



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:18 AM BST

PDB ID : 6PMW  
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with  
7-(4-(Aminomethyl)phenyl)-4-methylquinolin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2019-07-02  
Resolution : 1.75 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 : 2.14.6  
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) : 2.14.6

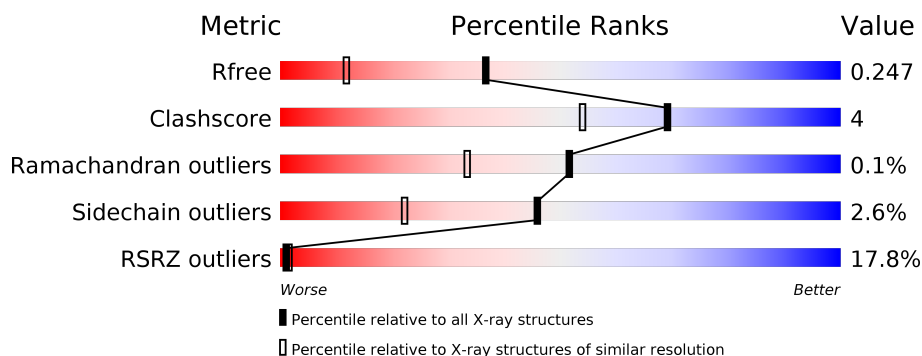
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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>23%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>••</div> </div> </div>
1	B	422	<div> <div>11%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>•</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7229 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	409	Total	C	N	O	S	0	3	0
			3340	2138	571	609	22			
1	B	411	Total	C	N	O	S	0	3	0
			3357	2148	574	614	21			

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



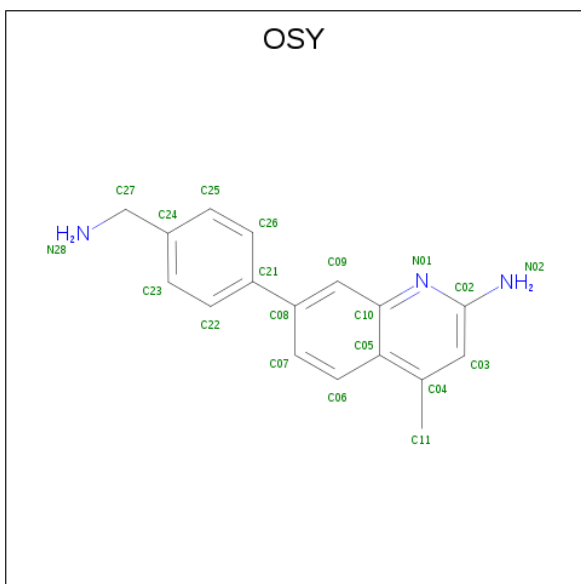
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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-[4-(aminomethyl)phenyl]-4-methylquinolin-2-amine (three-letter code: OSY) (formula: C<sub>17</sub>H<sub>17</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			20	17	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			20	17	3		

- 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	148	Total	O	0	0
			148	148		
7	B	215	Total	O	0	0
			215	215		

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.

- Chain A:
- 
- 23% 84% 13%
- CYS  
PRD  
R299  
F300  
D309  
V310  
V311  
K319  
S320  
T321  
L322  
E323  
I330  
F338  
SER  
GLN  
HIS  
THR  
ARG  
LYS  
PRD  
GLU  
ASP  
V348  
R349  
T350  
K351  
D352  
Q353  
L354  
F355  
E360  
Q364  
K370  
G373  
E382  
K385  
K386  
E387  
I388  
S389  
S390  
T391  
S392  
T393  
Y394  
R414  
C415  
V416  
I442  
V446  
T450  
L455  
I459  
R465  
T466  
D467  
Q468  
K469  
H470  
W475  
M476  
S477  
Q478  
L479  
I480  
R481  
Y485  
K486  
Q487  
F488  
D489  
Q490  
S491  
T492  
L493  
P496  
V499  
Q500  
E503  
I504  
C505  
I506  
Q507  
Q508  
S509  
W510  
K511  
R514  
P521  
L522  
L523  
P531  
P530  
I546  
R547  
H548  
P549  
K550  
P551  
W553  
F554  
K555  
K560  
A566  
V567  
F594  
Y588  
M589  
Q590  
T591  
E592  
I593  
G594  
V595  
C599  
Y604  
D608  
A611  
K612  
D615  
R619  
Q628  
A629  
L630  
V631  
E632  
I633  
W637  
S643  
D644  
K645  
K660  
B663  
N664  
P667  
G668  
W676  
V677  
W678  
I679  
V680  
P681  
P682  
M683  
S684  
G685  
S686  
F691  
F704  
E705  
Y706  
W711  
W712  
T713  
W714  
W715  
W716  
LYS  
GLY

- Chain B:
- 
- | Amino Acid | Category |
|------------|----------|
| CYS        | Red      |
| PRO        | Red      |
| R299       | Red      |
| F300       | Red      |
| I301       | Red      |
| K302       | Red      |
| V310       | Green    |
| V311       | Green    |
| L312       | Green    |
| T313       | Green    |
| L318       | Green    |
| T321       | Green    |
| L322       | Yellow   |
| Y332       | Yellow   |
| L337       | Green    |
| P338       | Green    |
| SER        | Red      |
| GLN        | Red      |
| HIS        | Red      |
| THR        | Red      |
| ARG        | Red      |
| LYS        | Red      |
| PRO        | Red      |
| GLU        | Red      |
| ASP        | Red      |
| V348       | Red      |
| R349       | Red      |
| T350       | Red      |
| K351       | Red      |
| D352       | Red      |
| F355       | Red      |
| Y356       | Yellow   |
| I359       | Yellow   |
| E389       | Red      |
| S390       | Red      |
| T391       | Red      |
| H407       | Yellow   |
| A408       | Yellow   |
| W409       | Yellow   |
| R410       | Yellow   |
| C415       | Red      |
| V416       | Red      |
| W421       | Yellow   |
| C443       | Red      |
| Q478       | Yellow   |
| L479       | Yellow   |
| I480       | Green    |
| R491       | Green    |
| Y495       | Yellow   |
| W510       | Yellow   |
| R514       | Green    |
| P521       | Yellow   |
| L540       | Green    |
| R547       | Green    |
| H548       | Green    |
| P549       | Yellow   |
| K550       | Red      |
| W561       | Red      |
| Y562       | Yellow   |
| A566       | Green    |
| Y567       | Yellow   |
| F584       | Red      |
| G590       | Green    |
| T591       | Green    |
| E592       | Green    |
| I593       | Green    |
| G594       | Green    |
| V595       | Green    |
| C599       | Yellow   |
| S602       | Red      |
| A611       | Green    |
| D615       | Red      |
| L616       | Green    |
| D617       | Green    |
| H618       | Red      |
| R619       | Red      |
| K620       | Red      |
| Q628       | Yellow   |
| E632       | Yellow   |
| H652       | Yellow   |
| R667       | Red      |
| W676       | Red      |
| V677       | Green    |
| W678       | Red      |
| I679       | Red      |
| W680       | Red      |
| D684       | Red      |
| F682       | Red      |
| S686       | Green    |
| F691       | Red      |
| L696       | Green    |
| R699       | Green    |
| Y706       | Green    |
| G718       | Red      |

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.99Å 111.78Å 164.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.07 – 1.75 38.07 – 1.75	Depositor EDS
% Data completeness (in resolution range)	94.2 (38.07-1.75) 94.9 (38.07-1.75)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.202 , 0.245 0.205 , 0.247	Depositor DCC
$R_{free}$ test set	4636 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.1	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	0.97	EDS
Total number of atoms	7229	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% 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: OSY, 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	0.36	0/3439	0.49	0/4665
1	B	0.38	0/3459	0.49	0/4689
All	All	0.37	0/6898	0.49	0/9354

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	3340	0	3254	29	0
1	B	3357	0	3275	17	0
2	A	43	0	30	6	0
2	B	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	20	0	0	1	0
4	B	20	0	0	2	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	148	0	0	2	0
7	B	215	0	0	1	0
All	All	7229	0	6625	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (50) 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	0.82
1:B:706:TYR:OH	2:B:801:HEM:O2D	1.98	0.79
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.70	0.73
2:A:801:HEM:HHC	2:A:801:HEM:HBB2	1.74	0.70
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.76	0.67
2:B:801:HEM:HBC2	2:B:801:HEM:HMC2	1.76	0.66
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.77	0.66
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.79	0.65
2:B:801:HEM:HBD1	4:B:803:OSY:C22	2.35	0.57
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.69	0.57
1:B:567:VAL:HG21	4:B:803:OSY:C07	2.35	0.56
1:A:706:TYR:OH	2:A:801:HEM:O2D	2.17	0.55
1:A:567:VAL:HG21	4:A:803:OSY:C07	2.43	0.49
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.46	0.48
1:A:393:THR:OG1	1:A:394:TYR:N	2.46	0.48
1:A:631:VAL:HG11	1:B:628:GLN:HG3	1.95	0.48
1:A:539:GLU:OE2	7:A:902:HOH:O	2.20	0.48
1:A:555:LYS:NZ	7:A:905:HOH:O	2.44	0.47
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.96	0.47
1:A:546:ILE:HG12	1:A:560:LYS:HA	1.97	0.47
1:A:608:GLU:H	1:A:608:GLU:HG2	1.44	0.47
1:A:664:ASN:OD1	1:A:667:ARG:NH2	2.48	0.46
1:B:366:TYR:HA	1:B:369:ILE:HG12	1.97	0.46
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.51	0.46
1:A:485:TYR:CE1	1:A:514:ARG:HA	2.51	0.45
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.99	0.45
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.77	0.45
2:A:801:HEM:HMD2	2:A:801:HEM:HBD2	1.99	0.45
1:A:686:SER:HA	1:A:691:PHE:CG	2.52	0.44
1:B:548:HIS:CG	1:B:549:PRO:HD2	2.53	0.44
1:B:652:HIS:ND1	7:B:904:HOH:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:VAL:O	1:B:599:CYS:HB2	2.17	0.44
1:A:548:HIS:CE1	1:A:551:PHE:HD1	2.35	0.44
1:A:360:GLU:O	1:A:364:GLN:HG2	2.18	0.44
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.98	0.44
1:A:595:VAL:O	1:A:599:CYS:HB2	2.18	0.43
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.53	0.43
1:A:551:PHE:HD2	1:A:553:TRP:HE1	1.67	0.42
1:A:414:ARG:HB2	2:A:801:HEM:HAD1	2.01	0.42
1:A:350:THR:N	1:A:353:GLN:OE1	2.50	0.42
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.55	0.42
1:A:450:THR:HA	1:A:455:LEU:HD22	2.01	0.42
1:B:686:SER:HA	1:B:691:PHE:CG	2.55	0.41
2:A:801:HEM:CMD	2:A:801:HEM:HBD2	2.50	0.41
1:B:485:TYR:CE1	1:B:514:ARG:HA	2.55	0.41
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.56	0.41
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.55	0.41
1:B:407:HIS:CE1	1:B:410:ARG:HH11	2.39	0.41
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.90	0.40
1:A:523:LEU:HA	1:A:523:LEU:HD23	1.92	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	407/422 (96%)	393 (97%)	13 (3%)	1 (0%)	47	29
1	B	410/422 (97%)	399 (97%)	11 (3%)	0	100	100
All	All	817/844 (97%)	792 (97%)	24 (3%)	1 (0%)	51	33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	491	SER

### 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	367/377 (97%)	352 (96%)	15 (4%)	30	9
1	B	369/377 (98%)	365 (99%)	4 (1%)	73	59
All	All	736/754 (98%)	717 (97%)	19 (3%)	46	22

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	LYS
1	A	348	VAL
1	A	382	GLU
1	A	476	ASN
1	A	489	ASP
1	A	508	GLN
1	A	523	LEU
1	A	547	ARG
1	A	555	LYS
1	A	608	GLU
1	A	612	LYS
1	A	615	ASP
1	A	645	LYS
1	A	663	GLU
1	A	715	VAL
1	B	332	MET
1	B	337	LEU
1	B	540	LEU
1	B	547	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	601	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 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	A	804	-	1,3,3	1.56	0	0,3,3	0.00	-
5	ACT	B	804	-	1,3,3	1.31	0	0,3,3	0.00	-
4	OSY	B	803	-	22,22,22	0.91	0	30,31,31	1.30	4 (13%)
2	HEM	B	801	1	27,50,50	2.17	7 (25%)	17,82,82	1.68	3 (17%)
2	HEM	A	801	1	27,50,50	2.24	6 (22%)	17,82,82	1.63	4 (23%)
4	OSY	A	803	-	22,22,22	0.89	1 (4%)	30,31,31	1.48	5 (16%)
3	H4B	A	802	-	16,18,18	0.85	0	11,26,26	2.60	6 (54%)
3	H4B	B	802	-	16,18,18	0.80	0	11,26,26	2.47	5 (45%)

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
4	OSY	B	803	-	-	4/6/6/6	0/3/3/3
2	HEM	B	801	1	-	1/6/54/54	-
2	HEM	A	801	1	-	2/6/54/54	-
4	OSY	A	803	-	-	6/6/6/6	0/3/3/3
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3D-C2D	5.48	1.53	1.37
2	B	801	HEM	C3D-C2D	5.02	1.52	1.37
2	A	801	HEM	C3B-C2B	-4.84	1.33	1.40
2	B	801	HEM	C3B-C2B	-4.76	1.33	1.40
2	B	801	HEM	C3C-C2C	-4.03	1.34	1.40
2	A	801	HEM	C3C-C2C	-3.80	1.35	1.40
2	A	801	HEM	C3B-CAB	3.73	1.55	1.47
2	B	801	HEM	C3C-CAC	3.54	1.55	1.47
2	A	801	HEM	C3C-CAC	3.54	1.55	1.47
2	B	801	HEM	C3B-CAB	3.24	1.54	1.47
2	A	801	HEM	C1D-ND	2.40	1.41	1.36
2	B	801	HEM	C1D-ND	2.34	1.41	1.36
4	A	803	OSY	C02-N01	2.17	1.36	1.33
2	B	801	HEM	C1C-C2C	2.02	1.47	1.42

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	H4B	C4-C4A-C8A	4.93	118.95	114.57
3	B	802	H4B	C4-C4A-C8A	4.57	118.63	114.57
4	A	803	OSY	C04-C05-C10	3.77	120.05	118.01
2	A	801	HEM	CBA-CAA-C2A	-3.61	105.83	112.49
4	B	803	OSY	C26-C21-C08	-3.54	115.23	121.36
2	B	801	HEM	CBA-CAA-C2A	-3.53	105.98	112.49
2	B	801	HEM	C1D-C2D-C3D	-3.43	104.61	107.00
3	A	802	H4B	C4-N3-C2	3.42	121.36	115.93
3	A	802	H4B	N3-C2-N1	-3.37	120.13	125.42
4	A	803	OSY	C05-C10-N01	-3.34	119.27	122.81
2	B	801	HEM	CAD-CBD-CGD	-3.16	107.37	112.67
3	B	802	H4B	C4-N3-C2	3.16	120.95	115.93
3	B	802	H4B	N3-C2-N1	-3.13	120.51	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	H4B	C4-C4A-N5	2.99	121.63	119.12
4	B	803	OSY	C04-C05-C10	2.75	119.50	118.01
4	A	803	OSY	N02-C02-N01	2.73	120.51	118.26
3	A	802	H4B	C2-N1-C8A	2.66	120.49	114.54
3	B	802	H4B	C2-N1-C8A	2.63	120.43	114.54
3	A	802	H4B	C4-C4A-N5	2.52	121.24	119.12
4	B	803	OSY	C05-C10-N01	-2.45	120.21	122.81
2	A	801	HEM	C3C-C4C-NC	-2.20	106.80	110.94
3	A	802	H4B	N2-C2-N3	2.15	120.60	117.25
4	B	803	OSY	C22-C21-C08	2.14	125.07	121.36
2	A	801	HEM	C1D-C2D-C3D	-2.14	105.51	107.00
4	A	803	OSY	C07-C08-C21	-2.10	117.71	121.36
4	A	803	OSY	C06-C05-C04	-2.10	119.66	123.66
2	A	801	HEM	CMC-C2C-C3C	2.09	128.60	124.68

There are no chirality outliers.

All (13) torsion outliers are listed below:

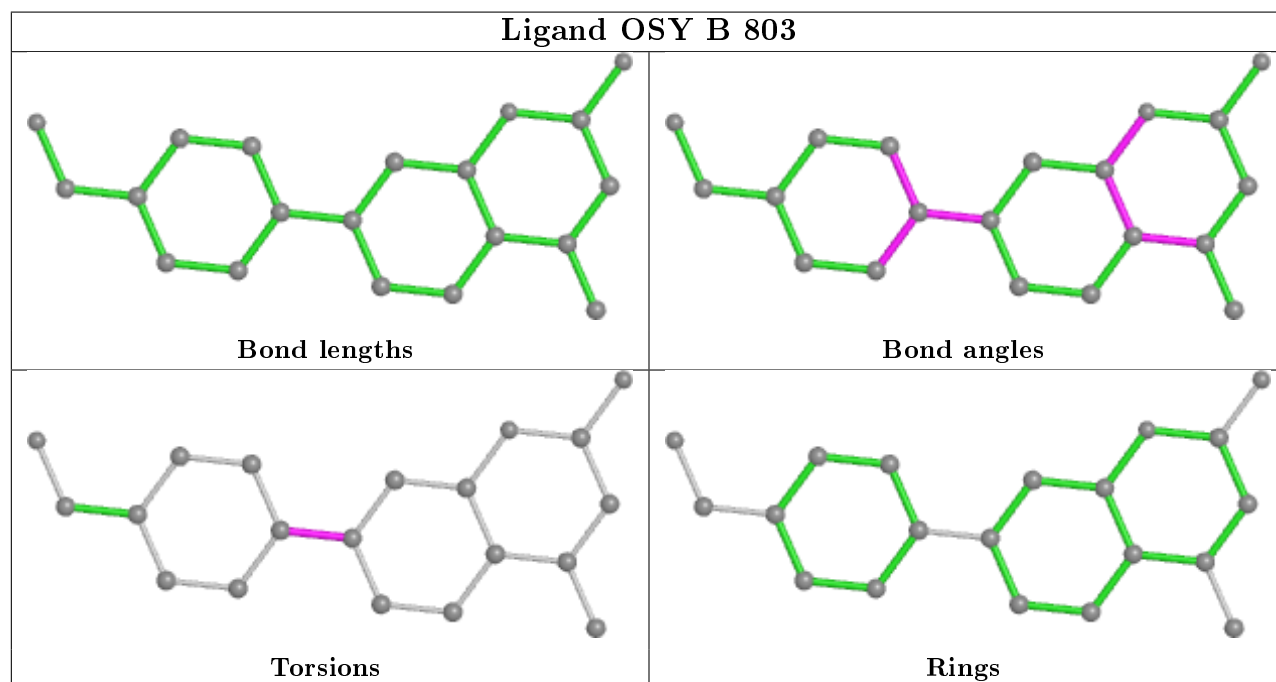
Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C2D-C3D-CAD-CBD
2	A	801	HEM	C4D-C3D-CAD-CBD
4	B	803	OSY	C07-C08-C21-C26
4	A	803	OSY	C07-C08-C21-C26
4	A	803	OSY	C09-C08-C21-C26
4	B	803	OSY	C07-C08-C21-C22
4	A	803	OSY	C07-C08-C21-C22
4	B	803	OSY	C09-C08-C21-C26
4	A	803	OSY	C09-C08-C21-C22
2	B	801	HEM	C2A-CAA-CBA-CGA
4	B	803	OSY	C09-C08-C21-C22
4	A	803	OSY	C23-C24-C27-N28
4	A	803	OSY	C25-C24-C27-N28

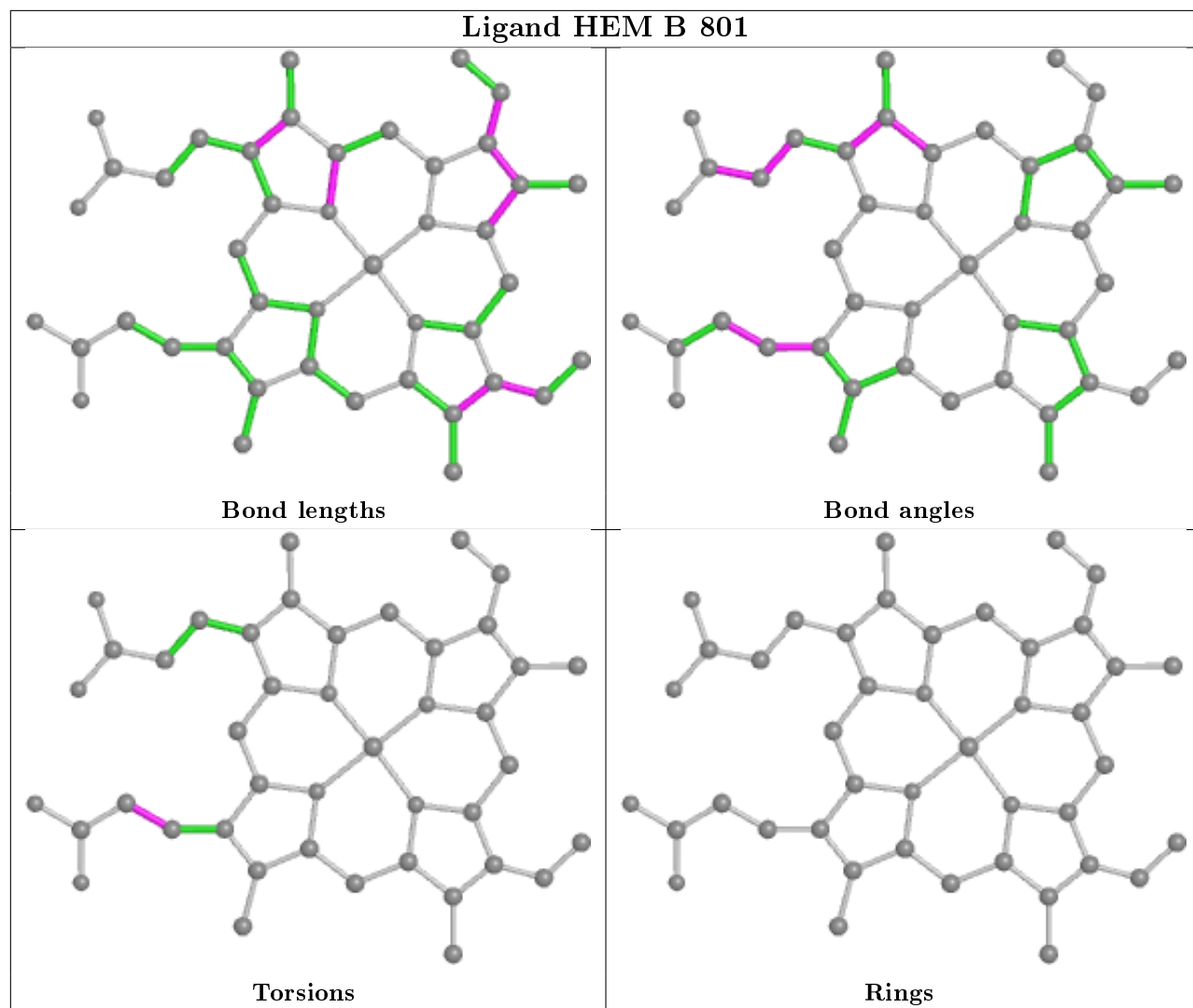
There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	803	OSY	2	0
2	B	801	HEM	4	0
2	A	801	HEM	6	0
4	A	803	OSY	1	0

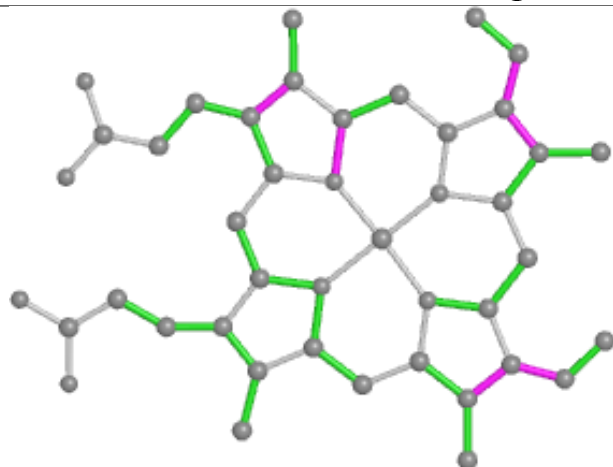
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



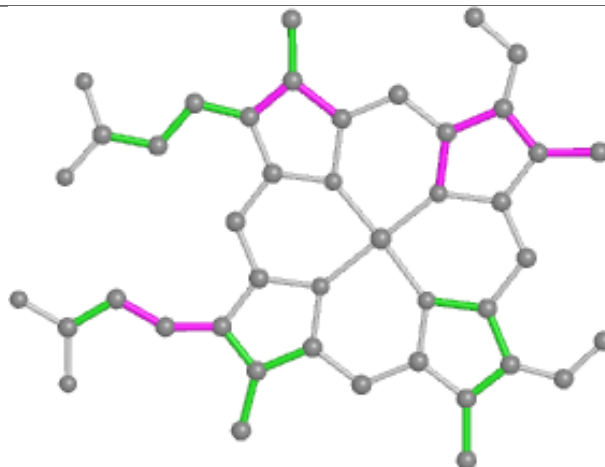




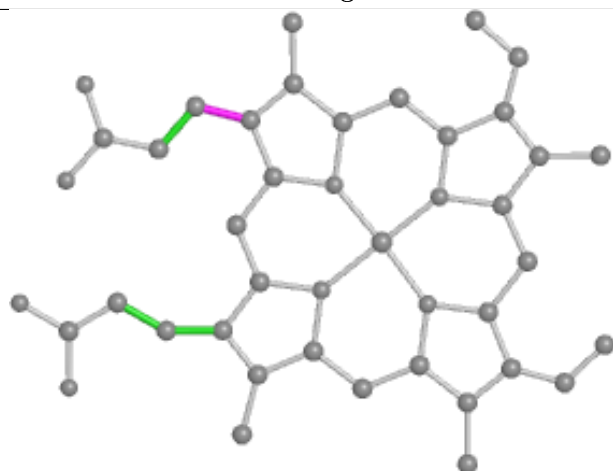
## Ligand HEM A 801



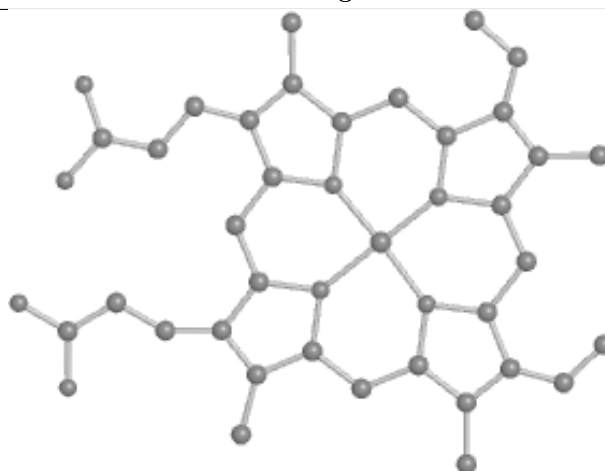
Bond lengths



Bond angles

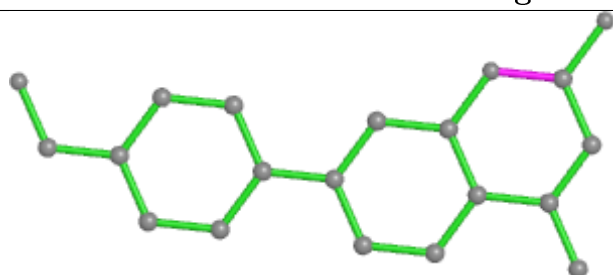


Torsions

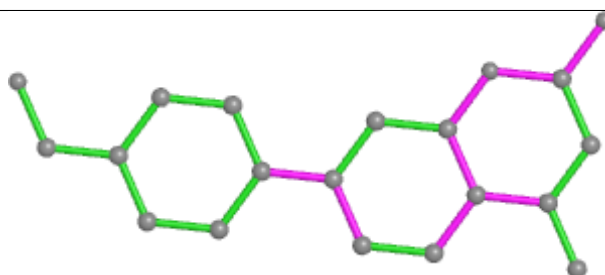


Rings

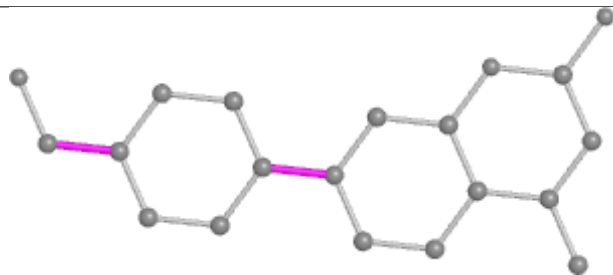
## Ligand OSY A 803



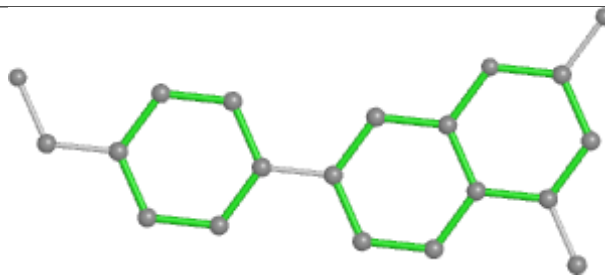
Bond lengths



Bond angles



Torsions



Rings

## 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	409/422 (96%)	1.23	99 (24%) <b>0</b> <b>0</b>	33, 59, 107, 148	0
1	B	411/422 (97%)	0.67	47 (11%) <b>5</b> <b>6</b>	30, 49, 85, 114	0
All	All	820/844 (97%)	0.95	146 (17%) <b>1</b> <b>1</b>	30, 54, 101, 148	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	10.9
1	A	716	TRP	8.6
1	A	715	VAL	8.0
1	A	506	ILE	6.8
1	A	488	PRO	6.5
1	A	388	ILE	5.9
1	A	355	PHE	5.8
1	A	299	ARG	5.8
1	A	348	VAL	5.7
1	A	349	ARG	5.0
1	A	486	LYS	4.9
1	A	551	PHE	4.9
1	B	299	ARG	4.8
1	A	300	PHE	4.8
1	A	499	VAL	4.6
1	A	490	GLY	4.6
1	A	711	TRP	4.6
1	A	391	THR	4.5
1	B	620	LYS	4.4
1	B	718	GLY	4.4
1	B	350	THR	4.4
1	B	348	VAL	4.3
1	A	714	HIS	4.2
1	A	713	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	593	ILE	4.1
1	A	322	LEU	4.1
1	A	678	TRP	4.0
1	A	352	ASP	4.0
1	A	679	ILE	4.0
1	A	584	PHE	4.0
1	B	351	LYS	4.0
1	B	301	LEU	3.9
1	A	677	VAL	3.9
1	B	677	VAL	3.9
1	A	567	VAL	3.9
1	A	489	ASP	3.9
1	B	352	ASP	3.9
1	A	385	ASN	3.9
1	B	313	THR	3.9
1	A	676	TRP	3.8
1	B	302	LYS	3.8
1	A	386	LYS	3.7
1	A	350	THR	3.6
1	A	712	ASN	3.6
1	A	311	VAL	3.6
1	B	318	LEU	3.6
1	A	351	LYS	3.5
1	A	470	HIS	3.5
1	A	685	GLY	3.5
1	B	321	THR	3.5
1	A	354	LEU	3.5
1	A	353	GLN	3.5
1	A	487	GLN	3.5
1	B	680	VAL	3.4
1	A	507	GLN	3.4
1	A	681	PRO	3.4
1	A	390	SER	3.4
1	B	678	TRP	3.4
1	A	508	GLN	3.4
1	A	591	THR	3.4
1	A	492	THR	3.3
1	A	566	ALA	3.3
1	A	373	GLY	3.3
1	A	643	SER	3.2
1	A	630	LEU	3.2
1	B	310	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	616	LEU	3.2
1	B	691	PHE	3.2
1	A	590	GLY	3.2
1	A	511	LYS	3.2
1	A	588	TYR	3.2
1	A	505	CYS	3.1
1	B	619	ARG	3.1
1	A	491	SER	3.1
1	B	679	ILE	3.1
1	A	503	GLU	3.1
1	A	479	LEU	3.0
1	B	567	VAL	3.0
1	A	415	CYS	2.9
1	B	676	TRP	2.9
1	A	389	GLU	2.9
1	A	480	ILE	2.9
1	B	682	PRO	2.8
1	B	602[A]	SER	2.8
1	A	485	TYR	2.8
1	A	309	ASP	2.8
1	B	615	ASP	2.8
1	A	469	LYS	2.8
1	B	667	ARG	2.7
1	A	310	VAL	2.7
1	A	682	PRO	2.7
1	A	466	THR	2.7
1	A	691	PHE	2.7
1	A	392	SER	2.7
1	A	393	THR	2.6
1	A	459	ILE	2.6
1	A	467	ASP	2.6
1	B	611	ALA	2.6
1	A	553	TRP	2.6
1	B	562	TYR	2.6
1	A	704	PHE	2.5
1	B	550	LYS	2.5
1	A	615	ASP	2.5
1	B	391	THR	2.5
1	B	355	PHE	2.5
1	A	633	ILE	2.5
1	A	611	ALA	2.5
1	B	311	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	493	LEU	2.5
1	A	321	THR	2.4
1	B	389	GLU	2.4
1	B	681	PRO	2.4
1	A	686	SER	2.4
1	A	382	GLU	2.4
1	A	680	VAL	2.3
1	A	619	ARG	2.3
1	A	667	ARG	2.3
1	B	566	ALA	2.3
1	A	500	GLN	2.3
1	B	479	LEU	2.3
1	A	683	MET	2.3
1	B	590	GLY	2.2
1	B	618	MET	2.2
1	A	504	ILE	2.2
1	B	561	TRP	2.2
1	A	323	GLU	2.2
1	B	593	ILE	2.2
1	A	394	TYR	2.1
1	B	312	LEU	2.1
1	B	416	VAL	2.1
1	B	443	CYS	2.1
1	A	442	ILE	2.1
1	A	589	MET	2.1
1	B	591	THR	2.1
1	A	595	VAL	2.1
1	A	550	LYS	2.1
1	B	584	PHE	2.1
1	A	604	TYR	2.0
1	A	706	TYR	2.0
1	A	660	LYS	2.0
1	A	668[A]	CYS	2.0
1	B	415	CYS	2.0
1	A	465	ARG	2.0
1	A	416	VAL	2.0
1	A	446	VAL	2.0
1	A	637	VAL	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

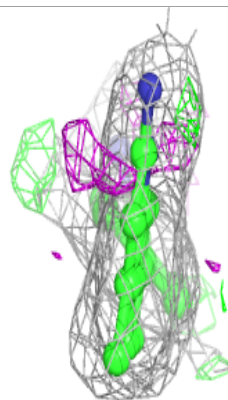
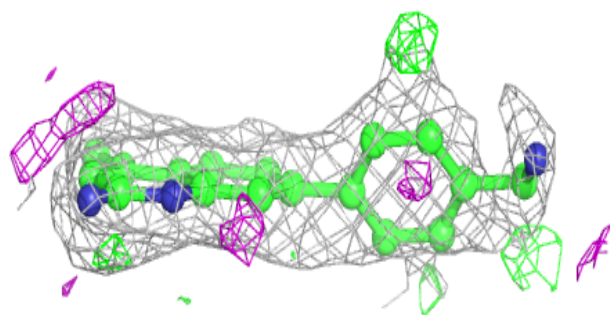
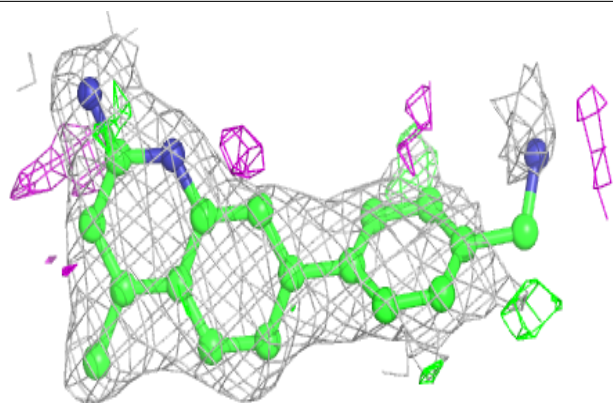
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	ACT	A	804	4/4	0.87	0.22	64,67,68,68	0
4	OSY	B	803	20/20	0.91	0.22	34,55,83,86	0
3	H4B	A	802	17/17	0.91	0.17	32,47,55,57	0
5	ACT	B	804	4/4	0.92	0.20	66,70,72,73	0
4	OSY	A	803	20/20	0.94	0.25	37,48,89,92	0
3	H4B	B	802	17/17	0.94	0.14	36,41,50,50	0
2	HEM	A	801	43/43	0.96	0.19	27,40,64,72	0
2	HEM	B	801	43/43	0.96	0.16	29,38,57,61	0
6	ZN	B	805	1/1	0.99	0.08	41,41,41,41	0

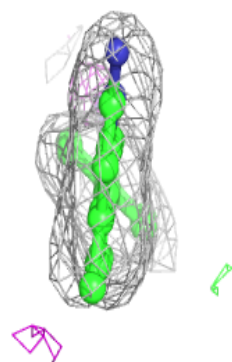
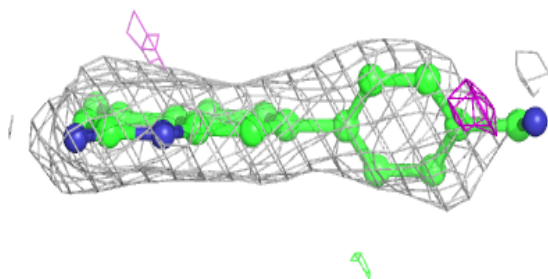
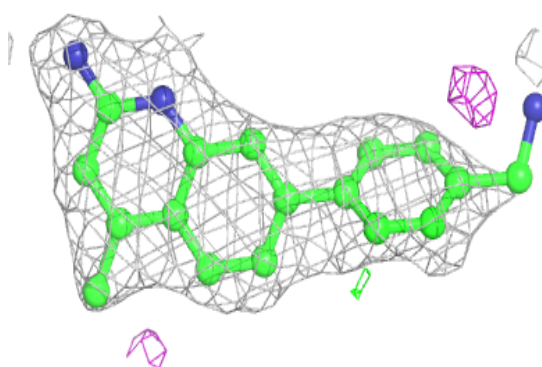
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around OSY 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 OSY A 803:**

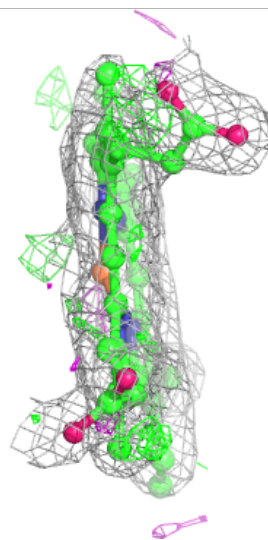
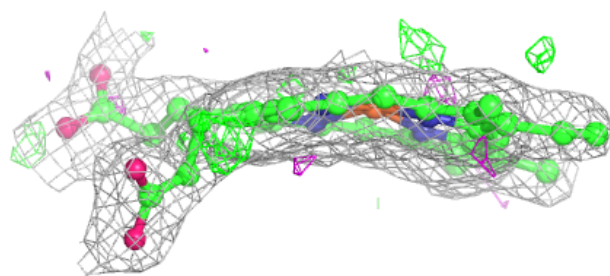
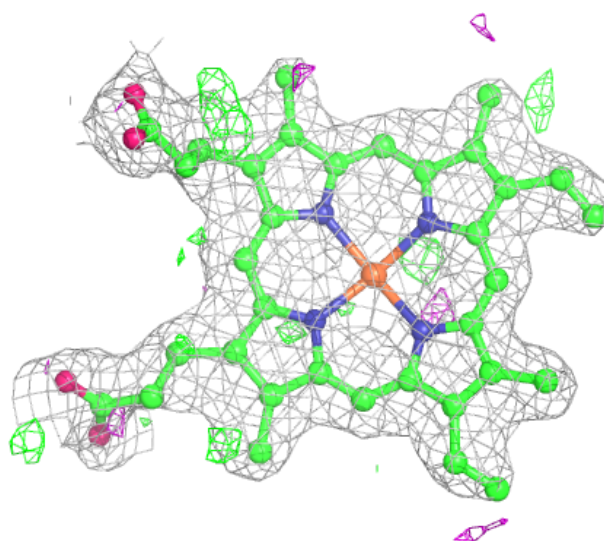
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





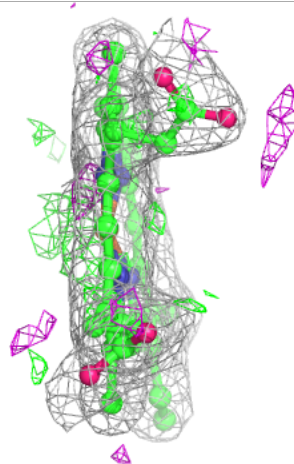
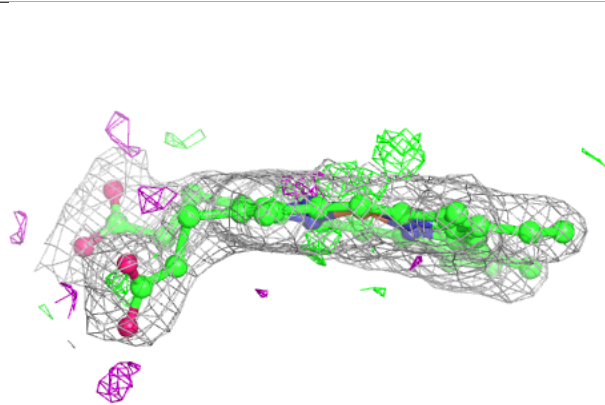
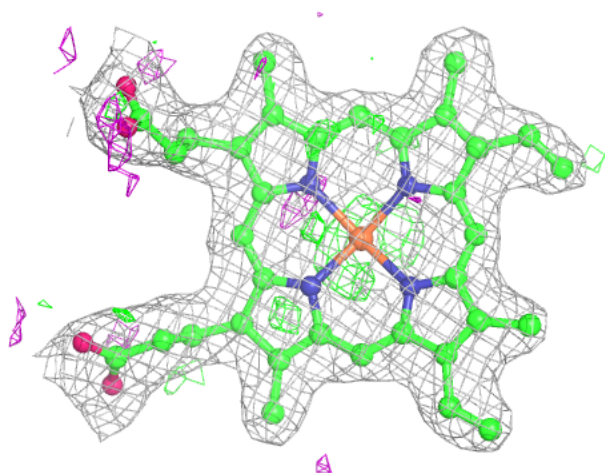
**Electron density around HEM A 801:**

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



**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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.