Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 12:26 AM EDT

PDB ID	:	3PNE
Title	:	Structure of rat neuronal nitric oxide synthase heme domain in complex with 6-(((3R,4R)-4-(2-((2,2-Difluoro-2-(3-chlorophenyl)ethyl)amino)ethoxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine
Authors	:	Li, H.; Delker, S.; Poulos, T.L.
Deposited on	:	2010-11-18
Resolution	:	1.97 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:

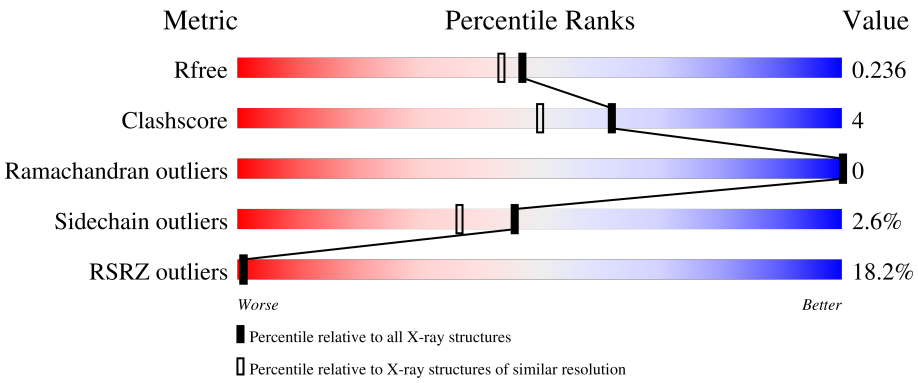
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.97 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	23% 87% 9% • •
1	B	422	13% 88% 9% •

2 Entry composition (i)

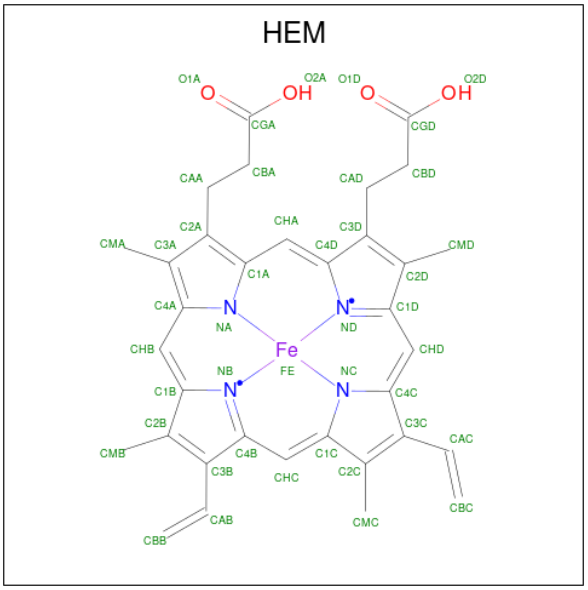
There are 7 unique types of molecules in this entry. The entry contains 7259 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

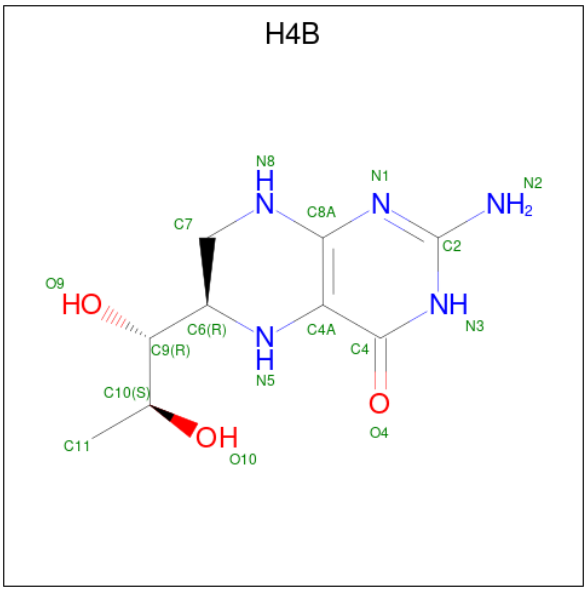
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	410	3348	2142	572	612	22	0	2	0
1	B	412	3365	2152	575	616	22	0	3	0

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



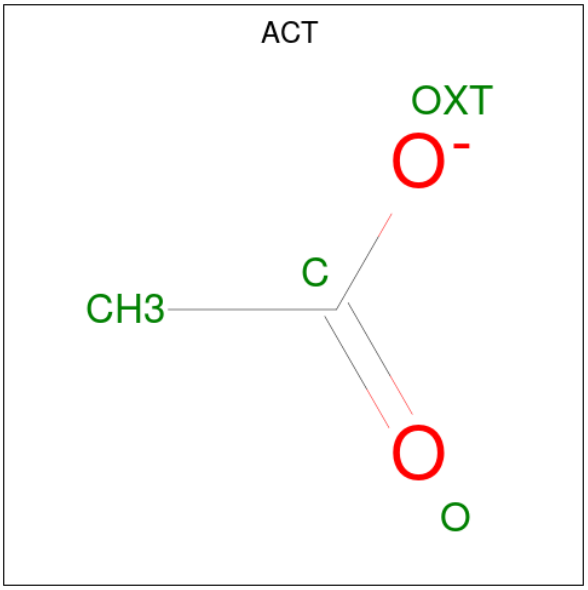
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0

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



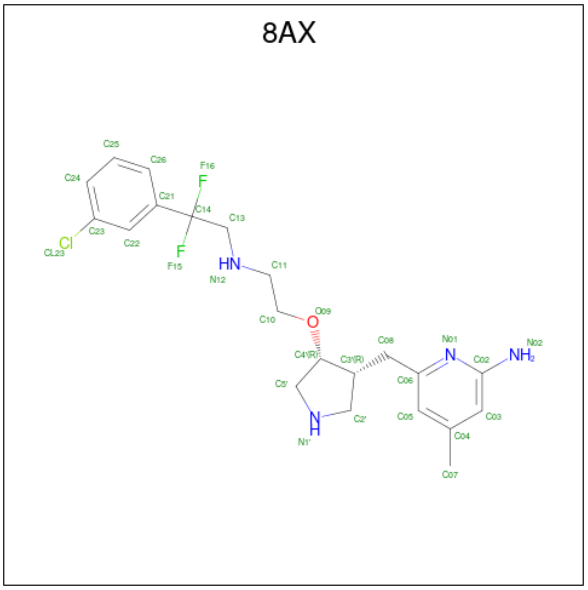
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	17	9	5	3	0	0
3	B	1	17	9	5	3	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is 6-{[(3R,4R)-4-(2-{[2-(3-chlorophenyl)-2,2-difluoroethyl]amino}ethoxy)pyrrolidin-3-yl]methyl}-4-methylpyridin-2-amine (three-letter code: 8AX) (formula: $C_{21}H_{27}ClF_2N_4O$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	F	N	O		
5	A	1	44	31	2	4	5	2	0	1
5	B	1	44	31	2	4	5	2	0	1

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

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

- Molecule 7 is water.

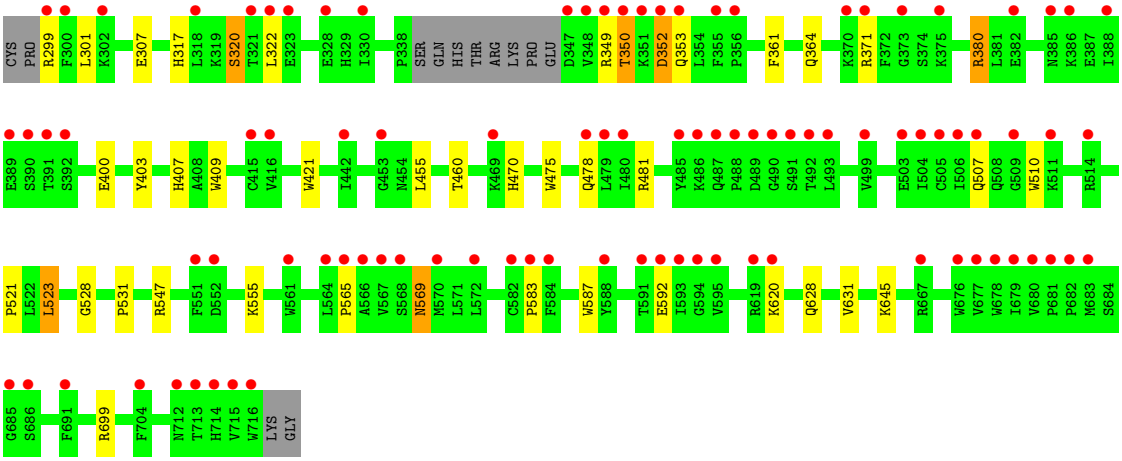
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	128	128	128	0	0
7	B	201	201	201	0	0

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.

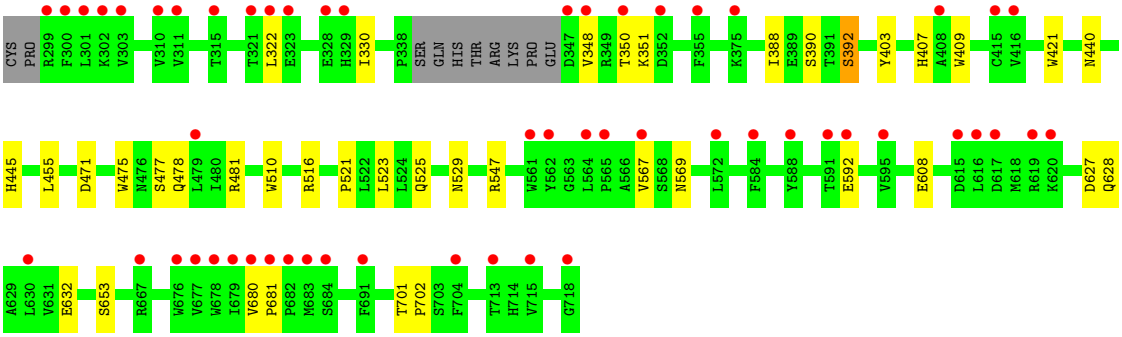
• Molecule 1: Nitric oxide synthase, brain

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	51.91Å 110.87Å 164.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.90 – 1.97 36.92 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.90-1.97) 99.2 (36.92-1.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 1.97Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.183 , 0.219 0.200 , 0.236	Depositor DCC
R_{free} test set	3329 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 42.3	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	0.96	EDS
Total number of atoms	7259	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% 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: 8AX, HEM, ACT, H4B, ZN

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	0.64	0/3447	0.68	0/4676
1	B	0.69	0/3467	0.69	1/4700 (0.0%)
All	All	0.66	0/6914	0.68	1/9376 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	471	ASP	CB-CG-OD2	5.14	122.92	118.30

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	3348	0	3258	33	0
1	B	3365	0	3279	20	0
2	A	43	0	30	3	0
2	B	43	0	30	5	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	44	0	24	6	0
5	B	44	0	24	6	0
6	A	1	0	0	0	0
7	A	128	0	0	1	0
7	B	201	0	0	5	0
All	All	7259	0	6681	60	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 (60) 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:A:750:HEM:HBA1	5:A:800[B]:8AX:F15	1.46	1.06
2:B:750:HEM:HBA1	5:B:800[B]:8AX:F15	1.41	1.06
2:B:750:HEM:CBA	5:B:800[B]:8AX:F15	1.95	1.05
1:B:592[A]:GLU:OE1	5:B:800[A]:8AX:H26	1.58	1.02
5:B:800[B]:8AX:N12	7:B:201:HOH:O	2.09	0.84
1:A:592[A]:GLU:OE1	5:A:800[A]:8AX:H26	1.85	0.77
2:B:750:HEM:HBA2	5:B:800[B]:8AX:F15	1.75	0.75
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.59	0.66
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.81	0.60
1:A:350:THR:H	1:A:353:GLN:HE21	1.49	0.58
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.85	0.58
1:A:307:GLU:HG3	7:B:48:HOH:O	2.03	0.58
1:A:349:ARG:HA	1:A:353:GLN:NE2	2.19	0.57
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.40	0.56
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.89	0.55
1:B:608:GLU:HG3	7:B:156:HOH:O	2.07	0.55
1:A:317:HIS:O	1:A:320:SER:HB3	2.09	0.53
1:B:440:ASN:ND2	7:B:181:HOH:O	2.41	0.52
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.92	0.52
1:A:350:THR:H	1:A:353:GLN:NE2	2.09	0.51
1:A:371:ARG:HH21	1:A:371:ARG:CG	2.24	0.51
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.93	0.50
1:B:350:THR:HG22	1:B:351:LYS:N	2.27	0.49
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.95	0.48
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.95	0.48
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.49	0.48
2:A:750:HEM:HBA1	5:A:800[B]:8AX:C14	2.42	0.47
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ARG:O	1:A:317:HIS:CE1	2.69	0.46
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.46	0.46
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.99	0.45
1:A:361:PHE:O	1:A:364:GLN:HG2	2.16	0.45
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.18	0.44
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.53	0.43
1:A:565:PRO:HB2	5:A:800[A]:8AX:C21	2.48	0.43
1:A:352:ASP:OD2	1:A:352:ASP:N	2.51	0.43
5:A:800[A]:8AX:H11	7:A:128:HOH:O	2.18	0.43
1:B:567:VAL:HG23	5:B:800[A]:8AX:H22	2.00	0.43
1:A:350:THR:N	1:A:353:GLN:HE21	2.16	0.43
1:A:460:THR:O	1:A:583:PRO:HD2	2.18	0.42
1:A:322:LEU:HB2	1:A:699:ARG:HB2	2.00	0.42
1:B:701:THR:HA	1:B:702:PRO:C	2.40	0.42
1:A:349:ARG:HA	1:A:353:GLN:HE21	1.82	0.42
1:A:301:LEU:CD1	1:B:330:ILE:HD13	2.50	0.42
1:A:470:HIS:HA	1:A:528:GLY:HA3	2.02	0.42
1:B:388:ILE:O	1:B:392:SER:HA	2.19	0.42
1:A:592[A]:GLU:CD	5:A:800[A]:8AX:H26	2.39	0.42
1:B:525:GLN:HG3	1:B:529:ASN:O	2.20	0.42
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.81	0.41
1:B:445:HIS:CD2	1:B:445:HIS:C	2.94	0.41
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.84	0.41
1:A:510:TRP:CG	1:A:521:PRO:HG3	2.56	0.41
1:B:477:SER:HA	1:B:569:ASN:HB3	2.02	0.41
2:B:750:HEM:HHC	2:B:750:HEM:CBB	2.50	0.41
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.09	0.41
1:A:569:ASN:HD22	1:A:569:ASN:H	1.69	0.40
1:B:322:LEU:HD21	7:B:129:HOH:O	2.20	0.40
1:B:475:TRP:HB2	1:B:523:LEU:HB3	2.03	0.40
1:A:322:LEU:HD13	1:A:699:ARG:NH2	2.36	0.40
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	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	408/422 (97%)	394 (97%)	14 (3%)	0	100	100
1	B	411/422 (97%)	404 (98%)	7 (2%)	0	100	100
All	All	819/844 (97%)	798 (97%)	21 (3%)	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	368/377 (98%)	357 (97%)	11 (3%)	41	29
1	B	370/377 (98%)	362 (98%)	8 (2%)	52	46
All	All	738/754 (98%)	719 (97%)	19 (3%)	46	37

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	SER
1	A	350	THR
1	A	352	ASP
1	A	380	ARG
1	A	507	GLN
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	B	348	VAL
1	B	390	SER
1	B	392	SER

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Mol	Chain	Res	Type
1	B	455	LEU
1	B	516	ARG
1	B	547	ARG
1	B	627	ASP
1	B	653	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	454	ASN
1	A	569	ASN
1	A	697	ASN
1	B	364	GLN
1	B	440	ASN
1	B	454	ASN
1	B	507	GLN
1	B	508	GLN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
1	B	642	GLN
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	$\#\|Z\| > 2$
3	H4B	B	760	-	16,18,18	1.16	2 (12%)	11,26,26	2.42	5 (45%)
4	ACT	B	860	-	3,3,3	0.54	0	3,3,3	1.34	0
5	8AX	B	800[B]	-	29,31,31	0.97	3 (10%)	31,43,43	1.55	3 (9%)
5	8AX	B	800[A]	-	29,31,31	0.82	1 (3%)	31,43,43	1.63	5 (16%)
5	8AX	A	800[B]	-	29,31,31	1.08	3 (10%)	31,43,43	1.83	5 (16%)
2	HEM	A	750	1	41,50,50	2.03	8 (19%)	45,82,82	2.00	10 (22%)
3	H4B	A	760	-	16,18,18	0.94	1 (6%)	11,26,26	2.79	6 (54%)
2	HEM	B	750	1	41,50,50	1.97	11 (26%)	45,82,82	1.98	7 (15%)
5	8AX	A	800[A]	-	29,31,31	0.95	1 (3%)	31,43,43	2.16	9 (29%)
4	ACT	A	860	-	3,3,3	0.83	0	3,3,3	0.73	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
5	8AX	B	800[B]	-	-	2/18/29/29	0/3/3/3
5	8AX	A	800[B]	-	-	3/18/29/29	0/3/3/3
2	HEM	A	750	1	-	1/12/54/54	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
2	HEM	B	750	1	-	0/12/54/54	-
5	8AX	A	800[A]	-	-	4/18/29/29	0/3/3/3
5	8AX	B	800[A]	-	-	5/18/29/29	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C2D	7.88	1.53	1.36
2	B	750	HEM	C3D-C2D	6.15	1.49	1.36
2	B	750	HEM	C3C-C2C	-4.65	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3C-CAC	4.23	1.56	1.47
2	A	750	HEM	C3C-C2C	-4.23	1.34	1.40
2	A	750	HEM	C3C-CAC	3.56	1.55	1.47
2	B	750	HEM	FE-ND	2.99	2.11	1.96
2	B	750	HEM	CAA-C2A	2.85	1.56	1.52
5	A	800[B]	8AX	C23-CL23	2.70	1.80	1.74
2	A	750	HEM	CAB-C3B	2.68	1.54	1.47
2	A	750	HEM	FE-ND	2.66	2.10	1.96
3	B	760	H4B	C7-N8	2.65	1.49	1.44
2	A	750	HEM	CMB-C2B	2.65	1.56	1.50
5	A	800[B]	8AX	F15-C14	-2.61	1.31	1.37
5	B	800[B]	8AX	F15-C14	-2.60	1.31	1.37
2	A	750	HEM	FE-NB	2.48	2.09	1.96
5	B	800[B]	8AX	F16-C14	-2.47	1.32	1.37
5	B	800[B]	8AX	C23-CL23	2.45	1.79	1.74
2	B	750	HEM	CMC-C2C	2.40	1.57	1.51
5	A	800[B]	8AX	F16-C14	-2.38	1.32	1.37
2	A	750	HEM	CMD-C2D	2.35	1.55	1.50
2	B	750	HEM	CMB-C2B	2.31	1.55	1.50
2	B	750	HEM	CAB-C3B	2.19	1.53	1.47
3	B	760	H4B	C7-C6	2.18	1.54	1.52
2	B	750	HEM	FE-NB	2.17	2.07	1.96
5	B	800[A]	8AX	F16-C14	-2.12	1.32	1.37
2	B	750	HEM	CMA-C3A	2.12	1.56	1.51
2	B	750	HEM	C4A-NA	2.11	1.40	1.36
5	A	800[A]	8AX	C23-CL23	2.02	1.78	1.74
3	A	760	H4B	C7-N8	2.02	1.48	1.44

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	750	HEM	CBA-CAA-C2A	-7.44	99.92	112.62
2	A	750	HEM	C4D-ND-C1D	6.45	111.74	105.07
2	A	750	HEM	CBA-CAA-C2A	-6.00	102.37	112.62
2	B	750	HEM	C4D-ND-C1D	5.86	111.13	105.07
5	A	800[A]	8AX	C02-N01-C06	5.78	122.48	118.10
5	A	800[B]	8AX	C02-N01-C06	5.78	122.48	118.10
3	B	760	H4B	C8A-C4A-C4	5.69	119.62	114.57
5	B	800[A]	8AX	C02-N01-C06	5.14	122.00	118.10
5	B	800[B]	8AX	C02-N01-C06	5.14	122.00	118.10
5	A	800[A]	8AX	C11-N12-C13	4.74	122.94	113.35
3	A	760	H4B	C2-N3-C4	4.35	122.84	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	750	HEM	C4B-CHC-C1C	4.18	128.08	122.56
3	A	760	H4B	N1-C2-N3	-3.96	119.21	125.42
2	B	750	HEM	CBD-CAD-C3D	-3.90	101.80	112.63
5	A	800[A]	8AX	C22-C23-CL23	-3.79	114.42	119.15
3	A	760	H4B	C4-C4A-N5	3.65	122.19	119.12
2	A	750	HEM	C4B-CHC-C1C	3.64	127.36	122.56
3	A	760	H4B	N2-C2-N1	3.50	122.69	117.25
2	A	750	HEM	CMD-C2D-C1D	3.49	130.35	125.04
2	A	750	HEM	CBD-CAD-C3D	-3.49	102.94	112.63
3	A	760	H4B	C8A-C4A-C4	3.43	117.61	114.57
5	A	800[A]	8AX	C5'-N1'-C2'	3.39	113.43	105.42
5	A	800[B]	8AX	C5'-N1'-C2'	3.39	113.43	105.42
5	A	800[A]	8AX	N02-C02-N01	3.37	121.82	116.49
5	A	800[B]	8AX	N02-C02-N01	3.37	121.82	116.49
3	B	760	H4B	C2-N3-C4	2.96	120.63	115.93
5	A	800[A]	8AX	C05-C06-N01	-2.93	119.80	122.90
5	A	800[B]	8AX	C05-C06-N01	-2.93	119.80	122.90
5	B	800[A]	8AX	C11-N12-C13	2.84	119.09	113.35
2	B	750	HEM	C2C-C3C-C4C	2.76	108.83	106.90
5	B	800[A]	8AX	C5'-N1'-C2'	2.70	111.79	105.42
5	B	800[B]	8AX	C5'-N1'-C2'	2.70	111.79	105.42
3	A	760	H4B	C2-N1-C8A	2.64	120.46	114.54
5	A	800[A]	8AX	C04-C05-C06	-2.64	118.59	120.32
5	A	800[B]	8AX	C04-C05-C06	-2.64	118.59	120.32
2	B	750	HEM	CAD-C3D-C4D	2.56	129.13	124.66
5	B	800[A]	8AX	C05-C06-N01	-2.55	120.20	122.90
5	B	800[B]	8AX	C05-C06-N01	-2.55	120.20	122.90
2	A	750	HEM	CMC-C2C-C3C	2.45	129.27	124.68
5	A	800[A]	8AX	C24-C23-CL23	2.43	123.16	119.35
2	A	750	HEM	CHA-C4D-ND	2.34	127.27	124.38
3	B	760	H4B	N1-C2-N3	-2.33	121.76	125.42
2	A	750	HEM	C4B-C3B-C2B	2.30	108.94	107.11
2	A	750	HEM	C4C-CHD-C1D	2.29	125.58	122.56
3	B	760	H4B	C2-N1-C8A	2.18	119.42	114.54
3	B	760	H4B	C4-C4A-N5	2.13	120.91	119.12
2	B	750	HEM	C4B-C3B-C2B	2.10	108.78	107.11
5	A	800[A]	8AX	C26-C25-C24	-2.09	117.28	120.25
2	A	750	HEM	CHC-C4B-C3B	2.06	127.72	124.57
5	B	800[A]	8AX	C25-C26-C21	2.01	122.87	120.76

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	800[A]	8AX	N01-C06-C08-C3'
5	A	800[B]	8AX	N01-C06-C08-C3'
5	A	800[B]	8AX	C5'-C4'-O09-C10
5	B	800[A]	8AX	N01-C06-C08-C3'
5	B	800[A]	8AX	C5'-C4'-O09-C10
5	B	800[B]	8AX	N01-C06-C08-C3'
5	B	800[B]	8AX	C10-C11-N12-C13
5	A	800[A]	8AX	C14-C13-N12-C11
5	B	800[A]	8AX	C14-C13-N12-C11
5	A	800[A]	8AX	C5'-C4'-O09-C10
5	B	800[A]	8AX	N12-C13-C14-F16
5	A	800[B]	8AX	F15-C14-C21-C26
2	A	750	HEM	C2A-CAA-CBA-CGA
5	A	800[A]	8AX	C3'-C4'-O09-C10
5	B	800[A]	8AX	C3'-C4'-O09-C10

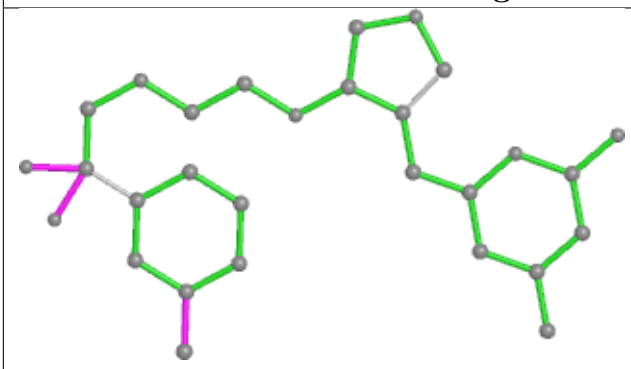
There are no ring outliers.

6 monomers are involved in 15 short contacts:

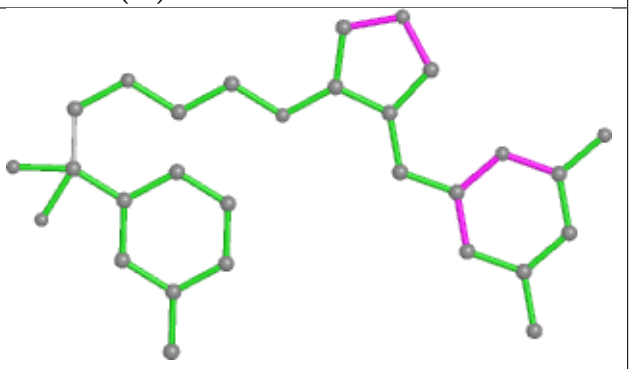
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	800[B]	8AX	4	0
5	B	800[A]	8AX	2	0
5	A	800[B]	8AX	2	0
2	A	750	HEM	3	0
2	B	750	HEM	5	0
5	A	800[A]	8AX	4	0

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.

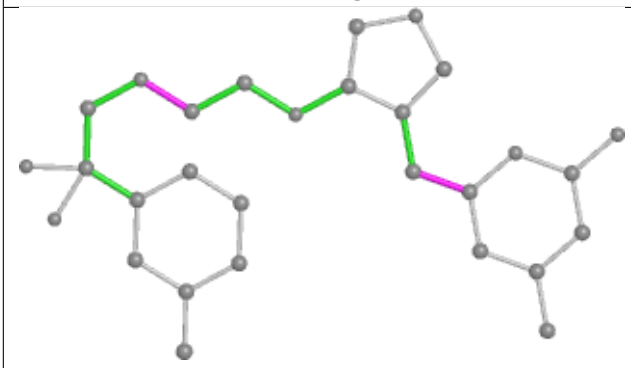
Ligand 8AX B 800 (B)



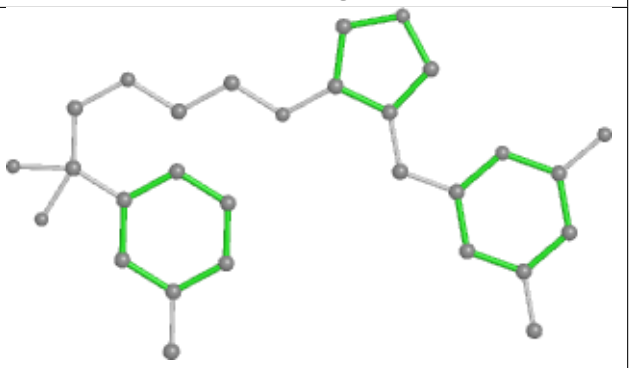
Bond lengths



Bond angles

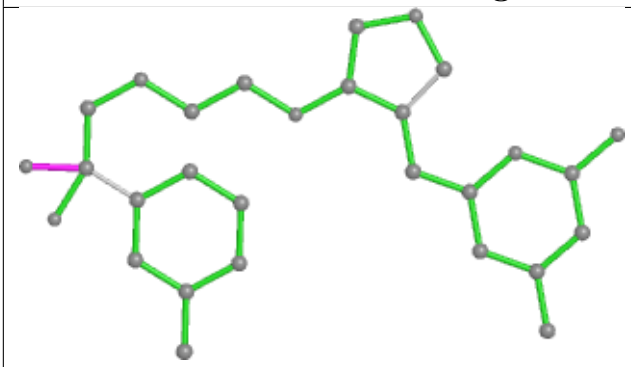


Torsions

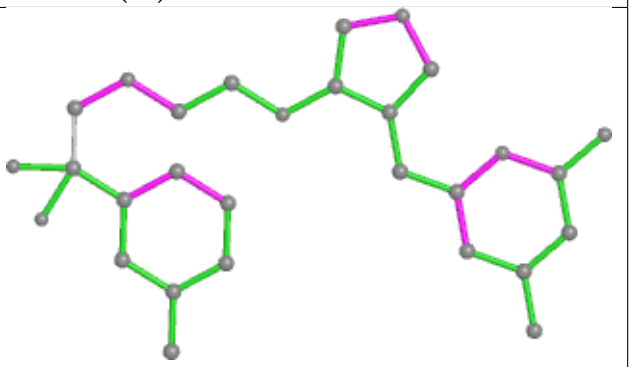


Rings

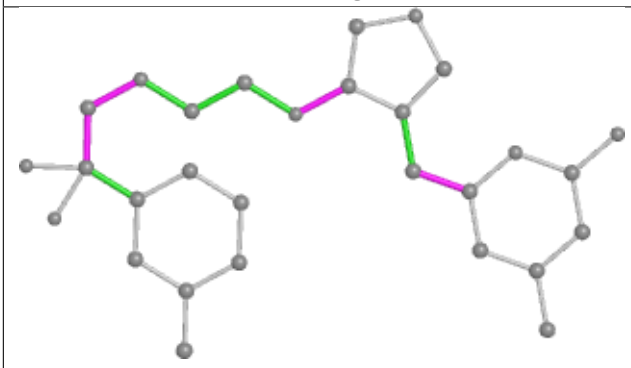
Ligand 8AX B 800 (A)



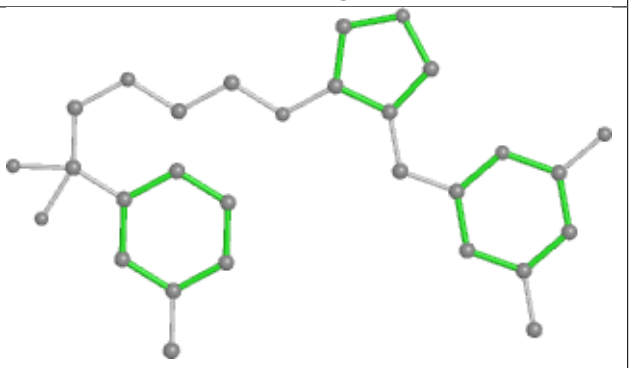
Bond lengths



Bond angles

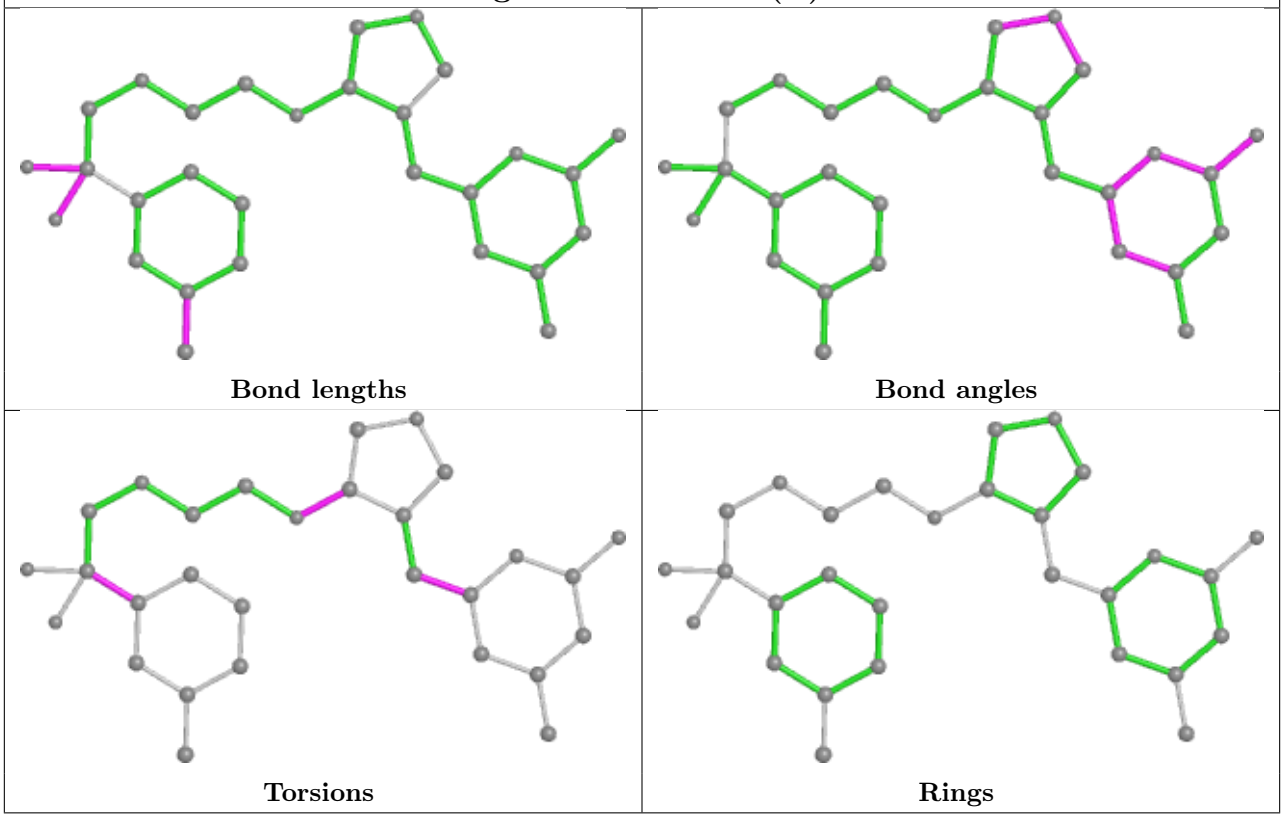


Torsions

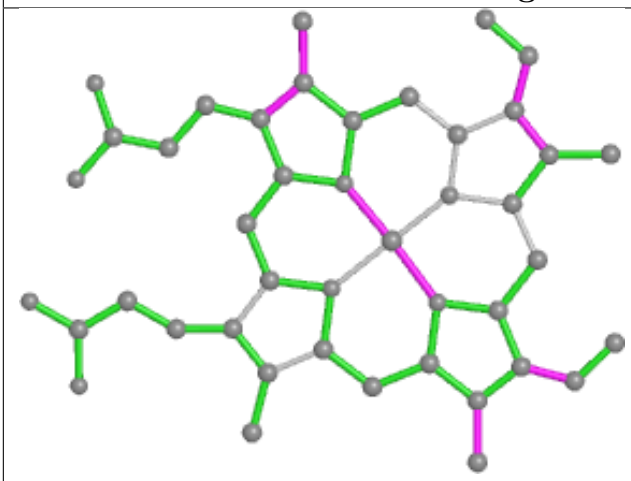


Rings

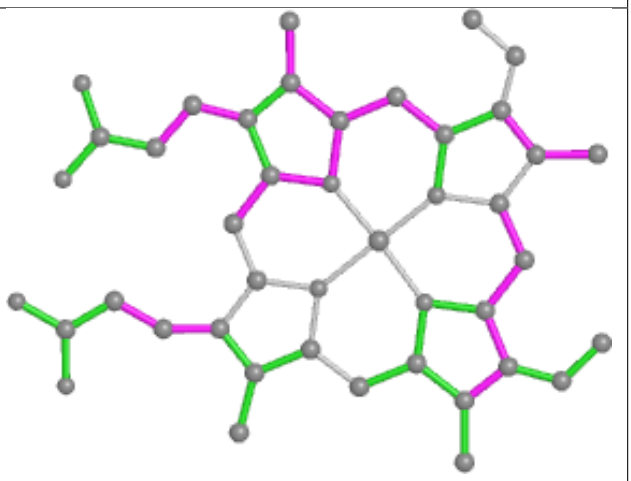
Ligand 8AX A 800 (B)



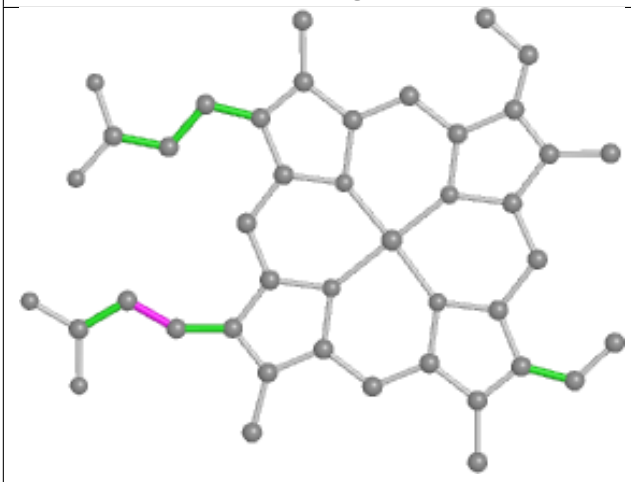
Ligand HEM A 750



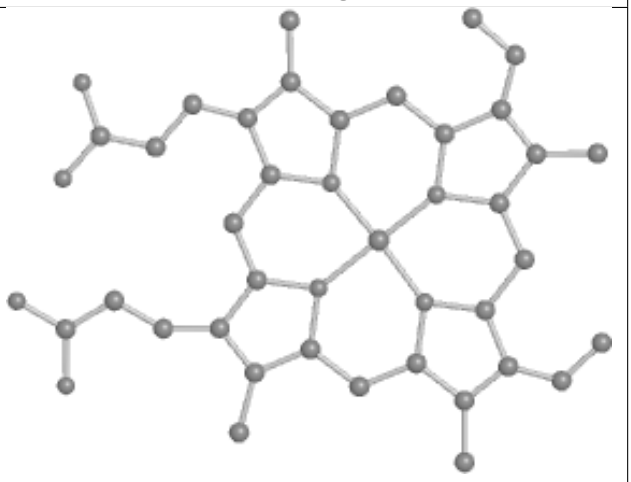
Bond lengths



Bond angles

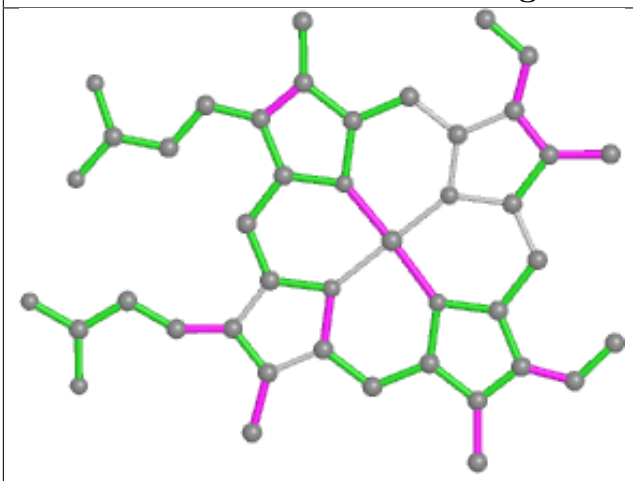


Torsions

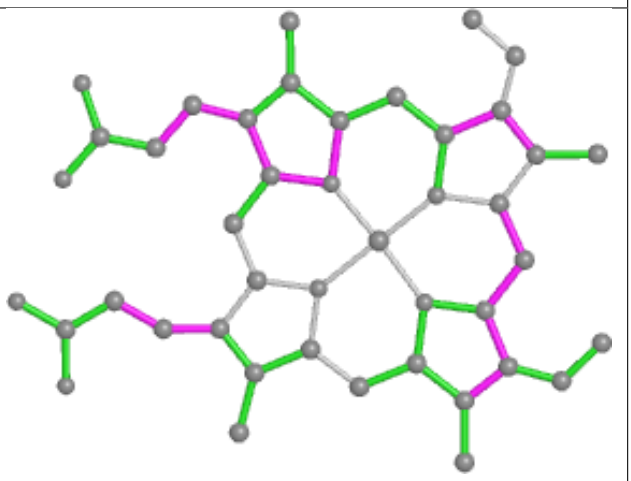


Rings

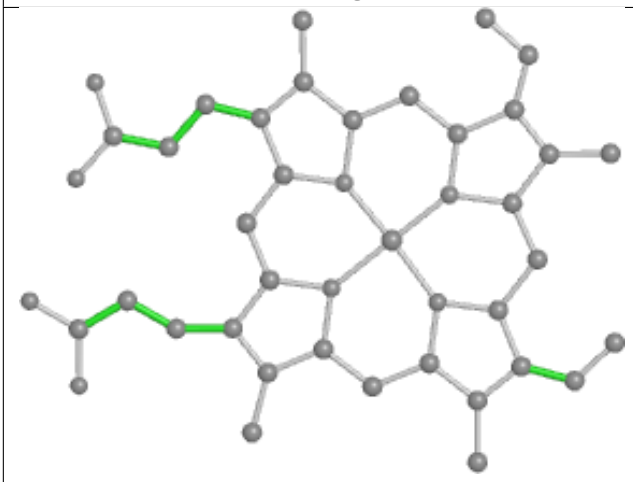
Ligand HEM B 750



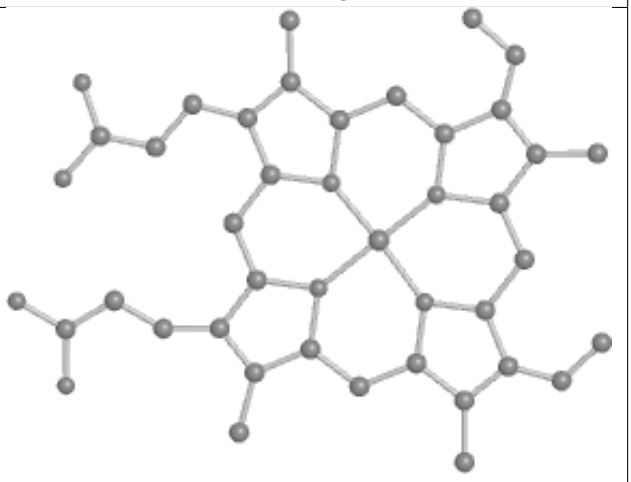
Bond lengths



Bond angles

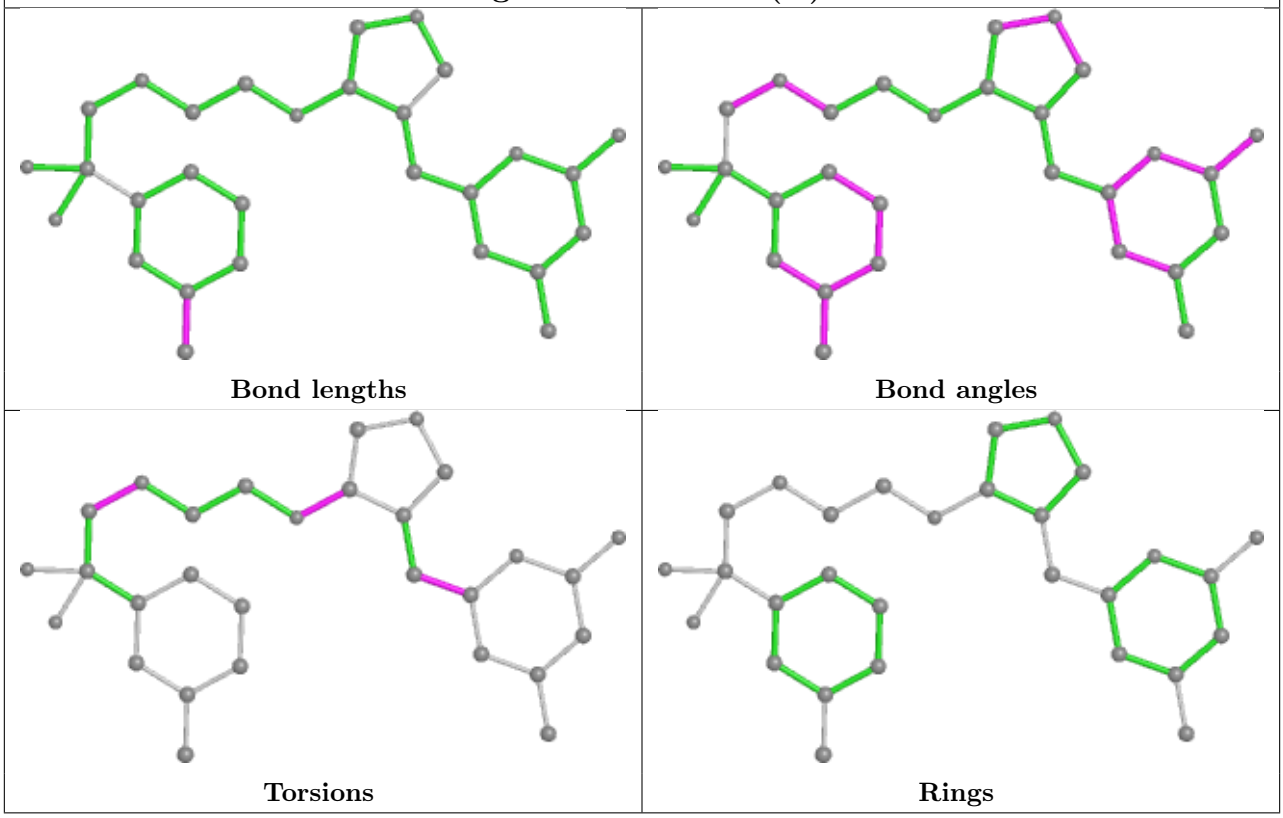


Torsions



Rings

Ligand 8AX A 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	410/422 (97%)	1.20	95 (23%)	0	0	31, 53, 89, 113	0
1	B	412/422 (97%)	0.68	55 (13%)	3	3	29, 43, 68, 82	0
All	All	822/844 (97%)	0.94	150 (18%)	1	1	29, 47, 83, 113	0

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	488	PRO	9.4
1	B	300	PHE	8.8
1	A	348	VAL	7.9
1	A	716	TRP	7.2
1	B	348	VAL	6.6
1	A	486	LYS	6.5
1	A	355	PHE	6.2
1	A	351	LYS	6.0
1	B	715	VAL	5.5
1	A	352	ASP	5.3
1	A	299	ARG	5.1
1	A	567	VAL	4.9
1	A	678	TRP	4.6
1	A	680	VAL	4.6
1	A	300	PHE	4.5
1	A	511	LYS	4.4
1	A	713	THR	4.3
1	A	390	SER	4.3
1	A	506	ILE	4.2
1	B	619	ARG	4.2
1	A	592[A]	GLU	4.1
1	A	715	VAL	4.1
1	A	507	GLN	4.1
1	A	347	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	491	SER	3.9
1	A	514	ARG	3.8
1	A	388	ILE	3.7
1	B	299	ARG	3.7
1	B	667	ARG	3.7
1	A	479	LEU	3.7
1	B	347	ASP	3.7
1	A	492	THR	3.6
1	A	386	LYS	3.6
1	A	619	ARG	3.6
1	A	480	ILE	3.5
1	A	505	CYS	3.5
1	A	391	THR	3.5
1	B	680	VAL	3.4
1	A	490	GLY	3.4
1	B	567	VAL	3.4
1	B	718	GLY	3.4
1	A	682	PRO	3.4
1	A	392	SER	3.4
1	A	679	ILE	3.3
1	B	620	LYS	3.3
1	B	677	VAL	3.3
1	B	584	PHE	3.2
1	A	568	SER	3.2
1	A	389	GLU	3.2
1	A	503	GLU	3.2
1	A	683	MET	3.2
1	A	350	THR	3.2
1	A	328	GLU	3.2
1	B	310	VAL	3.2
1	A	485	TYR	3.1
1	B	691	PHE	3.1
1	A	681	PRO	3.1
1	A	588	TYR	3.1
1	A	591	THR	3.1
1	A	677	VAL	3.1
1	A	322	LEU	3.1
1	A	584	PHE	3.0
1	A	469	LYS	3.0
1	B	591	THR	3.0
1	A	385	ASN	3.0
1	A	714	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	356	PRO	2.9
1	A	593	ILE	2.9
1	A	686	SER	2.9
1	A	373	GLY	2.8
1	A	489	ASP	2.8
1	A	667	ARG	2.8
1	A	330	ILE	2.8
1	A	415	CYS	2.8
1	A	416	VAL	2.8
1	A	565	PRO	2.7
1	B	679	ILE	2.7
1	A	487	GLN	2.7
1	B	572	LEU	2.7
1	B	678	TRP	2.7
1	A	552	ASP	2.7
1	B	301	LEU	2.7
1	A	676	TRP	2.7
1	B	561	TRP	2.7
1	A	620	LYS	2.7
1	A	504	ILE	2.6
1	A	704	PHE	2.6
1	A	685	GLY	2.6
1	A	353	GLN	2.6
1	A	349	ARG	2.6
1	B	352	ASP	2.6
1	A	302	LYS	2.6
1	A	370	LYS	2.6
1	A	570	MET	2.6
1	B	682	PRO	2.6
1	B	321	THR	2.6
1	B	350	THR	2.6
1	B	328	GLU	2.5
1	B	592[A]	GLU	2.5
1	A	499	VAL	2.5
1	B	595	VAL	2.5
1	A	712	ASN	2.5
1	B	713	THR	2.4
1	B	616	LEU	2.4
1	B	683	MET	2.4
1	A	323	GLU	2.4
1	A	551	PHE	2.4
1	B	415	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	617	ASP	2.3
1	B	375	LYS	2.3
1	A	382	GLU	2.3
1	A	509	GLY	2.3
1	B	323	GLU	2.3
1	A	566	ALA	2.3
1	A	691	PHE	2.3
1	A	442	ILE	2.3
1	A	453	GLY	2.3
1	A	493	LEU	2.3
1	A	564	LEU	2.2
1	B	630	LEU	2.2
1	A	321	THR	2.2
1	B	315	THR	2.2
1	B	564	LEU	2.2
1	A	594	GLY	2.2
1	B	416	VAL	2.2
1	B	303	VAL	2.2
1	B	676	TRP	2.2
1	A	318	LEU	2.1
1	B	479	LEU	2.1
1	B	322	LEU	2.1
1	A	371	ARG	2.1
1	B	302	LYS	2.1
1	A	583	PRO	2.1
1	A	561	TRP	2.1
1	B	704	PHE	2.1
1	A	478	GLN	2.1
1	B	681	PRO	2.1
1	A	375	LYS	2.1
1	B	684	SER	2.1
1	B	408	ALA	2.1
1	B	565	PRO	2.1
1	A	582	CYS	2.1
1	B	562	TYR	2.0
1	B	615	ASP	2.0
1	A	572	LEU	2.0
1	B	329	HIS	2.0
1	B	588	TYR	2.0
1	A	595	VAL	2.0
1	B	311	VAL	2.0
1	B	355	PHE	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)

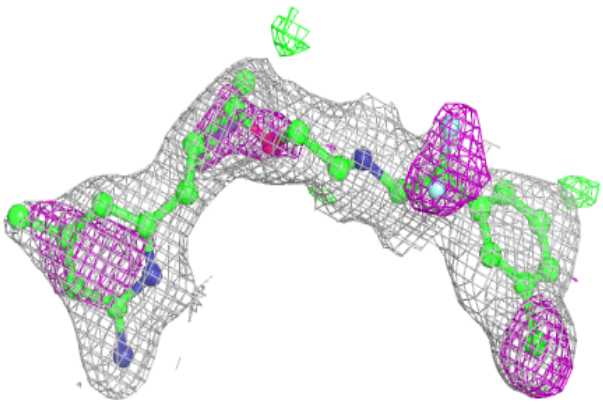
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

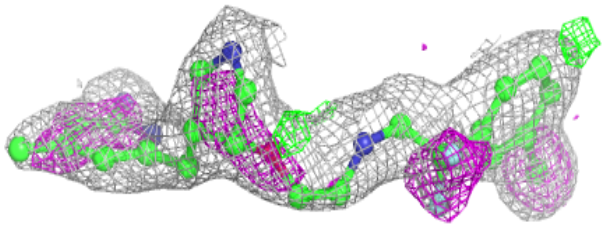
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	8AX	A	800[A]	29/29	0.88	0.20	22,31,35,37	15
5	8AX	A	800[B]	29/29	0.88	0.20	32,35,37,39	15
5	8AX	B	800[A]	29/29	0.91	0.17	29,31,34,37	15
5	8AX	B	800[B]	29/29	0.91	0.17	25,30,32,34	15
4	ACT	B	860	4/4	0.93	0.14	47,48,48,49	0
4	ACT	A	860	4/4	0.95	0.28	59,60,60,61	0
3	H4B	A	760	17/17	0.95	0.18	34,39,43,45	0
2	HEM	A	750	43/43	0.97	0.24	32,36,43,46	0
3	H4B	B	760	17/17	0.97	0.20	32,38,40,43	0
2	HEM	B	750	43/43	0.98	0.20	27,33,41,48	0
6	ZN	A	900	1/1	0.99	0.06	41,41,41,41	0

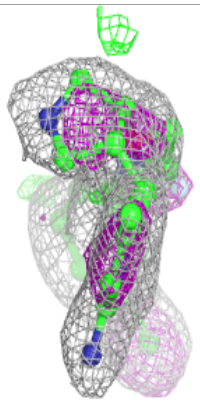
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 8AX 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)

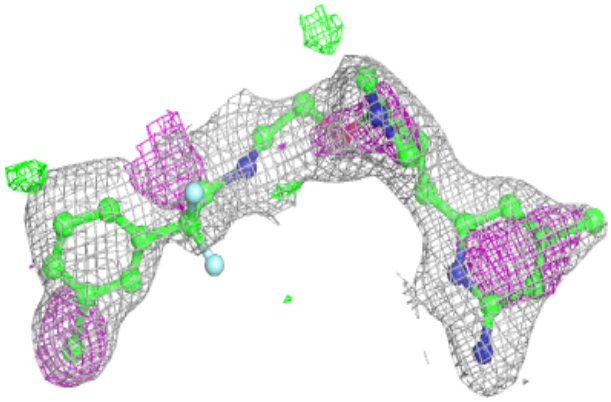


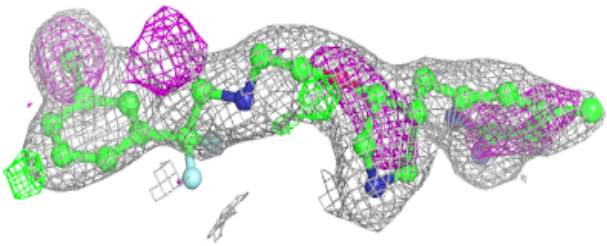


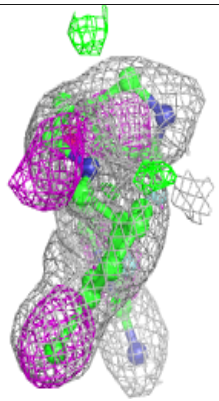


Electron density around 8AX A 800 (B):

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

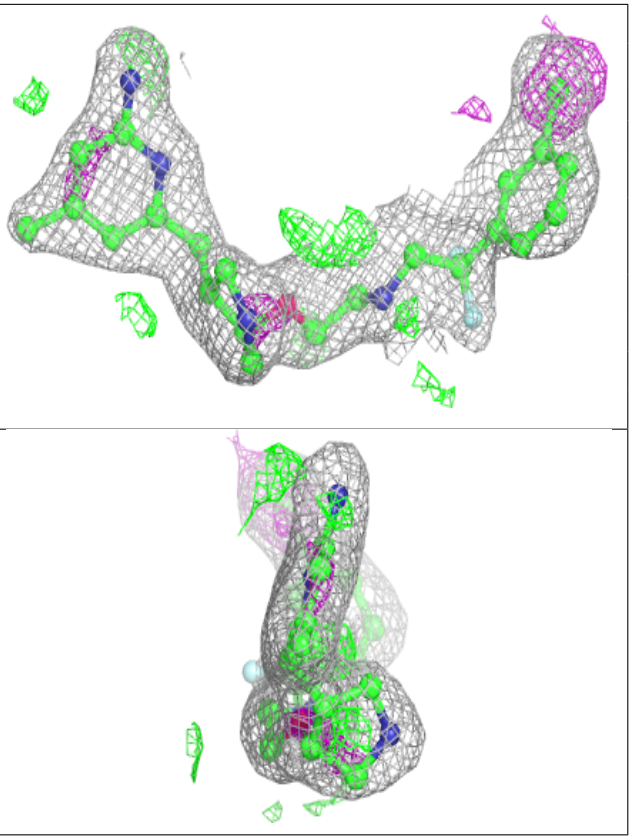






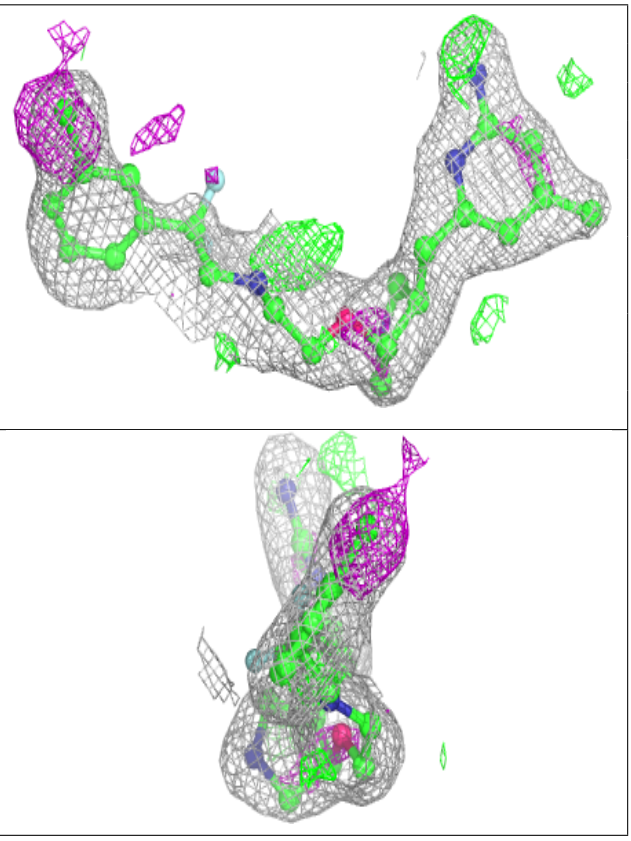
Electron density around 8AX B 800 (A):

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



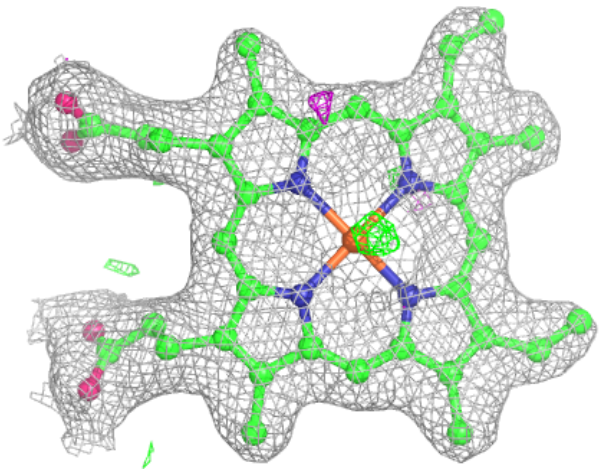
Electron density around 8AX B 800 (B):

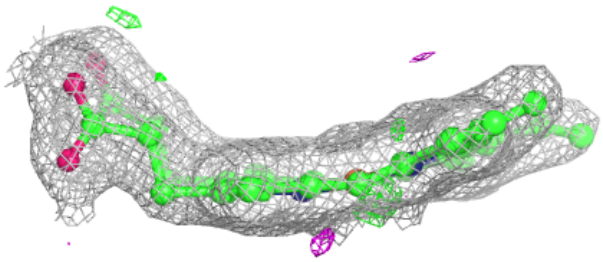
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

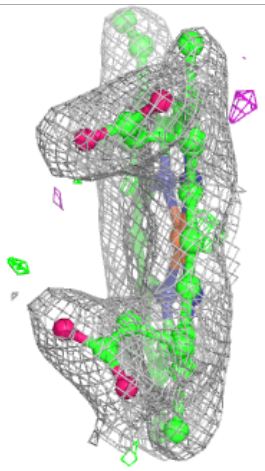


Electron density around HEM A 750:

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

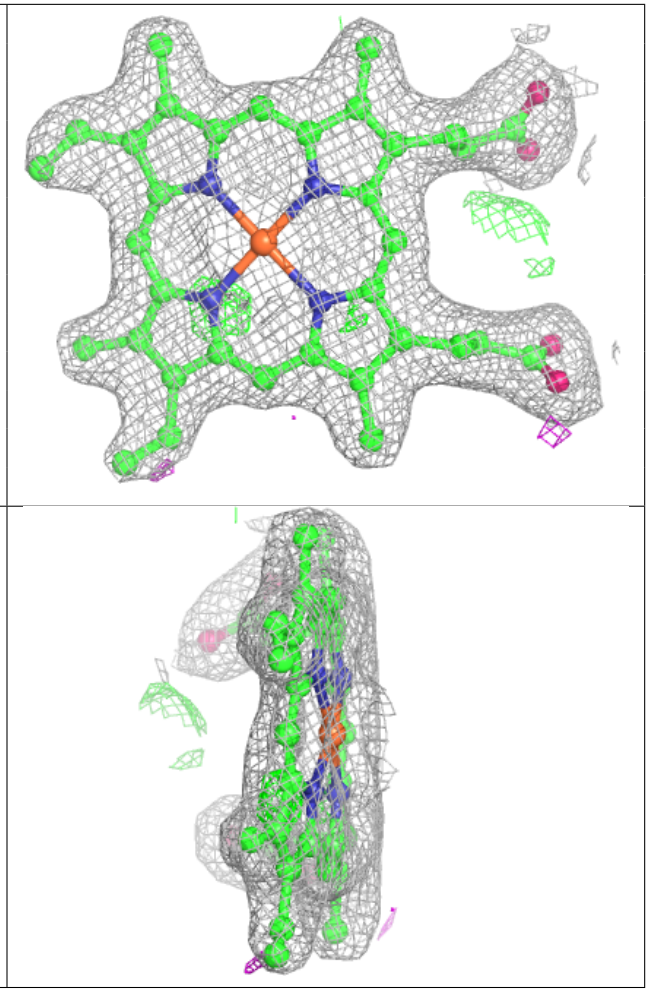






Electron density around HEM B 750:

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 (i)

There are no such residues in this entry.