Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 03:17 am BST

PDB ID	:	4CAM
Title	:	Structure of rat neuronal nitric oxide synthase heme domain in complex with 7-((3-Fluorophenethylamino)methyl)quinolin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2013-10-08
Resolution	:	1.83 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:

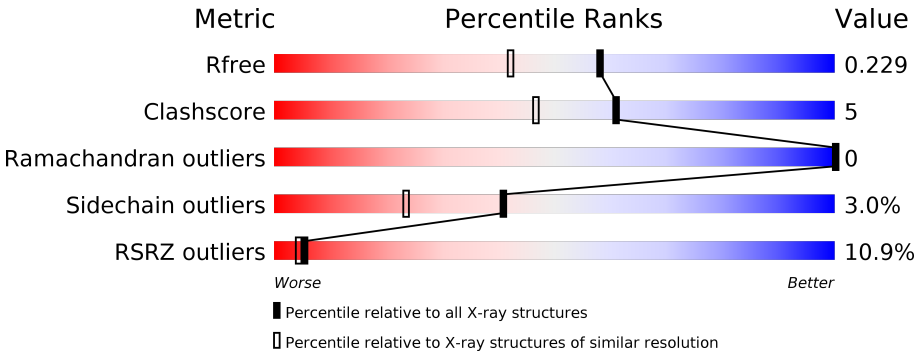
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.83 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	422	15% 83% 13%
1	B	422	6% 90% 7%

2 Entry composition

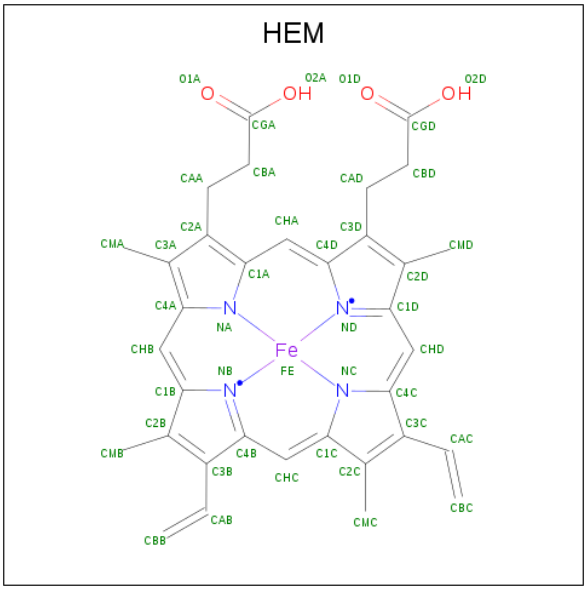
There are 7 unique types of molecules in this entry. The entry contains 7180 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

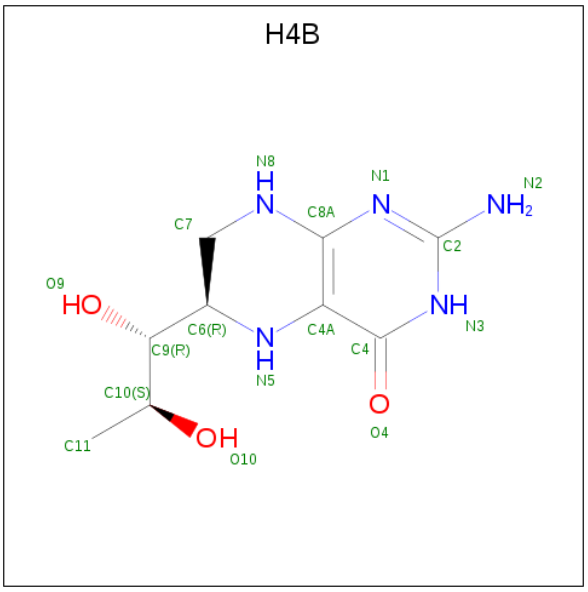
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	4	0
			3331	2133	567	609	22			
1	B	411	Total	C	N	O	S	0	3	0
			3359	2152	574	611	22			

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



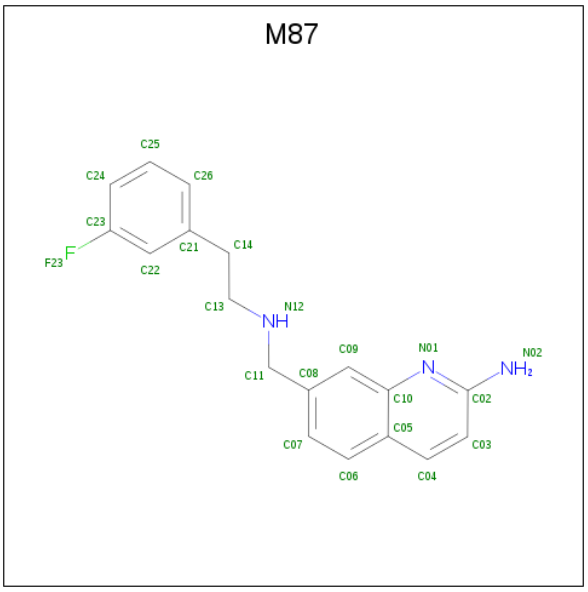
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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 7-[[2-(3-fluorophenyl)ethylamino]methyl]quinolin-2-amine (three-letter code: M87) (formula: $C_{18}H_{18}FN_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			22	18	1	3		

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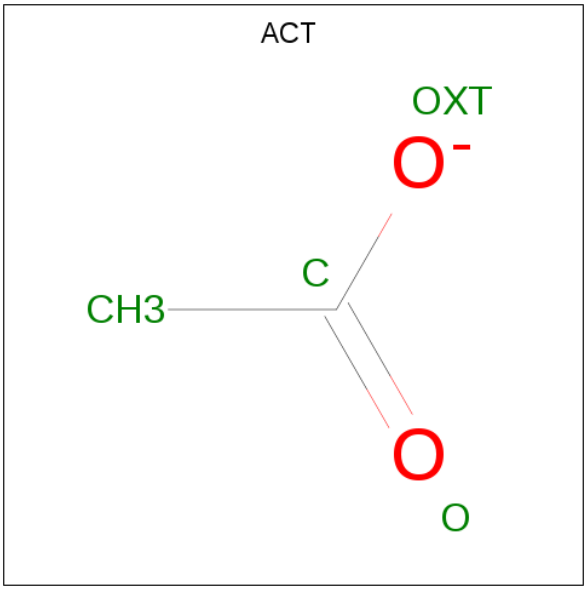
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C F N 22 18 1 3	0	0

- 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 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	A	1	Total Zn 1 1	0	0

- Molecule 7 is water.

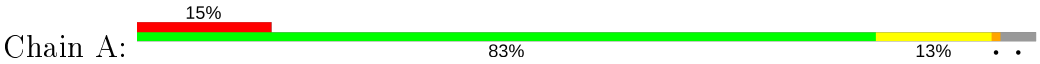
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	141	Total O 141 141	0	0
7	B	176	Total O 176 176	0	0

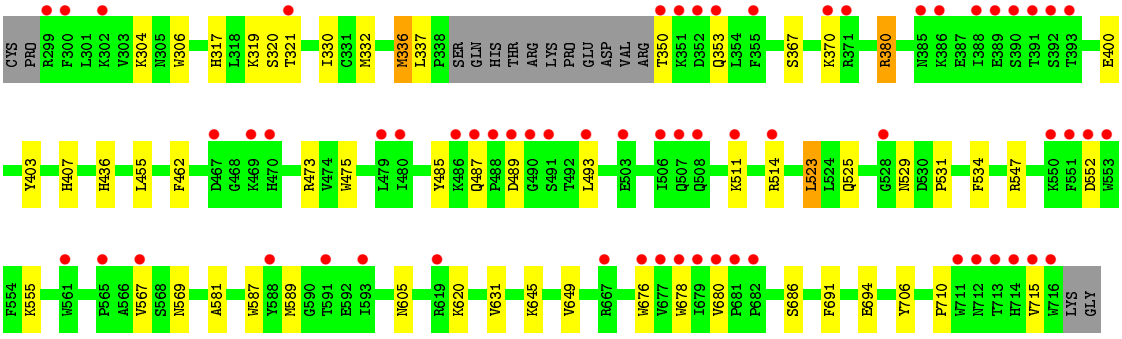
3 Residue-property plots (i)

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, BRAIN

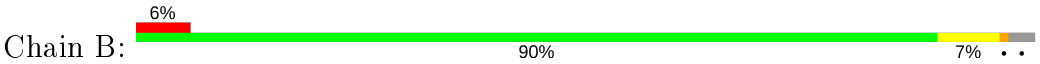
Chain A:

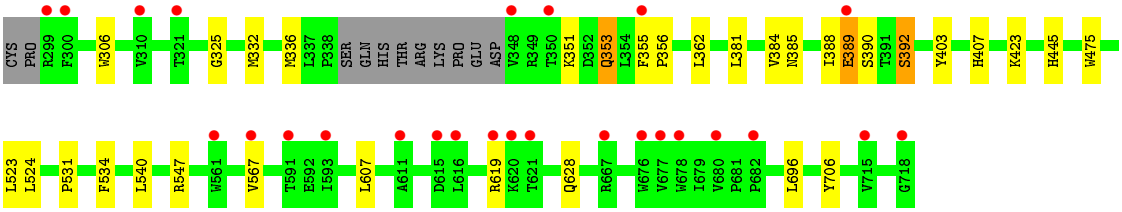




- Molecule 1: NITRIC OXIDE SYNTHASE, BRAIN

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	51.93Å 111.13Å 164.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.11 – 1.83 39.08 – 1.83	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.11-1.83) 99.4 (39.08-1.83)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.194 , 0.230 0.193 , 0.229	Depositor DCC
R_{free} test set	4196 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7180	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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: M87, ZN, H4B, HEM, ACT

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	0.52	0/3436	0.65	0/4663
1	B	0.60	0/3462	0.70	0/4694
All	All	0.56	0/6898	0.68	0/9357

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

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	3331	0	3245	36	0
1	B	3359	0	3278	26	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	22	0	18	3	0
4	B	22	0	18	2	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	141	0	0	4	0
7	B	176	0	0	0	0
All	All	7180	0	6655	61	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 (61) 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:336:MET:CE	1:A:678:TRP:HZ2	1.85	0.89
1:A:567:VAL:HG21	4:A:800:M87:C07	2.11	0.81
1:A:336:MET:CE	1:A:678:TRP:CZ2	2.68	0.77
1:B:567:VAL:HG21	4:B:800:M87:C07	2.14	0.76
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.68	0.74
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.70	0.72
1:B:355[A]:PHE:CE1	1:B:385:ASN:HB2	2.29	0.68
4:A:800:M87:H26	7:A:2069:HOH:O	1.95	0.67
1:A:321:THR:HG22	7:A:2006:HOH:O	1.98	0.62
1:A:336:MET:HE3	1:A:678:TRP:HZ2	1.62	0.62
1:A:380:ARG:HD3	1:A:400:GLU:OE2	2.01	0.60
1:A:332:MET:HE2	1:B:696:LEU:HD22	1.84	0.59
1:B:355[B]:PHE:HB2	1:B:356:PRO:CD	2.33	0.58
1:A:332:MET:HE2	1:B:696:LEU:CD2	2.33	0.57
1:B:706:TYR:OH	2:B:750:HEM:O2D	2.20	0.57
1:A:336:MET:HE1	1:A:678:TRP:CZ2	2.39	0.56
1:A:706:TYR:OH	2:A:750:HEM:O2D	2.18	0.56
1:A:620:LYS:HB2	1:A:620:LYS:NZ	2.20	0.55
1:B:351:LYS:HE2	1:B:389:GLU:HA	1.89	0.55
1:B:403:TYR:CE1	1:B:407:HIS:CE1	2.94	0.55
1:A:321:THR:HG21	7:A:2007:HOH:O	2.06	0.55
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.88	0.55
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.23	0.53
1:B:362:LEU:HD12	1:B:381:LEU:HD23	1.91	0.53
1:A:485:TYR:HB3	1:A:514:ARG:NH2	2.25	0.52
2:B:750:HEM:HHC	2:B:750:HEM:CBB	2.38	0.52
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.92	0.51
1:A:605:ASN:ND2	7:A:2111:HOH:O	2.46	0.48
1:A:336:MET:HG3	1:B:306:TRP:NE1	2.29	0.47
1:A:525:GLN:HG3	1:A:529:ASN:O	2.15	0.47
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:MET:HE3	1:A:678:TRP:CZ2	2.45	0.46
1:B:388:ILE:O	1:B:392:SER:N	2.45	0.46
1:A:462:PHE:HB2	1:A:581:ALA:HB3	1.97	0.45
1:B:325:GLY:O	1:B:332:MET:HG3	2.16	0.45
1:A:306:TRP:CD2	1:B:336:MET:HE3	2.52	0.45
1:A:304:LYS:O	1:A:694:GLU:HG3	2.17	0.45
1:B:355[B]:PHE:HB2	1:B:356:PRO:HD3	1.99	0.44
1:B:524:LEU:HD12	1:B:534:PHE:CD2	2.52	0.44
1:A:436:HIS:CD2	1:A:534:PHE:HE2	2.36	0.44
1:B:353:GLN:HB3	1:B:353:GLN:HE21	1.64	0.43
1:A:330:ILE:HD11	1:B:696:LEU:HB3	2.01	0.43
1:A:686:SER:HA	1:A:691:PHE:CG	2.53	0.43
2:A:750:HEM:C4B	4:A:800:M87:H03	2.54	0.42
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.07	0.42
1:A:589:MET:HA	1:A:649:VAL:O	2.19	0.42
2:B:750:HEM:CHC	2:B:750:HEM:HBB2	2.40	0.42
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.55	0.41
1:A:487:GLN:HE21	1:A:493:LEU:HB2	1.85	0.41
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.01	0.41
1:B:445:HIS:C	1:B:445:HIS:CD2	2.93	0.41
1:B:619:ARG:HB2	1:B:619:ARG:HE	1.62	0.41
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.01	0.41
1:B:351:LYS:HE3	1:B:392:SER:OG	2.21	0.41
1:A:317:HIS:O	1:A:320:SER:HB3	2.20	0.41
1:A:350:THR:N	1:A:353:GLN:HE21	2.19	0.41
1:B:567:VAL:HG21	4:B:800:M87:C06	2.49	0.41
1:B:607:LEU:HA	1:B:607:LEU:HD23	1.94	0.41
1:B:524:LEU:O	1:B:531:PRO:HA	2.20	0.41
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.56	0.41
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.56	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%)	396 (97%)	11 (3%)	0	100	100
1	B	410/422 (97%)	403 (98%)	7 (2%)	0	100	100
All	All	817/844 (97%)	799 (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	367/377 (97%)	352 (96%)	15 (4%)	30	13
1	B	369/377 (98%)	362 (98%)	7 (2%)	57	42
All	All	736/754 (98%)	714 (97%)	22 (3%)	41	23

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	LYS
1	A	336	MET
1	A	337	LEU
1	A	367	SER
1	A	370	LYS
1	A	380	ARG
1	A	489	ASP
1	A	511	LYS
1	A	523	LEU
1	A	547	ARG
1	A	552	ASP
1	A	555	LYS
1	A	569	ASN
1	A	645	LYS
1	A	715	VAL

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Mol	Chain	Res	Type
1	B	353	GLN
1	B	389	GLU
1	B	390	SER
1	B	392	SER
1	B	423	LYS
1	B	540	LEU
1	B	547	ARG

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

Mol	Chain	Res	Type
1	A	425	GLN
1	A	454	ASN
1	A	569	ASN
1	A	605	ASN
1	A	697	ASN
1	B	364	GLN
1	B	454	ASN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
1	B	697	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\#\|Z\| > 2$
5	ACT	B	860	-	1,3,3	1.14	0	0,3,3	0.00	-
5	ACT	A	860	-	1,3,3	1.67	0	0,3,3	0.00	-
4	M87	B	800	-	24,24,24	1.11	3 (12%)	30,32,32	1.73	8 (26%)
3	H4B	A	760	-	16,18,18	1.32	3 (18%)	11,26,26	2.82	6 (54%)
2	HEM	A	750	1	27,50,50	0.96	2 (7%)	17,82,82	1.32	3 (17%)
4	M87	A	800	-	24,24,24	1.11	3 (12%)	30,32,32	1.07	3 (10%)
3	H4B	B	760	-	16,18,18	1.41	2 (12%)	11,26,26	2.69	5 (45%)
2	HEM	B	750	1	27,50,50	1.03	1 (3%)	17,82,82	1.71	5 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	750	1	-	0/6/54/54	-
4	M87	B	800	-	-	2/7/7/7	0/3/3/3
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	M87	A	800	-	-	1/7/7/7	0/3/3/3
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
2	HEM	B	750	1	-	0/6/54/54	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	760	H4B	C7-C6	3.96	1.56	1.52
4	A	800	M87	C06-C07	2.89	1.42	1.36
4	B	800	M87	C06-C07	2.66	1.42	1.36
3	A	760	H4B	C2-N2	2.64	1.39	1.33
2	A	750	HEM	C3B-C2B	-2.61	1.36	1.40
2	B	750	HEM	C4D-C3D	2.53	1.48	1.42
2	A	750	HEM	C4D-C3D	2.42	1.48	1.42
3	B	760	H4B	C7-N8	2.25	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	760	H4B	C7-N8	2.23	1.48	1.44
4	A	800	M87	C04-C03	2.20	1.41	1.36
4	B	800	M87	C24-C23	2.19	1.41	1.37
4	B	800	M87	C04-C03	2.10	1.41	1.36
4	A	800	M87	C02-N01	2.06	1.36	1.33
3	A	760	H4B	C4-N3	2.05	1.36	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	760	H4B	C4-C4A-C8A	5.89	119.81	114.57
3	A	760	H4B	C4-C4A-C8A	5.63	119.57	114.57
4	B	800	M87	C03-C02-N01	-3.98	117.30	122.08
3	A	760	H4B	C4-N3-C2	3.89	122.10	115.93
3	A	760	H4B	N3-C2-N1	-3.50	119.92	125.42
4	B	800	M87	C04-C03-C02	3.43	122.16	119.48
4	B	800	M87	C14-C21-C22	-3.38	114.99	120.54
3	B	760	H4B	N3-C2-N1	-3.26	120.30	125.42
3	B	760	H4B	C4-N3-C2	3.11	120.87	115.93
3	B	760	H4B	C2-N1-C8A	3.01	121.30	114.54
2	B	750	HEM	C1D-C2D-C3D	-2.99	104.91	107.00
2	B	750	HEM	CBA-CAA-C2A	-2.84	107.24	112.49
2	B	750	HEM	CMA-C3A-C4A	-2.79	124.17	128.46
4	B	800	M87	C11-C08-C09	-2.74	116.61	121.51
3	A	760	H4B	C2-N1-C8A	2.71	120.61	114.54
4	A	800	M87	C11-C08-C09	-2.63	116.80	121.51
4	B	800	M87	N02-C02-N01	2.60	120.41	118.26
4	B	800	M87	C08-C11-N12	2.55	119.41	112.80
2	A	750	HEM	CBD-CAD-C3D	-2.48	107.91	112.48
2	A	750	HEM	CBA-CAA-C2A	-2.47	107.93	112.49
3	A	760	H4B	C4-C4A-N5	2.40	121.13	119.12
2	A	750	HEM	CMC-C2C-C3C	2.37	129.11	124.68
4	A	800	M87	C03-C02-N01	-2.37	119.23	122.08
2	B	750	HEM	C3B-C4B-NB	-2.18	106.39	109.21
3	A	760	H4B	N2-C2-N1	2.17	120.63	117.25
4	B	800	M87	C24-C23-C22	-2.17	120.47	123.29
2	B	750	HEM	CMA-C3A-C2A	2.15	129.00	124.94
4	A	800	M87	C24-C23-C22	-2.14	120.52	123.29
4	B	800	M87	F23-C23-C24	2.07	122.05	118.54
3	B	760	H4B	C4-C4A-N5	2.02	120.82	119.12

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	800	M87	C14-C13-N12-C11
4	B	800	M87	C13-C14-C21-C22
4	B	800	M87	C13-C14-C21-C26

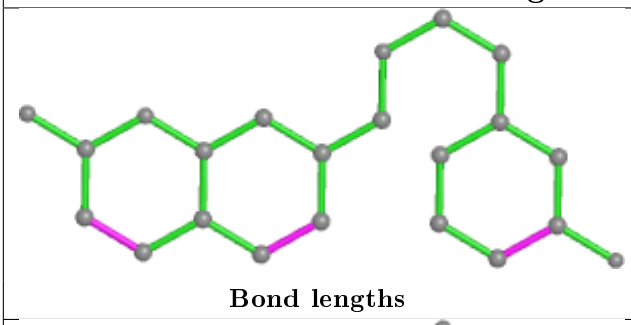
There are no ring outliers.

4 monomers are involved in 10 short contacts:

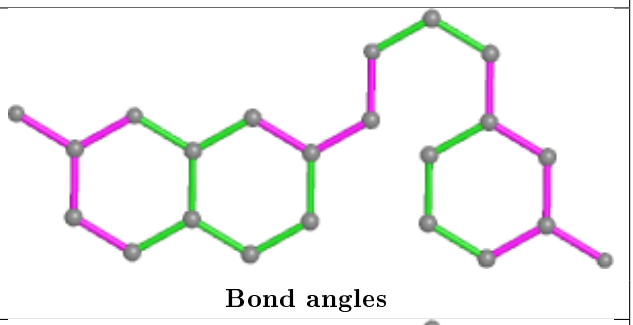
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	800	M87	2	0
2	A	750	HEM	2	0
4	A	800	M87	3	0
2	B	750	HEM	4	0

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.

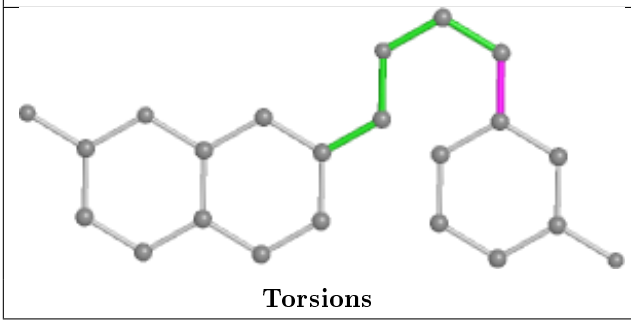
Ligand M87 B 800



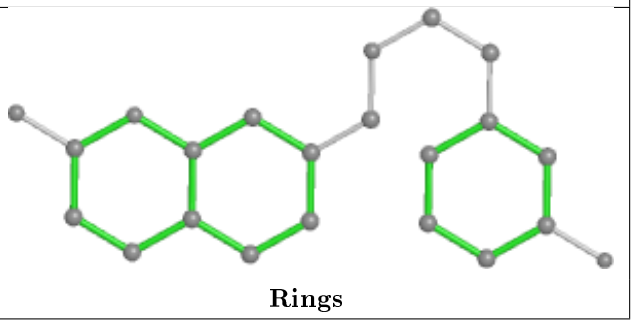
Bond lengths



Bond angles

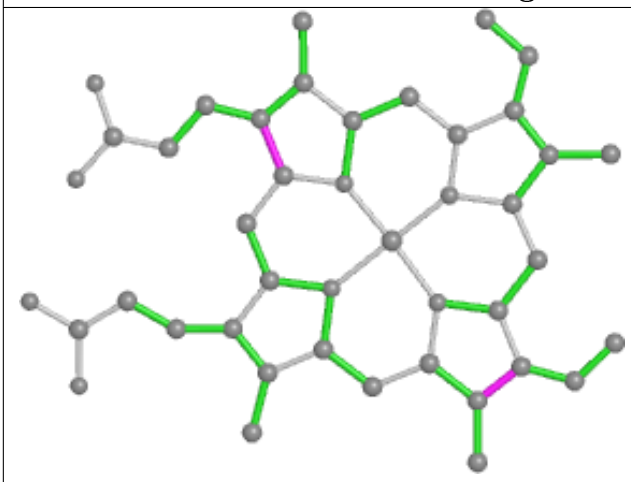


Torsions

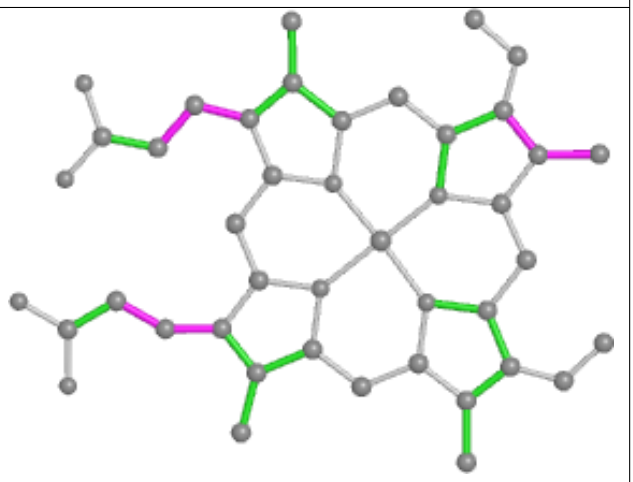


Rings

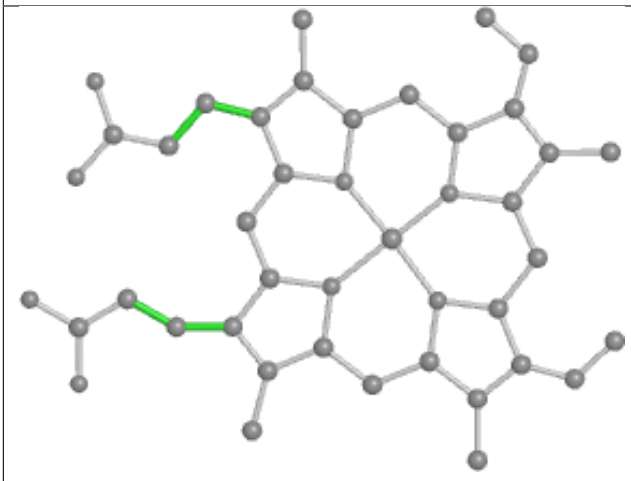
Ligand HEM A 750



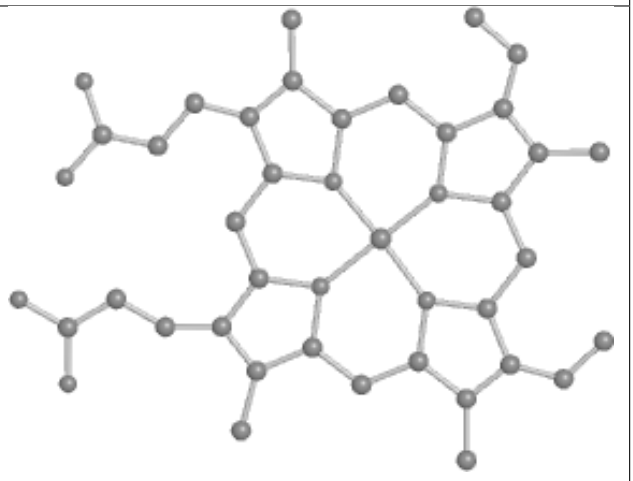
Bond lengths



Bond angles

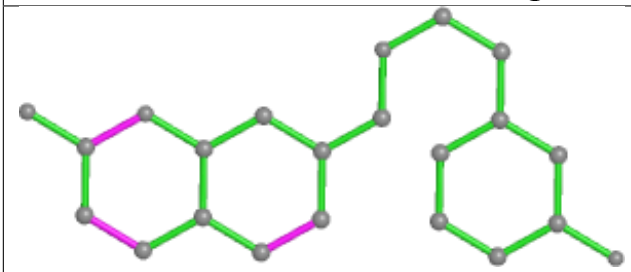


Torsions

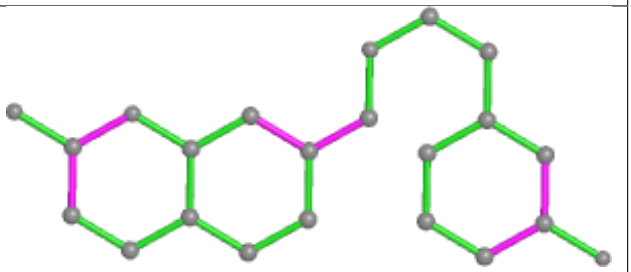


Rings

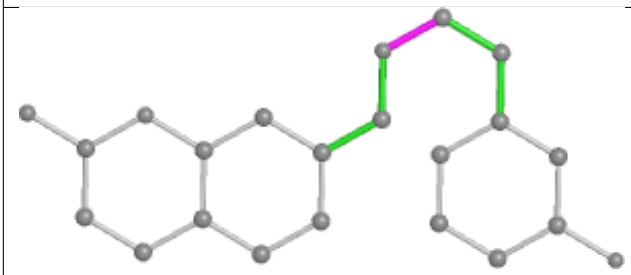
Ligand M87 A 800



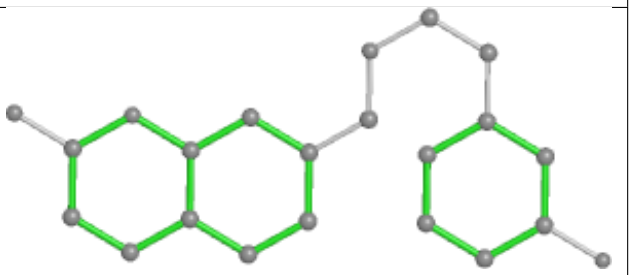
Bond lengths



Bond angles

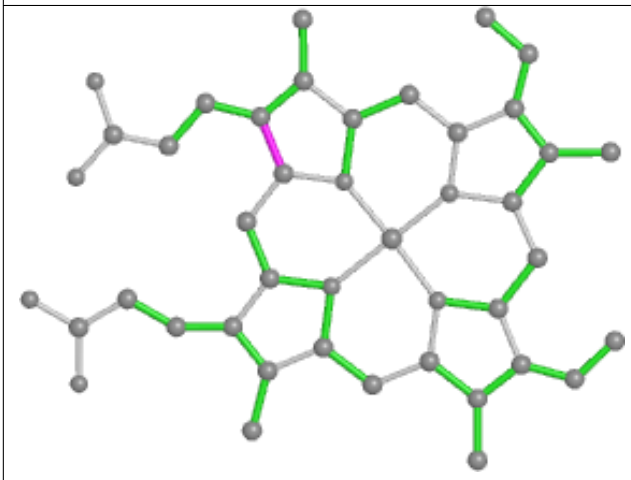


Torsions

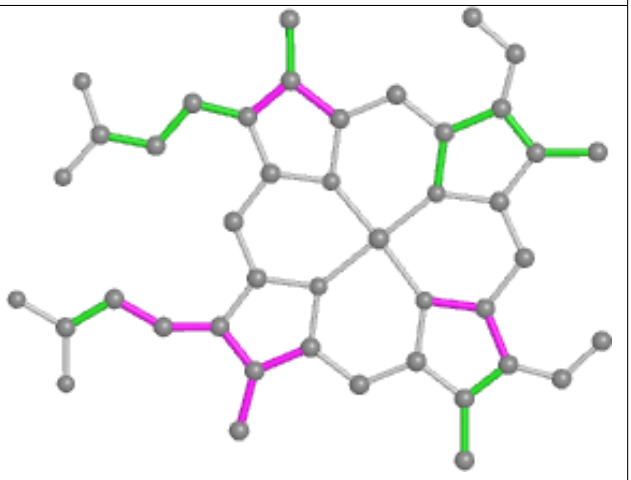


Rings

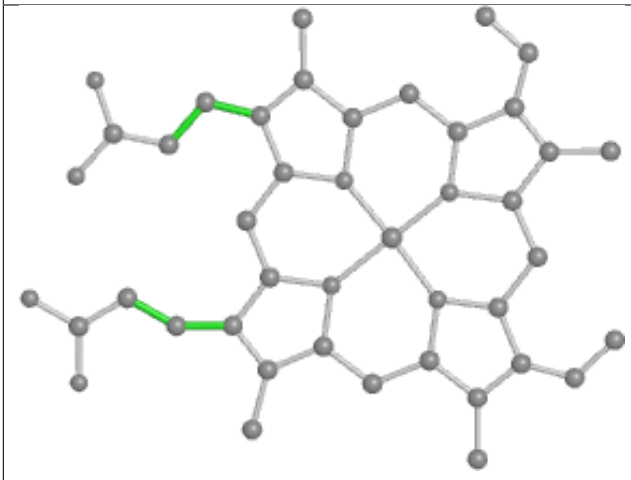
Ligand HEM B 750



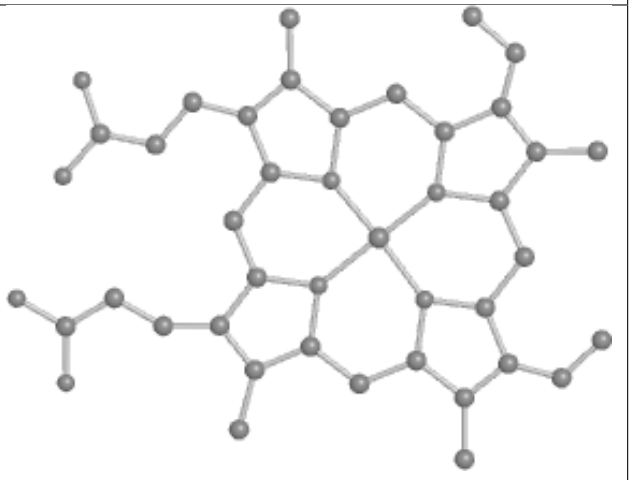
Bond lengths



Bond angles



Torsions



Rings

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	407/422 (96%)	0.75	63 (15%) 2 1	26, 49, 86, 117	0
1	B	411/422 (97%)	0.22	26 (6%) 20 17	24, 38, 66, 89	0
All	All	818/844 (96%)	0.49	89 (10%) 5 4	24, 43, 81, 117	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	VAL	8.2
1	A	715	VAL	7.6
1	A	488	PRO	7.4
1	B	300	PHE	7.2
1	A	716	TRP	6.6
1	A	355	PHE	5.7
1	A	713	THR	5.3
1	B	619	ARG	4.9
1	B	718	GLY	4.8
1	A	507	GLN	4.7
1	A	352	ASP	4.5
1	A	489	ASP	4.5
1	A	391	THR	4.5
1	A	392	SER	4.3
1	A	486	LYS	4.2
1	A	491	SER	4.2
1	A	712	ASN	4.1
1	B	350	THR	4.1
1	A	487	GLN	4.0
1	A	490	GLY	4.0
1	B	616	LEU	3.9
1	A	388	ILE	3.9
1	A	390	SER	3.9
1	A	386	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	551	PHE	3.3
1	A	300	PHE	3.3
1	A	503	GLU	3.3
1	A	677	VAL	3.3
1	B	620	LYS	3.3
1	B	677	VAL	3.2
1	B	321	THR	3.2
1	A	680	VAL	3.2
1	A	511	LYS	3.1
1	A	469	LYS	3.1
1	A	350	THR	3.1
1	A	619	ARG	3.0
1	A	528	GLY	3.0
1	A	676	TRP	3.0
1	A	506	ILE	3.0
1	A	679	ILE	3.0
1	A	479	LEU	2.9
1	A	714	HIS	2.9
1	B	611	ALA	2.9
1	B	591	THR	2.8
1	B	615	ASP	2.8
1	B	680	VAL	2.8
1	A	351	LYS	2.8
1	B	355[A]	PHE	2.8
1	A	711	TRP	2.8
1	A	385	ASN	2.7
1	A	593	ILE	2.7
1	A	667	ARG	2.7
1	A	508	GLN	2.7
1	A	389	GLU	2.7
1	B	389	GLU	2.7
1	B	667	ARG	2.7
1	A	299	ARG	2.6
1	A	678	TRP	2.6
1	A	480	ILE	2.6
1	A	588	TYR	2.6
1	A	353	GLN	2.6
1	A	467	ASP	2.6
1	B	676	TRP	2.5
1	B	678	TRP	2.5
1	B	299	ARG	2.5
1	A	682	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	567	VAL	2.5
1	A	321	THR	2.4
1	A	470	HIS	2.4
1	A	550	LYS	2.3
1	A	514	ARG	2.3
1	A	552	ASP	2.3
1	A	561	TRP	2.3
1	A	565	PRO	2.3
1	A	371	ARG	2.3
1	B	621	THR	2.3
1	B	715	VAL	2.2
1	A	393	THR	2.2
1	A	591	THR	2.2
1	B	310	VAL	2.2
1	B	567	VAL	2.2
1	A	553	TRP	2.1
1	B	682	PRO	2.1
1	A	302	LYS	2.1
1	A	370	LYS	2.0
1	A	681	PRO	2.0
1	B	561	TRP	2.0
1	A	493	LEU	2.0
1	B	593	ILE	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 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.

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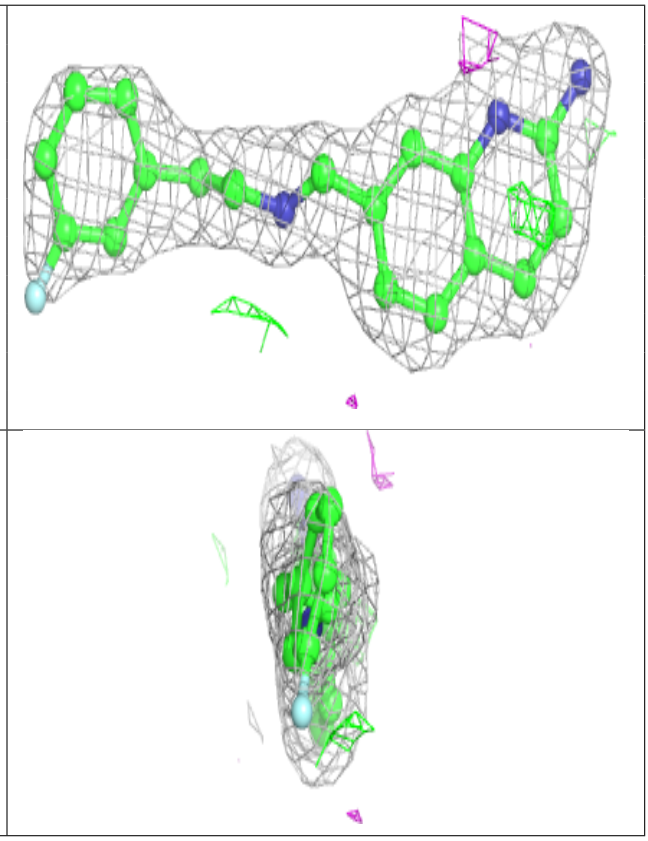
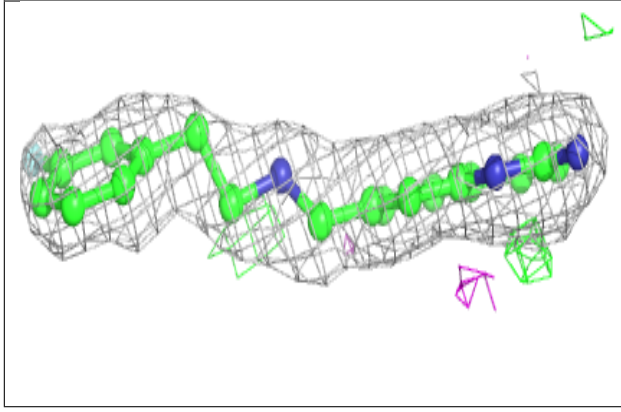
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	M87	A	800	22/22	0.92	0.23	29,34,74,83	0
4	M87	B	800	22/22	0.93	0.18	28,35,60,64	0
5	ACT	B	860	4/4	0.95	0.08	52,53,54,56	0
5	ACT	A	860	4/4	0.96	0.13	60,61,64,66	0
3	H4B	A	760	17/17	0.96	0.16	27,30,35,36	0
3	H4B	B	760	17/17	0.96	0.17	28,31,35,37	0
2	HEM	A	750	43/43	0.97	0.18	28,30,37,45	0
2	HEM	B	750	43/43	0.97	0.16	23,27,36,38	0
6	ZN	A	1717	1/1	1.00	0.09	36,36,36,36	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 M87 A 800:

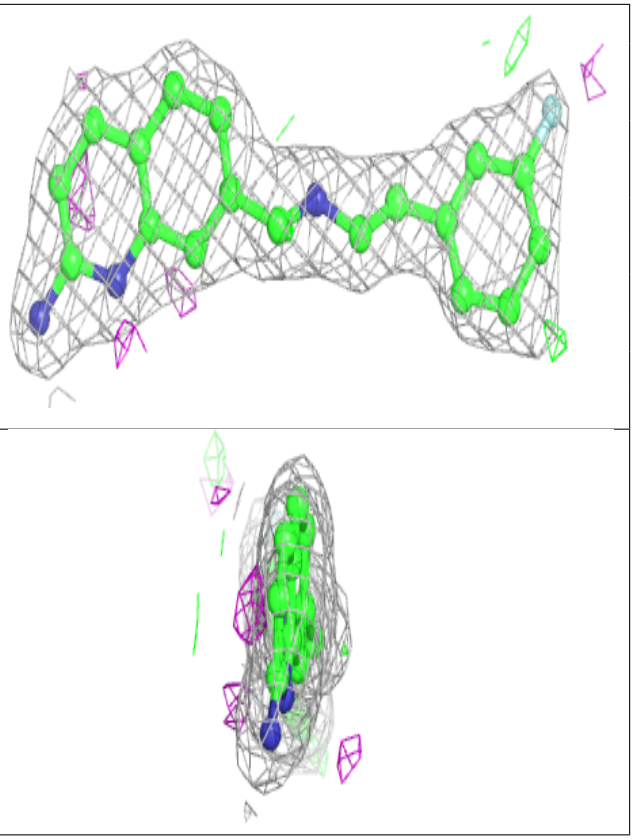
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





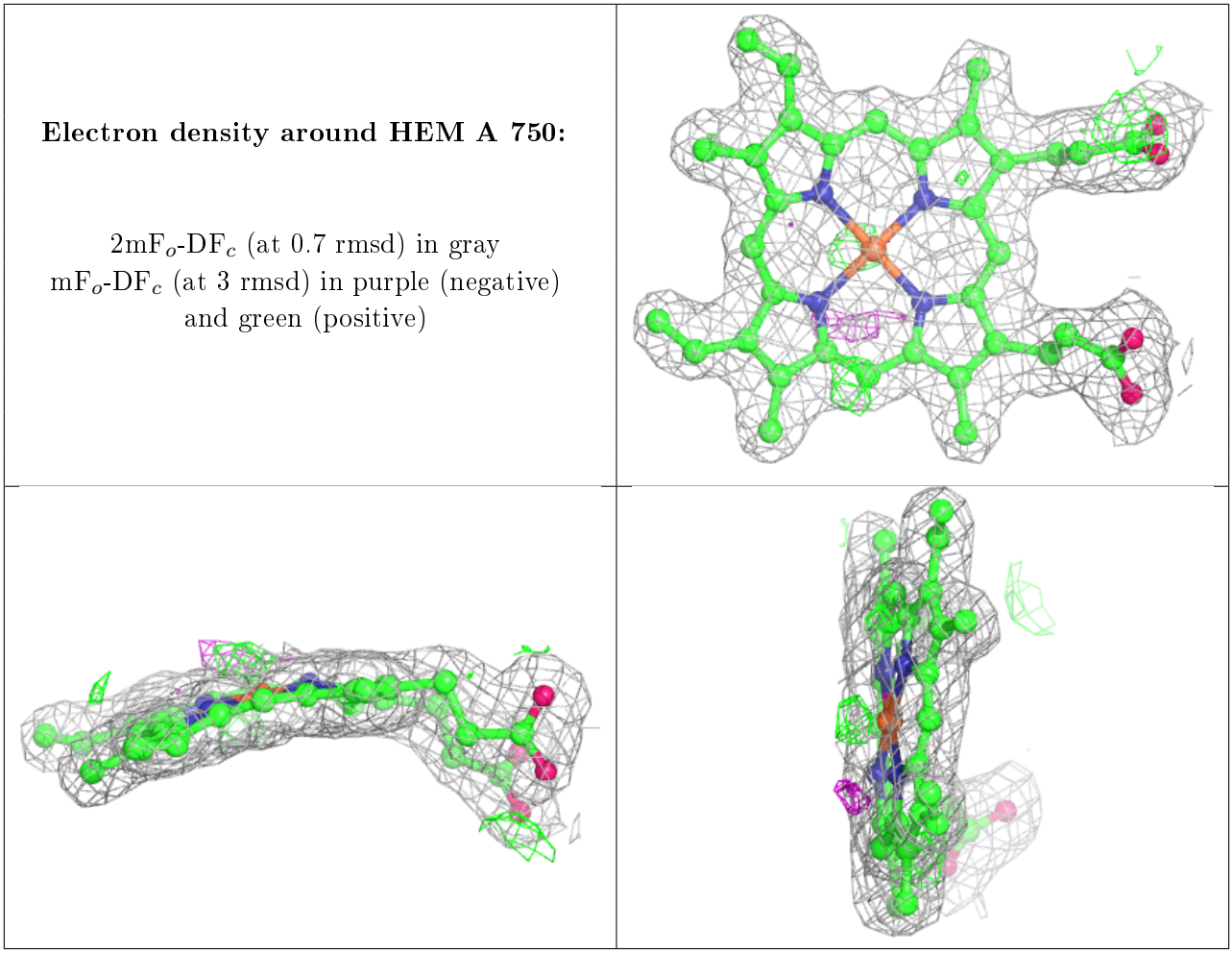
Electron density around M87 B 800:

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



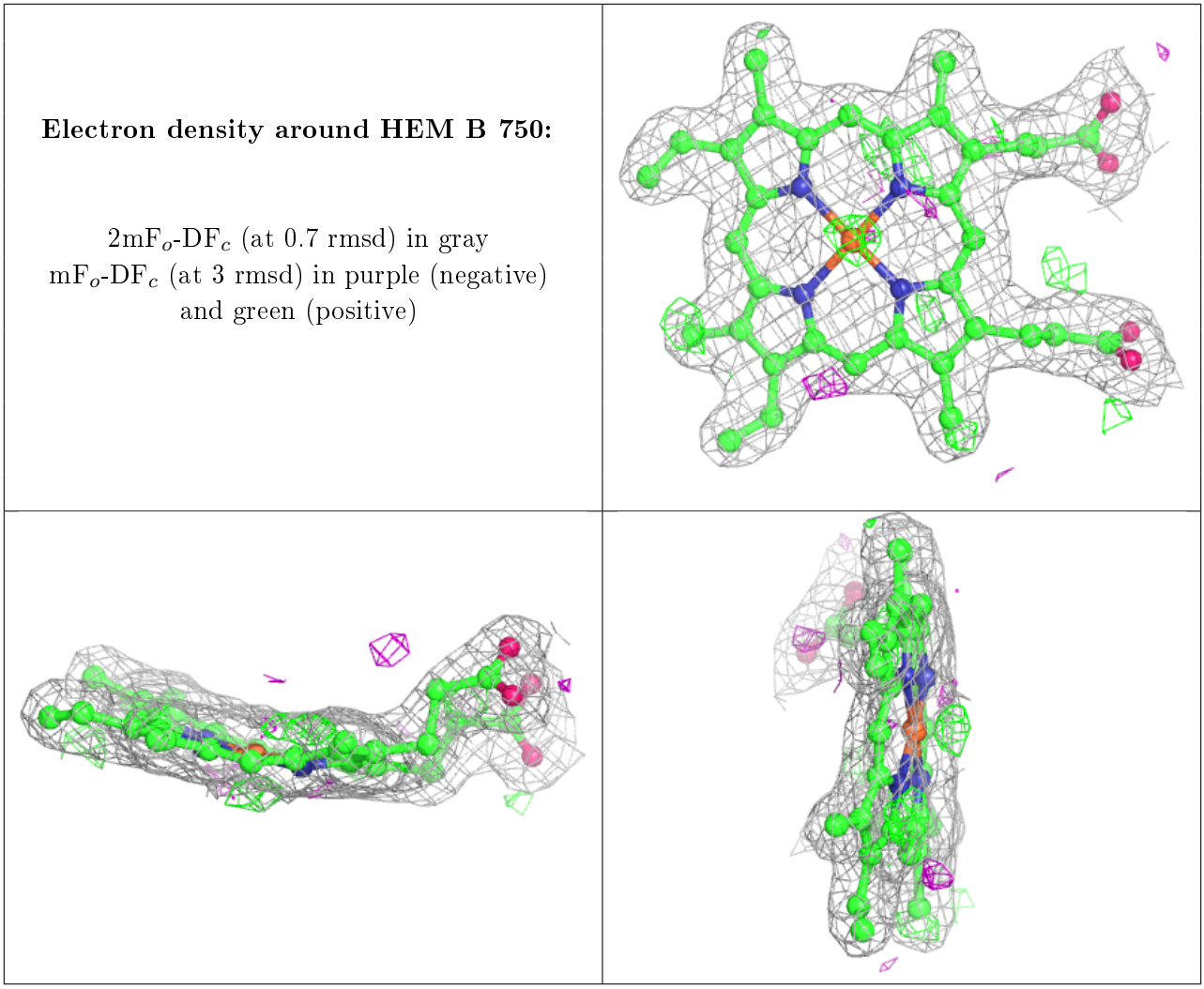
Electron density around HEM A 750:

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



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)



6.5 Other polymers

There are no such residues in this entry.