



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:50 am BST

PDB ID : 6AV3
Title : Structure of human neuronal nitric oxide synthase R354A/G357D mutant 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 : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

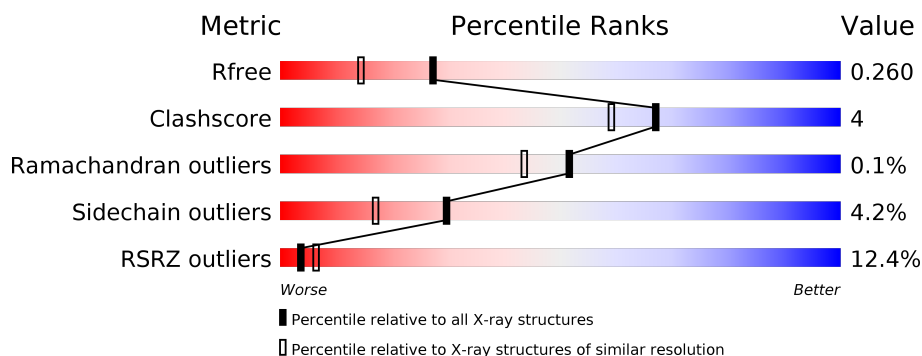
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	421	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	B	421	<div> <div>18%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7212 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	413	Total	C	N	O	S	0	2	0
			3371	2159	574	616	22			
1	B	408	Total	C	N	O	S	0	2	0
			3333	2136	568	608	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	engineered mutation	UNP P29475
A	357	ASP	GLY	engineered mutation	UNP P29475
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475

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



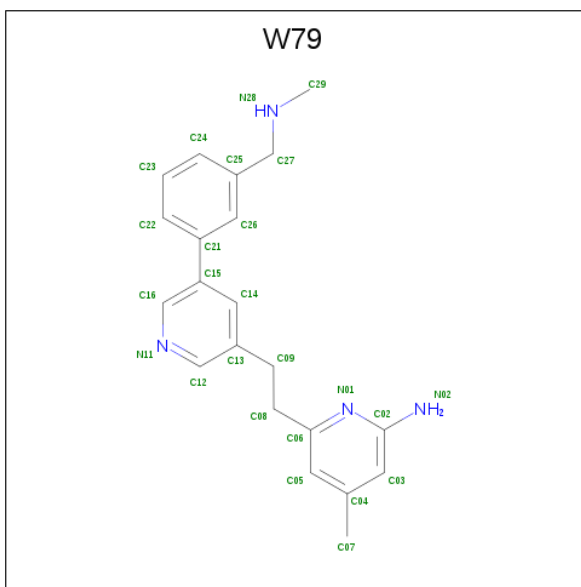
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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

- 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	0	0
			25	21	4		
4	B	1	Total	C	N	0	0
			25	21	4		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

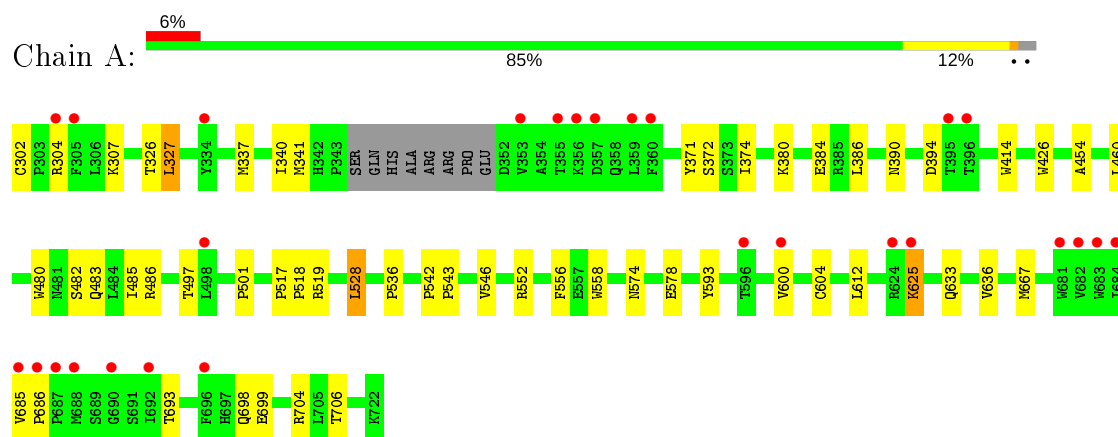
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	195	Total	O	0	0
			195	195		
6	B	142	Total	O	0	0
			142	142		

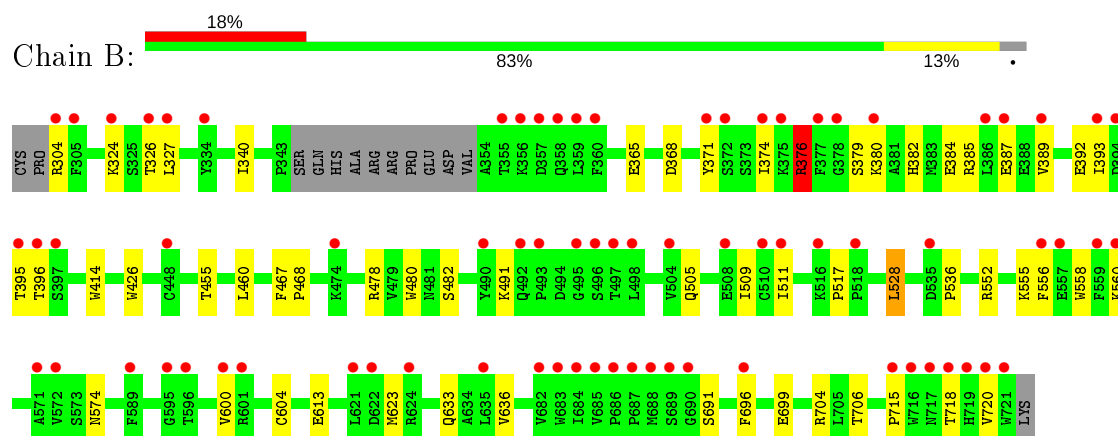
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitric oxide synthase, brain



- Molecule 1: Nitric oxide synthase, brain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.49Å 122.25Å 163.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.87 – 1.95 38.87 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.1 (38.87-1.95) 95.8 (38.87-1.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.203 , 0.259 0.205 , 0.260	Depositor DCC
R_{free} test set	3698 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7212	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: HEM, ZN, W79, H4B

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	0.37	0/3473	0.49	0/4712
1	B	0.36	0/3434	0.48	0/4660
All	All	0.36	0/6907	0.49	0/9372

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	3371	0	3282	26	0
1	B	3333	0	3244	28	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	0	0
4	B	25	0	0	0	0
5	A	1	0	0	0	0
6	A	195	0	0	0	0
6	B	142	0	0	0	0
All	All	7212	0	6616	53	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 (53) 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:528:LEU:HD22	1:A:536:PRO:HB2	1.67	0.76
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.68	0.75
1:B:482:SER:HA	1:B:574:ASN:HB3	1.71	0.72
1:B:380:LYS:NZ	1:B:384:GLU:OE2	2.26	0.68
1:A:482:SER:HA	1:A:574:ASN:HB3	1.77	0.67
2:B:801:HEM:HBC2	2:B:801:HEM:HMC2	1.80	0.64
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.81	0.63
1:A:667:MET:HE1	1:A:698:GLN:HG2	1.81	0.62
1:B:511:ILE:HG12	1:B:517:PRO:HG3	1.81	0.61
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.83	0.60
1:A:633:GLN:HG3	1:B:636:VAL:HG11	1.85	0.59
1:A:326:THR:HG21	1:A:706:THR:HG22	1.86	0.57
1:A:480:TRP:HB2	1:A:528:LEU:HB3	1.87	0.57
1:B:480:TRP:CE2	1:B:715:PRO:HB2	2.44	0.53
1:B:392:GLU:O	1:B:396:THR:OG1	2.25	0.52
1:B:389:VAL:O	1:B:393:ILE:HG13	2.11	0.51
1:B:455:THR:HA	1:B:460:LEU:HD13	1.94	0.48
1:A:636:VAL:HG11	1:B:633:GLN:HG3	1.96	0.48
2:A:801:HEM:HHC	2:A:801:HEM:HBB2	1.96	0.47
1:A:483:GLN:HB2	1:A:486:ARG:HG2	1.98	0.46
1:B:556:PHE:HB3	1:B:558:TRP:CE2	2.51	0.46
1:A:686:PRO:HG2	1:A:693:THR:HG21	1.98	0.46
1:B:613:GLU:HG3	1:B:623:MET:HE3	1.97	0.45
1:B:414:TRP:CE3	1:B:426:TRP:HA	2.52	0.45
1:B:327:LEU:HD12	1:B:704:ARG:HG2	1.99	0.45
1:B:376:ARG:HB2	1:B:379:SER:HB3	1.99	0.45
1:A:371:TYR:HA	1:A:374:ILE:HG12	2.00	0.44
1:A:600:VAL:O	1:A:604:CYS:HB2	2.17	0.44
1:A:497:THR:HG21	1:A:501:PRO:HA	2.00	0.44
1:A:517:PRO:HA	1:A:518:PRO:HD2	1.88	0.44
1:B:371:TYR:HA	1:B:374:ILE:HG12	1.99	0.43
1:B:505:GLN:O	1:B:509:ILE:HG13	2.18	0.43
1:B:478:ARG:NH2	1:B:715:PRO:HD3	2.32	0.43
1:B:480:TRP:HB2	1:B:528:LEU:HB3	1.99	0.43
1:A:625:LYS:HB2	1:A:625:LYS:HE3	1.71	0.42
1:B:368:ASP:OD1	1:B:382:HIS:NE2	2.45	0.42
1:A:556:PHE:HB3	1:A:558:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:LEU:HA	1:A:612:LEU:HD23	1.92	0.42
1:A:633:GLN:HG3	1:B:636:VAL:CG1	2.49	0.42
1:B:385:ARG:HD2	1:B:385:ARG:HA	1.85	0.42
1:B:600:VAL:O	1:B:604:CYS:HB2	2.19	0.42
1:A:327:LEU:HD11	1:A:704:ARG:NH1	2.35	0.41
1:A:685:VAL:HA	1:A:686:PRO:HD3	1.89	0.41
1:A:542:PRO:HA	1:A:543:PRO:HD3	1.90	0.41
1:A:340:ILE:HD13	1:B:699:GLU:HB3	2.03	0.41
1:A:414:TRP:CE3	1:A:426:TRP:HA	2.56	0.40
1:A:699:GLU:HB3	1:B:340:ILE:HD13	2.03	0.40
1:B:467:PHE:HB3	1:B:468:PRO:HD2	2.03	0.40
1:B:691:SER:HA	1:B:696:PHE:CB	2.51	0.40
1:A:454:ALA:O	1:A:460:LEU:HA	2.22	0.40
1:A:485:ILE:HD13	1:A:546:VAL:HG13	2.02	0.40
1:B:385:ARG:O	1:B:389:VAL:HG23	2.21	0.40
1:A:380:LYS:NZ	1:A:384:GLU:OE2	2.46	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	411/421 (98%)	404 (98%)	7 (2%)	0	100	100
1	B	406/421 (96%)	392 (97%)	13 (3%)	1 (0%)	47	38
All	All	817/842 (97%)	796 (97%)	20 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	376	ARG

5.3.2 Protein sidechains ⓘ

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	371/376 (99%)	355 (96%)	16 (4%)	29	16
1	B	366/376 (97%)	351 (96%)	15 (4%)	30	18
All	All	737/752 (98%)	706 (96%)	31 (4%)	30	17

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	CYS
1	A	304	ARG
1	A	307	LYS
1	A	327	LEU
1	A	337	MET
1	A	341	MET
1	A	372	SER
1	A	386	LEU
1	A	390	ASN
1	A	394	ASP
1	A	519	ARG
1	A	528	LEU
1	A	552	ARG
1	A	578	GLU
1	A	593	TYR
1	A	625	LYS
1	B	304	ARG
1	B	324	LYS
1	B	326	THR
1	B	365	GLU
1	B	376	ARG
1	B	387	GLU
1	B	395	THR
1	B	491	LYS
1	B	528	LEU
1	B	552	ARG
1	B	555	LYS

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Mol	Chain	Res	Type
1	B	560	LYS
1	B	706	THR
1	B	718	THR
1	B	720	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	H4B	A	802	-	16,18,18	0.73	0	11,26,26	2.51	6 (54%)
3	H4B	B	802	-	16,18,18	0.78	0	11,26,26	2.59	6 (54%)
4	W79	A	803	-	27,27,27	0.38	0	35,36,36	1.62	8 (22%)
2	HEM	B	801	1	27,50,50	2.21	6 (22%)	17,82,82	1.70	4 (23%)
2	HEM	A	801	1	27,50,50	2.15	5 (18%)	17,82,82	1.87	5 (29%)
4	W79	B	803	-	27,27,27	0.39	0	35,36,36	1.62	8 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
4	W79	A	803	-	-	2/11/12/12	0/3/3/3
2	HEM	B	801	1	-	0/6/54/54	-
2	HEM	A	801	1	-	0/6/54/54	-
4	W79	B	803	-	-	2/11/12/12	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3B-C2B	-5.32	1.33	1.40
2	B	801	HEM	C3D-C2D	5.25	1.53	1.37
2	A	801	HEM	C3B-C2B	-5.12	1.33	1.40
2	A	801	HEM	C3D-C2D	5.10	1.52	1.37
2	A	801	HEM	C3C-C2C	-3.78	1.35	1.40
2	A	801	HEM	C3B-CAB	3.70	1.55	1.47
2	B	801	HEM	C3C-C2C	-3.69	1.35	1.40
2	B	801	HEM	C3B-CAB	3.64	1.55	1.47
2	B	801	HEM	C3C-CAC	3.60	1.55	1.47
2	A	801	HEM	C3C-CAC	3.27	1.54	1.47
2	B	801	HEM	C1D-ND	2.20	1.40	1.36

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	H4B	C4-C4A-C8A	5.30	119.28	114.57
3	A	802	H4B	C4-C4A-C8A	4.85	118.87	114.57
4	B	803	W79	C02-N01-C06	4.65	121.63	118.10
4	A	803	W79	C09-C08-C06	-4.35	103.23	112.99
2	A	801	HEM	CBD-CAD-C3D	-4.13	104.87	112.48
4	A	803	W79	C02-N01-C06	4.06	121.18	118.10
4	B	803	W79	C09-C08-C06	-3.87	104.31	112.99
2	A	801	HEM	CBA-CAA-C2A	-3.86	105.36	112.49
2	B	801	HEM	CBA-CAA-C2A	-3.60	105.84	112.49
2	B	801	HEM	CBD-CAD-C3D	-3.60	105.84	112.48
3	A	802	H4B	C4-N3-C2	3.51	121.51	115.93
3	B	802	H4B	C4-N3-C2	3.25	121.09	115.93
3	B	802	H4B	C4-C4A-N5	3.06	121.69	119.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	H4B	C4-C4A-N5	3.01	121.65	119.12
4	B	803	W79	C14-C13-C12	3.00	119.61	116.71
3	B	802	H4B	N3-C2-N1	-2.99	120.72	125.42
3	A	802	H4B	N3-C2-N1	-2.99	120.74	125.42
4	B	803	W79	C05-C06-N01	-2.98	119.74	122.90
2	A	801	HEM	C1D-C2D-C3D	-2.85	105.01	107.00
4	A	803	W79	C05-C06-N01	-2.62	120.13	122.90
2	B	801	HEM	C1D-C2D-C3D	-2.58	105.20	107.00
4	B	803	W79	C16-N11-C12	2.53	120.94	117.48
3	B	802	H4B	C2-N1-C8A	2.53	120.21	114.54
4	A	803	W79	C09-C13-C12	-2.43	117.92	121.83
4	B	803	W79	C08-C06-N01	2.42	119.55	115.95
4	A	803	W79	C16-N11-C12	2.35	120.68	117.48
2	A	801	HEM	CMC-C2C-C3C	2.31	129.00	124.68
3	A	802	H4B	C2-N1-C8A	2.24	119.57	114.54
4	A	803	W79	C08-C06-N01	2.22	119.26	115.95
4	A	803	W79	C14-C15-C16	2.21	119.31	117.11
4	A	803	W79	C14-C13-C12	2.17	118.81	116.71
2	A	801	HEM	CMA-C3A-C4A	-2.13	125.19	128.46
3	B	802	H4B	N2-C2-N1	2.10	120.51	117.25
4	B	803	W79	C09-C13-C12	-2.09	118.47	121.83
4	B	803	W79	C14-C15-C16	2.07	119.17	117.11
3	A	802	H4B	N2-C2-N1	2.06	120.45	117.25
2	B	801	HEM	CMA-C3A-C4A	-2.04	125.33	128.46

There are no chirality outliers.

All (4) torsion outliers are listed below:

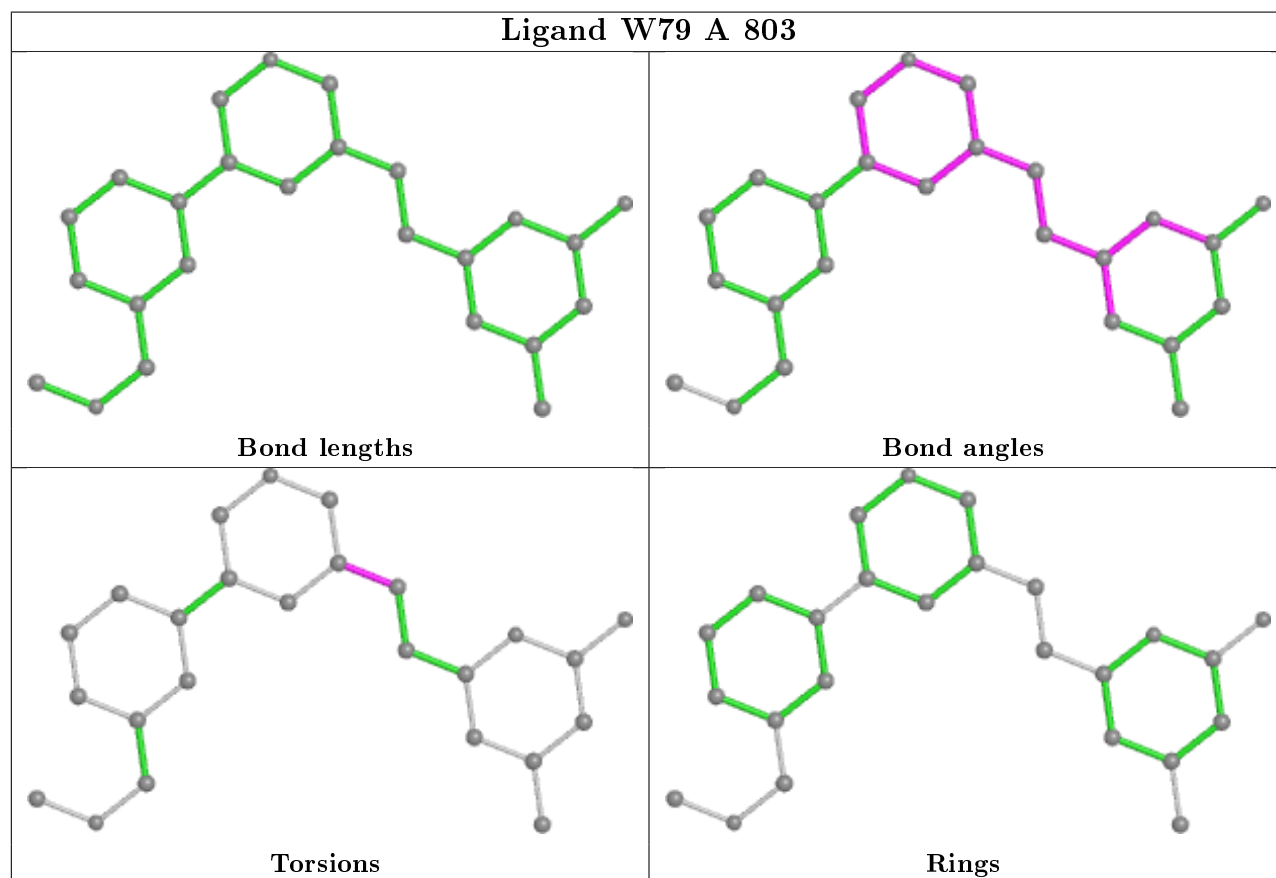
Mol	Chain	Res	Type	Atoms
4	B	803	W79	C08-C09-C13-C12
4	A	803	W79	C08-C09-C13-C12
4	B	803	W79	C08-C09-C13-C14
4	A	803	W79	C08-C09-C13-C14

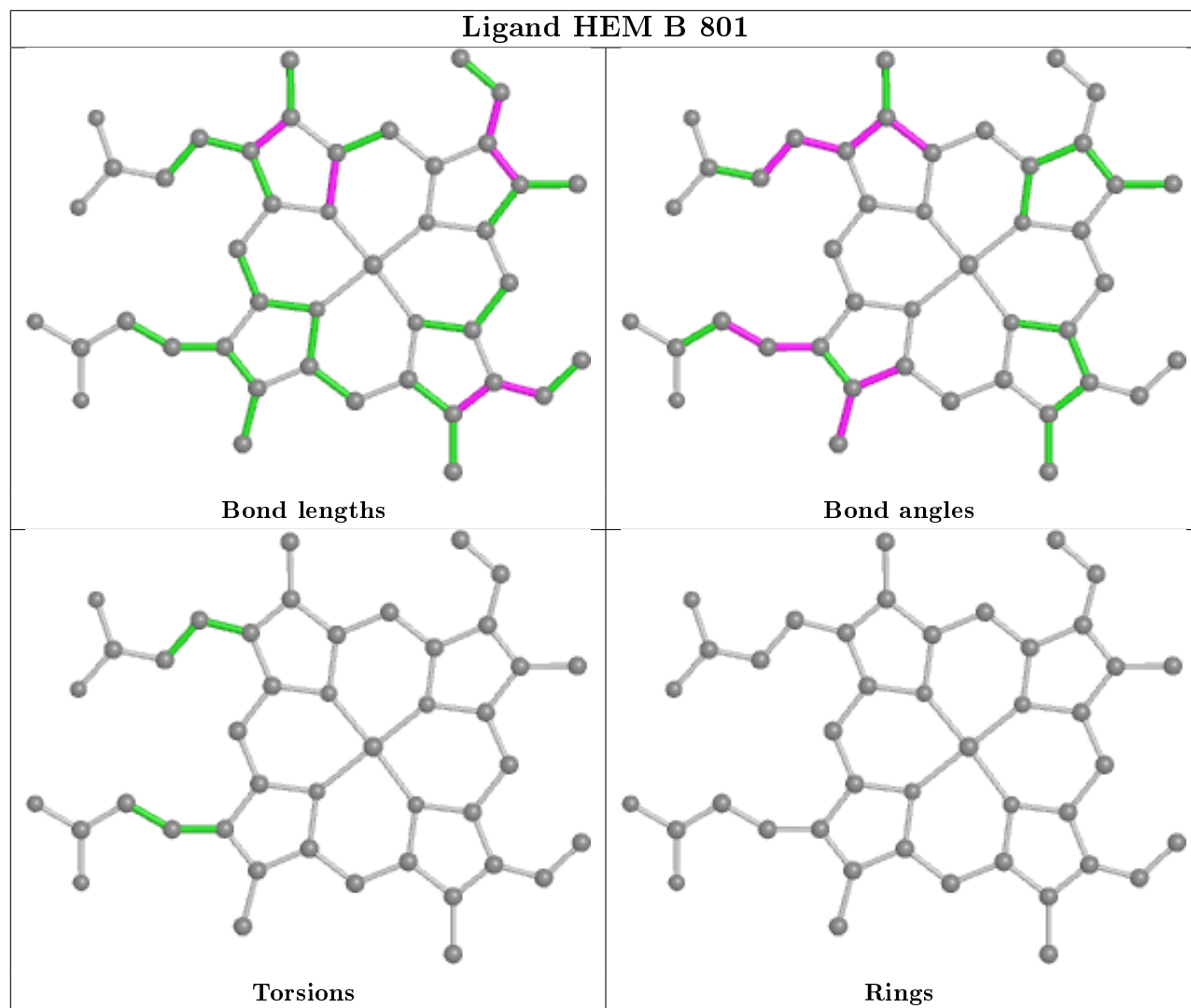
There are no ring outliers.

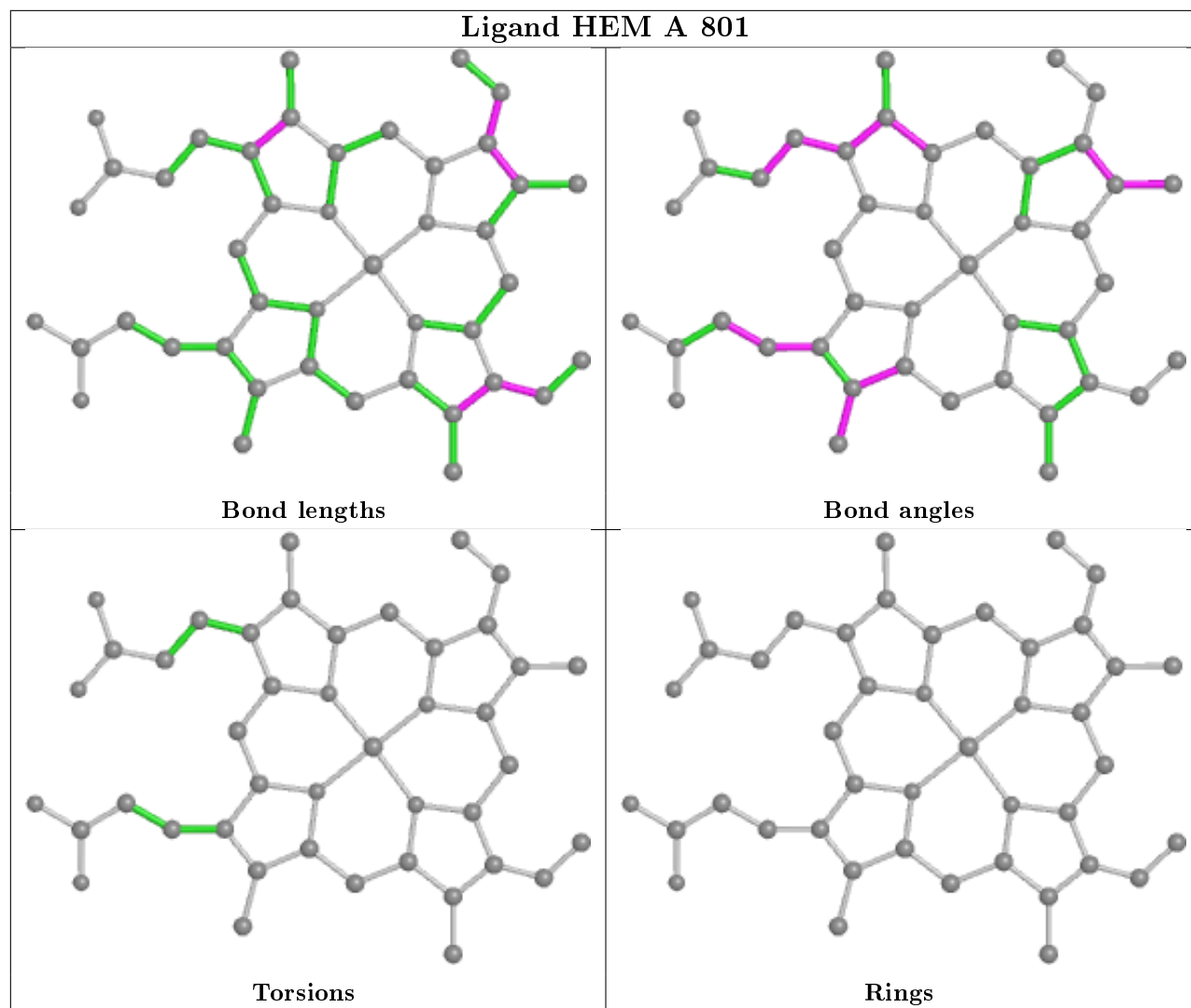
2 monomers are involved in 4 short contacts:

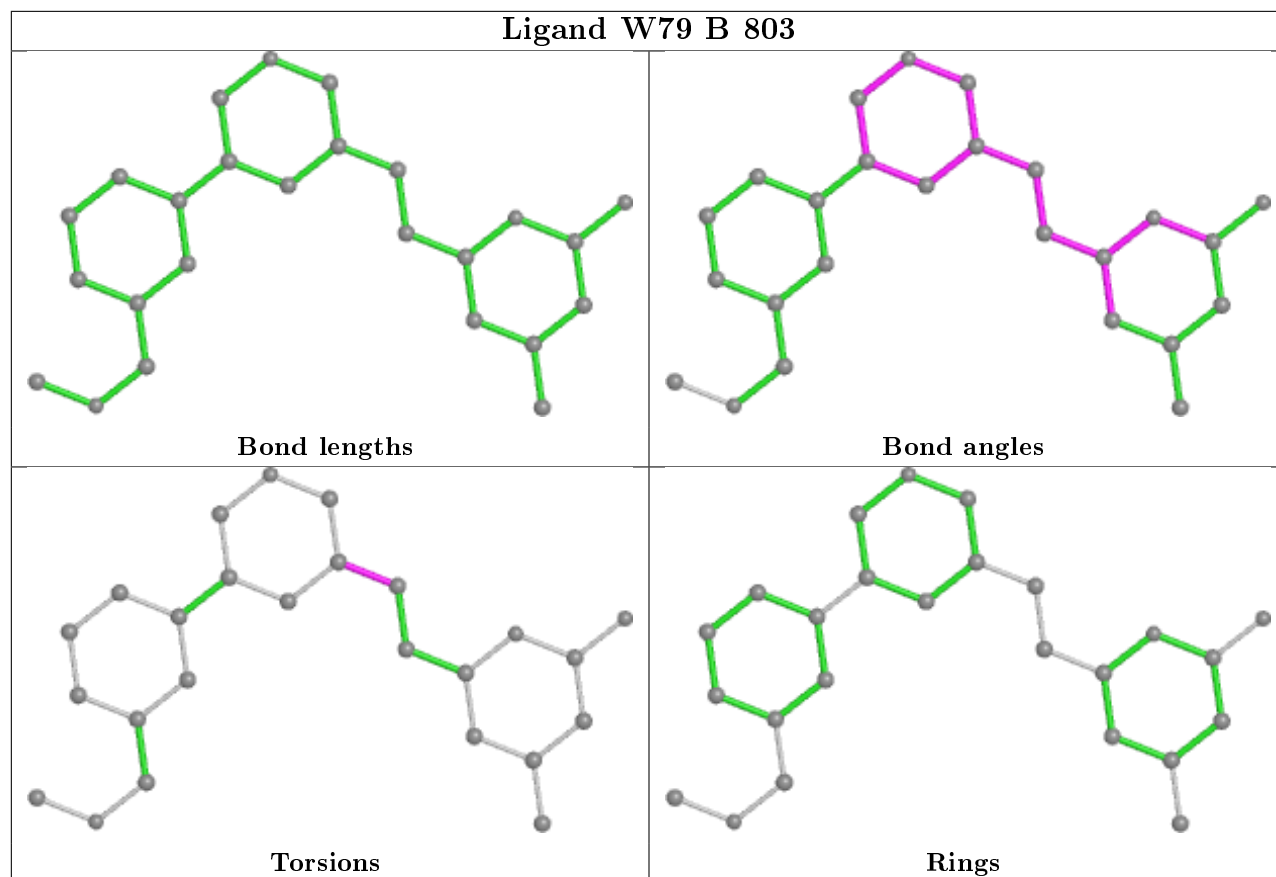
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HEM	2	0
2	A	801	HEM	2	0

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 than 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.









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, 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	413/421 (98%)	0.39	27 (6%) 18 27	31, 53, 87, 111	0
1	B	408/421 (96%)	0.93	75 (18%) 1 1	33, 64, 111, 144	0
All	All	821/842 (97%)	0.66	102 (12%) 4 6	31, 57, 104, 144	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	721	TRP	7.1
1	B	720	VAL	5.3
1	B	511	ILE	5.1
1	B	360	PHE	4.9
1	A	305	PHE	4.8
1	A	353	VAL	4.8
1	B	493	PRO	4.7
1	B	304	ARG	4.7
1	B	498	LEU	4.6
1	B	393	ILE	4.5
1	B	386	LEU	4.5
1	B	396	THR	4.4
1	B	504	VAL	4.1
1	B	397	SER	4.1
1	B	716	TRP	4.0
1	B	682	VAL	4.0
1	B	474	LYS	3.9
1	B	683	TRP	3.9
1	A	624	ARG	3.9
1	B	356	LYS	3.9
1	B	557	GLU	3.8
1	B	357	ASP	3.7
1	B	490	TYR	3.6
1	B	305	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	374	ILE	3.6
1	B	510	CYS	3.6
1	A	684	ILE	3.5
1	B	326	THR	3.5
1	B	624	ARG	3.5
1	B	719	HIS	3.5
1	B	497	THR	3.4
1	B	560	LYS	3.4
1	B	718	THR	3.4
1	B	355	THR	3.3
1	B	375	LYS	3.3
1	B	600	VAL	3.2
1	A	681	TRP	3.2
1	B	358	GLN	3.1
1	B	686	PRO	3.1
1	B	687	PRO	3.1
1	B	685	VAL	3.1
1	B	571	ALA	3.1
1	B	596	THR	3.0
1	B	690	GLY	3.0
1	B	492	GLN	3.0
1	A	360	PHE	2.9
1	B	395	THR	2.9
1	B	371	TYR	2.9
1	B	508	GLU	2.8
1	A	685	VAL	2.8
1	B	359	LEU	2.8
1	B	556	PHE	2.8
1	A	355	THR	2.7
1	B	380	LYS	2.7
1	A	683	TRP	2.7
1	B	621	LEU	2.7
1	B	589	PHE	2.7
1	A	690	GLY	2.7
1	B	516	LYS	2.6
1	B	717	ASN	2.6
1	A	682	VAL	2.6
1	B	689	SER	2.6
1	B	496	SER	2.5
1	A	687	PRO	2.5
1	A	356	LYS	2.5
1	B	572	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	377	PHE	2.5
1	A	357	ASP	2.4
1	A	692	ILE	2.4
1	B	635	LEU	2.4
1	B	387	GLU	2.4
1	B	715	PRO	2.3
1	B	688	MET	2.3
1	A	395	THR	2.3
1	A	600	VAL	2.3
1	B	684	ILE	2.3
1	A	625	LYS	2.3
1	A	696	PHE	2.2
1	A	686	PRO	2.2
1	B	622	ASP	2.2
1	B	495	GLY	2.2
1	B	334	TYR	2.2
1	A	359	LEU	2.2
1	A	498	LEU	2.2
1	A	334	TYR	2.2
1	A	596	THR	2.2
1	B	535	ASP	2.2
1	A	688	MET	2.1
1	B	696	PHE	2.1
1	A	396	THR	2.1
1	A	304	ARG	2.1
1	B	389	VAL	2.1
1	B	559	PHE	2.1
1	B	378	GLY	2.1
1	B	324	LYS	2.1
1	B	372	SER	2.0
1	B	595	GLY	2.0
1	B	394	ASP	2.0
1	B	601	ARG	2.0
1	B	518	PRO	2.0
1	B	327	LEU	2.0
1	B	448	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

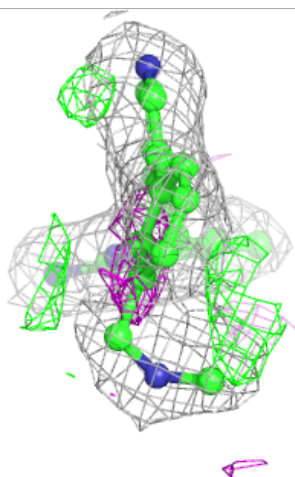
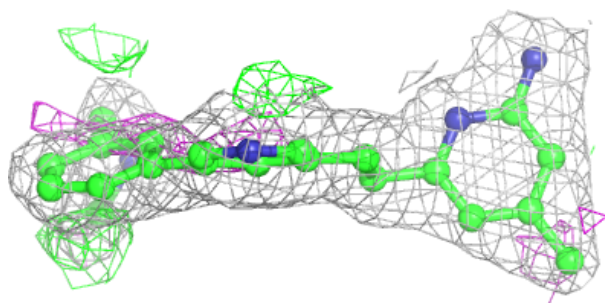
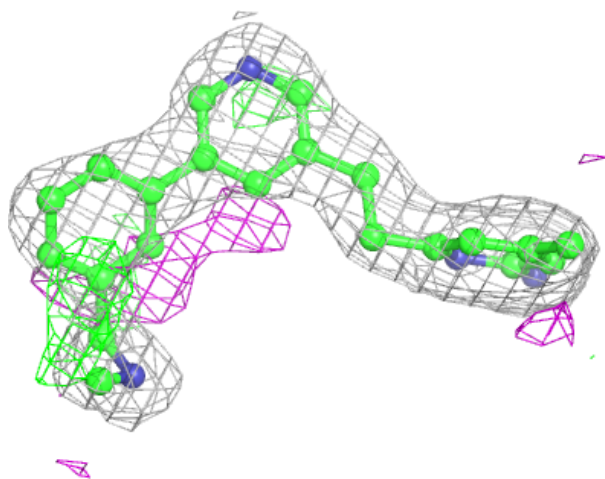
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	W79	A	803	25/25	0.91	0.19	32,42,58,63	0
4	W79	B	803	25/25	0.92	0.25	32,43,53,64	0
3	H4B	B	802	17/17	0.96	0.23	31,40,48,49	0
3	H4B	A	802	17/17	0.97	0.16	31,39,46,47	0
2	HEM	A	801	43/43	0.98	0.18	25,35,45,52	0
2	HEM	B	801	43/43	0.98	0.20	28,39,48,51	0
5	ZN	A	804	1/1	0.99	0.10	42,42,42,42	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.

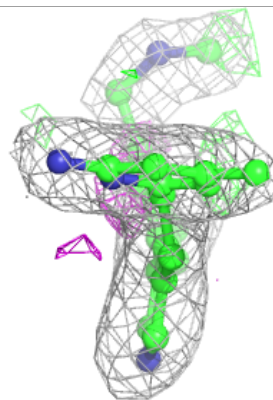
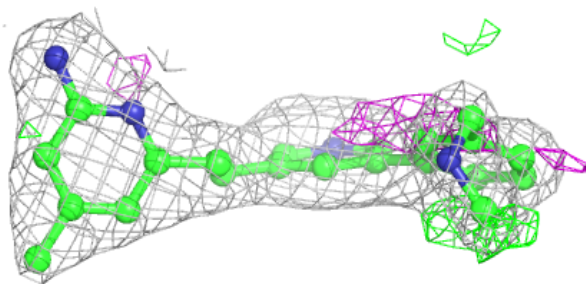
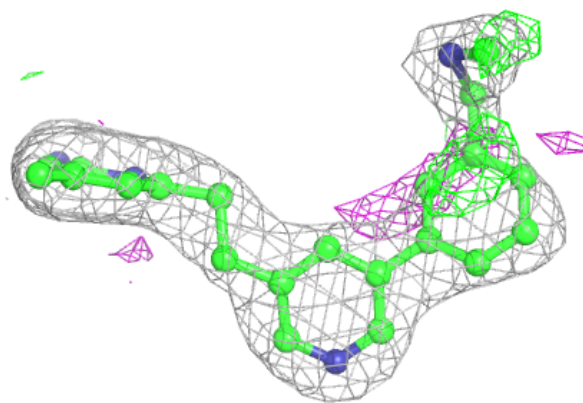
Electron density around W79 A 803:

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



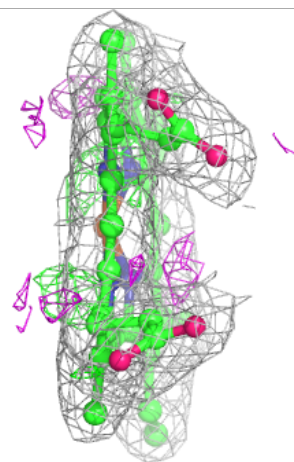
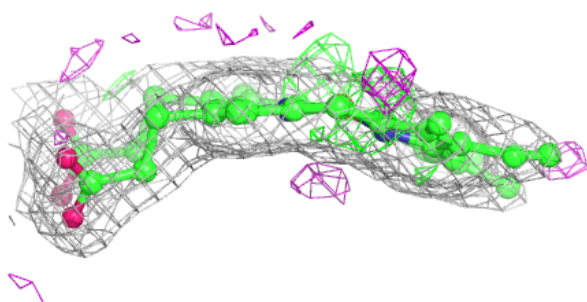
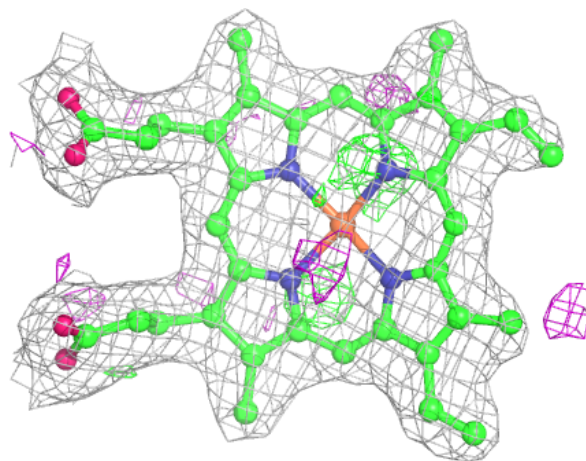
Electron density around W79 B 803:

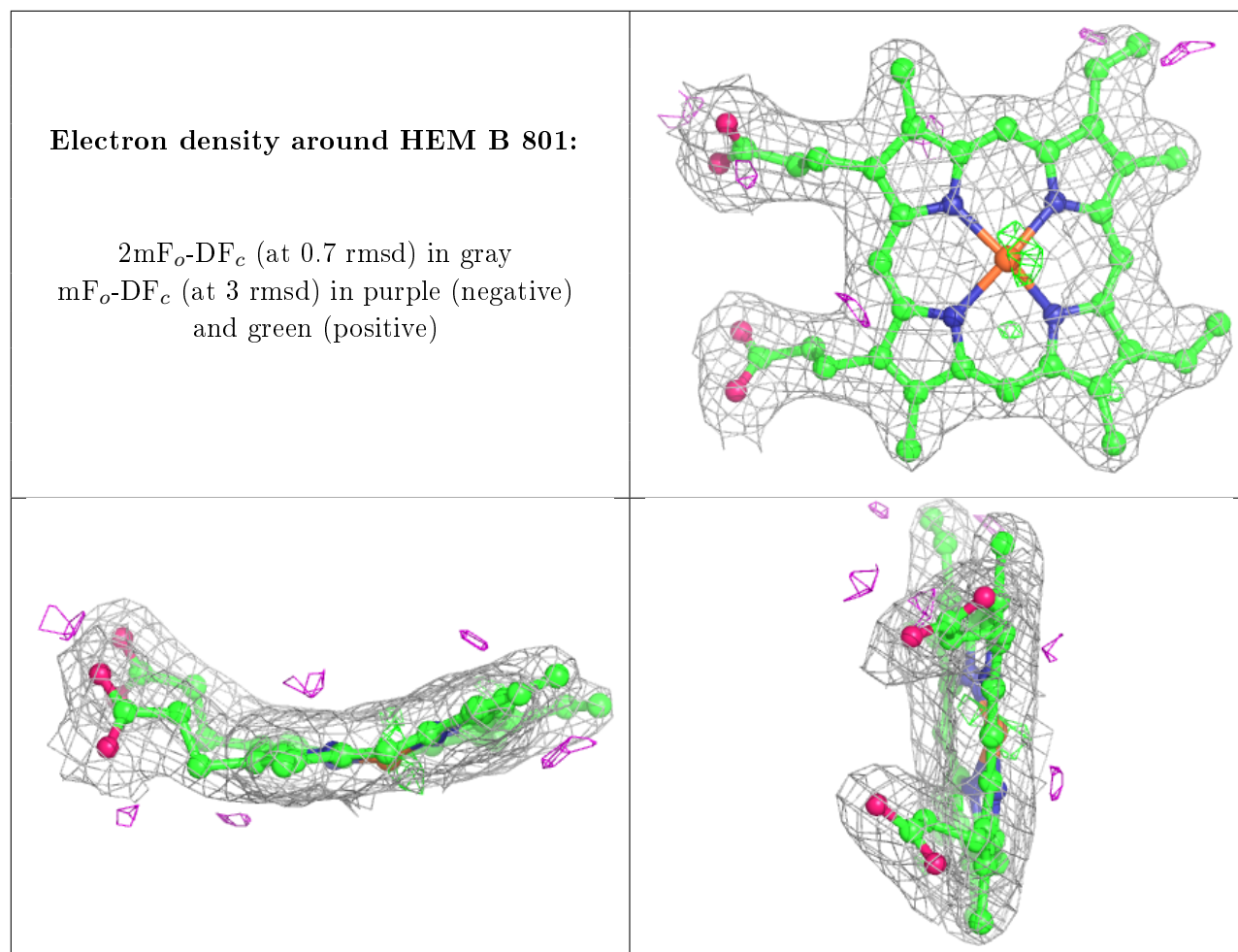
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.