



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:37 AM BST

PDB ID : 6PN6  
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with 7-(3-(Aminomethyl)-4-(pyridin-3-ylmethoxy)phenyl)-4-methylquinolin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2019-07-02  
Resolution : 1.84 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 : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

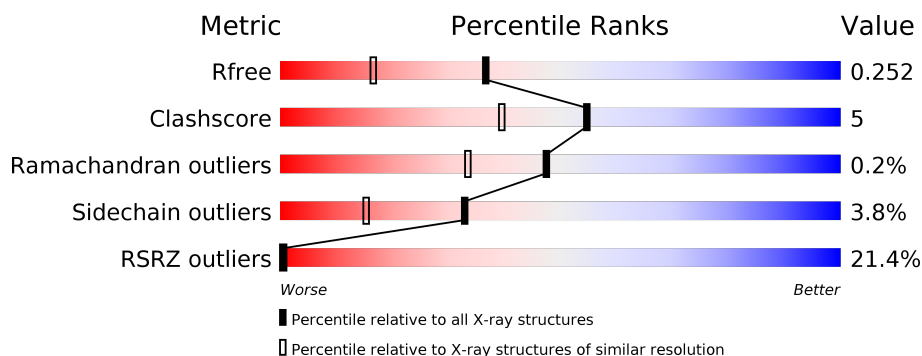
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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>27%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>••</div> </div> </div>
1	B	422	<div> <div>14%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>•</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7064 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	410	Total	C	N	O	S	0	2	0
			3340	2137	572	609	22			
1	B	411	Total	C	N	O	S	0	2	0
			3351	2144	574	612	21			

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



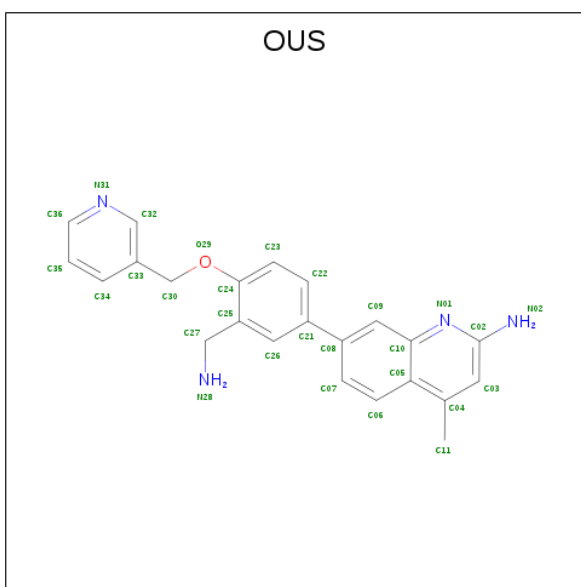
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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 7-{3-(aminomethyl)-4-[(pyridin-3-yl)methoxy]phenyl}-4-methylquinolin-2-amine (three-letter code: OUS) (formula:  $C_{23}H_{22}N_4O$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			28	23	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			28	23	4	1		

- 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	B	1	Total	Zn	0	0
			1	1		

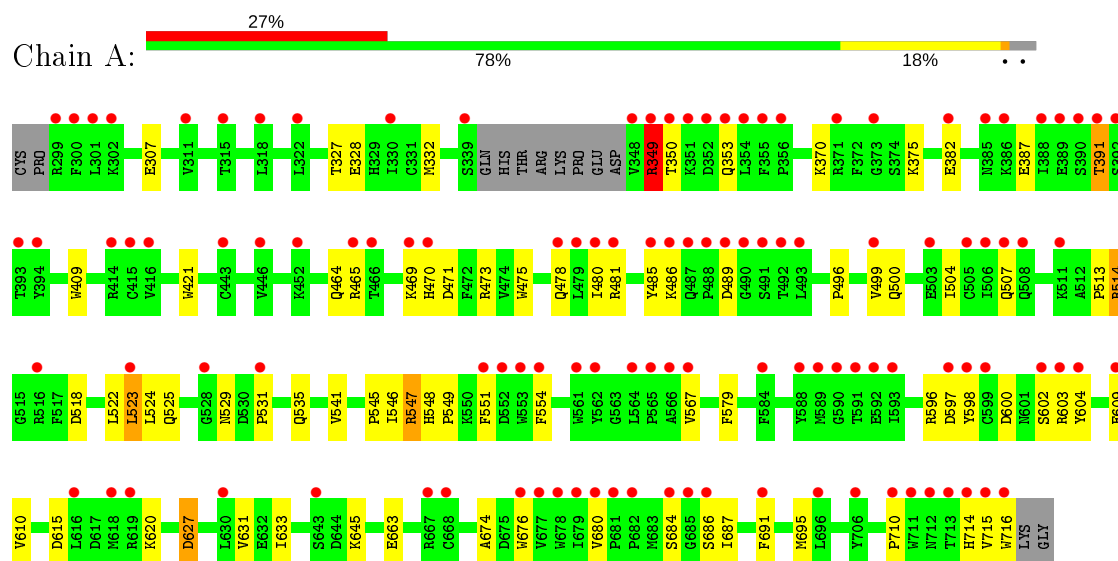
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	71	Total	O	0	0
			71	71		
7	B	117	Total	O	0	0
			117	117		

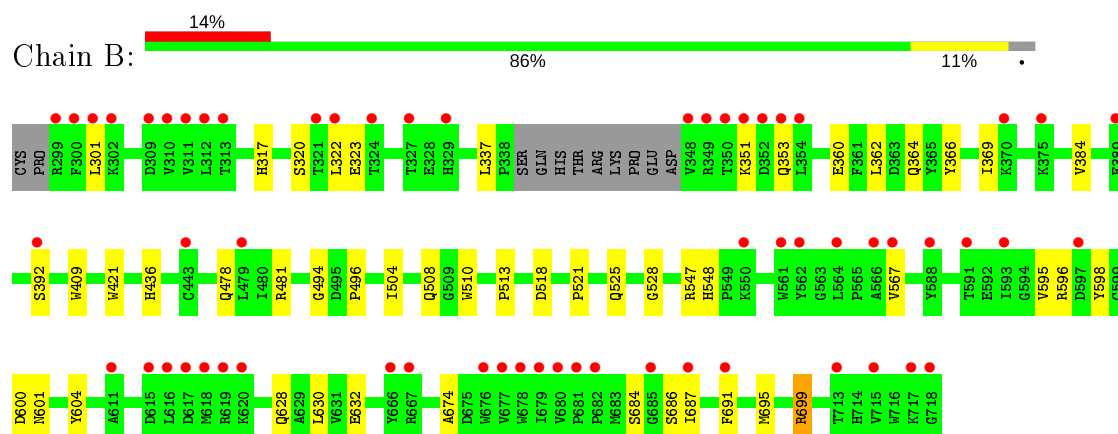
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	51.55Å 111.17Å 164.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.02 – 1.84 39.02 – 1.84	Depositor EDS
% Data completeness (in resolution range)	95.4 (39.02-1.84) 96.8 (39.02-1.84)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575_1496: ???)	Depositor
R, $R_{free}$	0.206 , 0.248 0.208 , 0.252	Depositor DCC
$R_{free}$ test set	3937 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtriage
Anisotropy	1.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 70.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: OUS, HEM, ZN, H4B, 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	0.35	0/3436	0.52	1/4661 (0.0%)
1	B	0.38	0/3450	0.51	0/4677
All	All	0.37	0/6886	0.51	1/9338 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	ARG	NE-CZ-NH1	5.88	123.24	120.30

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	3340	0	3253	39	0
1	B	3351	0	3269	28	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	17	0	15	1	0
3	B	17	0	15	0	0
4	A	28	0	0	1	0
4	B	28	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	B	1	0	0	0	0
7	A	71	0	0	0	0
7	B	117	0	0	2	0
All	All	7064	0	6618	70	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 5.

All (70) 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:523:LEU:HD22	1:A:531:PRO:HB2	1.62	0.81
1:A:349:ARG:HH11	1:A:349:ARG:HG3	1.53	0.73
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.72	0.70
2:B:801:HEM:HBC2	2:B:801:HEM:HMC2	1.77	0.67
1:A:465:ARG:NH2	1:A:471:ASP:OD2	2.28	0.67
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.77	0.66
1:B:436:HIS:ND1	7:B:903:HOH:O	2.27	0.66
2:A:801:HEM:HHC	2:A:801:HEM:HBB2	1.78	0.65
2:A:801:HEM:HBC2	2:A:801:HEM:HMC2	1.80	0.64
1:A:387:GLU:O	1:A:391:THR:OG1	2.14	0.63
1:B:364:GLN:OE1	7:B:901:HOH:O	2.16	0.58
1:B:525:GLN:HE21	1:B:528:GLY:HA2	1.67	0.58
1:A:480:ILE:HD13	1:A:541:VAL:HG13	1.85	0.57
1:B:595:VAL:HA	1:B:630:LEU:HD11	1.87	0.56
2:B:801:HEM:HBD1	4:B:803:OUS:C22	2.35	0.56
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.88	0.55
1:A:567:VAL:HG21	4:A:803:OUS:C07	2.37	0.54
1:B:567:VAL:HG21	4:B:803:OUS:C07	2.37	0.54
1:A:349:ARG:HG3	1:A:349:ARG:NH1	2.22	0.54
1:A:714:HIS:CE1	1:A:716:TRP:HA	2.45	0.51
1:A:546:ILE:HG22	1:A:554:PHE:HE2	1.76	0.51
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.94	0.50
1:A:596:ARG:NH2	1:A:600:ASP:OD2	2.45	0.49
1:A:349:ARG:HH11	1:A:349:ARG:CG	2.22	0.49
1:A:684:SER:HB3	1:A:687:ILE:HD11	1.94	0.48
1:B:362:LEU:HD11	1:B:384:VAL:HG21	1.96	0.48
1:A:548:HIS:CG	1:A:549:PRO:HD2	2.49	0.48
1:B:686:SER:HA	1:B:691:PHE:CG	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:PRO:HG2	1:B:518:ASP:OD2	2.14	0.48
1:B:504:ILE:O	1:B:508:GLN:HG2	2.14	0.47
1:A:686:SER:HA	1:A:691:PHE:CG	2.49	0.47
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.50	0.47
1:B:323:GLU:O	1:B:699:ARG:HD2	2.15	0.47
1:B:596:ARG:NH2	1:B:600:ASP:OD1	2.42	0.47
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.50	0.46
1:A:620:LYS:HB2	1:A:620:LYS:NZ	2.30	0.46
1:A:610:VAL:HG21	1:A:633:ILE:HD11	1.98	0.46
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.98	0.46
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.98	0.46
1:A:522:LEU:HB3	1:A:524:LEU:HD21	1.98	0.46
1:B:548:HIS:NE2	1:B:632:GLU:OE1	2.48	0.45
1:A:307:GLU:OE2	1:B:601:ASN:HB2	2.17	0.45
1:A:548:HIS:ND1	1:A:551:PHE:HD2	2.15	0.45
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.51	0.44
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.77	0.44
1:A:500:GLN:O	1:A:504:ILE:HG13	2.17	0.44
1:B:366:TYR:HA	1:B:369:ILE:HG12	2.00	0.44
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.53	0.44
3:A:802:H4B:H71	3:A:802:H4B:H10	1.70	0.44
1:B:598:TYR:HA	1:B:604:TYR:HB2	1.98	0.44
1:B:699:ARG:HH11	1:B:699:ARG:HB3	1.83	0.44
1:A:598:TYR:HA	1:A:604:TYR:HB2	1.99	0.44
1:A:545:PRO:HG2	1:A:547:ARG:NH2	2.33	0.43
1:A:627:ASP:O	1:A:631:VAL:HG23	2.18	0.43
1:A:676:TRP:CE2	1:A:680:VAL:HG21	2.54	0.43
1:A:473:ARG:NH2	1:A:710:PRO:HD3	2.34	0.43
1:A:523:LEU:HA	1:A:523:LEU:HD23	1.86	0.42
1:A:525:GLN:HG3	1:A:529:ASN:O	2.20	0.42
1:A:674:ALA:HB3	1:A:695:MET:HB3	2.00	0.42
1:A:513:PRO:HG2	1:A:518:ASP:CG	2.40	0.42
1:A:597:ASP:OD1	1:A:603:ARG:NH2	2.53	0.42
1:B:674:ALA:HB3	1:B:695:MET:HB3	2.00	0.42
1:A:332:MET:HE1	1:B:301:LEU:HD13	2.02	0.42
1:B:684:SER:HB3	1:B:687:ILE:HD11	2.02	0.41
1:A:485:TYR:CZ	1:A:514:ARG:HA	2.56	0.41
1:B:353:GLN:N	1:B:353:GLN:OE1	2.54	0.41
1:B:317:HIS:O	1:B:320:SER:HB3	2.21	0.40
1:A:496:PRO:HA	1:A:499:VAL:HG23	2.02	0.40
1:B:513:PRO:HG2	1:B:518:ASP:CG	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:GLY:O	1:B:496:PRO:HD3	2.22	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	407/422 (96%)	389 (96%)	16 (4%)	2 (0%)	29	15
1	B	409/422 (97%)	397 (97%)	12 (3%)	0	100	100
All	All	816/844 (97%)	786 (96%)	28 (3%)	2 (0%)	47	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	LYS
1	A	514	ARG

### 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	367/377 (97%)	345 (94%)	22 (6%)	19	5
1	B	368/377 (98%)	362 (98%)	6 (2%)	62	49
All	All	735/754 (98%)	707 (96%)	28 (4%)	33	15

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	THR
1	A	328	GLU
1	A	349	ARG
1	A	350	THR
1	A	353	GLN
1	A	382	GLU
1	A	391	THR
1	A	469	LYS
1	A	470	HIS
1	A	486	LYS
1	A	489	ASP
1	A	507	GLN
1	A	523	LEU
1	A	535	GLN
1	A	547	ARG
1	A	602	SER
1	A	609	GLU
1	A	615	ASP
1	A	627	ASP
1	A	645	LYS
1	A	663	GLU
1	A	715	VAL
1	B	337	LEU
1	B	351	LYS
1	B	360	GLU
1	B	392	SER
1	B	547	ARG
1	B	699	ARG

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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	B	801	1	27,50,50	1.97	7 (25%)	17,82,82	1.69	5 (29%)
2	HEM	A	801	1	27,50,50	1.90	7 (25%)	17,82,82	2.07	5 (29%)
5	ACT	A	804	-	1,3,3	1.39	0	0,3,3	0.00	-
5	ACT	B	804	-	1,3,3	1.11	0	0,3,3	0.00	-
3	H4B	A	802	-	16,18,18	0.85	0	11,26,26	2.67	7 (63%)
3	H4B	B	802	-	16,18,18	0.78	0	11,26,26	2.45	5 (45%)
4	OUS	B	803	-	31,31,31	0.78	1 (3%)	42,43,43	1.34	6 (14%)
4	OUS	A	803	-	31,31,31	0.84	1 (3%)	42,43,43	1.61	6 (14%)

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

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

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3B-C2B	-4.72	1.33	1.40
2	B	801	HEM	C3C-C2C	-4.41	1.34	1.40
2	B	801	HEM	C3B-C2B	-4.29	1.34	1.40
2	A	801	HEM	C3B-CAB	3.79	1.55	1.47
2	B	801	HEM	C3B-CAB	3.69	1.55	1.47
2	B	801	HEM	C3C-CAC	3.53	1.55	1.47
2	A	801	HEM	C3C-CAC	3.32	1.54	1.47
2	A	801	HEM	C3C-C2C	-3.23	1.35	1.40
2	A	801	HEM	CMC-C2C	2.22	1.56	1.51
2	B	801	HEM	CAD-C3D	2.18	1.56	1.52
2	A	801	HEM	C1D-ND	2.16	1.40	1.36
2	A	801	HEM	C4B-NB	2.12	1.40	1.36
2	B	801	HEM	CAA-C2A	2.09	1.55	1.52
2	B	801	HEM	CMD-C2D	2.08	1.56	1.51
4	B	803	OUS	C05-C10	-2.03	1.39	1.42
4	A	803	OUS	C02-N01	2.03	1.36	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	OUS	O29-C24-C25	4.98	122.29	115.78
3	A	802	H4B	C4-C4A-C8A	4.74	118.78	114.57
3	B	802	H4B	C4-C4A-C8A	4.45	118.52	114.57
2	A	801	HEM	CAD-CBD-CGD	-4.25	105.54	112.67
2	A	801	HEM	CMD-C2D-C1D	-4.12	122.13	128.46
4	B	803	OUS	O29-C24-C25	3.65	120.55	115.78
2	B	801	HEM	CMD-C2D-C1D	-3.44	123.18	128.46
3	A	802	H4B	C4-C4A-N5	3.42	121.99	119.12
3	B	802	H4B	C4-C4A-N5	3.37	121.95	119.12
3	A	802	H4B	N3-C2-N1	-3.30	120.25	125.42
4	A	803	OUS	C05-C10-N01	-3.29	119.33	122.81
3	A	802	H4B	C4-N3-C2	3.16	120.96	115.93
3	B	802	H4B	N3-C2-N1	-3.14	120.50	125.42
4	A	803	OUS	C04-C05-C10	3.13	119.70	118.01
3	B	802	H4B	C4-N3-C2	2.98	120.66	115.93
2	A	801	HEM	CMD-C2D-C3D	2.75	130.12	124.94
2	B	801	HEM	C4A-C3A-C2A	2.74	108.90	107.00
3	A	802	H4B	C2-N1-C8A	2.73	120.65	114.54
3	A	802	H4B	N2-C2-N3	2.71	121.47	117.25
3	B	802	H4B	C2-N1-C8A	2.69	120.57	114.54
2	B	801	HEM	CMA-C3A-C4A	-2.55	124.55	128.46
2	A	801	HEM	CBD-CAD-C3D	2.54	117.16	112.48
2	A	801	HEM	CMC-C2C-C3C	2.51	129.38	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	OUS	C36-N31-C32	2.49	121.16	116.85
4	A	803	OUS	O29-C24-C23	-2.42	118.74	123.97
3	A	802	H4B	C4A-N5-C6	-2.36	114.75	121.16
4	A	803	OUS	C03-C04-C05	2.31	120.06	117.78
4	A	803	OUS	C36-N31-C32	2.30	120.83	116.85
4	B	803	OUS	C04-C05-C10	2.28	119.25	118.01
2	B	801	HEM	CMD-C2D-C3D	2.25	129.19	124.94
2	B	801	HEM	CMC-C2C-C3C	2.21	128.82	124.68
4	B	803	OUS	N02-C02-N01	2.17	120.06	118.26
4	B	803	OUS	C05-C10-N01	-2.08	120.60	122.81
4	B	803	OUS	O29-C24-C23	-2.00	119.64	123.97

There are no chirality outliers.

All (15) torsion outliers are listed below:

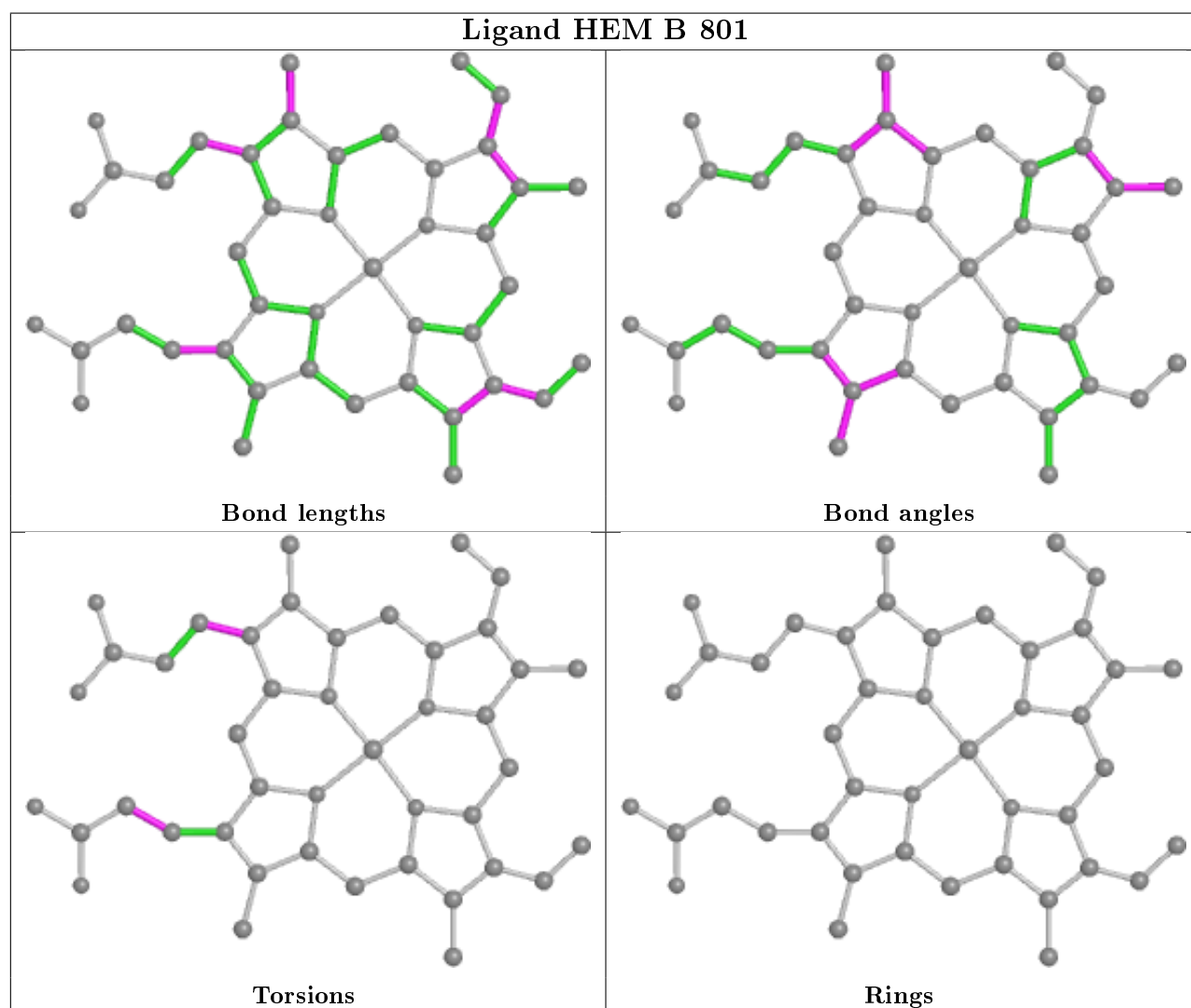
Mol	Chain	Res	Type	Atoms
2	B	801	HEM	C2A-CAA-CBA-CGA
2	B	801	HEM	C2D-C3D-CAD-CBD
2	B	801	HEM	C4D-C3D-CAD-CBD
2	A	801	HEM	C2A-CAA-CBA-CGA
2	A	801	HEM	C2D-C3D-CAD-CBD
2	A	801	HEM	C4D-C3D-CAD-CBD
4	B	803	OUS	C23-C24-O29-C30
4	A	803	OUS	C25-C24-O29-C30
4	B	803	OUS	C25-C24-O29-C30
4	A	803	OUS	C23-C24-O29-C30
3	A	802	H4B	C11-C10-C9-O9
3	A	802	H4B	O10-C10-C9-O9
3	A	802	H4B	C7-C6-C9-C10
3	B	802	H4B	C7-C6-C9-C10
3	A	802	H4B	N5-C6-C9-O9

There are no ring outliers.

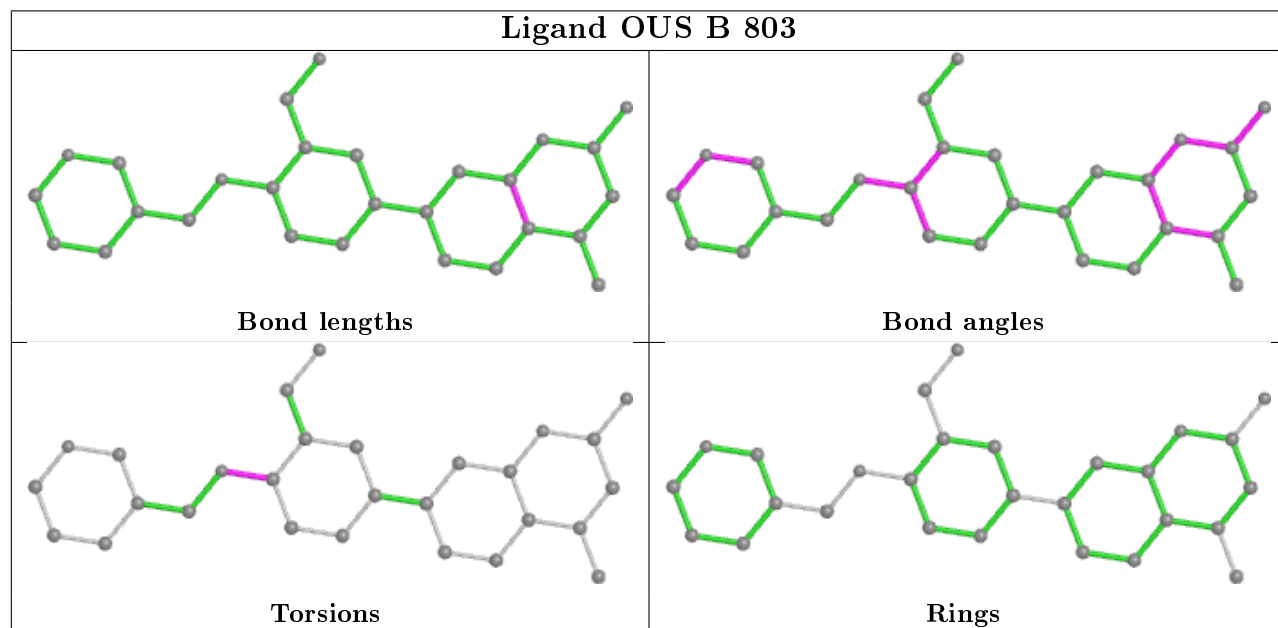
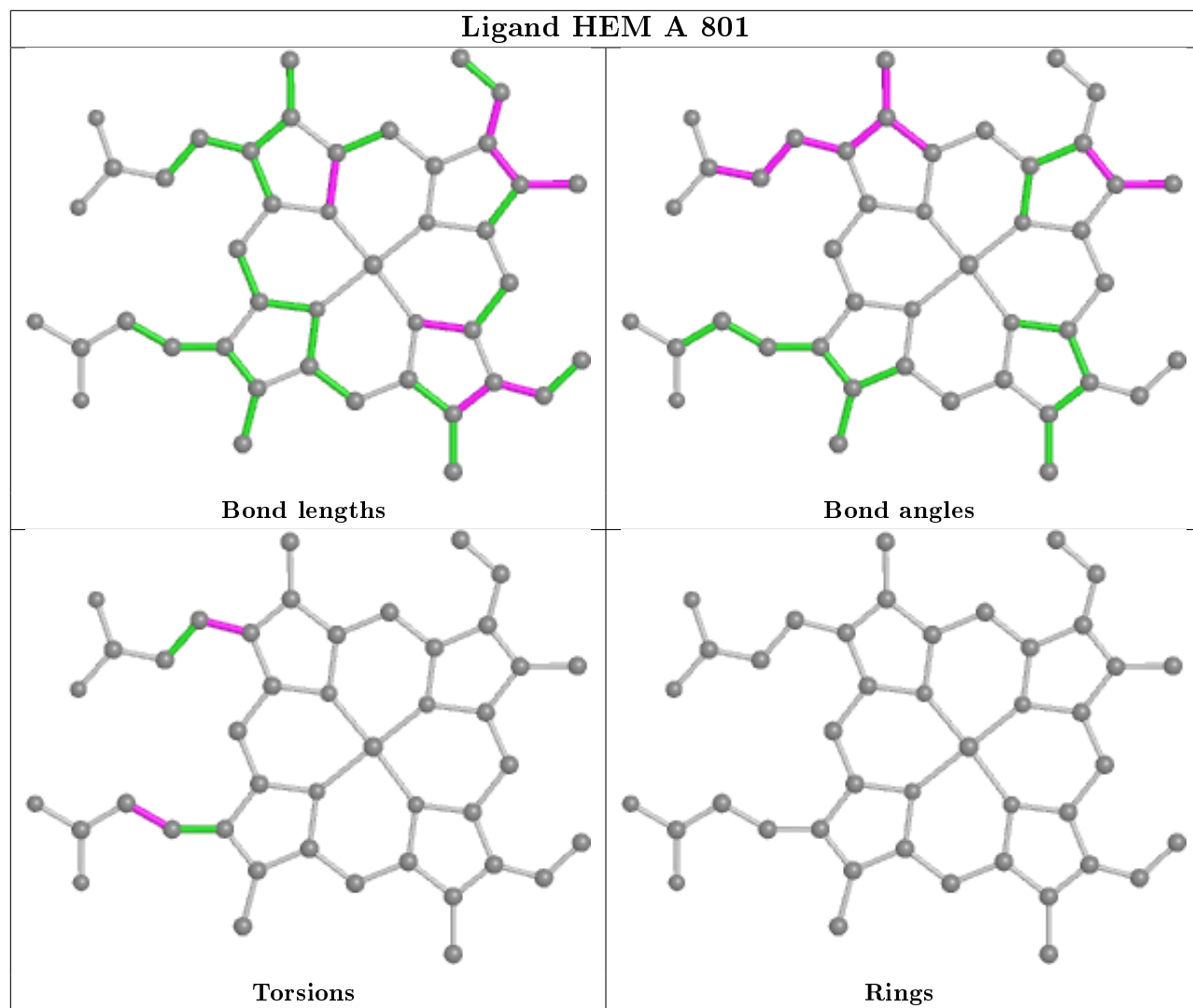
5 monomers are involved in 8 short contacts:

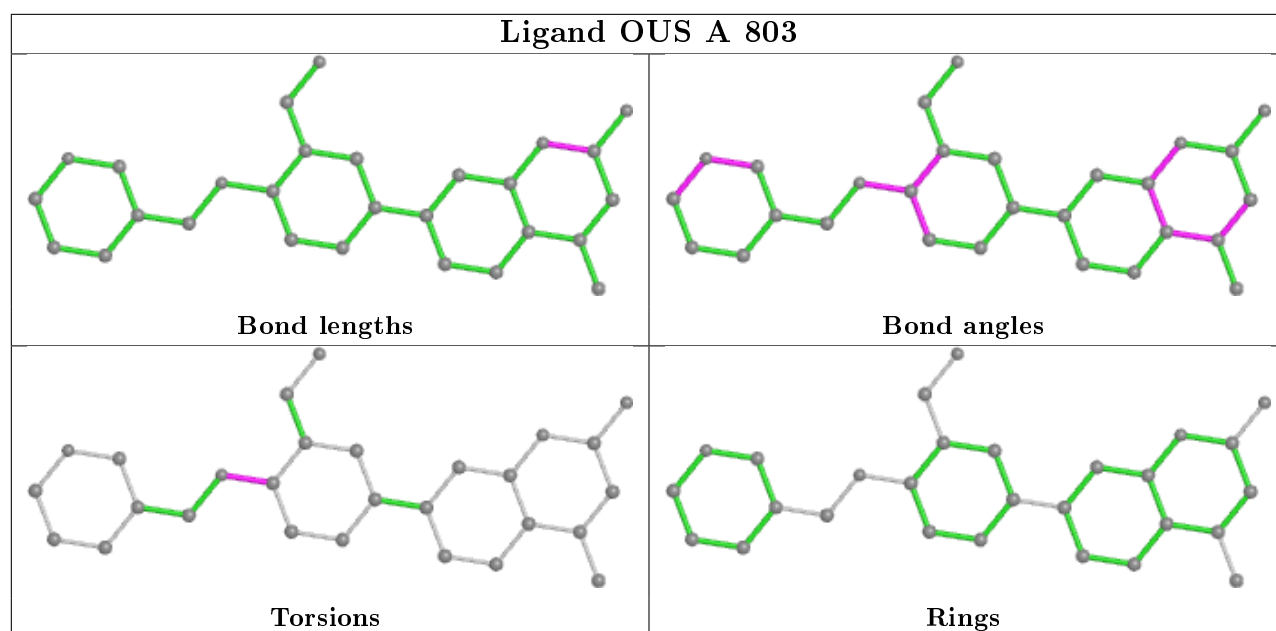
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HEM	3	0
2	A	801	HEM	2	0
3	A	802	H4B	1	0
4	B	803	OUS	2	0
4	A	803	OUS	1	0

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.









## 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	410/422 (97%)	1.38	116 (28%) 0 0	45, 83, 139, 177	0
1	B	411/422 (97%)	0.87	60 (14%) 2 2	43, 72, 115, 152	0
All	All	821/844 (97%)	1.12	176 (21%) 0 0	43, 76, 133, 177	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	715	VAL	11.5
1	B	300	PHE	10.3
1	A	322	LEU	9.3
1	A	716	TRP	7.8
1	B	348	VAL	7.0
1	A	352	ASP	6.7
1	A	713	THR	6.5
1	A	299	ARG	6.2
1	A	355	PHE	6.0
1	A	488	PRO	5.9
1	A	349	ARG	5.6
1	B	350	THR	5.5
1	A	678	TRP	5.5
1	A	348	VAL	5.4
1	A	351	LYS	5.3
1	A	503	GLU	5.3
1	A	677	VAL	5.0
1	A	489	ASP	4.9
1	A	551	PHE	4.8
1	A	388	ILE	4.8
1	A	506	ILE	4.8
1	B	619	ARG	4.6
1	B	351	LYS	4.6
1	B	718	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	680	VAL	4.6
1	A	566	ALA	4.5
1	B	302	LYS	4.5
1	B	677	VAL	4.5
1	B	566	ALA	4.5
1	A	318	LEU	4.4
1	A	679	ILE	4.4
1	A	389	GLU	4.4
1	A	676	TRP	4.3
1	A	486	LYS	4.3
1	B	678	TRP	4.3
1	B	389	GLU	4.3
1	A	567	VAL	4.2
1	B	301	LEU	4.2
1	A	685	GLY	4.2
1	B	349	ARG	4.1
1	A	711	TRP	4.1
1	A	714	HIS	4.0
1	A	554	PHE	4.0
1	A	339	SER	4.0
1	A	390	SER	4.0
1	A	505	CYS	4.0
1	B	717	LYS	3.9
1	B	679	ILE	3.9
1	A	593	ILE	3.9
1	A	603	ARG	3.9
1	A	300	PHE	3.8
1	B	329	HIS	3.8
1	A	508	GLN	3.8
1	B	352	ASP	3.7
1	A	588	TYR	3.7
1	B	667	ARG	3.7
1	A	354	LEU	3.7
1	A	392	SER	3.7
1	B	562	TYR	3.7
1	B	715	VAL	3.7
1	A	353	GLN	3.7
1	A	480	ILE	3.7
1	A	712	ASN	3.6
1	A	350	THR	3.6
1	B	611	ALA	3.5
1	B	299	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	493	LEU	3.5
1	A	565	PRO	3.5
1	A	584	PHE	3.5
1	A	415	CYS	3.4
1	A	591	THR	3.4
1	A	681	PRO	3.4
1	B	567	VAL	3.4
1	B	676	TRP	3.4
1	B	310	VAL	3.3
1	B	597	ASP	3.3
1	A	491	SER	3.3
1	A	597	ASP	3.3
1	A	382	GLU	3.2
1	A	680	VAL	3.2
1	A	553	TRP	3.2
1	A	490	GLY	3.2
1	A	616	LEU	3.1
1	B	620	LYS	3.1
1	A	416	VAL	3.1
1	A	691	PHE	3.1
1	B	616	LEU	3.1
1	A	373	GLY	3.1
1	A	481	ARG	3.1
1	A	479	LEU	3.1
1	B	615	ASP	3.1
1	A	667	ARG	3.1
1	A	492	THR	3.0
1	A	507	GLN	3.0
1	B	561	TRP	3.0
1	B	593	ILE	3.0
1	A	682	PRO	3.0
1	B	375	LYS	3.0
1	A	487	GLN	2.9
1	A	446	VAL	2.9
1	B	321	THR	2.9
1	A	528	GLY	2.9
1	A	391	THR	2.9
1	B	691	PHE	2.9
1	B	327	THR	2.8
1	A	311	VAL	2.8
1	A	552	ASP	2.8
1	A	604	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	706	TYR	2.8
1	A	564	LEU	2.8
1	A	385	ASN	2.8
1	A	561	TRP	2.7
1	A	414	ARG	2.7
1	B	591	THR	2.7
1	A	394	TYR	2.7
1	A	393	THR	2.7
1	A	516	ARG	2.7
1	A	386	LYS	2.7
1	B	618	MET	2.7
1	A	686	SER	2.7
1	A	562	TYR	2.6
1	B	311	VAL	2.6
1	B	312	LEU	2.6
1	B	322	LEU	2.6
1	A	511	LYS	2.6
1	A	470	HIS	2.6
1	B	682	PRO	2.6
1	A	619	ARG	2.5
1	A	618	MET	2.5
1	B	617	ASP	2.5
1	B	443	CYS	2.4
1	B	370	LYS	2.4
1	A	630	LEU	2.4
1	A	485	TYR	2.4
1	A	643	SER	2.4
1	B	392	SER	2.4
1	B	479	LEU	2.4
1	B	309	ASP	2.4
1	B	564	LEU	2.3
1	A	592	GLU	2.3
1	B	666	TYR	2.3
1	A	469	LYS	2.3
1	A	330	ILE	2.3
1	A	466	THR	2.3
1	A	478	GLN	2.3
1	A	684	SER	2.3
1	B	685	GLY	2.3
1	B	681	PRO	2.3
1	A	590	GLY	2.2
1	A	599	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	499	VAL	2.2
1	A	696	LEU	2.2
1	A	443	CYS	2.2
1	A	602	SER	2.2
1	A	452	LYS	2.2
1	B	588	TYR	2.2
1	A	598	TYR	2.2
1	A	523	LEU	2.1
1	B	313	THR	2.1
1	A	356	PRO	2.1
1	A	710	PRO	2.1
1	A	668[A]	CYS	2.1
1	B	324	THR	2.1
1	A	301	LEU	2.1
1	A	531	PRO	2.1
1	A	302	LYS	2.1
1	A	589	MET	2.1
1	A	315	THR	2.1
1	B	353	GLN	2.1
1	A	609	GLU	2.1
1	B	550	LYS	2.1
1	B	713	THR	2.1
1	A	371	ARG	2.0
1	A	465	ARG	2.0
1	B	354	LEU	2.0
1	B	687	ILE	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](#)

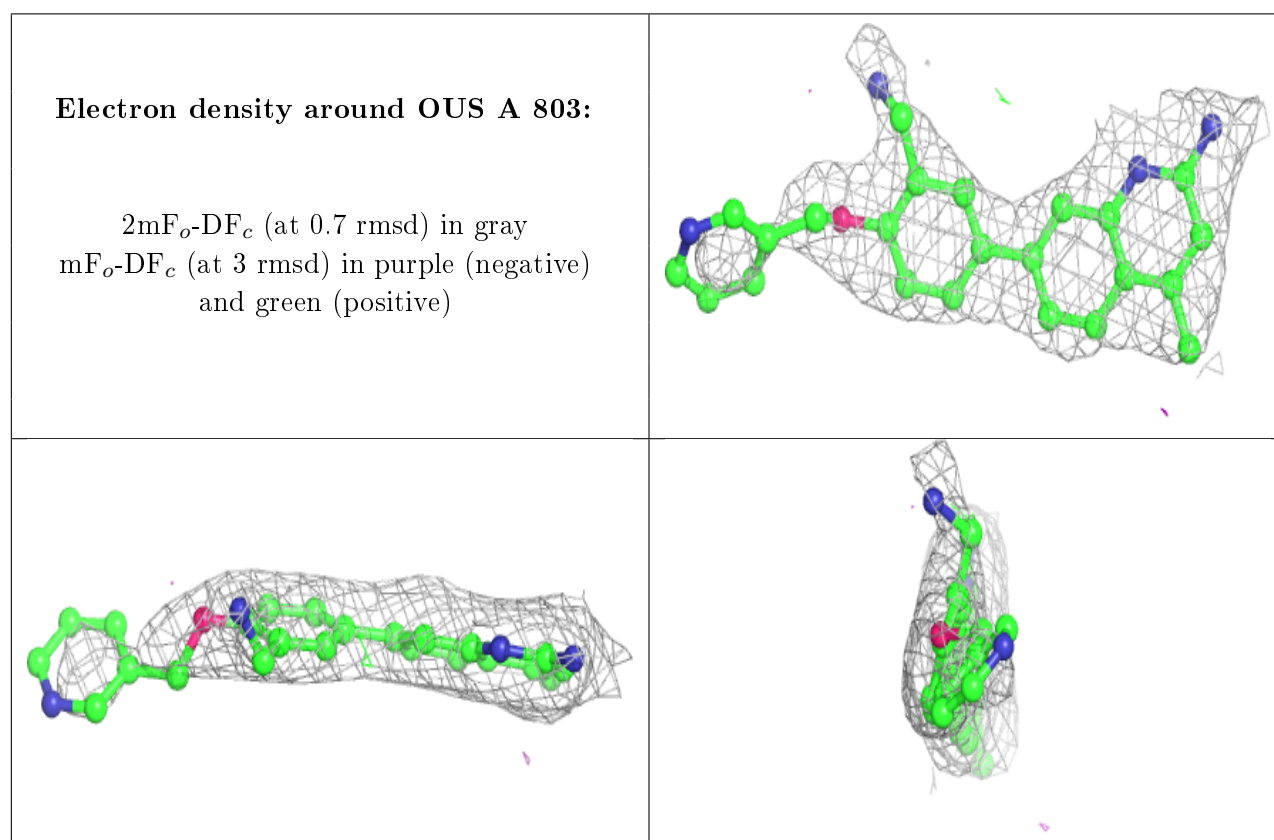
There are no monosaccharides in this entry.

## 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
3	H4B	A	802	17/17	0.90	0.29	68,93,102,104	0
3	H4B	B	802	17/17	0.92	0.28	65,76,93,95	0
4	OUS	A	803	28/28	0.93	0.36	53,78,138,140	0
4	OUS	B	803	28/28	0.93	0.28	50,78,128,130	0
5	ACT	A	804	4/4	0.94	0.14	80,81,81,82	0
5	ACT	B	804	4/4	0.96	0.14	88,90,91,96	0
2	HEM	B	801	43/43	0.97	0.23	46,53,78,89	0
2	HEM	A	801	43/43	0.97	0.26	43,54,76,96	0
6	ZN	B	805	1/1	0.99	0.06	61,61,61,61	0

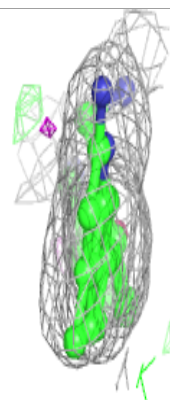
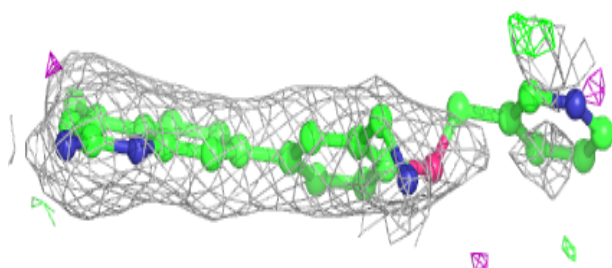
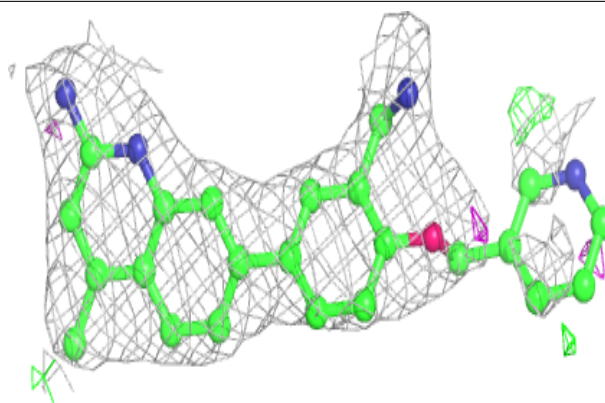
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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





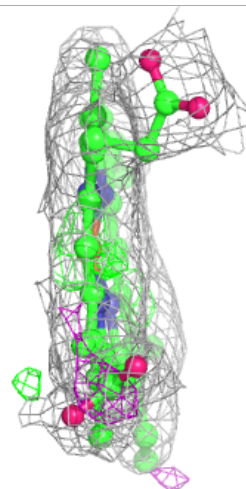
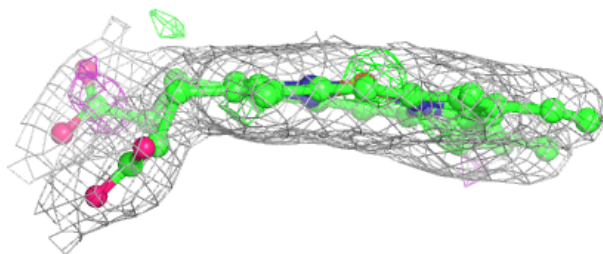
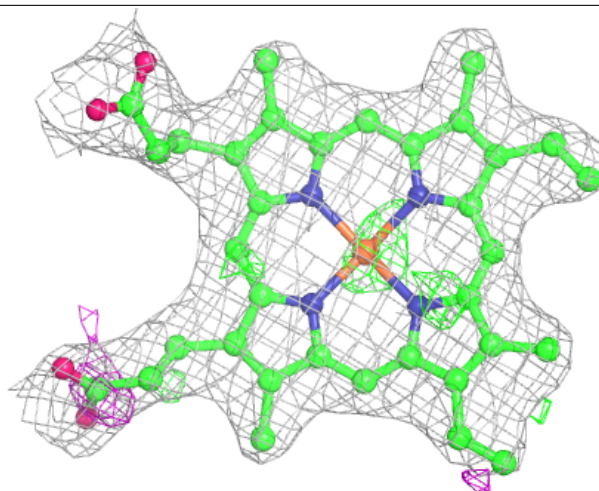
**Electron density around OUS B 803:**

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



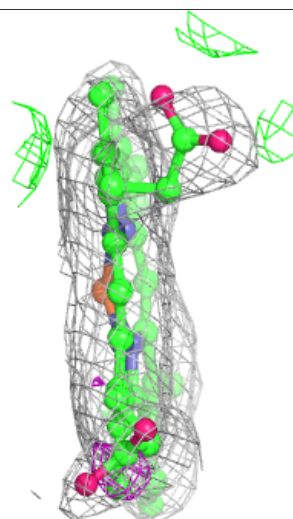
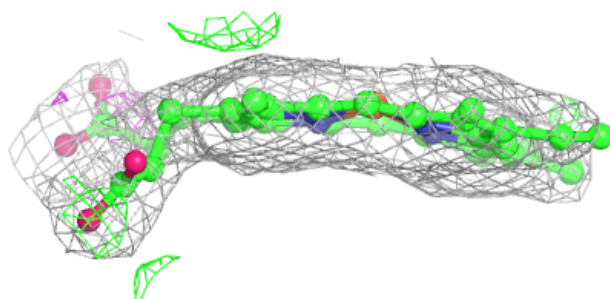
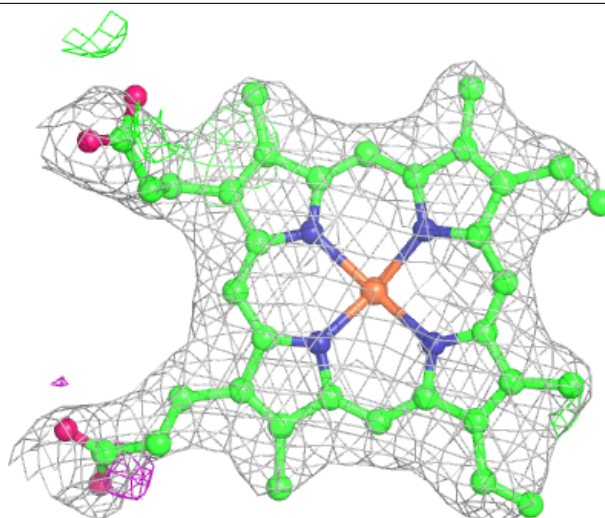
**Electron density around HEM B 801:**

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



**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.