



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:30 PM UTC

PDB ID : 1WNV / pdb_00001wnv
Title : D136A mutant of Heme Oxygenase from *Corynebacterium diphtheriae* (HmuO)
Authors : Matsui, T.; Unno, M.; Ikeda-Saito, M.
Deposited on : 2004-08-10
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

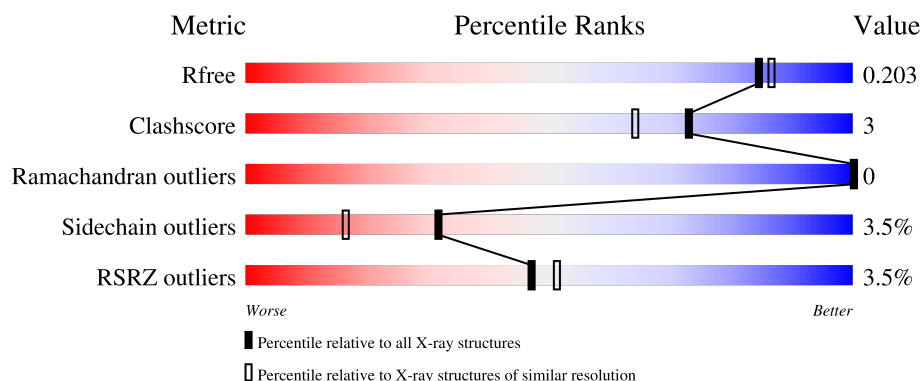
1 Overall quality at a glance

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	3% 87% 9% .
1	B	215	5% 88% 8% ..
1	C	215	3% 88% 7% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5426 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Heme oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1649	1041	293	312	3			
1	B	210	Total	C	N	O	S	0	0	0
			1666	1052	296	315	3			
1	C	207	Total	C	N	O	S	0	0	0
			1649	1041	293	312	3			

There are 18 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	136	ALA	ASP	engineered mutation	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	436	ALA	ASP	engineered mutation	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	736	ALA	ASP	engineered mutation	UNP P71119
C	792	HIS	ASN	SEE REMARK 999	UNP P71119

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- 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	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

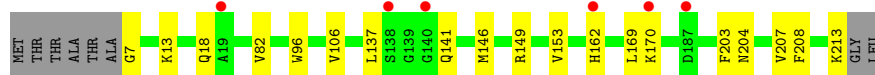
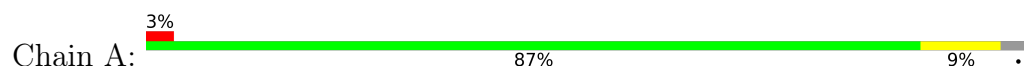
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total	O	0	0
			65	65		
4	B	119	Total	O	0	0
			119	119		
4	C	124	Total	O	0	0
			124	124		

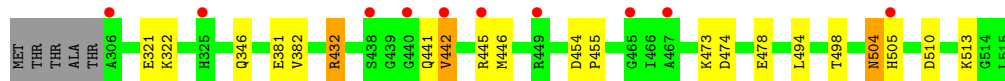
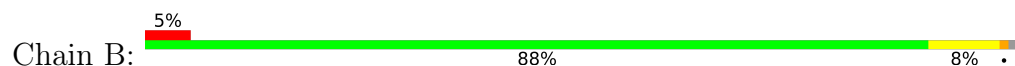
3 Residue-property plots [i](#)

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.

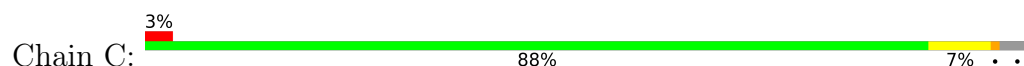
- Molecule 1: Heme oxygenase



- 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	54.13Å 62.78Å 107.99Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.85 20.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-1.85) 98.0 (20.00-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.164 , 0.204 (Not available) , 0.203	Depositor DCC
R_{free} test set	6049 reflections (10.13%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 41.7	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	0.95	EDS
Total number of atoms	5426	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, HEM

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	1.13	2/1681 (0.1%)	1.13	3/2270 (0.1%)
1	B	1.26	3/1698 (0.2%)	1.14	1/2293 (0.0%)
1	C	1.25	0/1681	1.10	0/2270
All	All	1.21	5/5060 (0.1%)	1.12	4/6833 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	VAL	CA-CB	-5.82	1.47	1.54
1	B	494	LEU	C-O	5.77	1.30	1.24
1	B	382	VAL	CA-CB	5.23	1.60	1.54
1	B	381	GLU	CD-OE2	5.16	1.35	1.25
1	A	7	GLY	N-CA	5.02	1.53	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	TRP	N-CA-C	5.74	117.54	111.28
1	A	153	VAL	CA-C-N	5.33	127.81	120.67
1	A	153	VAL	C-N-CA	5.33	127.81	120.67
1	B	504	ASN	N-CA-C	5.02	116.44	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1649	0	1612	8	0
1	B	1666	0	1631	8	0
1	C	1649	0	1612	13	0
2	A	5	0	0	0	0
2	B	10	0	0	1	0
2	C	10	0	0	0	0
3	A	43	0	30	1	0
3	B	43	0	30	1	0
3	C	43	0	30	2	0
4	A	65	0	0	4	0
4	B	119	0	0	0	0
4	C	124	0	0	2	0
All	All	5426	0	4945	32	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 3.

All (32) 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:634:LYS:HG3	4:C:44:HOH:O	1.68	0.92
1:C:642:PHE:CG	1:C:747:MET:HE2	2.30	0.67
1:A:204:ASN:ND2	1:A:208:PHE:CE2	2.68	0.62
1:B:473:LYS:NZ	2:B:2011:SO4:O2	2.33	0.60
1:A:82:VAL:HG23	4:A:2022:HOH:O	2.02	0.58
1:A:208:PHE:CD2	4:A:2056:HOH:O	2.53	0.58
1:B:442:VAL:HG13	1:B:446:MET:HE3	1.86	0.57
1:C:646:GLN:HE21	1:C:646:GLN:HA	1.72	0.55
3:C:903:HEM:HBB2	3:C:903:HEM:HHC	1.89	0.53
1:C:646:GLN:HA	1:C:646:GLN:NE2	2.24	0.52
3:A:901:HEM:HBD1	4:A:2072:HOH:O	2.10	0.51
1:C:741:GLN:HG3	4:C:77:HOH:O	2.11	0.51
1:C:704:PRO:HD2	1:C:810:ASP:OD2	2.11	0.50
1:B:442:VAL:HG13	1:B:446:MET:CE	2.42	0.49
1:A:137:LEU:HD22	1:A:169:LEU:HD11	1.94	0.49
1:A:13:LYS:NZ	4:A:2072:HOH:O	2.46	0.48
1:C:738:SER:HB3	3:C:903:HEM:HBD1	1.95	0.48
1:B:432:ARG:NH1	1:B:504:ASN:OD1	2.46	0.48
3:B:902:HEM:HBC2	3:B:902:HEM:HHD	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:ASP:HA	1:B:513:LYS:HE3	1.97	0.47
1:A:146:MET:HA	1:A:146:MET:HE2	1.97	0.46
1:B:454:ASP:OD2	1:B:455:PRO:HD2	2.15	0.46
1:C:642:PHE:HB2	1:C:747:MET:HE1	1.98	0.46
1:C:642:PHE:HB2	1:C:747:MET:CE	2.46	0.45
1:B:322:LYS:HG2	1:B:505:HIS:CD2	2.52	0.45
1:B:474:ASP:O	1:B:478:GLU:HG3	2.17	0.43
1:A:146:MET:HE1	1:A:149:ARG:CZ	2.50	0.42
1:C:689:LYS:HE2	1:C:689:LYS:HB3	1.68	0.42
1:C:793:LEU:C	1:C:793:LEU:HD23	2.46	0.41
1:C:695:GLU:OE2	1:C:699:ARG:HD3	2.21	0.41
1:C:700:ILE:HD13	1:C:700:ILE:HG21	1.75	0.41
1:A:203:PHE:O	1:A:207:VAL:HG23	2.22	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	205/215 (95%)	200 (98%)	5 (2%)	0	100	100
1	B	208/215 (97%)	205 (99%)	3 (1%)	0	100	100
1	C	205/215 (95%)	203 (99%)	2 (1%)	0	100	100
All	All	618/645 (96%)	608 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/174 (97%)	164 (97%)	5 (3%)	36	21
1	B	170/174 (98%)	163 (96%)	7 (4%)	27	12
1	C	169/174 (97%)	163 (96%)	6 (4%)	31	16
All	All	508/522 (97%)	490 (96%)	18 (4%)	32	16

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	141	GLN
1	A	162	HIS
1	A	170	LYS
1	A	213	LYS
1	B	321	GLU
1	B	346	GLN
1	B	432	ARG
1	B	441	GLN
1	B	442	VAL
1	B	445	ARG
1	B	498	THR
1	C	614	GLN
1	C	646	GLN
1	C	689	LYS
1	C	708	ASP
1	C	783	LEU
1	C	798	THR

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

Mol	Chain	Res	Type
1	A	78	ASN
1	A	182	ASN
1	B	325	HIS
1	B	378	ASN
1	B	448	GLN
1	B	505	HIS
1	B	506	GLN
1	C	646	GLN

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Mol	Chain	Res	Type
1	C	678	ASN
1	C	741	GLN
1	C	748	GLN
1	C	762	HIS
1	C	806	GLN

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](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	HEM	C	903	1,4	50,50,50	1.67	9 (18%)	67,82,82	1.48	13 (19%)
2	SO4	B	2012	-	4,4,4	0.46	0	6,6,6	0.74	0
2	SO4	C	2014	-	4,4,4	0.29	0	6,6,6	0.81	0
2	SO4	B	2011	-	4,4,4	0.28	0	6,6,6	0.84	0
2	SO4	C	2015	-	4,4,4	0.31	0	6,6,6	0.63	0
3	HEM	A	901	1,4	50,50,50	1.74	7 (14%)	67,82,82	1.45	11 (16%)
3	HEM	B	902	1,4	50,50,50	1.80	12 (24%)	67,82,82	1.35	8 (11%)
2	SO4	A	2013	-	4,4,4	0.21	0	6,6,6	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	C	903	1,4	-	2/14/54/54	-
3	HEM	A	901	1,4	-	9/14/54/54	-
3	HEM	B	902	1,4	-	3/14/54/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	HEM	C3D-C2D	6.75	1.51	1.36
3	B	902	HEM	C3D-C2D	6.54	1.50	1.36
3	C	903	HEM	C3D-C2D	5.92	1.49	1.36
3	A	901	HEM	FE-NA	4.35	2.09	1.95
3	B	902	HEM	FE-NC	4.18	2.09	1.95
3	C	903	HEM	FE-ND	3.82	2.06	1.94
3	A	901	HEM	FE-ND	3.51	2.05	1.94
3	A	901	HEM	FE-NB	3.10	2.04	1.94
3	B	902	HEM	CAC-C3C	3.05	1.55	1.47
3	B	902	HEM	CMB-C2B	2.95	1.56	1.50
3	C	903	HEM	FE-NB	2.89	2.03	1.94
3	A	901	HEM	CAB-C3B	2.84	1.55	1.47
3	C	903	HEM	CAB-C3B	2.78	1.54	1.47
3	B	902	HEM	FE-ND	2.77	2.03	1.94
3	A	901	HEM	CAC-C3C	2.72	1.54	1.47
3	C	903	HEM	CAC-C3C	2.56	1.54	1.47
3	B	902	HEM	C4D-ND	-2.45	1.36	1.40
3	B	902	HEM	CMC-C2C	2.32	1.55	1.50
3	A	901	HEM	C1B-NB	-2.30	1.36	1.40
3	C	903	HEM	C1B-NB	-2.30	1.36	1.40
3	B	902	HEM	CAB-C3B	2.19	1.53	1.47
3	B	902	HEM	C4B-NB	-2.17	1.34	1.38
3	B	902	HEM	C3B-C2B	-2.16	1.32	1.37
3	C	903	HEM	CHA-C4D	-2.16	1.34	1.38
3	C	903	HEM	CMA-C3A	2.15	1.55	1.50
3	B	902	HEM	FE-NB	2.11	2.01	1.94
3	B	902	HEM	C2A-C3A	-2.09	1.33	1.38
3	C	903	HEM	C2A-C3A	-2.04	1.33	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	HEM	C4D-ND-C1D	4.89	110.99	105.21
3	A	901	HEM	CAD-C3D-C4D	4.09	131.82	124.70
3	B	902	HEM	C4D-ND-C1D	3.96	109.90	105.21
3	B	902	HEM	CHC-C4B-NB	3.80	128.51	124.42
3	C	903	HEM	C1B-NB-C4B	3.72	109.62	105.21
3	B	902	HEM	C3B-C4B-NB	-3.43	107.00	109.47
3	C	903	HEM	C3B-C4B-NB	-3.35	107.06	109.47
3	B	902	HEM	C4B-C3B-C2B	3.34	110.35	107.28
3	A	901	HEM	O2D-CGD-CBD	3.27	124.33	114.00
3	C	903	HEM	CAD-C3D-C4D	3.10	130.09	124.70
3	C	903	HEM	O1A-CGA-CBA	-2.92	113.83	123.09
3	B	902	HEM	CAA-CBA-CGA	-2.75	106.36	113.67
3	B	902	HEM	CHD-C1D-ND	2.73	127.36	124.42
3	C	903	HEM	C4D-C3D-C2D	-2.69	102.97	106.89
3	C	903	HEM	CAA-CBA-CGA	-2.68	106.56	113.67
3	A	901	HEM	CHD-C1D-ND	2.68	127.30	124.42
3	C	903	HEM	C4D-ND-C1D	2.66	108.36	105.21
3	C	903	HEM	CHB-C1B-NB	2.62	127.61	124.37
3	B	902	HEM	C1B-NB-C4B	2.54	108.21	105.21
3	A	901	HEM	O1D-CGD-CBD	-2.49	115.19	123.09
3	C	903	HEM	CMD-C2D-C1D	2.46	128.88	125.03
3	C	903	HEM	CMB-C2B-C1B	2.43	128.83	125.03
3	A	901	HEM	CAA-CBA-CGA	-2.40	107.29	113.67
3	A	901	HEM	CBB-CAB-C3B	-2.36	115.73	127.53
3	A	901	HEM	C1B-NB-C4B	2.34	107.98	105.21
3	C	903	HEM	O2A-CGA-CBA	2.23	121.04	114.00
3	A	901	HEM	CAD-C3D-C2D	-2.12	123.89	127.87
3	C	903	HEM	C2B-C1B-NB	-2.12	107.41	109.84
3	A	901	HEM	C3B-C4B-NB	-2.11	107.95	109.47
3	A	901	HEM	C3B-C2B-C1B	2.09	107.98	106.41
3	C	903	HEM	O1D-CGD-CBD	-2.08	116.50	123.09
3	B	902	HEM	CMB-C2B-C1B	2.06	128.25	125.03

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	HEM	C2C-C3C-CAC-CBC
3	A	901	HEM	C4D-C3D-CAD-CBD
3	A	901	HEM	C2D-C3D-CAD-CBD
3	A	901	HEM	C3D-CAD-CBD-CGD
3	A	901	HEM	C2B-C3B-CAB-CBB
3	A	901	HEM	C4C-C3C-CAC-CBC

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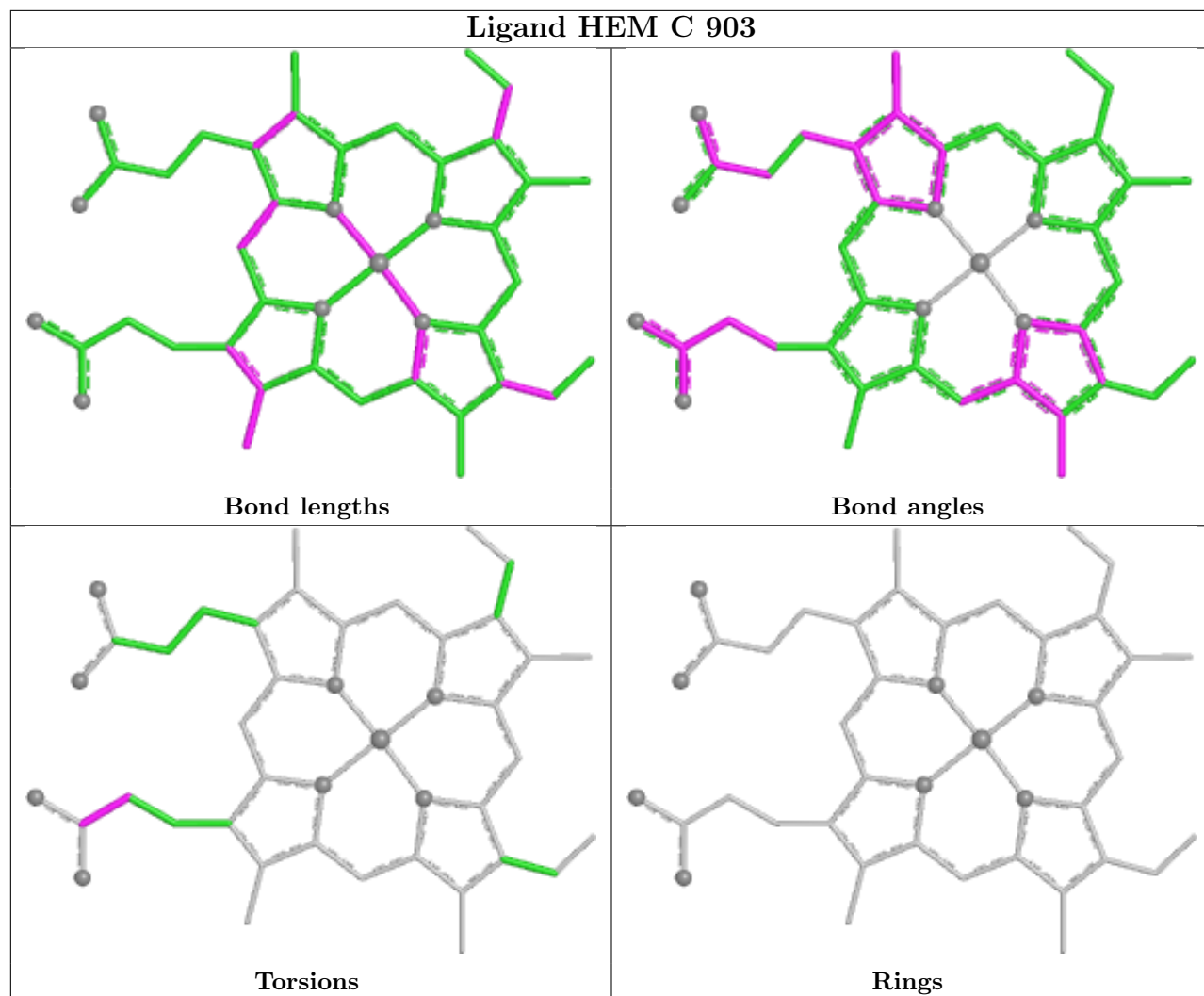
Mol	Chain	Res	Type	Atoms
3	C	903	HEM	CAA-CBA-CGA-O1A
3	B	902	HEM	CAA-CBA-CGA-O1A
3	C	903	HEM	CAA-CBA-CGA-O2A
3	B	902	HEM	CAA-CBA-CGA-O2A
3	A	901	HEM	CAA-CBA-CGA-O2A
3	A	901	HEM	CAA-CBA-CGA-O1A
3	A	901	HEM	C4B-C3B-CAB-CBB
3	B	902	HEM	C2B-C3B-CAB-CBB

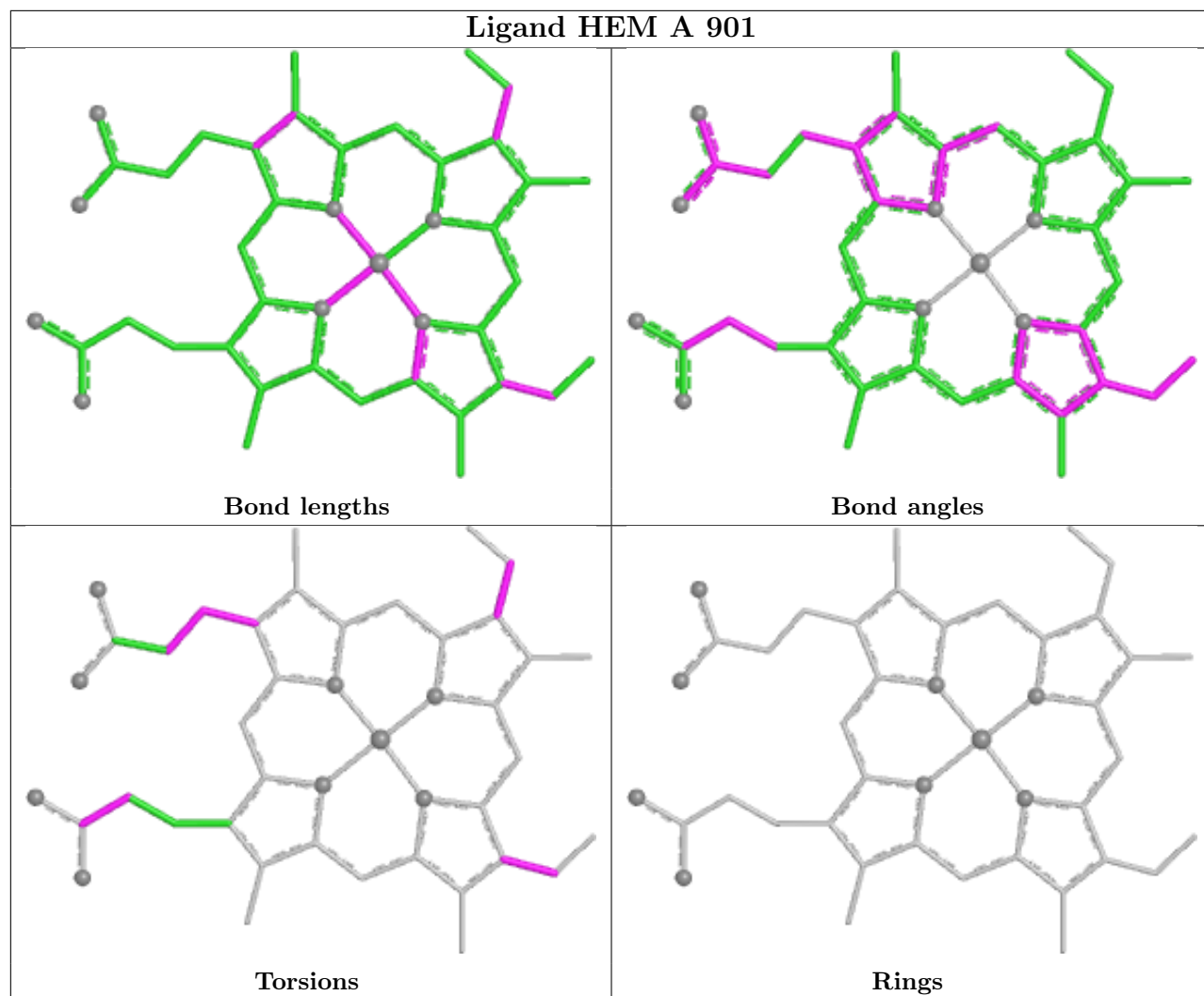
There are no ring outliers.

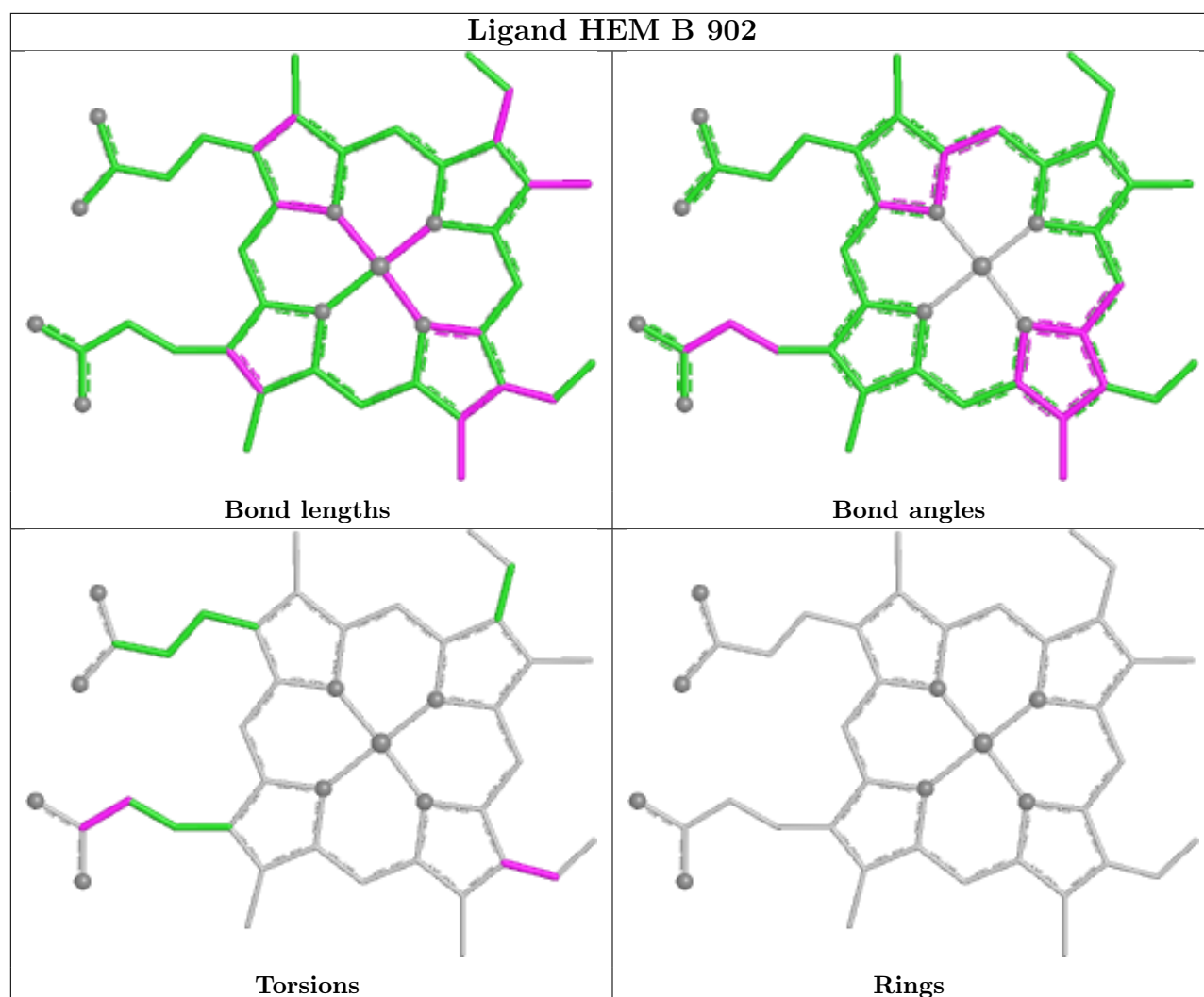
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	903	HEM	2	0
2	B	2011	SO4	1	0
3	A	901	HEM	1	0
3	B	902	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	207/215 (96%)	0.35	6 (2%) 53 57	25, 37, 55, 60	0
1	B	210/215 (97%)	0.08	10 (4%) 35 39	20, 29, 48, 58	0
1	C	207/215 (96%)	0.12	6 (2%) 53 57	20, 30, 46, 58	0
All	All	624/645 (96%)	0.18	22 (3%) 47 51	20, 32, 52, 60	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	325	HIS	3.4
1	A	138	SER	2.9
1	C	765	GLY	2.9
1	B	445	ARG	2.8
1	B	467	ALA	2.8
1	B	440	GLY	2.7
1	A	187	ASP	2.6
1	C	767	ALA	2.6
1	A	170	LYS	2.5
1	A	162	HIS	2.5
1	B	438	SER	2.4
1	B	306	ALA	2.4
1	B	465	GLY	2.4
1	C	762	HIS	2.3
1	C	621	GLU	2.2
1	B	505	HIS	2.2
1	C	813	LYS	2.2
1	A	140	GLY	2.1
1	B	449	ARG	2.1
1	C	739	GLY	2.0
1	A	19	ALA	2.0
1	B	442	VAL	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](#)

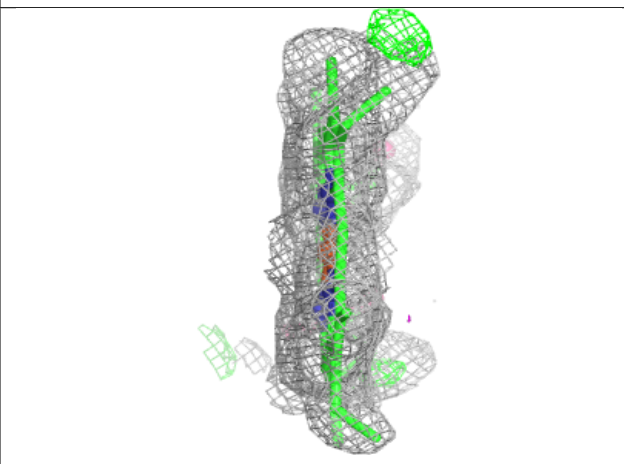
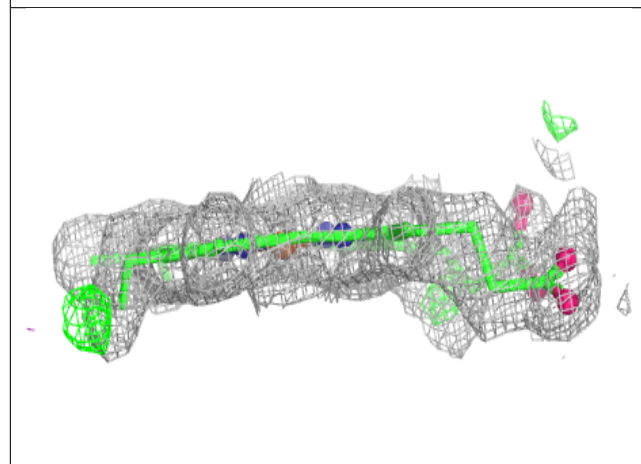
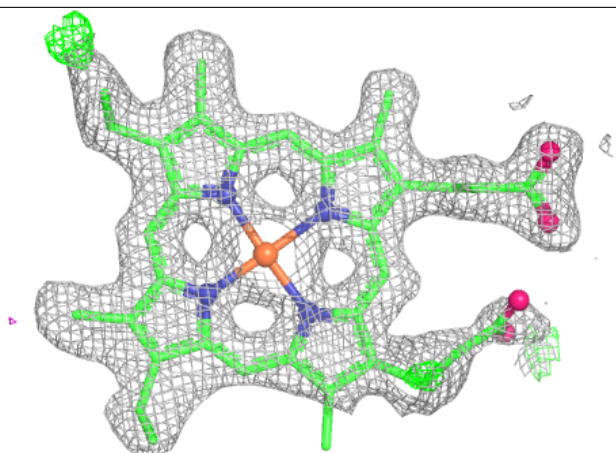
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	2014	5/5	0.84	0.15	38,39,41,42	5
2	SO4	A	2013	5/5	0.86	0.14	44,44,45,46	5
2	SO4	B	2011	5/5	0.91	0.09	32,32,36,37	5
2	SO4	C	2015	5/5	0.93	0.10	28,28,34,34	5
2	SO4	B	2012	5/5	0.95	0.11	25,26,30,32	5
3	HEM	A	901	43/43	0.96	0.10	30,43,86,88	0
3	HEM	B	902	43/43	0.97	0.09	27,36,57,69	0
3	HEM	C	903	43/43	0.97	0.09	23,34,49,52	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.

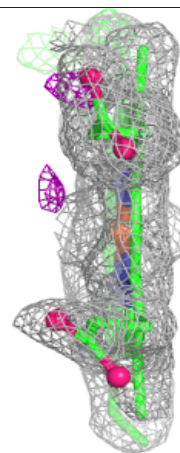
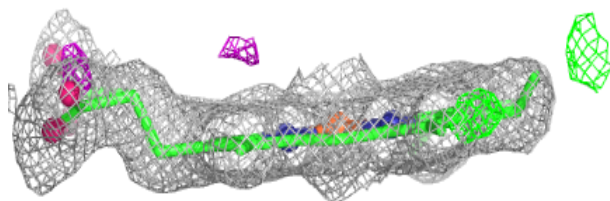
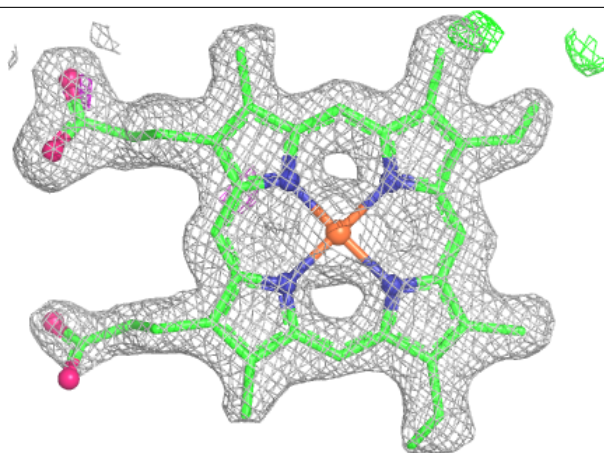
Electron density around HEM A 901:

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

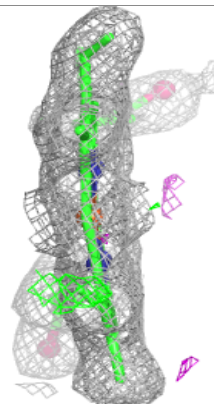
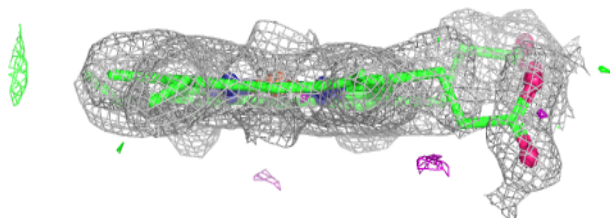
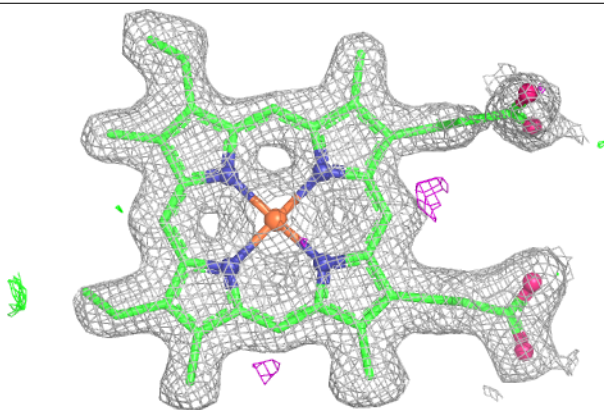


Electron density around HEM B 902:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.