Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:28 am BST

PDB ID	:	4CX1
Title	:	Structure of bovine endothelial nitric oxide synthase L111A 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	:	2.13 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

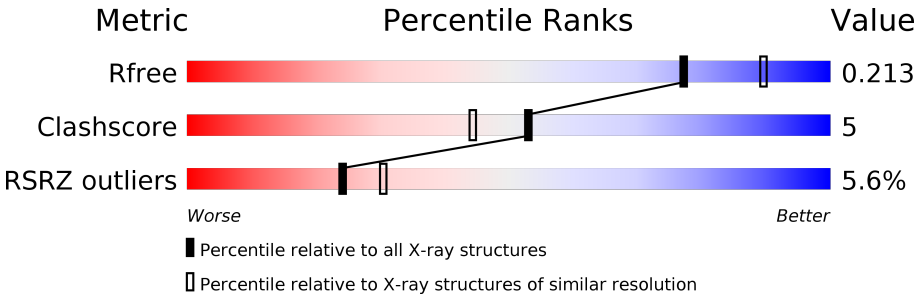
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	443	6% 83% 8% 9%
1	B	443	5% 81% 11% 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6997 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.

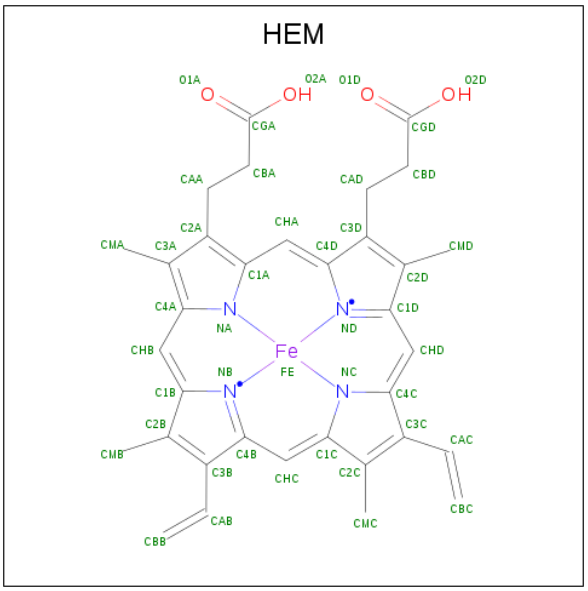
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	0	0
			3223	1	2049	568	589	16			
1	B	404	Total	As	C	N	O	S	0	0	0
			3221	1	2048	568	588	16			

There are 4 discrepancies between the modelled and reference sequences:

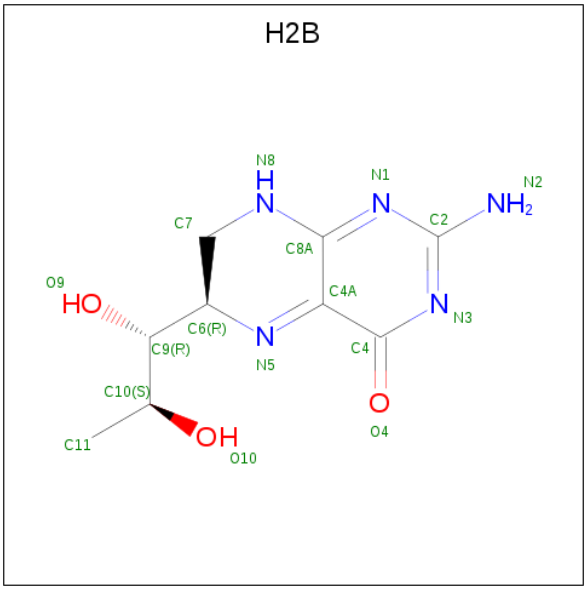
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	conflict	UNP P29473
A	111	ALA	LEU	engineered mutation	UNP P29473
B	100	ARG	CYS	conflict	UNP P29473
B	111	ALA	LEU	engineered mutation	UNP P29473

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



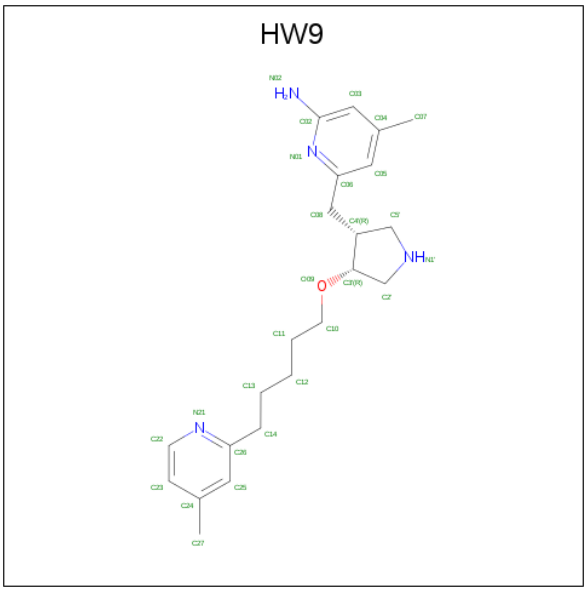
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 2-AMINO-6-(1,2-DIHYDROXY-PROPYL)-7,8-DIHYDRO-6H-PTERIDIN-4-ONE (three-letter code: H2B) (formula: $C_9H_{13}N_5O_3$).



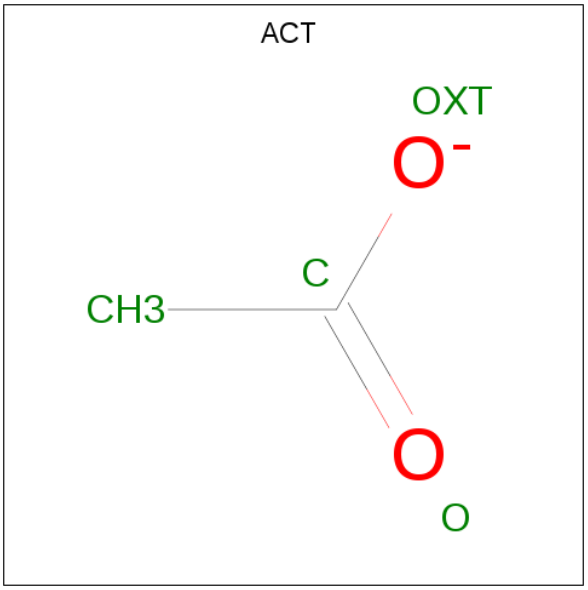
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- 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
4	A	1	Total	C	N	O	0	0
			27	22	4	1		
4	B	1	Total	C	N	O	0	0
			27	22	4	1		

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



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

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

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

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

- Molecule 7 is water.

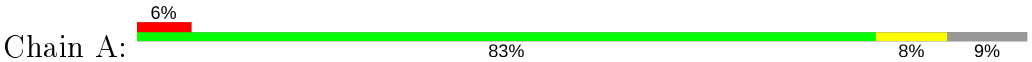
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	209	Total O 209 209	0	0
7	B	153	Total O 153 153	0	0

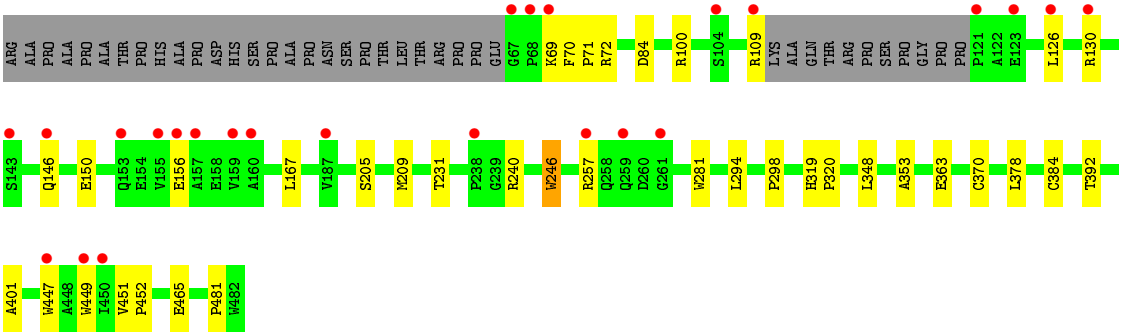
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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, ENDOTHELIAL

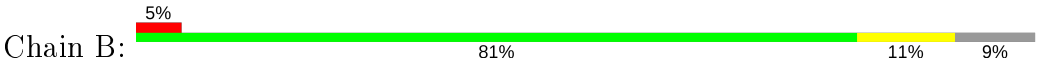
Chain A:

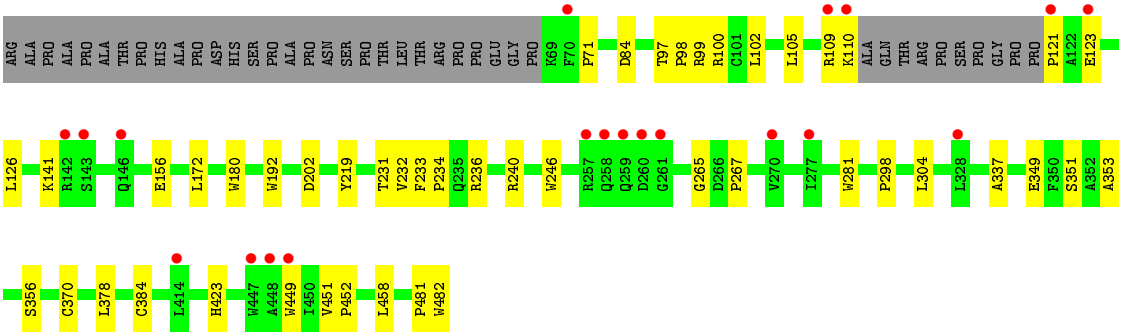




- Molecule 1: NITRIC OXIDE SYNTHASE, ENDOTHELIAL

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	57.73Å 106.20Å 156.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.19 – 2.13 48.23 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.9 (92.19-2.13) 97.8 (48.23-2.12)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.172 , 0.214 0.171 , 0.213	Depositor DCC
R_{free} test set	2712 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6997	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CAS, HW9, ACT, HEM, H2B

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	3/3303 (0.1%)	0.72	0/4497
1	B	0.68	1/3300 (0.0%)	0.70	0/4491
All	All	0.69	4/6603 (0.1%)	0.71	0/8988

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	TRP	CD2-CE2	5.66	1.48	1.41
1	A	281	TRP	CD2-CE2	5.62	1.48	1.41
1	B	482	TRP	CD2-CE2	5.54	1.48	1.41
1	A	246	TRP	CD2-CE2	5.02	1.47	1.41

There are no bond angle outliers.

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	3223	0	3127	34	0
1	B	3221	0	3130	35	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
3	A	17	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	13	1	0
4	A	27	0	32	2	0
4	B	27	0	32	1	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
6	B	1	0	0	0	0
7	A	209	0	0	3	0
7	B	153	0	0	1	0
All	All	6997	0	6419	70	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 5.

All (70) 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:A:384:CAS:AS	1:A:384:CAS:SG	2.49	1.31
1:B:384:CAS:AS	1:B:384:CAS:SG	2.57	1.22
1:A:72:ARG:HD3	7:A:2002:HOH:O	1.77	0.84
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.62	0.81
1:A:72:ARG:H	1:B:109:ARG:HE	1.37	0.70
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.74	0.70
1:A:384:CAS:CB	1:A:384:CAS:AS	3.02	0.67
2:B:500:HEM:HBC2	2:B:500:HEM:HMC1	1.78	0.66
1:A:109:ARG:H	1:A:109:ARG:HH11	1.44	0.64
2:B:500:HEM:HBC2	2:B:500:HEM:CMC	2.29	0.63
1:B:240:ARG:HD3	1:B:298:PRO:HB3	1.82	0.62
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.82	0.61
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.68	0.58
1:A:146:GLN:O	1:A:150:GLU:CG	2.53	0.56
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.35	0.56
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.87	0.56
1:A:449:TRP:HA	3:A:600:H2B:N1	2.21	0.55
1:B:110:LYS:C	1:B:110:LYS:HD2	2.28	0.54
1:A:72:ARG:H	1:B:109:ARG:NE	2.05	0.53
1:B:236:ARG:HG3	1:B:349:GLU:HB2	1.90	0.53
1:B:231:THR:O	1:B:353:ALA:HA	2.08	0.53
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.47	0.53
1:A:146:GLN:O	1:A:150:GLU:HG2	2.09	0.53
1:A:384:CAS:HB2	1:A:384:CAS:AS	2.70	0.51
1:A:384:CAS:SG	1:A:384:CAS:CE1	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.93	0.49
1:A:257:ARG:NH1	1:A:257:ARG:HG3	2.27	0.48
1:B:97:THR:HB	1:B:98:PRO:HD2	1.94	0.48
1:B:172:LEU:HD11	1:B:232:VAL:HG11	1.95	0.47
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.96	0.47
1:A:146:GLN:O	1:A:150:GLU:HG3	2.12	0.47
1:A:205:SER:O	1:A:209:MET:HG3	2.15	0.47
1:A:69:LYS:HG3	1:A:69:LYS:O	2.14	0.47
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.55	0.46
1:B:378:LEU:HB2	7:B:2118:HOH:O	2.16	0.46
2:A:500:HEM:CMC	2:A:500:HEM:HBC2	2.46	0.45
1:B:219:TYR:CD1	1:B:219:TYR:C	2.90	0.45
1:B:449:TRP:HA	3:B:600:H2B:N1	2.32	0.45
1:B:99:ARG:HG2	1:B:100:ARG:HD2	1.97	0.45
1:A:167:LEU:HG	1:A:348:LEU:HD12	1.99	0.45
1:B:246:TRP:CD1	1:B:481:PRO:HG2	2.52	0.44
1:B:121:PRO:HB2	1:B:123:GLU:OE1	2.17	0.44
1:B:84:ASP:C	1:B:84:ASP:OD1	2.56	0.44
1:B:109:ARG:HD2	1:B:109:ARG:HA	1.72	0.44
1:A:392:THR:HB	1:B:423:HIS:HB2	2.00	0.43
2:B:500:HEM:C1C	4:B:800:HW9:H33	2.53	0.43
1:B:71:PRO:HG2	1:B:84:ASP:HB3	2.00	0.43
1:A:100:ARG:NE	7:A:2027:HOH:O	2.37	0.43
1:A:126:LEU:HD23	1:A:130:ARG:NH2	2.34	0.43
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.81	0.43
2:A:500:HEM:C1C	4:A:800:HW9:H33	2.54	0.43
1:B:141:LYS:HA	1:B:141:LYS:HD3	1.86	0.43
1:A:401:ALA:CB	1:B:458:LEU:HD21	2.49	0.42
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.55	0.42
1:A:71:PRO:HB3	1:B:102:LEU:HD21	2.01	0.42
1:A:465:GLU:HB3	1:B:105:LEU:HD22	2.02	0.42
1:B:451:VAL:HA	1:B:452:PRO:HD3	1.92	0.41
1:A:231:THR:O	1:A:353:ALA:HA	2.19	0.41
2:B:500:HEM:HMC1	2:B:500:HEM:CBC	2.47	0.41
1:A:378:LEU:HB2	7:A:2153:HOH:O	2.19	0.41
1:A:70:PHE:HB3	1:A:84:ASP:O	2.21	0.41
1:B:202:ASP:CG	1:B:202:ASP:O	2.58	0.41
2:A:500:HEM:CBB	2:A:500:HEM:HHC	2.51	0.41
1:A:246:TRP:CD1	1:A:481:PRO:HG2	2.56	0.41
1:B:110:LYS:CD	1:B:110:LYS:C	2.89	0.41
1:B:97:THR:HB	1:B:98:PRO:CD	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:GLU:OE1	4:A:800:HW9:N21	2.55	0.40
1:B:126:LEU:HD11	1:B:156:GLU:HA	2.03	0.40
1:B:265:GLY:O	1:B:267:PRO:HD3	2.21	0.40
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CAS	B	384	1	5,8,9	1.35	1 (20%)	1,9,11	0.22	0
1	CAS	A	384	1	5,8,9	1.04	0	1,9,11	0.33	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
1	CAS	B	384	1	-	0/0/7/9	-
1	CAS	A	384	1	-	0/0/7/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	CAS	AS-CE2	2.01	2.01	1.96

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	384	CAS	1	0
1	A	384	CAS	4	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	-	28,29,29	0.69	0	32,38,38	2.17	10 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	ACT	A	860	-	1,3,3	1.36	0	0,3,3	0.00	-
5	ACT	B	860	-	1,3,3	1.68	0	0,3,3	0.00	-
4	HW9	A	800	-	28,29,29	0.73	0	32,38,38	1.82	5 (15%)
2	HEM	A	500	1	27,50,50	2.36	9 (33%)	17,82,82	3.35	8 (47%)
5	ACT	A	861	-	1,3,3	2.20	1 (100%)	0,3,3	0.00	-
2	HEM	B	500	1	27,50,50	2.36	11 (40%)	17,82,82	3.18	7 (41%)
5	ACT	B	861	-	1,3,3	1.92	0	0,3,3	0.00	-
3	H2B	A	600	-	13,18,18	1.29	1 (7%)	11,26,26	2.04	3 (27%)
3	H2B	B	600	-	13,18,18	1.43	2 (15%)	11,26,26	1.86	3 (27%)

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	-	-	0/13/23/23	0/3/3/3
2	HEM	B	500	1	-	0/6/54/54	-
2	HEM	A	500	1	-	0/6/54/54	-
4	HW9	A	800	-	-	0/13/23/23	0/3/3/3
3	H2B	A	600	-	-	0/8/33/33	0/2/2/2
3	H2B	B	600	-	-	0/8/33/33	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3C-C2C	5.78	1.48	1.40
2	B	500	HEM	C3C-C2C	5.48	1.48	1.40
2	A	500	HEM	C4A-NA	5.11	1.46	1.36
2	B	500	HEM	C4A-NA	4.50	1.45	1.36
2	B	500	HEM	C3B-C2B	4.05	1.46	1.40
2	B	500	HEM	C1A-NA	4.03	1.44	1.36
3	B	600	H2B	C4A-N5	3.82	1.37	1.28
2	A	500	HEM	C3B-C2B	3.73	1.45	1.40
2	B	500	HEM	C1C-C2C	3.66	1.50	1.42
2	A	500	HEM	C4D-C3D	3.59	1.50	1.42
2	A	500	HEM	C1A-NA	3.58	1.43	1.36
3	A	600	H2B	C4A-N5	3.55	1.37	1.28
2	B	500	HEM	C2A-C3A	3.44	1.47	1.37
2	A	500	HEM	C2A-C3A	3.12	1.46	1.37
2	A	500	HEM	C1B-C2B	3.10	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3D-C2D	3.06	1.46	1.37
2	B	500	HEM	C3D-C2D	2.93	1.46	1.37
2	A	500	HEM	C1C-C2C	2.63	1.48	1.42
2	B	500	HEM	C4D-C3D	2.57	1.48	1.42
2	B	500	HEM	C1B-C2B	2.45	1.48	1.42
3	B	600	H2B	C8A-N1	2.44	1.37	1.32
2	B	500	HEM	C4A-CHB	2.21	1.47	1.41
5	A	861	ACT	CH3-C	2.20	1.51	1.48
2	B	500	HEM	C4B-CHC	2.15	1.47	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	C1D-C2D-C3D	-8.68	100.96	107.00
2	B	500	HEM	C1D-C2D-C3D	-7.83	101.55	107.00
4	B	800	HW9	C02-N01-C06	7.39	123.70	118.10
4	A	800	HW9	C02-N01-C06	6.30	122.87	118.10
2	B	500	HEM	CBA-CAA-C2A	-6.22	101.01	112.49
2	A	500	HEM	C4A-C3A-C2A	-5.55	103.13	107.00
2	A	500	HEM	C3B-C4B-NB	5.04	115.73	109.21
2	B	500	HEM	C3B-C4B-NB	4.74	115.33	109.21
3	A	600	H2B	C4-C4A-N5	4.73	123.25	118.06
3	B	600	H2B	C4-C4A-N5	4.05	122.51	118.06
2	A	500	HEM	CMD-C2D-C3D	3.85	132.20	124.94
4	A	800	HW9	C05-C06-N01	-3.61	119.07	122.90
3	A	600	H2B	N1-C2-N3	-3.47	120.80	126.43
2	A	500	HEM	CMB-C2B-C3B	3.40	131.04	124.68
2	B	500	HEM	CBD-CAD-C3D	-3.39	106.23	112.48
4	B	800	HW9	C05-C06-N01	-3.38	119.32	122.90
4	B	800	HW9	C5'-N1'-C2'	3.33	113.27	105.42
4	A	800	HW9	C5'-N1'-C2'	3.31	113.24	105.42
3	B	600	H2B	N1-C2-N3	-3.29	121.08	126.43
4	B	800	HW9	C22-N21-C26	3.27	121.90	117.42
4	B	800	HW9	C23-C22-N21	-3.17	120.03	123.96
4	A	800	HW9	C3'-C2'-N1'	-3.07	100.05	105.20
2	B	500	HEM	CMB-C2B-C3B	3.01	130.31	124.68
2	A	500	HEM	CBA-CAA-C2A	-2.96	107.04	112.49
4	B	800	HW9	C24-C25-C26	-2.94	118.39	120.32
2	A	500	HEM	CBD-CAD-C3D	-2.88	107.17	112.48
4	B	800	HW9	C06-C08-C4'	-2.86	106.14	115.55
2	B	500	HEM	CMD-C2D-C3D	2.77	130.16	124.94
4	A	800	HW9	C22-N21-C26	2.74	121.18	117.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	HEM	C4A-C3A-C2A	-2.55	105.22	107.00
4	B	800	HW9	C3'-C2'-N1'	-2.54	100.94	105.20
3	A	600	H2B	N2-C2-N1	2.51	120.64	116.57
3	B	600	H2B	N2-C2-N1	2.44	120.53	116.57
4	B	800	HW9	C04-C05-C06	-2.37	118.77	120.32
4	B	800	HW9	C10-O09-C3'	2.31	119.23	113.87
2	A	500	HEM	CMC-C2C-C3C	2.21	128.82	124.68

There are no chirality outliers.

There are no torsion outliers.

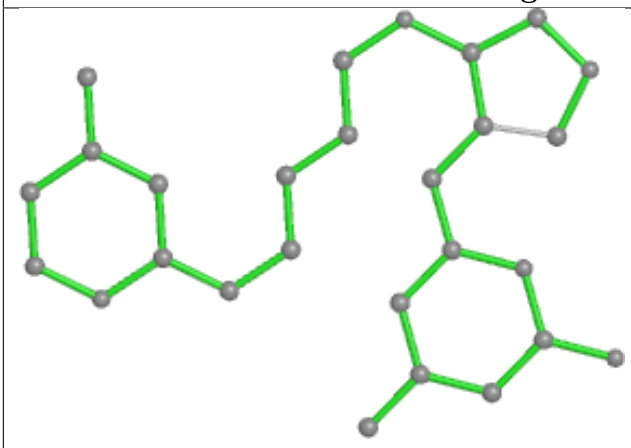
There are no ring outliers.

6 monomers are involved in 10 short contacts:

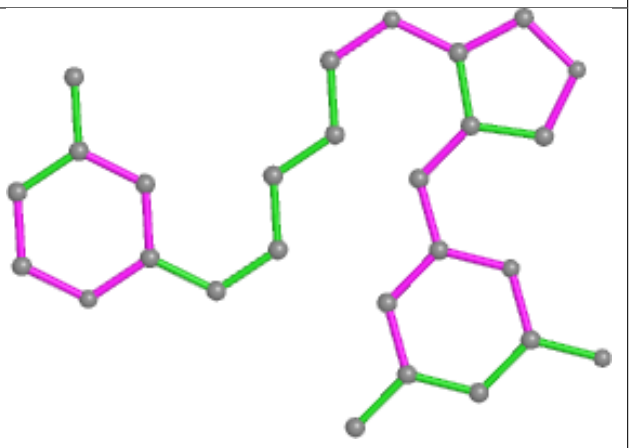
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	800	HW9	1	0
4	A	800	HW9	2	0
2	A	500	HEM	3	0
2	B	500	HEM	4	0
3	A	600	H2B	1	0
3	B	600	H2B	1	0

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 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.

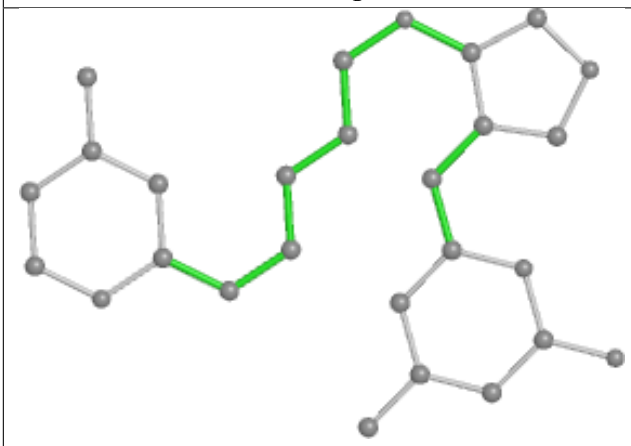
Ligand HW9 B 800



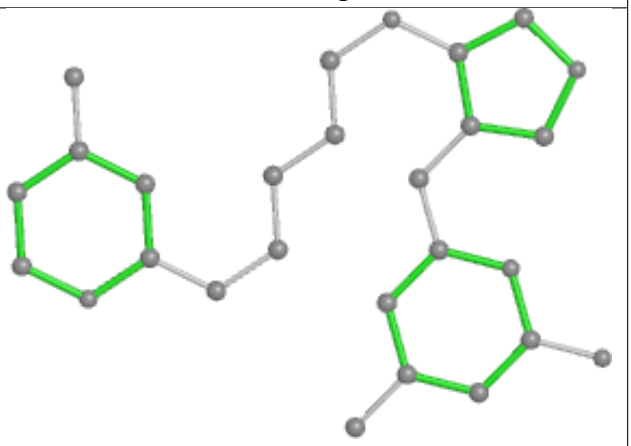
Bond lengths



Bond angles

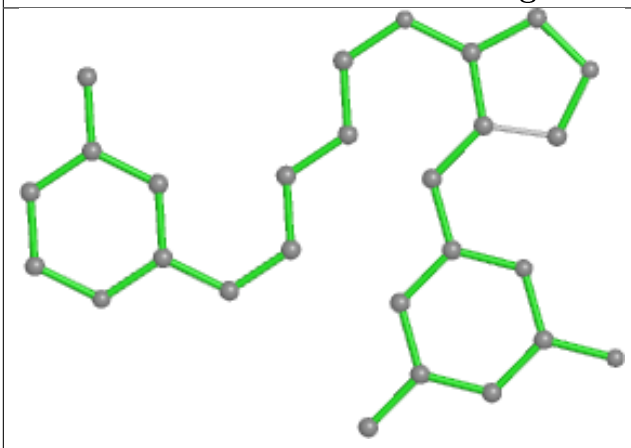


Torsions

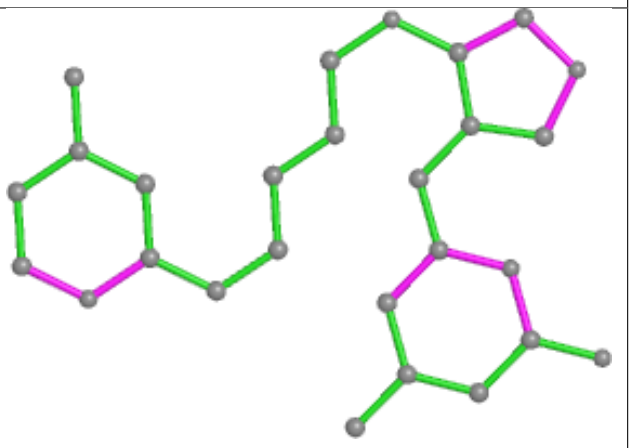


Rings

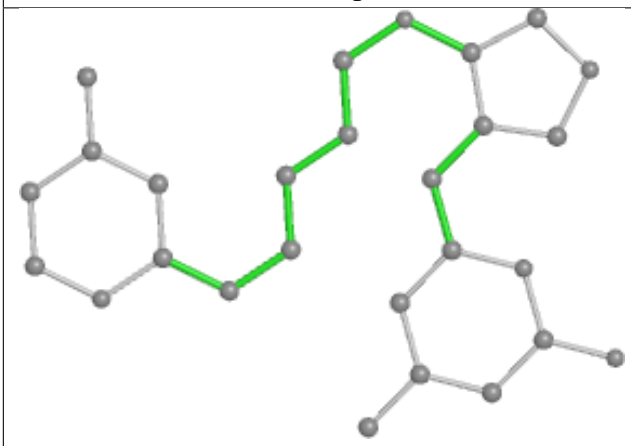
Ligand HW9 A 800



Bond lengths



Bond angles



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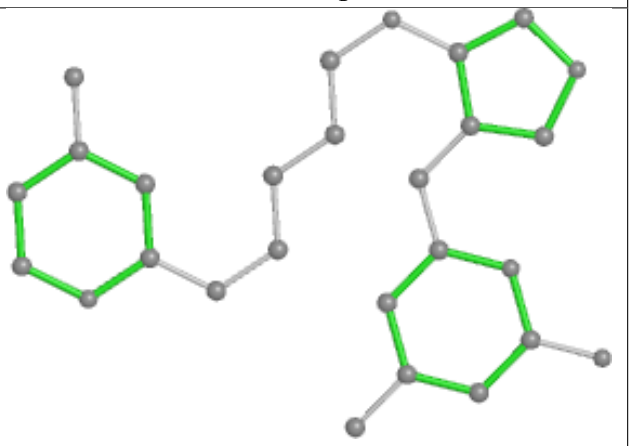
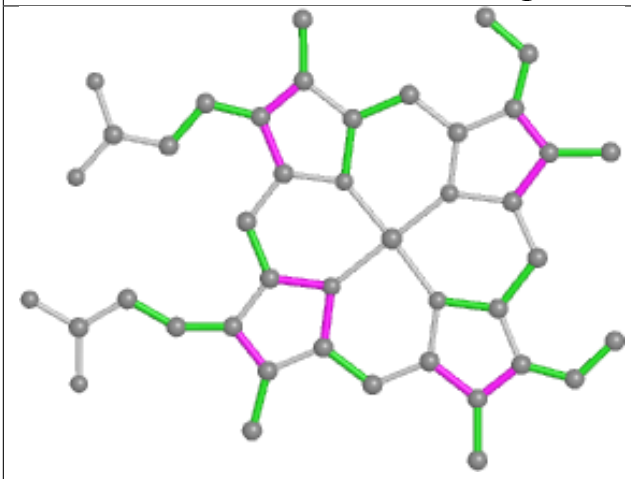
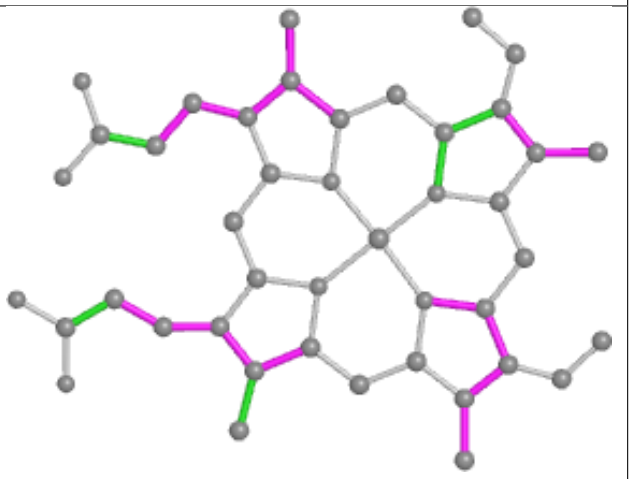


Rings

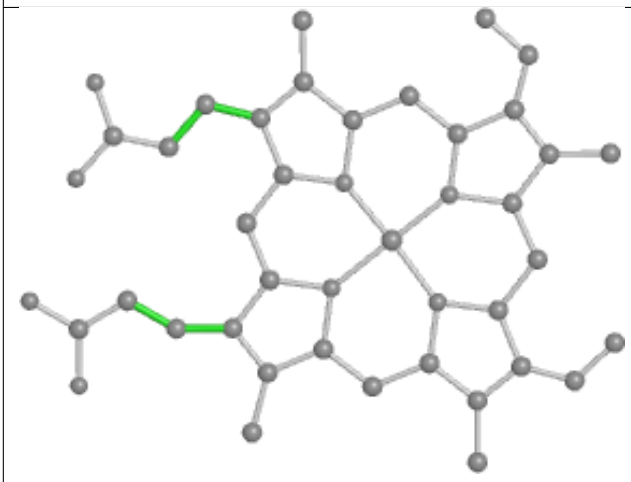
Ligand HEM A 500



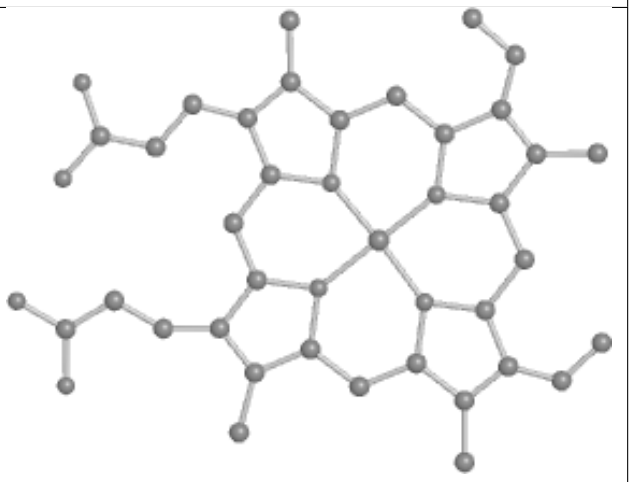
Bond lengths



Bond angles

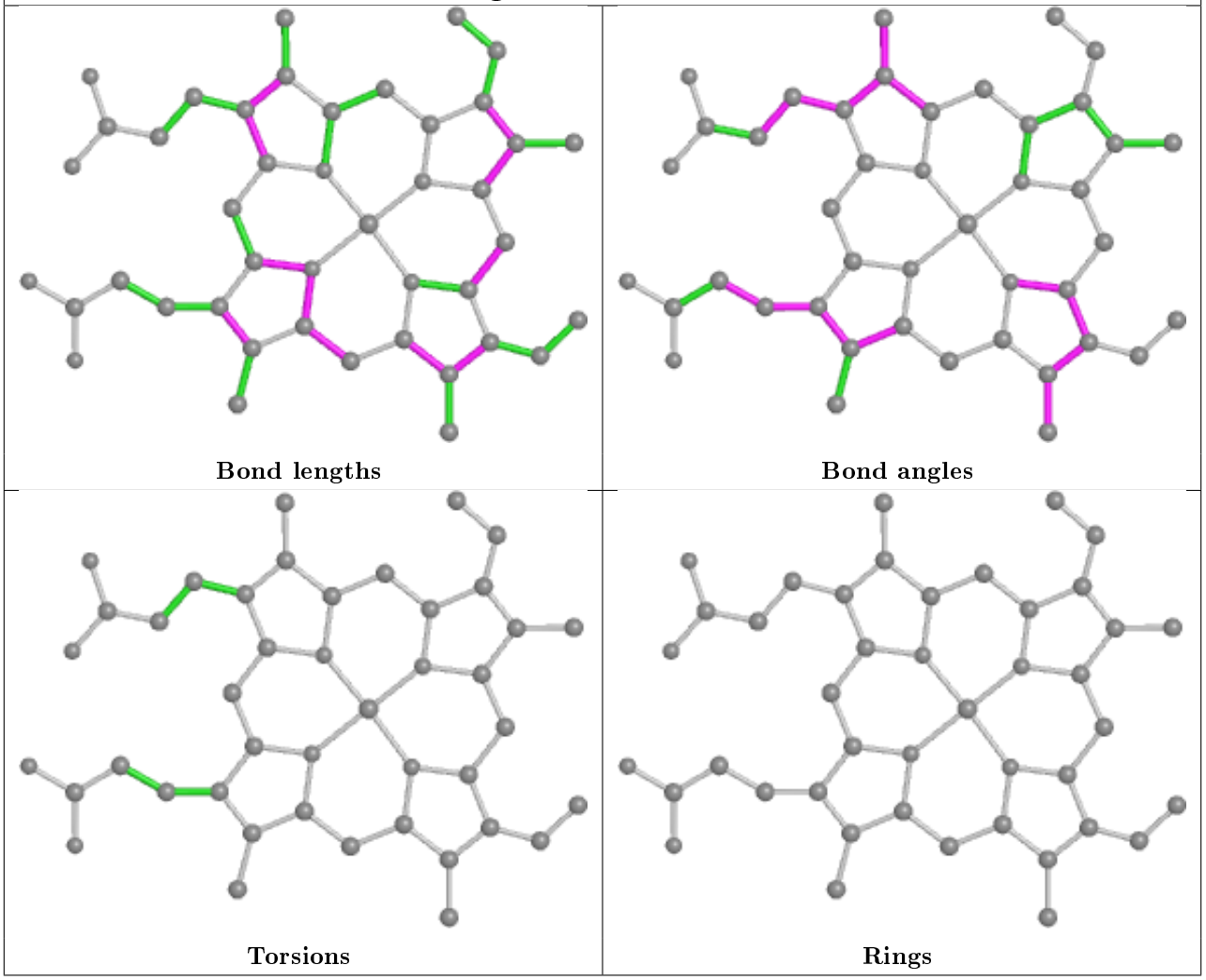


Torsions



Rings

Ligand HEM B 500



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, 95^{th} 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	404/443 (91%)	0.39	25 (6%)	20	25	26, 38, 67, 95	0
1	B	403/443 (90%)	0.23	20 (4%)	28	35	25, 41, 69, 99	0
All	All	807/886 (91%)	0.31	45 (5%)	24	30	25, 40, 68, 99	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	6.0
1	A	67	GLY	5.2
1	A	126	LEU	4.2
1	A	121	PRO	3.7
1	A	259	GLN	3.6
1	B	270	VAL	3.5
1	A	160	ALA	3.4
1	A	261	GLY	3.3
1	A	146	GLN	3.3
1	A	450	ILE	3.1
1	A	157	ALA	3.1
1	B	142	ARG	3.0
1	A	156	GLU	3.0
1	A	123	GLU	2.9
1	A	109	ARG	2.9
1	B	109	ARG	2.9
1	B	261	GLY	2.8
1	B	110	LYS	2.8
1	A	449	TRP	2.7
1	A	69	LYS	2.7
1	A	153	GLN	2.7
1	B	328	LEU	2.6
1	B	70	PHE	2.5
1	B	414	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	277	ILE	2.5
1	B	146	GLN	2.5
1	B	448	ALA	2.4
1	A	238	PRO	2.4
1	B	121	PRO	2.4
1	A	257	ARG	2.4
1	B	260	ASP	2.4
1	B	447	TRP	2.3
1	B	258	GLN	2.3
1	A	187	VAL	2.2
1	A	159	VAL	2.2
1	A	68	PRO	2.2
1	B	449	TRP	2.1
1	B	143	SER	2.1
1	B	257	ARG	2.1
1	A	143	SER	2.1
1	A	130	ARG	2.1
1	A	155	VAL	2.1
1	A	447	TRP	2.1
1	A	104	SER	2.0
1	B	123	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	CAS	B	384	9/10	0.94	0.11	51,57,86,91	0
1	CAS	A	384	9/10	0.95	0.11	39,41,56,65	0

6.3 Carbohydrates (i)

There are no carbohydrates 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,

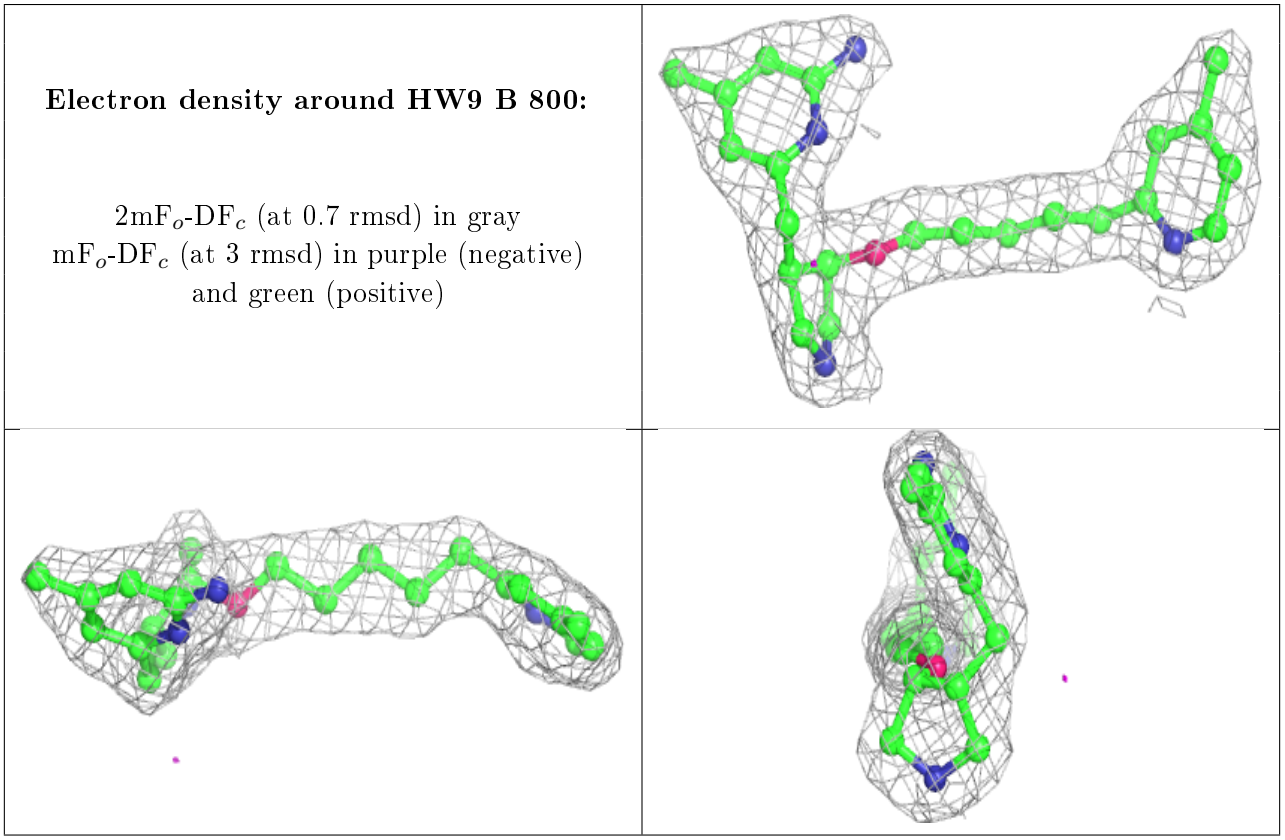
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	B	860	4/4	0.94	0.28	49,53,55,56	0
5	ACT	A	860	4/4	0.97	0.16	47,48,49,52	0
4	HW9	B	800	27/27	0.97	0.14	29,32,35,36	0
4	HW9	A	800	27/27	0.97	0.16	26,30,34,35	0
2	HEM	A	500	43/43	0.98	0.20	24,26,32,34	0
5	ACT	A	861	4/4	0.98	0.11	29,30,32,32	0
2	HEM	B	500	43/43	0.98	0.14	28,30,34,34	0
5	ACT	B	861	4/4	0.98	0.10	34,35,38,38	0
3	H2B	B	600	17/17	0.98	0.17	23,27,28,28	0
3	H2B	A	600	17/17	0.99	0.19	25,28,30,30	0
6	ZN	B	900	1/1	1.00	0.12	33,33,33,33	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.

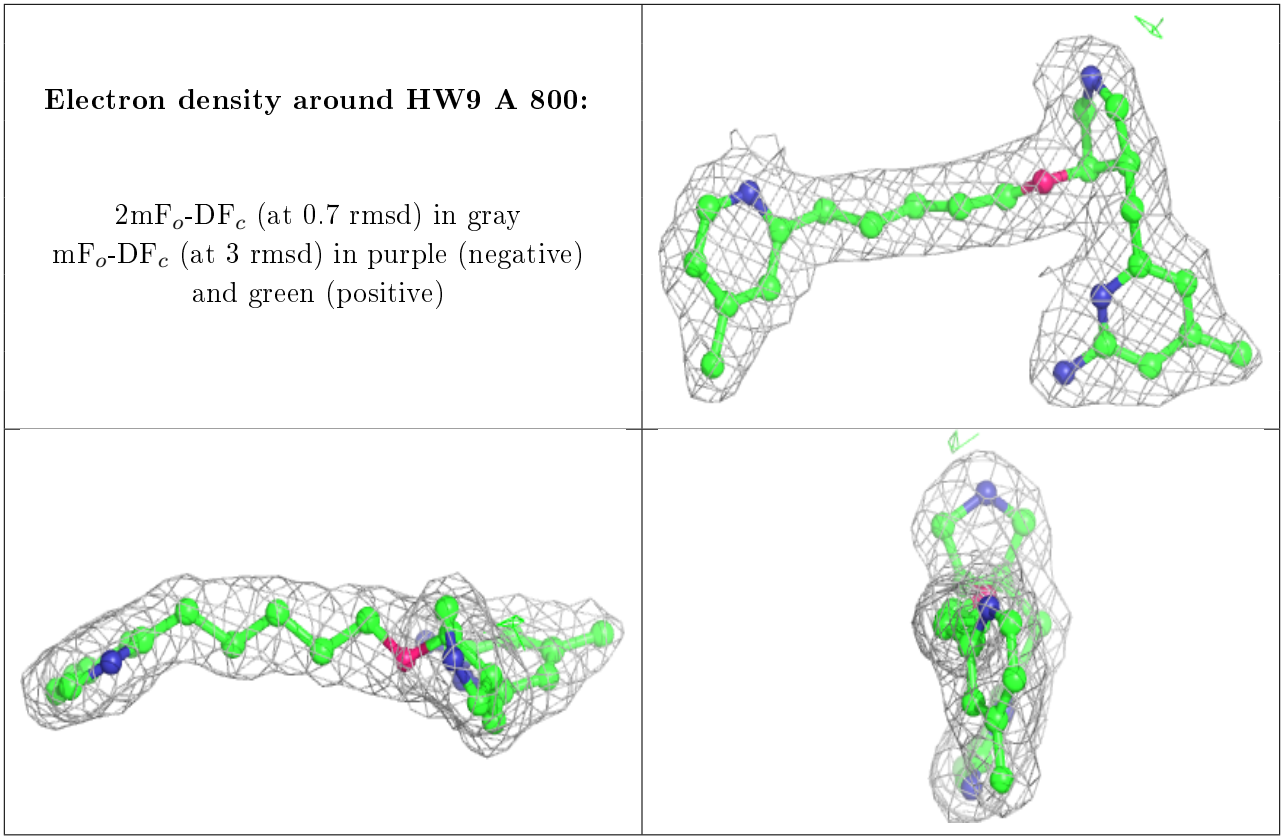
Electron density around HW9 B 800:

$2mF_o$-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:

$2mF_o$-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 500:

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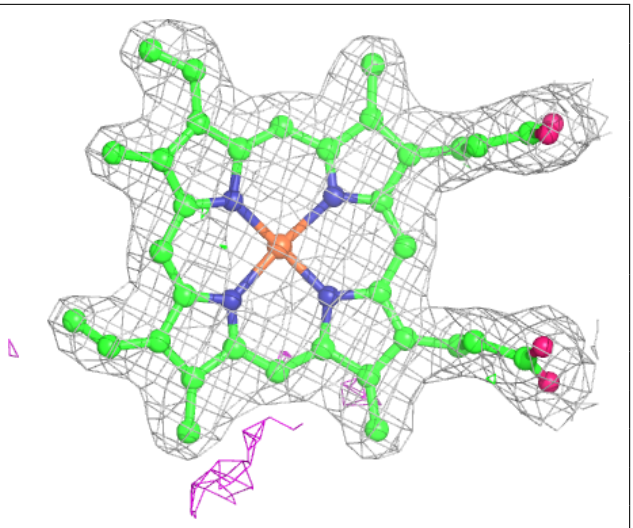
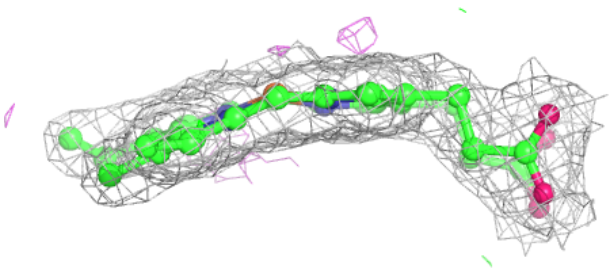
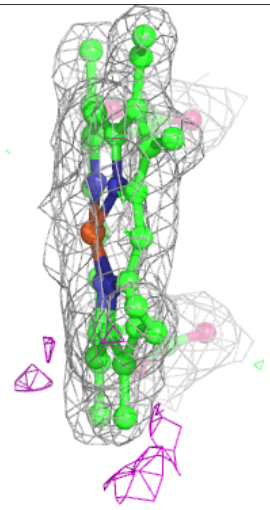
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

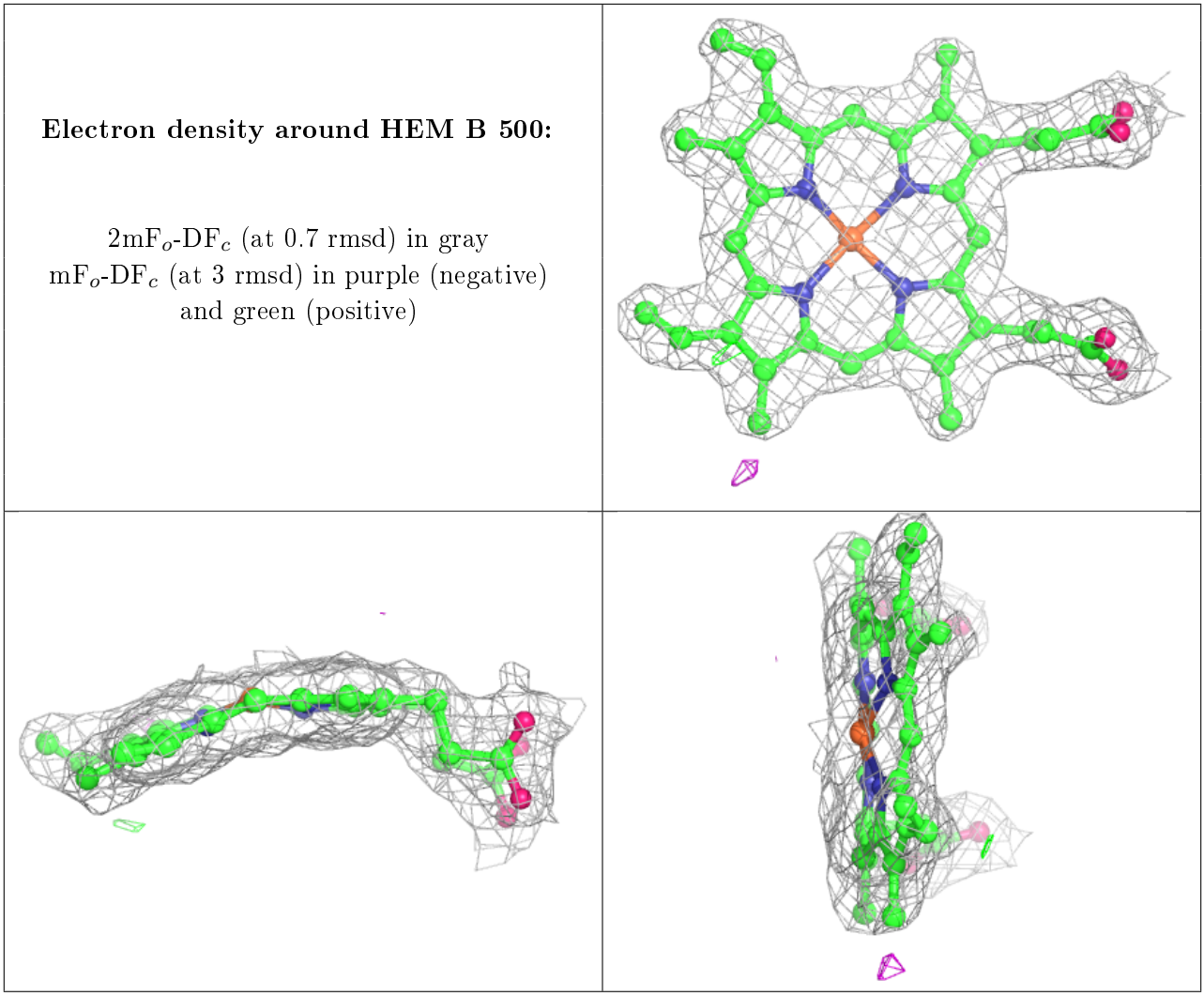






Electron density around HEM B 500:

$2mF_o$-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

There are no such residues in this entry.