Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 09:14 pm BST

PDB ID	:	4CX4
Title	:	Structure of rat neuronal nitric oxide synthase M336V D597N mutant heme domain in complex with 4-METHYL-6-(((3R,4R)-4-((5-(4- METHYLPYRIDIN-2-YL)PENTYL)OXY)PYRROLIDIN-3-YL)METHYL)PYRIDIN-2-AMINE
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2014-04-03
Resolution	:	1.98 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 (i) 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 (i)) were used in the production of this report:

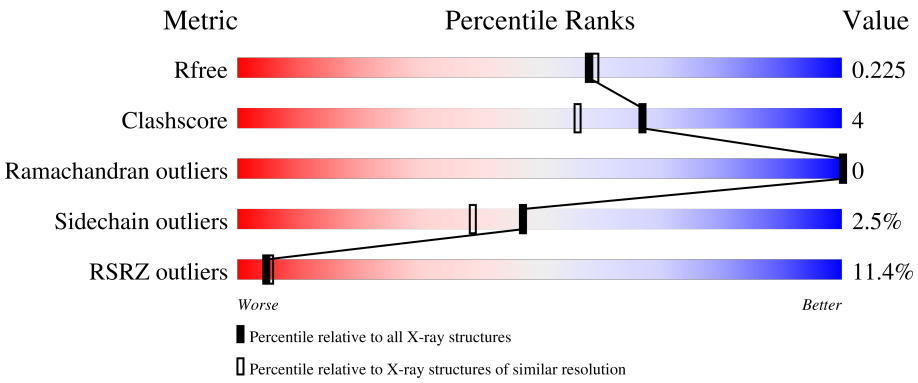
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 <=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	422	13% 87% 8% • •
1	B	422	9% 91% 6% •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7330 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.

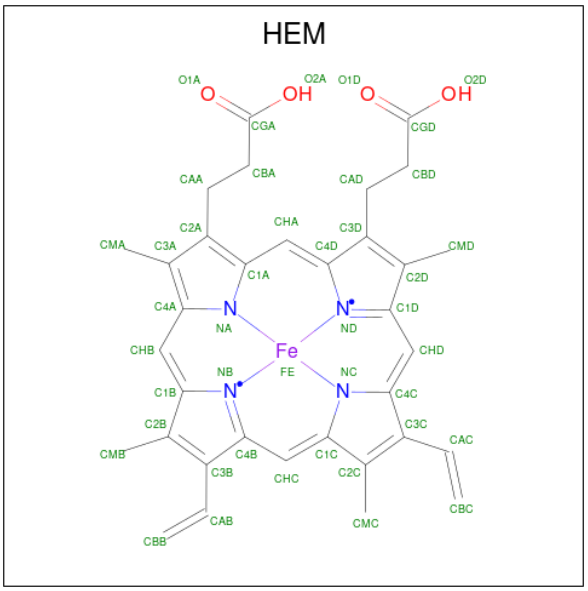
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, BRAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	408	3333	2136	569	608	20	0	3	1
1	B	411	3367	2158	575	613	21	0	5	0

There are 4 discrepancies between the modelled and reference sequences:

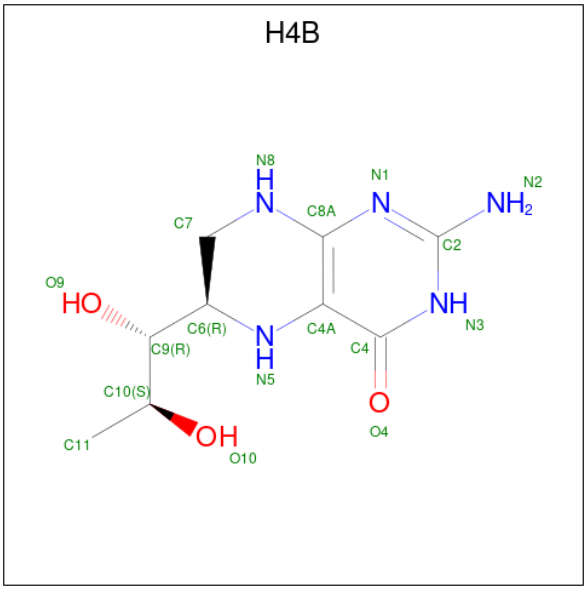
Chain	Residue	Modelled	Actual	Comment	Reference
A	336	VAL	MET	engineered mutation	UNP P29476
A	597	ASN	ASP	engineered mutation	UNP P29476
B	336	VAL	MET	engineered mutation	UNP P29476
B	597	ASN	ASP	engineered mutation	UNP P29476

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



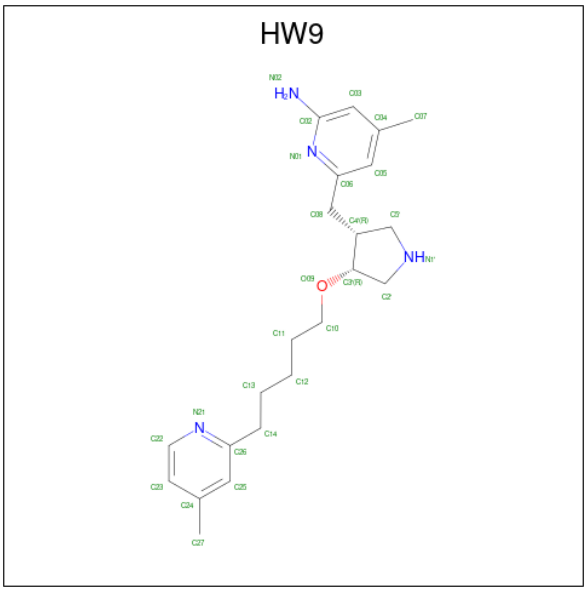
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



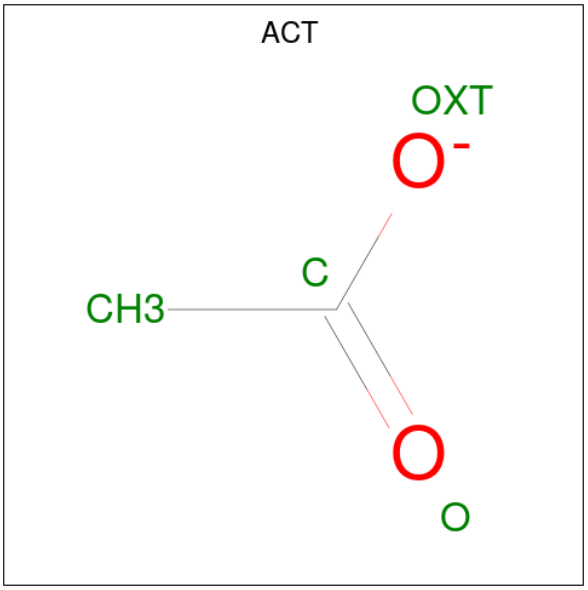
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O			
3	A	1	17	9	5	3		0	0
3	B	1	17	9	5	3		0	0

- Molecule 4 is 4-methyl-6-{[(3R,4R)-4-{[5-(4-methylpyridin-2-yl)pentyl]oxy}pyrrolidin-3-yl]methyl}pyridin-2-amine (three-letter code: HW9) (formula: $C_{22}H_{32}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	44	35	7	2	0	1
			Total	C	N	O		
4	B	1	44	35	7	2	0	1

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	B	1	1	1	0	0

- Molecule 7 is water.

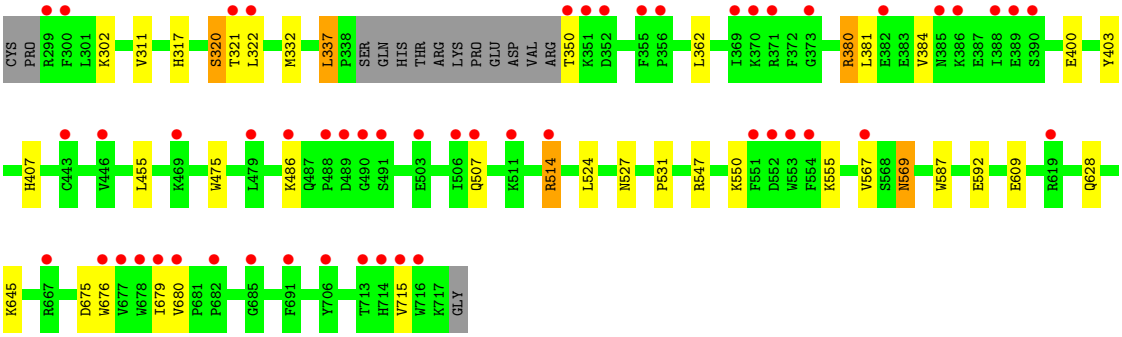
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	185	185	185	0	0
			Total	O		
7	B	228	228	228	0	0

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.

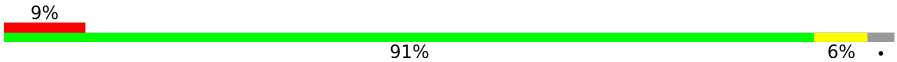
• Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

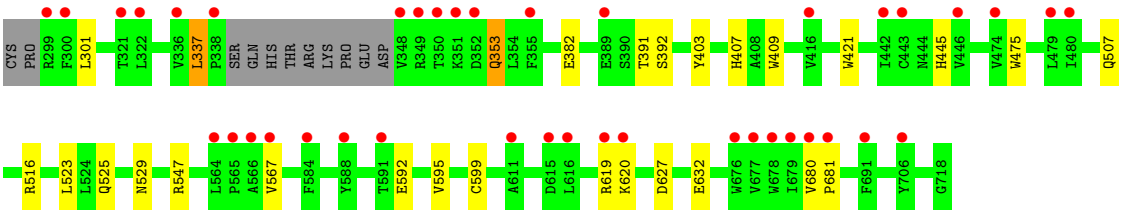
Chain A:



• Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	51.83Å 110.63Å 164.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.84 – 1.98 43.84 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.9 (43.84-1.98) 98.9 (43.84-1.98)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.47 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.175 , 0.212 0.196 , 0.225	Depositor DCC
R_{free} test set	3272 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7330	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: HW9, ACT, ZN, H4B, 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	0.69	0/3436	0.69	0/4664
1	B	0.77	0/3476	0.70	0/4715
All	All	0.73	0/6912	0.70	0/9379

There are no bond length outliers.

There are no bond angle outliers.

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	3333	0	3244	27	0
1	B	3367	0	3291	19	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	44	0	44	8	0
4	B	44	0	44	1	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	185	0	0	2	0
7	B	228	0	0	4	0
All	All	7330	0	6719	53	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 (53) 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)
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.72	0.72
1:B:382:GLU:HG3	7:B:2026:HOH:O	1.90	0.70
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.75	0.68
1:A:302:LYS:HD3	1:A:311:VAL:HG11	1.76	0.67
1:A:337:LEU:HD21	4:A:800[A]:HW9:C07	2.24	0.66
1:A:337:LEU:HD23	4:A:800[A]:HW9:H3	1.77	0.66
1:A:569:ASN:HD21	4:A:800[B]:HW9:H1	1.44	0.64
1:A:337:LEU:HD21	4:A:800[A]:HW9:H6	1.85	0.59
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.85	0.58
1:A:337:LEU:CD2	4:A:800[A]:HW9:H3	2.34	0.58
1:A:380:ARG:HD3	1:A:400:GLU:OE2	2.06	0.56
1:A:317:HIS:O	1:A:320:SER:HB3	2.06	0.56
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.41	0.53
1:B:595:VAL:O	1:B:599:CYS:HB2	2.10	0.52
1:A:403:TYR:CE1	1:A:407:HIS:CE1	2.98	0.51
7:A:2178:HOH:O	1:B:337:LEU:HD12	2.10	0.50
2:A:750:HEM:O2D	4:A:800[B]:HW9:N01	2.45	0.50
1:A:302:LYS:HD3	1:A:311:VAL:CG1	2.42	0.50
1:A:609:GLU:HG3	7:A:2149:HOH:O	2.12	0.49
1:B:516:ARG:HD2	7:B:2133:HOH:O	2.13	0.47
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.44	0.47
1:A:550:LYS:HB2	1:A:550:LYS:HE3	1.85	0.46
1:B:507:GLN:NE2	7:B:2139:HOH:O	2.48	0.46
1:A:332:MET:CE	1:B:301:LEU:HD22	2.47	0.45
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.99	0.45
1:A:675:ASP:O	1:A:679:ILE:HG12	2.18	0.44
1:A:362:LEU:HD11	1:A:384:VAL:HG21	2.00	0.44
1:A:321:THR:HG23	1:A:322:LEU:HG	1.97	0.44
4:A:800[A]:HW9:H4	4:A:800[A]:HW9:H10	1.47	0.44
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.05	0.44
4:B:800[B]:HW9:H19	4:B:800[B]:HW9:H12	1.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:THR:O	1:B:392:SER:HB2	2.19	0.43
1:A:527:ASN:HD22	1:A:527:ASN:HA	1.73	0.43
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.54	0.43
1:B:525:GLN:HG3	1:B:529:ASN:O	2.19	0.43
1:A:337:LEU:HD21	4:A:800[A]:HW9:H7	2.01	0.42
1:B:475:TRP:HB2	1:B:523:LEU:HB3	2.00	0.42
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.54	0.42
1:A:514:ARG:HH11	1:A:514:ARG:HG2	1.84	0.42
2:B:750:HEM:CMC	2:B:750:HEM:HBC2	2.50	0.42
1:B:516:ARG:CD	7:B:2133:HOH:O	2.67	0.42
1:B:445:HIS:CD2	1:B:445:HIS:C	2.94	0.41
1:A:524:LEU:O	1:A:531:PRO:HA	2.21	0.41
1:B:353:GLN:H	1:B:353:GLN:HG2	1.65	0.40
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.95	0.40
2:B:750:HEM:HBB2	2:B:750:HEM:CHC	2.46	0.40
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.56	0.40
1:B:619:ARG:HE	1:B:619:ARG:HB2	1.27	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	407/422 (96%)	397 (98%)	10 (2%)	0	100	100
1	B	412/422 (98%)	404 (98%)	8 (2%)	0	100	100
All	All	819/844 (97%)	801 (98%)	18 (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	366/377 (97%)	353 (96%)	13 (4%)	35	23
1	B	371/377 (98%)	366 (99%)	5 (1%)	69	64
All	All	737/754 (98%)	719 (98%)	18 (2%)	47	41

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

Mol	Chain	Res	Type
1	A	320	SER
1	A	337	LEU
1	A	350	THR
1	A	380	ARG
1	A	381	LEU
1	A	486	LYS
1	A	507	GLN
1	A	514	ARG
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	645	LYS
1	A	715	VAL
1	B	337	LEU
1	B	353	GLN
1	B	547	ARG
1	B	620	LYS
1	B	627	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	454	ASN
1	A	507	GLN
1	A	527	ASN
1	A	569	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	605	ASN
1	A	628	GLN
1	A	697	ASN
1	B	364	GLN
1	B	425	GLN
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	601	ASN
1	B	605	ASN
1	B	697	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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	HW9	B	800[B]	-	28,29,29	0.88	1 (3%)	32,38,38	1.91	6 (18%)
5	ACT	B	860	-	3,3,3	0.68	0	3,3,3	1.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	HW9	A	800[B]	-	28,29,29	0.77	1 (3%)	32,38,38	2.25	9 (28%)
5	ACT	A	860	-	3,3,3	0.80	0	3,3,3	0.76	0
2	HEM	A	750	1	41,50,50	1.87	10 (24%)	45,82,82	1.91	8 (17%)
2	HEM	B	750	1	41,50,50	1.95	11 (26%)	45,82,82	1.74	8 (17%)
4	HW9	A	800[A]	-	28,29,29	0.74	1 (3%)	32,38,38	1.99	10 (31%)
4	HW9	B	800[A]	-	28,29,29	0.86	1 (3%)	32,38,38	1.86	8 (25%)
3	H4B	B	760	-	16,18,18	1.36	2 (12%)	11,26,26	2.38	5 (45%)
3	H4B	A	760	-	16,18,18	1.11	2 (12%)	11,26,26	2.75	6 (54%)

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
4	HW9	B	800[B]	-	-	1/13/23/23	0/3/3/3
4	HW9	A	800[B]	-	-	2/13/23/23	0/3/3/3
2	HEM	A	750	1	-	0/12/54/54	-
2	HEM	B	750	1	-	1/12/54/54	-
4	HW9	A	800[A]	-	-	4/13/23/23	0/3/3/3
4	HW9	B	800[A]	-	-	4/13/23/23	0/3/3/3
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C2D	7.07	1.51	1.36
2	B	750	HEM	C3D-C2D	6.15	1.49	1.36
2	B	750	HEM	C3C-C2C	-5.02	1.33	1.40
2	A	750	HEM	C3C-CAC	3.59	1.55	1.47
2	B	750	HEM	C3C-CAC	3.38	1.54	1.47
3	B	760	H4B	C7-C6	3.29	1.55	1.52
2	A	750	HEM	C3C-C2C	-3.14	1.36	1.40
4	B	800[A]	HW9	C14-C26	3.06	1.57	1.51
4	B	800[B]	HW9	C14-C26	3.06	1.57	1.51
2	B	750	HEM	CMD-C2D	2.97	1.57	1.50
2	B	750	HEM	CAD-C3D	2.70	1.58	1.51
2	A	750	HEM	CMD-C2D	2.58	1.56	1.50
2	A	750	HEM	CAB-C3B	2.53	1.54	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	CAA-C2A	2.53	1.55	1.52
2	A	750	HEM	CMB-C2B	2.52	1.56	1.50
2	B	750	HEM	CMA-C3A	2.49	1.56	1.51
2	A	750	HEM	CMC-C2C	2.43	1.57	1.51
2	A	750	HEM	FE-ND	2.38	2.08	1.96
4	A	800[A]	HW9	C14-C26	2.37	1.56	1.51
4	A	800[B]	HW9	C14-C26	2.37	1.56	1.51
2	B	750	HEM	CAB-C3B	2.35	1.53	1.47
3	B	760	H4B	C7-N8	2.23	1.48	1.44
3	A	760	H4B	C7-N8	2.18	1.48	1.44
2	B	750	HEM	CMB-C2B	2.14	1.55	1.50
2	A	750	HEM	FE-NB	2.12	2.07	1.96
2	B	750	HEM	CHA-C4D	2.08	1.40	1.35
2	B	750	HEM	FE-ND	2.08	2.07	1.96
3	A	760	H4B	C2-N2	2.04	1.38	1.33
2	A	750	HEM	CMA-C3A	2.04	1.55	1.51

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	800[B]	HW9	C02-N01-C06	6.14	122.75	118.10
2	B	750	HEM	CBA-CAA-C2A	-6.00	102.39	112.62
4	B	800[B]	HW9	C02-N01-C06	5.88	122.55	118.10
2	A	750	HEM	C4D-ND-C1D	5.86	111.12	105.07
3	B	760	H4B	C8A-C4A-C4	5.64	119.58	114.57
2	A	750	HEM	CBA-CAA-C2A	-5.14	103.84	112.62
4	B	800[A]	HW9	C02-N01-C06	4.96	121.86	118.10
4	A	800[B]	HW9	C04-C05-C06	-4.82	117.16	120.32
3	A	760	H4B	C4-C4A-N5	4.47	122.87	119.12
2	A	750	HEM	CBD-CAD-C3D	-4.30	100.68	112.63
2	B	750	HEM	C4D-ND-C1D	4.20	109.42	105.07
2	A	750	HEM	CMC-C2C-C3C	4.08	132.31	124.68
3	A	760	H4B	N1-C2-N3	-4.02	119.11	125.42
4	A	800[A]	HW9	C02-N01-C06	4.01	121.14	118.10
4	A	800[B]	HW9	C5'-N1'-C2'	3.88	114.58	105.42
4	A	800[A]	HW9	C23-C22-N21	-3.85	119.17	123.96
4	A	800[B]	HW9	C23-C22-N21	-3.85	119.17	123.96
2	B	750	HEM	CBD-CAD-C3D	-3.84	101.95	112.63
4	A	800[B]	HW9	C06-C08-C4'	-3.84	102.90	115.55
4	A	800[A]	HW9	C22-N21-C26	3.84	122.67	117.42
4	A	800[B]	HW9	C22-N21-C26	3.84	122.67	117.42
4	B	800[B]	HW9	C5'-N1'-C2'	3.77	114.33	105.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	800[A]	HW9	C22-N21-C26	3.68	122.46	117.42
4	B	800[B]	HW9	C22-N21-C26	3.68	122.46	117.42
4	A	800[A]	HW9	C5'-N1'-C2'	3.57	113.85	105.42
3	A	760	H4B	C8A-C4A-C4	3.57	117.74	114.57
4	A	800[A]	HW9	C06-C08-C4'	-3.51	103.99	115.55
4	B	800[A]	HW9	C5'-N1'-C2'	3.30	113.20	105.42
3	A	760	H4B	C2-N1-C8A	3.25	121.83	114.54
3	A	760	H4B	C2-N3-C4	3.22	121.05	115.93
4	B	800[A]	HW9	C23-C22-N21	-3.13	120.06	123.96
4	B	800[B]	HW9	C23-C22-N21	-3.13	120.06	123.96
4	B	800[A]	HW9	C25-C26-N21	-3.04	117.50	121.78
4	B	800[B]	HW9	C25-C26-N21	-3.04	117.50	121.78
2	B	750	HEM	CAD-C3D-C4D	2.95	129.82	124.66
3	B	760	H4B	C2-N3-C4	2.84	120.44	115.93
4	B	800[B]	HW9	C05-C06-N01	-2.83	119.90	122.90
4	B	800[A]	HW9	C05-C06-N01	-2.75	119.98	122.90
4	A	800[A]	HW9	C07-C04-C05	-2.75	116.87	120.94
2	A	750	HEM	C4B-CHC-C1C	2.71	126.14	122.56
2	A	750	HEM	C2C-C3C-C4C	2.70	108.78	106.90
2	A	750	HEM	CHA-C4D-ND	2.59	127.58	124.38
3	B	760	H4B	N1-C2-N3	-2.48	121.53	125.42
4	A	800[A]	HW9	C07-C04-C03	2.40	124.49	120.94
3	A	760	H4B	N2-C2-N1	2.35	120.91	117.25
4	B	800[A]	HW9	C07-C04-C05	-2.33	117.48	120.94
3	B	760	H4B	N2-C2-N3	2.30	120.83	117.25
4	A	800[A]	HW9	C27-C24-C25	-2.25	117.61	120.94
4	A	800[B]	HW9	C27-C24-C25	-2.25	117.61	120.94
2	B	750	HEM	CMD-C2D-C1D	2.24	128.44	125.04
2	A	750	HEM	CHC-C4B-C3B	2.24	127.99	124.57
2	B	750	HEM	C4B-CHC-C1C	2.20	125.47	122.56
3	B	760	H4B	C2-N1-C8A	2.20	119.48	114.54
2	B	750	HEM	C1B-NB-C4B	2.18	107.32	105.07
4	A	800[B]	HW9	C3'-C2'-N1'	-2.15	101.59	105.20
4	A	800[A]	HW9	C12-C11-C10	-2.11	104.12	113.49
4	B	800[A]	HW9	N02-C02-N01	2.11	119.82	116.49
2	B	750	HEM	CAD-C3D-C2D	-2.05	124.06	127.88
4	A	800[A]	HW9	C25-C26-N21	-2.04	118.91	121.78
4	A	800[B]	HW9	C25-C26-N21	-2.04	118.91	121.78

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	800[A]	HW9	C05-C06-C08-C4'
4	A	800[A]	HW9	N01-C06-C08-C4'
4	A	800[B]	HW9	C2'-C3'-O09-C10
4	B	800[A]	HW9	C05-C06-C08-C4'
4	B	800[A]	HW9	N01-C06-C08-C4'
4	B	800[B]	HW9	C2'-C3'-O09-C10
4	A	800[A]	HW9	O09-C10-C11-C12
4	B	800[A]	HW9	C2'-C3'-O09-C10
4	B	800[A]	HW9	C4'-C3'-O09-C10
4	A	800[B]	HW9	C10-C11-C12-C13
4	A	800[A]	HW9	C11-C10-O09-C3'
2	B	750	HEM	C4B-C3B-CAB-CBB

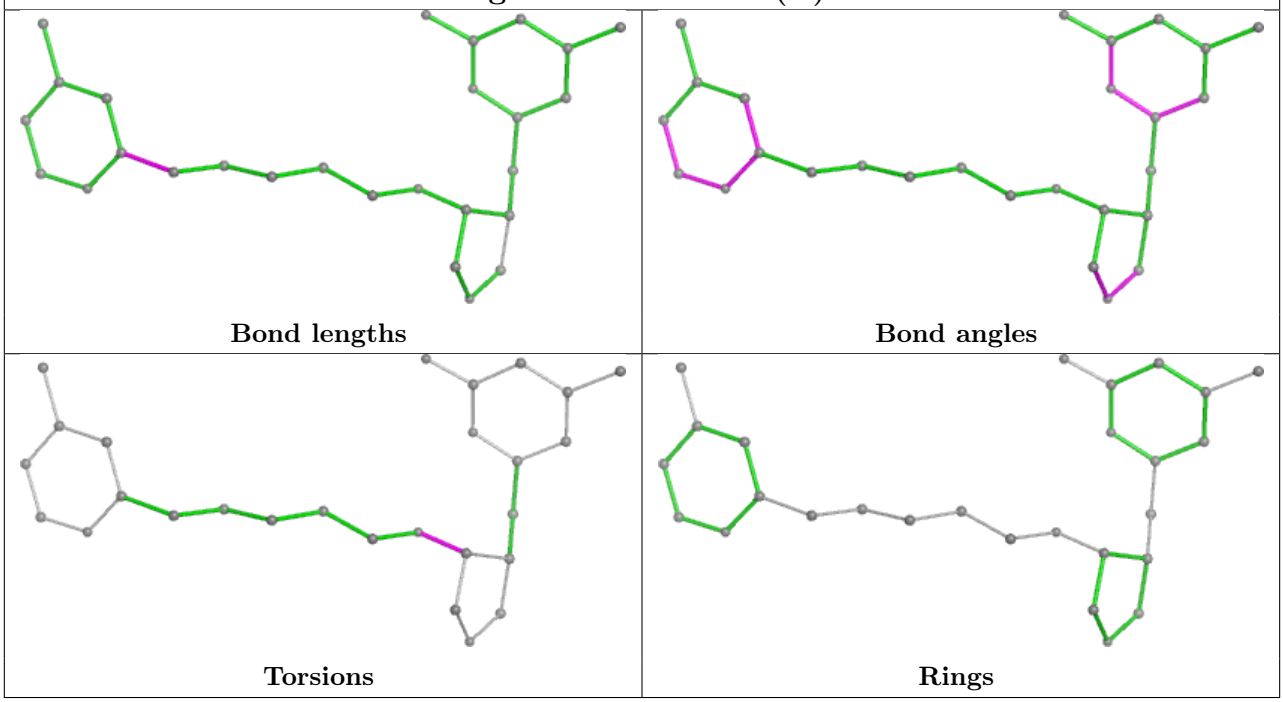
There are no ring outliers.

5 monomers are involved in 15 short contacts:

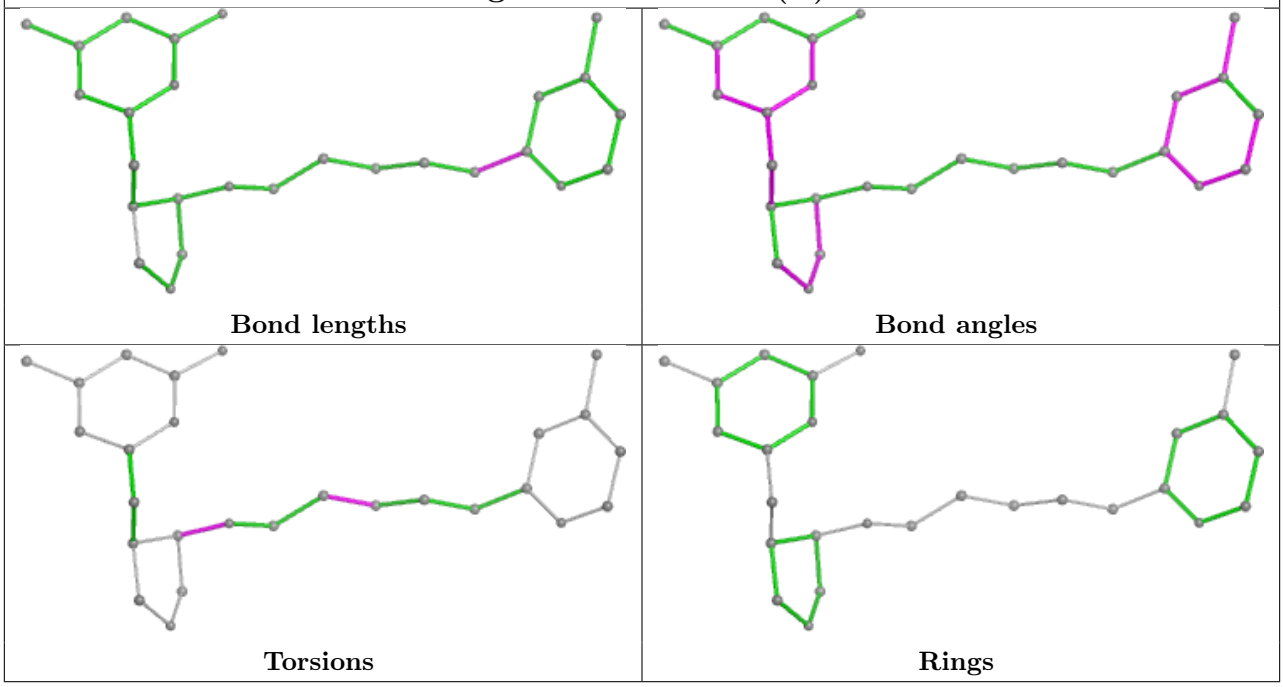
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	800[B]	HW9	1	0
4	A	800[B]	HW9	2	0
2	A	750	HEM	3	0
2	B	750	HEM	4	0
4	A	800[A]	HW9	6	0

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 then 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.

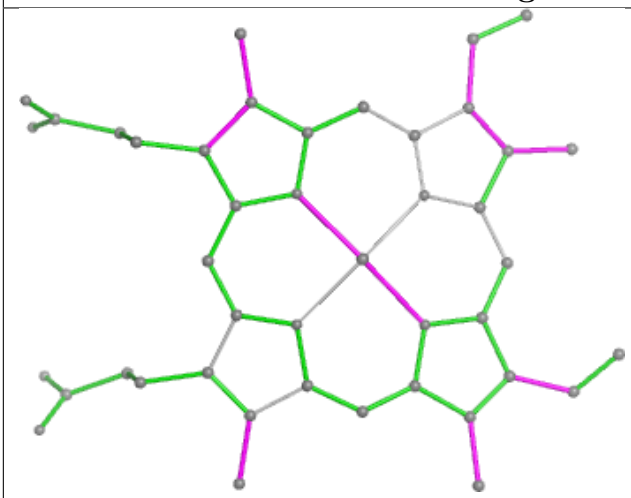
Ligand HW9 B 800 (B)



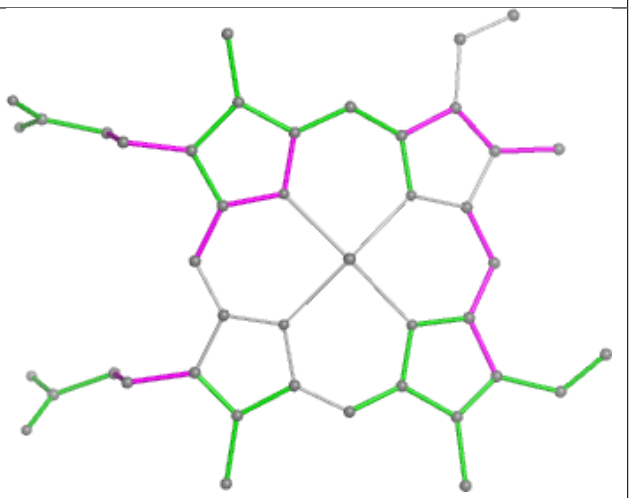
Ligand HW9 A 800 (B)



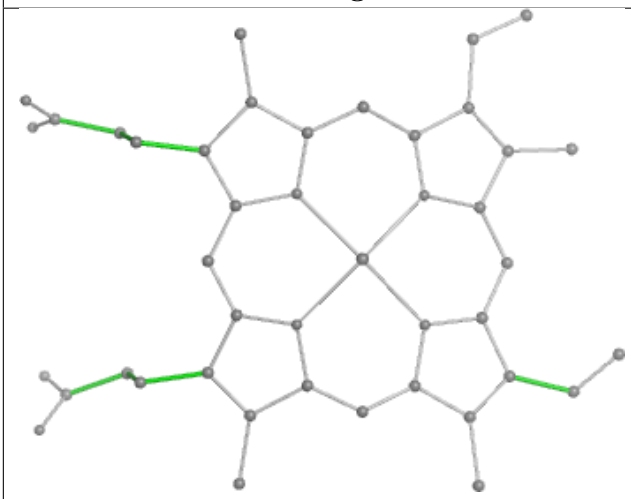
Ligand HEM A 750



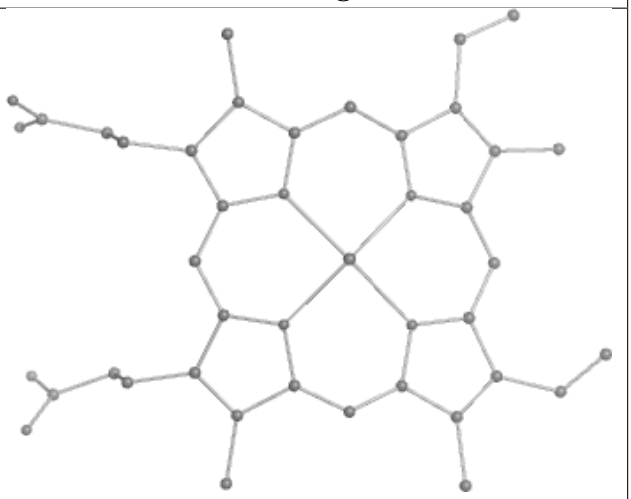
Bond lengths



Bond angles

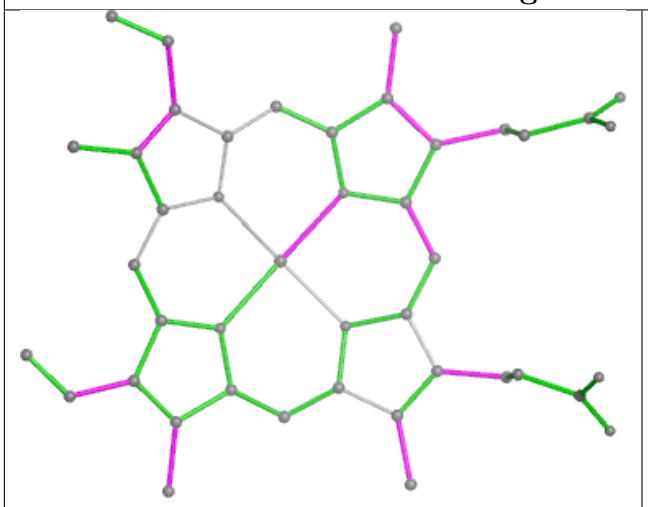


Torsions

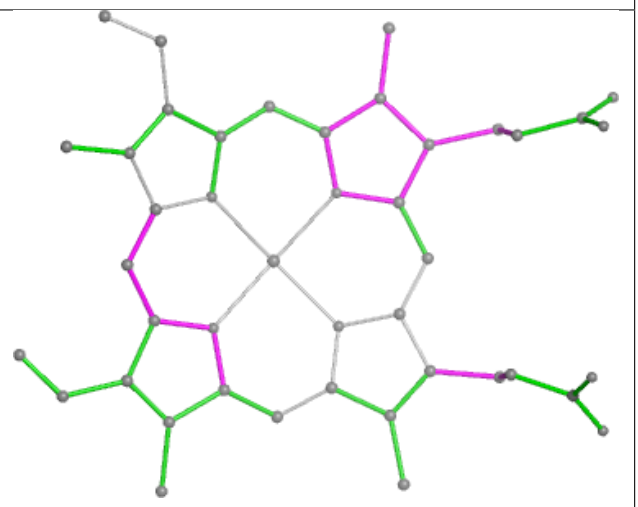


Rings

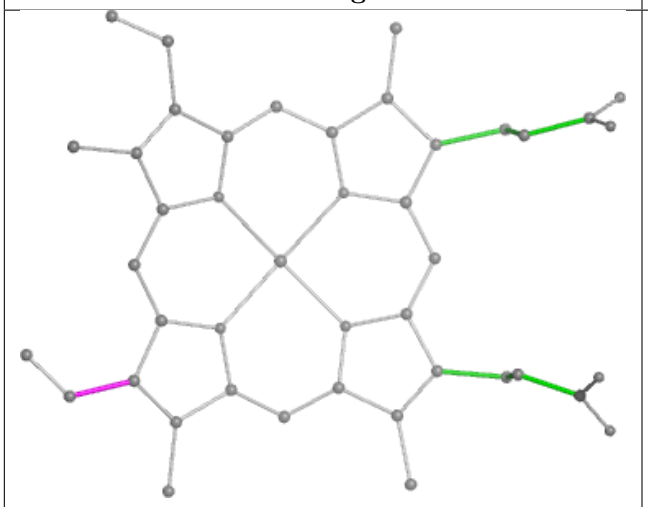
Ligand HEM B 750



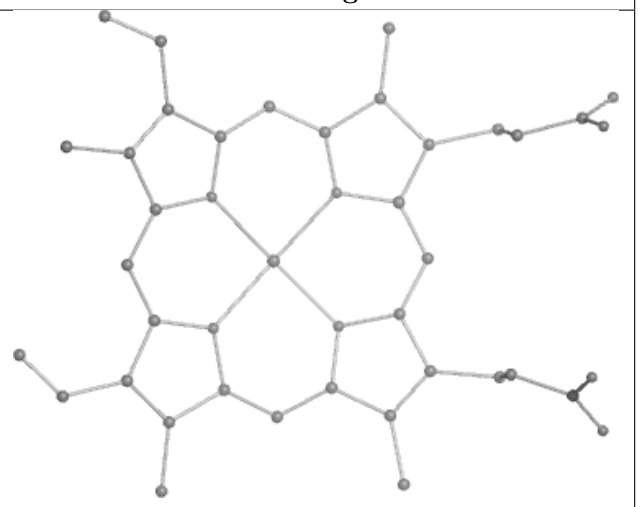
Bond lengths



Bond angles

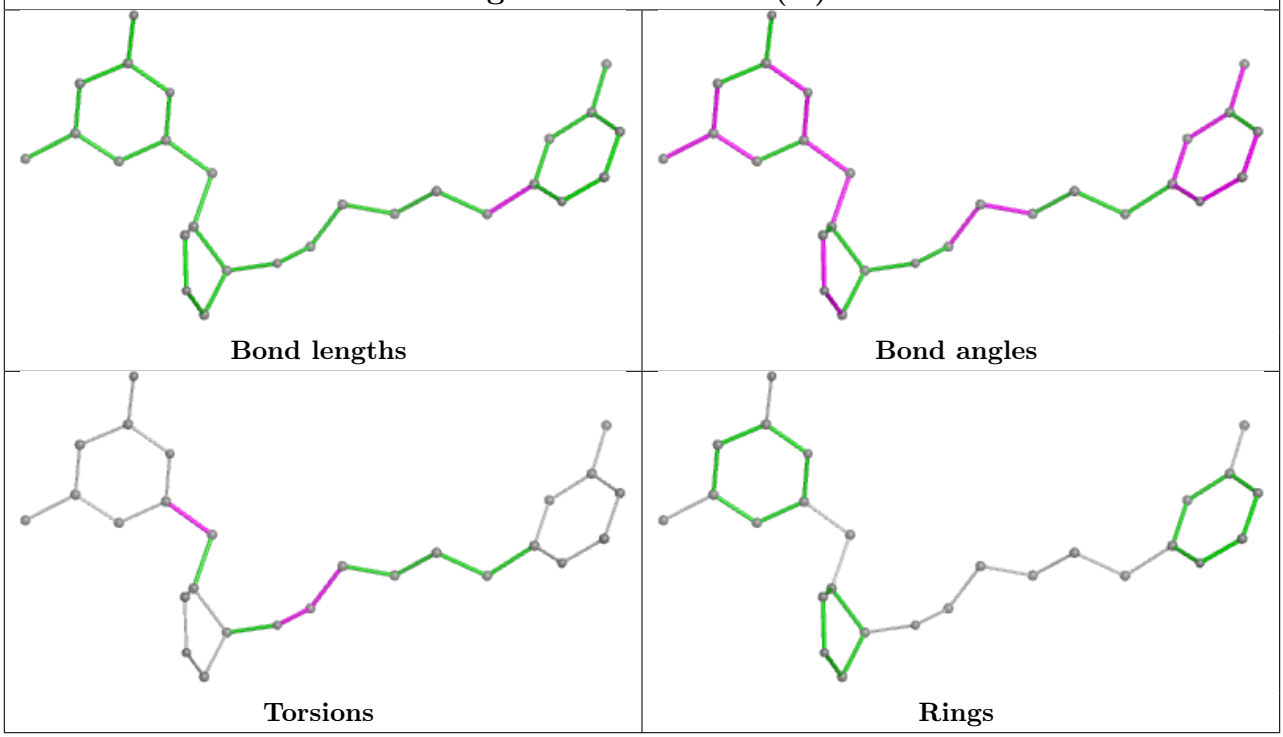


Torsions

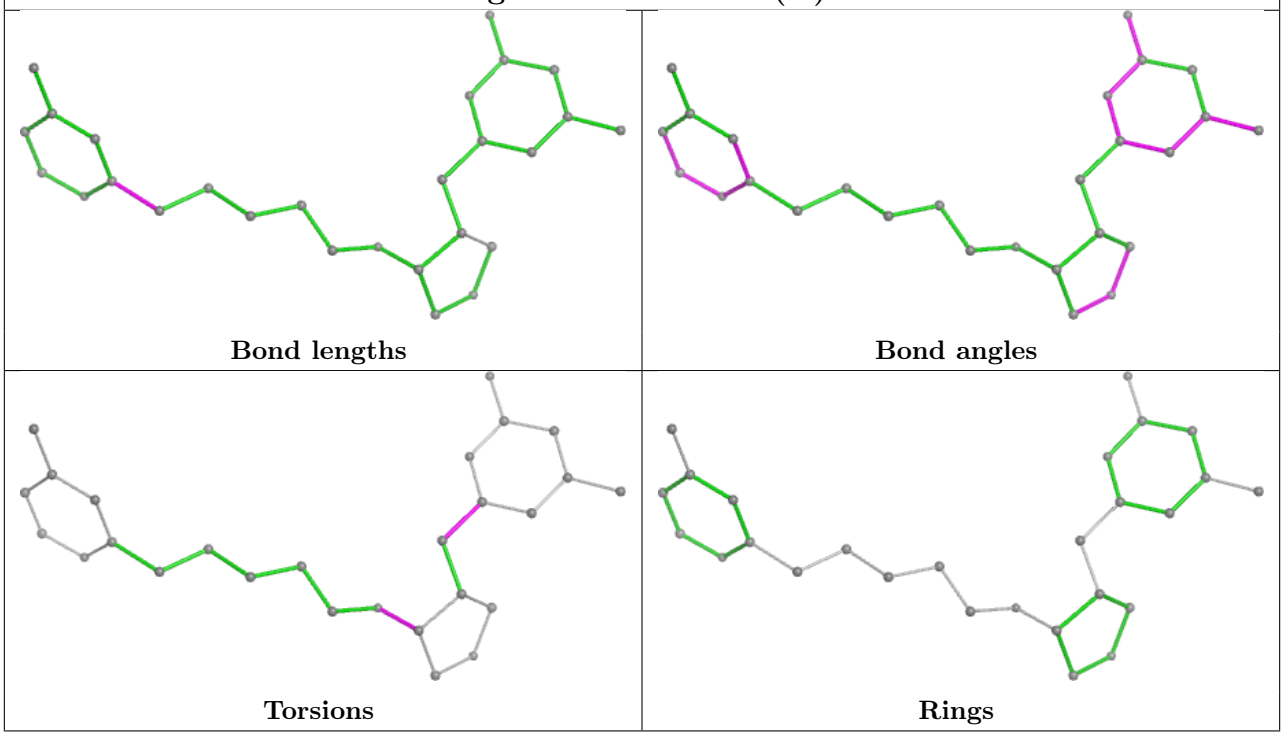


Rings

Ligand HW9 A 800 (A)



Ligand HW9 B 800 (A)



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	408/422 (96%)	0.83	53 (12%)	3	3	22, 43, 78, 99	0
1	B	411/422 (97%)	0.60	40 (9%)	7	8	22, 34, 58, 82	0
All	All	819/844 (97%)	0.71	93 (11%)	5	5	22, 38, 72, 99	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	716	TRP	7.9
1	A	488	PRO	7.3
1	B	300	PHE	6.4
1	A	355	PHE	6.0
1	B	350	THR	5.9
1	A	715	VAL	5.4
1	A	706[A]	TYR	4.6
1	B	352	ASP	4.6
1	A	352	ASP	4.5
1	B	321	THR	4.3
1	A	351	LYS	4.3
1	B	348	VAL	4.2
1	A	300	PHE	4.1
1	B	619	ARG	4.0
1	A	714	HIS	3.7
1	A	388	ILE	3.7
1	A	490	GLY	3.6
1	B	677	VAL	3.6
1	A	507	GLN	3.5
1	A	321	THR	3.4
1	A	386	LYS	3.4
1	A	486	LYS	3.4
1	A	677	VAL	3.3
1	A	678	TRP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	706[A]	TYR	3.3
1	B	611	ALA	3.3
1	A	350	THR	3.2
1	A	552	ASP	3.2
1	B	616	LEU	3.2
1	B	567	VAL	3.2
1	A	713	THR	3.2
1	A	551	PHE	3.1
1	B	479	LEU	3.1
1	A	676	TRP	3.0
1	B	678	TRP	3.0
1	A	503	GLU	3.0
1	A	373	GLY	3.0
1	B	351	LYS	3.0
1	A	680	VAL	2.9
1	B	442	ILE	2.9
1	A	506	ILE	2.8
1	A	299	ARG	2.8
1	B	349	ARG	2.8
1	B	336	VAL	2.7
1	B	564	LEU	2.7
1	B	620	LYS	2.7
1	B	691	PHE	2.7
1	B	389	GLU	2.6
1	A	554	PHE	2.6
1	B	679	ILE	2.6
1	B	591	THR	2.6
1	B	615	ASP	2.6
1	A	514	ARG	2.5
1	B	565	PRO	2.5
1	A	469	LYS	2.5
1	B	588	TYR	2.5
1	A	322	LEU	2.5
1	A	356	PRO	2.4
1	B	416	VAL	2.4
1	A	491	SER	2.4
1	A	369	ILE	2.4
1	B	680	VAL	2.4
1	A	619	ARG	2.4
1	B	566	ALA	2.4
1	B	480	ILE	2.4
1	B	446	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	489	ASP	2.4
1	B	443	CYS	2.4
1	A	691	PHE	2.3
1	B	338	PRO	2.3
1	A	679	ILE	2.3
1	A	667	ARG	2.3
1	B	676	TRP	2.3
1	A	389	GLU	2.3
1	A	443	CYS	2.3
1	B	322	LEU	2.3
1	B	355	PHE	2.2
1	A	390	SER	2.2
1	A	370	LYS	2.2
1	A	371	ARG	2.2
1	B	584	PHE	2.2
1	B	474	VAL	2.2
1	A	479	LEU	2.2
1	A	553	TRP	2.2
1	A	682	PRO	2.1
1	A	685	GLY	2.1
1	B	681	PRO	2.1
1	A	511	LYS	2.1
1	A	446	VAL	2.1
1	A	382	GLU	2.1
1	A	385	ASN	2.0
1	A	567	VAL	2.0
1	B	299	ARG	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,

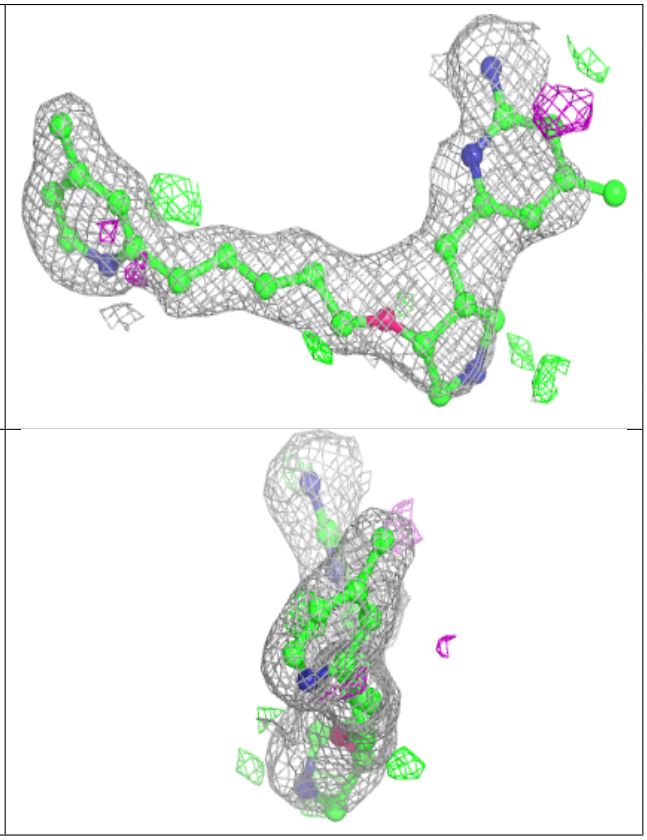
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	HW9	B	800[A]	27/27	0.90	0.30	26,41,51,53	17
4	HW9	B	800[B]	27/27	0.90	0.30	26,30,34,36	17
4	HW9	A	800[A]	27/27	0.91	0.24	27,48,53,54	17
4	HW9	A	800[B]	27/27	0.91	0.24	24,30,33,35	17
5	ACT	B	860	4/4	0.96	0.10	39,39,41,42	0
5	ACT	A	860	4/4	0.97	0.16	48,49,49,50	0
3	H4B	A	760	17/17	0.97	0.19	22,26,30,33	0
2	HEM	B	750	43/43	0.98	0.18	23,26,34,39	0
2	HEM	A	750	43/43	0.98	0.16	23,27,34,36	0
3	H4B	B	760	17/17	0.98	0.22	24,27,32,33	0
6	ZN	B	900	1/1	1.00	0.09	32,32,32,32	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.

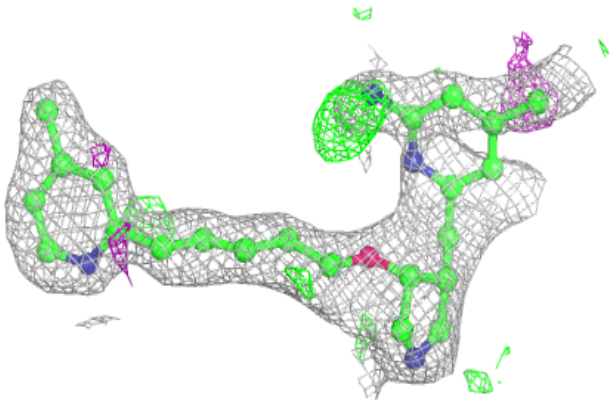
Electron density around HW9 B 800 (A):

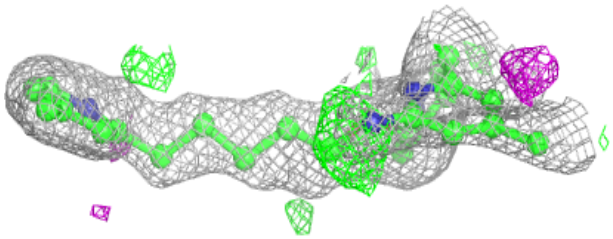
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

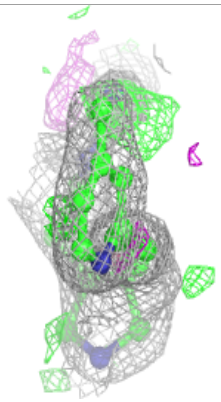


Electron density around HW9 B 800 (B):

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

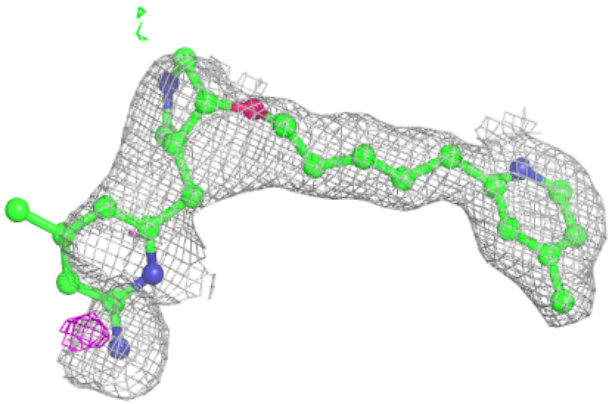


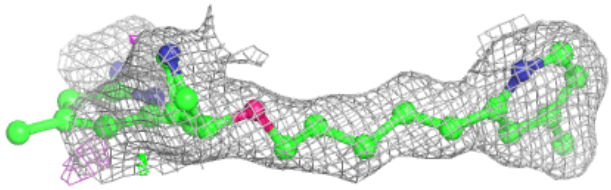


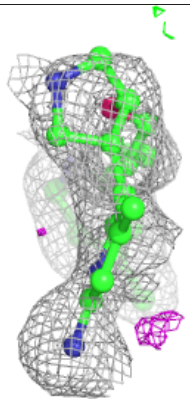


Electron density around HW9 A 800 (A):

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

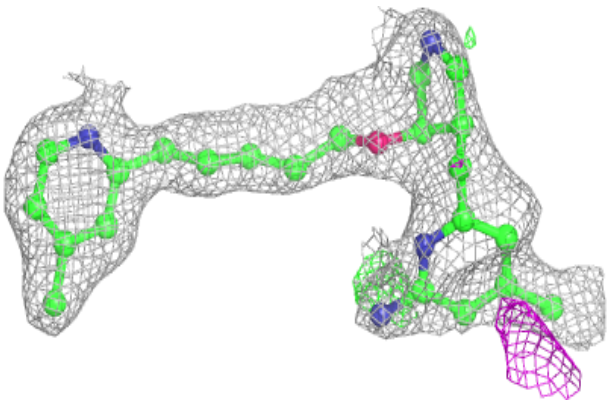


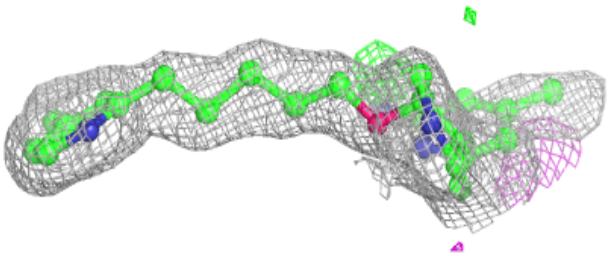


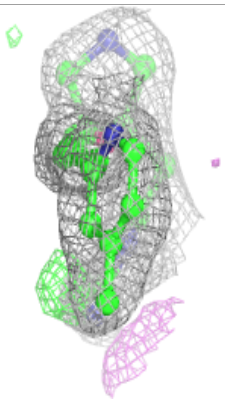


Electron density around HW9 A 800 (B):

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

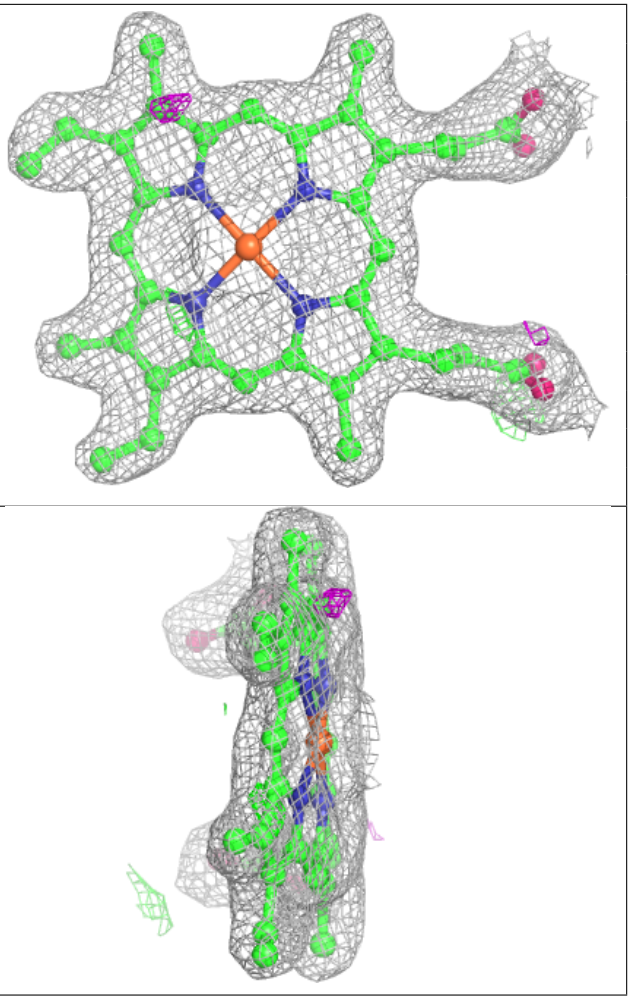






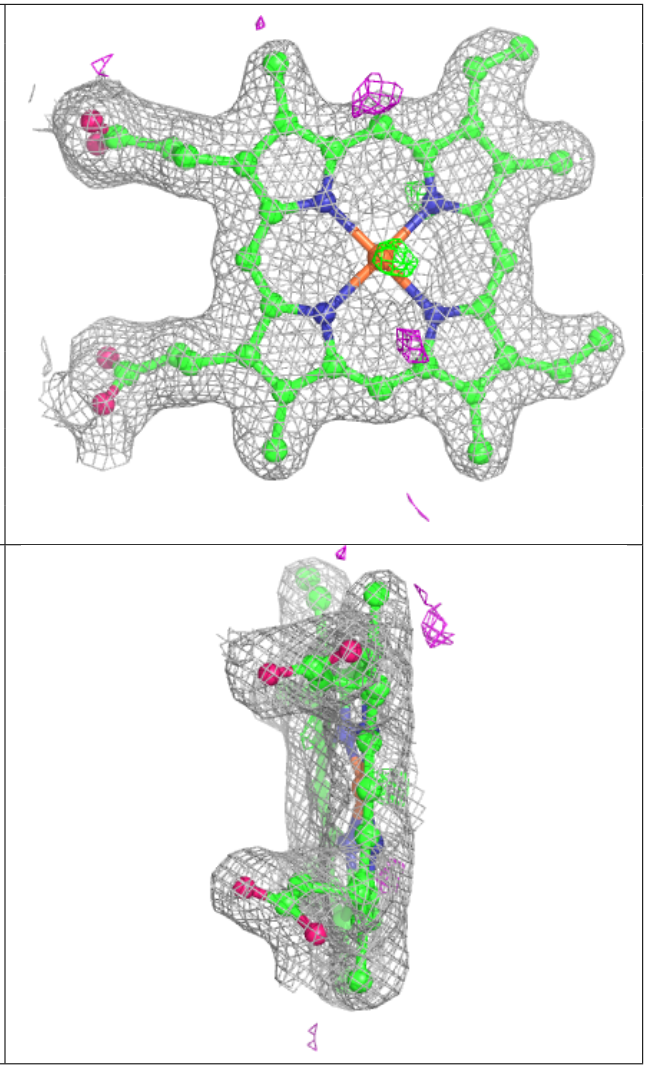
Electron density around HEM B 750:

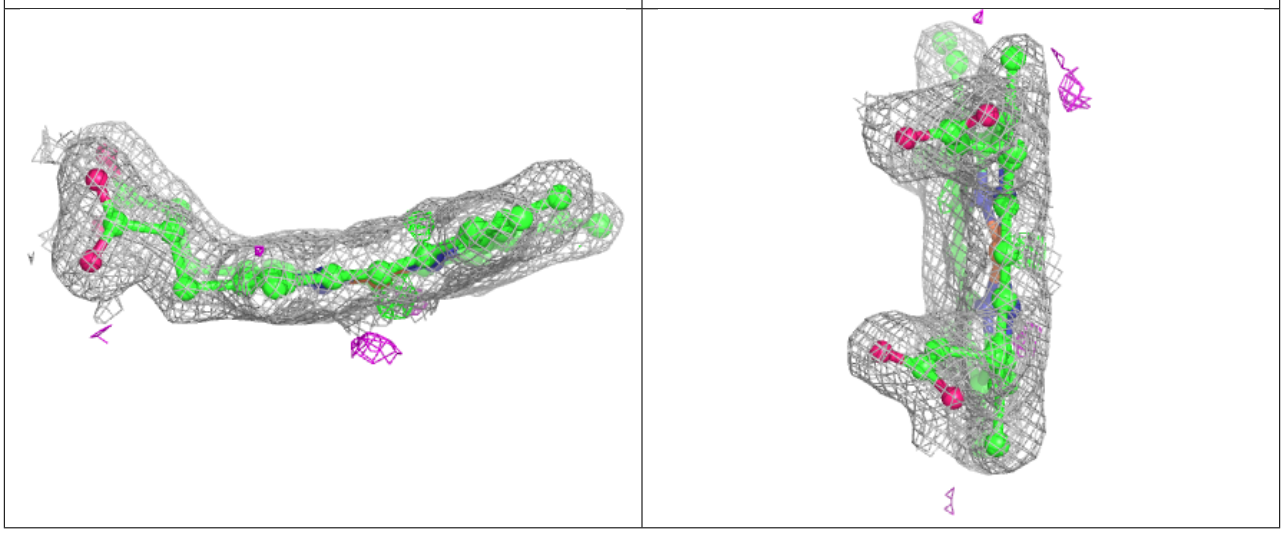
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 750:

$2mF_o$-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.