



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2020 – 10:13 pm BST

PDB ID : 5VUU  
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with 4-(2-(((2-Amino-4-methylquinolin-7-yl)methyl)amino)ethyl)-2-methylbenzoni-  
trile  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2017-05-19  
Resolution : 1.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

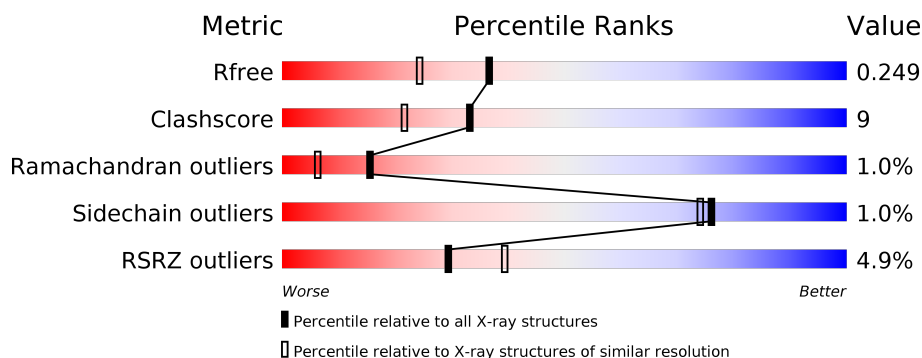
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	<div> <div>9%</div> <div>74%</div> <div>21%</div> <div>...</div> </div>
1	B	422	<div> <div>%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7233 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	3	0
			3354	2145	573	614	22			
1	B	412	Total	C	N	O	S	0	4	0
			3370	2159	575	615	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 ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



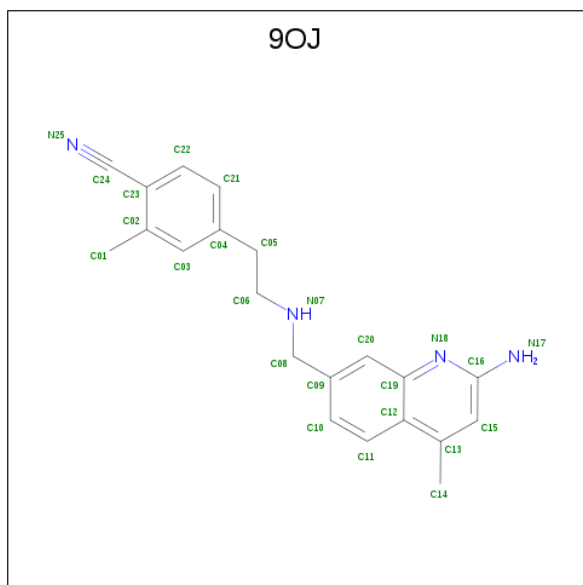
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is 4-(2-[[[(2-amino-4-methylquinolin-7-yl)methyl]amino}ethyl)-2-methylbenzonitrile (three-letter code: 9OJ) (formula: C<sub>21</sub>H<sub>22</sub>N<sub>4</sub>).



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

- 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		

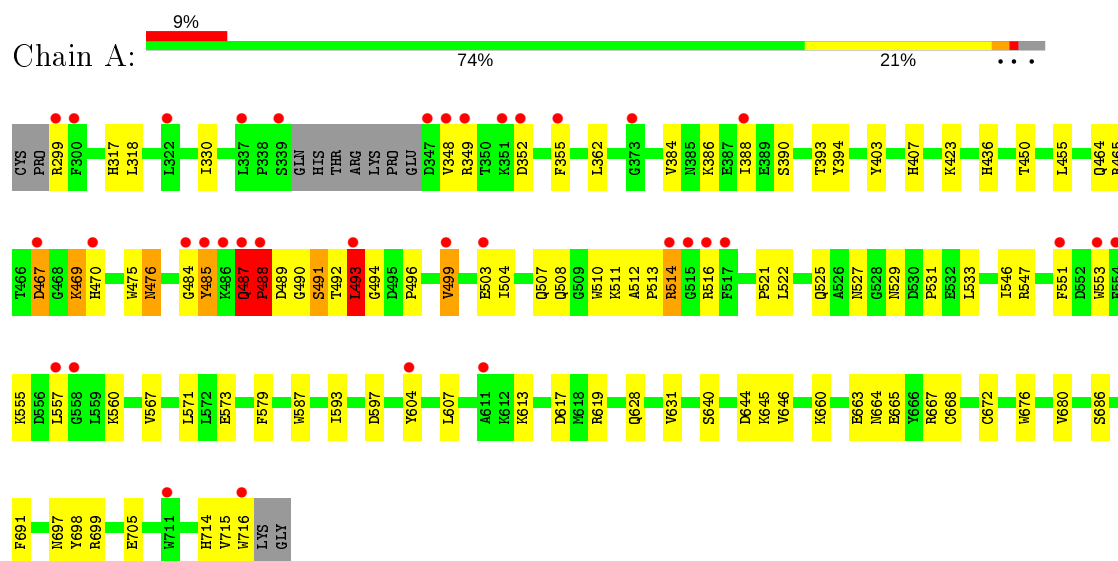
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	137	Total	O	0	0
			137	137		
7	B	189	Total	O	0	0
			189	189		

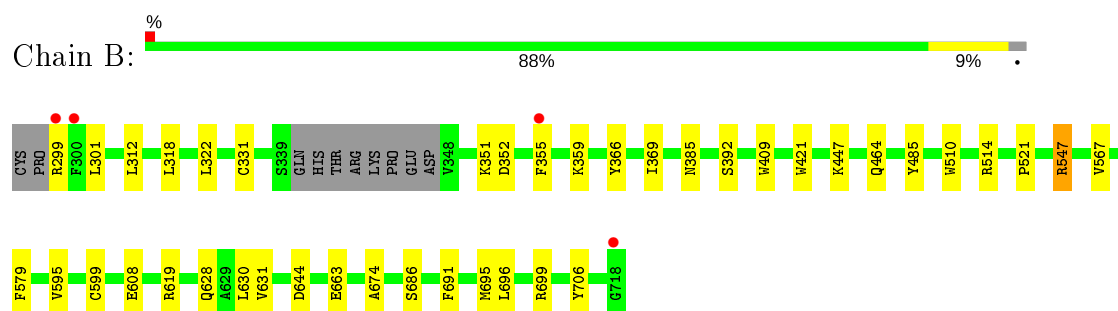
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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 111.07Å 164.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.62 – 1.96 92.06 – 1.96	Depositor EDS
% Data completeness (in resolution range)	97.6 (52.62-1.96) 98.4 (92.06-1.96)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.195 , 0.244 0.196 , 0.249	Depositor DCC
$R_{free}$ test set	3370 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	1.010	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7233	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% 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: H4B, HEM, ZN, 9OJ, 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	0.41	0/3453	0.60	1/4684 (0.0%)
1	B	0.41	0/3476	0.54	0/4713
All	All	0.41	0/6929	0.57	1/9397 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	493	LEU	CA-CB-CG	7.37	132.25	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	352	ASP	Peptide
1	A	487	GLN	Peptide
1	A	488	PRO	Peptide



## 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	3354	0	3263	84	1
1	B	3370	0	3286	33	1
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	8	0	6	0	0
4	B	4	0	3	0	0
5	A	25	0	0	1	0
5	B	25	0	0	1	0
6	A	1	0	0	0	0
7	A	137	0	0	4	0
7	B	189	0	0	2	0
All	All	7233	0	6648	116	1

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 9.

All (116) 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:514:ARG:NH1	7:A:901:HOH:O	2.02	0.92
1:B:322:LEU:HD13	1:B:699:ARG:HH21	1.37	0.88
1:A:557:LEU:HD11	1:A:613:LYS:HZ1	1.55	0.71
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.75	0.68
1:A:476:ASN:HD21	1:A:522:LEU:HA	1.57	0.68
1:A:488:PRO:C	1:A:490:GLY:H	1.96	0.68
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.75	0.66
1:A:469:LYS:HB3	1:A:470:HIS:ND1	2.10	0.66
1:A:487:GLN:HB3	1:A:488:PRO:HD3	1.77	0.66
2:B:801:HEM:HBC2	2:B:801:HEM:HMC2	1.78	0.65
2:A:801:HEM:HHC	2:A:801:HEM:HBB2	1.78	0.65
1:A:484:GLY:HA2	1:A:494:GLY:HA3	1.78	0.64
1:A:348:VAL:HG11	1:A:467:ASP:HA	1.79	0.64
1:A:714:HIS:HD1	1:A:716:TRP:HE3	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:VAL:CG1	1:A:467:ASP:HA	2.29	0.63
1:A:617:ASP:OD1	1:A:619:ARG:HG3	1.99	0.63
1:A:299:ARG:HG3	1:A:318:LEU:HD21	1.82	0.61
1:A:494:GLY:HA2	1:A:516:ARG:HG3	1.81	0.61
1:A:488:PRO:O	1:A:490:GLY:N	2.35	0.59
1:A:484:GLY:O	1:A:499:VAL:HA	2.03	0.58
1:A:465:ARG:HH12	1:A:571:LEU:HD11	1.71	0.56
1:A:494:GLY:CA	1:A:516:ARG:HG3	2.37	0.55
1:A:567:VAL:HG21	5:A:805:9OJ:C10	2.37	0.54
1:B:355[A]:PHE:CD1	1:B:385:ASN:ND2	2.75	0.54
1:B:567:VAL:HG21	5:B:803:9OJ:C10	2.38	0.54
1:A:393:THR:OG1	1:A:394:TYR:N	2.40	0.54
1:A:508:GLN:NE2	1:A:716:TRP:HH2	2.05	0.54
1:A:488:PRO:C	1:A:490:GLY:N	2.62	0.53
1:A:487:GLN:HB2	1:A:493:LEU:HD12	1.89	0.53
1:A:714:HIS:HD2	7:A:1030:HOH:O	1.91	0.53
1:A:485:TYR:HB2	1:A:493:LEU:CD1	2.39	0.52
1:A:644:ASP:O	1:A:645:LYS:HG2	2.10	0.52
1:A:660:LYS:O	1:A:663:GLU:HG2	2.10	0.52
1:A:557:LEU:CD1	1:A:613:LYS:HZ1	2.22	0.51
1:A:546:ILE:HG12	1:A:560:LYS:HA	1.92	0.51
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.45	0.51
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.93	0.51
1:A:423:LYS:HG2	1:A:423:LYS:O	2.10	0.51
1:A:491:SER:OG	1:A:492:THR:N	2.45	0.50
1:A:403:TYR:CE1	1:A:407:HIS:CE1	3.00	0.50
1:A:697:ASN:HB3	1:B:331:CYS:HB3	1.94	0.50
1:A:476:ASN:ND2	1:A:522:LEU:HD23	2.27	0.50
1:A:349:ARG:NH2	1:A:573:GLU:OE2	2.41	0.49
1:A:467:ASP:OD1	1:A:469:LYS:HD3	2.11	0.49
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.93	0.49
1:A:628:GLN:HG3	1:B:631:VAL:HG11	1.93	0.49
1:A:663:GLU:HB3	7:A:936:HOH:O	2.11	0.49
1:B:464:GLN:HB3	1:B:579:PHE:CE2	2.48	0.49
1:B:547:ARG:HH22	1:B:644:ASP:CG	2.15	0.48
1:A:470:HIS:HB3	1:A:527:ASN:OD1	2.12	0.48
1:B:619:ARG:HH11	1:B:619:ARG:HG2	1.77	0.48
1:B:595:VAL:O	1:B:599:CYS:HB2	2.13	0.47
1:B:299:ARG:HB3	1:B:318:LEU:HD21	1.96	0.47
1:A:699:ARG:NH1	1:A:705:GLU:OE1	2.47	0.47
1:A:469:LYS:HE3	1:A:470:HIS:HE1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:TRP:CE2	1:A:521:PRO:HD3	2.50	0.47
1:A:504:ILE:HA	1:A:507:GLN:HB3	1.96	0.47
1:A:355:PHE:HD1	1:A:388:ILE:HD12	1.80	0.47
1:A:485:TYR:HB2	1:A:493:LEU:HD13	1.97	0.46
1:A:547:ARG:NH2	1:A:640:SER:HA	2.30	0.46
1:A:436:HIS:ND1	7:A:904:HOH:O	2.36	0.46
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.51	0.46
1:A:386:LYS:O	1:A:390:SER:OG	2.26	0.46
1:B:322:LEU:HB2	1:B:699:ARG:HB2	1.98	0.46
1:B:706:TYR:OH	2:B:801:HEM:O2D	2.30	0.46
1:A:513:PRO:O	1:A:514:ARG:CB	2.65	0.45
1:A:525:GLN:HG3	1:A:529:ASN:O	2.17	0.45
1:A:644:ASP:C	1:A:645:LYS:HG2	2.37	0.45
1:B:355[A]:PHE:CE1	1:B:359:LYS:HB2	2.51	0.45
1:A:513:PRO:O	1:A:514:ARG:HB2	2.15	0.45
1:B:366:TYR:HA	1:B:369:ILE:HG12	1.98	0.45
1:A:494:GLY:N	1:A:516:ARG:HG3	2.31	0.45
1:A:362:LEU:HD11	1:A:384:VAL:HG21	1.99	0.44
1:A:487:GLN:CB	1:A:488:PRO:HD3	2.47	0.44
1:B:608:GLU:HG3	7:B:908:HOH:O	2.16	0.44
1:B:674:ALA:HB3	1:B:695:MET:HB3	1.99	0.44
1:A:386:LYS:HE3	1:A:386:LYS:HB2	1.72	0.44
1:A:476:ASN:N	1:A:476:ASN:OD1	2.51	0.44
1:A:667:ARG:NH1	1:A:668[A]:CYS:SG	2.91	0.44
1:B:510:TRP:CE2	1:B:521:PRO:HD3	2.53	0.44
1:B:351:LYS:HE2	1:B:392:SER:OG	2.18	0.43
1:A:555:LYS:HB2	1:A:555:LYS:HE3	1.71	0.43
1:B:447:LYS:NZ	7:B:907:HOH:O	2.51	0.43
1:A:450:THR:HA	1:A:455:LEU:HD22	2.00	0.43
1:B:301:LEU:HA	1:B:301:LEU:HD23	1.85	0.43
1:A:330:ILE:HD11	1:B:696:LEU:HD22	2.01	0.42
1:A:557:LEU:HD11	1:A:613:LYS:NZ	2.28	0.42
1:A:664:ASN:OD1	1:A:667:ARG:NH2	2.51	0.42
1:A:676:TRP:CZ2	1:A:680:VAL:HG21	2.54	0.42
1:B:619:ARG:HG2	1:B:619:ARG:NH1	2.34	0.42
1:A:455:LEU:HD12	1:A:587:TRP:CB	2.49	0.42
1:B:355[A]:PHE:CZ	1:B:359:LYS:HB2	2.54	0.42
1:A:330:ILE:HD11	1:B:696:LEU:HB3	2.01	0.42
1:A:464:GLN:HB3	1:A:579:PHE:CE2	2.55	0.42
1:A:512:ALA:HA	1:A:513:PRO:HD3	1.69	0.42
1:A:467:ASP:N	1:A:467:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:LEU:HD11	1:B:663:GLU:HG2	2.02	0.42
1:B:547:ARG:NH2	1:B:644:ASP:OD1	2.49	0.42
1:B:385:ASN:HA	1:B:385:ASN:HD22	1.54	0.41
1:B:485:TYR:CZ	1:B:514:ARG:HA	2.55	0.41
1:A:644:ASP:O	1:A:646:VAL:HG23	2.21	0.41
1:A:551:PHE:N	1:A:551:PHE:CD1	2.88	0.41
1:A:593:ILE:HA	1:A:597:ASP:HB2	2.03	0.41
1:B:686:SER:HA	1:B:691:PHE:CG	2.55	0.41
1:A:533:LEU:HA	1:A:533:LEU:HD23	1.84	0.41
1:A:516:ARG:HG2	1:A:604:TYR:HE2	1.86	0.41
1:A:607:LEU:HD23	1:A:607:LEU:HA	1.95	0.41
1:A:317:HIS:HA	1:A:698:TYR:CE1	2.56	0.41
1:A:631:VAL:HG11	1:B:628:GLN:HG3	2.02	0.41
1:A:551:PHE:HD2	1:A:553:TRP:CZ2	2.39	0.41
1:A:686:SER:HA	1:A:691:PHE:CG	2.55	0.41
1:A:547:ARG:NH1	1:A:644:ASP:OD1	2.54	0.40
1:A:665:GLU:HB2	1:A:672:CYS:HB2	2.04	0.40
1:B:595:VAL:HA	1:B:630:LEU:HD11	2.04	0.40
1:A:492:THR:HG21	1:A:496:PRO:HG3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:ARG:NH2	1:B:352:ASP:OD1[3_545]	2.15	0.05

## 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	409/422 (97%)	384 (94%)	17 (4%)	8 (2%)	<b>7</b> <b>1</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	412/422 (98%)	402 (98%)	10 (2%)	0	100	100
All	All	821/844 (97%)	786 (96%)	27 (3%)	8 (1%)	15	6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	487	GLN
1	A	488	PRO
1	A	489	ASP
1	A	467	ASP
1	A	469	LYS
1	A	491	SER
1	A	715	VAL
1	A	499	VAL

### 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	369/377 (98%)	363 (98%)	6 (2%)	62	58
1	B	370/377 (98%)	369 (100%)	1 (0%)	92	92
All	All	739/754 (98%)	732 (99%)	7 (1%)	76	77

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	476	ASN
1	A	485	TYR
1	A	493	LEU
1	A	503	GLU
1	A	511	LYS
1	A	514	ARG
1	B	547	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	508	GLN
1	B	385	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	2.18	7 (25%)	17,82,82	1.36	2 (11%)
5	9OJ	B	803	-	27,27,27	2.14	1 (3%)	35,37,37	1.44	5 (14%)
5	9OJ	A	805	-	27,27,27	2.23	1 (3%)	35,37,37	1.39	6 (17%)
3	H4B	A	802	-	16,18,18	0.83	0	11,26,26	2.60	7 (63%)
2	HEM	A	801	1	27,50,50	2.11	6 (22%)	17,82,82	1.69	5 (29%)
4	ACT	B	804	-	1,3,3	1.30	0	0,3,3	0.00	-
4	ACT	A	804	-	1,3,3	1.47	0	0,3,3	0.00	-
4	ACT	A	803	-	1,3,3	1.67	0	0,3,3	0.00	-
3	H4B	B	802	-	16,18,18	1.05	1 (6%)	11,26,26	2.48	4 (36%)

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	-	1/6/54/54	-
5	9OJ	B	803	-	-	3/9/9/9	0/3/3/3
5	9OJ	A	805	-	-	4/9/9/9	0/3/3/3
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
2	HEM	A	801	1	-	3/6/54/54	-
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	805	9OJ	C23-C24	-10.60	1.28	1.44
5	B	803	9OJ	C23-C24	-10.22	1.28	1.44
2	B	801	HEM	C3D-C2D	5.06	1.52	1.37
2	A	801	HEM	C3D-C2D	4.96	1.52	1.37
2	A	801	HEM	C3B-C2B	-4.63	1.33	1.40
2	B	801	HEM	C3B-C2B	-4.62	1.34	1.40
2	B	801	HEM	C3C-C2C	-3.92	1.34	1.40
2	A	801	HEM	C3B-CAB	3.85	1.55	1.47
2	B	801	HEM	C3B-CAB	3.71	1.55	1.47
2	A	801	HEM	C3C-CAC	3.63	1.55	1.47
2	B	801	HEM	C3C-CAC	3.59	1.55	1.47
2	A	801	HEM	C3C-C2C	-3.44	1.35	1.40
2	A	801	HEM	C1D-ND	2.30	1.40	1.36
3	B	802	H4B	C4-C4A	-2.08	1.38	1.41
2	B	801	HEM	CAA-C2A	2.04	1.55	1.52
2	B	801	HEM	CMA-C3A	2.03	1.55	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	802	H4B	C4-C4A-C8A	5.96	119.86	114.57
3	A	802	H4B	C4-C4A-C8A	5.46	119.42	114.57
5	B	803	9OJ	C13-C12-C19	3.96	120.16	118.01
5	A	805	9OJ	C13-C12-C19	3.85	120.10	118.01
2	A	801	HEM	CBD-CAD-C3D	-3.65	105.75	112.48
5	B	803	9OJ	C02-C23-C24	3.24	122.47	119.06
3	A	802	H4B	N3-C2-N1	-3.04	120.66	125.42
2	B	801	HEM	C1D-C2D-C3D	-2.96	104.94	107.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	805	9OJ	C12-C19-N18	-2.95	119.69	122.81
5	B	803	9OJ	C12-C19-N18	-2.93	119.70	122.81
3	A	802	H4B	C4-N3-C2	2.85	120.46	115.93
3	B	802	H4B	C4-N3-C2	2.81	120.39	115.93
5	A	805	9OJ	C02-C03-C04	-2.80	118.97	122.21
3	B	802	H4B	N3-C2-N1	-2.77	121.08	125.42
3	A	802	H4B	C2-N1-C8A	2.75	120.71	114.54
2	A	801	HEM	CMC-C2C-C3C	2.65	129.64	124.68
2	A	801	HEM	CAD-CBD-CGD	-2.53	108.42	112.67
5	B	803	9OJ	N17-C16-N18	2.53	120.35	118.26
5	A	805	9OJ	C03-C02-C23	2.52	121.11	117.40
3	B	802	H4B	C2-N1-C8A	2.50	120.15	114.54
3	A	802	H4B	C4-C4A-N5	2.49	121.21	119.12
3	A	802	H4B	N2-C2-N3	2.40	120.99	117.25
2	B	801	HEM	CBD-CAD-C3D	-2.39	108.07	112.48
5	A	805	9OJ	C01-C02-C23	-2.31	118.69	121.58
5	B	803	9OJ	C02-C03-C04	-2.26	119.60	122.21
2	A	801	HEM	C1D-C2D-C3D	-2.25	105.43	107.00
3	A	802	H4B	C4A-N5-C6	-2.06	115.54	121.16
5	A	805	9OJ	N17-C16-N18	2.05	119.95	118.26
2	A	801	HEM	CBA-CAA-C2A	-2.04	108.73	112.49

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	HEM	C2A-CAA-CBA-CGA
2	A	801	HEM	C1A-C2A-CAA-CBA
2	A	801	HEM	C2A-CAA-CBA-CGA
5	A	805	9OJ	C04-C05-C06-N07
5	B	803	9OJ	C04-C05-C06-N07
5	B	803	9OJ	C21-C04-C05-C06
5	B	803	9OJ	C03-C04-C05-C06
5	A	805	9OJ	C21-C04-C05-C06
2	A	801	HEM	C3A-C2A-CAA-CBA
5	A	805	9OJ	C03-C04-C05-C06
5	A	805	9OJ	C09-C08-N07-C06

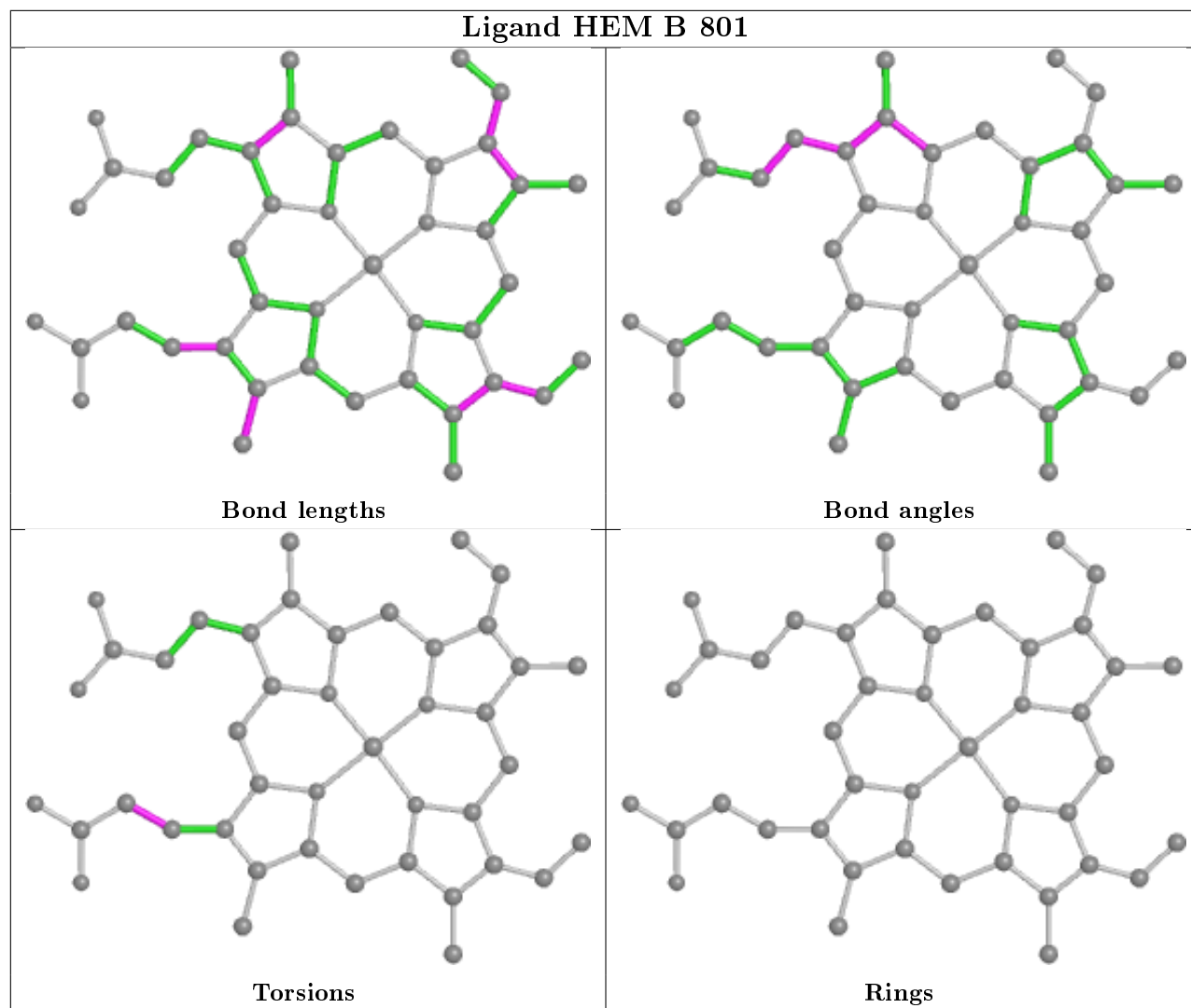
There are no ring outliers.

4 monomers are involved in 7 short contacts:

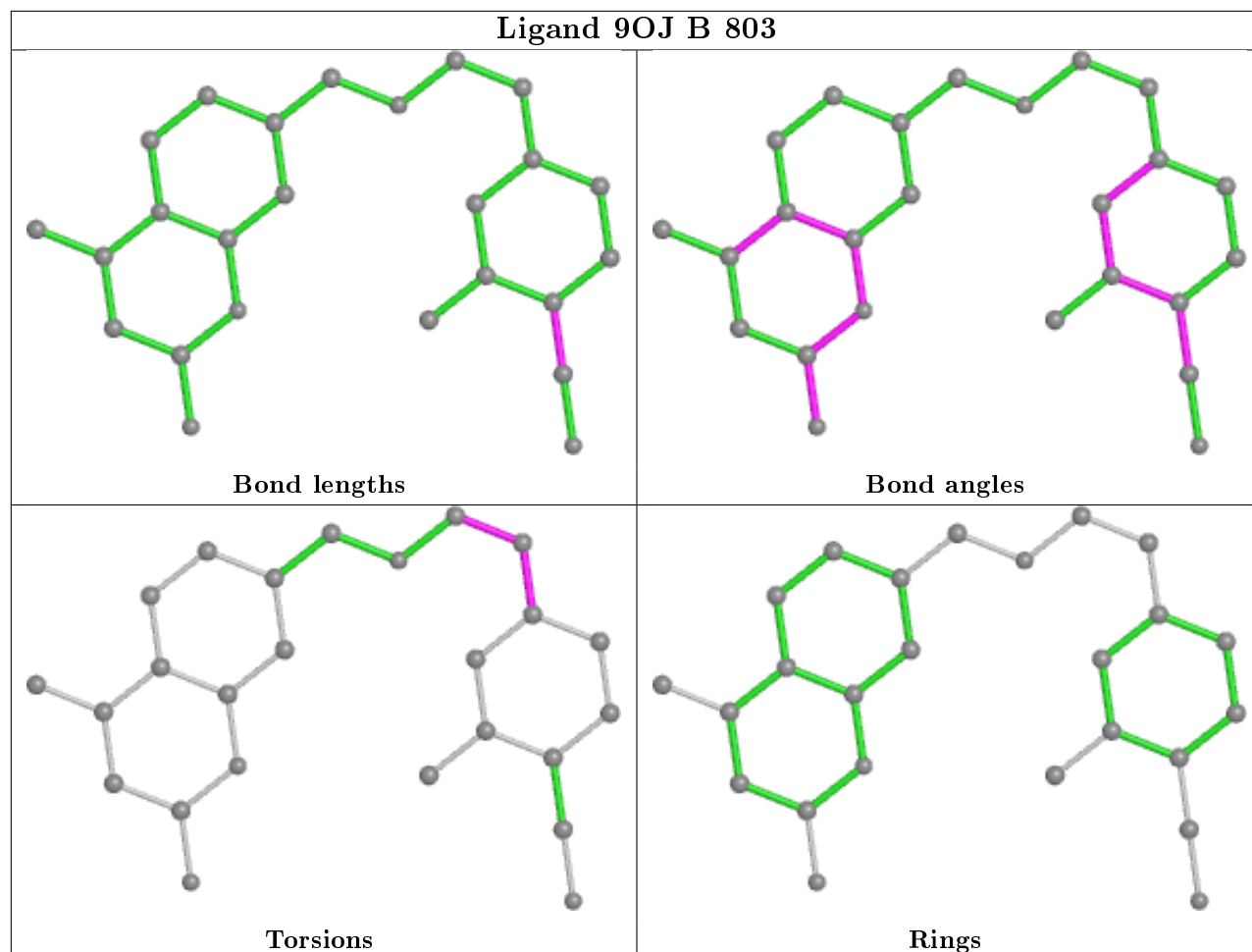


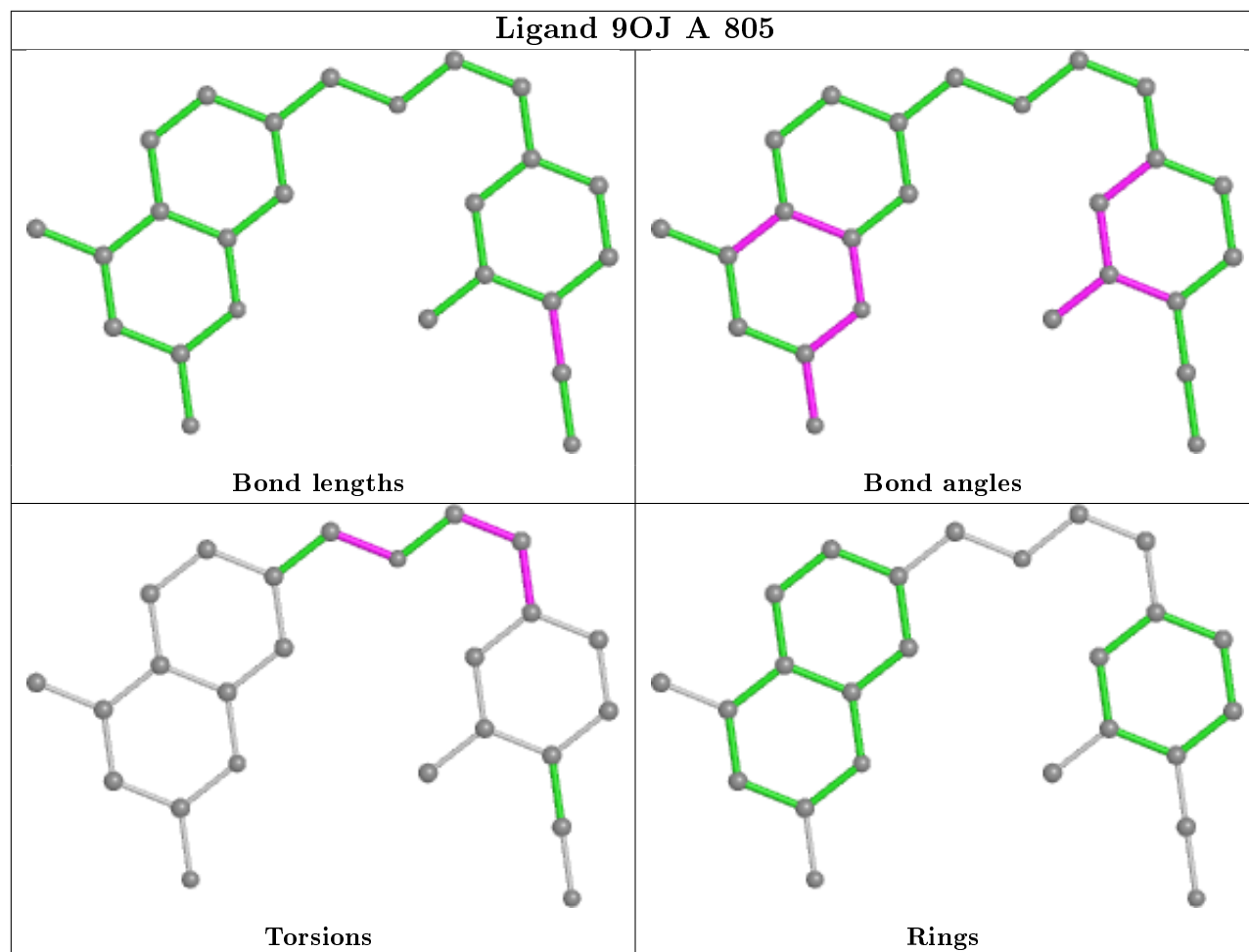
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HEM	3	0
5	B	803	9OJ	1	0
5	A	805	9OJ	1	0
2	A	801	HEM	2	0

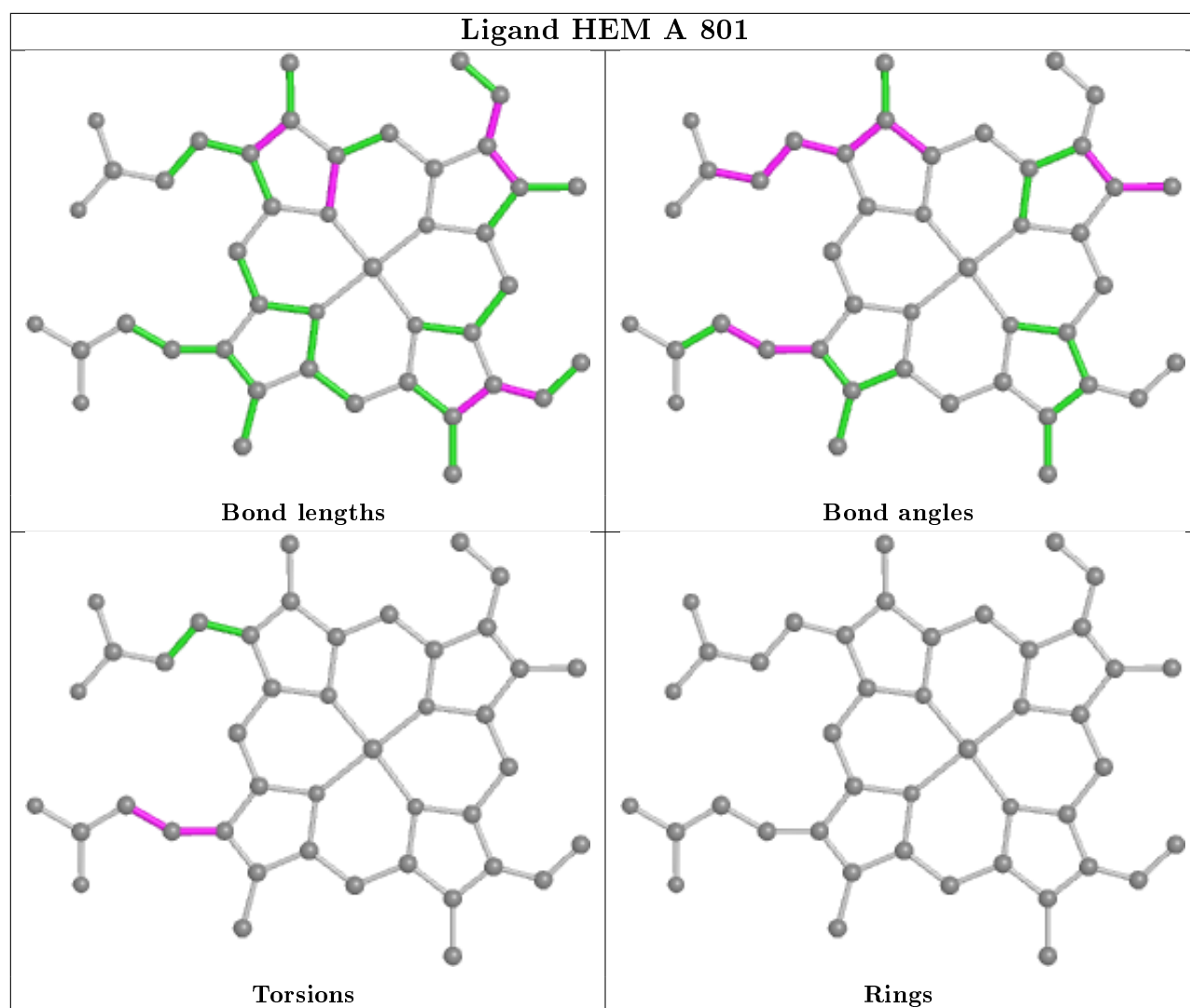
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## Ligand 9OJ B 803







## 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	411/422 (97%)	0.60	36 (8%) 10 16	30, 62, 117, 174	0
1	B	412/422 (97%)	0.22	4 (0%) 82 87	30, 49, 80, 113	0
All	All	823/844 (97%)	0.41	40 (4%) 29 39	30, 54, 108, 174	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	514	ARG	7.4
1	A	486	LYS	6.5
1	A	348	VAL	5.5
1	A	716	TRP	4.4
1	B	300	PHE	4.3
1	A	373	GLY	4.3
1	A	551	PHE	4.2
1	A	493	LEU	4.1
1	A	516	ARG	3.9
1	A	470	HIS	3.6
1	A	553	TRP	3.5
1	A	352	ASP	3.4
1	B	355[A]	PHE	3.4
1	A	355	PHE	3.4
1	B	299	ARG	3.3
1	A	499	VAL	3.2
1	A	339	SER	3.0
1	A	467	ASP	3.0
1	A	322	LEU	2.9
1	A	349	ARG	2.9
1	A	337	LEU	2.9
1	A	558	GLY	2.7
1	A	604	TYR	2.7
1	A	503	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	554	PHE	2.5
1	A	299	ARG	2.3
1	A	488	PRO	2.3
1	A	351	LYS	2.3
1	B	718	GLY	2.2
1	A	515	GLY	2.2
1	A	557	LEU	2.2
1	A	611	ALA	2.1
1	A	485	TYR	2.1
1	A	487	GLN	2.1
1	A	517	PHE	2.0
1	A	484	GLY	2.0
1	A	388	ILE	2.0
1	A	300	PHE	2.0
1	A	711	TRP	2.0
1	A	347	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	H4B	A	802	17/17	0.91	0.14	37,47,50,51	0
5	9OJ	B	803	25/25	0.92	0.15	35,55,97,100	0
5	9OJ	A	805	25/25	0.93	0.16	29,58,96,102	0
4	ACT	B	804	4/4	0.93	0.23	62,64,65,66	0
3	H4B	B	802	17/17	0.94	0.12	34,42,53,59	0
4	ACT	A	803	4/4	0.96	0.24	59,62,63,66	0
2	HEM	B	801	43/43	0.97	0.12	31,41,62,69	0

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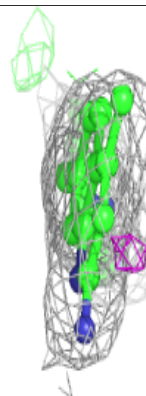
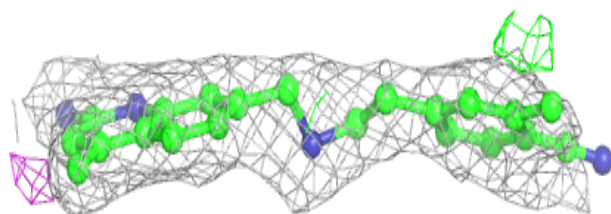
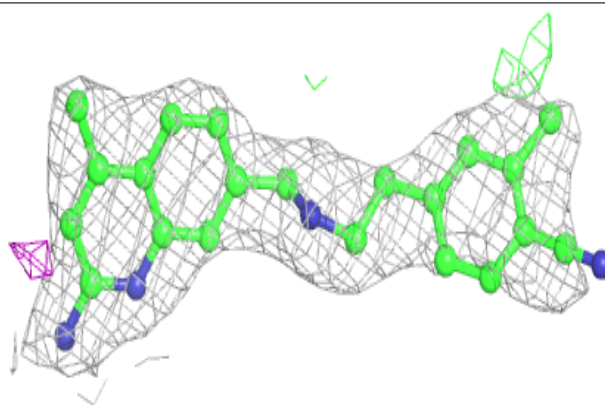
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	801	43/43	0.97	0.12	30,41,66,73	0
4	ACT	A	804	4/4	0.98	0.13	44,47,51,55	0
6	ZN	A	806	1/1	0.99	0.11	46,46,46,46	0

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 9OJ B 803:**

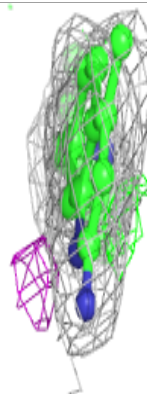
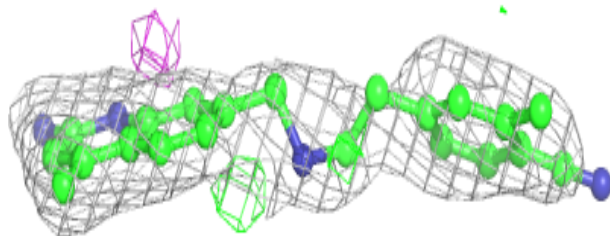
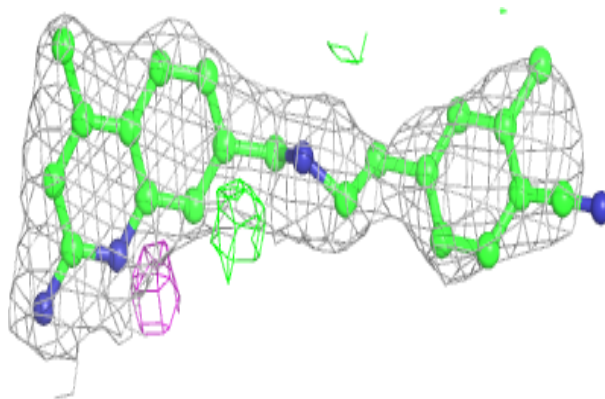
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





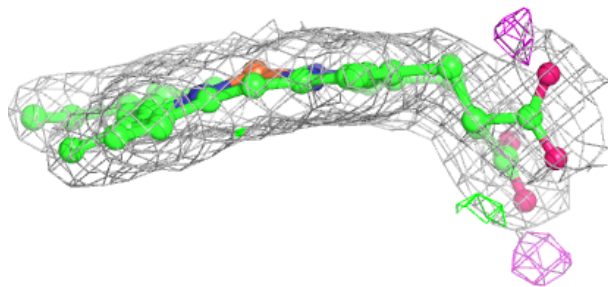
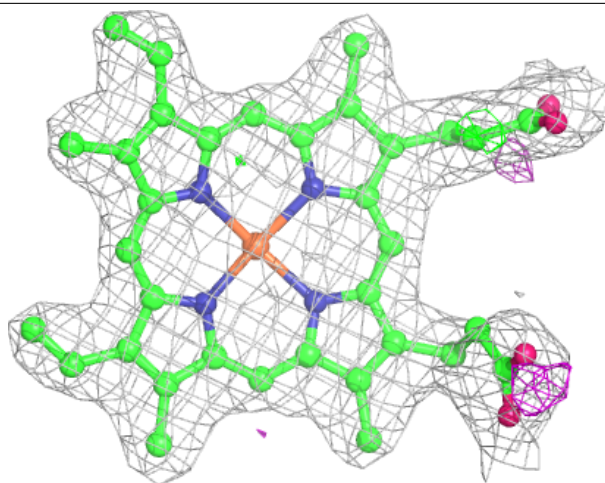
**Electron density around 9OJ A 805:**

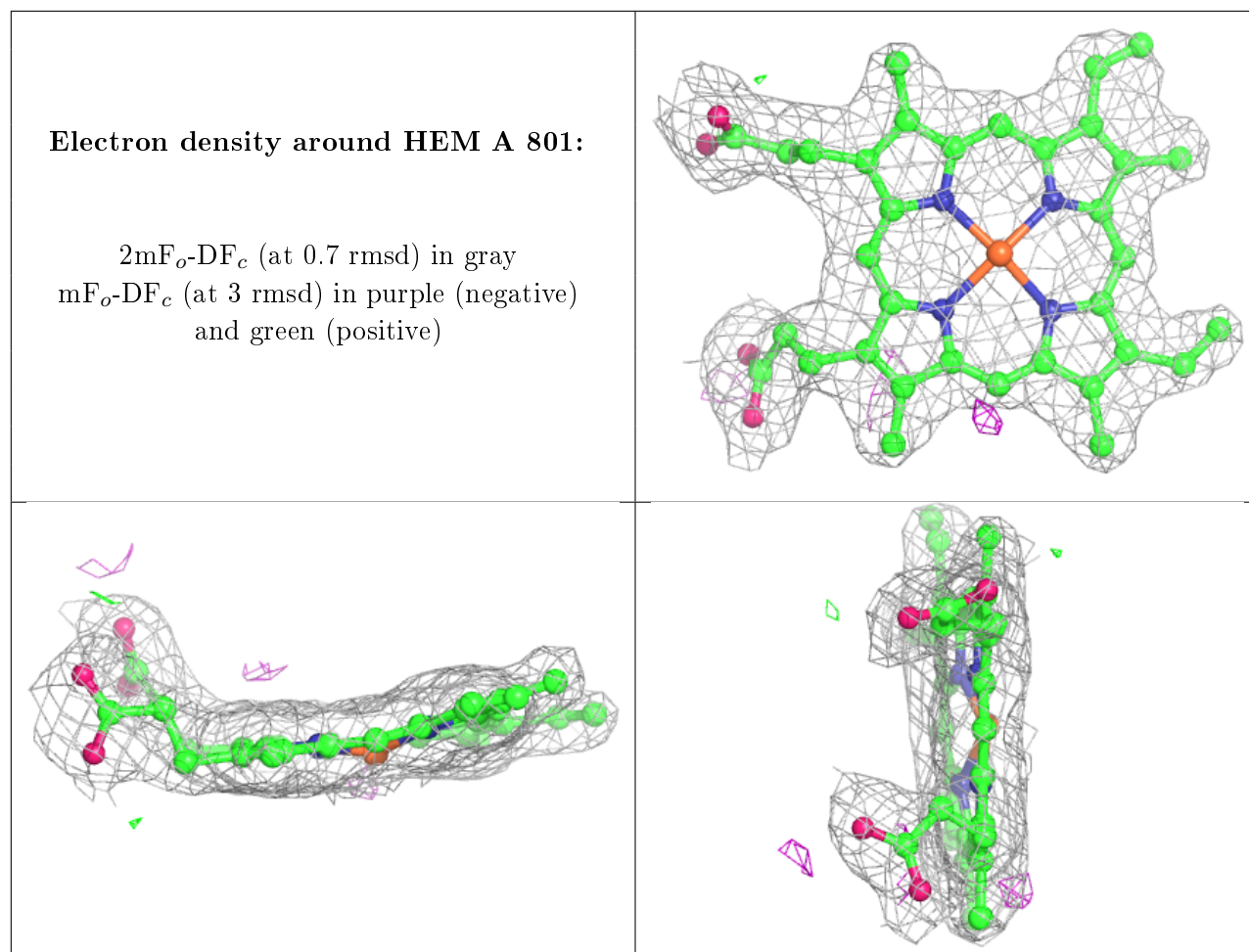
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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.