



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:19 pm BST

PDB ID : 3NNZ  
Title : Structure of rat neuronal nitric oxide synthase heme domain complexed with 6-(((3S,4S)-4-(2-(3-Fluorophenethylamino)ethoxy)pyrrolidin-3-yl)methyl)pyridin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2010-06-24  
Resolution : 1.97 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](mailto: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.

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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

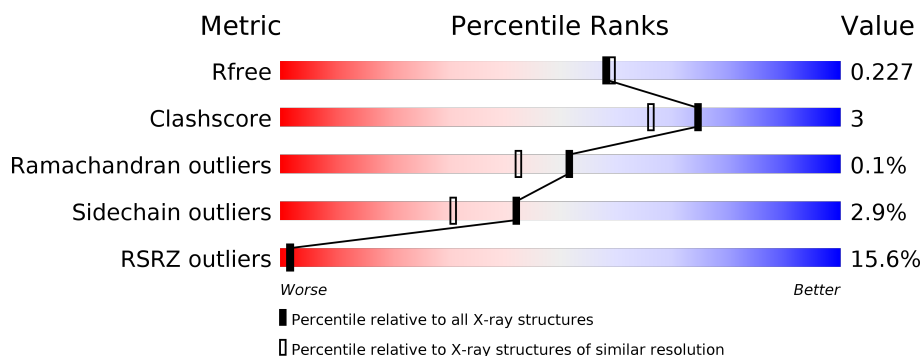
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.97 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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  $\geq 3$ , 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	<div> <div>21%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>••</div> </div> </div>
1	B	422	<div> <div>10%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>•</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7312 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
			3316	2123	566	605	22			
1	B	411	Total	C	N	O	S	0	3	0
			3354	2146	574	612	22			

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



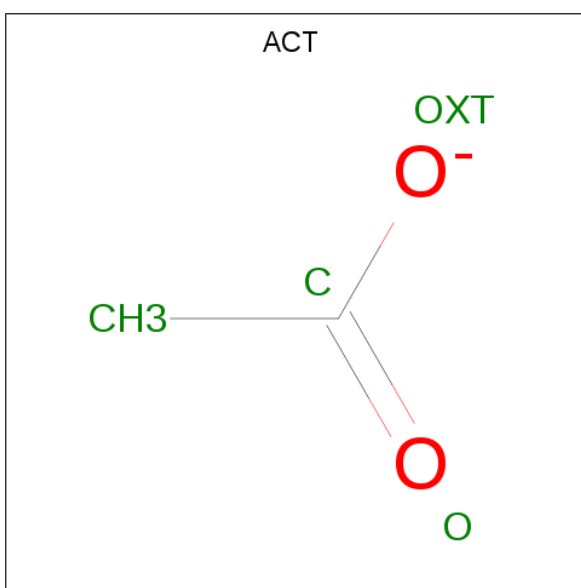
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



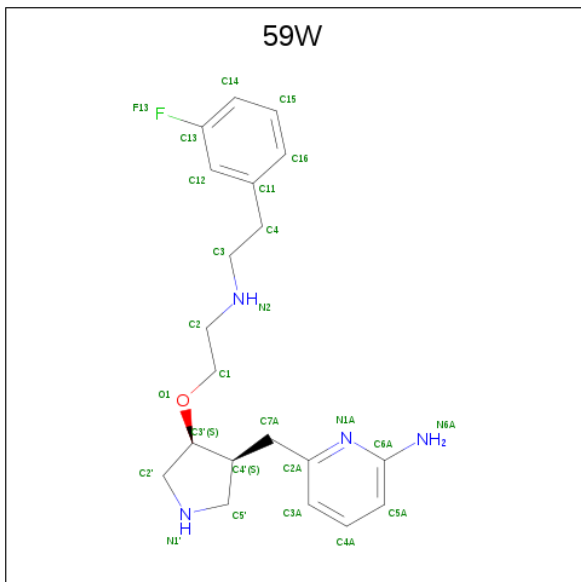
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 5 is 6-{{[(3S,4S)-4-(2-{{[2-(3-fluorophenyl)ethyl]amino}ethoxy)pyrrolidin-3-yl]methyl}pyridin-2-amine (three-letter code: 59W) (formula: C<sub>20</sub>H<sub>27</sub>FN<sub>4</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	N	O	0	0
			26	20	1	4	1		
5	B	1	Total	C	F	N	O	0	0
			26	20	1	4	1		

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

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

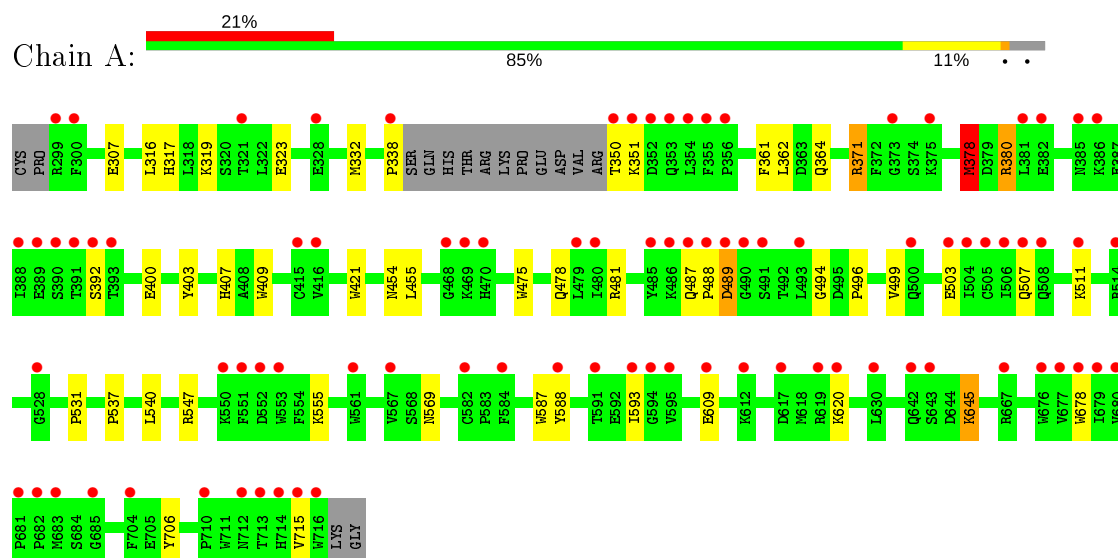
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	199	Total	O	0	0
			199	199		
7	B	262	Total	O	0	0
			262	262		

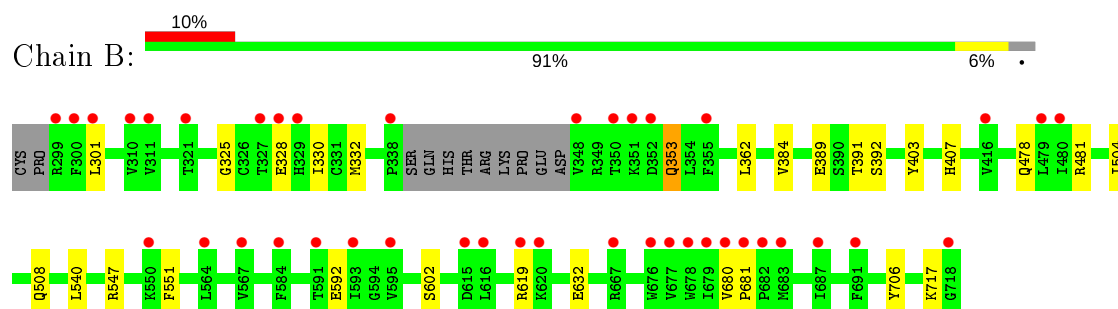
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	52.05Å 110.98Å 164.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.64 – 1.97 37.96 – 1.97	Depositor EDS
% Data completeness (in resolution range)	97.8 (38.64-1.97) 97.8 (37.96-1.97)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.78 (at 1.97Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.179 , 0.213 0.197 , 0.227	Depositor DCC
$R_{free}$ test set	3313 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7312	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, ZN, H4B, 59W, ACT

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	0/3412	0.63	0/4629
1	B	0.66	0/3456	0.65	0/4685
All	All	0.63	0/6868	0.64	0/9314

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	378	MET	Mainchain

### 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	3316	0	3226	28	0
1	B	3354	0	3274	16	0
2	A	43	0	30	1	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	26	0	27	1	0
5	B	26	0	27	2	0
6	A	1	0	0	0	0
7	A	199	0	0	0	0
7	B	262	0	0	2	0
All	All	7312	0	6650	43	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 (43) 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:B:706:TYR:OH	2:B:750:HEM:O1D	2.02	0.77
1:A:371:ARG:HH21	1:A:371:ARG:HG3	1.50	0.76
1:A:371:ARG:HH21	1:A:371:ARG:CG	2.07	0.67
1:B:717:LYS:NZ	7:B:1177:HOH:O	2.31	0.63
1:A:307:GLU:HG3	7:B:1260:HOH:O	1.98	0.62
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.82	0.62
1:A:499:VAL:O	1:A:503:GLU:HG3	2.03	0.59
1:A:380:ARG:HD3	1:A:400:GLU:OE1	2.04	0.58
1:A:351:LYS:HE2	1:A:392:SER:HB3	1.87	0.57
1:B:592:GLU:OE1	5:B:800:59W:H5'A	2.05	0.57
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.87	0.56
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.89	0.55
1:A:371:ARG:CG	1:A:371:ARG:NH2	2.68	0.53
1:A:487:GLN:HB3	1:A:488:PRO:HD2	1.91	0.53
2:B:750:HEM:HBB2	2:B:750:HEM:HHC	1.90	0.53
1:A:378:MET:HA	1:A:378:MET:CE	2.40	0.52
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.41	0.51
1:A:537:PRO:HB2	1:A:540:LEU:HG	1.94	0.49
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.01	0.49
1:A:706:TYR:OH	2:A:750:HEM:O1D	2.19	0.47
1:B:619:ARG:HE	1:B:619:ARG:HB2	1.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PHE:O	1:A:364:GLN:HG2	2.15	0.46
1:A:487:GLN:HB3	1:A:488:PRO:CD	2.46	0.46
1:A:316:LEU:HD12	1:A:319:LYS:HD2	1.96	0.46
1:B:391:THR:O	1:B:392:SER:HB2	2.15	0.46
1:A:475:TRP:CE2	1:A:531:PRO:HG3	2.52	0.45
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.53	0.44
1:A:332:MET:CE	1:B:301:LEU:HD22	2.48	0.43
1:B:504:ILE:O	1:B:508:GLN:HG2	2.18	0.43
1:B:551:PHE:HE2	1:B:632:GLU:HG3	1.83	0.42
1:A:494:GLY:O	1:A:496:PRO:HD3	2.20	0.41
1:B:353:GLN:HE21	1:B:353:GLN:HB3	1.68	0.41
1:A:317:HIS:HB2	1:B:330:ILE:HD12	2.03	0.41
1:B:362:LEU:HD11	1:B:384:VAL:HG21	2.01	0.41
1:B:325:GLY:O	1:B:332:MET:HG3	2.21	0.41
2:B:750:HEM:HBA2	5:B:800:59W:H7AA	2.03	0.41
1:A:678:TRP:HH2	5:A:800:59W:H3	1.85	0.41
1:A:323:GLU:HG2	1:B:328:GLU:HB3	2.01	0.41
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.09	0.40
1:A:645:LYS:HE3	1:A:645:LYS:HB2	1.89	0.40
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.93	0.40
1:A:362:LEU:HA	1:A:362:LEU:HD23	1.93	0.40
1:A:588:TYR:CD1	1:A:593:ILE:HD11	2.56	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%)	395 (98%)	8 (2%)	1 (0%)	47	38
1	B	410/422 (97%)	406 (99%)	4 (1%)	0	100	100
All	All	814/844 (96%)	801 (98%)	12 (2%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	ASP

### 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	364/377 (97%)	348 (96%)	16 (4%)	28	16
1	B	369/377 (98%)	363 (98%)	6 (2%)	62	56
All	All	733/754 (97%)	711 (97%)	22 (3%)	42	29

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	PRO
1	A	350	THR
1	A	371	ARG
1	A	378	MET
1	A	380	ARG
1	A	454	ASN
1	A	489	ASP
1	A	507	GLN
1	A	511	LYS
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	609	GLU
1	A	620	LYS
1	A	645	LYS
1	A	715	VAL
1	B	353	GLN
1	B	389	GLU
1	B	540	LEU
1	B	547	ARG
1	B	602[A]	SER
1	B	602[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	353	GLN
1	A	454	ASN
1	A	569	ASN
1	A	601	ASN
1	A	605	ASN
1	A	697	ASN
1	B	364	GLN
1	B	454	ASN
1	B	507	GLN
1	B	601	ASN
1	B	605	ASN
1	B	642	GLN
1	B	697	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	760	-	16,18,18	0.95	0	11,26,26	3.01	7 (63%)
5	59W	A	800	-	27,28,28	0.69	1 (3%)	29,36,36	1.61	6 (20%)
3	H4B	B	760	-	16,18,18	1.33	2 (12%)	11,26,26	2.64	7 (63%)
5	59W	B	800	-	27,28,28	0.85	1 (3%)	29,36,36	1.54	4 (13%)
4	ACT	A	860	-	1,3,3	1.27	0	0,3,3	0.00	-
2	HEM	B	750	1	27,50,50	2.25	9 (33%)	17,82,82	2.24	7 (41%)
2	HEM	A	750	1	27,50,50	2.14	7 (25%)	17,82,82	2.09	6 (35%)
4	ACT	B	860	-	1,3,3	1.21	0	0,3,3	0.00	-

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	760	-	-	0/8/17/17	0/2/2/2
5	59W	A	800	-	-	2/13/23/23	0/3/3/3
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
5	59W	B	800	-	-	2/13/23/23	0/3/3/3
2	HEM	B	750	1	-	0/6/54/54	-
2	HEM	A	750	1	-	0/6/54/54	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3B-C2B	-4.81	1.33	1.40
2	A	750	HEM	C3D-C2D	4.73	1.51	1.37
2	B	750	HEM	C3C-C2C	-4.72	1.33	1.40
2	B	750	HEM	C3B-C2B	-4.47	1.34	1.40
2	B	750	HEM	C3C-CAC	3.87	1.55	1.47
2	A	750	HEM	C3C-C2C	-3.81	1.35	1.40
2	B	750	HEM	C3D-C2D	3.59	1.48	1.37
2	B	750	HEM	C3B-CAB	3.54	1.55	1.47
2	A	750	HEM	C3C-CAC	3.54	1.55	1.47
2	A	750	HEM	C3B-CAB	3.53	1.55	1.47
2	B	750	HEM	CAA-C2A	3.36	1.57	1.52
3	B	760	H4B	C7-C6	3.27	1.55	1.52
5	B	800	59W	C7A-C4'	2.35	1.57	1.53
2	B	750	HEM	CAD-C3D	2.31	1.56	1.52
3	B	760	H4B	C7-N8	2.24	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	CMA-C3A	2.22	1.56	1.51
2	B	750	HEM	CMD-C2D	2.18	1.56	1.51
2	A	750	HEM	CMB-C2B	2.10	1.56	1.51
5	A	800	59W	C14-C13	2.07	1.41	1.37
2	A	750	HEM	CAA-C2A	2.05	1.55	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	H4B	C4-C4A-C8A	5.51	119.46	114.57
2	A	750	HEM	CBD-CAD-C3D	-5.40	102.53	112.48
3	B	760	H4B	C4-C4A-C8A	5.12	119.12	114.57
5	B	800	59W	C6A-N1A-C2A	4.99	121.88	118.10
2	B	750	HEM	CBD-CAD-C3D	-4.94	103.38	112.48
5	A	800	59W	C6A-N1A-C2A	4.70	121.67	118.10
2	B	750	HEM	CBA-CAA-C2A	-4.55	104.09	112.49
3	B	760	H4B	C4-N3-C2	4.10	122.45	115.93
3	A	760	H4B	C4-N3-C2	4.05	122.37	115.93
3	A	760	H4B	N3-C2-N1	-3.82	119.43	125.42
2	A	750	HEM	CBA-CAA-C2A	-3.66	105.73	112.49
2	B	750	HEM	CMA-C3A-C4A	-3.28	123.42	128.46
5	A	800	59W	C5'-N1'-C2'	3.25	113.10	105.42
3	B	760	H4B	N3-C2-N1	-3.19	120.41	125.42
3	A	760	H4B	C4-C4A-N5	3.19	121.80	119.12
5	B	800	59W	C3A-C2A-N1A	-3.16	118.41	122.41
5	A	800	59W	C3A-C2A-N1A	-3.15	118.42	122.41
3	A	760	H4B	N2-C2-N3	3.13	122.12	117.25
3	A	760	H4B	C2-N1-C8A	2.93	121.10	114.54
2	A	750	HEM	CMC-C2C-C3C	2.87	130.04	124.68
5	B	800	59W	C5'-N1'-C2'	2.57	111.48	105.42
2	B	750	HEM	C1D-C2D-C3D	-2.49	105.26	107.00
5	A	800	59W	C14-C13-C12	-2.28	120.33	123.29
3	B	760	H4B	C2-N1-C8A	2.22	119.51	114.54
2	A	750	HEM	C4C-C3C-C2C	2.21	108.44	106.90
3	B	760	H4B	N2-C2-N3	2.19	120.67	117.25
2	B	750	HEM	CMA-C3A-C2A	2.18	129.05	124.94
3	B	760	H4B	C4-C4A-N5	2.18	120.95	119.12
5	A	800	59W	F13-C13-C14	2.17	122.23	118.54
3	A	760	H4B	C4A-C4-N3	-2.16	117.87	124.01
5	B	800	59W	C14-C13-C12	-2.15	120.50	123.29
2	B	750	HEM	C4C-C3C-C2C	2.14	108.39	106.90
2	B	750	HEM	CMC-C2C-C3C	2.09	128.58	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	750	HEM	CAA-CBA-CGA	-2.05	109.23	112.67
3	B	760	H4B	C4A-C4-N3	-2.04	118.22	124.01
2	A	750	HEM	C1D-C2D-C3D	-2.02	105.59	107.00
5	A	800	59W	C2A-C7A-C4'	-2.01	108.92	115.55

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	800	59W	C4'-C3'-O1-C1
5	B	800	59W	C4'-C3'-O1-C1
5	A	800	59W	C2'-C3'-O1-C1
5	B	800	59W	C2'-C3'-O1-C1

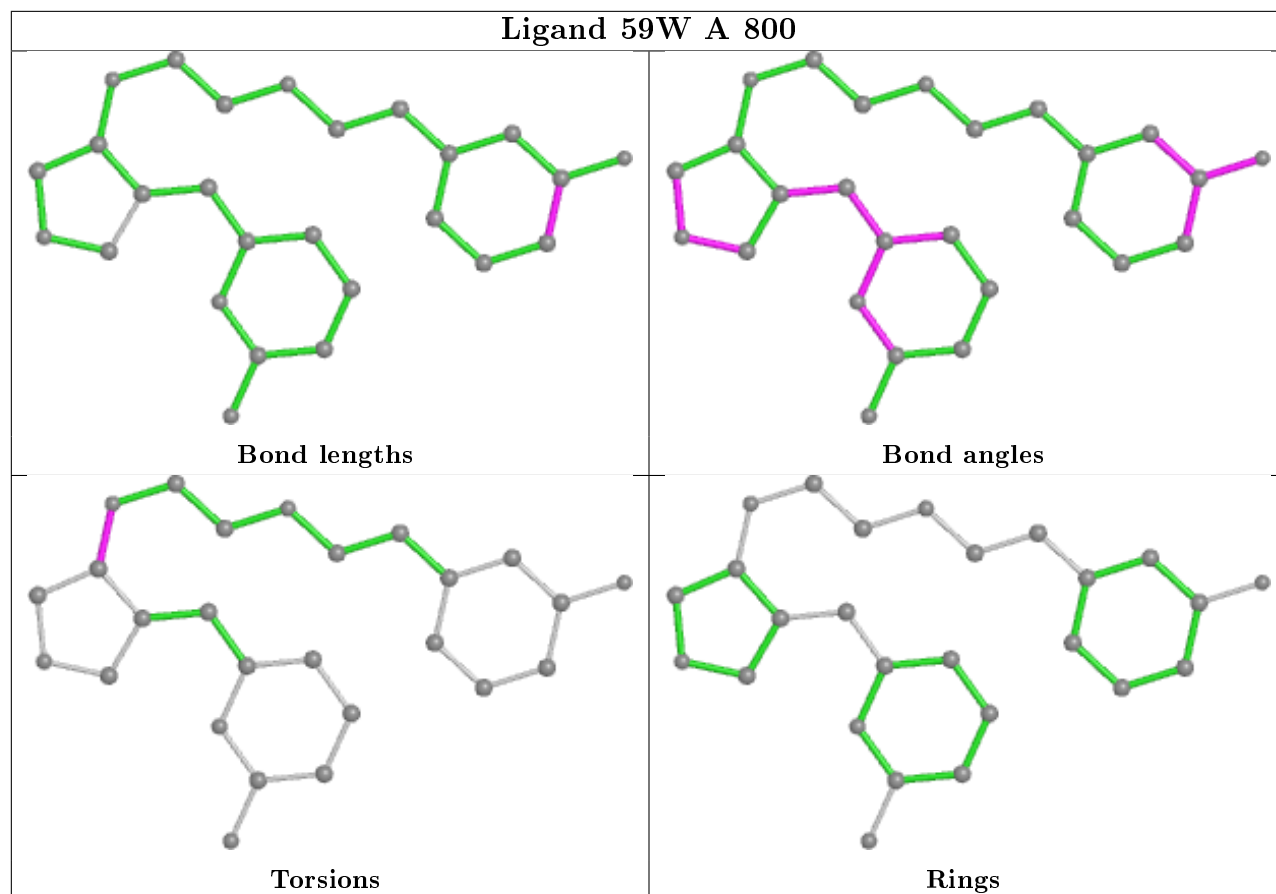
There are no ring outliers.

4 monomers are involved in 6 short contacts:

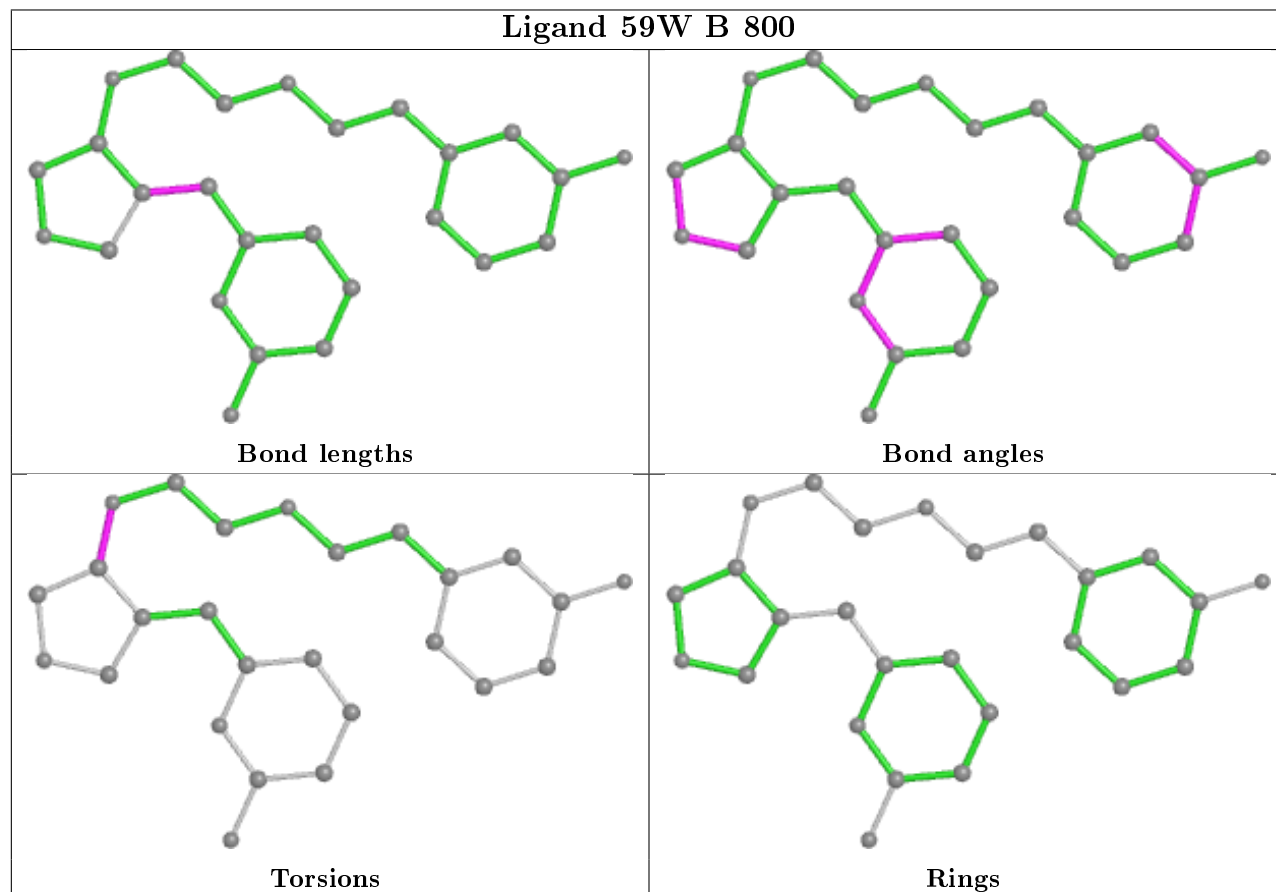
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	59W	1	0
5	B	800	59W	2	0
2	B	750	HEM	3	0
2	A	750	HEM	1	0

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

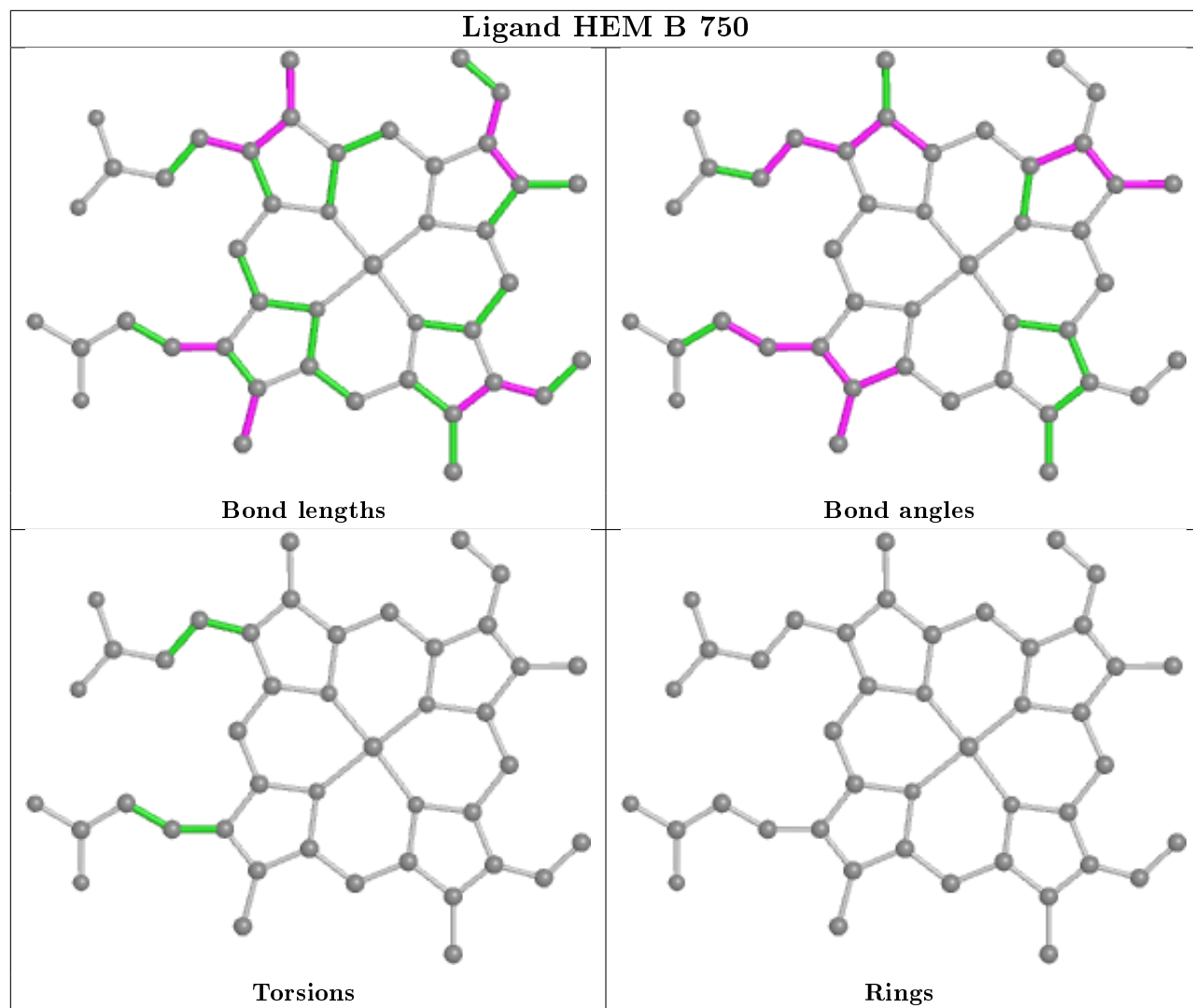
## Ligand 59W A 800

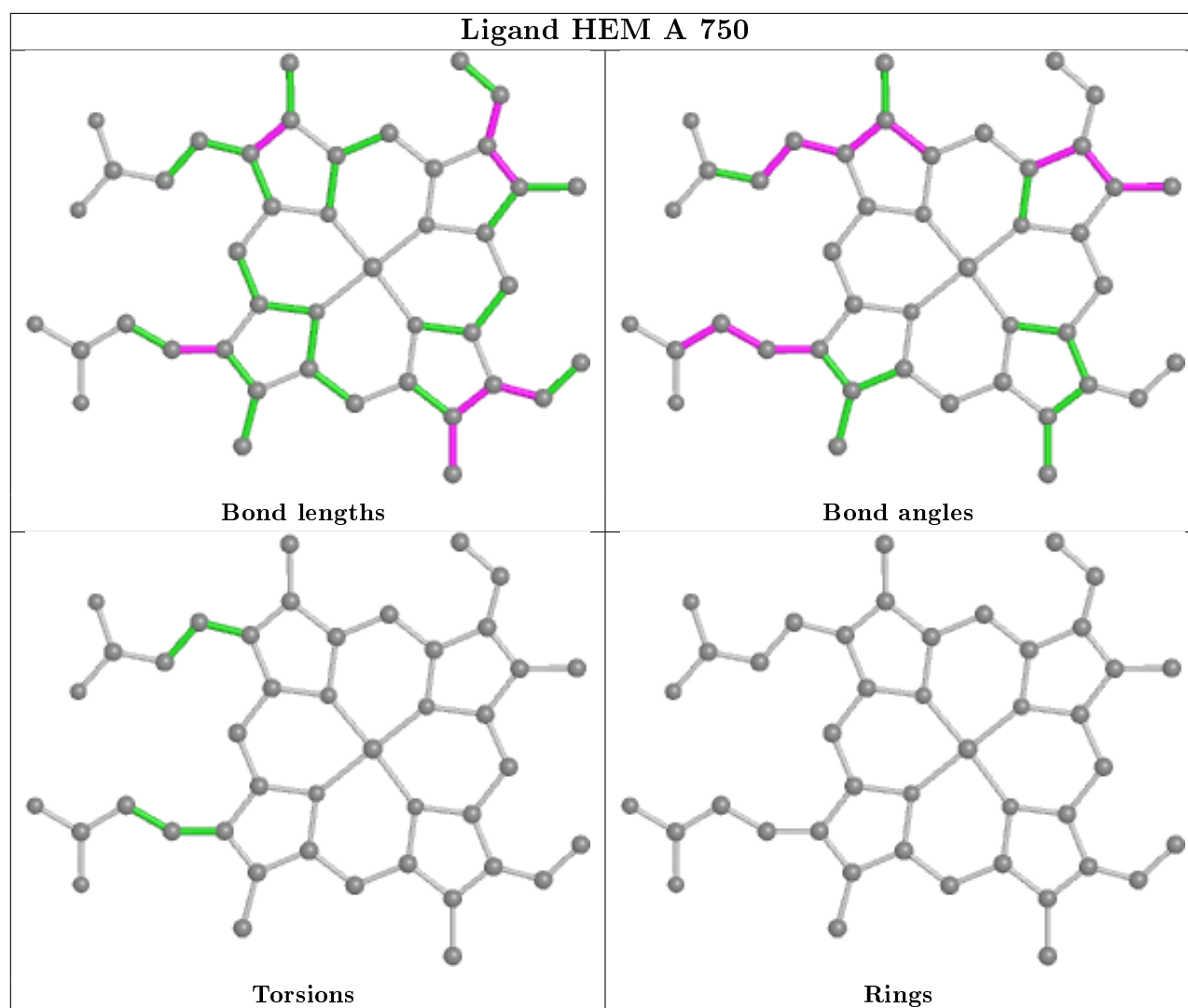


## Ligand 59W B 800









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	407/422 (96%)	1.14	87 (21%) <b>0</b> <b>0</b>	24, 49, 90, 117	0
1	B	411/422 (97%)	0.51	41 (9%) <b>7</b> <b>8</b>	24, 37, 61, 78	0
All	All	818/844 (96%)	0.82	128 (15%) <b>2</b> <b>2</b>	24, 41, 83, 117	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	8.9
1	A	715	VAL	8.0
1	A	355	PHE	7.5
1	A	716	TRP	7.1
1	A	488	PRO	6.7
1	A	506	ILE	5.9
1	A	388	ILE	5.3
1	B	619	ARG	5.3
1	A	392	SER	5.2
1	A	486	LYS	5.2
1	A	503	GLU	5.2
1	A	491	SER	5.1
1	A	300	PHE	5.0
1	A	386	LYS	5.0
1	B	350	THR	4.9
1	A	350	THR	4.6
1	A	351	LYS	4.5
1	A	385	ASN	4.5
1	A	490	GLY	4.4
1	A	619	ARG	4.2
1	A	352	ASP	4.2
1	B	620	LYS	4.1
1	B	348	VAL	4.0
1	A	391	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	507	GLN	3.9
1	A	354	LEU	3.8
1	A	470	HIS	3.8
1	A	567	VAL	3.6
1	A	682	PRO	3.6
1	A	677	VAL	3.5
1	A	713	THR	3.5
1	B	479	LEU	3.5
1	A	393	THR	3.4
1	A	712	ASN	3.4
1	A	714	HIS	3.4
1	A	584	PHE	3.3
1	A	479	LEU	3.3
1	B	667	ARG	3.1
1	A	489	ASP	3.1
1	A	680	VAL	3.0
1	B	616	LEU	3.0
1	B	299	ARG	3.0
1	A	511	LYS	3.0
1	A	643	SER	3.0
1	B	679	ILE	3.0
1	B	567	VAL	3.0
1	A	550	LYS	2.9
1	B	310	VAL	2.9
1	B	691	PHE	2.9
1	A	595	VAL	2.9
1	A	389	GLU	2.9
1	A	469	LYS	2.9
1	A	514	ARG	2.9
1	A	416	VAL	2.9
1	A	353	GLN	2.8
1	A	678	TRP	2.8
1	A	617	ASP	2.8
1	A	667	ARG	2.8
1	A	504	ILE	2.8
1	A	487	GLN	2.8
1	A	679	ILE	2.8
1	A	390	SER	2.7
1	A	593	ILE	2.7
1	B	682	PRO	2.7
1	B	677	VAL	2.7
1	A	356	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	676	TRP	2.7
1	A	382	GLU	2.7
1	A	321	THR	2.7
1	B	680	VAL	2.7
1	A	480	ILE	2.6
1	A	552	ASP	2.6
1	A	642	GLN	2.6
1	A	681	PRO	2.6
1	B	355	PHE	2.6
1	B	595	VAL	2.6
1	B	718	GLY	2.6
1	A	508	GLN	2.6
1	A	683	MET	2.6
1	B	681	PRO	2.6
1	B	301	LEU	2.5
1	A	299	ARG	2.5
1	A	415	CYS	2.5
1	B	615	ASP	2.5
1	B	683	MET	2.5
1	B	591	THR	2.5
1	A	594	GLY	2.5
1	A	704	PHE	2.5
1	A	553	TRP	2.4
1	B	327	THR	2.4
1	A	685	GLY	2.4
1	A	338	PRO	2.4
1	A	551	PHE	2.3
1	B	311	VAL	2.3
1	B	351	LYS	2.3
1	A	485	TYR	2.3
1	A	328	GLU	2.3
1	A	612	LYS	2.3
1	B	550	LYS	2.3
1	B	328	GLU	2.2
1	B	352	ASP	2.2
1	B	416	VAL	2.2
1	A	505	CYS	2.2
1	B	329	HIS	2.2
1	B	480	ILE	2.2
1	B	321	THR	2.2
1	B	593	ILE	2.2
1	B	687	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	338	PRO	2.2
1	A	630	LEU	2.2
1	B	564	LEU	2.2
1	A	591	THR	2.2
1	B	676	TRP	2.2
1	A	373	GLY	2.1
1	A	609	GLU	2.1
1	A	381	LEU	2.1
1	A	561	TRP	2.1
1	B	678	TRP	2.1
1	A	710	PRO	2.1
1	A	500	GLN	2.1
1	A	375	LYS	2.1
1	A	468	GLY	2.1
1	A	620	LYS	2.1
1	A	588	TYR	2.0
1	A	528	GLY	2.0
1	A	493	LEU	2.0
1	B	584	PHE	2.0
1	A	582	CYS	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 carbohydrates 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	59W	B	800	26/26	0.88	0.23	32,41,53,55	0
4	ACT	A	860	4/4	0.90	0.17	53,55,56,56	0
5	59W	A	800	26/26	0.91	0.23	31,40,57,60	0

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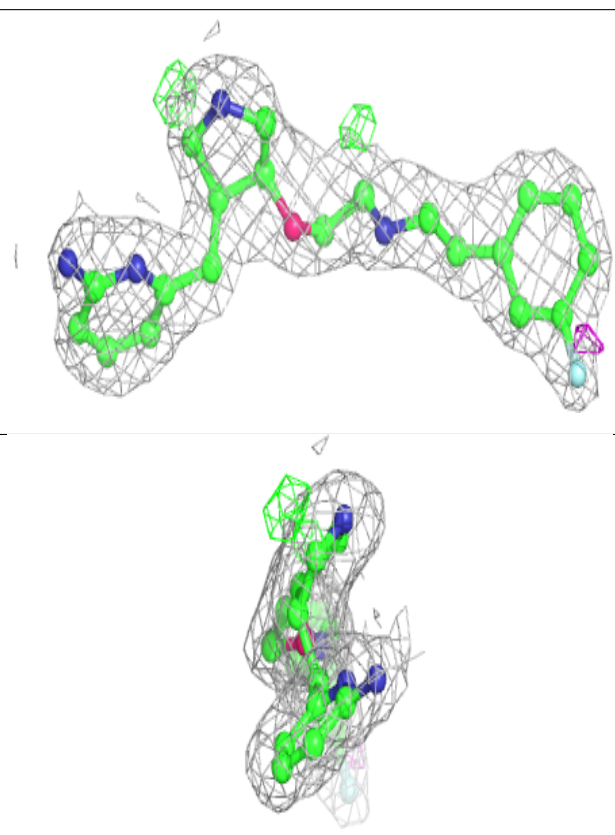
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	H4B	A	760	17/17	0.96	0.21	27,29,33,33	0
3	H4B	B	760	17/17	0.97	0.19	24,29,31,34	0
2	HEM	B	750	43/43	0.97	0.18	21,26,36,44	0
2	HEM	A	750	43/43	0.97	0.20	23,29,39,41	0
4	ACT	B	860	4/4	0.97	0.12	40,42,44,44	0
6	ZN	A	900	1/1	1.00	0.04	33,33,33,33	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.

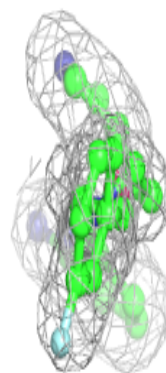
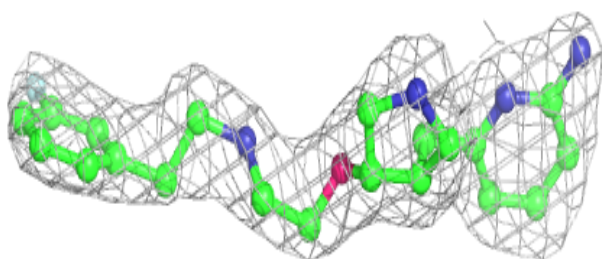
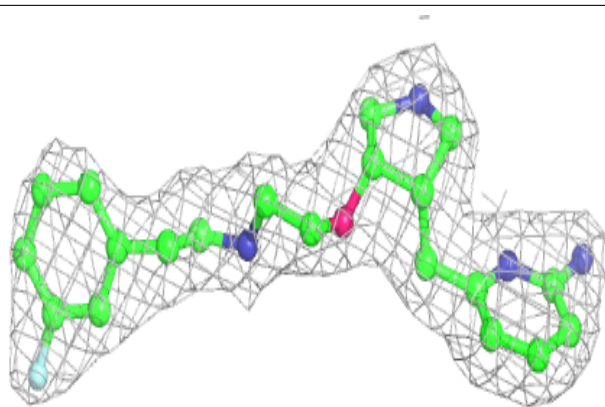
**Electron density around 59W B 800:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 59W A 800:**

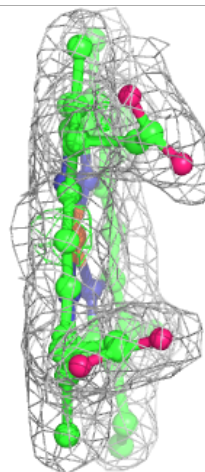
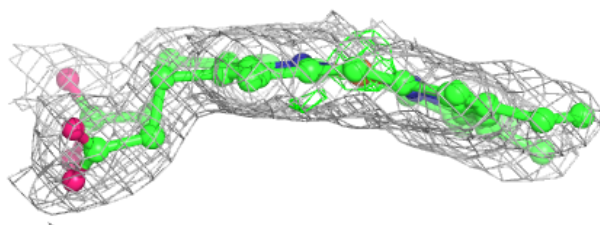
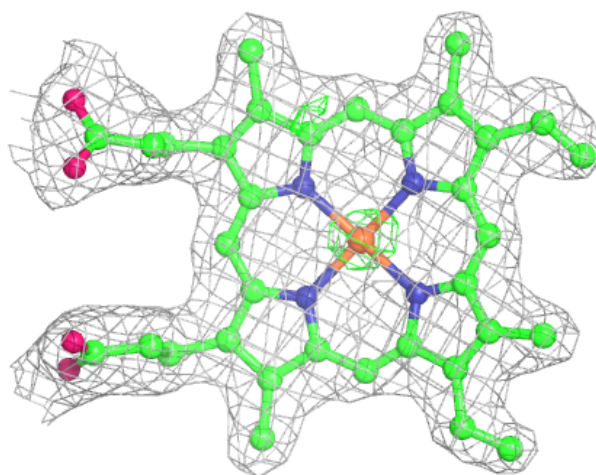
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





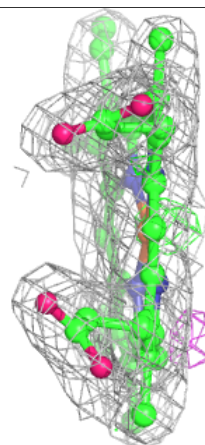
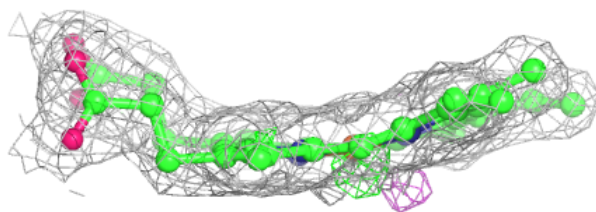
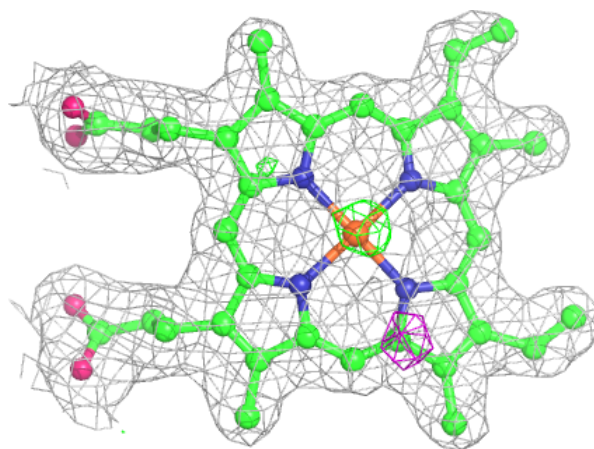
**Electron density around HEM B 750:**

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



**Electron density around HEM A 750:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.