Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2023 – 03:10 PM EDT

PDB ID	:	4JSI
Title	:	Structure of rat neuronal nitric oxide synthase heme domain in complex with 6-((3-(((3-fluorophenethyl)amino)methyl)phenoxy)methyl)-4-methylpyridin-2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2013-03-22
Resolution	:	2.09 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

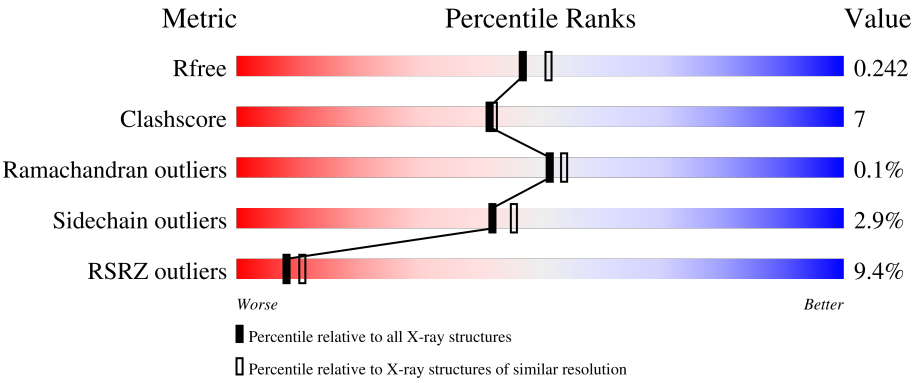
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	13% 76% 18%
1	B	422	5% 84% 13%

2 Entry composition

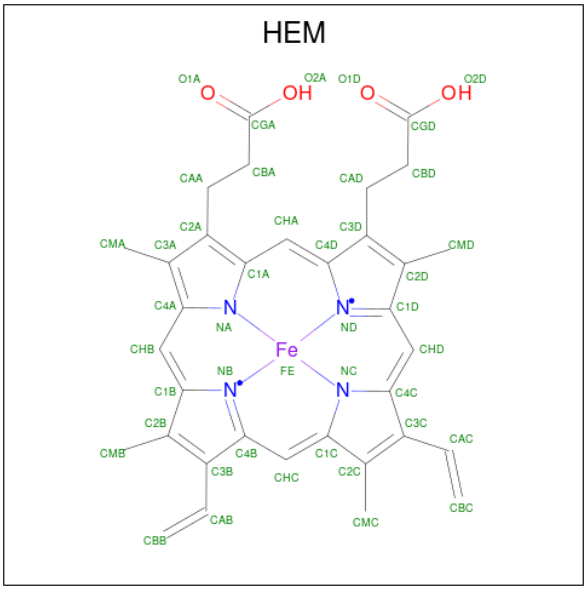
There are 7 unique types of molecules in this entry. The entry contains 7072 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

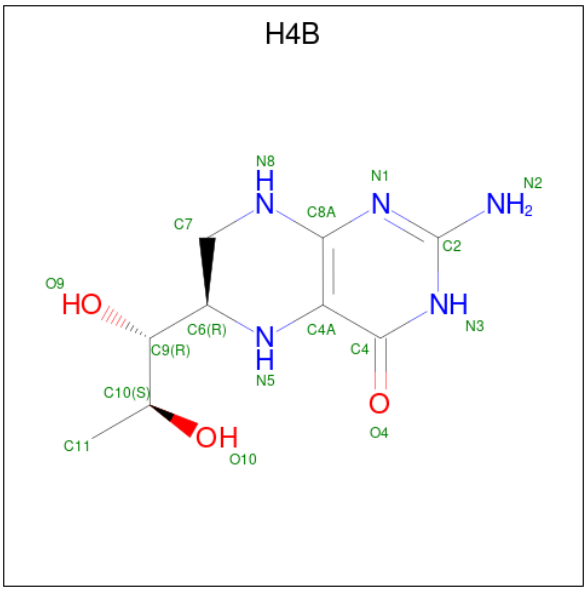
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	1	0
			3319	2125	566	607	21			
1	B	411	Total	C	N	O	S	0	1	0
			3348	2142	574	610	22			

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



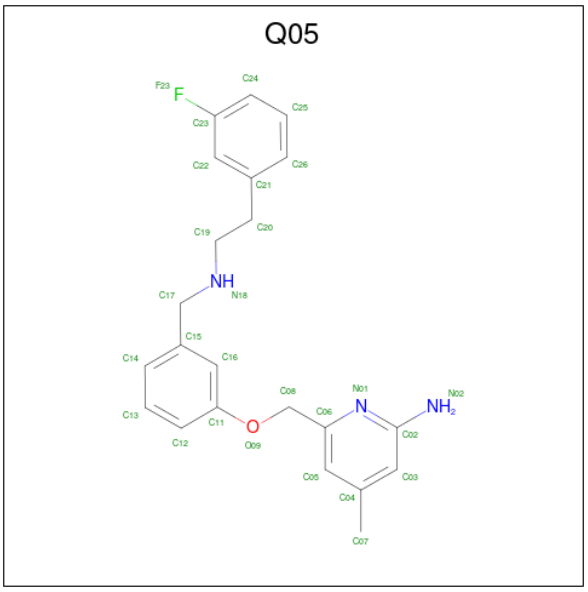
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 17 9 5 3	0	0
3	B	1	Total C N O 17 9 5 3	0	0

- Molecule 4 is 6-{[3-({[2-(3-fluorophenyl)ethyl]amino}methyl)phenoxy]methyl}-4-methylpyridin-2-amine (three-letter code: Q05) (formula: $C_{22}H_{24}FN_3O$).



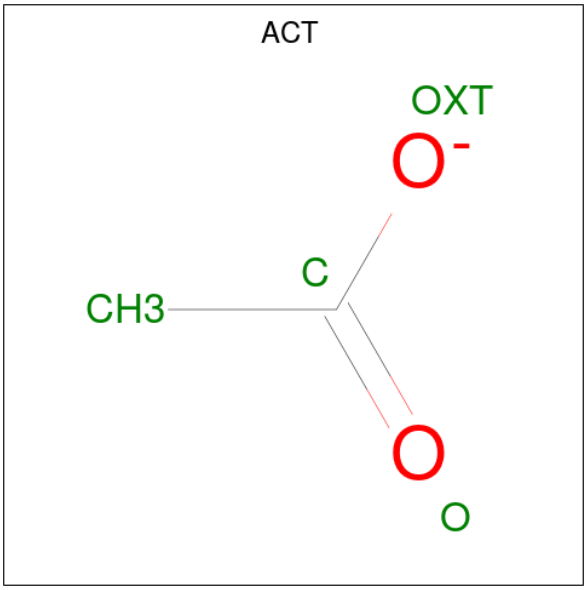
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O 27 22 1 3 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	0	0
			27	22	1	3	1		

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



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

- 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.

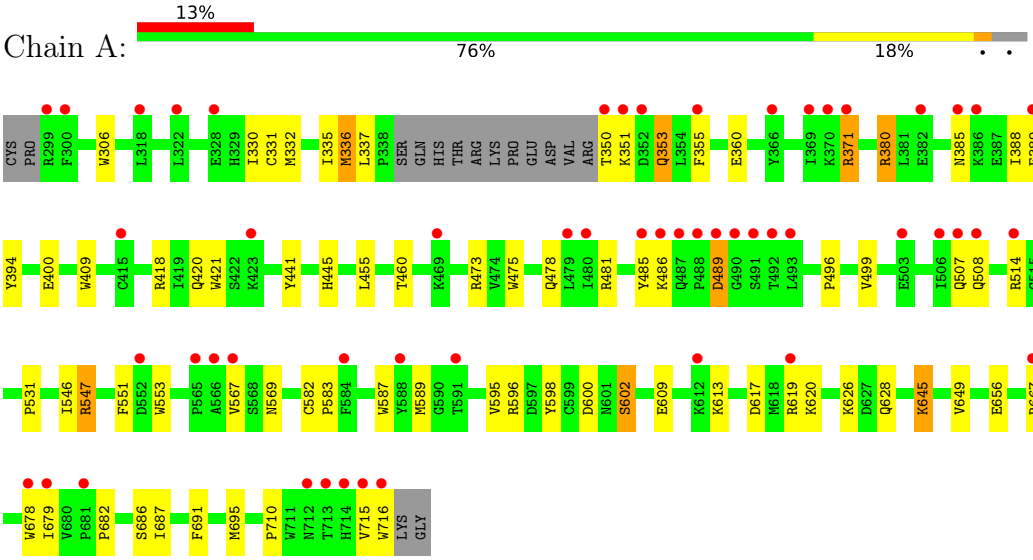
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	95	Total	O	0	0
			95	95		
7	B	127	Total	O	0	0
			127	127		

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.

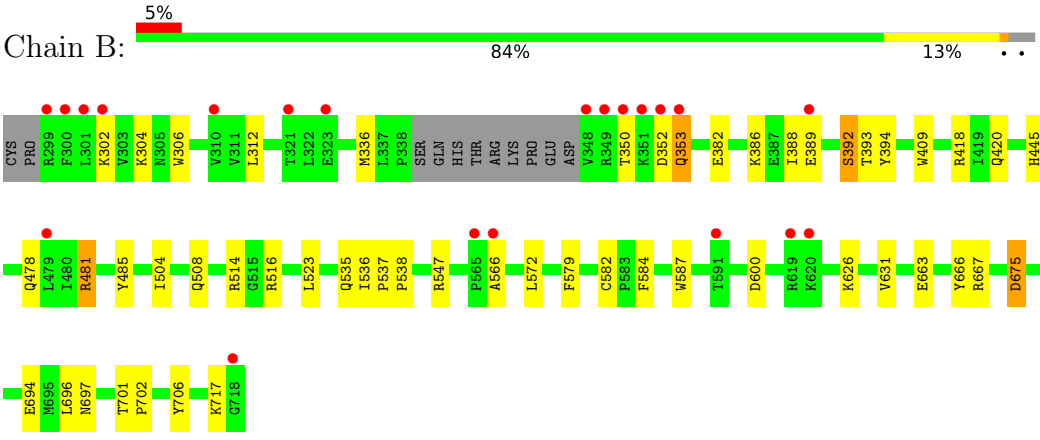
• Molecule 1: Nitric oxide synthase, brain

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	51.60Å 110.78Å 164.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.70 – 2.09 40.66 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.70-2.09) 99.1 (40.66-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.08Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.241 0.192 , 0.242	Depositor DCC
R_{free} test set	2792 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.839	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.9	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	7072	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, Q05, H4B, ACT, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.60	1/3415 (0.0%)	0.70	0/4633
1	B	0.73	0/3444	0.79	3/4669 (0.1%)
All	All	0.67	1/6859 (0.0%)	0.75	3/9302 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	TYR	CG-CD2	5.24	1.46	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	600	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	675	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	675	ASP	CB-CG-OD2	-5.34	113.50	118.30

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	3319	0	3227	55	0
1	B	3348	0	3264	44	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	3	0
2	B	43	0	30	8	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	27	0	24	4	0
4	B	27	0	24	2	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0
7	A	95	0	0	0	0
7	B	127	0	0	4	0
All	All	7072	0	6635	94	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 7.

All (94) 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:337:LEU:HD21	4:A:803:Q05:H2	1.60	0.82
1:A:371:ARG:CG	1:A:371:ARG:HH21	2.01	0.74
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.70	0.72
1:B:536:ILE:HG13	7:B:921:HOH:O	1.89	0.71
1:A:380:ARG:HD3	1:A:400:GLU:OE1	1.91	0.70
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.58	0.69
1:B:350:THR:HG22	1:B:352:ASP:H	1.60	0.66
1:B:353:GLN:HE21	1:B:353:GLN:H	1.46	0.62
1:B:504:ILE:O	1:B:508:GLN:HG2	2.01	0.60
1:A:596:ARG:NH2	1:A:600:ASP:OD2	2.33	0.58
2:B:801:HEM:C1C	4:B:803:Q05:H25	2.37	0.58
1:B:508:GLN:NE2	7:B:1014:HOH:O	2.38	0.57
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.87	0.56
1:A:485:TYR:HB3	1:A:514:ARG:NH1	2.20	0.56
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.42	0.55
1:B:475:TRP:HB2	1:B:523:LEU:HB3	1.89	0.55
1:B:535:GLN:HG3	7:B:1015:HOH:O	2.07	0.54
1:A:626:LYS:HB3	1:B:687:ILE:HD12	1.90	0.54
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.66	0.53
1:A:628:GLN:HG3	1:B:631:VAL:HG11	1.91	0.52
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.41	0.51
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:ASP:O	1:B:679:ILE:HG12	2.10	0.51
1:A:675:ASP:O	1:A:679:ILE:HG12	2.11	0.51
1:B:584:PHE:CD1	2:B:801:HEM:HAC	2.45	0.51
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.93	0.51
1:B:353:GLN:H	1:B:353:GLN:NE2	2.09	0.50
1:B:587:TRP:H	2:B:801:HEM:HAB	1.76	0.50
1:A:337:LEU:CD2	4:A:803:Q05:H2	2.38	0.50
1:A:567:VAL:HG21	4:A:803:Q05:C12	2.42	0.50
1:A:460:THR:O	1:A:583:PRO:HD2	2.13	0.49
1:A:445:HIS:C	1:A:445:HIS:CD2	2.86	0.49
1:B:386:LYS:O	1:B:389:GLU:HG2	2.12	0.49
1:A:393:THR:OG1	1:A:394:TYR:N	2.47	0.48
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.95	0.48
1:B:706:TYR:OH	2:B:801:HEM:O1D	2.19	0.48
1:A:486:LYS:HD2	1:A:499:VAL:HG11	1.94	0.47
1:B:701:THR:HA	1:B:702:PRO:C	2.35	0.47
1:A:351:LYS:NZ	1:A:389:GLU:O	2.43	0.47
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.48	0.47
1:A:674:ALA:HB3	1:A:695:MET:HB3	1.96	0.47
1:B:409:TRP:CD2	2:B:801:HEM:HBC2	2.49	0.47
1:A:547:ARG:HD3	1:A:547:ARG:H	1.80	0.47
1:A:682:PRO:HB2	1:B:686:SER:HB3	1.98	0.46
1:B:388:ILE:O	1:B:392:SER:HA	2.16	0.46
1:B:516:ARG:HD2	7:B:1011:HOH:O	2.15	0.46
1:A:332:MET:HB3	1:A:335:ILE:HG13	1.97	0.46
1:A:595:VAL:CG1	1:B:686:SER:OG	2.64	0.46
1:A:667:ARG:NH1	1:A:668:CYS:SG	2.89	0.45
1:B:445:HIS:C	1:B:445:HIS:CD2	2.90	0.45
1:A:645:LYS:HE3	1:A:645:LYS:HB2	1.69	0.45
1:B:566:ALA:HA	1:B:584:PHE:O	2.17	0.45
1:A:617:ASP:OD2	1:A:619:ARG:HB2	2.17	0.45
1:B:302:LYS:HE3	1:B:302:LYS:HB2	1.52	0.44
1:A:353:GLN:NE2	1:A:353:GLN:H	2.16	0.44
1:A:496:PRO:HB2	1:A:602:SER:O	2.17	0.44
1:A:306:TRP:CD1	1:B:336:MET:HE2	2.53	0.44
2:B:801:HEM:HHA	2:B:801:HEM:HAD2	1.81	0.44
1:A:391:THR:O	1:A:392:SER:OG	2.31	0.43
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.32	0.43
1:A:524:LEU:O	1:A:531:PRO:HA	2.18	0.43
1:A:351:LYS:HE2	1:A:392:SER:HB3	2.00	0.43
1:B:312:LEU:HB3	1:B:666:TYR:CD2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:TYR:OH	4:B:803:Q05:H5	2.18	0.43
1:B:537:PRO:HA	1:B:538:PRO:HD3	1.92	0.43
1:A:678:TRP:CE3	2:A:801:HEM:HBA2	2.53	0.43
1:B:418:ARG:C	1:B:420:GLN:N	2.73	0.43
1:A:350:THR:N	1:A:353:GLN:HE22	2.17	0.42
1:B:409:TRP:CH2	2:B:801:HEM:HMC3	2.54	0.42
1:B:460:THR:O	1:B:582:CYS:HA	2.19	0.42
1:B:572:LEU:HB3	1:B:579:PHE:HB2	2.00	0.42
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.54	0.42
1:A:336:MET:HE3	1:A:678:TRP:HZ2	1.84	0.42
1:B:584:PHE:CD1	2:B:801:HEM:CAC	3.03	0.42
1:A:336:MET:HG3	1:B:306:TRP:NE1	2.35	0.42
1:A:337:LEU:HD21	4:A:803:Q05:C25	2.42	0.42
1:A:686:SER:HA	1:A:691:PHE:CG	2.54	0.42
1:B:393:THR:OG1	1:B:394:TYR:N	2.52	0.42
1:A:460:THR:O	1:A:582:CYS:HA	2.20	0.42
1:A:546:ILE:HG13	1:A:598:TYR:OH	2.20	0.41
1:A:687:ILE:HD12	1:B:626:LYS:HB3	2.02	0.41
2:A:801:HEM:HHA	2:A:801:HEM:HAD2	1.89	0.41
1:B:478:GLN:HA	1:B:566:ALA:O	2.21	0.41
1:A:508:GLN:OE1	1:A:716:TRP:CH2	2.75	0.41
1:B:302:LYS:HA	1:B:312:LEU:O	2.21	0.41
1:B:304:LYS:O	1:B:694:GLU:HG3	2.21	0.41
1:A:388:ILE:O	1:A:392:SER:HA	2.21	0.40
1:A:589:MET:HA	1:A:649:VAL:O	2.20	0.40
1:A:609:GLU:O	1:A:613:LYS:HG2	2.21	0.40
1:A:355:PHE:CE1	1:A:385:ASN:HB2	2.55	0.40
1:A:418:ARG:C	1:A:420:GLN:N	2.74	0.40
1:A:475:TRP:HB2	1:A:523:LEU:HB3	2.03	0.40
1:B:663:GLU:HB3	1:B:667:ARG:NH1	2.37	0.40
1:A:331:CYS:HB3	1:B:697:ASN:HB3	2.03	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	404/422 (96%)	388 (96%)	15 (4%)	1 (0%)	47 49
1	B	408/422 (97%)	392 (96%)	16 (4%)	0	100 100
All	All	812/844 (96%)	780 (96%)	31 (4%)	1 (0%)	51 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ASP

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	364/377 (97%)	349 (96%)	15 (4%)	30 31
1	B	367/377 (97%)	361 (98%)	6 (2%)	62 69
All	All	731/754 (97%)	710 (97%)	21 (3%)	42 46

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	336	MET
1	A	353	GLN
1	A	360	GLU
1	A	371	ARG
1	A	380	ARG
1	A	489	ASP
1	A	507	GLN
1	A	516	ARG
1	A	547	ARG
1	A	569	ASN
1	A	602	SER
1	A	620	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	645	LYS
1	A	656	GLU
1	A	715	VAL
1	B	353	GLN
1	B	382	GLU
1	B	392	SER
1	B	481	ARG
1	B	547	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	317	HIS
1	A	436	HIS
1	A	454	ASN
1	A	527	ASN
1	A	569	ASN
1	A	642	GLN
1	A	697	ASN
1	B	364	GLN
1	B	385	ASN
1	B	454	ASN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
1	B	642	GLN
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 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	$\#\|Z\| > 2$
4	Q05	B	803	-	29,29,29	0.75	0	37,38,38	1.53	6 (16%)
3	H4B	A	802	-	16,18,18	0.76	0	11,26,26	3.02	6 (54%)
5	ACT	A	804	-	3,3,3	0.85	0	3,3,3	0.65	0
5	ACT	B	804	-	3,3,3	0.89	0	3,3,3	0.33	0
2	HEM	A	801	1	41,50,50	1.35	5 (12%)	45,82,82	1.95	11 (24%)
3	H4B	B	802	-	16,18,18	1.26	2 (12%)	11,26,26	2.99	6 (54%)
4	Q05	A	803	-	29,29,29	0.62	0	37,38,38	1.42	7 (18%)
2	HEM	B	801	1	41,50,50	1.40	4 (9%)	45,82,82	2.22	16 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	Q05	B	803	-	-	7/12/12/12	0/3/3/3
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
2	HEM	A	801	1	-	7/12/54/54	-
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
4	Q05	A	803	-	-	3/12/12/12	0/3/3/3
2	HEM	B	801	1	-	6/12/54/54	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C1B-NB	-4.50	1.32	1.40
2	B	801	HEM	C1B-NB	-2.85	1.35	1.40
2	A	801	HEM	FE-NB	2.81	2.10	1.96
3	B	802	H4B	C4-N3	2.68	1.37	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	H4B	C2-N2	2.48	1.38	1.33
2	A	801	HEM	CHA-C4D	2.46	1.41	1.35
2	B	801	HEM	C3B-C4B	2.45	1.49	1.44
2	A	801	HEM	C4B-NB	-2.42	1.33	1.38
2	A	801	HEM	C3B-C4B	2.28	1.49	1.44
2	B	801	HEM	CHA-C4D	2.25	1.40	1.35
2	B	801	HEM	C4D-ND	-2.06	1.36	1.40

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802	H4B	C4-C4A-N5	5.58	123.80	119.12
2	A	801	HEM	CHA-C4D-ND	4.97	130.52	124.38
2	B	801	HEM	CHA-C4D-ND	4.97	130.52	124.38
2	B	801	HEM	CHC-C4B-NB	4.83	129.68	124.43
2	B	801	HEM	CHA-C4D-C3D	-4.79	116.35	125.33
3	B	802	H4B	C8A-C4A-C4	4.61	118.67	114.57
2	A	801	HEM	CAD-CBD-CGD	-4.48	103.97	113.60
2	B	801	HEM	C1B-NB-C4B	4.38	109.59	105.07
2	B	801	HEM	CBD-CAD-C3D	4.38	124.79	112.63
3	B	802	H4B	N1-C2-N3	-4.35	118.60	125.42
4	B	803	Q05	C02-N01-C06	4.29	121.35	118.10
3	B	802	H4B	C4-C4A-N5	3.95	122.43	119.12
3	B	802	H4B	C2-N3-C4	3.93	122.18	115.93
3	A	802	H4B	N1-C2-N3	-3.90	119.30	125.42
2	A	801	HEM	C1B-NB-C4B	3.77	108.96	105.07
3	A	802	H4B	C2-N3-C4	3.67	121.76	115.93
3	A	802	H4B	C2-N1-C8A	3.54	122.47	114.54
2	A	801	HEM	C2C-C3C-C4C	3.52	109.35	106.90
2	A	801	HEM	CHA-C4D-C3D	-3.50	118.75	125.33
2	B	801	HEM	CHD-C1D-C2D	-3.42	119.64	124.98
2	B	801	HEM	C4C-CHD-C1D	-3.41	118.06	122.56
3	A	802	H4B	C8A-C4A-C4	3.40	117.59	114.57
4	A	803	Q05	C15-C17-N18	-3.39	104.01	112.80
4	A	803	Q05	C02-N01-C06	3.35	120.64	118.10
4	B	803	Q05	C24-C23-C22	-3.35	118.94	123.29
3	B	802	H4B	C2-N1-C8A	3.27	121.86	114.54
2	B	801	HEM	O2D-CGD-CBD	3.17	124.22	114.03
2	B	801	HEM	CHB-C1B-NB	3.15	128.27	124.38
2	B	801	HEM	CHD-C1D-ND	3.15	127.85	124.43
4	B	803	Q05	C05-C06-N01	-3.14	119.57	122.90
3	B	802	H4B	N2-C2-N3	2.83	121.66	117.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	HEM	CHC-C4B-NB	2.82	127.50	124.43
4	A	803	Q05	C08-O09-C11	2.71	124.35	117.65
4	A	803	Q05	C05-C06-N01	-2.66	120.08	122.90
4	A	803	Q05	C24-C23-C22	-2.65	119.84	123.29
2	A	801	HEM	O2D-CGD-CBD	2.63	122.47	114.03
3	A	802	H4B	N2-C2-N3	2.51	121.16	117.25
2	A	801	HEM	CHD-C1D-ND	2.51	127.16	124.43
2	B	801	HEM	C3D-C4D-ND	2.42	112.86	110.17
4	A	803	Q05	C17-N18-C19	2.42	121.68	113.41
2	A	801	HEM	CAA-C2A-C3A	-2.37	120.44	127.25
4	A	803	Q05	C21-C22-C23	2.30	120.90	118.81
4	B	803	Q05	C08-O09-C11	2.23	123.16	117.65
2	B	801	HEM	C4D-ND-C1D	-2.22	102.78	105.07
2	B	801	HEM	CHB-C1B-C2B	-2.17	120.72	126.72
4	B	803	Q05	C07-C04-C05	-2.17	117.73	120.94
2	B	801	HEM	CAD-CBD-CGD	-2.16	108.96	113.60
4	B	803	Q05	C17-N18-C19	2.12	120.67	113.41
2	A	801	HEM	C4B-CHC-C1C	2.11	125.34	122.56
2	B	801	HEM	CMD-C2D-C1D	2.02	128.11	125.04
2	A	801	HEM	CHD-C1D-C2D	-2.01	121.84	124.98
2	B	801	HEM	C2D-C1D-ND	2.01	112.29	109.88

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C1A-C2A-CAA-CBA
2	A	801	HEM	C3A-C2A-CAA-CBA
2	A	801	HEM	C2A-CAA-CBA-CGA
2	A	801	HEM	C2D-C3D-CAD-CBD
2	A	801	HEM	C4D-C3D-CAD-CBD
2	B	801	HEM	C2A-CAA-CBA-CGA
4	B	803	Q05	N18-C19-C20-C21
4	A	803	Q05	C20-C19-N18-C17
4	B	803	Q05	C20-C19-N18-C17
4	A	803	Q05	C15-C17-N18-C19
2	B	801	HEM	C2B-C3B-CAB-CBB
2	B	801	HEM	C4B-C3B-CAB-CBB
4	B	803	Q05	C06-C08-O09-C11
4	B	803	Q05	C12-C11-O09-C08
4	A	803	Q05	C06-C08-O09-C11
4	B	803	Q05	C16-C11-O09-C08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	801	HEM	CAD-CBD-CGD-O1D
2	A	801	HEM	CAD-CBD-CGD-O2D
2	B	801	HEM	C2D-C3D-CAD-CBD
2	B	801	HEM	CAD-CBD-CGD-O2D
2	A	801	HEM	CAD-CBD-CGD-O1D
4	B	803	Q05	C19-C20-C21-C22
4	B	803	Q05	C19-C20-C21-C26

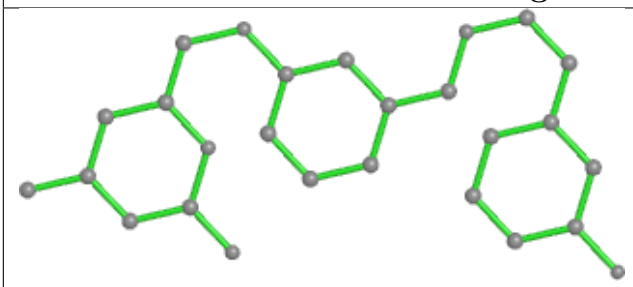
There are no ring outliers.

4 monomers are involved in 16 short contacts:

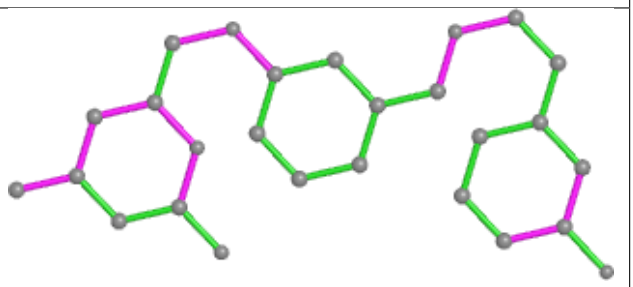
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	803	Q05	2	0
2	A	801	HEM	3	0
4	A	803	Q05	4	0
2	B	801	HEM	8	0

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.

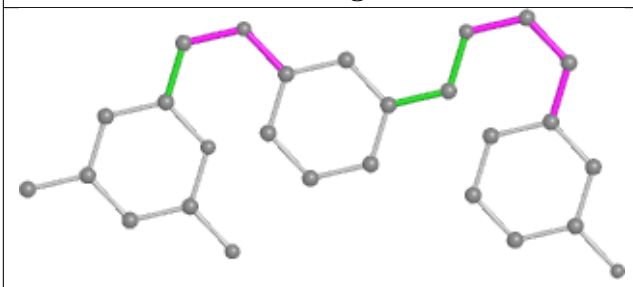
Ligand Q05 B 803



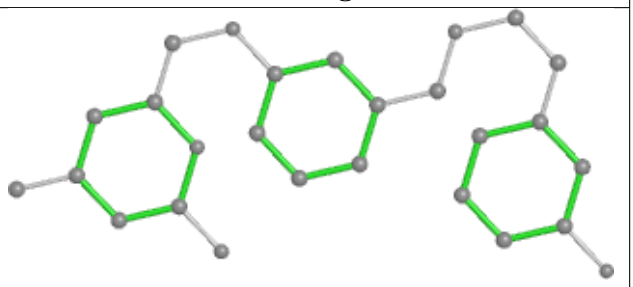
Bond lengths



Bond angles

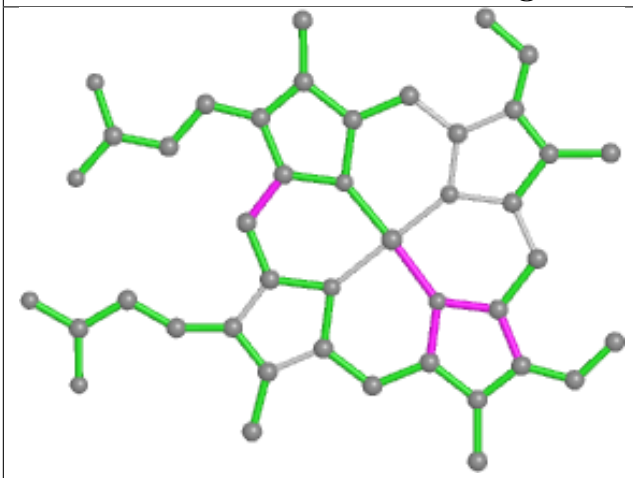


Torsions

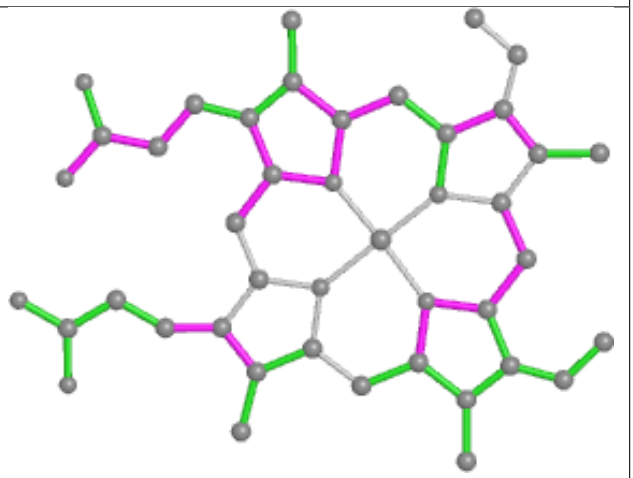


Rings

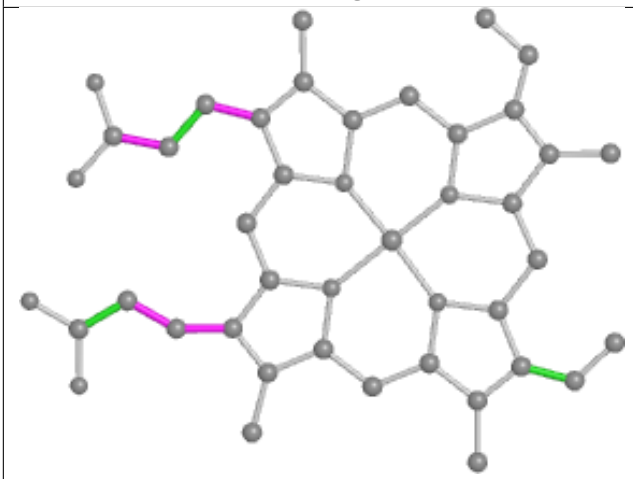
Ligand HEM A 801



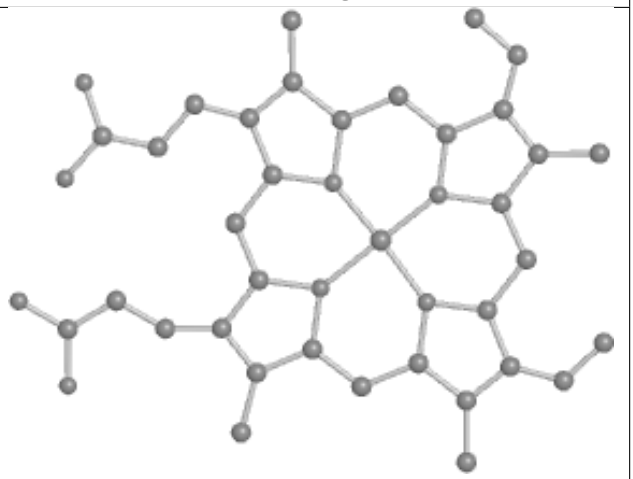
Bond lengths



Bond angles

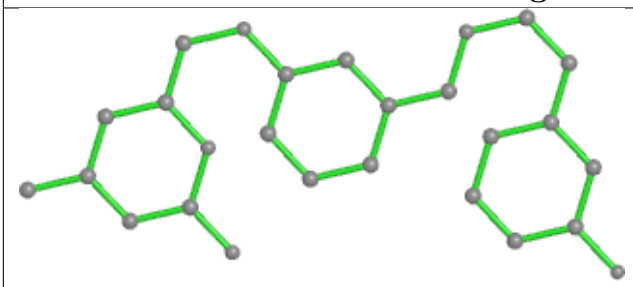


Torsions

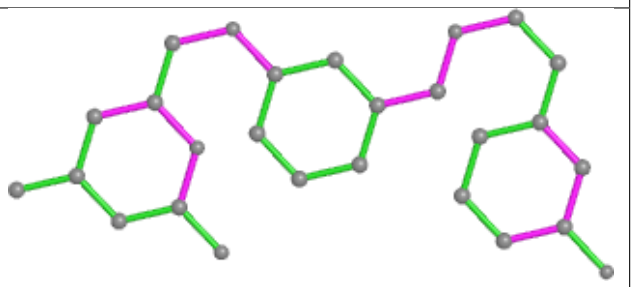


Rings

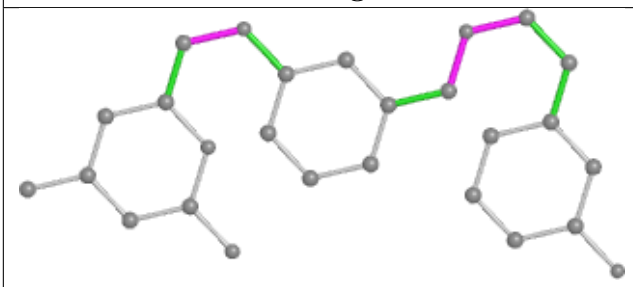
Ligand Q05 A 803



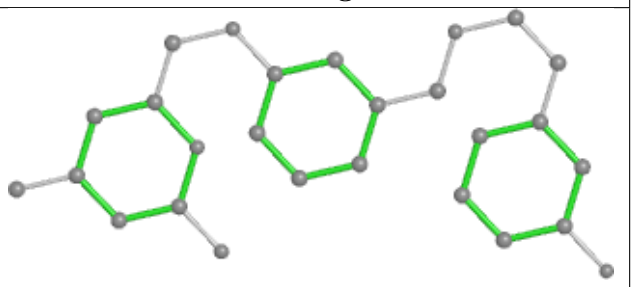
Bond lengths



Bond angles

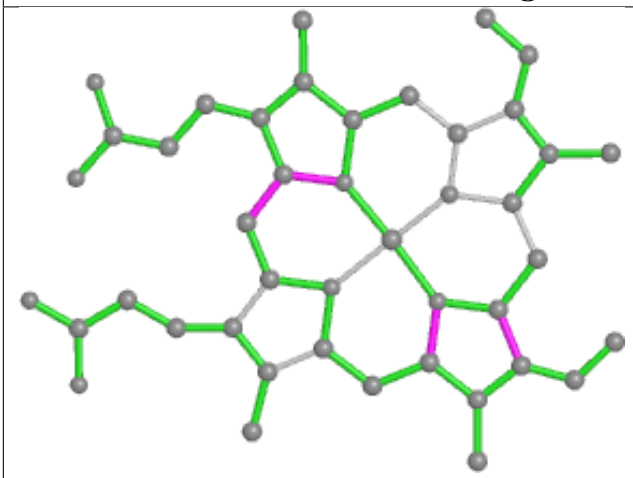


Torsions

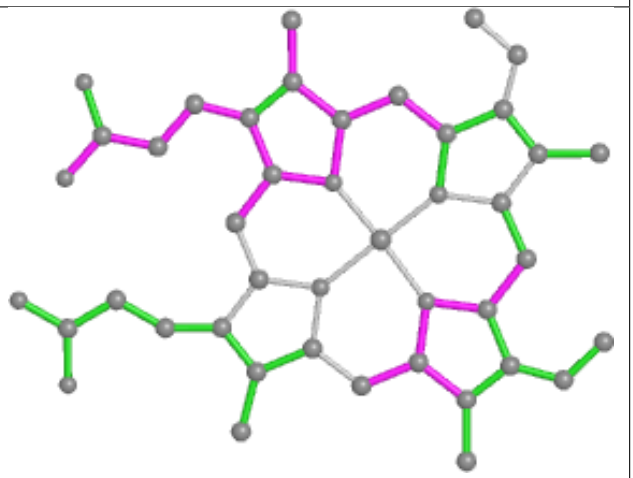


Rings

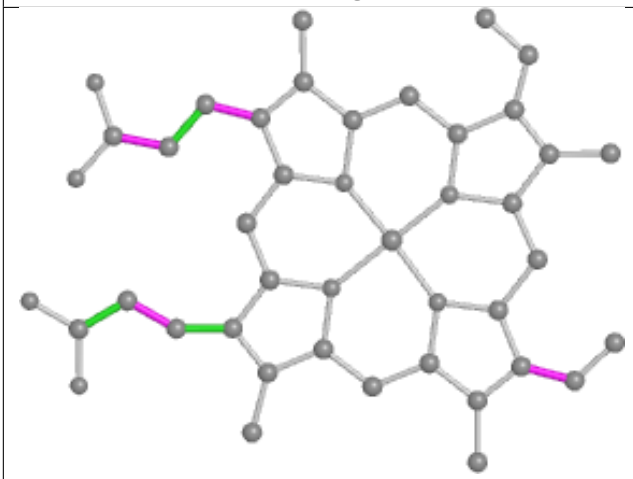
Ligand HEM B 801



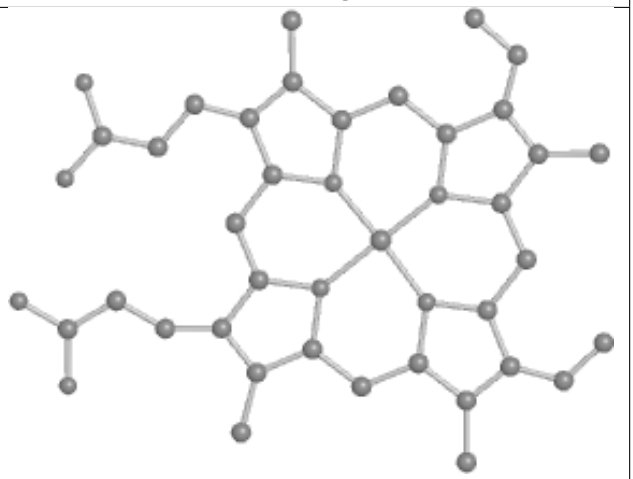
Bond lengths



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%)	0.82	56 (13%) 2 4	28, 52, 84, 117	0
1	B	411/422 (97%)	0.36	21 (5%) 28 33	25, 42, 70, 104	0
All	All	818/844 (96%)	0.59	77 (9%) 8 11	25, 46, 81, 117	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	9.3
1	A	716	TRP	7.6
1	A	488	PRO	6.9
1	B	350	THR	6.1
1	B	348	VAL	5.7
1	A	715	VAL	5.6
1	A	352	ASP	5.0
1	A	350	THR	4.9
1	B	352	ASP	4.8
1	B	351	LYS	4.8
1	A	351	LYS	4.7
1	A	355	PHE	4.1
1	B	718	GLY	4.1
1	A	486	LYS	4.0
1	A	386	LYS	4.0
1	A	567	VAL	3.8
1	A	493	LEU	3.6
1	A	714	HIS	3.6
1	B	353	GLN	3.5
1	A	713	THR	3.4
1	A	490	GLY	3.4
1	A	300	PHE	3.3
1	A	491	SER	3.3
1	A	299	ARG	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	390	SER	3.2
1	A	492	THR	3.1
1	A	667	ARG	3.1
1	B	619	ARG	3.1
1	A	508	GLN	3.0
1	A	480	ILE	3.0
1	A	385	ASN	2.9
1	B	301	LEU	2.9
1	A	503	GLU	2.9
1	B	321	THR	2.9
1	B	299	ARG	2.9
1	B	349	ARG	2.8
1	A	507	GLN	2.8
1	A	389	GLU	2.8
1	B	479	LEU	2.8
1	A	712	ASN	2.8
1	A	487	GLN	2.7
1	A	485	TYR	2.7
1	A	382	GLU	2.7
1	A	678	TRP	2.7
1	A	514	ARG	2.7
1	A	371	ARG	2.6
1	B	620	LYS	2.6
1	A	565	PRO	2.5
1	A	369	ILE	2.5
1	A	370	LYS	2.5
1	A	322	LEU	2.5
1	A	393	THR	2.4
1	A	415	CYS	2.4
1	A	366	TYR	2.4
1	A	679	ILE	2.4
1	A	489	ASP	2.4
1	A	328	GLU	2.4
1	B	389	GLU	2.4
1	A	612	LYS	2.4
1	A	681	PRO	2.3
1	A	588	TYR	2.3
1	A	423	LYS	2.3
1	A	584	PHE	2.3
1	A	591	THR	2.3
1	B	310	VAL	2.2
1	A	506	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	566	ALA	2.2
1	A	479	LEU	2.1
1	B	323	GLU	2.1
1	A	552	ASP	2.1
1	A	619	ARG	2.1
1	A	318	LEU	2.1
1	B	591	THR	2.1
1	B	302	LYS	2.0
1	B	565	PRO	2.0
1	B	566	ALA	2.0
1	A	469	LYS	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

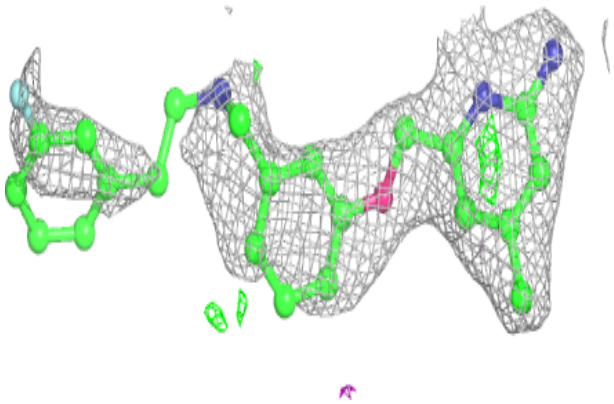
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	Q05	A	803	27/27	0.91	0.32	36,69,102,103	0
4	Q05	B	803	27/27	0.92	0.24	31,63,101,104	0
3	H4B	A	802	17/17	0.95	0.17	45,49,53,55	0
3	H4B	B	802	17/17	0.95	0.17	40,44,50,50	0
2	HEM	A	801	43/43	0.97	0.22	31,36,53,56	0
2	HEM	B	801	43/43	0.98	0.17	30,32,49,58	0
5	ACT	A	804	4/4	0.98	0.21	58,62,62,64	0
5	ACT	B	804	4/4	0.98	0.09	46,46,46,46	0
6	ZN	A	805	1/1	1.00	0.11	44,44,44,44	0

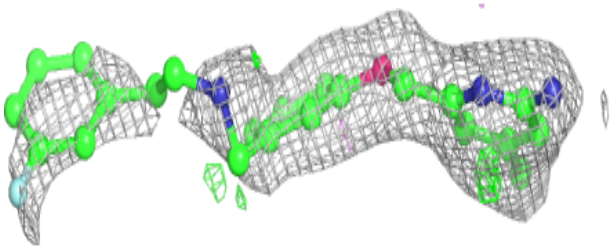
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

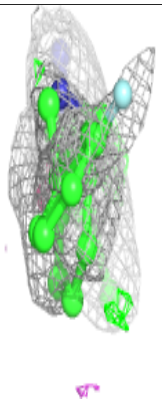
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Q05 A 803:

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

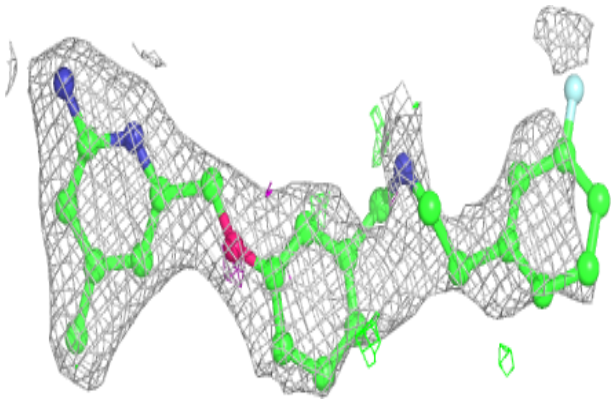


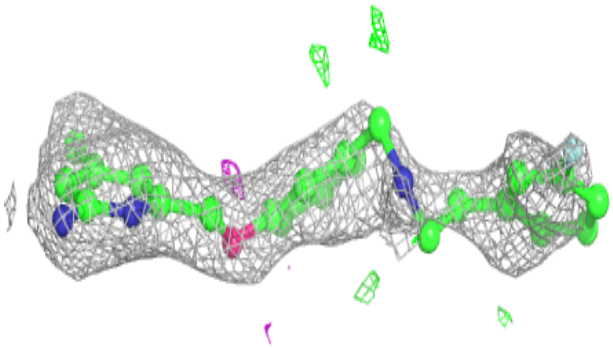


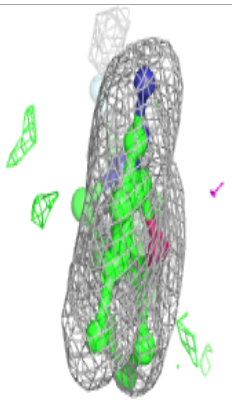


Electron density around Q05 B 803:

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

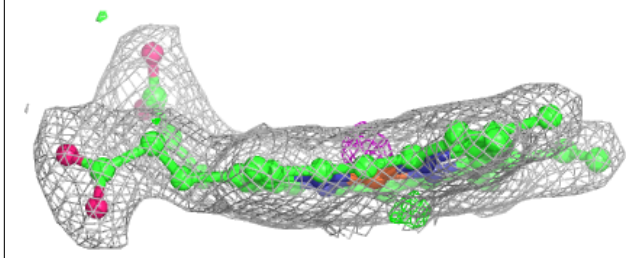


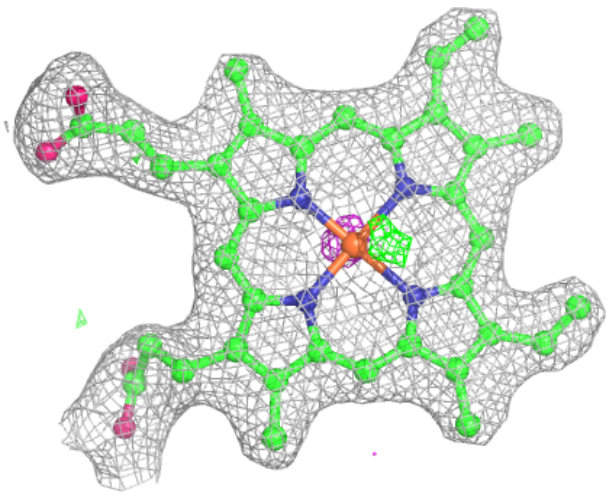


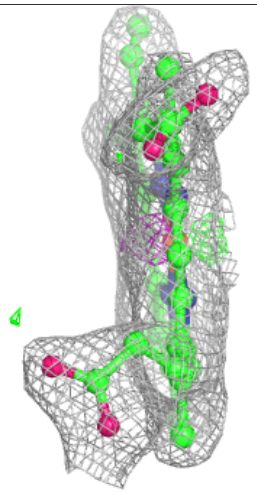


Electron density around HEM A 801:

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

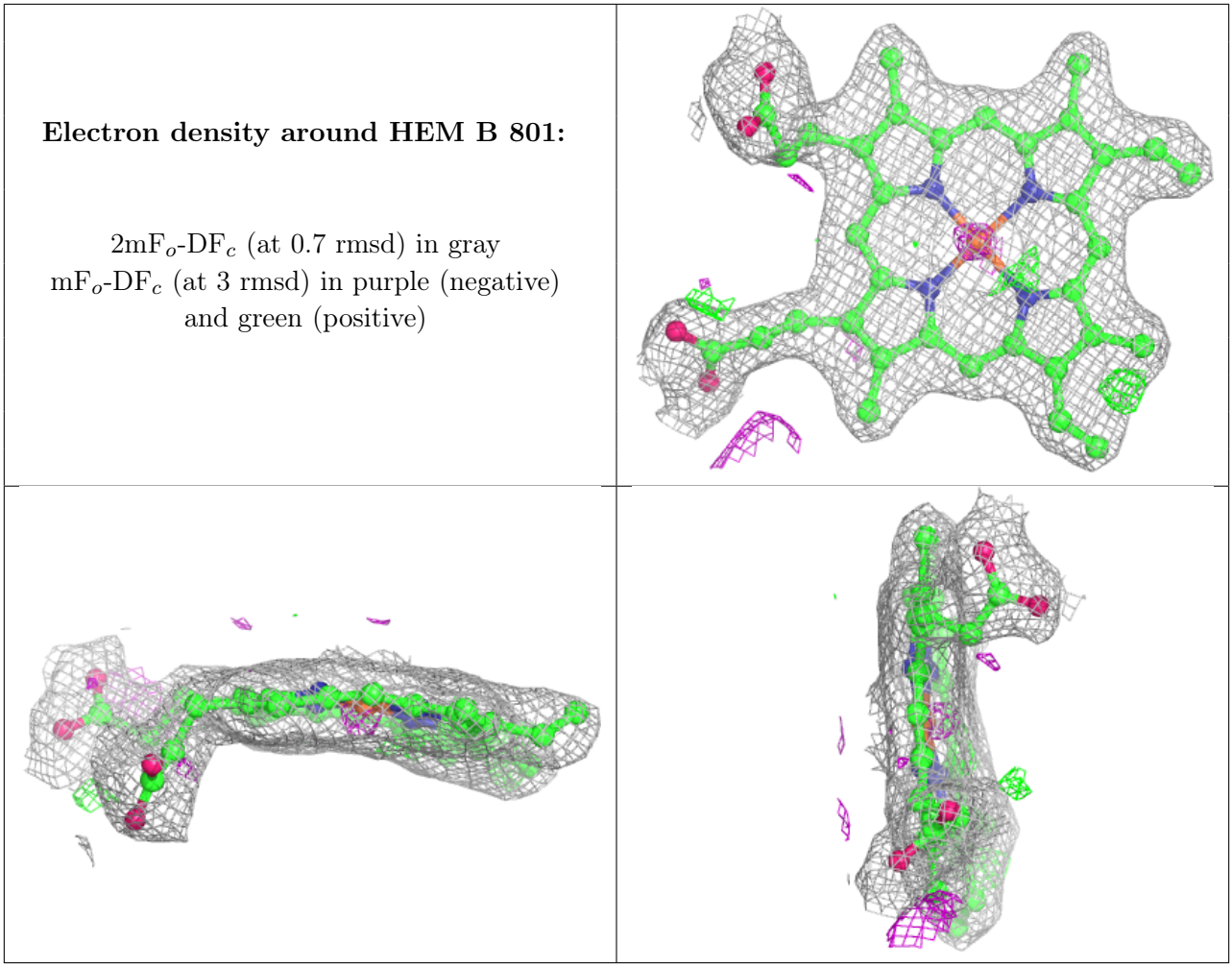






Electron density around HEM B 801:

$2mF_o$-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.