Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 04:56 AM EDT

PDB ID	:	3NLY
Title	:	Structure of rat neuronal nitric oxide synthase heme domain in complex with 6-(((3R,4R)-4-(2- (2,2-Difluoro-2-(4-fluorophenyl)ethylamino)ethoxy)pyrrolidin-3-yl)methyl)-4-methylpyridin-2-amine
Authors	:	Li, H.; Delker, S.L.; Poulos, T.L.
Deposited on	:	2010-06-21
Resolution	:	1.99 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:

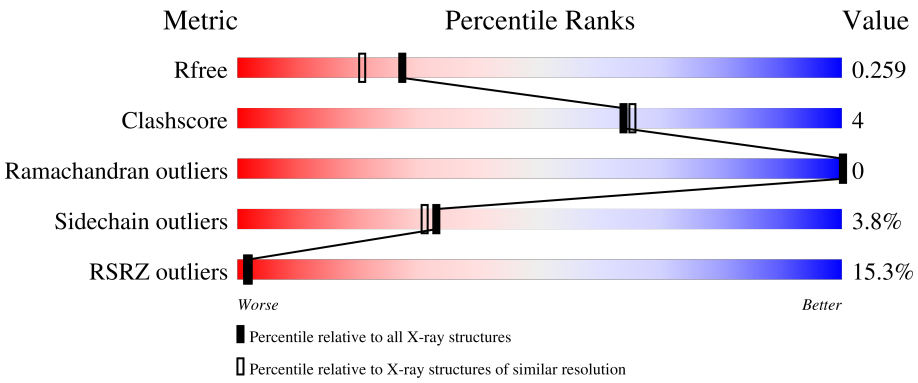
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.99 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	21% 85% 10% • •
1	B	422	9% 85% 12% •

2 Entry composition (i)

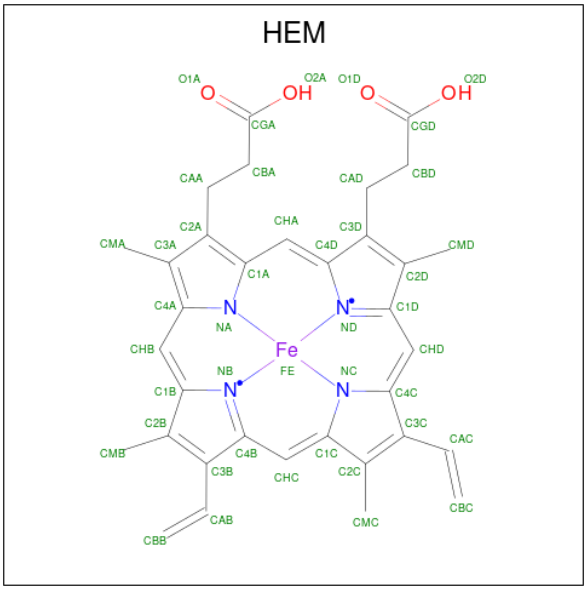
There are 7 unique types of molecules in this entry. The entry contains 7052 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

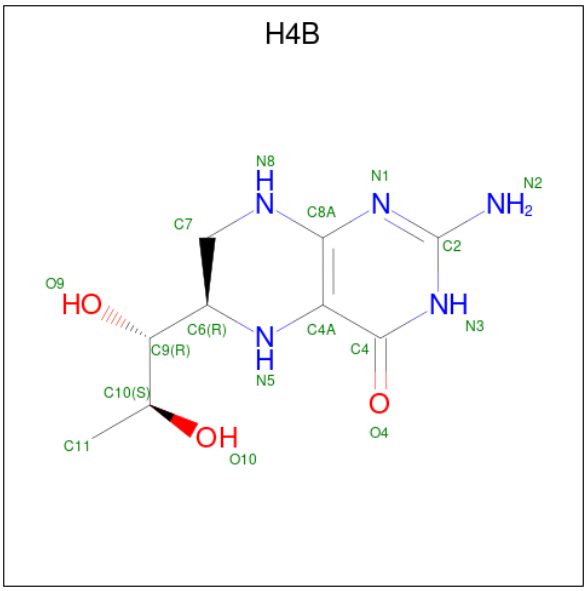
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	407	3321	2126	567	607	21	0	2	0
1	B	411	3354	2146	574	613	21	0	3	0

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



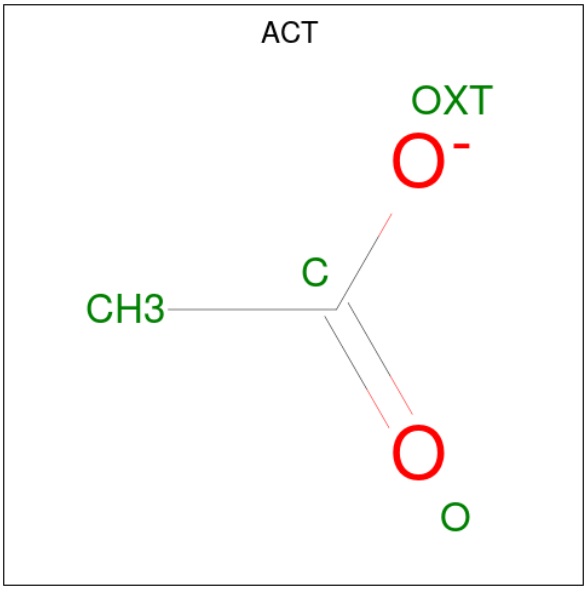
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0

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



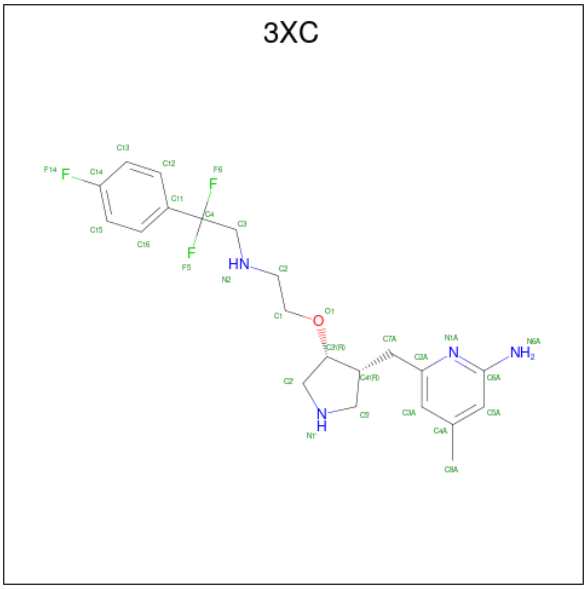
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	17	9	5	3	0	0
3	B	1	17	9	5	3	0	0

- 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-{[2,2-difluoro-2-(4-fluorophenyl)ethyl]amino}ethoxy)pyrrolidin-3-yl]methyl}-4-methylpyridin-2-amine (three-letter code: 3XC) (formula: $C_{21}H_{27}F_3N_4O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			29	21	3	4	1		
5	B	1	Total	C	F	N	O	0	0
			29	21	3	4	1		

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

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

- Molecule 7 is water.

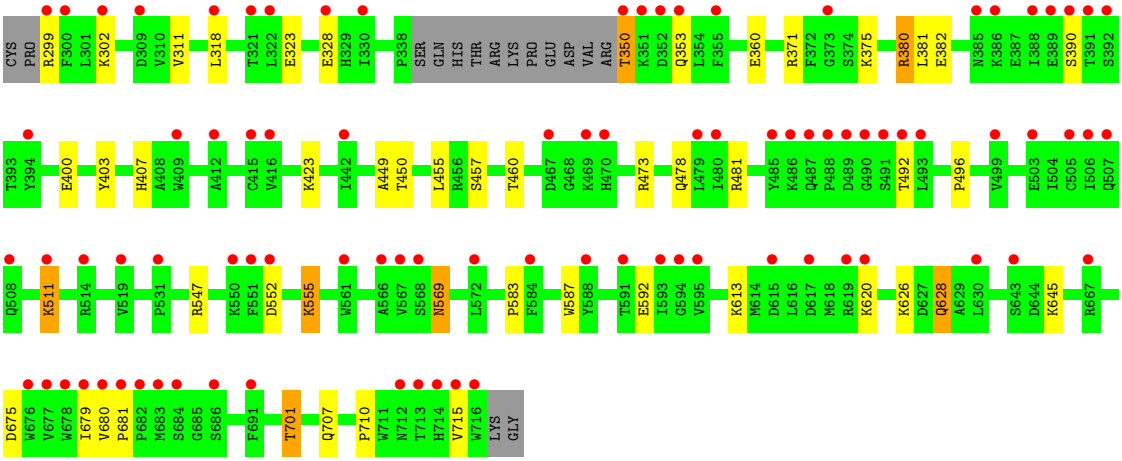
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	84	Total	O	0	0
			84	84		
7	B	106	Total	O	0	0
			106	106		

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.

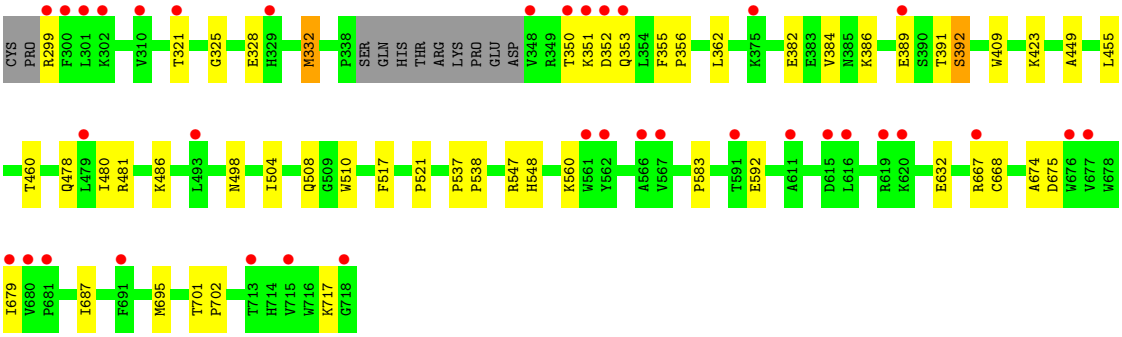
- Molecule 1: Nitric oxide synthase, brain

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	51.79Å 111.22Å 164.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.64 – 1.99 38.49 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.5 (38.64-1.99) 96.5 (38.49-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.249 0.212 , 0.259	Depositor DCC
R_{free} test set	3122 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.6	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	7052	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.94% 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: ACT, H4B, 3XC, HEM, 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	0.67	0/3420	0.69	0/4640
1	B	0.74	0/3456	0.71	0/4685
All	All	0.71	0/6876	0.70	0/9325

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3321	0	3232	28	0
1	B	3354	0	3274	28	0
2	A	43	0	30	3	0
2	B	43	0	30	3	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
5	A	29	0	27	1	0
5	B	29	0	27	1	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	84	0	0	1	0
7	B	106	0	0	2	0
All	All	7052	0	6656	57	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 (57) 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:511:LYS:H	1:A:511:LYS:HD3	1.23	0.99
1:A:350:THR:N	1:A:353:GLN:HE21	1.81	0.78
2:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.64	0.77
1:A:511:LYS:HD3	1:A:511:LYS:N	1.98	0.76
1:A:302:LYS:HD3	1:A:311:VAL:CG1	2.19	0.72
1:A:302:LYS:HD3	1:A:311:VAL:HG11	1.75	0.69
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.79	0.64
1:A:350:THR:N	1:A:353:GLN:NE2	2.46	0.63
1:B:668:CYS:HB3	7:B:1004:HOH:O	1.98	0.63
1:B:350:THR:HG22	1:B:352:ASP:H	1.67	0.60
1:A:460:THR:O	1:A:583:PRO:HD2	2.03	0.57
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.38	0.57
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.03	0.57
1:B:675:ASP:O	1:B:679:ILE:HG12	2.06	0.55
1:A:592:GLU:OE1	5:A:800:3XC:H16	2.08	0.54
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.89	0.54
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.44	0.52
1:A:403:TYR:CE1	1:A:407:HIS:CE1	2.97	0.52
1:A:449:ALA:HB1	7:A:1004:HOH:O	2.11	0.50
1:B:355:PHE:N	1:B:356:PRO:HD2	2.27	0.49
1:A:423:LYS:O	1:A:457[B]:SER:OG	2.30	0.49
1:B:409:TRP:CZ3	2:B:750:HEM:HMC3	2.48	0.48
1:B:391:THR:O	1:B:392:SER:HB2	2.13	0.48
1:B:409:TRP:CH2	2:B:750:HEM:HMC3	2.49	0.48
1:A:569:ASN:O	1:A:707:GLN:HG2	2.14	0.47
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.96	0.47
1:A:360:GLU:OE1	1:A:701:THR:HG22	2.16	0.46
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.96	0.46
1:B:504:ILE:O	1:B:508:GLN:HG2	2.16	0.46
1:B:701:THR:HA	1:B:702:PRO:C	2.36	0.46
1:A:626:LYS:HB3	1:B:687:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLU:HA	1:B:328:GLU:O	2.16	0.45
2:A:750:HEM:HBC2	2:A:750:HEM:CMC	2.39	0.45
1:B:325:GLY:O	1:B:332:MET:HG3	2.16	0.45
1:B:299:ARG:HB3	1:B:299:ARG:CZ	2.45	0.45
1:A:492:THR:HG21	1:A:496:PRO:HG3	1.98	0.45
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.32	0.45
1:B:386:LYS:O	1:B:389:GLU:HG2	2.17	0.45
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.98	0.45
1:A:555:LYS:NZ	1:A:555:LYS:HB3	2.32	0.44
1:B:517:PHE:HB2	1:B:560:LYS:HE3	2.00	0.43
1:A:511:LYS:H	1:A:511:LYS:CD	2.11	0.43
1:A:450:THR:HA	1:A:455:LEU:HD22	2.00	0.43
1:B:460:THR:O	1:B:583:PRO:HD2	2.20	0.42
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.50	0.42
1:B:537:PRO:HA	1:B:538:PRO:HD3	1.87	0.42
1:B:480:ILE:HA	7:B:1021:HOH:O	2.20	0.41
1:A:382:GLU:OE2	1:A:382:GLU:HA	2.20	0.41
1:B:353:GLN:H	1:B:353:GLN:HG2	1.74	0.41
1:B:674:ALA:HB3	1:B:695:MET:HB3	2.03	0.41
1:B:481:ARG:NH1	1:B:498:ASN:OD1	2.53	0.41
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.92	0.41
1:A:675:ASP:O	1:A:679:ILE:HG12	2.21	0.41
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.02	0.40
1:B:592:GLU:OE1	5:B:800:3XC:H16	2.21	0.40
1:A:455:LEU:HD12	1:A:587:TRP:HB3	2.03	0.40
1:B:449:ALA:O	1:B:455:LEU:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	405/422 (96%)	389 (96%)	16 (4%)	0	100	100
1	B	410/422 (97%)	396 (97%)	14 (3%)	0	100	100
All	All	815/844 (97%)	785 (96%)	30 (4%)	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	365/377 (97%)	347 (95%)	18 (5%)	25	21
1	B	369/377 (98%)	359 (97%)	10 (3%)	44	46
All	All	734/754 (97%)	706 (96%)	28 (4%)	33	31

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	328	GLU
1	A	350	THR
1	A	371	ARG
1	A	375	LYS
1	A	380	ARG
1	A	381	LEU
1	A	390	SER
1	A	511	LYS
1	A	547	ARG
1	A	552	ASP
1	A	555	LYS
1	A	569	ASN
1	A	613	LYS
1	A	620	LYS
1	A	628	GLN
1	A	645	LYS
1	A	701	THR
1	A	715	VAL

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Mol	Chain	Res	Type
1	B	321	THR
1	B	332	MET
1	B	351	LYS
1	B	382	GLU
1	B	392	SER
1	B	423	LYS
1	B	486	LYS
1	B	547	ARG
1	B	667	ARG
1	B	717	LYS

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

Mol	Chain	Res	Type
1	A	329	HIS
1	A	407	HIS
1	A	454	ASN
1	A	569	ASN
1	A	628	GLN
1	A	697	ASN
1	A	712	ASN
1	B	364	GLN
1	B	385	ASN
1	B	454	ASN
1	B	527	ASN
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 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	$\#\|Z\| > 2$
2	HEM	A	750	1	41,50,50	1.94	9 (21%)	45,82,82	1.81	11 (24%)
5	3XC	B	800	-	29,31,31	0.85	0	30,43,43	1.92	8 (26%)
3	H4B	A	760	-	16,18,18	0.81	0	11,26,26	2.89	7 (63%)
4	ACT	A	860	-	3,3,3	0.80	0	3,3,3	0.77	0
2	HEM	B	750	1	41,50,50	1.78	8 (19%)	45,82,82	1.84	8 (17%)
3	H4B	B	760	-	16,18,18	1.09	1 (6%)	11,26,26	2.63	3 (27%)
5	3XC	A	800	-	29,31,31	1.04	3 (10%)	30,43,43	2.09	9 (30%)
4	ACT	B	860	-	3,3,3	0.65	0	3,3,3	1.14	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
2	HEM	A	750	1	-	3/12/54/54	-
5	3XC	B	800	-	-	2/18/29/29	0/3/3/3
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2
2	HEM	B	750	1	-	3/12/54/54	-
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
5	3XC	A	800	-	-	1/18/29/29	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C2D	7.25	1.52	1.36
2	B	750	HEM	C3D-C2D	6.49	1.50	1.36
2	A	750	HEM	C3C-CAC	4.04	1.56	1.47
2	B	750	HEM	C3C-C2C	-3.67	1.35	1.40
2	A	750	HEM	C3C-C2C	-3.66	1.35	1.40
2	B	750	HEM	C3C-CAC	3.48	1.54	1.47
2	A	750	HEM	CAB-C3B	2.71	1.54	1.47
3	B	760	H4B	C7-N8	2.70	1.49	1.44
5	A	800	3XC	C3-N2	-2.67	1.43	1.46
2	B	750	HEM	FE-NB	2.63	2.09	1.96
2	B	750	HEM	CMB-C2B	2.49	1.56	1.50
2	A	750	HEM	CMC-C2C	2.36	1.57	1.51
2	A	750	HEM	CMD-C2D	2.36	1.55	1.50
2	A	750	HEM	CMB-C2B	2.35	1.55	1.50
2	B	750	HEM	CAB-C3B	2.33	1.53	1.47
5	A	800	3XC	F6-C4	-2.27	1.32	1.37
2	A	750	HEM	C3B-C2B	-2.26	1.32	1.37
2	A	750	HEM	FE-NB	2.14	2.07	1.96
2	B	750	HEM	CMD-C2D	2.05	1.55	1.50
5	A	800	3XC	C13-C14	2.02	1.41	1.37
2	B	750	HEM	C4A-NA	2.01	1.40	1.36

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	760	H4B	C8A-C4A-C4	6.98	120.77	114.57
5	B	800	3XC	C6A-N1A-C2A	6.22	122.82	118.10
2	B	750	HEM	C4D-ND-C1D	5.86	111.12	105.07
5	A	800	3XC	C6A-N1A-C2A	5.84	122.52	118.10
2	A	750	HEM	C4D-ND-C1D	5.08	110.33	105.07
5	A	800	3XC	F5-C4-C11	4.83	116.26	110.34
2	B	750	HEM	C4B-CHC-C1C	4.59	128.61	122.56
3	A	760	H4B	C2-N3-C4	4.33	122.81	115.93
2	A	750	HEM	CBD-CAD-C3D	-4.07	101.31	112.63
3	A	760	H4B	C4-C4A-N5	4.05	122.52	119.12
3	A	760	H4B	N1-C2-N3	-3.99	119.17	125.42
3	A	760	H4B	C8A-C4A-C4	3.91	118.05	114.57
2	B	750	HEM	CBD-CAD-C3D	-3.88	101.85	112.63
5	A	800	3XC	C4A-C3A-C2A	-3.70	117.90	120.32
2	A	750	HEM	CHA-C4D-ND	3.48	128.68	124.38
2	A	750	HEM	C4B-CHC-C1C	3.32	126.94	122.56
5	B	800	3XC	C4A-C3A-C2A	-3.30	118.16	120.32
2	A	750	HEM	CMA-C3A-C4A	-3.30	123.39	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	800	3XC	C5'-N1'-C2'	3.12	112.79	105.42
3	A	760	H4B	C2-N1-C8A	2.96	121.18	114.54
5	B	800	3XC	C3A-C2A-N1A	-2.91	119.82	122.90
3	B	760	H4B	C2-N3-C4	2.84	120.44	115.93
5	B	800	3XC	C5'-N1'-C2'	2.80	112.02	105.42
5	A	800	3XC	C13-C12-C11	-2.65	117.67	121.22
5	A	800	3XC	C12-C13-C14	2.63	121.08	118.36
2	B	750	HEM	CHC-C4B-NB	2.57	127.23	124.43
2	B	750	HEM	CMA-C3A-C4A	-2.57	124.52	128.46
5	B	800	3XC	F5-C4-C11	2.56	113.48	110.34
2	A	750	HEM	C4C-CHD-C1D	2.53	125.89	122.56
2	B	750	HEM	CAA-CBA-CGA	-2.48	106.81	113.76
2	A	750	HEM	CMC-C2C-C3C	2.44	129.24	124.68
5	B	800	3XC	C3'-C2'-N1'	-2.37	101.22	105.20
3	A	760	H4B	N2-C2-N1	2.34	120.89	117.25
5	A	800	3XC	N6A-C6A-N1A	2.30	120.12	116.49
2	A	750	HEM	CMA-C3A-C2A	2.23	129.15	124.94
2	B	750	HEM	CHA-C4D-ND	2.22	127.12	124.38
5	A	800	3XC	C3A-C2A-N1A	-2.22	120.55	122.90
5	A	800	3XC	C2A-C7A-C4'	-2.17	108.39	115.55
2	B	750	HEM	C2C-C3C-C4C	2.16	108.41	106.90
3	A	760	H4B	C4A-N5-C6	-2.15	115.30	121.16
5	B	800	3XC	C2-N2-C3	2.12	117.64	113.35
5	B	800	3XC	N6A-C6A-N1A	2.11	119.82	116.49
2	A	750	HEM	CAB-C3B-C2B	-2.08	121.74	128.60
2	A	750	HEM	C1D-C2D-C3D	-2.07	104.78	106.96
3	B	760	H4B	C4A-C4-N3	-2.05	118.17	124.01
2	A	750	HEM	CMD-C2D-C1D	2.05	128.17	125.04

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	750	HEM	C1A-C2A-CAA-CBA
2	A	750	HEM	C3A-C2A-CAA-CBA
2	B	750	HEM	C3A-C2A-CAA-CBA
2	A	750	HEM	C2A-CAA-CBA-CGA
2	B	750	HEM	C2A-CAA-CBA-CGA
5	A	800	3XC	C1-C2-N2-C3
5	B	800	3XC	C1-C2-N2-C3
2	B	750	HEM	C1A-C2A-CAA-CBA
5	B	800	3XC	C12-C11-C4-F5

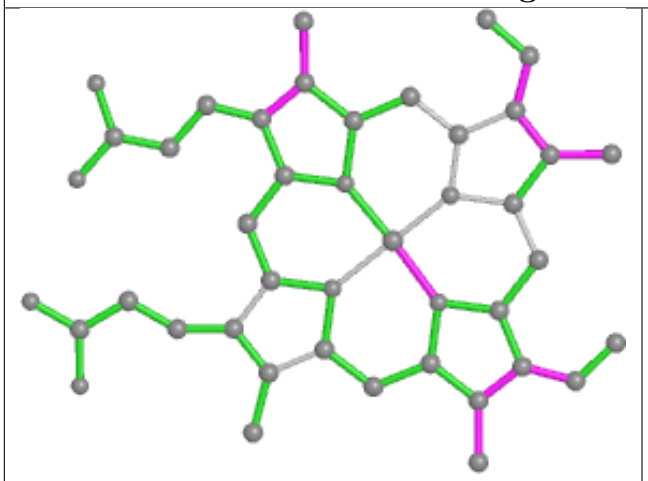
There are no ring outliers.

4 monomers are involved in 8 short contacts:

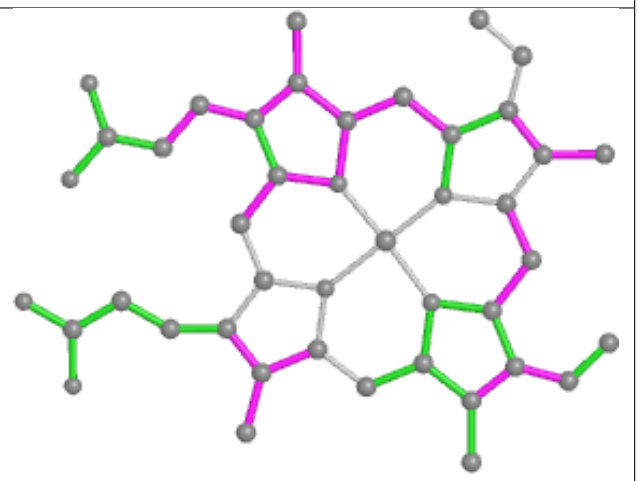
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	750	HEM	3	0
5	B	800	3XC	1	0
2	B	750	HEM	3	0
5	A	800	3XC	1	0

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.

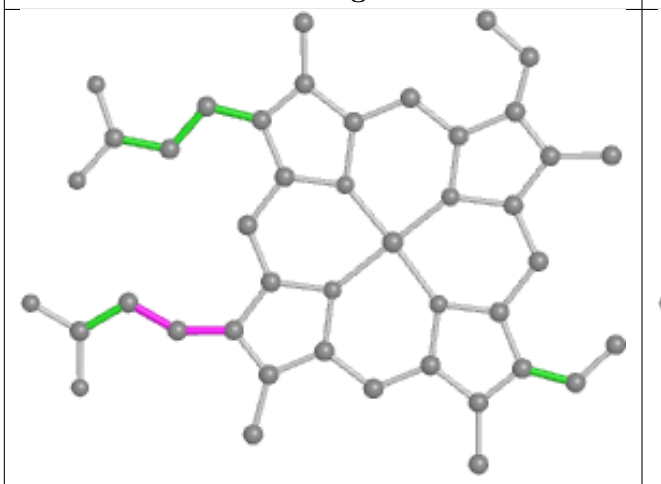
Ligand HEM A 750



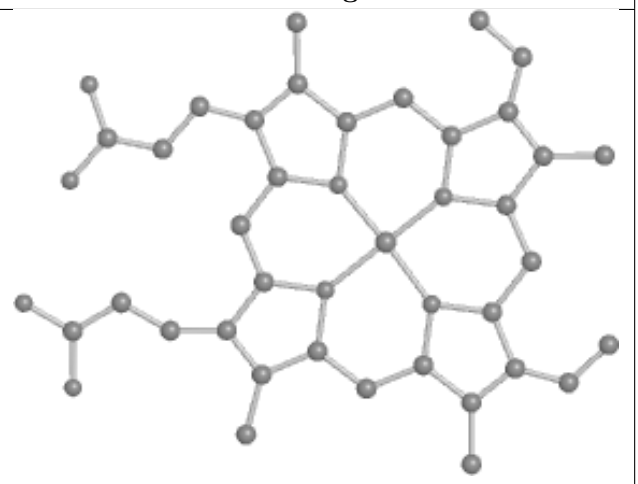
Bond lengths



Bond angles

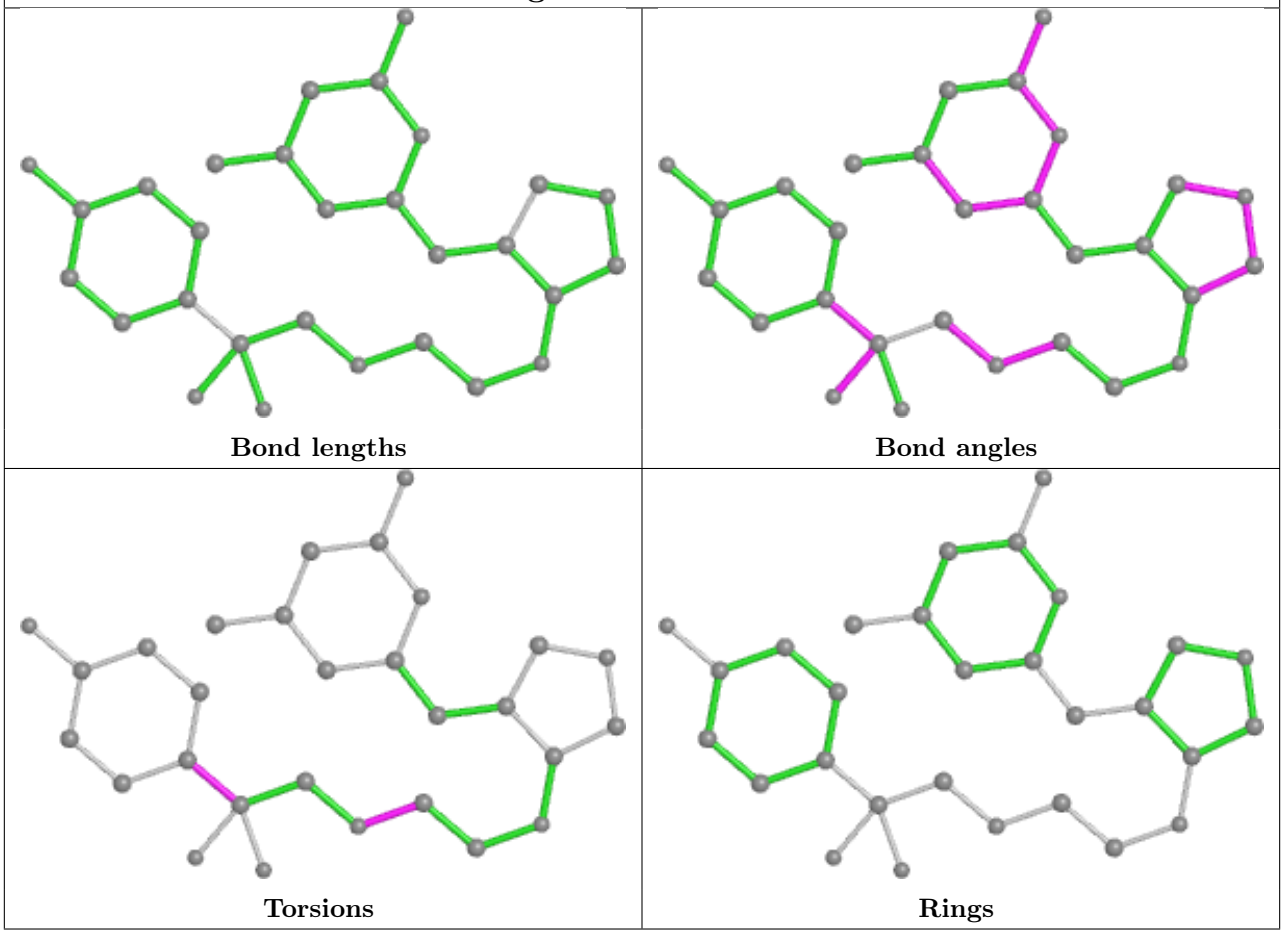


Torsions

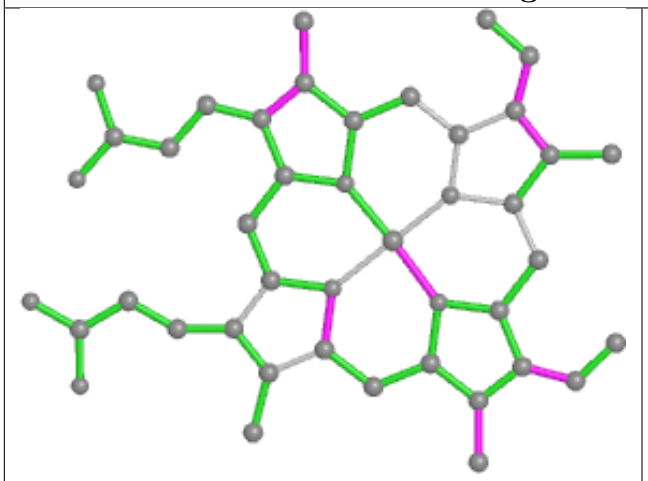


Rings

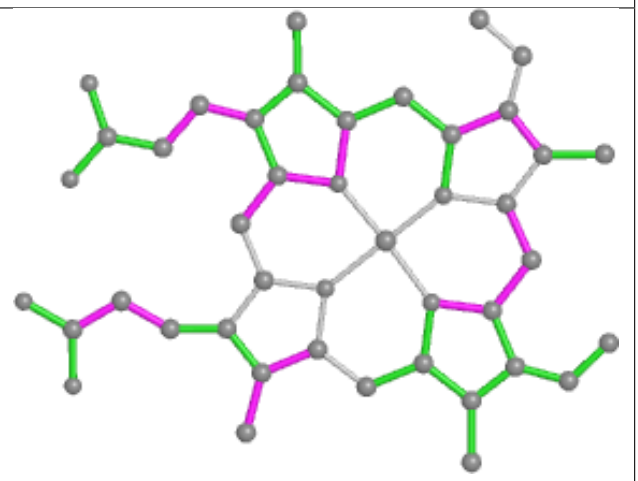
Ligand 3XC B 800



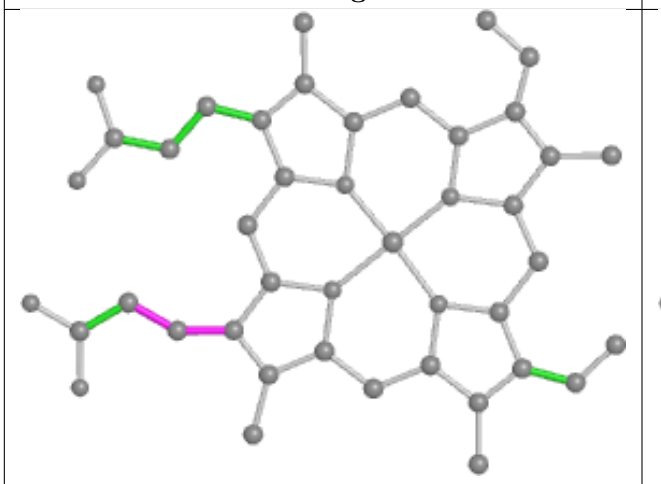
Ligand HEM B 750



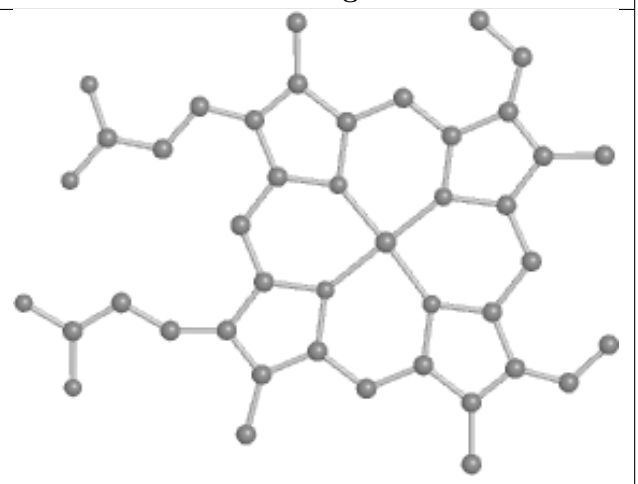
Bond lengths



Bond angles

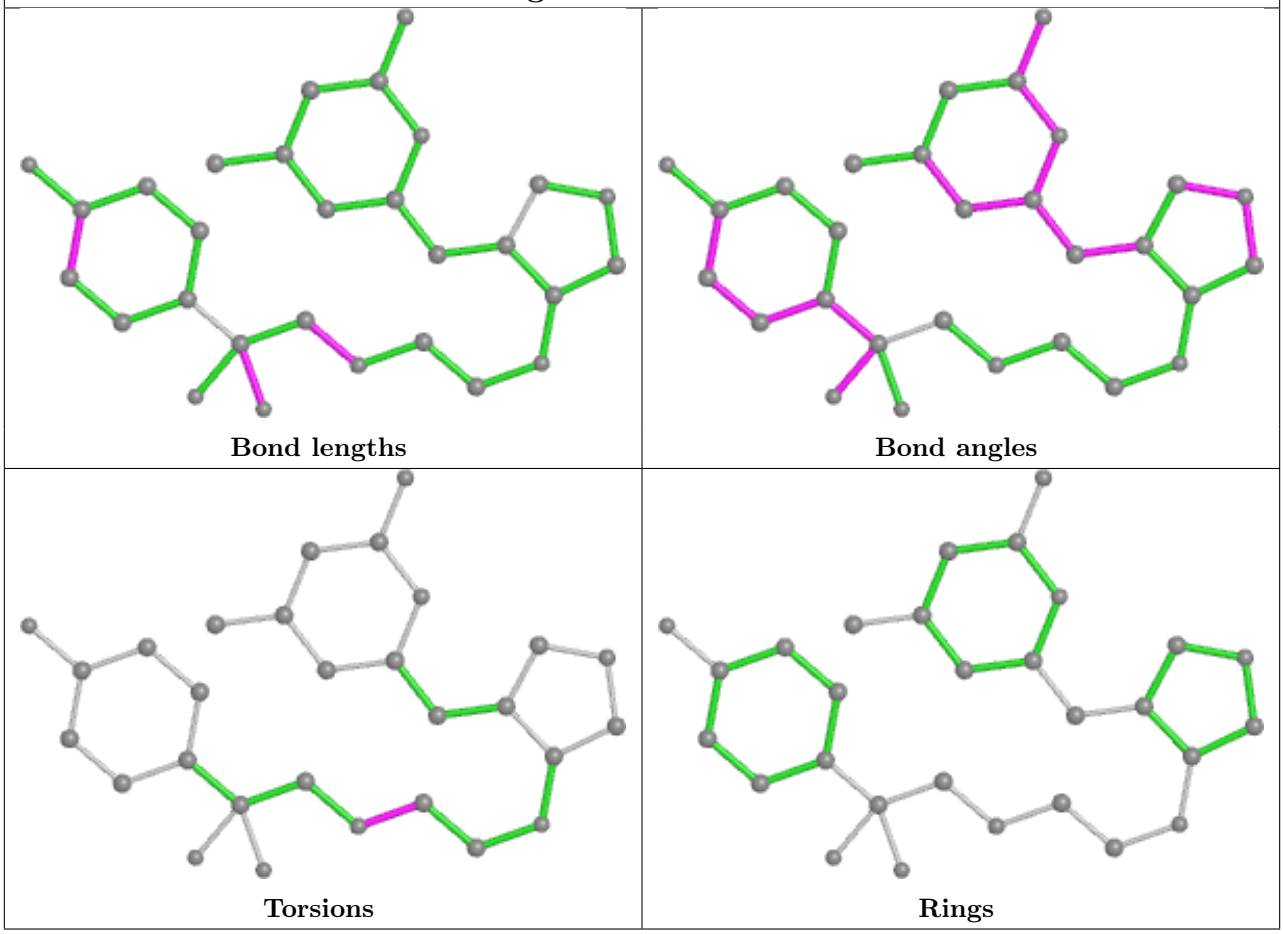


Torsions



Rings

Ligand 3XC A 800



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	407/422 (96%)	1.16	89 (21%)	0	0	33, 60, 101, 132	0
1	B	411/422 (97%)	0.65	36 (8%)	10	9	32, 50, 77, 100	0
All	All	818/844 (96%)	0.90	125 (15%)	2	1	32, 54, 95, 132	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	9.2
1	A	716	TRP	8.9
1	A	488	PRO	8.4
1	B	348	VAL	7.0
1	A	506	ILE	6.6
1	B	718	GLY	6.2
1	A	355	PHE	6.0
1	A	351	LYS	5.5
1	B	619	ARG	5.4
1	A	300	PHE	5.0
1	A	713	THR	4.9
1	A	619	ARG	4.4
1	A	715	VAL	4.2
1	B	299	ARG	4.1
1	B	350	THR	4.1
1	A	486	LYS	4.0
1	A	352	ASP	4.0
1	A	391	THR	4.0
1	A	591	THR	4.0
1	A	322	LEU	3.8
1	B	301	LEU	3.8
1	A	302	LYS	3.8
1	A	480	ILE	3.8
1	A	566	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	350	THR	3.8
1	A	507	GLN	3.7
1	A	551	PHE	3.7
1	A	567	VAL	3.7
1	A	385	ASN	3.6
1	A	503	GLU	3.6
1	A	415	CYS	3.6
1	A	677	VAL	3.6
1	A	299	ARG	3.5
1	A	469	LYS	3.5
1	B	616	LEU	3.5
1	B	351	LYS	3.4
1	A	712	ASN	3.4
1	A	643	SER	3.4
1	A	489	ASP	3.3
1	B	591	THR	3.3
1	A	667	ARG	3.3
1	A	390	SER	3.2
1	B	667	ARG	3.2
1	A	388	ILE	3.2
1	A	353	GLN	3.1
1	B	567	VAL	3.1
1	B	715	VAL	3.0
1	B	566	ALA	3.0
1	A	682	PRO	3.0
1	A	595	VAL	3.0
1	B	321	THR	3.0
1	B	353	GLN	2.9
1	A	679	ILE	2.9
1	A	588	TYR	2.9
1	A	479	LEU	2.9
1	B	375	LYS	2.9
1	A	552	ASP	2.8
1	A	678	TRP	2.8
1	B	352	ASP	2.8
1	A	487	GLN	2.8
1	A	561	TRP	2.8
1	A	676	TRP	2.8
1	B	691	PHE	2.8
1	A	416	VAL	2.8
1	B	615	ASP	2.8
1	A	617	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	491	SER	2.7
1	A	493	LEU	2.7
1	B	677	VAL	2.6
1	A	514	ARG	2.6
1	A	499	VAL	2.6
1	A	681	PRO	2.6
1	A	328	GLU	2.6
1	A	680	VAL	2.6
1	A	318	LEU	2.6
1	B	479	LEU	2.6
1	A	389	GLU	2.6
1	A	714	HIS	2.6
1	A	409	TRP	2.6
1	A	568	SER	2.6
1	A	686	SER	2.6
1	A	584	PHE	2.5
1	B	389	GLU	2.5
1	B	713	THR	2.5
1	A	594	GLY	2.5
1	A	615	ASP	2.5
1	A	531	PRO	2.4
1	B	310	VAL	2.4
1	A	386	LYS	2.4
1	A	492	THR	2.4
1	B	680	VAL	2.4
1	B	620	LYS	2.4
1	B	493	LEU	2.4
1	A	505	CYS	2.4
1	A	508	GLN	2.3
1	A	392	SER	2.3
1	B	562	TYR	2.3
1	A	684	SER	2.3
1	A	593	ILE	2.3
1	A	550	LYS	2.3
1	A	412	ALA	2.3
1	B	681	PRO	2.3
1	A	691	PHE	2.2
1	B	329	HIS	2.2
1	A	321	THR	2.2
1	A	630	LEU	2.2
1	A	485	TYR	2.2
1	B	611	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	519	VAL	2.1
1	B	302	LYS	2.1
1	A	330	ILE	2.1
1	B	679	ILE	2.1
1	A	620	LYS	2.1
1	B	676	TRP	2.1
1	A	683	MET	2.1
1	A	467	ASP	2.1
1	A	470	HIS	2.1
1	A	511	LYS	2.1
1	B	561	TRP	2.1
1	A	572	LEU	2.1
1	A	373	GLY	2.1
1	A	309	ASP	2.0
1	A	394	TYR	2.0
1	A	490	GLY	2.0
1	A	442	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 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	3XC	A	800	29/29	0.85	0.20	33,41,49,51	0
5	3XC	B	800	29/29	0.90	0.17	33,43,46,51	0
4	ACT	B	860	4/4	0.95	0.17	61,62,62,62	0
3	H4B	A	760	17/17	0.96	0.20	37,40,47,51	0
4	ACT	A	860	4/4	0.97	0.23	72,72,73,76	0
3	H4B	B	760	17/17	0.97	0.18	30,38,44,44	0

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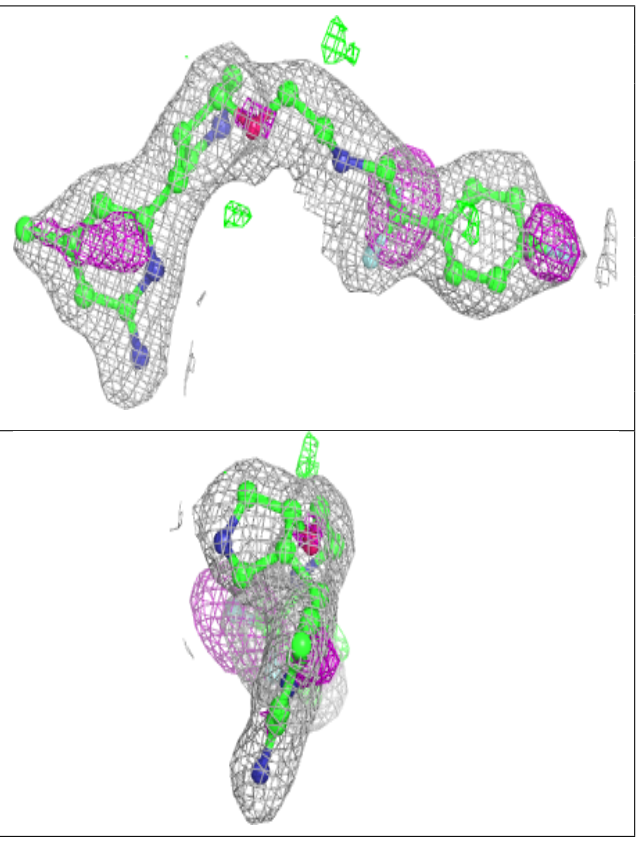
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	A	750	43/43	0.98	0.22	36,40,45,52	0
2	HEM	B	750	43/43	0.98	0.18	33,38,49,53	0
6	ZN	A	900	1/1	1.00	0.09	47,47,47,47	0

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.

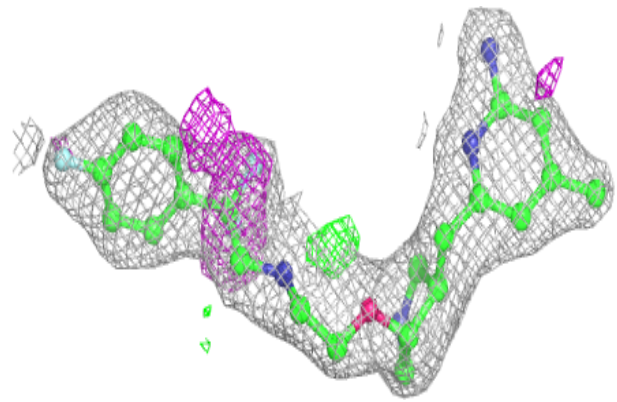
Electron density around 3XC A 800:

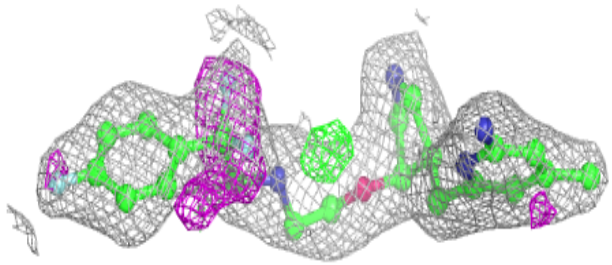
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

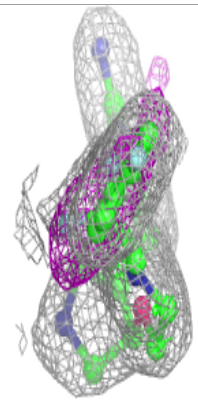


Electron density around 3XC B 800:

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

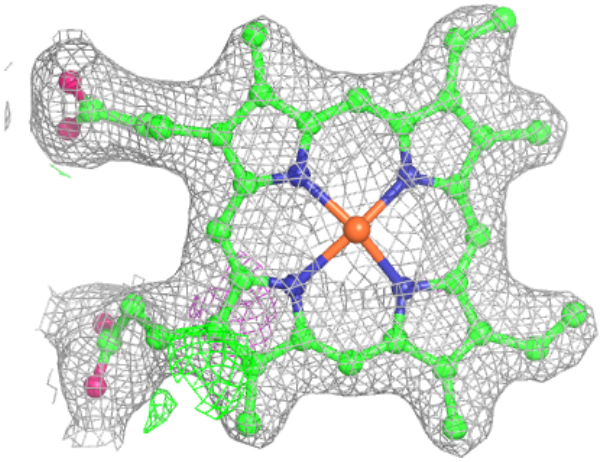


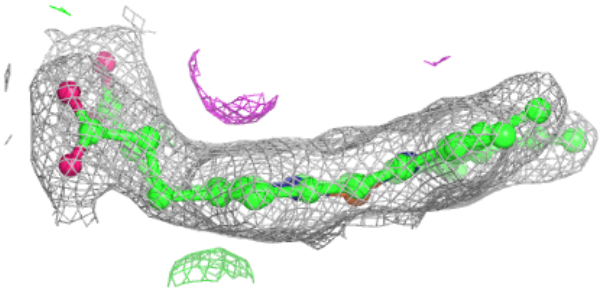


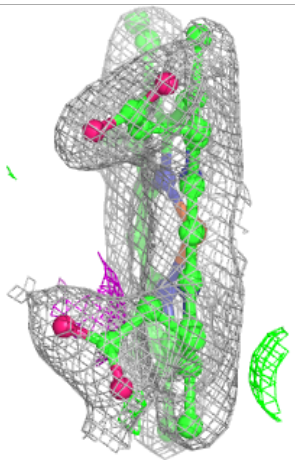


Electron density around HEM A 750:

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

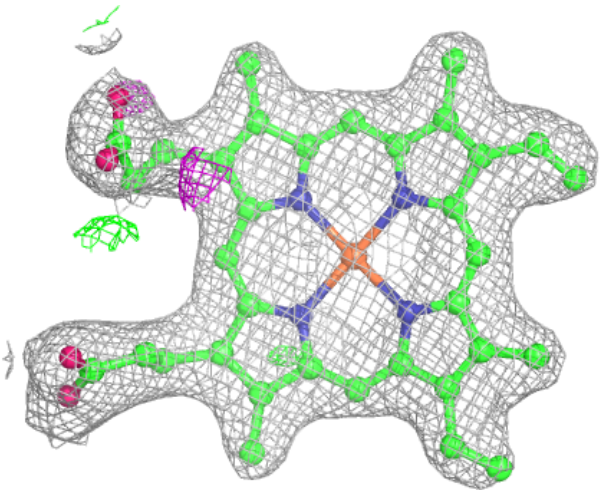


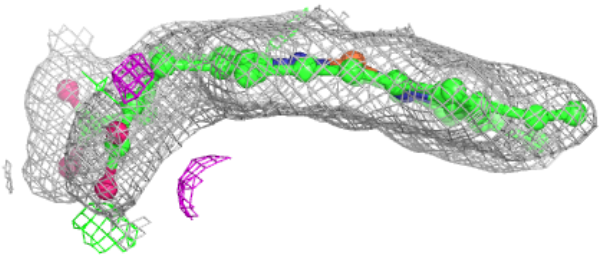


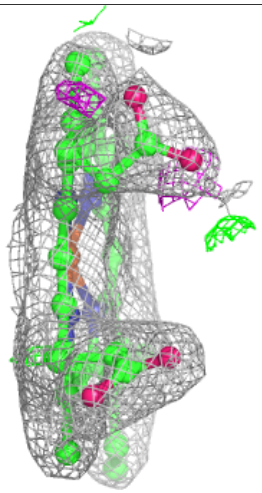


Electron density around HEM B 750:

$2mF_o$-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 (i)

There are no such residues in this entry.