Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 02:08 AM EDT

PDB ID	:	6AUV
Title	:	Structure of rat neuronal nitric oxide synthase heme domain in complex with 4-Methyl-6-(2-(5-(3-((methylamino)methyl)phenyl)pyridin-3-yl)ethyl)pyridin -2-amine
Authors	:	Li, H.; Poulos, T.L.
Deposited on	:	2017-09-01
Resolution	:	1.76 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:

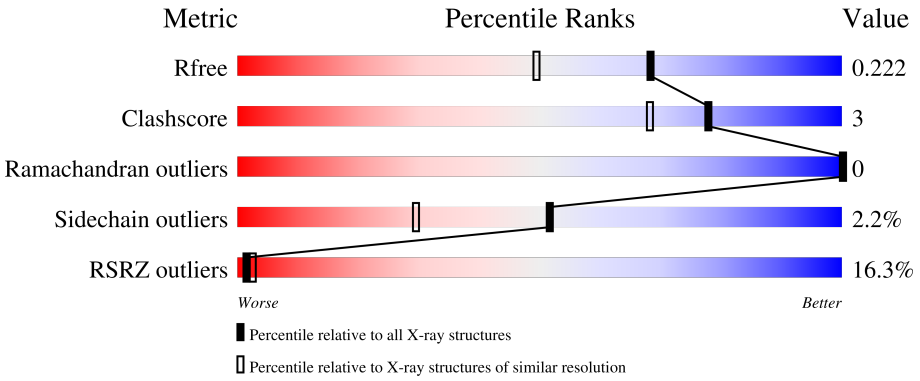
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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% 88% 9% .
1	B	422	9% 90% 8% .

2 Entry composition

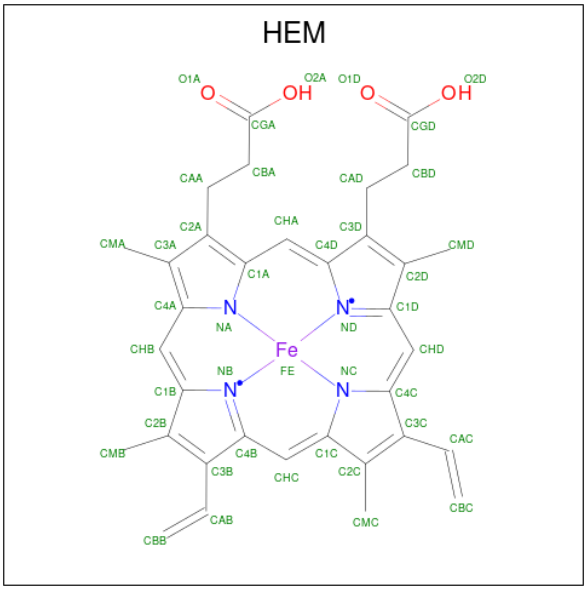
There are 7 unique types of molecules in this entry. The entry contains 7472 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

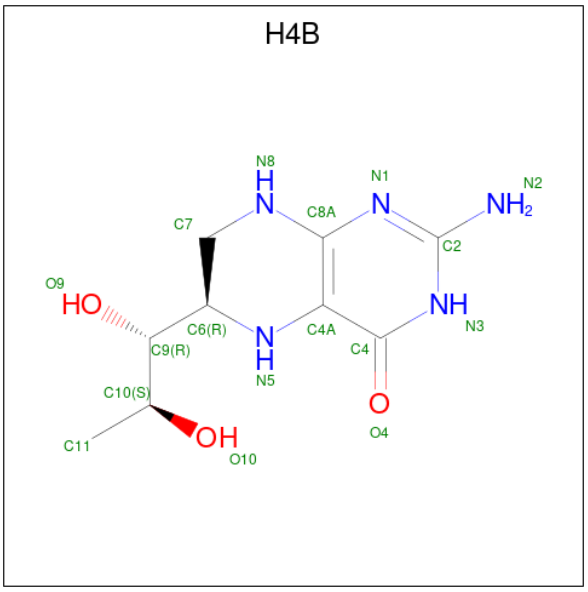
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	4	0
			3361	2149	574	616	22			
1	B	413	Total	C	N	O	S	0	5	0
			3381	2166	576	616	23			

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



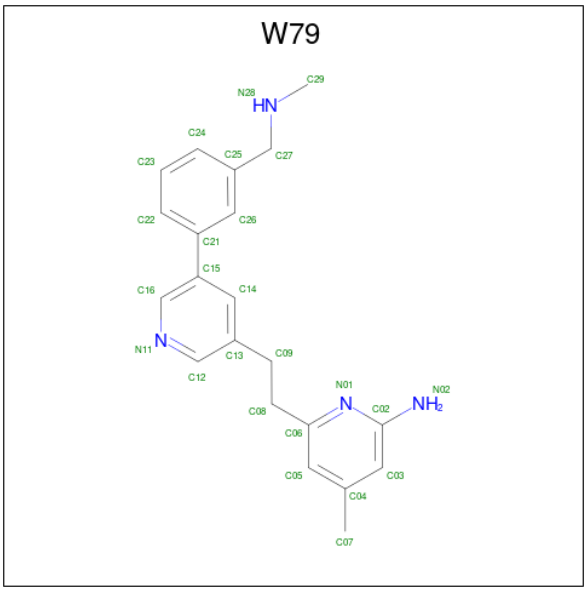
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 4-methyl-6-[2-(5-{3-[(methylamino)methyl]phenyl}pyridin-3-yl)ethyl]pyridin-2-amine (three-letter code: W79) (formula: $C_{21}H_{24}N_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N 25 21 4	0	0

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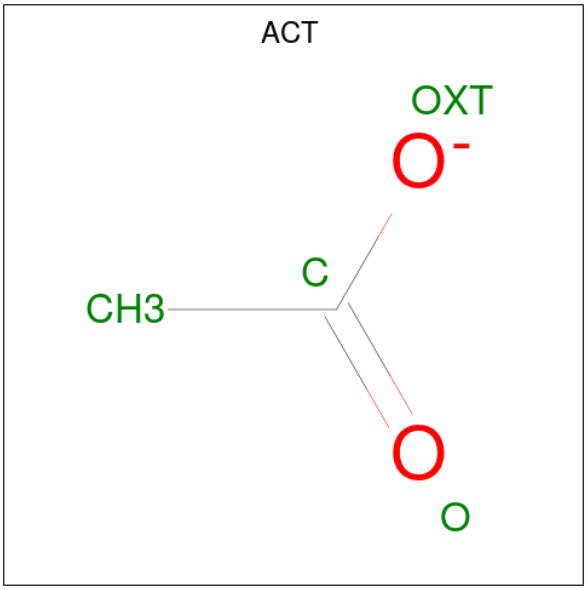
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N 25 21 4	0	0

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



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

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

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

- Molecule 7 is water.

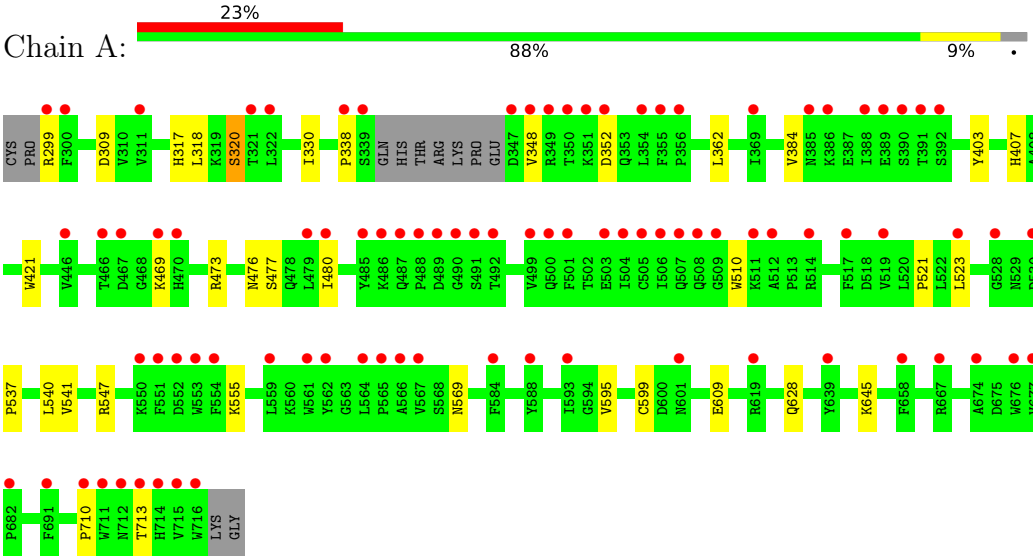
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	239	Total O 239 239	0	0
7	B	312	Total O 312 312	0	0

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.

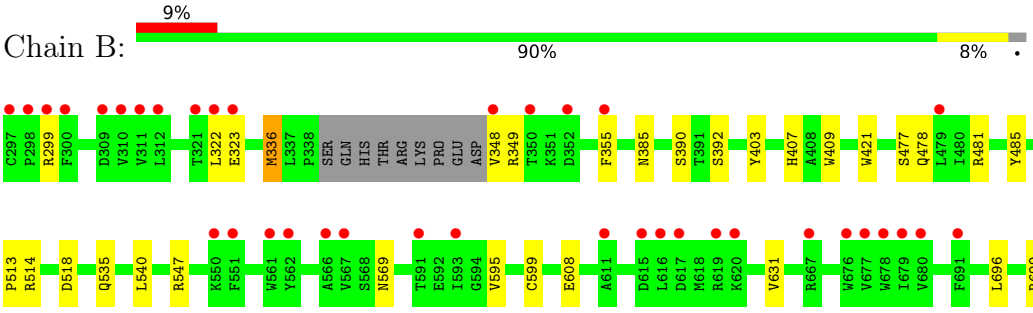
• Molecule 1: Nitric oxide synthase, brain

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	52.12Å 111.18Å 164.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.00 – 1.76 39.00 – 1.76	Depositor EDS
% Data completeness (in resolution range)	96.7 (39.00-1.76) 97.5 (39.00-1.76)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.184 , 0.222 0.185 , 0.222	Depositor DCC
R_{free} test set	4642 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.6	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	0.94	EDS
Total number of atoms	7472	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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: H4B, ZN, HEM, ACT, W79

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	0.34	0/3460	0.49	0/4695
1	B	0.39	0/3491	0.51	0/4734
All	All	0.37	0/6951	0.50	0/9429

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3361	0	3270	18	0
1	B	3381	0	3301	17	0
2	A	43	0	30	2	0
2	B	43	0	30	2	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	25	0	0	1	0
4	B	25	0	0	1	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	239	0	0	4	0
7	B	312	0	0	3	0
All	All	7472	0	6667	39	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 3.

All (39) 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:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.72	0.71
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.72	0.70
2:B:801:HEM:HMC2	2:B:801:HEM:HBC2	1.74	0.70
4:A:803:W79:N28	7:A:902:HOH:O	2.25	0.69
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.75	0.68
1:B:478:GLN:OE1	1:B:481:ARG:HD2	1.95	0.67
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.78	0.66
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.81	0.63
1:A:628:GLN:HG3	1:B:631:VAL:HG11	1.82	0.61
1:A:477:SER:HA	1:A:569:ASN:HB3	1.88	0.55
1:A:535:GLN:NE2	7:A:903:HOH:O	2.40	0.54
1:B:403:TYR:CE1	1:B:407:HIS:CE1	2.99	0.50
1:B:355[A]:PHE:CE1	1:B:385:ASN:HB2	2.47	0.49
1:B:595:VAL:O	1:B:599:CYS:HB2	2.12	0.49
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.94	0.49
1:A:330:ILE:HD11	1:B:696:LEU:HB3	1.95	0.48
4:B:803:W79:N28	7:B:901:HOH:O	2.35	0.48
1:B:608:GLU:HB2	7:B:1077:HOH:O	2.14	0.48
1:B:477:SER:HA	1:B:569:ASN:HB3	1.96	0.47
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.97	0.47
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.36	0.47
1:B:348:VAL:HG22	1:B:349:ARG:H	1.79	0.46
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.30	0.46
1:B:336:MET:HB2	1:B:336:MET:HE2	1.78	0.45
1:B:322:LEU:HB2	1:B:699:ARG:HD3	1.99	0.45
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.05	0.44
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.52	0.44
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.53	0.44
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.52	0.43
1:A:609:GLU:HG3	7:A:947:HOH:O	2.19	0.42
1:A:299:ARG:HE	1:A:318:LEU:HD13	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.55	0.42
1:B:323:GLU:O	1:B:699:ARG:HD2	2.20	0.41
1:A:362:LEU:HD11	1:A:384:VAL:HG21	2.02	0.41
1:A:595:VAL:O	1:A:599:CYS:HB2	2.21	0.41
1:A:317:HIS:O	1:A:320:SER:HB3	2.21	0.41
1:A:338:PRO:O	7:A:901:HOH:O	2.22	0.41
1:B:492:THR:HG21	1:B:496:PRO:HA	2.02	0.41
1:B:535:GLN:HG3	7:B:1128:HOH:O	2.20	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	410/422 (97%)	400 (98%)	10 (2%)	0	100	100
1	B	414/422 (98%)	409 (99%)	5 (1%)	0	100	100
All	All	824/844 (98%)	809 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/377 (98%)	360 (97%)	10 (3%)	44	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	373/377 (99%)	367 (98%)	6 (2%)	62 45
All	All	743/754 (98%)	727 (98%)	16 (2%)	52 29

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	ASP
1	A	320	SER
1	A	348	VAL
1	A	352	ASP
1	A	469	LYS
1	A	476	ASN
1	A	547	ARG
1	A	555	LYS
1	A	645	LYS
1	A	713	THR
1	B	299	ARG
1	B	336	MET
1	B	390	SER
1	B	392	SER
1	B	540	LEU
1	B	547	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	425	GLN

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	$\#\|Z\| > 2$
2	HEM	B	801	1	41,50,50	1.89	8 (19%)	45,82,82	1.73	6 (13%)
4	W79	A	803	-	27,27,27	0.36	0	35,36,36	1.96	11 (31%)
5	ACT	A	804	-	3,3,3	0.78	0	3,3,3	0.67	0
5	ACT	B	804	-	3,3,3	0.80	0	3,3,3	0.65	0
3	H4B	B	802	-	16,18,18	0.97	0	11,26,26	2.53	4 (36%)
4	W79	B	803	-	27,27,27	0.41	0	35,36,36	1.90	10 (28%)
3	H4B	A	802	-	16,18,18	0.76	0	11,26,26	2.64	5 (45%)
2	HEM	A	801	1	41,50,50	1.90	8 (19%)	45,82,82	1.85	7 (15%)

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	B	801	1	-	1/12/54/54	-
4	W79	A	803	-	-	2/11/12/12	0/3/3/3
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
4	W79	B	803	-	-	2/11/12/12	0/3/3/3
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
2	HEM	A	801	1	-	1/12/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3D-C2D	7.52	1.52	1.36
2	B	801	HEM	C3D-C2D	7.45	1.52	1.36
2	B	801	HEM	C3C-CAC	3.64	1.55	1.47
2	B	801	HEM	C3C-C2C	-3.57	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3C-C2C	-3.54	1.35	1.40
2	A	801	HEM	C3C-CAC	3.38	1.54	1.47
2	A	801	HEM	FE-NB	3.07	2.12	1.96
2	A	801	HEM	CAB-C3B	2.99	1.55	1.47
2	B	801	HEM	CAB-C3B	2.89	1.55	1.47
2	B	801	HEM	FE-NB	2.51	2.09	1.96
2	B	801	HEM	FE-ND	2.28	2.08	1.96
2	A	801	HEM	CMD-C2D	2.15	1.55	1.50
2	A	801	HEM	CMB-C2B	2.14	1.55	1.50
2	B	801	HEM	CMD-C2D	2.07	1.55	1.50
2	B	801	HEM	CMB-C2B	2.01	1.55	1.50
2	A	801	HEM	FE-ND	2.01	2.06	1.96

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	HEM	C4D-ND-C1D	5.90	111.16	105.07
2	A	801	HEM	C4D-ND-C1D	5.50	110.76	105.07
3	A	802	H4B	C8A-C4A-C4	5.45	119.41	114.57
3	B	802	H4B	C8A-C4A-C4	5.27	119.25	114.57
4	A	803	W79	C02-N01-C06	5.24	122.07	118.10
4	B	803	W79	C02-N01-C06	4.97	121.87	118.10
4	A	803	W79	C09-C08-C06	-4.84	102.13	112.99
2	A	801	HEM	CBA-CAA-C2A	-4.75	104.52	112.62
4	B	803	W79	C09-C08-C06	-4.71	102.42	112.99
2	B	801	HEM	CBA-CAA-C2A	-4.13	105.58	112.62
2	A	801	HEM	C4B-CHC-C1C	3.97	127.79	122.56
2	A	801	HEM	CBD-CAD-C3D	-3.81	102.03	112.63
4	A	803	W79	C05-C06-N01	-3.39	119.31	122.90
3	B	802	H4B	N1-C2-N3	-3.38	120.12	125.42
4	B	803	W79	C05-C06-N01	-3.36	119.34	122.90
2	B	801	HEM	CBD-CAD-C3D	-3.35	103.31	112.63
2	B	801	HEM	C4B-CHC-C1C	3.22	126.81	122.56
4	B	803	W79	C08-C06-N01	3.16	120.65	115.95
3	A	802	H4B	N1-C2-N3	-3.15	120.47	125.42
4	A	803	W79	C09-C13-C12	-3.09	116.85	121.83
4	B	803	W79	C14-C15-C16	3.06	120.15	117.11
3	B	802	H4B	C2-N1-C8A	2.98	121.21	114.54
3	A	802	H4B	C2-N3-C4	2.98	120.66	115.93
3	A	802	H4B	C2-N1-C8A	2.96	121.17	114.54
4	A	803	W79	C14-C15-C16	2.90	119.98	117.11
3	B	802	H4B	C2-N3-C4	2.89	120.52	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	HEM	CMD-C2D-C1D	2.83	129.35	125.04
2	A	801	HEM	CMC-C2C-C3C	2.80	129.91	124.68
3	A	802	H4B	C4-C4A-N5	2.77	121.45	119.12
4	A	803	W79	C08-C06-N01	2.64	119.88	115.95
4	A	803	W79	C14-C13-C12	2.59	119.22	116.71
4	B	803	W79	C14-C13-C12	2.57	119.19	116.71
2	B	801	HEM	CMC-C2C-C3C	2.55	129.45	124.68
4	A	803	W79	C16-N11-C12	2.43	120.80	117.48
4	B	803	W79	C09-C13-C12	-2.41	117.95	121.83
4	A	803	W79	C15-C14-C13	-2.39	117.93	121.19
4	B	803	W79	C15-C14-C13	-2.32	118.02	121.19
2	B	801	HEM	C4C-CHD-C1D	2.25	125.53	122.56
4	B	803	W79	C25-C27-N28	-2.16	107.33	112.67
4	A	803	W79	C25-C27-N28	-2.10	107.48	112.67
4	A	803	W79	C09-C13-C14	2.07	123.94	120.54
2	A	801	HEM	CHC-C4B-C3B	2.05	127.71	124.57
4	B	803	W79	C16-N11-C12	2.02	120.24	117.48

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C4B-C3B-CAB-CBB
2	B	801	HEM	C4B-C3B-CAB-CBB
4	A	803	W79	C08-C09-C13-C12
4	B	803	W79	C08-C09-C13-C12
4	A	803	W79	C08-C09-C13-C14
4	B	803	W79	C08-C09-C13-C14

There are no ring outliers.

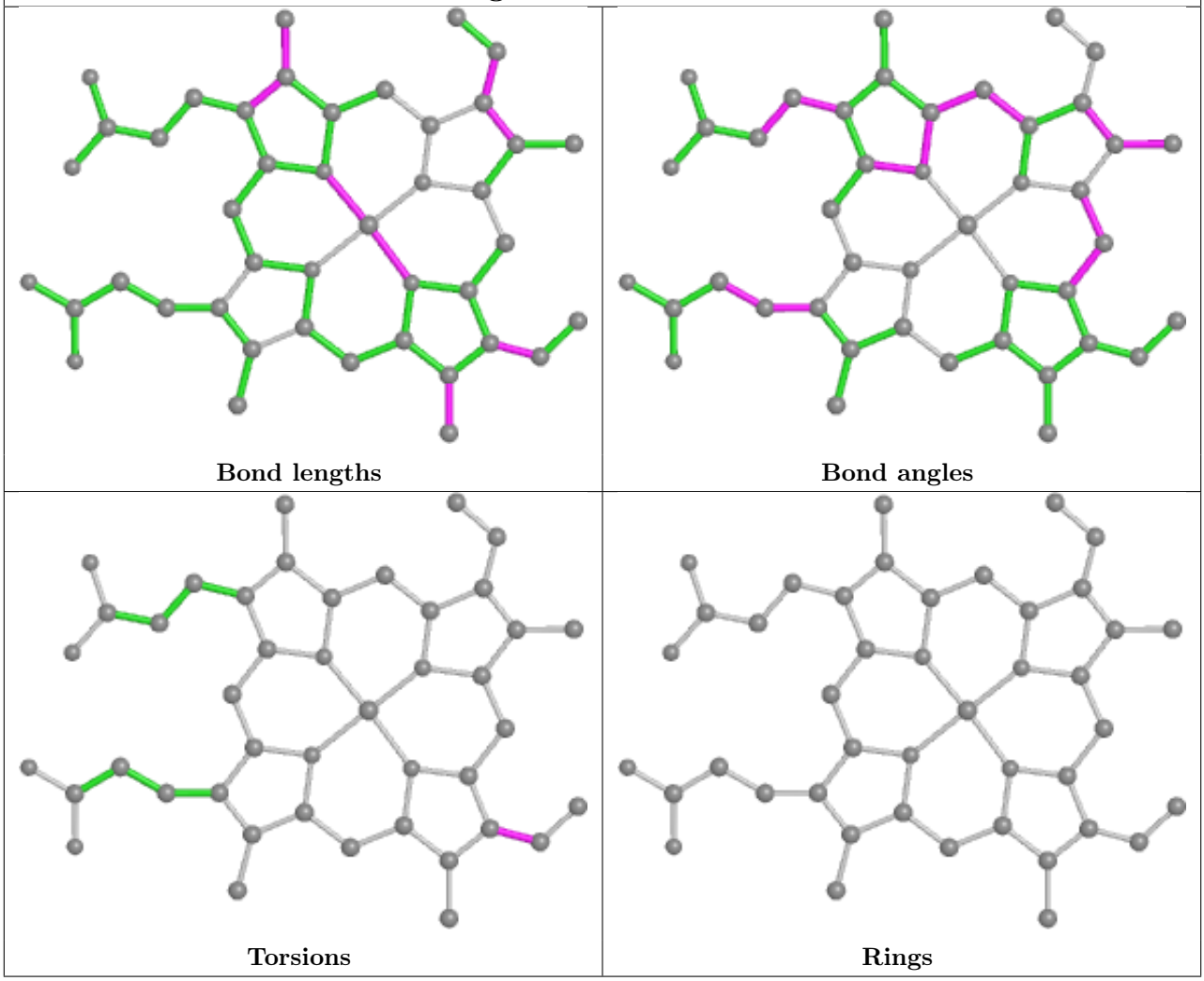
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HEM	2	0
4	A	803	W79	1	0
4	B	803	W79	1	0
2	A	801	HEM	2	0

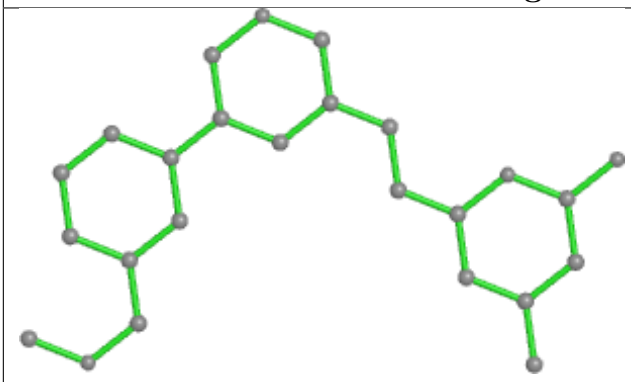
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

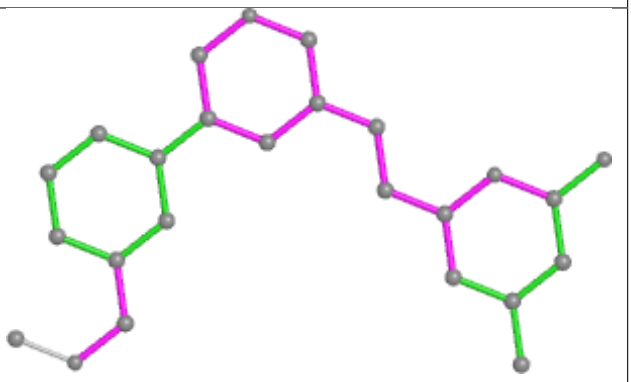
Ligand HEM B 801



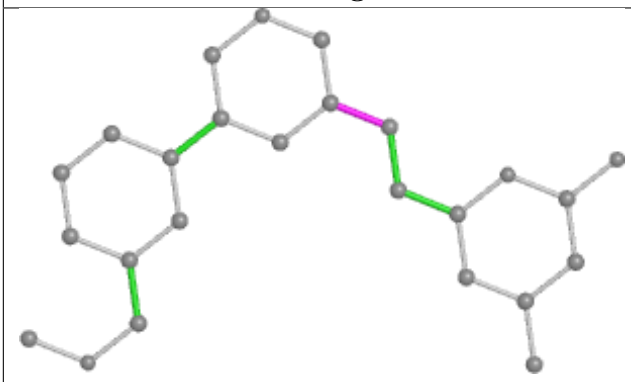
Ligand W79 A 803



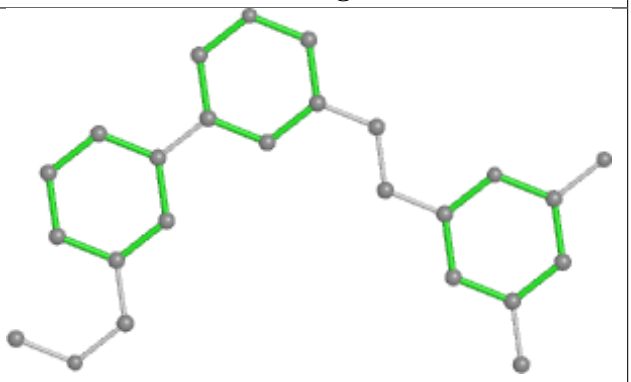
Bond lengths



Bond angles

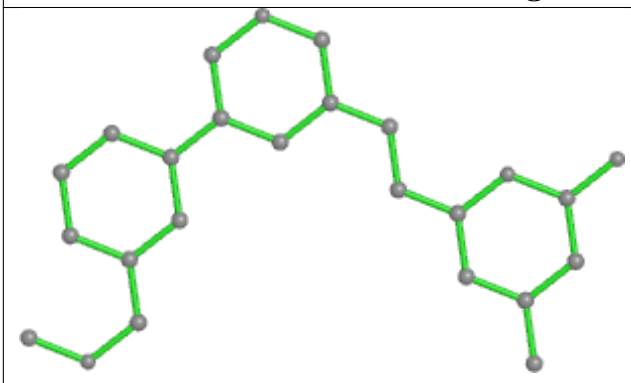


Torsions

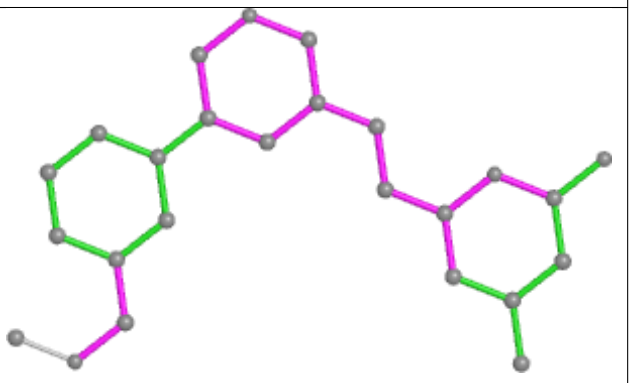


Rings

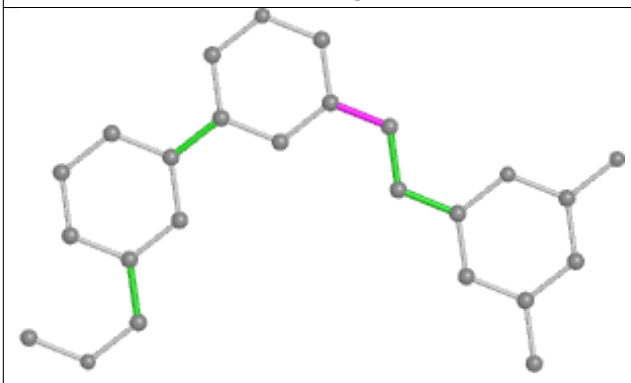
Ligand W79 B 803



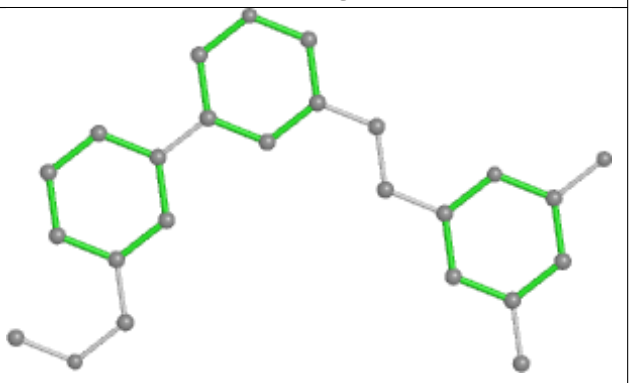
Bond lengths



Bond angles

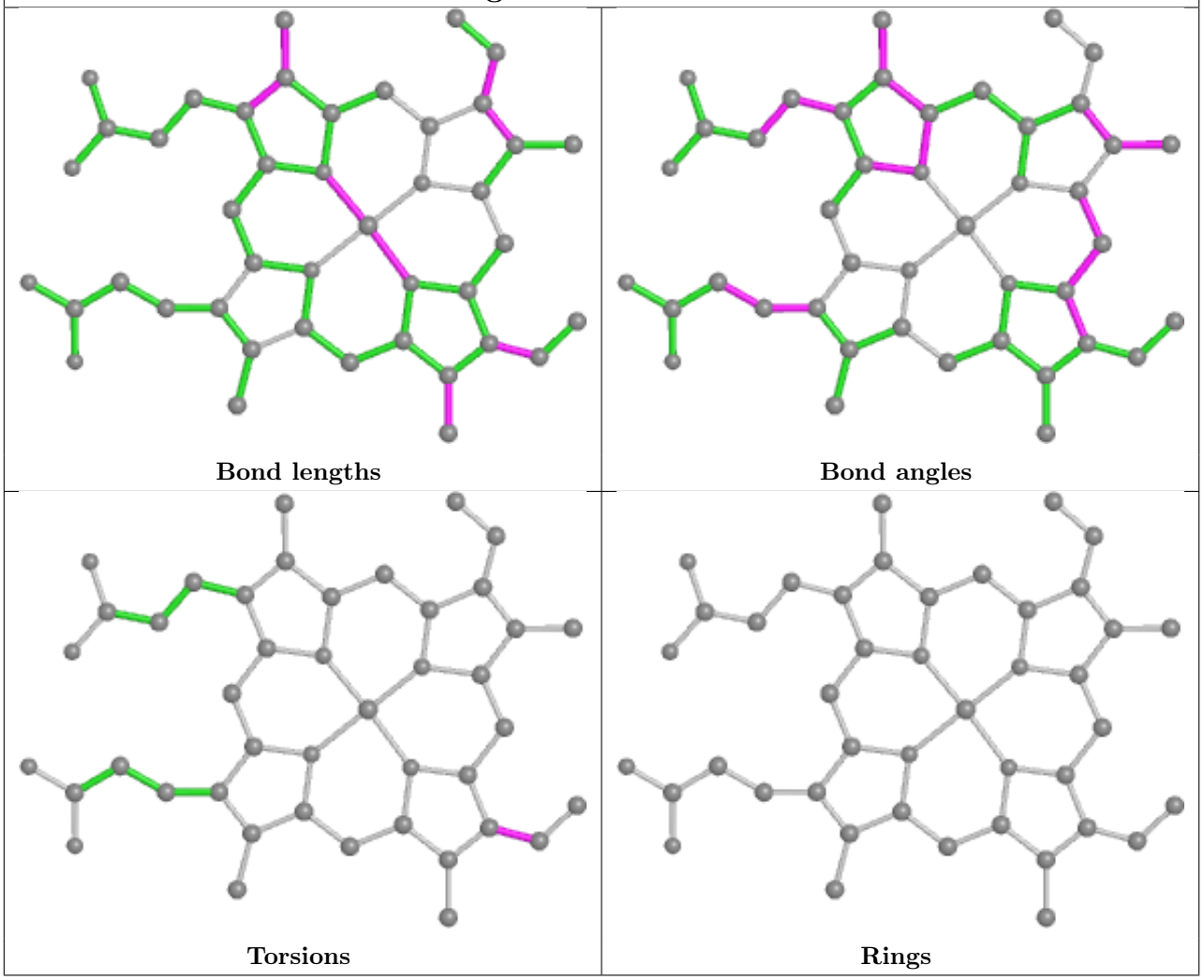


Torsions



Rings

Ligand HEM A 801



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	411/422 (97%)	1.36	95 (23%) 0 0	26, 48, 88, 126	0
1	B	413/422 (97%)	0.78	39 (9%) 8 11	24, 37, 67, 107	0
All	All	824/844 (97%)	1.07	134 (16%) 1 2	24, 42, 82, 126	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	VAL	10.8
1	A	715	VAL	9.5
1	B	297	CYS	9.3
1	A	347	ASP	8.2
1	B	300	PHE	7.6
1	A	488	PRO	6.7
1	B	299	ARG	6.6
1	A	300	PHE	6.5
1	A	355	PHE	6.4
1	B	348	VAL	6.1
1	A	716	TRP	5.8
1	A	619	ARG	5.4
1	B	298	PRO	5.0
1	A	351	LYS	5.0
1	A	339	SER	5.0
1	A	388	ILE	4.9
1	A	392	SER	4.8
1	B	616	LEU	4.8
1	B	310	VAL	4.7
1	A	349	ARG	4.7
1	B	322	LEU	4.6
1	A	504	ILE	4.4
1	A	678	TRP	4.4
1	A	713	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	619	ARG	4.2
1	B	678	TRP	4.1
1	A	490	GLY	4.0
1	B	355[A]	PHE	3.9
1	A	486	LYS	3.9
1	B	677	VAL	3.9
1	A	712	ASN	3.9
1	A	391	THR	3.9
1	A	352	ASP	3.8
1	A	677	VAL	3.8
1	A	679	ILE	3.8
1	A	551	PHE	3.7
1	A	505	CYS	3.7
1	A	489	ASP	3.7
1	A	491	SER	3.6
1	B	718	GLY	3.6
1	A	511	LYS	3.6
1	A	369	ILE	3.6
1	A	503	GLU	3.6
1	A	528	GLY	3.5
1	A	711	TRP	3.4
1	A	389	GLU	3.4
1	A	680	VAL	3.4
1	A	487	GLN	3.4
1	A	480	ILE	3.4
1	A	507	GLN	3.4
1	A	350	THR	3.4
1	A	479	LEU	3.3
1	A	492	THR	3.2
1	A	322	LEU	3.2
1	B	680	VAL	3.2
1	B	611	ALA	3.2
1	A	710	PRO	3.2
1	A	567	VAL	3.2
1	B	321	THR	3.2
1	A	390	SER	3.1
1	A	553	TRP	3.1
1	A	311	VAL	3.1
1	A	321	THR	3.1
1	A	561	TRP	3.1
1	B	620	LYS	3.0
1	A	506	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	676	TRP	3.0
1	B	617	ASP	2.9
1	A	550	LYS	2.9
1	A	299	ARG	2.9
1	B	667	ARG	2.9
1	B	679	ILE	2.9
1	A	681	PRO	2.8
1	A	470	HIS	2.8
1	B	615	ASP	2.8
1	A	415	CYS	2.8
1	A	639	TYR	2.8
1	A	467	ASP	2.8
1	A	446	VAL	2.7
1	B	551	PHE	2.7
1	B	350	THR	2.7
1	A	500	GLN	2.7
1	A	584	PHE	2.7
1	A	559	LEU	2.7
1	A	676	TRP	2.7
1	B	309	ASP	2.6
1	B	715	VAL	2.6
1	A	508	GLN	2.6
1	A	499	VAL	2.6
1	A	519	VAL	2.6
1	B	567	VAL	2.6
1	A	714	HIS	2.6
1	B	562	TYR	2.5
1	A	588	TYR	2.5
1	A	552	ASP	2.5
1	A	517	PHE	2.5
1	A	485	TYR	2.5
1	A	562	TYR	2.5
1	B	691	PHE	2.5
1	A	564	LEU	2.4
1	B	593	ILE	2.4
1	A	530	ASP	2.4
1	A	682	PRO	2.3
1	A	385	ASN	2.3
1	A	501	PHE	2.3
1	A	658	PHE	2.3
1	A	469	LYS	2.3
1	A	338	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	593	ILE	2.3
1	A	691	PHE	2.3
1	B	311	VAL	2.2
1	A	523	LEU	2.2
1	A	386	LYS	2.2
1	A	466	THR	2.2
1	A	667	ARG	2.2
1	B	561	TRP	2.2
1	A	554	PHE	2.2
1	A	566	ALA	2.2
1	A	601	ASN	2.2
1	B	312	LEU	2.2
1	B	550	LYS	2.2
1	A	674	ALA	2.2
1	A	354	LEU	2.2
1	A	356	PRO	2.2
1	B	323	GLU	2.2
1	A	512	ALA	2.2
1	A	416	VAL	2.1
1	B	352	ASP	2.1
1	A	514	ARG	2.1
1	A	509	GLY	2.1
1	A	565	PRO	2.0
1	B	566	ALA	2.0
1	B	479	LEU	2.0
1	B	591	THR	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)

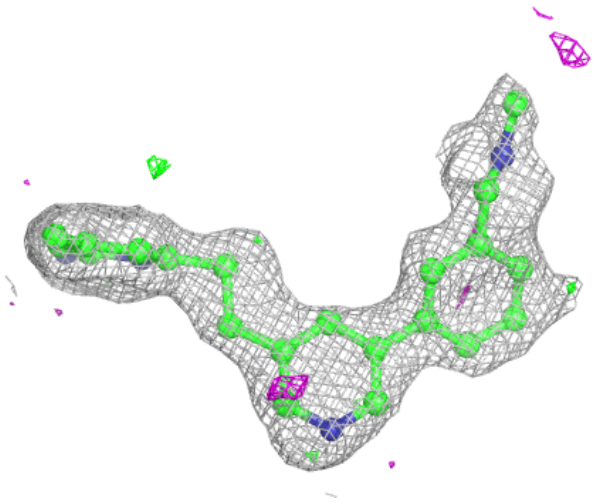
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

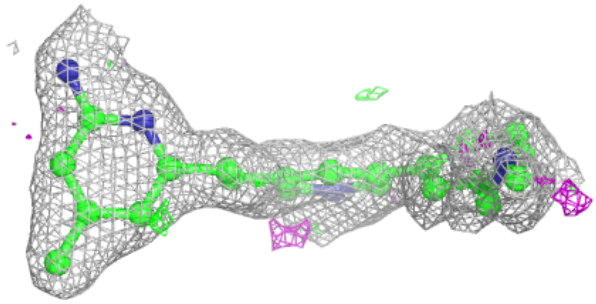
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	W79	B	803	25/25	0.86	0.21	26,50,65,66	0
4	W79	A	803	25/25	0.88	0.25	28,49,61,66	0
3	H4B	A	802	17/17	0.89	0.17	27,30,37,37	0
5	ACT	B	804	4/4	0.89	0.17	52,52,57,59	0
5	ACT	A	804	4/4	0.90	0.29	66,67,70,74	0
3	H4B	B	802	17/17	0.92	0.16	25,30,34,38	0
2	HEM	A	801	43/43	0.95	0.19	22,32,42,50	0
2	HEM	B	801	43/43	0.96	0.15	21,33,42,49	0
6	ZN	A	805	1/1	1.00	0.04	32,32,32,32	0

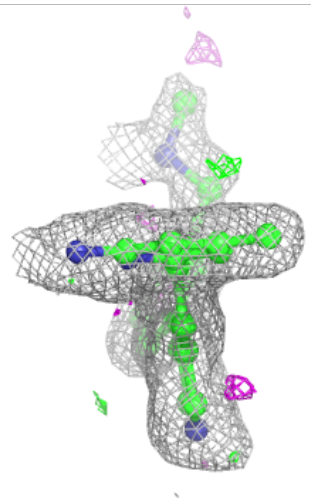
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around W79 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)

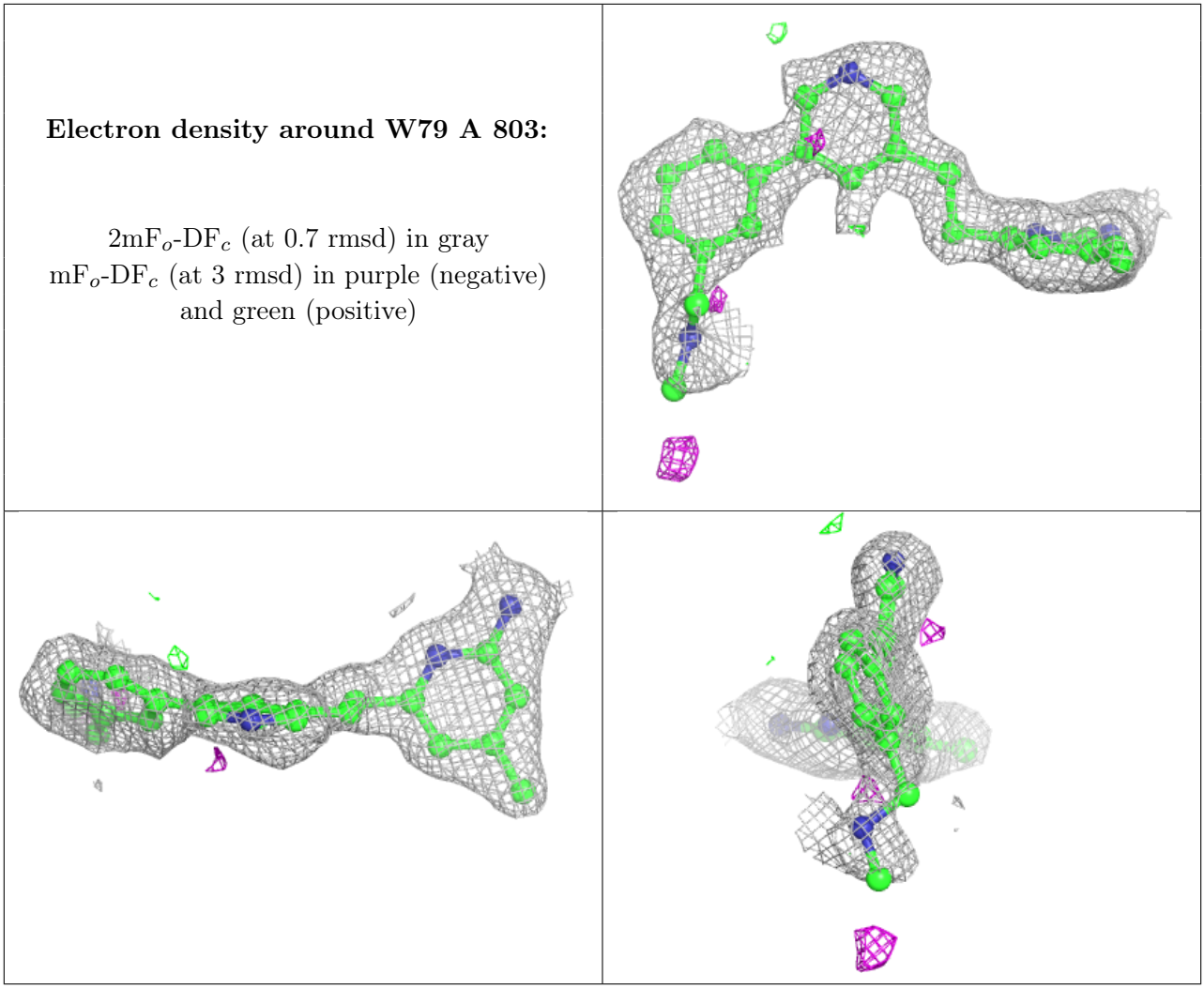






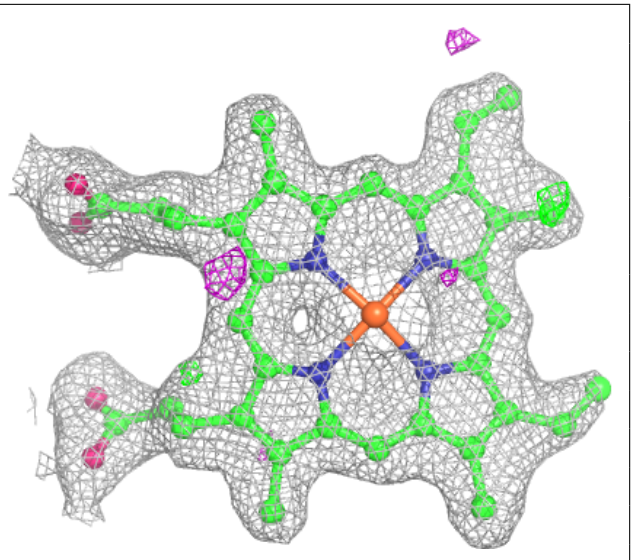
Electron density around W79 A 803:

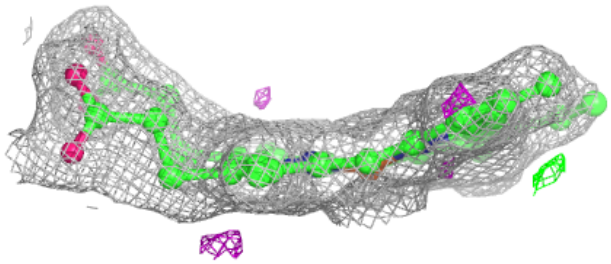
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

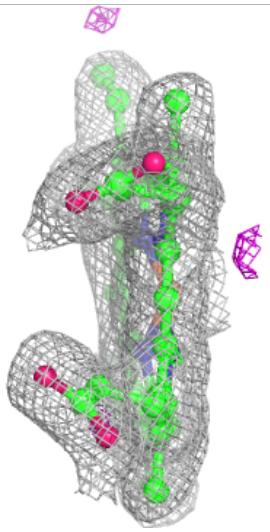


Electron density around HEM A 801:

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

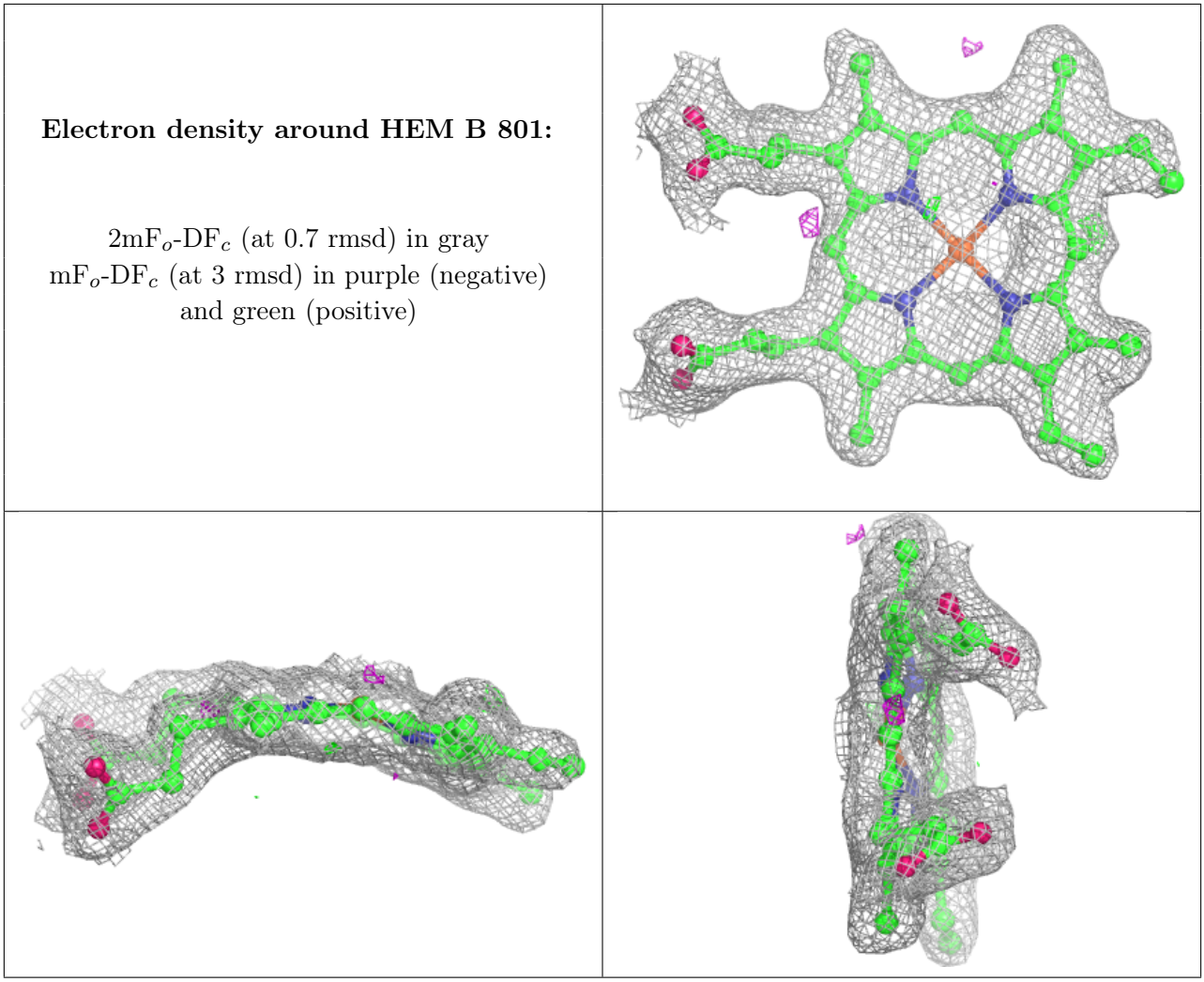






Electron density around HEM B 801:

$2mF_o$-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

There are no such residues in this entry.