



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 08:24 am BST

PDB ID : 4V3Z  
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with 2-(2-(1H-imidazol-1-yl)pyrimidin-4-yl)-N-(2-(3- fluorophenyl)cyclopropylmethyl)ethan-1-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2014-10-20  
Resolution : 2.05 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

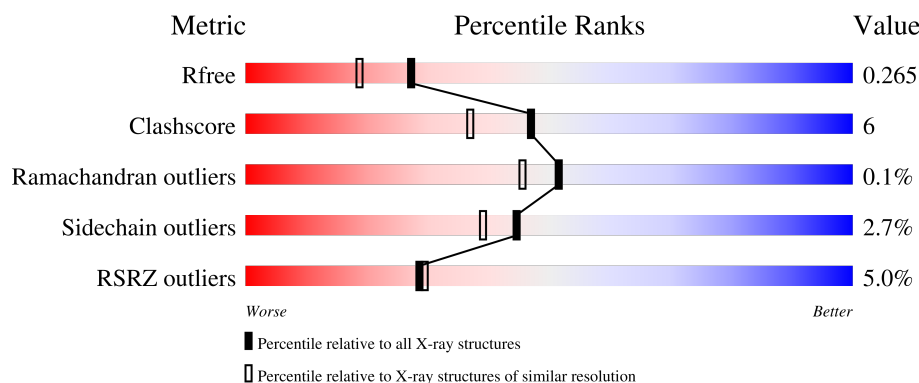
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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  $\geq 3$ , 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>7%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>
1	B	422	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7104 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.

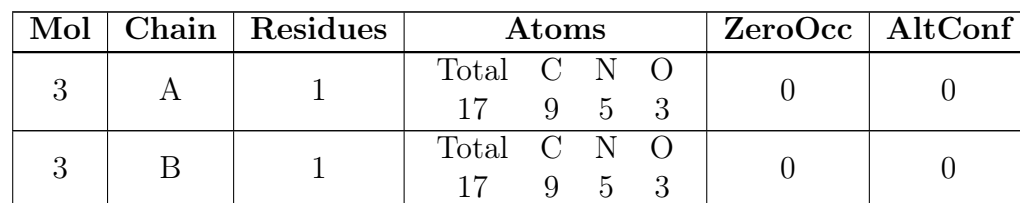
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	2	1
			3317	2123	567	605	22			
1	B	411	Total	C	N	O	S	0	2	0
			3354	2146	574	613	21			

- 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:  $C_9H_{15}N_5O_3$ ).



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- The chemical structure of 9HL is shown. It consists of a pyridine ring (N11, N13, C12, C14, C15, C16) connected via a methylene chain (C17, C18) to a secondary amine (N19). The amine is further connected to a carbonyl group (C20), which is linked to a cyclopropane ring (C21, C22, C23). The cyclopropane ring is substituted with a 4-fluorophenyl group (C1', C2', C3', C4', C5', C6') and a fluorine atom (F7).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			25	19	1	5		



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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	F	N	0	0
			25	19	1	5		

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



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

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

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

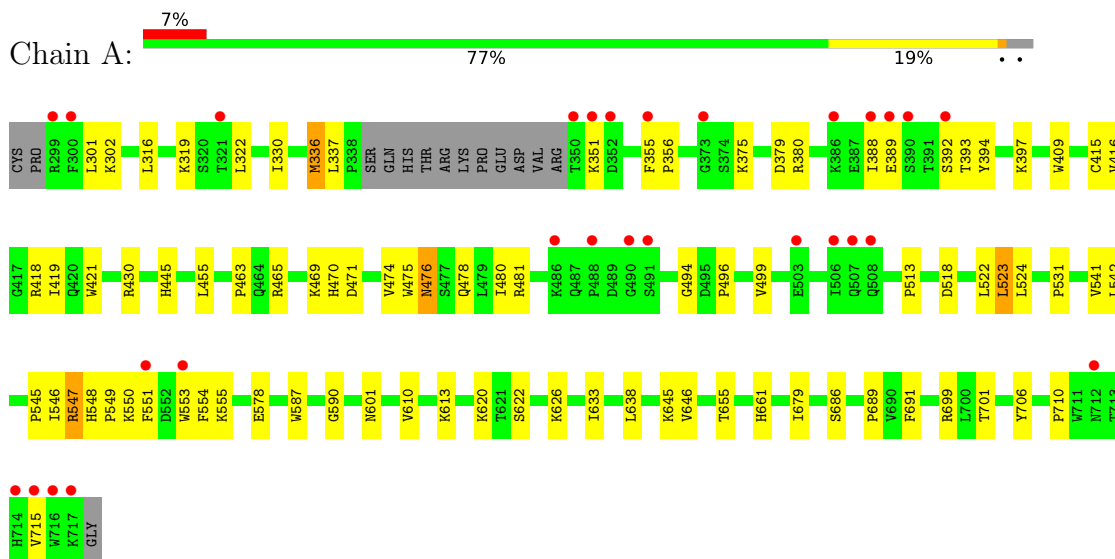
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	118	Total	O	0	0
			118	118		
7	B	136	Total	O	0	0
			136	136		

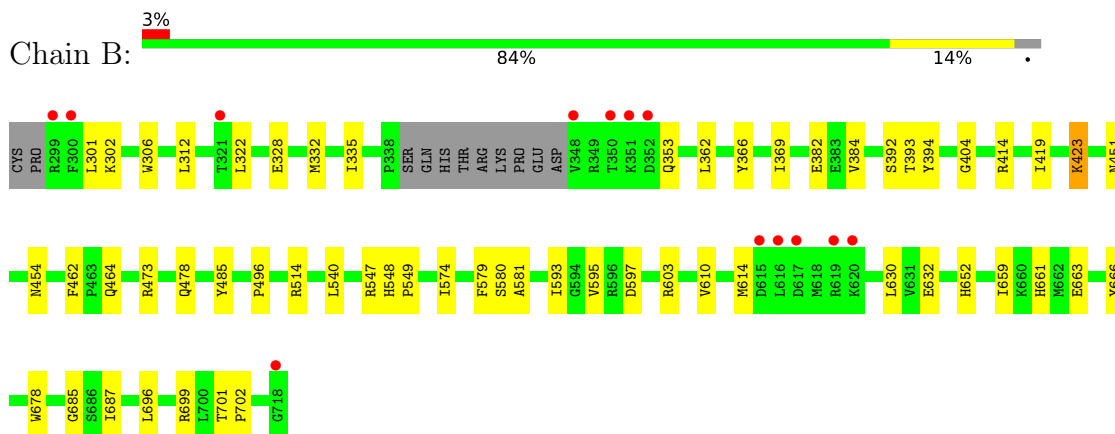
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	51.79Å 111.05Å 164.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.97 – 2.05 38.97 – 2.05	Depositor EDS
% Data completeness (in resolution range)	70.6 (38.97-2.05) 70.6 (38.97-2.05)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.42 (at 2.05Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.196 , 0.265 0.196 , 0.265	Depositor DCC
$R_{free}$ test set	2084 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.8	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	0.93	EDS
Total number of atoms	7104	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9HL, H4B, HEM, ACT, ZN

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	0/3413	0.57	0/4631
1	B	0.41	0/3453	0.57	0/4681
All	All	0.41	0/6866	0.57	0/9312

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	3317	0	3226	50	0
1	B	3354	0	3270	32	0
2	A	43	0	30	6	0
2	B	43	0	30	1	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	25	0	20	1	0
4	B	25	0	20	1	0
5	A	4	0	3	1	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	118	0	0	1	0
7	B	136	0	0	2	0
All	All	7104	0	6632	83	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 6.

All (83) 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:A:750:HEM:HMC2	2:A:750:HEM:HBC2	1.62	0.80
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.52	0.74
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.72	0.72
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.79	0.64
1:A:375:LYS:NZ	1:A:379:ASP:OD2	2.30	0.64
1:B:595:VAL:HG13	1:B:630:LEU:HD11	1.81	0.61
1:B:393:THR:OG1	1:B:394:TYR:N	2.34	0.61
1:B:652:HIS:ND1	7:B:2122:HOH:O	2.31	0.59
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.86	0.57
1:B:332:MET:HB3	1:B:335:ILE:HG13	1.87	0.56
1:A:465:ARG:NH1	1:A:578:GLU:OE1	2.38	0.56
1:A:554:PHE:HB3	7:A:2073:HOH:O	2.05	0.56
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.88	0.55
1:A:626:LYS:HB3	1:B:687:ILE:HD12	1.89	0.55
1:B:414:ARG:HD3	1:B:678:TRP:CD2	2.43	0.54
1:B:659:ILE:O	1:B:663:GLU:HG3	2.08	0.53
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.91	0.53
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.91	0.53
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.93	0.51
1:A:316:LEU:HD12	1:A:319:LYS:HE2	1.92	0.51
1:B:451:ASN:HB3	1:B:454:ASN:O	2.12	0.50
1:A:393:THR:OG1	1:A:394:TYR:N	2.43	0.50
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.47	0.50
1:A:336:MET:HG3	1:B:306:TRP:NE1	2.27	0.49
1:B:328:GLU:N	1:B:328:GLU:OE1	2.45	0.49
1:A:351:LYS:NZ	1:A:389:GLU:O	2.38	0.49
1:A:551:PHE:HB3	1:A:553:TRP:CE2	2.47	0.49
1:A:351:LYS:HE2	1:A:392:SER:HA	1.94	0.49
1:A:474:VAL:HG22	1:A:524:LEU:HD22	1.94	0.49
1:A:590:GLY:HA3	1:A:638:LEU:HD21	1.94	0.49
1:A:620:LYS:HB2	1:A:620:LYS:NZ	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.96	0.48
1:B:404:GLY:HA3	1:B:574:ILE:HD13	1.96	0.47
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.95	0.47
1:B:419:ILE:HG13	1:B:661:HIS:HB2	1.96	0.47
1:A:355:PHE:HD1	1:A:388:ILE:HD12	1.79	0.47
1:A:415:CYS:HB2	2:A:750:HEM:ND	2.29	0.47
1:B:366:TYR:HA	1:B:369:ILE:HG12	1.97	0.47
1:A:545:PRO:HG2	1:A:547:ARG:NH1	2.29	0.47
1:B:423:LYS:NZ	7:B:2029:HOH:O	2.47	0.47
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.49	0.46
1:B:302:LYS:HB2	1:B:302:LYS:HE3	1.82	0.46
1:B:610:VAL:O	1:B:614:MET:HG3	2.16	0.46
1:A:322:LEU:HB3	1:A:699:ARG:HH21	1.81	0.45
1:B:366:TYR:CD1	1:B:369:ILE:HD11	2.52	0.45
1:A:494:GLY:O	1:A:496:PRO:HD3	2.17	0.45
1:A:686:SER:HA	1:A:691:PHE:CG	2.51	0.45
1:B:701:THR:HA	1:B:702:PRO:C	2.37	0.45
1:A:551:PHE:HB3	1:A:553:TRP:NE1	2.32	0.44
1:B:312:LEU:HB3	1:B:666:TYR:CD2	2.52	0.44
1:B:593:ILE:HA	1:B:597:ASP:HB2	2.00	0.44
1:A:553:TRP:CZ3	1:A:613:LYS:HB3	2.53	0.44
1:B:462:PHE:HB2	1:B:581:ALA:HB3	1.99	0.43
1:A:548:HIS:HB2	1:A:554:PHE:CG	2.53	0.43
1:A:430:ARG:O	1:A:463:PRO:HG3	2.19	0.43
1:B:464:GLN:HB3	1:B:579:PHE:CE1	2.54	0.43
2:A:750:HEM:O1D	4:A:800:9HL:N19	2.52	0.42
1:B:301:LEU:HD23	1:B:301:LEU:HA	1.89	0.42
1:A:513:PRO:HG2	1:A:518:ASP:CG	2.40	0.42
1:A:409:TRP:CE2	2:A:750:HEM:C2C	3.07	0.42
1:B:473:ARG:HD3	1:B:580:SER:HB2	2.01	0.42
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.01	0.42
1:A:549:PRO:O	1:A:550:LYS:HG3	2.20	0.42
1:A:546:ILE:HG22	1:A:554:PHE:HE2	1.85	0.41
1:B:478:GLN:NE2	4:B:800:9HL:H15	2.35	0.41
1:B:496:PRO:HD2	1:B:603:ARG:HA	2.01	0.41
1:A:418:ARG:O	1:A:421:TRP:HB3	2.20	0.41
1:A:465:ARG:HG3	1:A:471:ASP:OD1	2.21	0.41
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.50	0.41
1:A:416:VAL:HG23	1:A:679:ILE:HG23	2.02	0.41
1:A:542:LEU:HD21	1:A:646:VAL:HG22	2.03	0.41
1:A:587:TRP:NE1	5:A:860:ACT:H1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:VAL:HG21	1:A:633:ILE:HD11	2.03	0.41
1:A:445:HIS:CD2	1:A:445:HIS:C	2.94	0.41
1:A:355:PHE:N	1:A:356:PRO:HD2	2.36	0.41
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.91	0.40
1:A:419:ILE:HB	1:A:661:HIS:HB2	2.03	0.40
1:A:476:ASN:HD21	1:A:522:LEU:HA	1.85	0.40
1:A:380:ARG:NH2	1:A:397:LYS:HG2	2.37	0.40
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.57	0.40
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.56	0.40
1:A:655:THR:OG1	1:A:689:PRO:HD2	2.21	0.40
1:A:706:TYR:OH	2:A:750:HEM:O2D	2.30	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	405/422 (96%)	382 (94%)	23 (6%)	0	100	100
1	B	409/422 (97%)	394 (96%)	14 (3%)	1 (0%)	47	39
All	All	814/844 (96%)	776 (95%)	37 (4%)	1 (0%)	51	45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	685	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	364/377 (97%)	350 (96%)	14 (4%)	33	26
1	B	368/377 (98%)	362 (98%)	6 (2%)	62	59
All	All	732/754 (97%)	712 (97%)	20 (3%)	44	39

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	LYS
1	A	336	MET
1	A	337	LEU
1	A	469	LYS
1	A	470	HIS
1	A	476	ASN
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	601	ASN
1	A	622	SER
1	A	645	LYS
1	A	701	THR
1	A	715	VAL
1	B	353	GLN
1	B	382	GLU
1	B	392	SER
1	B	423	LYS
1	B	540	LEU
1	B	547	ARG

Sometimes 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 [i](#)

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$
5	ACT	B	860	-	3,3,3	0.71	0	3,3,3	0.91	0
2	HEM	B	750	1,4	41,50,50	1.95	6 (14%)	45,82,82	1.48	4 (8%)
4	9HL	A	800	2	27,28,28	1.36	5 (18%)	32,38,38	2.73	13 (40%)
3	H4B	B	760	-	16,18,18	0.95	0	11,26,26	2.67	6 (54%)
4	9HL	B	800	2	27,28,28	1.34	3 (11%)	32,38,38	2.95	13 (40%)
5	ACT	A	860	-	3,3,3	0.77	0	3,3,3	0.75	0
2	HEM	A	750	1,4	41,50,50	1.88	7 (17%)	45,82,82	1.99	13 (28%)
3	H4B	A	760	-	16,18,18	0.79	0	11,26,26	2.80	6 (54%)

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	750	1,4	-	3/12/54/54	-
4	9HL	A	800	2	-	0/11/20/20	0/4/4/4
3	H4B	B	760	-	-	1/8/17/17	0/2/2/2
4	9HL	B	800	2	-	2/11/20/20	0/4/4/4
2	HEM	A	750	1,4	-	2/12/54/54	-
3	H4B	A	760	-	-	0/8/17/17	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	750	HEM	C3D-C2D	7.68	1.53	1.36
2	A	750	HEM	C3D-C2D	7.59	1.52	1.36
2	B	750	HEM	C3C-C2C	-4.90	1.33	1.40
2	A	750	HEM	C3C-C2C	-4.17	1.34	1.40
2	B	750	HEM	C3C-CAC	3.82	1.55	1.47
4	A	800	9HL	C04-N03	-3.81	1.33	1.39
2	A	750	HEM	C3C-CAC	3.51	1.55	1.47
4	B	800	9HL	C04-N03	-3.51	1.34	1.39
4	B	800	9HL	C12-N13	2.90	1.36	1.31
4	A	800	9HL	C12-N13	2.84	1.36	1.31
2	B	750	HEM	CAA-C2A	2.70	1.56	1.52
2	A	750	HEM	CAB-C3B	2.63	1.54	1.47
4	B	800	9HL	C12-N11	2.63	1.36	1.32
2	B	750	HEM	CAB-C3B	2.60	1.54	1.47
4	A	800	9HL	C12-N11	2.40	1.35	1.32
4	A	800	9HL	C02-N03	-2.33	1.34	1.36
4	A	800	9HL	C1'-C23	-2.24	1.48	1.51
2	B	750	HEM	CMD-C2D	2.23	1.55	1.50
2	A	750	HEM	CAA-C2A	2.12	1.55	1.52
2	A	750	HEM	FE-NB	2.04	2.06	1.96
2	A	750	HEM	CMC-C2C	2.01	1.56	1.51

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	9HL	C22-C23-C1'	-7.54	107.74	122.24
4	A	800	9HL	C22-C23-C1'	-6.91	108.95	122.24
4	B	800	9HL	C1'-C23-C21	-6.70	111.31	121.31
2	A	750	HEM	C4D-ND-C1D	6.61	111.90	105.07
3	B	760	H4B	C8A-C4A-C4	5.91	119.82	114.57
2	A	750	HEM	CBA-CAA-C2A	-5.77	102.77	112.62
4	B	800	9HL	C14-N13-C12	5.63	121.50	114.04
4	B	800	9HL	N13-C12-N11	-5.62	119.71	126.08
4	A	800	9HL	C1'-C23-C21	-5.50	113.09	121.31
4	A	800	9HL	N13-C12-N11	-5.14	120.26	126.08
4	A	800	9HL	C14-N13-C12	5.10	120.80	114.04
3	A	760	H4B	C4-C4A-N5	4.83	123.17	119.12
4	B	800	9HL	N11-C12-N03	4.64	120.79	114.78
2	B	750	HEM	C4D-ND-C1D	4.51	109.73	105.07
4	A	800	9HL	N11-C12-N03	4.37	120.44	114.78
3	A	760	H4B	C8A-C4A-C4	4.26	118.35	114.57
4	B	800	9HL	C04-N03-C12	-3.90	121.09	125.50
3	A	760	H4B	N1-C2-N3	-3.75	119.55	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	9HL	C04-N03-C12	-3.56	121.48	125.50
4	A	800	9HL	C02-N03-C04	3.52	114.88	108.50
4	A	800	9HL	C15-C14-N13	-3.45	119.67	123.96
4	B	800	9HL	C15-C14-N13	-3.40	119.74	123.96
4	B	800	9HL	C02-N03-C04	3.19	114.28	108.50
3	A	760	H4B	C2-N1-C8A	3.10	121.50	114.54
3	B	760	H4B	C2-N3-C4	3.10	120.85	115.93
3	A	760	H4B	C2-N3-C4	3.09	120.84	115.93
3	B	760	H4B	N1-C2-N3	-3.07	120.60	125.42
4	B	800	9HL	C17-C16-N11	3.03	120.46	115.95
4	B	800	9HL	N13-C12-N03	3.02	119.49	114.81
4	B	800	9HL	C4'-C3'-C2'	-2.95	119.45	123.29
4	A	800	9HL	N13-C12-N03	2.90	119.30	114.81
4	A	800	9HL	C17-C16-N11	2.89	120.25	115.95
3	B	760	H4B	C4-C4A-N5	2.84	121.50	119.12
2	A	750	HEM	CAD-CBD-CGD	-2.73	107.73	113.60
2	B	750	HEM	C1D-C2D-C3D	-2.71	104.11	106.96
2	B	750	HEM	CBD-CAD-C3D	-2.70	105.12	112.63
4	A	800	9HL	C14-C15-C16	2.66	119.12	116.62
2	A	750	HEM	C1B-NB-C4B	2.66	107.82	105.07
3	B	760	H4B	C2-N1-C8A	2.61	120.38	114.54
3	A	760	H4B	N2-C2-N3	2.58	121.26	117.25
2	A	750	HEM	C3B-C2B-C1B	2.57	108.39	106.49
4	A	800	9HL	C15-C16-N11	-2.47	119.28	122.41
2	A	750	HEM	CHD-C1D-ND	2.39	127.03	124.43
4	A	800	9HL	C4'-C3'-C2'	-2.35	120.24	123.29
2	A	750	HEM	C4B-CHC-C1C	2.34	125.65	122.56
2	A	750	HEM	CHA-C4D-ND	2.30	127.22	124.38
2	A	750	HEM	CBD-CAD-C3D	-2.28	106.28	112.63
2	A	750	HEM	C3D-C4D-ND	-2.25	107.66	110.17
2	A	750	HEM	CMD-C2D-C1D	2.21	128.41	125.04
4	B	800	9HL	C15-C16-N11	-2.17	119.65	122.41
3	B	760	H4B	N2-C2-N1	2.16	120.61	117.25
4	B	800	9HL	C14-C15-C16	2.12	118.61	116.62
2	A	750	HEM	CAD-C3D-C4D	2.09	128.32	124.66
2	B	750	HEM	C3B-C2B-C1B	2.07	108.02	106.49
2	A	750	HEM	C2C-C3C-C4C	2.02	108.31	106.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	800	9HL	C2'-C1'-C23-C21
4	B	800	9HL	C6'-C1'-C23-C21
2	A	750	HEM	C4B-C3B-CAB-CBB
2	B	750	HEM	C4B-C3B-CAB-CBB
3	B	760	H4B	N5-C6-C9-O9
2	B	750	HEM	CAD-CBD-CGD-O2D
2	A	750	HEM	CAD-CBD-CGD-O1D
2	B	750	HEM	CAD-CBD-CGD-O1D

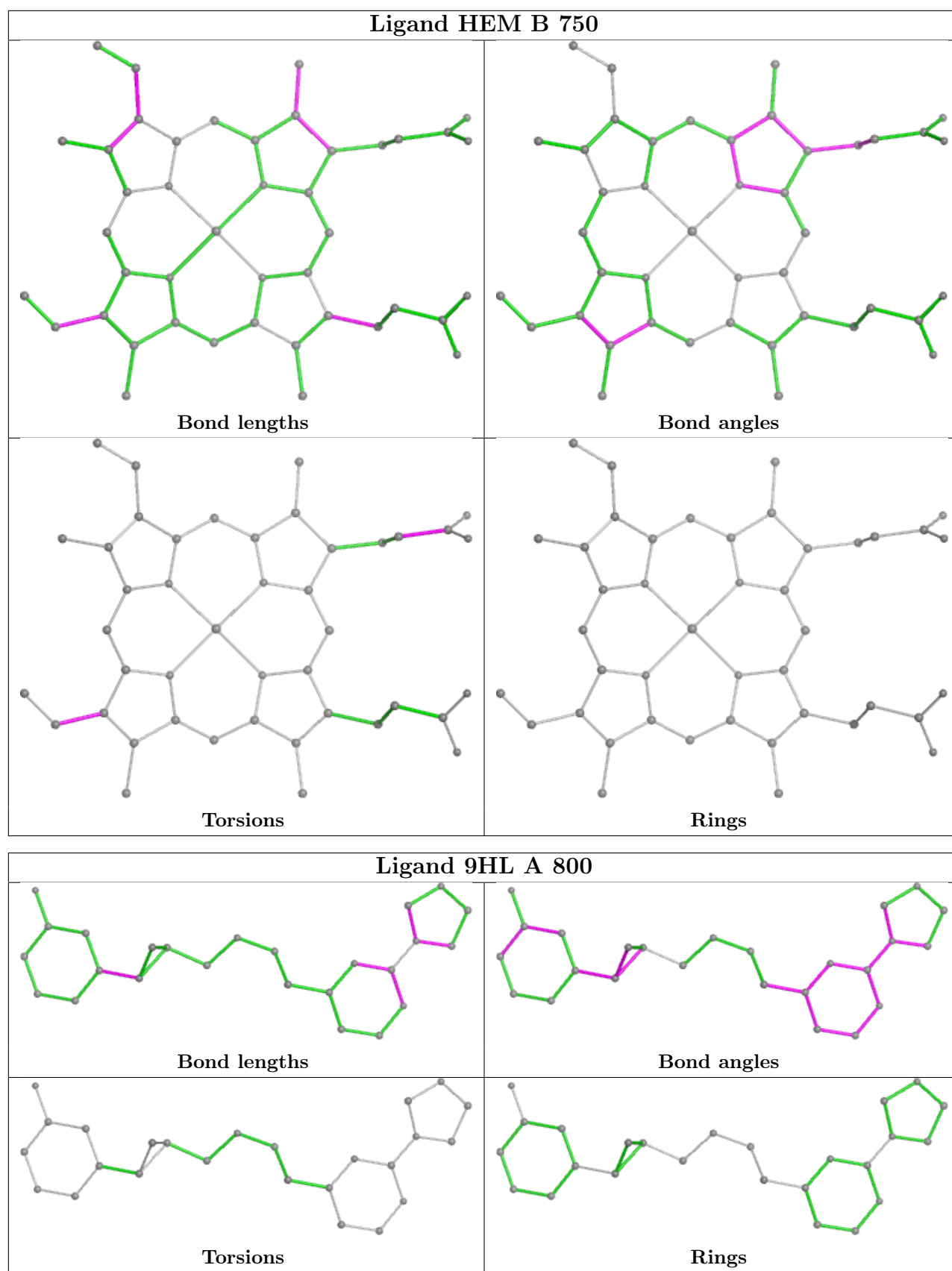
There are no ring outliers.

5 monomers are involved in 9 short contacts:

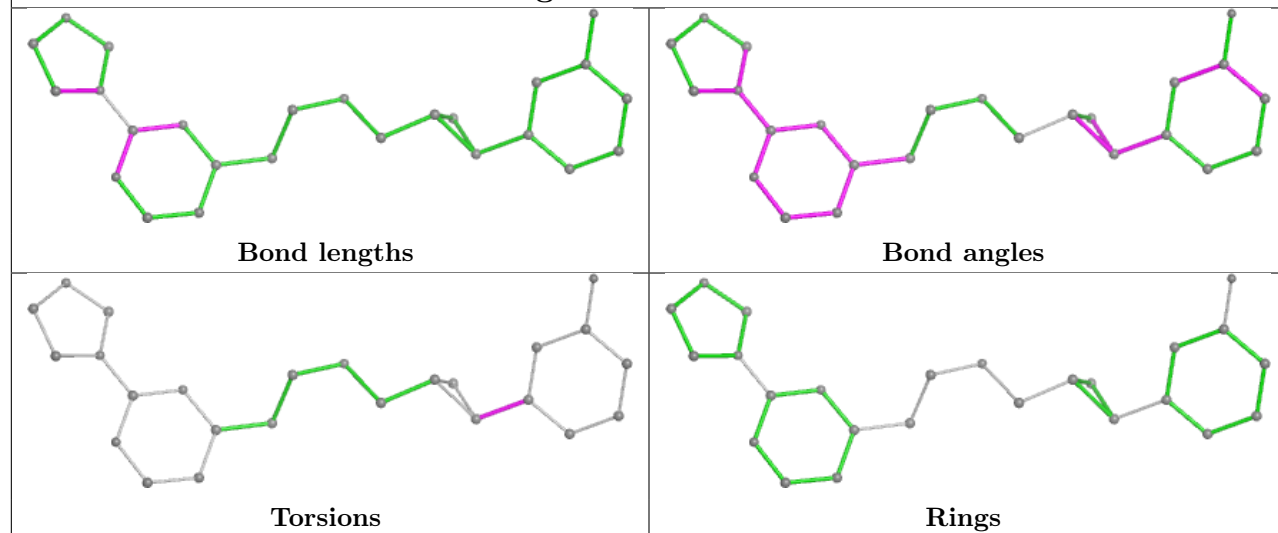
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	750	HEM	1	0
4	A	800	9HL	1	0
4	B	800	9HL	1	0
5	A	860	ACT	1	0
2	A	750	HEM	6	0

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.

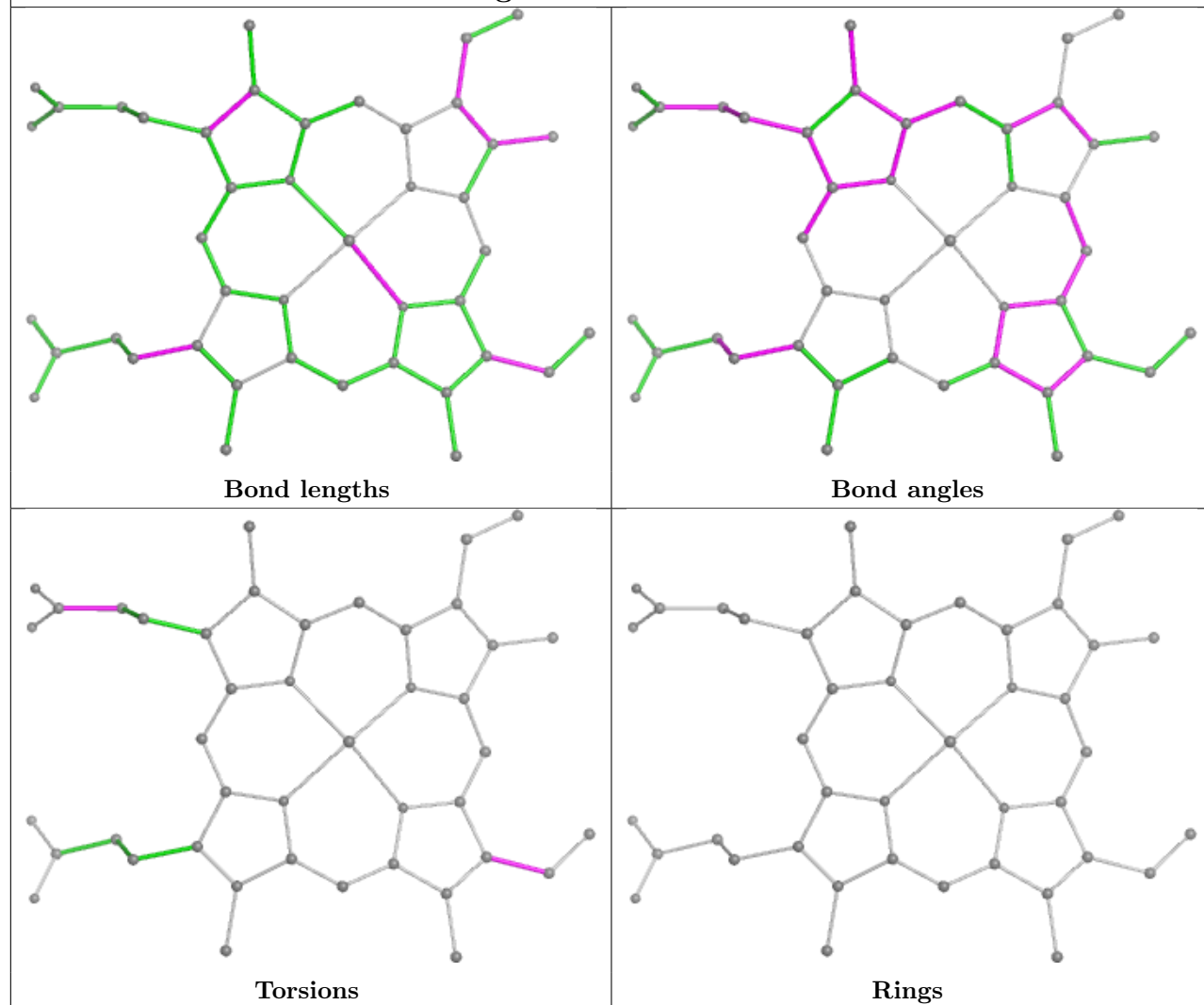




## Ligand 9HL B 800



## Ligand HEM A 750



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	408/422 (96%)	0.24	28 (6%) 16 17	17, 41, 77, 109	0
1	B	411/422 (97%)	-0.22	13 (3%) 47 50	13, 33, 63, 96	0
All	All	819/844 (97%)	0.01	41 (5%) 28 29	13, 36, 75, 109	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	717	LYS	10.4
1	A	490	GLY	5.9
1	A	715	VAL	5.8
1	A	352	ASP	5.0
1	A	488	PRO	4.5
1	A	716	TRP	4.5
1	B	348	VAL	4.3
1	A	300	PHE	3.9
1	A	506	ILE	3.6
1	B	300	PHE	3.5
1	A	486	LYS	3.3
1	B	350	THR	3.2
1	A	351	LYS	3.2
1	A	507	GLN	3.2
1	B	619	ARG	3.2
1	A	390	SER	3.1
1	B	718	GLY	3.0
1	A	508	GLN	2.8
1	A	712	ASN	2.8
1	A	388	ILE	2.7
1	A	553	TRP	2.7
1	A	386	LYS	2.7
1	B	321	THR	2.7
1	A	491	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	620	LYS	2.6
1	A	299	ARG	2.5
1	B	299	ARG	2.5
1	A	373	GLY	2.4
1	A	551	PHE	2.4
1	A	321	THR	2.4
1	B	351	LYS	2.3
1	A	714	HIS	2.3
1	A	392	SER	2.2
1	B	352	ASP	2.2
1	B	616	LEU	2.2
1	A	355	PHE	2.1
1	B	615	ASP	2.1
1	A	389	GLU	2.1
1	A	503	GLU	2.1
1	A	350	THR	2.1
1	B	617	ASP	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<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	ACT	A	860	4/4	0.90	0.19	60,61,62,62	0
4	9HL	A	800	25/25	0.93	0.18	15,33,60,62	0
3	H4B	A	760	17/17	0.96	0.12	19,24,38,40	0
4	9HL	B	800	25/25	0.96	0.17	13,38,73,77	0
3	H4B	B	760	17/17	0.96	0.15	19,26,36,36	0
2	HEM	A	750	43/43	0.97	0.16	3,25,35,37	0

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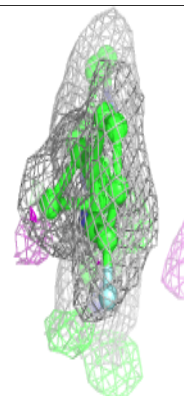
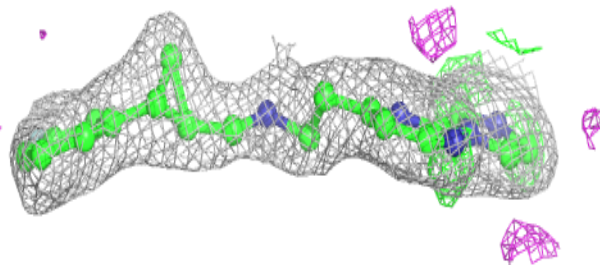
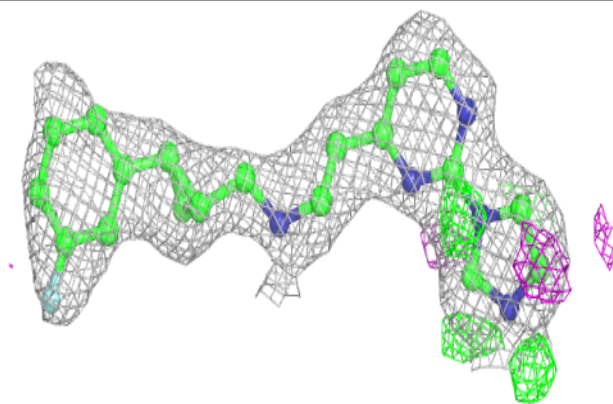
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ACT	B	860	4/4	0.97	0.12	49,50,52,53	0
2	HEM	B	750	43/43	0.98	0.15	10,28,38,45	0
6	ZN	A	1717	1/1	0.99	0.08	34,34,34,34	0

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.

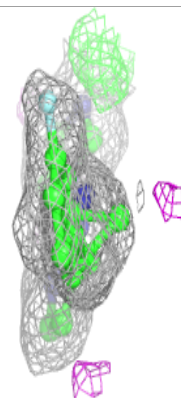
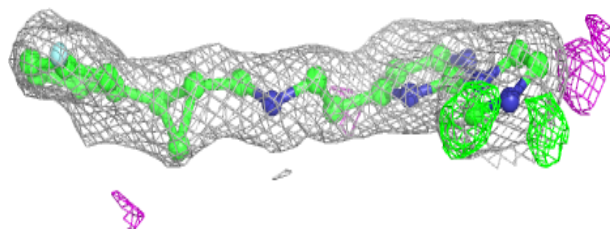
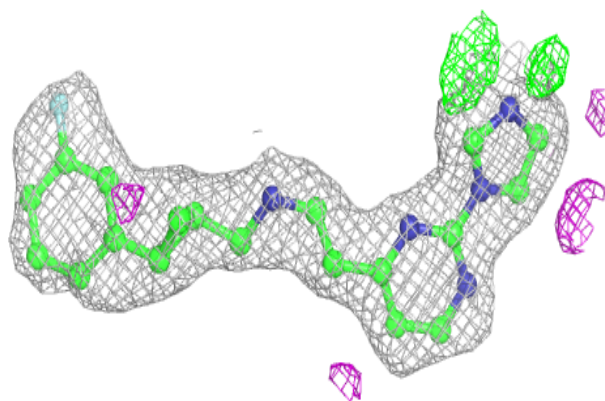
**Electron density around 9HL A 800:**

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)

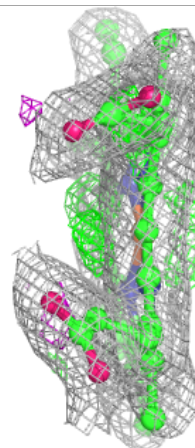
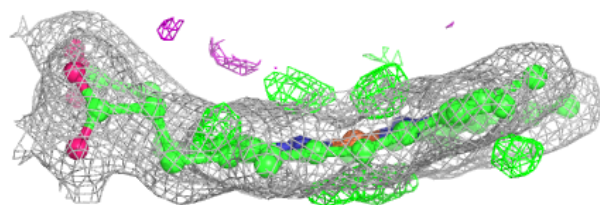
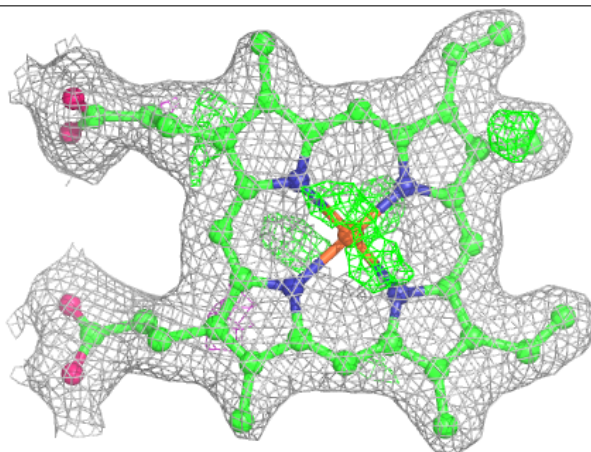


**Electron density around 9HL B 800:**

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

**Electron density around HEM A 750:**

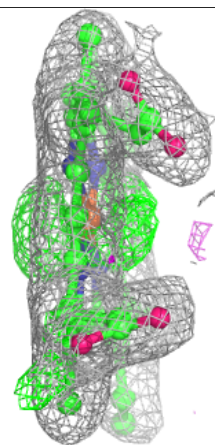
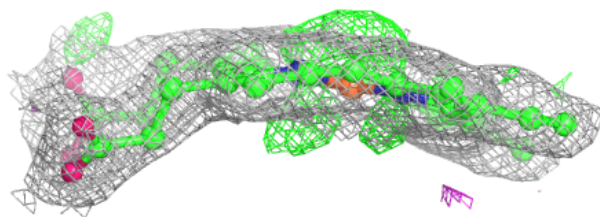
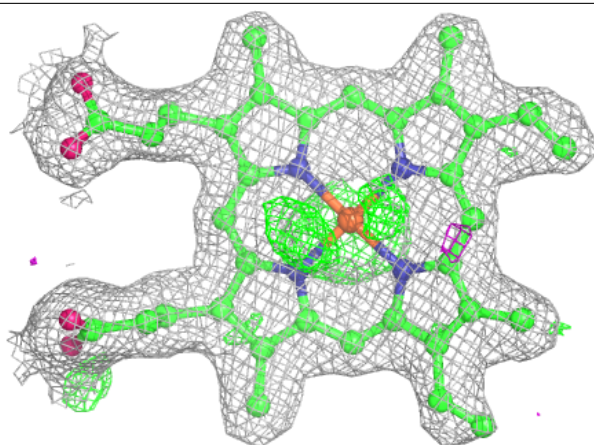
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**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)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.