



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 06:58 PM UTC

PDB ID : 6AUV / pdb_00006auv
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

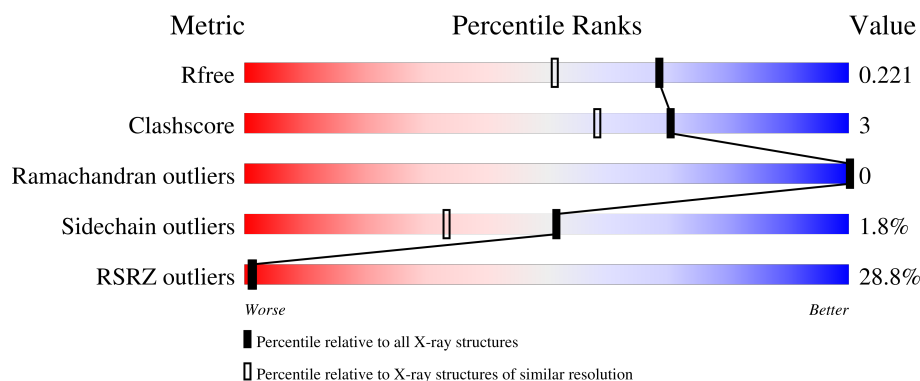
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.76 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 $\leq 5\%$. 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	422	37% 87% 10% .
1	B	422	19% 89% 9% .

2 Entry composition [i](#)

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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



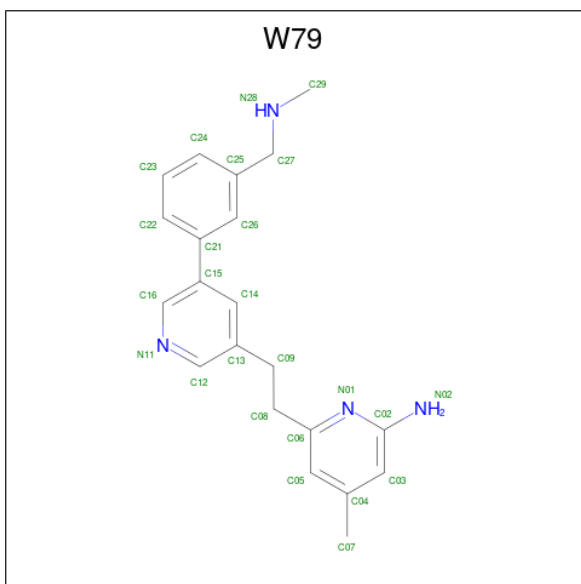
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 4 is 4-methyl-6-[2-(5-{3-[(methylamino)methyl]phenyl}pyridin-3-yl)ethyl]pyridin-2-amine (CCD ID: 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			

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

- Molecule 5 is ACETATE ION (CCD ID: 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 (CCD ID: ZN) (formula: Zn).

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

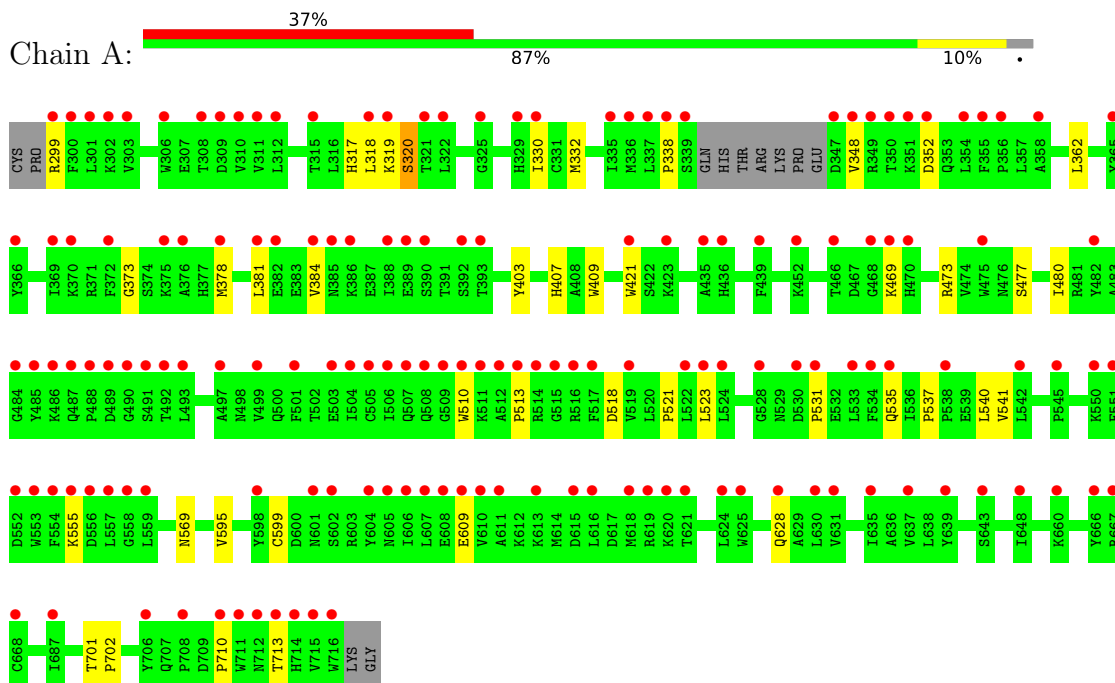
- Molecule 7 is water.

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

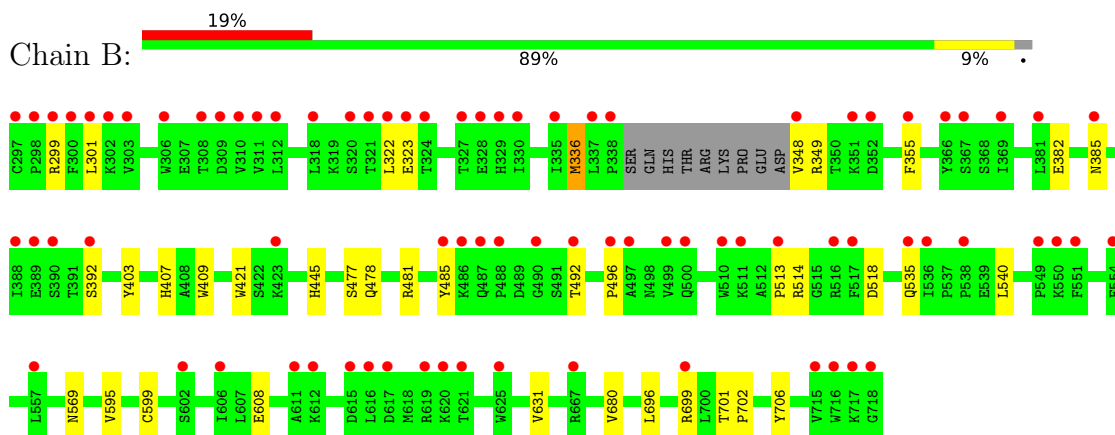
3 Residue-property plots [i](#)

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



- 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	52.12Å 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) 97.6 (39.00-1.76)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.184 , 0.222 0.185 , 0.221	Depositor DCC
R_{free} test set	4642 reflections (4.58%)	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 , 49.9	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	0.94	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.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, W79, ZN, ACT, 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	0.41	0/3460	0.75	0/4695
1	B	0.47	0/3491	0.75	2/4734 (0.0%)
All	All	0.44	0/6951	0.75	2/9429 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	680	VAL	CA-C-N	5.80	123.89	119.66
1	B	680	VAL	C-N-CA	5.80	123.89	119.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3361	0	3270	22	0
1	B	3381	0	3301	21	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	25	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
7	A	239	0	0	4	0
7	B	312	0	0	3	0
All	All	7472	0	6667	46	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 (46) 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:513:PRO:HG2	1:B:518:ASP:CG	2.36	0.51
1:B:706:TYR:OH	2:B:801:HEM:O1D	2.21	0.50
1:B:403:TYR:CE1	1:B:407:HIS:CE1	2.99	0.50
1:A:332:MET:HE1	1:B:301:LEU:HD22	1.94	0.49
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:348:VAL:HG22	1:B:349:ARG:H	1.79	0.46
1:B:336:MET:HE2	1:B:336:MET:HB2	1.86	0.46
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.30	0.46
1:B:322:LEU:HB2	1:B:699:ARG:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:373:GLY:HA2	1:A:378:MET:HE3	1.99	0.44
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.53	0.44
1:B:445:HIS:C	1:B:445:HIS:CD2	2.97	0.43
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
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:A:513:PRO:HG2	1:A:518:ASP:CG	2.46	0.41
1:A:701[B]:THR:HA	1:A:702:PRO:C	2.46	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
1:B:701:THR:HA	1:B:702:PRO:C	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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%)	362 (98%)	8 (2%)	45	26
1	B	373/377 (99%)	368 (99%)	5 (1%)	61	46
All	All	743/754 (98%)	730 (98%)	13 (2%)	51	36

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	LYS
1	A	320	SER
1	A	348	VAL
1	A	352	ASP
1	A	381	LEU
1	A	469	LYS
1	A	555	LYS
1	A	713	THR
1	B	299	ARG
1	B	336	MET
1	B	382	GLU
1	B	392	SER
1	B	540	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	385	ASN
1	A	407	HIS
1	B	407	HIS
1	B	425	GLN
1	B	664	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
3	H4B	A	802	-	17,18,18	0.76	0	14,26,26	1.88	4 (28%)
4	W79	B	803	-	27,27,27	0.40	0	34,36,36	1.90	10 (29%)
4	W79	A	803	-	27,27,27	0.35	0	34,36,36	1.96	11 (32%)
2	HEM	B	801	1	50,50,50	1.97	11 (22%)	67,82,82	1.30	5 (7%)
5	ACT	B	804	-	3,3,3	0.85	0	3,3,3	0.66	0
3	H4B	B	802	-	17,18,18	0.78	0	14,26,26	1.95	4 (28%)
5	ACT	A	804	-	3,3,3	0.83	0	3,3,3	0.68	0
2	HEM	A	801	1	50,50,50	2.01	11 (22%)	67,82,82	1.34	6 (8%)

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
4	W79	B	803	-	-	2/12/12/12	0/3/3/3
4	W79	A	803	-	-	2/12/12/12	0/3/3/3
2	HEM	B	801	1	-	1/14/54/54	-
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	801	1	-	1/14/54/54	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3D-C2D	7.40	1.52	1.36
2	B	801	HEM	C3D-C2D	7.33	1.52	1.36
2	A	801	HEM	FE-NB	5.57	2.12	1.94
2	B	801	HEM	FE-NB	4.66	2.09	1.94
2	A	801	HEM	FE-NA	4.66	2.10	1.95
2	B	801	HEM	FE-ND	4.29	2.08	1.94
2	B	801	HEM	FE-NA	4.12	2.08	1.95
2	B	801	HEM	FE-NC	3.88	2.08	1.95
2	A	801	HEM	FE-ND	3.86	2.06	1.94
2	A	801	HEM	FE-NC	3.47	2.06	1.95
2	A	801	HEM	CAB-C3B	3.07	1.55	1.47
2	B	801	HEM	CAB-C3B	2.97	1.55	1.47
2	B	801	HEM	CAC-C3C	2.95	1.55	1.47
2	A	801	HEM	CAC-C3C	2.76	1.54	1.47
2	B	801	HEM	CMC-C2C	2.61	1.56	1.50
2	A	801	HEM	CMC-C2C	2.44	1.55	1.50
2	A	801	HEM	CMD-C2D	2.23	1.55	1.50
2	A	801	HEM	CMB-C2B	2.23	1.55	1.50
2	A	801	HEM	CMA-C3A	2.20	1.55	1.50
2	B	801	HEM	CMA-C3A	2.16	1.55	1.50
2	B	801	HEM	CMD-C2D	2.15	1.55	1.50
2	B	801	HEM	CMB-C2B	2.09	1.55	1.50

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	W79	C02-N01-C06	5.35	122.07	118.07
4	B	803	W79	C02-N01-C06	5.08	121.87	118.07
2	B	801	HEM	C4D-ND-C1D	5.03	111.16	105.21
4	A	803	W79	C09-C08-C06	-4.89	102.13	113.01
4	B	803	W79	C09-C08-C06	-4.76	102.42	113.01
2	A	801	HEM	C4D-ND-C1D	4.69	110.76	105.21
3	B	802	H4B	C2-N1-C8A	4.45	121.21	113.36
3	A	802	H4B	C2-N1-C8A	4.42	121.17	113.36
2	A	801	HEM	CBD-CAD-C3D	-3.80	102.03	112.53
2	B	801	HEM	CBD-CAD-C3D	-3.33	103.31	112.53
4	B	803	W79	C08-C06-N01	3.03	120.65	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	W79	C05-C06-N01	-3.00	119.31	122.73
3	B	802	H4B	O4-C4-C4A	-3.00	120.02	127.26
4	B	803	W79	C05-C06-N01	-2.98	119.34	122.73
2	A	801	HEM	CBA-CAA-C2A	-2.90	104.52	112.53
4	B	803	W79	C14-C15-C16	2.84	120.15	117.10
2	A	801	HEM	CMD-C2D-C1D	2.76	129.35	125.03
3	B	802	H4B	C4A-C4-N3	2.76	119.71	112.13
4	A	803	W79	C09-C13-C12	-2.75	116.85	121.73
4	A	803	W79	C14-C15-C16	2.69	119.98	117.10
3	A	802	H4B	C4A-C4-N3	2.60	119.27	112.13
3	B	802	H4B	C2-N3-C4	-2.53	120.52	125.11
4	A	803	W79	C08-C06-N01	2.52	119.88	116.06
2	B	801	HEM	CBA-CAA-C2A	-2.51	105.58	112.53
4	A	803	W79	C14-C13-C12	2.50	119.22	116.90
4	B	803	W79	C14-C13-C12	2.47	119.19	116.90
3	A	802	H4B	C2-N3-C4	-2.46	120.66	125.11
4	A	803	W79	C15-C14-C13	-2.45	117.93	121.20
4	A	803	W79	C16-N11-C12	2.42	120.80	117.51
2	B	801	HEM	C2A-C1A-NA	-2.42	107.47	110.15
4	B	803	W79	C15-C14-C13	-2.38	118.02	121.20
3	A	802	H4B	O4-C4-C4A	-2.37	121.55	127.26
4	B	803	W79	C25-C27-N28	-2.22	107.33	112.67
4	A	803	W79	C25-C27-N28	-2.16	107.48	112.67
2	A	801	HEM	C4C-NC-C1C	2.16	109.34	105.82
4	B	803	W79	C09-C13-C12	-2.13	117.95	121.73
2	B	801	HEM	C3B-C2B-C1B	2.03	107.94	106.41
4	A	803	W79	C09-C13-C14	2.02	123.94	120.54
2	A	801	HEM	CHC-C1C-NC	2.02	126.65	124.45
4	B	803	W79	C16-N11-C12	2.01	120.24	117.51

There are no chirality outliers.

All (6) torsion outliers are listed below:

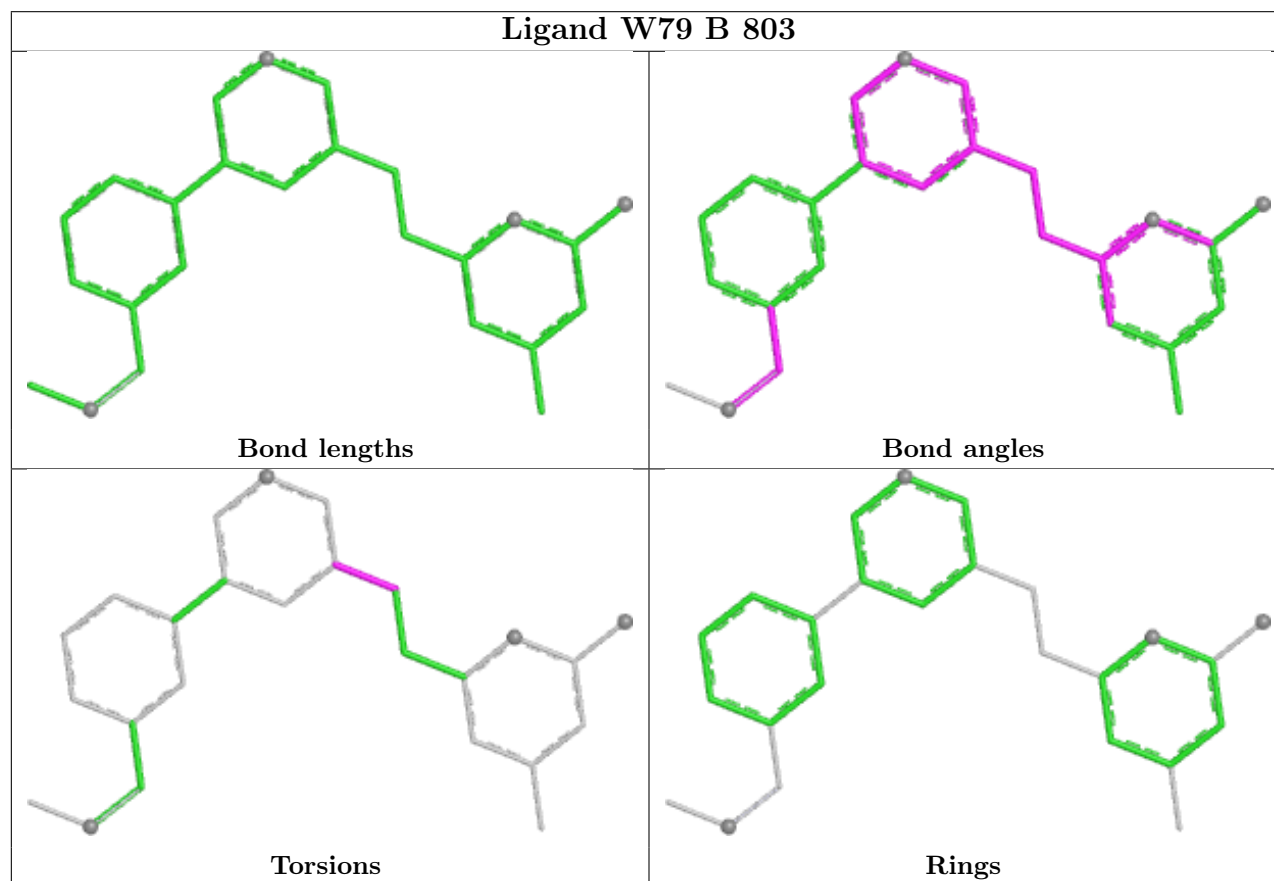
Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C4B-C3B-CAB-CBB
2	B	801	HEM	C4B-C3B-CAB-CBB
4	A	803	W79	C08-C09-C13-C12
4	B	803	W79	C08-C09-C13-C12
4	A	803	W79	C08-C09-C13-C14
4	B	803	W79	C08-C09-C13-C14

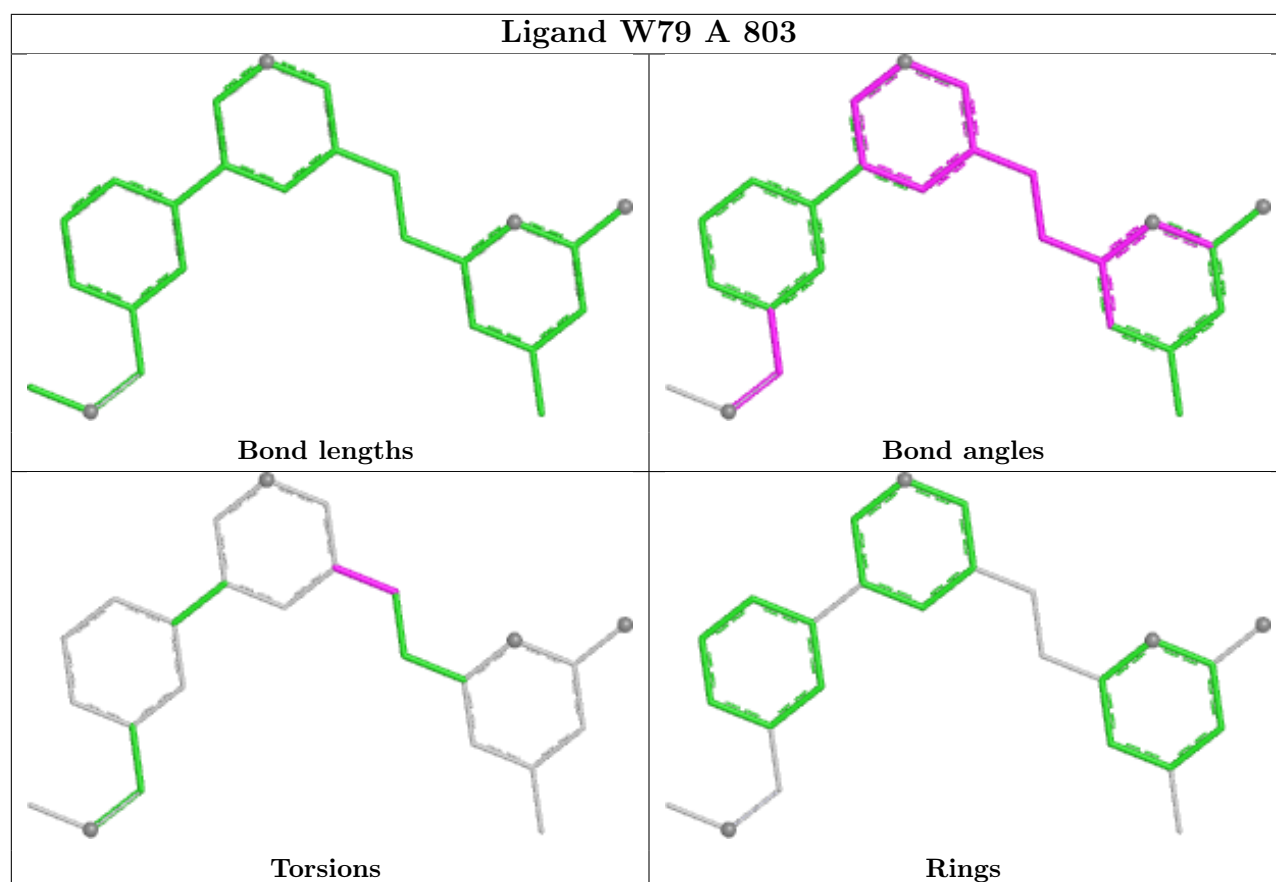
There are no ring outliers.

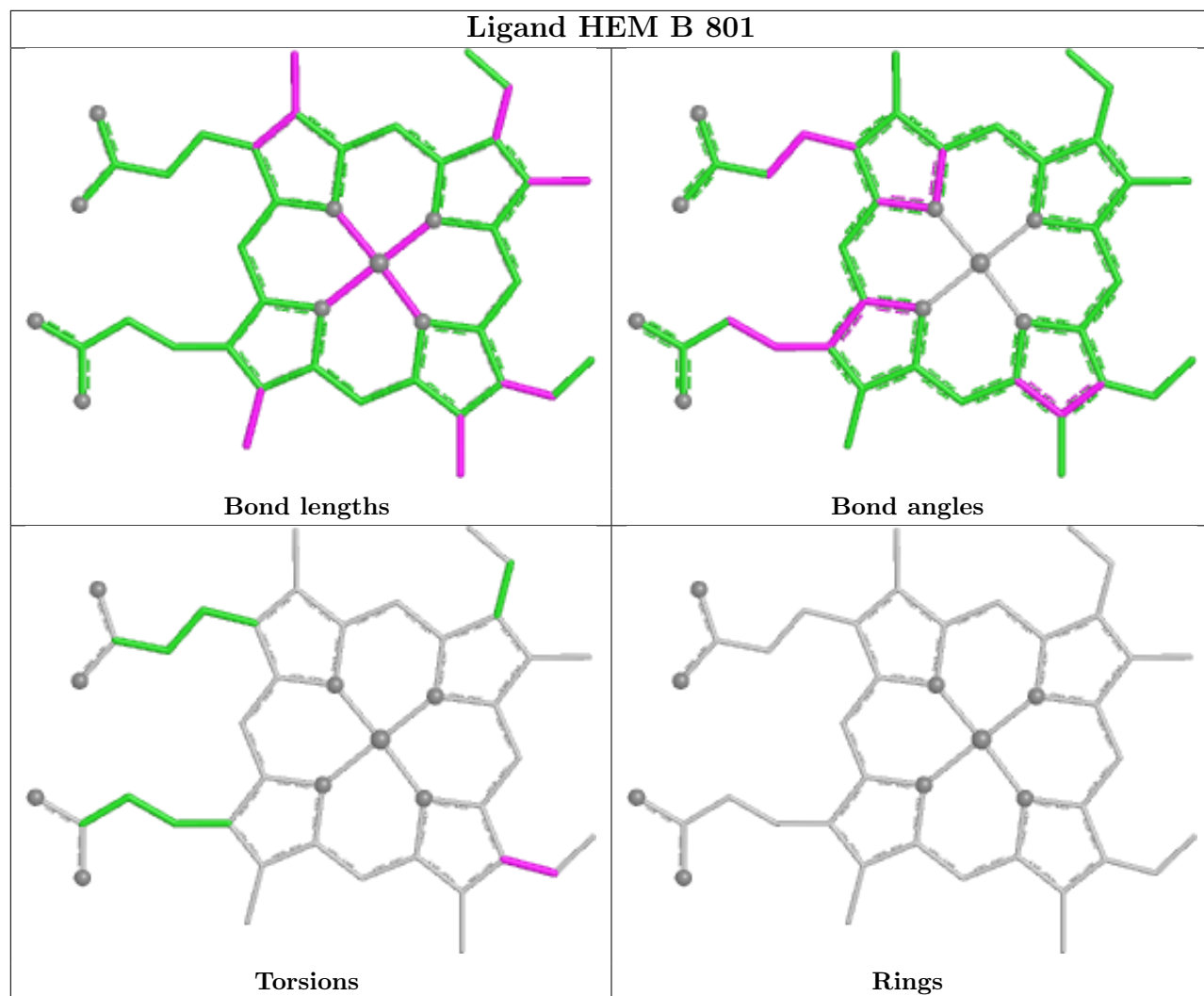
4 monomers are involved in 7 short contacts:

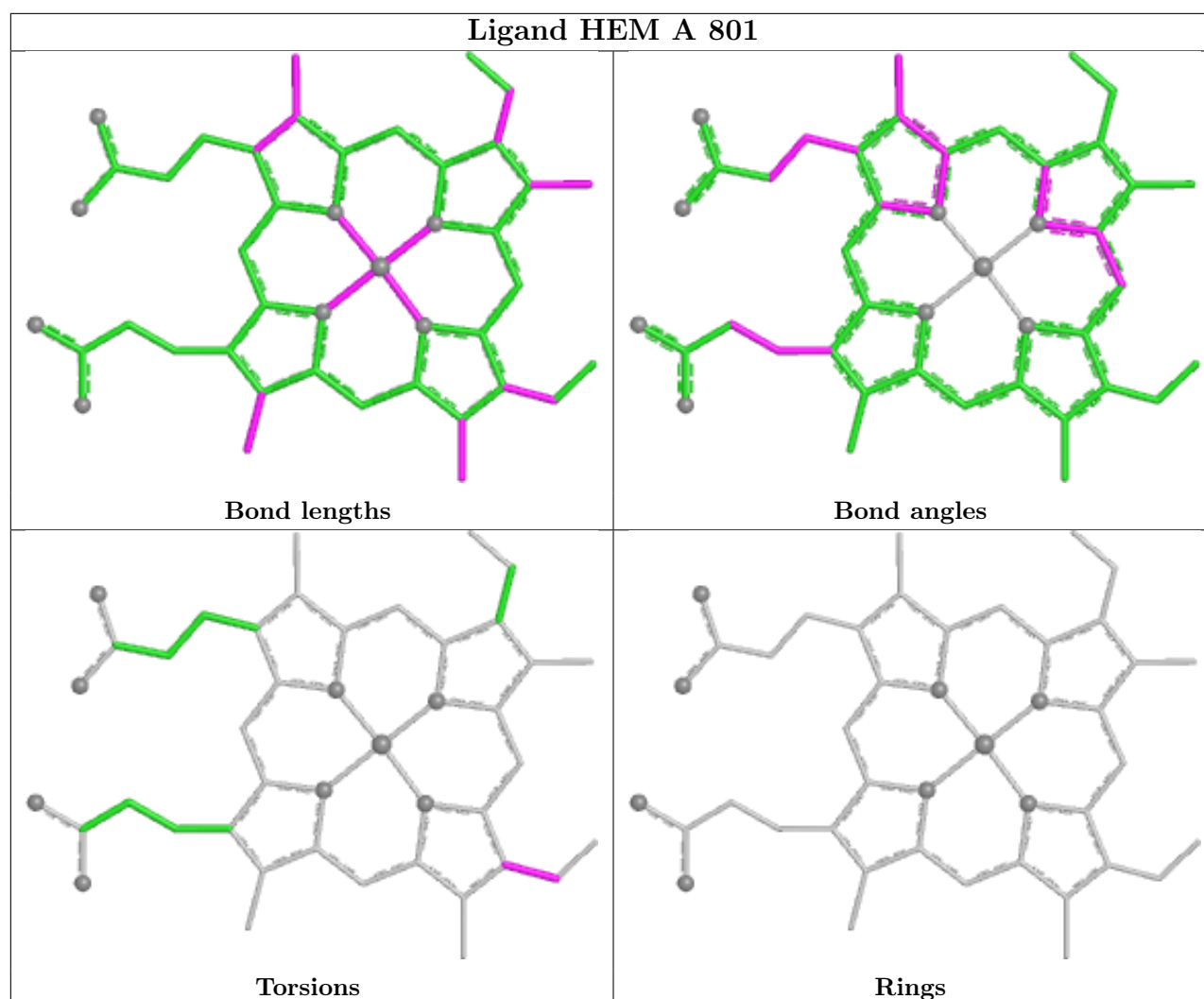
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	803	W79	1	0
4	A	803	W79	1	0
2	B	801	HEM	3	0
2	A	801	HEM	2	0

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	411/422 (97%)	1.80	157 (38%)	1 1	18, 48, 88, 126	3 (0%)
1	B	413/422 (97%)	1.32	80 (19%)	3 3	22, 37, 67, 107	5 (1%)
All	All	824/844 (97%)	1.56	237 (28%)	1 1	18, 42, 82, 126	8 (0%)

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	VAL	7.3
1	A	300	PHE	6.7
1	A	355	PHE	6.4
1	A	488	PRO	6.2
1	A	715	VAL	5.4
1	A	716	TRP	5.4
1	B	300	PHE	5.3
1	B	297	CYS	5.3
1	B	355[A]	PHE	5.2
1	B	321	THR	5.0
1	B	322	LEU	4.9
1	B	338	PRO	4.9
1	A	322	LEU	4.6
1	B	348	VAL	4.5
1	A	486	LYS	4.5
1	A	339	SER	4.3
1	A	321	THR	4.2
1	A	499	VAL	4.1
1	B	299	ARG	4.1
1	A	713	THR	4.1
1	A	616	LEU	4.0
1	B	298	PRO	3.9
1	B	311	VAL	3.9
1	B	718	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	338	PRO	3.8
1	A	490	GLY	3.7
1	A	711	TRP	3.7
1	A	310	VAL	3.7
1	A	337	LEU	3.6
1	A	553	TRP	3.6
1	A	507	GLN	3.6
1	B	616	LEU	3.6
1	B	667	ARG	3.5
1	A	392	SER	3.5
1	A	318	LEU	3.5
1	A	489	ASP	3.5
1	A	485	TYR	3.5
1	B	492	THR	3.5
1	A	668[A]	CYS	3.5
1	A	554	PHE	3.4
1	A	492	THR	3.4
1	B	621	THR	3.4
1	A	506	ILE	3.4
1	A	351	LYS	3.3
1	A	369	ILE	3.3
1	B	310	VAL	3.3
1	A	372	PHE	3.3
1	A	347	ASP	3.3
1	A	350	THR	3.2
1	A	330	ILE	3.2
1	A	552	ASP	3.2
1	A	551	PHE	3.2
1	A	514	ARG	3.2
1	A	619	ARG	3.2
1	A	466	THR	3.2
1	A	301	LEU	3.2
1	A	487	GLN	3.2
1	B	351	LYS	3.2
1	A	558	GLY	3.2
1	B	318	LEU	3.1
1	B	381	LEU	3.1
1	B	352	ASP	3.1
1	A	533	LEU	3.1
1	A	376	ALA	3.1
1	B	611	ALA	3.1
1	A	319	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	493	LEU	3.1
1	A	349	ARG	3.1
1	A	385	ASN	3.0
1	B	301	LEU	3.0
1	B	309	ASP	3.0
1	A	299	ARG	3.0
1	B	486	LYS	3.0
1	A	604	TYR	3.0
1	A	436	HIS	3.0
1	A	511	LYS	3.0
1	A	555	LYS	3.0
1	B	323	GLU	3.0
1	A	423	LYS	3.0
1	A	303	VAL	2.9
1	A	491	SER	2.9
1	A	501	PHE	2.9
1	A	517	PHE	2.9
1	A	557	LEU	2.9
1	A	510	TRP	2.9
1	A	375	LYS	2.9
1	A	469	LYS	2.9
1	A	497	ALA	2.9
1	A	559	LEU	2.9
1	A	550	LYS	2.9
1	A	708	PRO	2.9
1	B	302	LYS	2.9
1	B	550	LYS	2.9
1	A	621	THR	2.8
1	A	512	ALA	2.8
1	A	613	LYS	2.8
1	A	620	LYS	2.8
1	A	335	ILE	2.8
1	B	535	GLN	2.8
1	A	388	ILE	2.8
1	A	624	LEU	2.8
1	B	389	GLU	2.8
1	A	352	ASP	2.8
1	A	468	GLY	2.8
1	A	484	GLY	2.8
1	A	519	VAL	2.7
1	B	303	VAL	2.7
1	B	717	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	312	LEU	2.7
1	B	551	PHE	2.7
1	A	475	TRP	2.7
1	A	384	VAL	2.7
1	A	354	LEU	2.7
1	A	523	LEU	2.7
1	A	607	LEU	2.7
1	A	509	GLY	2.7
1	B	487	GLN	2.7
1	A	309	ASP	2.7
1	B	488	PRO	2.7
1	A	329	HIS	2.7
1	A	534	PHE	2.6
1	A	712	ASN	2.6
1	B	619	ARG	2.6
1	B	496	PRO	2.6
1	B	516	ARG	2.6
1	A	706	TYR	2.6
1	B	330	ILE	2.6
1	A	386	LYS	2.6
1	B	699	ARG	2.6
1	A	421	TRP	2.6
1	A	667	ARG	2.6
1	A	601	ASN	2.5
1	A	528	GLY	2.5
1	B	329	HIS	2.5
1	B	390	SER	2.5
1	A	358	ALA	2.5
1	B	499	VAL	2.5
1	B	715	VAL	2.5
1	B	517	PHE	2.5
1	A	311	VAL	2.5
1	B	385	ASN	2.4
1	A	302	LYS	2.4
1	A	598	TYR	2.4
1	A	306	TRP	2.4
1	A	522	LEU	2.4
1	B	490	GLY	2.4
1	B	538	PRO	2.4
1	A	535	GLN	2.4
1	B	606	ILE	2.4
1	B	497	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	510	TRP	2.4
1	A	530	ASP	2.4
1	B	620	LYS	2.4
1	A	648	ILE	2.4
1	A	524	LEU	2.3
1	A	556	ASP	2.3
1	B	367	SER	2.3
1	A	452	LYS	2.3
1	A	545	PRO	2.3
1	A	378	MET	2.3
1	A	611	ALA	2.3
1	A	366	TYR	2.3
1	A	639	TYR	2.3
1	A	631	VAL	2.3
1	A	615	ASP	2.3
1	A	513	PRO	2.3
1	B	549	PRO	2.3
1	A	435	ALA	2.3
1	A	505	CYS	2.3
1	A	381	LEU	2.3
1	B	557	LEU	2.3
1	B	554	PHE	2.3
1	A	687	ILE	2.3
1	B	388	ILE	2.3
1	A	637	VAL	2.3
1	B	337	LEU	2.2
1	B	392	SER	2.2
1	B	602[A]	SER	2.2
1	B	617	ASP	2.2
1	A	504	ILE	2.2
1	B	327	THR	2.2
1	B	625	TRP	2.2
1	B	716	TRP	2.2
1	A	605	ASN	2.2
1	A	370	LYS	2.2
1	A	542	LEU	2.2
1	A	365	TYR	2.2
1	B	366	TYR	2.2
1	A	710	PRO	2.2
1	B	511	LYS	2.2
1	B	500	GLN	2.2
1	A	312	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	423	LYS	2.2
1	A	336	MET	2.1
1	A	382	GLU	2.1
1	A	508	GLN	2.1
1	B	328	GLU	2.1
1	B	612	LYS	2.1
1	B	320	SER	2.1
1	A	356	PRO	2.1
1	A	439	PHE	2.1
1	B	324	THR	2.1
1	B	615	ASP	2.1
1	B	513	PRO	2.1
1	A	635	ILE	2.1
1	A	610	VAL	2.1
1	A	630	LEU	2.1
1	A	602	SER	2.1
1	A	608	GLU	2.1
1	A	609	GLU	2.1
1	A	625	TRP	2.1
1	A	643	SER	2.1
1	A	315	THR	2.1
1	A	393	THR	2.1
1	A	516	ARG	2.1
1	A	531	PRO	2.1
1	A	606	ILE	2.1
1	A	666	TYR	2.1
1	B	536	ILE	2.1
1	A	325	GLY	2.1
1	A	515	GLY	2.1
1	A	503	GLU	2.1
1	A	618	MET	2.1
1	A	308	THR	2.1
1	A	714	HIS	2.1
1	A	482	TYR	2.1
1	B	335	ILE	2.1
1	B	369	ILE	2.1
1	B	485	TYR	2.1
1	A	389	GLU	2.0
1	A	390	SER	2.0
1	B	308	THR	2.0
1	A	538	PRO	2.0
1	A	628	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	306	TRP	2.0
1	A	470	HIS	2.0
1	A	660	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

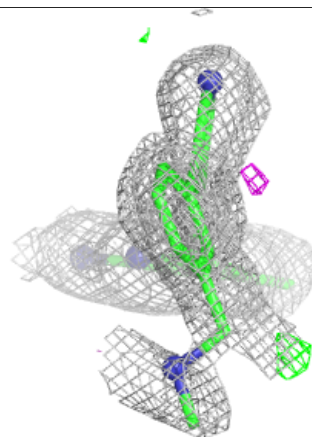
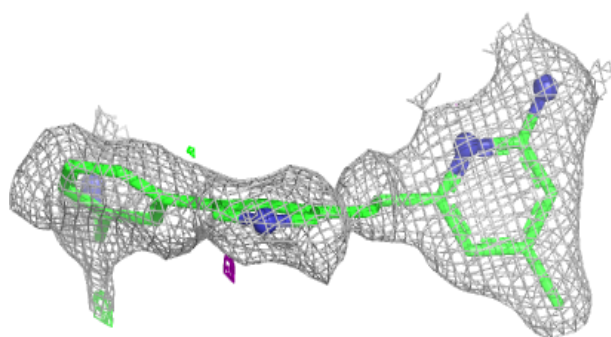
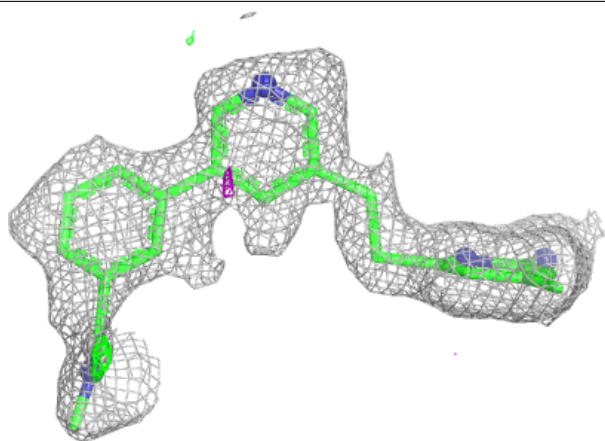
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	A	804	4/4	0.80	0.22	66,67,70,74	0
5	ACT	B	804	4/4	0.83	0.17	52,52,57,59	0
4	W79	A	803	25/25	0.85	0.16	28,49,61,66	0
3	H4B	A	802	17/17	0.86	0.11	27,30,37,37	0
4	W79	B	803	25/25	0.86	0.15	26,50,65,66	0
3	H4B	B	802	17/17	0.89	0.10	25,30,34,38	0
2	HEM	A	801	43/43	0.95	0.10	22,32,42,50	0
2	HEM	B	801	43/43	0.95	0.10	21,33,42,49	0
6	ZN	A	805	1/1	0.99	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.

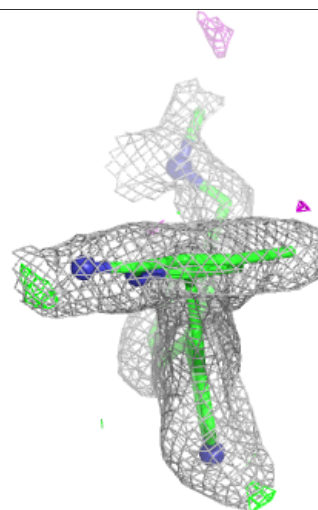
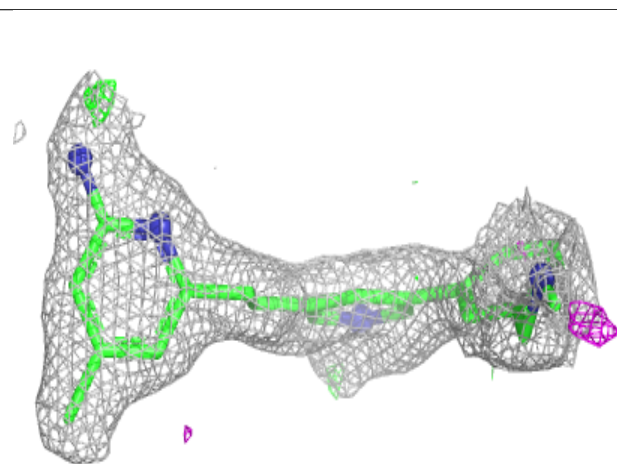
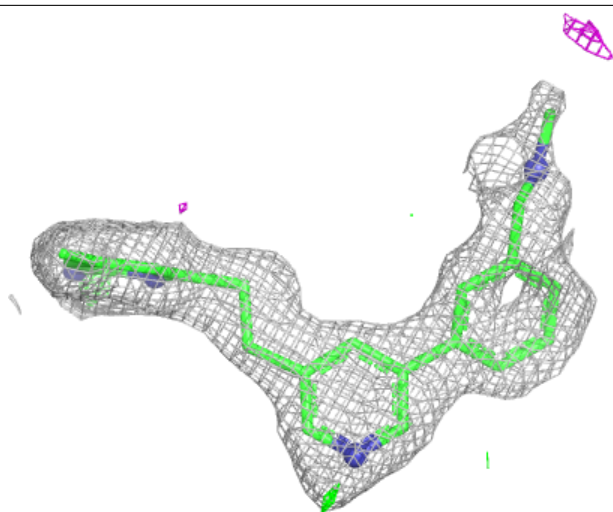
Electron density around W79 A 803:

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



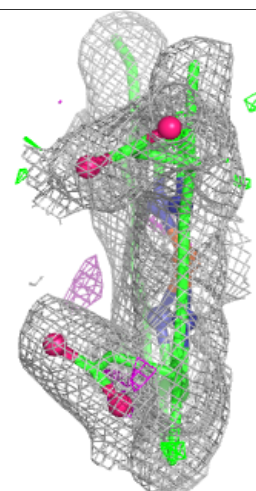
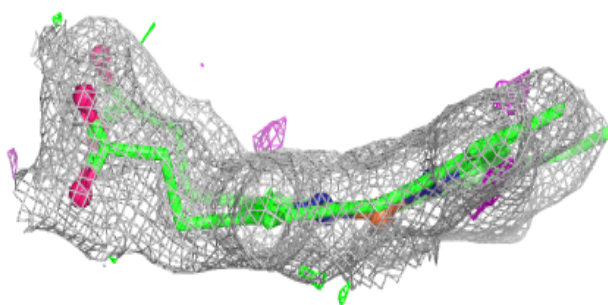
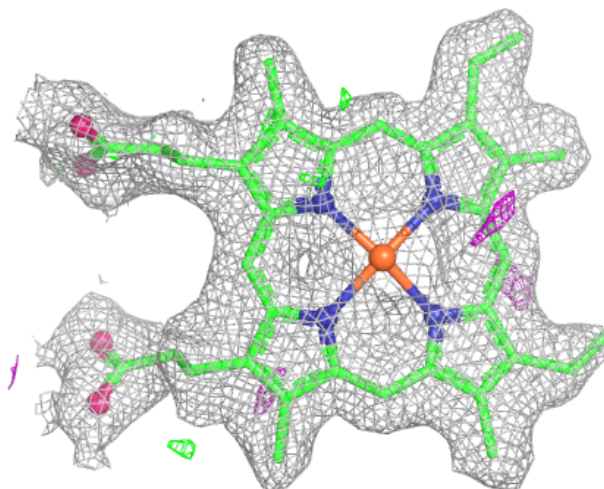
Electron density around W79 B 803:

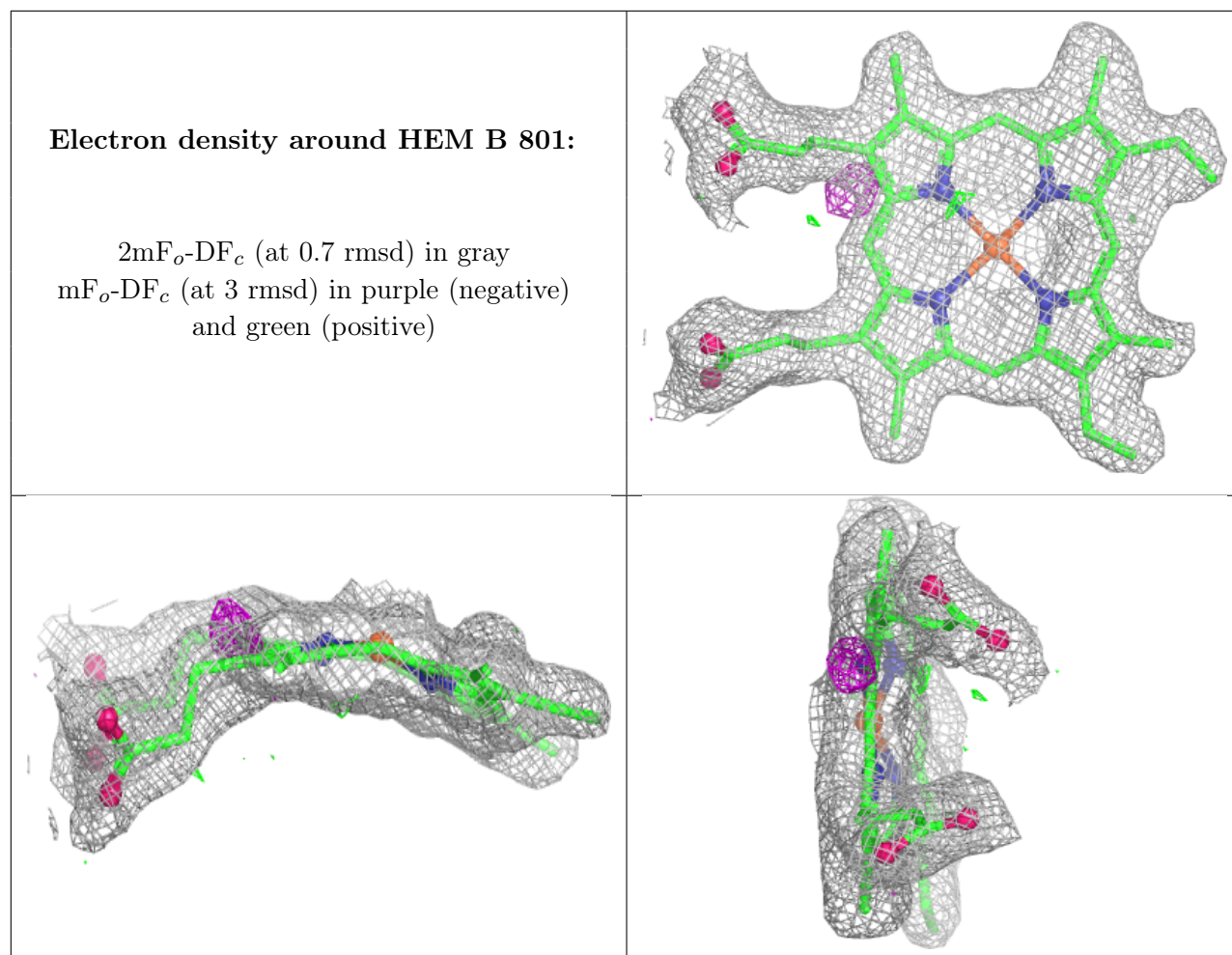
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

There are no such residues in this entry.