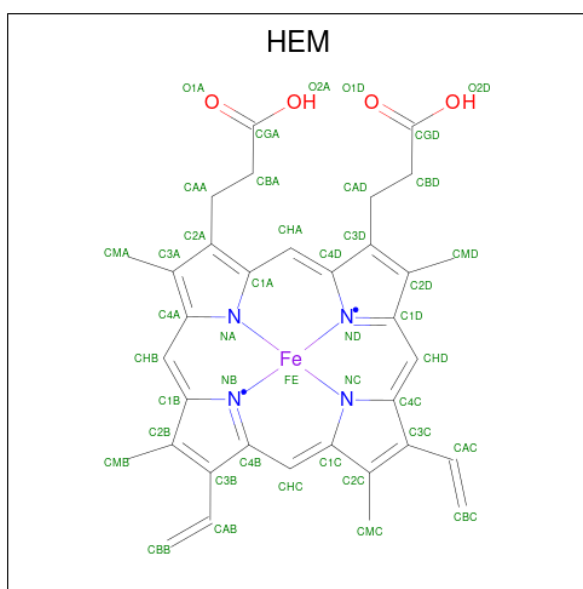
There are 5 unique types of molecules in this entry. The entry contains 5643 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



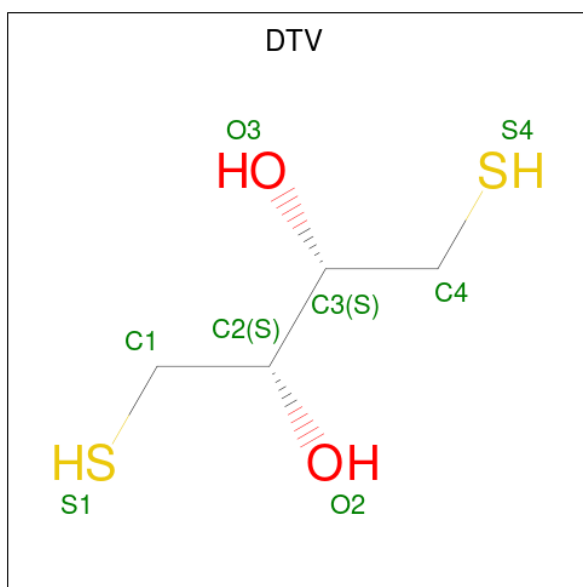
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is SULFATE ION (CCD ID: 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	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 (CCD ID: 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		

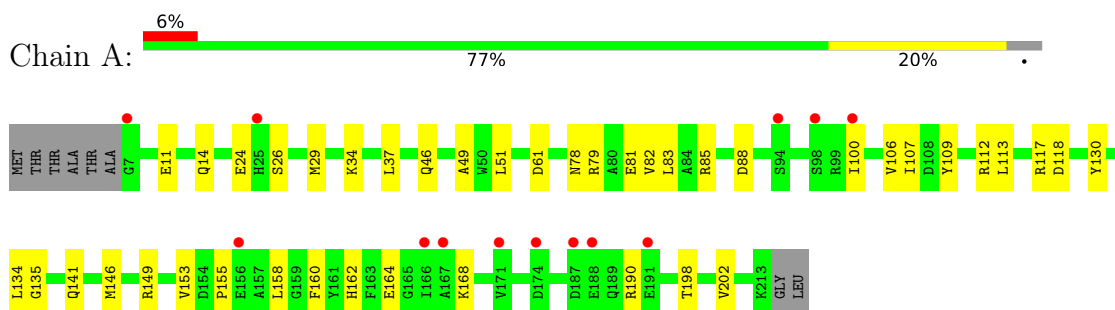
- Molecule 5 is water.

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		

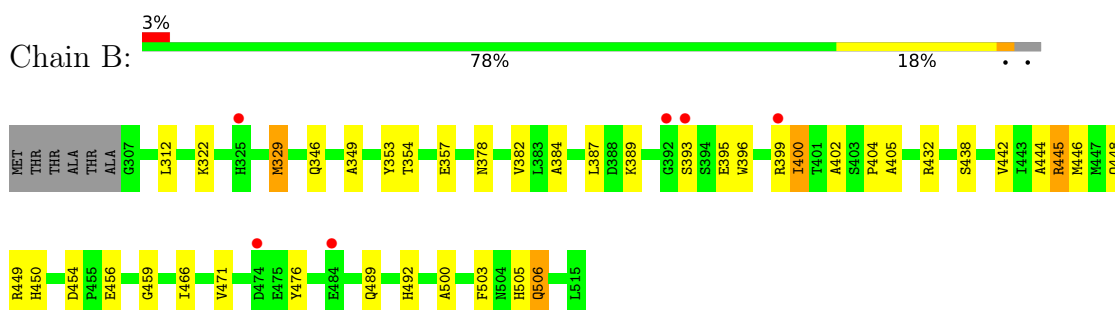
3 Residue-property plots [i](#)

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.

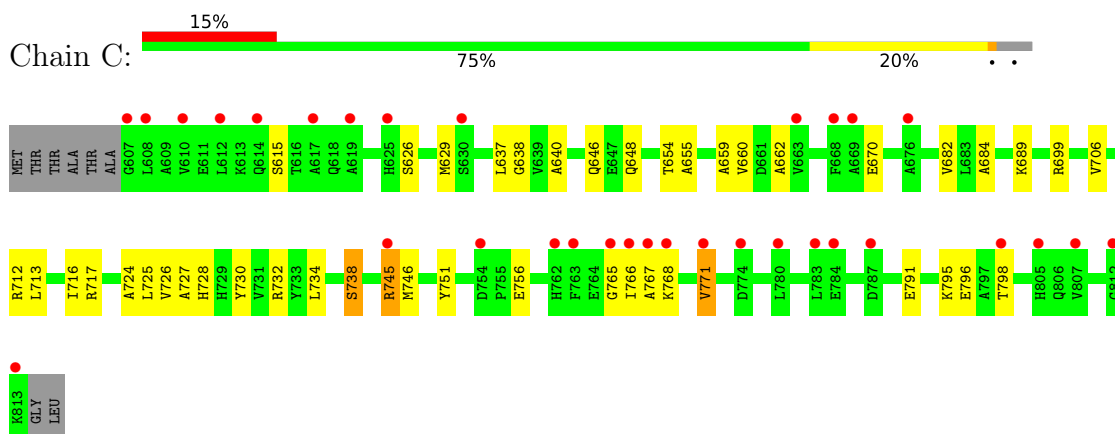
- Molecule 1: Heme oxygenase



- 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	54.12Å 62.56Å 108.00Å 90.00° 100.67° 90.00°	Depositor
Resolution (Å)	30.00 – 1.50 30.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-1.50) 98.0 (30.00-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.50Å)	Xtriage
Refinement program	CNS, REFMAC 5.1.24	Depositor
R, R_{free}	0.194 , 0.224 0.200 , 0.227	Depositor DCC
R_{free} test set	11109 reflections (9.81%)	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)	0.40 , 38.9	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: SO4, HEM, 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	1.77	21/1695 (1.2%)	1.55	14/2288 (0.6%)
1	B	1.79	18/1697 (1.1%)	1.62	18/2290 (0.8%)
1	C	1.70	17/1672 (1.0%)	1.45	10/2261 (0.4%)
All	All	1.75	56/5064 (1.1%)	1.54	42/6839 (0.6%)

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	VAL	CA-CB	8.77	1.63	1.54
1	A	37	LEU	CA-C	-8.57	1.48	1.53
1	B	402	ALA	C-O	8.23	1.33	1.23
1	C	716	ILE	CA-CB	8.09	1.64	1.54
1	A	49	ALA	CA-CB	7.77	1.66	1.53
1	C	662	ALA	N-CA	7.75	1.55	1.46
1	B	312	LEU	C-O	-7.63	1.15	1.24
1	A	79	ARG	CA-C	-7.55	1.43	1.52
1	A	164	GLU	C-O	7.13	1.32	1.23
1	C	732	ARG	CA-C	-6.92	1.44	1.52
1	A	83	LEU	N-CA	-6.91	1.38	1.46
1	B	432	ARG	CZ-NH2	6.84	1.42	1.33
1	B	400	ILE	CA-CB	6.70	1.63	1.54
1	C	727	ALA	CA-CB	-6.64	1.43	1.53
1	A	88	ASP	N-CA	6.59	1.54	1.46
1	C	682	VAL	C-O	6.57	1.31	1.24
1	B	354	THR	N-CA	6.25	1.53	1.46
1	B	349	ALA	CA-CB	6.25	1.63	1.53
1	B	378	ASN	C-O	6.22	1.31	1.23
1	C	732	ARG	C-O	6.14	1.31	1.24
1	A	141	GLN	CA-C	-6.12	1.44	1.52
1	A	202	VAL	N-CA	-6.10	1.39	1.46
1	A	34	LYS	N-CA	6.08	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	640	ALA	N-CA	5.91	1.53	1.46
1	C	730	TYR	C-O	5.86	1.30	1.24
1	C	662	ALA	CA-CB	-5.79	1.44	1.53
1	B	432	ARG	C-O	5.75	1.30	1.24
1	C	712	ARG	CA-CB	5.74	1.62	1.53
1	C	659	ALA	N-CA	5.71	1.53	1.46
1	B	503	PHE	C-O	-5.66	1.17	1.24
1	B	500	ALA	CA-CB	-5.52	1.44	1.53
1	A	130	TYR	C-O	5.45	1.30	1.24
1	A	160	PHE	C-O	-5.42	1.17	1.24
1	B	438	SER	CA-CB	5.32	1.61	1.53
1	A	135	GLY	C-O	5.29	1.30	1.23
1	A	61	ASP	CA-C	5.28	1.59	1.52
1	A	46	GLN	C-O	-5.28	1.17	1.24
1	C	726	VAL	C-O	5.27	1.30	1.24
1	B	444	ALA	CA-CB	5.26	1.61	1.53
1	C	738	SER	C-O	5.25	1.31	1.23
1	A	24	GLU	N-CA	5.24	1.52	1.46
1	C	724	ALA	N-CA	5.24	1.52	1.46
1	A	158	LEU	N-CA	5.19	1.52	1.46
1	B	353	TYR	C-O	-5.18	1.17	1.24
1	B	476	TYR	C-O	5.16	1.30	1.24
1	A	78	ASN	C-O	5.15	1.30	1.23
1	B	382	VAL	CA-CB	5.13	1.60	1.54
1	C	717	ARG	CA-C	5.07	1.59	1.52
1	B	449	ARG	CA-CB	-5.06	1.45	1.53
1	C	654	THR	CA-C	5.05	1.59	1.52
1	B	329	MET	CG-SD	-5.04	1.68	1.80
1	B	444	ALA	CA-C	5.03	1.59	1.52
1	A	51	LEU	N-CA	5.01	1.52	1.46
1	A	79	ARG	CA-CB	5.01	1.61	1.54
1	C	655	ALA	CA-CB	-5.01	1.45	1.53
1	A	29	MET	CA-CB	5.00	1.61	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	492	HIS	O-C-N	7.61	130.19	122.12
1	B	448	GLN	O-C-N	7.46	129.75	122.07
1	A	100	ILE	N-CA-C	7.41	119.65	109.80
1	C	637	LEU	CA-C-O	7.03	122.02	117.94
1	B	387	LEU	CA-C-O	-7.03	113.10	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	LEU	O-C-N	6.74	129.27	122.12
1	C	732	ARG	CA-C-O	-6.73	113.73	120.80
1	B	506	GLN	N-CA-C	6.29	118.95	111.71
1	A	117	ARG	O-C-N	6.26	128.78	122.08
1	A	14	GLN	N-CA-C	6.20	118.03	111.28
1	B	384	ALA	O-C-N	6.12	128.60	122.12
1	B	444	ALA	O-C-N	5.88	128.35	122.12
1	B	450	HIS	N-CA-C	5.82	117.71	111.36
1	B	357	GLU	O-C-N	5.73	129.31	122.27
1	A	46	GLN	O-C-N	5.71	128.90	122.22
1	A	107	ILE	N-CA-C	-5.69	104.98	110.72
1	A	112[A]	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	A	112[B]	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	C	670	GLU	N-CA-C	5.62	117.08	111.07
1	A	134	LEU	N-CA-C	-5.56	105.38	111.82
1	B	489	GLN	O-C-N	5.50	127.96	122.12
1	A	113	LEU	O-C-N	5.49	127.94	122.12
1	C	684	ALA	O-C-N	5.48	127.93	122.12
1	C	717	ARG	O-C-N	5.42	127.65	122.07
1	A	109	TYR	N-CA-CB	-5.40	102.24	110.07
1	B	400	ILE	CB-CG1-CD1	-5.38	102.51	113.80
1	C	654	THR	O-C-N	5.37	127.60	122.07
1	C	771	VAL	CA-C-O	-5.31	115.22	120.85
1	B	471	VAL	N-CA-C	-5.29	105.56	110.53
1	A	106	VAL	O-C-N	5.28	127.76	121.80
1	C	660	VAL	N-CA-C	5.26	115.99	110.62
1	B	445	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	B	354	THR	O-C-N	5.17	127.39	122.07
1	B	459	GLY	O-C-N	5.16	127.50	122.19
1	B	438	SER	CA-C-O	5.14	122.70	119.77
1	B	395	GLU	N-CA-C	5.13	118.79	112.54
1	C	713	LEU	O-C-N	5.11	128.20	122.22
1	B	466	ILE	N-CA-C	5.11	113.73	106.53
1	A	112[A]	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	A	112[B]	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	A	135	GLY	O-C-N	-5.06	117.32	122.18
1	C	615	SER	N-CA-C	5.03	117.49	111.71

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	9	0
1	B	1665	0	1625	15	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
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:C:745:ARG:HG3	1:C:746:MET:HE2	1.34	1.08
1:B:454:ASP:HB3	1:B:456:GLU:OE2	1.77	0.84
1:B:442:VAL:HG22	1:B:446:MET:HE3	1.61	0.83
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:CG	1:C:746:MET:HE2	2.19	0.69
1:A:146:MET:HA	1:A:146:MET:HE2	1.74	0.69
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:A:118:ASP:OD2	1:B:445:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:CE	2.79	0.56
2:B:902:HEM:HBC2	2:B:902:HEM:HHD	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:456:GLU:H	1:B:456:GLU:CD	2.17	0.52
1:A:146:MET:HE2	1:A:146:MET:CA	2.40	0.51
1:B:322:LYS:HE3	1:B:505:HIS:CE1	2.47	0.49
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:HG21	1:B:400:ILE:HD13	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
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:C:725:LEU:C	1:C:725:LEU:HD13	2.43	0.43
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:HD12	1:C:734:LEU:HA	1.93	0.41
1:C:768:LYS:CB	1:C:771:VAL:CG1	2.95	0.40
1:C:646:GLN:HA	1:C:646:GLN:NE2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	24	8
All	All	618/645 (96%)	604 (98%)	13 (2%)	1 (0%)	43	22

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%)	167 (98%)	4 (2%)	44	16
1	B	171/175 (98%)	168 (98%)	3 (2%)	51	24
1	C	167/175 (95%)	164 (98%)	3 (2%)	51	24
All	All	509/525 (97%)	499 (98%)	10 (2%)	48	20

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

Mol	Chain	Res	Type
1	A	26	SER
1	A	81	GLU
1	A	168	LYS
1	A	198	THR
1	B	329	MET
1	B	393	SER
1	B	404	PRO
1	C	699	ARG
1	C	745	ARG
1	C	798	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	119	ASN
1	A	182	ASN
1	B	346	GLN
1	B	378	ASN
1	B	448	GLN
1	B	505	HIS
1	C	678	ASN
1	C	691	ASN
1	C	728	HIS
1	C	762	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	4,1	50,50,50	2.05	17 (34%)	67,82,82	3.16	30 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	1001	-	4,4,4	0.50	0	6,6,6	0.60	0
3	SO4	C	1009	-	4,4,4	0.38	0	6,6,6	0.60	0
4	DTV	C	2003	2	7,7,7	1.27	1 (14%)	4,8,8	1.67	1 (25%)
3	SO4	C	1011	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	B	1002	-	4,4,4	0.48	0	6,6,6	0.38	0
2	HEM	C	903	4,1	50,50,50	2.04	17 (34%)	67,82,82	2.68	26 (38%)
3	SO4	C	1010	-	4,4,4	0.62	0	6,6,6	0.50	0
2	HEM	B	902	4,1	50,50,50	1.99	15 (30%)	67,82,82	2.93	31 (46%)
3	SO4	B	1004	-	4,4,4	0.42	0	6,6,6	0.87	0
4	DTV	B	2002	2	7,7,7	1.16	0	4,8,8	1.63	1 (25%)
3	SO4	B	1003	-	4,4,4	0.35	0	6,6,6	0.83	0
3	SO4	A	1005	-	4,4,4	0.21	0	6,6,6	0.31	0
4	DTV	A	2001	2	7,7,7	1.90	1 (14%)	4,8,8	4.74	2 (50%)
3	SO4	B	1008	-	4,4,4	0.74	0	6,6,6	0.74	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	4,1	-	7/14/54/54	-
4	DTV	C	2003	2	-	1/8/8/8	-
2	HEM	C	903	4,1	-	4/14/54/54	-
2	HEM	B	902	4,1	-	4/14/54/54	-
4	DTV	B	2002	2	-	0/8/8/8	-
4	DTV	A	2001	2	-	6/8/8/8	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEM	C3D-C2D	6.39	1.50	1.36
2	B	902	HEM	C3D-C2D	5.43	1.48	1.36
2	C	903	HEM	C4C-NC	5.14	1.49	1.39
2	B	902	HEM	FE-NC	4.86	2.11	1.95
2	C	903	HEM	FE-ND	4.67	2.09	1.94
2	C	903	HEM	C3D-C2D	4.45	1.46	1.36
2	C	903	HEM	CMA-C3A	4.26	1.59	1.50
4	A	2001	DTV	O3-C3	-4.10	1.34	1.43
2	C	903	HEM	C1B-C2B	-4.00	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	HEM	FE-NB	3.87	2.06	1.94
2	B	902	HEM	FE-ND	3.72	2.06	1.94
2	A	901	HEM	C4D-ND	-3.66	1.33	1.40
2	B	902	HEM	C3C-C4C	-3.58	1.39	1.46
2	C	903	HEM	CAC-C3C	3.46	1.56	1.47
2	A	901	HEM	CBD-CGD	3.41	1.58	1.50
2	B	902	HEM	CMD-C2D	3.35	1.57	1.50
2	A	901	HEM	O1A-CGA	3.34	1.33	1.22
2	C	903	HEM	CMB-C2B	3.13	1.57	1.50
2	A	901	HEM	C3B-C4B	3.11	1.51	1.44
2	B	902	HEM	CAC-C3C	3.06	1.55	1.47
2	A	901	HEM	C1B-C2B	-2.97	1.38	1.44
2	B	902	HEM	C1D-C2D	-2.97	1.38	1.44
2	A	901	HEM	CMB-C2B	2.87	1.56	1.50
2	A	901	HEM	FE-NA	2.83	2.04	1.95
4	C	2003	DTV	C4-C3	2.82	1.59	1.51
2	B	902	HEM	C3B-C2B	-2.79	1.31	1.37
2	A	901	HEM	FE-ND	2.79	2.03	1.94
2	C	903	HEM	CMD-C2D	2.72	1.56	1.50
2	B	902	HEM	C1B-NB	2.61	1.44	1.40
2	C	903	HEM	O1A-CGA	2.56	1.30	1.22
2	B	902	HEM	CMA-C3A	2.55	1.56	1.50
2	B	902	HEM	CMB-C2B	2.51	1.55	1.50
2	A	901	HEM	CAB-C3B	2.50	1.54	1.47
2	B	902	HEM	C4A-NA	2.48	1.44	1.39
2	A	901	HEM	CBD-CAD	2.38	1.60	1.51
2	C	903	HEM	FE-NA	2.30	2.02	1.95
2	C	903	HEM	C4B-NB	-2.26	1.34	1.38
2	A	901	HEM	CAC-C3C	2.25	1.53	1.47
2	A	901	HEM	FE-NC	2.24	2.02	1.95
2	C	903	HEM	C1A-NA	-2.24	1.35	1.39
2	A	901	HEM	C3C-C2C	-2.23	1.32	1.37
2	C	903	HEM	CMC-C2C	2.21	1.55	1.50
2	C	903	HEM	C1D-ND	2.21	1.43	1.38
2	B	902	HEM	C1D-ND	2.15	1.43	1.38
2	C	903	HEM	C4A-NA	2.14	1.43	1.39
2	C	903	HEM	CAB-C3B	2.13	1.53	1.47
2	C	903	HEM	O1D-CGD	2.07	1.28	1.22
2	A	901	HEM	O1D-CGD	2.05	1.28	1.22
2	B	902	HEM	C1B-C2B	-2.04	1.40	1.44
2	B	902	HEM	CMC-C2C	-2.02	1.46	1.50
2	A	901	HEM	C1D-C2D	-2.01	1.40	1.44

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	HEM	C3B-C2B-C1B	12.76	115.99	106.41
2	B	902	HEM	C3B-C2B-C1B	8.08	112.48	106.41
2	C	903	HEM	C3B-C2B-C1B	7.94	112.38	106.41
2	B	902	HEM	CHA-C4D-ND	7.88	134.12	124.37
2	C	903	HEM	C4D-ND-C1D	7.59	114.19	105.21
2	C	903	HEM	CHC-C4B-NB	7.20	132.17	124.42
2	C	903	HEM	CHA-C4D-ND	7.07	133.12	124.37
2	B	902	HEM	C4D-ND-C1D	7.06	113.57	105.21
4	A	2001	DTV	C3-C4-S4	-6.91	95.13	114.43
2	A	901	HEM	C4B-C3B-C2B	-6.74	101.09	107.28
2	A	901	HEM	C4C-C3C-C2C	6.61	112.55	106.81
2	B	902	HEM	CMA-C3A-C4A	-6.59	115.38	125.42
2	A	901	HEM	C4D-ND-C1D	6.06	112.39	105.21
2	B	902	HEM	C4A-C3A-C2A	6.01	113.70	106.82
4	A	2001	DTV	C2-C1-S1	-5.95	97.80	114.43
2	A	901	HEM	CHC-C4B-NB	5.94	130.81	124.42
2	B	902	HEM	CHC-C4B-NB	5.77	130.63	124.42
2	C	903	HEM	C2D-C1D-ND	-5.71	103.30	109.90
2	A	901	HEM	CHD-C1D-ND	4.91	129.71	124.42
2	A	901	HEM	CHA-C4D-ND	4.84	130.36	124.37
2	A	901	HEM	CAD-CBD-CGD	4.76	126.30	113.67
2	A	901	HEM	O2D-CGD-O1D	-4.69	111.27	123.33
2	B	902	HEM	C3D-C4D-ND	-4.59	105.14	110.17
2	B	902	HEM	C2B-C1B-NB	-4.57	104.58	109.84
2	A	901	HEM	CBD-CAD-C3D	-4.47	100.16	112.53
2	B	902	HEM	CMB-C2B-C1B	-4.36	118.22	125.03
2	B	902	HEM	CHC-C1C-NC	4.34	129.18	124.45
2	A	901	HEM	C2B-C1B-NB	-4.28	104.92	109.84
2	C	903	HEM	C3D-C4D-ND	-4.25	105.51	110.17
2	C	903	HEM	C1D-C2D-C3D	4.24	111.44	106.98
2	A	901	HEM	C4A-C3A-C2A	3.95	111.34	106.82
2	B	902	HEM	C2D-C1D-ND	-3.95	105.34	109.90
2	A	901	HEM	C2D-C1D-ND	-3.93	105.36	109.90
2	B	902	HEM	CHD-C1D-C2D	3.84	131.09	125.03
2	C	903	HEM	CHD-C1D-C2D	3.83	131.07	125.03
2	C	903	HEM	C2B-C1B-NB	-3.73	105.55	109.84
2	B	902	HEM	CHD-C4C-NC	-3.56	120.58	124.45
2	C	903	HEM	C1C-CHC-C4B	-3.50	118.57	126.02
2	C	903	HEM	C1B-NB-C4B	3.41	109.25	105.21
2	A	901	HEM	C1B-NB-C4B	3.41	109.24	105.21
2	C	903	HEM	C4C-NC-C1C	-3.39	100.29	105.82
2	A	901	HEM	CAD-C3D-C4D	3.34	130.53	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	HEM	CHA-C4D-C3D	-3.29	119.16	125.23
2	B	902	HEM	CAA-CBA-CGA	-3.29	104.95	113.67
2	A	901	HEM	CHA-C1A-NA	3.22	129.70	123.86
2	B	902	HEM	C1A-C2A-C3A	-3.14	102.01	106.87
2	A	901	HEM	CMB-C2B-C1B	-3.00	120.35	125.03
2	A	901	HEM	C3C-C2C-C1C	-2.99	104.21	107.05
4	B	2002	DTV	O3-C3-C2	-2.91	103.47	109.57
2	C	903	HEM	C4A-C3A-C2A	2.91	110.15	106.82
2	A	901	HEM	C4D-C3D-C2D	-2.89	102.68	106.89
2	B	902	HEM	CHD-C4C-C3C	2.87	130.05	125.21
2	B	902	HEM	C1C-CHC-C4B	-2.86	119.93	126.02
4	C	2003	DTV	C2-C1-S1	-2.85	106.48	114.43
2	A	901	HEM	C3A-C4A-NA	-2.82	105.62	110.14
2	A	901	HEM	CMA-C3A-C4A	-2.78	121.18	125.42
2	B	902	HEM	CAA-C2A-C1A	2.78	130.37	124.94
2	C	903	HEM	C3B-C4B-NB	-2.76	107.49	109.47
2	B	902	HEM	C1D-C2D-C3D	2.74	109.87	106.98
2	B	902	HEM	O2D-CGD-CBD	2.72	122.59	114.00
2	C	903	HEM	CHC-C1C-NC	-2.69	121.53	124.45
2	A	901	HEM	CBC-CAC-C3C	-2.68	114.11	127.53
2	B	902	HEM	C3A-C4A-NA	-2.68	105.85	110.14
2	A	901	HEM	C1A-CHA-C4D	-2.67	119.97	126.25
2	A	901	HEM	O2D-CGD-CBD	2.54	122.03	114.00
2	A	901	HEM	CHD-C4C-C3C	2.50	129.43	125.21
2	C	903	HEM	C1A-CHA-C4D	-2.47	120.43	126.25
2	B	902	HEM	CMA-C3A-C2A	2.46	130.84	125.62
2	B	902	HEM	C1B-NB-C4B	2.44	108.09	105.21
2	B	902	HEM	CHA-C4D-C3D	-2.43	120.74	125.23
2	C	903	HEM	CHC-C4B-C3B	-2.42	120.25	125.07
2	C	903	HEM	C2C-C1C-NC	2.36	114.01	109.64
2	C	903	HEM	CHA-C4D-C3D	-2.36	120.87	125.23
2	A	901	HEM	CHC-C4B-C3B	-2.29	120.51	125.07
2	B	902	HEM	C2C-C1C-NC	-2.28	105.43	109.64
2	C	903	HEM	C3A-C4A-NA	-2.26	106.51	110.14
2	C	903	HEM	C4B-C3B-C2B	-2.25	105.21	107.28
2	B	902	HEM	O2A-CGA-CBA	2.24	121.07	114.00
2	C	903	HEM	CAA-CBA-CGA	-2.21	107.80	113.67
2	A	901	HEM	O2A-CGA-CBA	2.19	120.93	114.00
2	B	902	HEM	C3C-C2C-C1C	2.18	109.11	107.05
2	B	902	HEM	CBD-CAD-C3D	-2.16	106.57	112.53
2	A	901	HEM	C1D-C2D-C3D	2.12	109.22	106.98
2	C	903	HEM	CHD-C4C-NC	2.10	126.74	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	903	HEM	CHD-C4C-C3C	-2.10	121.67	125.21
2	B	902	HEM	O2A-CGA-O1A	-2.09	117.95	123.33
2	C	903	HEM	CBC-CAC-C3C	-2.08	117.14	127.53
2	B	902	HEM	C4C-CHD-C1D	2.06	130.40	126.02
2	C	903	HEM	O2D-CGD-O1D	-2.04	118.08	123.33
2	B	902	HEM	C2A-C1A-NA	2.04	112.41	110.15
2	A	901	HEM	O2A-CGA-O1A	-2.01	118.15	123.33

There are no chirality outliers.

All (22) 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
2	A	901	HEM	C2C-C3C-CAC-CBC
2	C	903	HEM	C2C-C3C-CAC-CBC
2	C	903	HEM	C4C-C3C-CAC-CBC
4	A	2001	DTV	O3-C3-C4-S4
2	A	901	HEM	C4C-C3C-CAC-CBC
2	B	902	HEM	CAA-CBA-CGA-O1A
2	B	902	HEM	CAD-CBD-CGD-O1D
2	C	903	HEM	CAA-CBA-CGA-O2A
2	B	902	HEM	CAA-CBA-CGA-O2A
2	C	903	HEM	CAA-CBA-CGA-O1A
2	A	901	HEM	CAD-CBD-CGD-O1D
2	B	902	HEM	CAD-CBD-CGD-O2D
2	A	901	HEM	CAD-CBD-CGD-O2D
2	A	901	HEM	CAA-CBA-CGA-O2A
2	A	901	HEM	CAA-CBA-CGA-O1A
4	C	2003	DTV	C1-C2-C3-C4
2	A	901	HEM	C3D-CAD-CBD-CGD

There are no ring outliers.

3 monomers are involved in 4 short contacts:

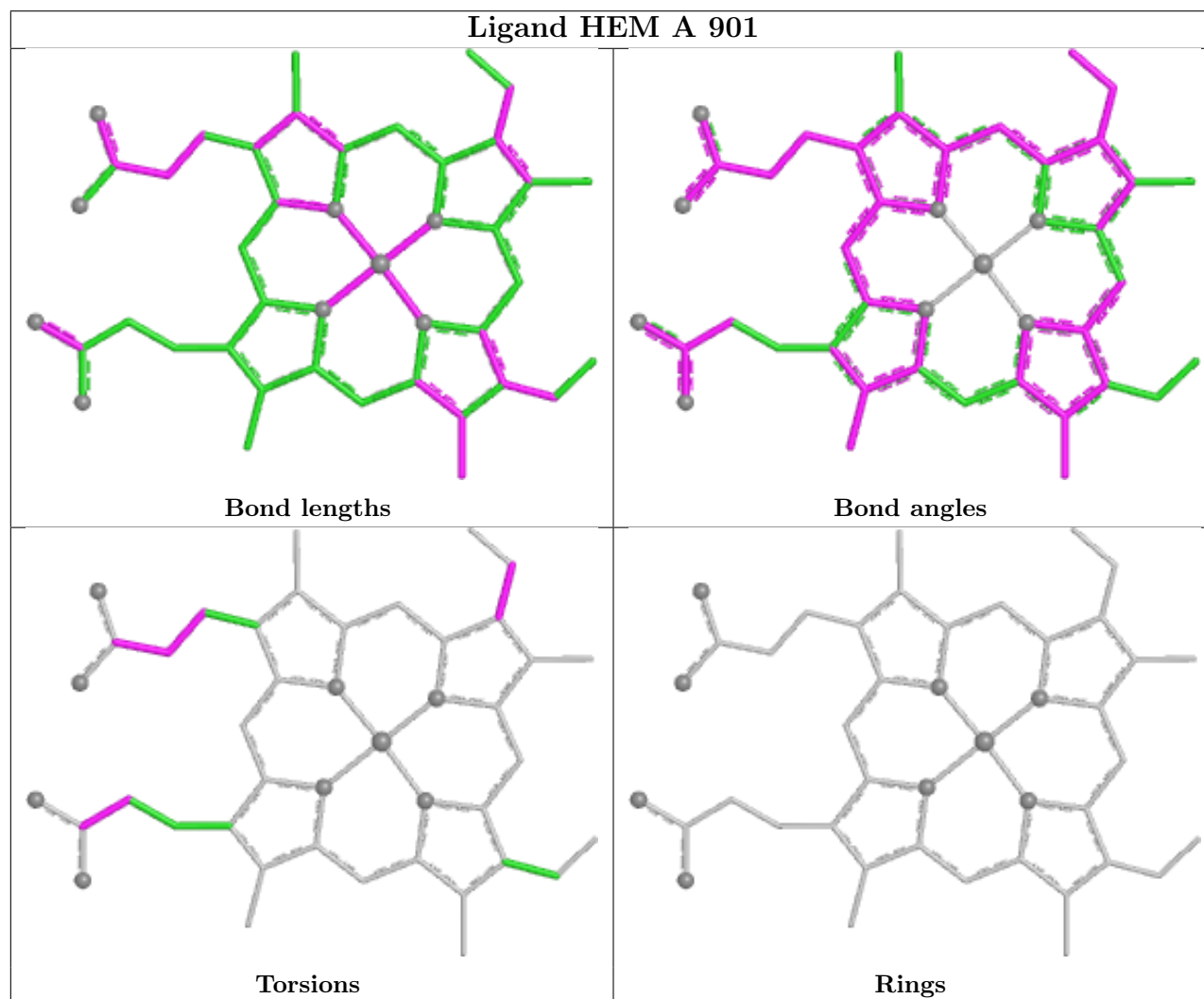
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2003	DTV	1	0
2	C	903	HEM	2	0

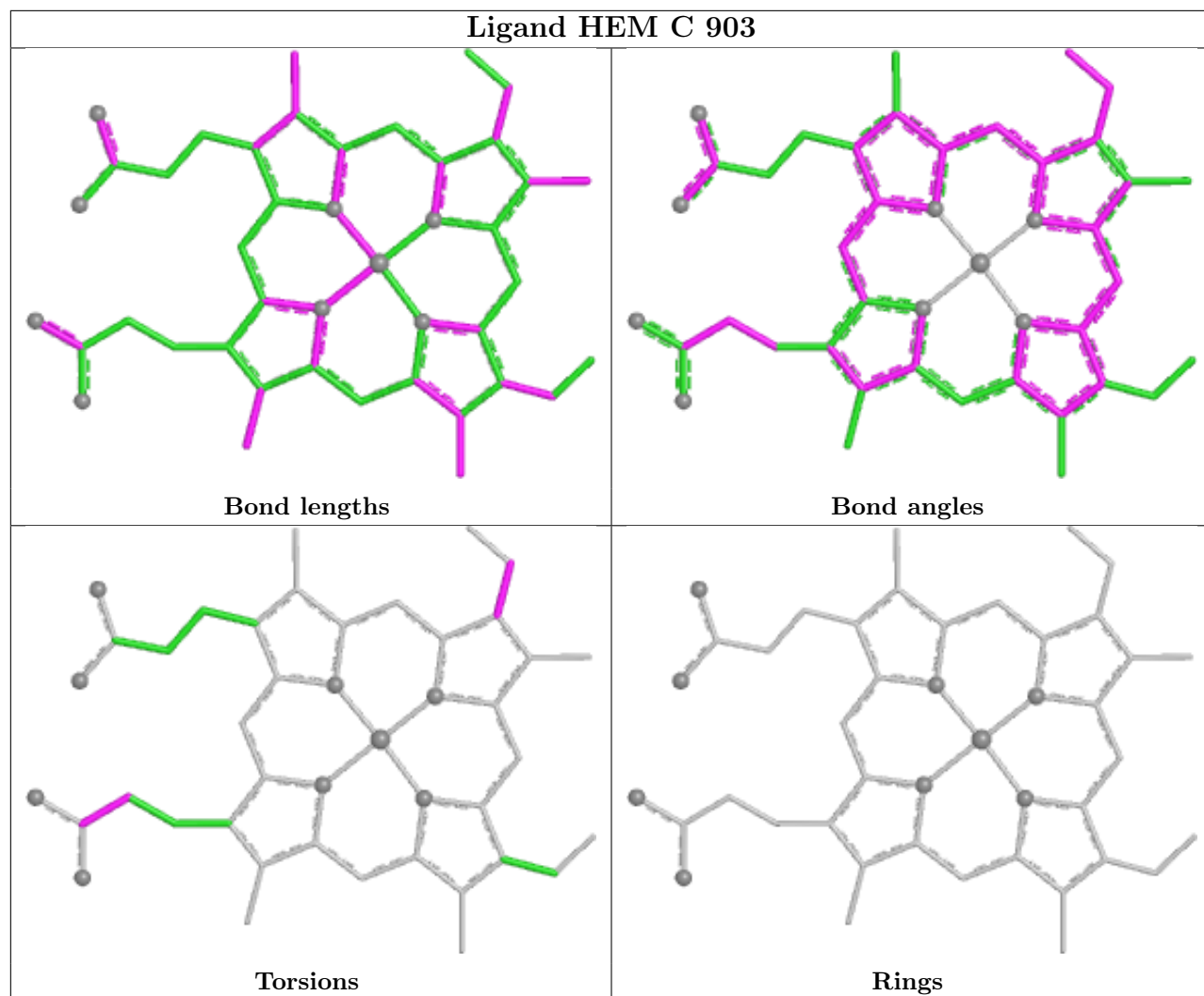
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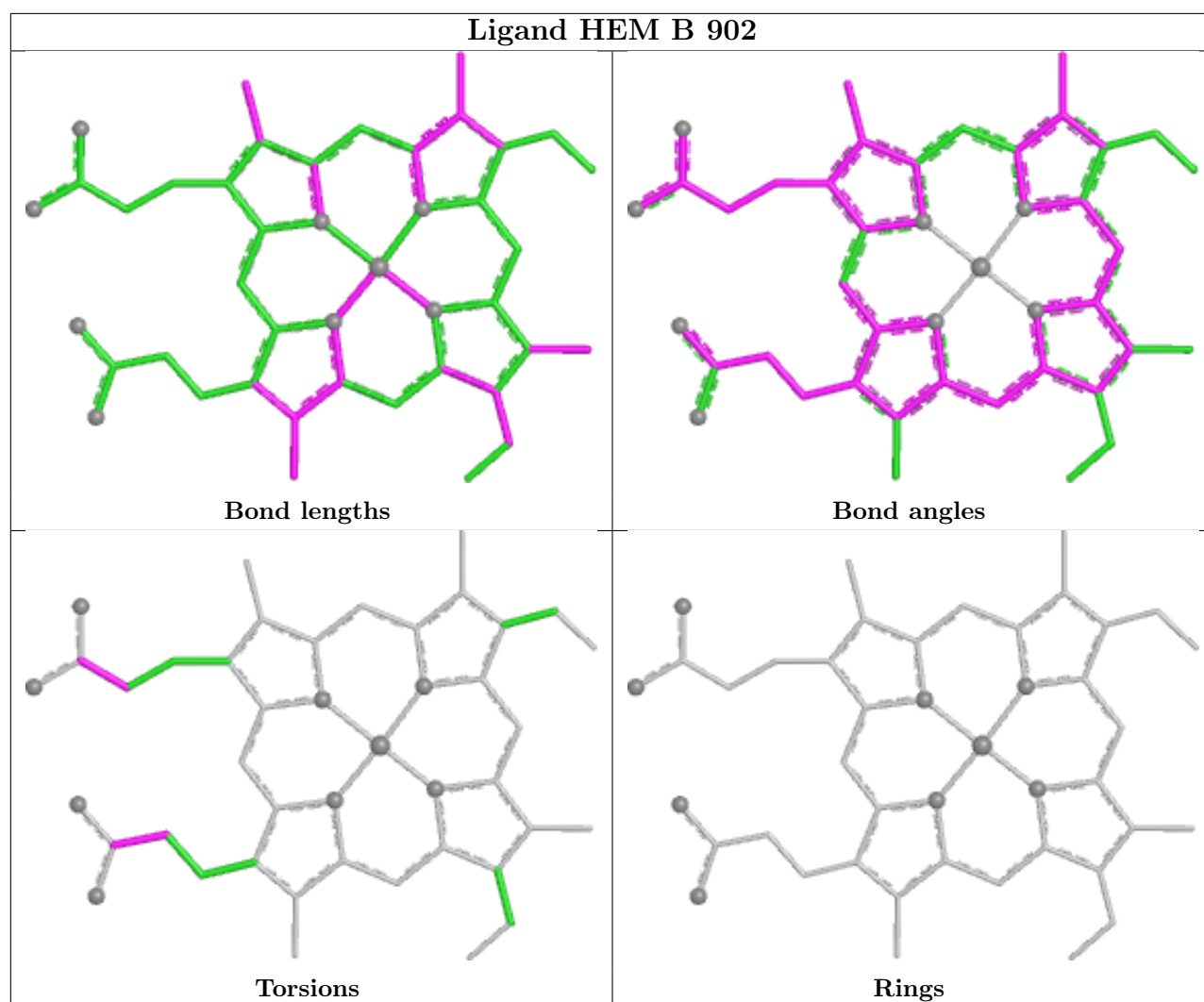
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	902	HEM	2	0

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%)	0.64	13 (6%) 26 28	13, 22, 36, 42	1 (0%)
1	B	209/215 (97%)	0.27	6 (2%) 53 58	12, 21, 33, 42	0
1	C	207/215 (96%)	1.07	32 (15%) 5 5	16, 26, 42, 54	0
All	All	623/645 (96%)	0.66	51 (8%) 17 19	12, 23, 37, 54	1 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	771	VAL	4.6
1	C	767	ALA	4.5
1	C	765	GLY	4.5
1	C	754	ASP	3.3
1	C	762	HIS	3.3
1	B	325	HIS	2.9
1	C	610	VAL	2.9
1	A	174	ASP	2.8
1	C	608	LEU	2.8
1	A	100	ILE	2.7
1	C	630	SER	2.6
1	A	191	GLU	2.6
1	A	25	HIS	2.5
1	C	625	HIS	2.5
1	A	94	SER	2.4
1	C	676	ALA	2.4
1	C	766	ILE	2.4
1	C	813	LYS	2.4
1	C	774	ASP	2.3
1	C	763	PHE	2.3
1	A	166	ILE	2.3
1	C	768	LYS	2.3
1	C	812	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	787	ASP	2.2
1	B	399	ARG	2.2
1	C	668	PHE	2.2
1	C	807	VAL	2.2
1	C	783	LEU	2.2
1	A	7	GLY	2.2
1	A	156	GLU	2.2
1	A	171	VAL	2.2
1	C	784	GLU	2.2
1	A	188	GLU	2.1
1	C	669	ALA	2.1
1	B	474	ASP	2.1
1	C	607	GLY	2.1
1	A	167	ALA	2.1
1	C	619	ALA	2.1
1	C	745	ARG	2.1
1	B	393	SER	2.1
1	A	187	ASP	2.1
1	C	617	ALA	2.0
1	C	614	GLN	2.0
1	B	392	GLY	2.0
1	C	798	THR	2.0
1	C	805	HIS	2.0
1	B	484	GLU	2.0
1	C	663	VAL	2.0
1	C	612	LEU	2.0
1	C	780	LEU	2.0
1	A	98	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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,

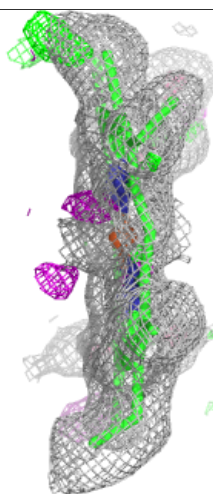
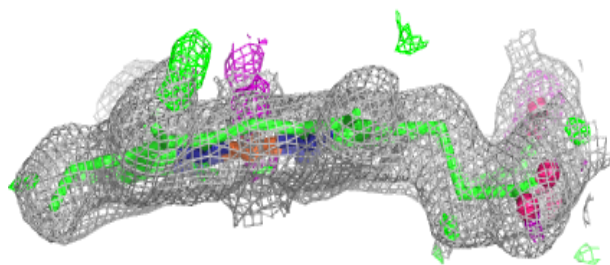
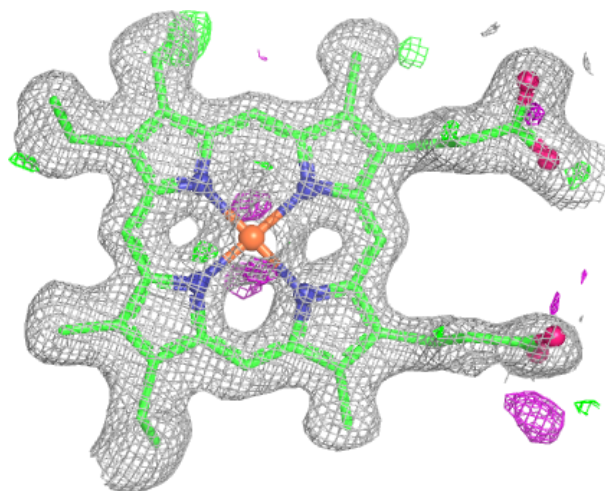
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	1010	5/5	0.65	0.18	55,58,61,62	0
3	SO4	A	1005	5/5	0.67	0.17	108,109,109,109	0
3	SO4	C	1009	5/5	0.80	0.16	56,58,60,60	0
3	SO4	C	1011	5/5	0.84	0.13	95,96,97,97	0
3	SO4	B	1008	5/5	0.85	0.12	35,35,44,46	0
3	SO4	B	1002	5/5	0.88	0.12	45,49,51,52	0
3	SO4	B	1004	5/5	0.88	0.12	41,44,47,51	0
3	SO4	A	1001	5/5	0.92	0.08	43,43,46,51	0
3	SO4	B	1003	5/5	0.93	0.09	35,37,41,42	0
4	DTV	C	2003	8/8	0.94	0.10	27,30,39,45	0
4	DTV	A	2001	8/8	0.95	0.11	20,30,32,32	0
2	HEM	C	903	43/43	0.95	0.11	18,26,39,50	0
2	HEM	A	901	43/43	0.96	0.09	16,22,33,39	0
2	HEM	B	902	43/43	0.97	0.08	14,19,30,51	0
4	DTV	B	2002	8/8	0.98	0.06	18,21,24,28	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.

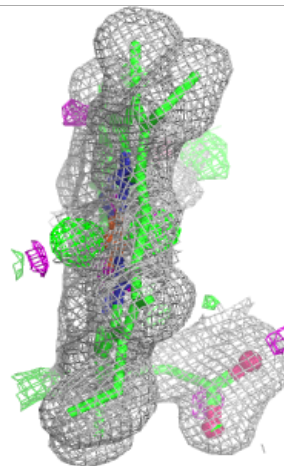
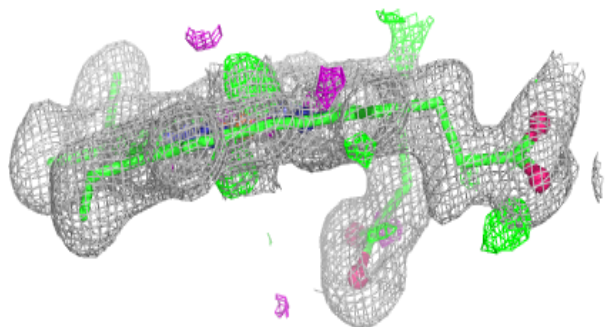
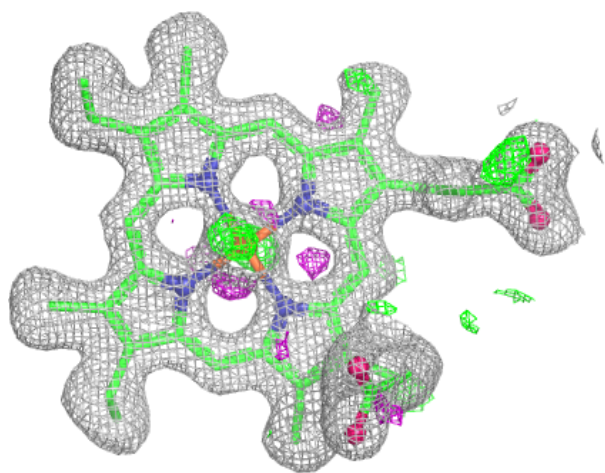
Electron density around HEM C 903:

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



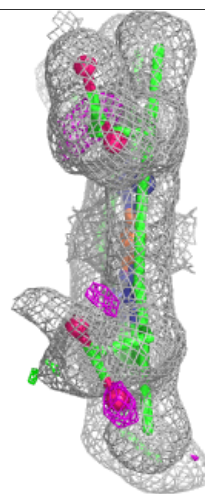
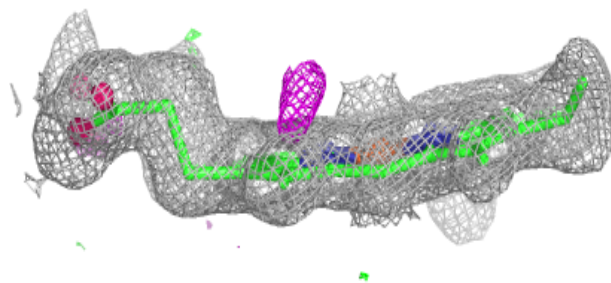
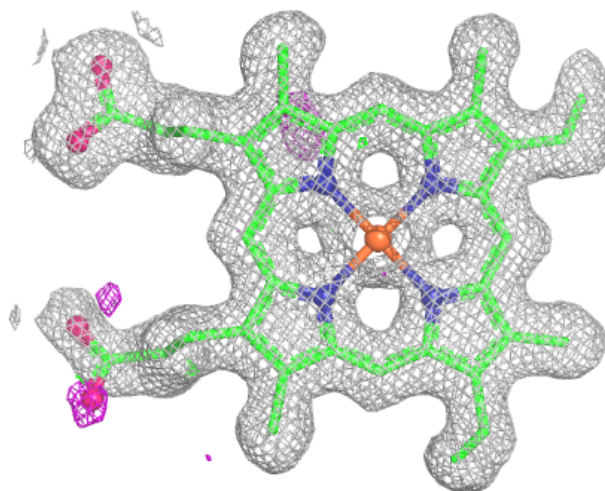
Electron density around HEM A 901:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.