



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:55 PM BST

PDB ID : 5UNY  
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with (RS)-3-[(2-amino-4-methylquinolin-7-yl)methoxy]-5-(2-(methylamino)propyl) benzonitrile  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2017-01-31  
Resolution : 1.82 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

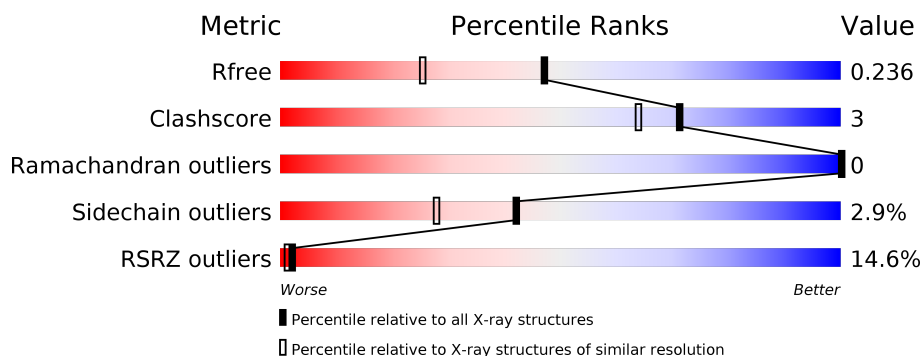
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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>20%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>••</div> </div> </div>
1	B	422	<div> <div>9%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>•</div> </div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7354 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.

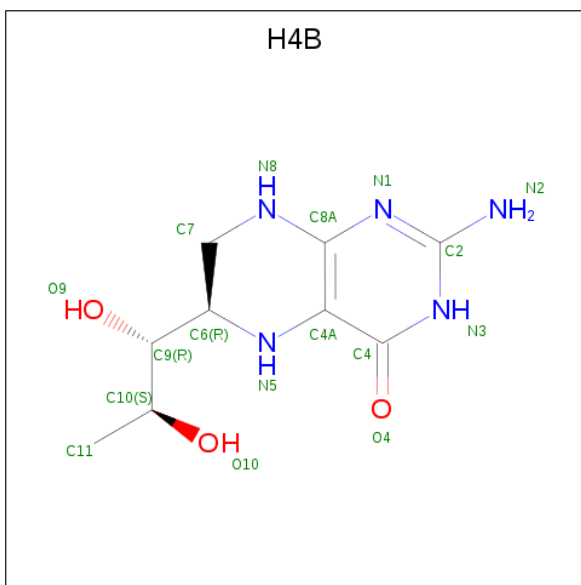
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	4	0
			3354	2146	572	614	22			
1	B	411	Total	C	N	O	S	0	3	0
			3357	2148	574	614	21			

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



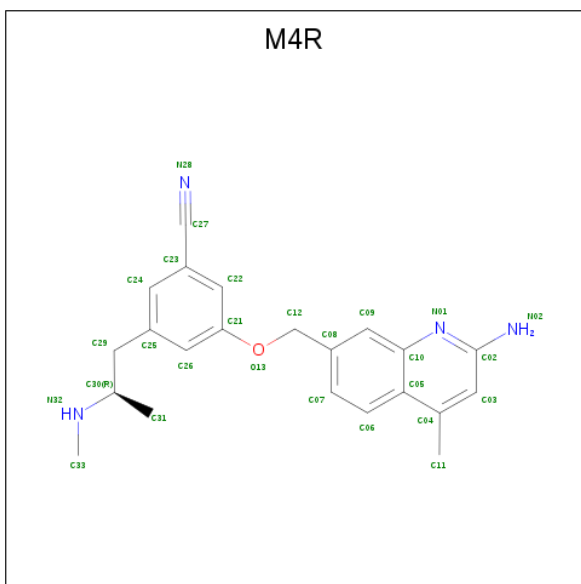
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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 17	C 9	N 5	O 3	0	0
3	B	1	Total 17	C 9	N 5	O 3	0	0

- Molecule 4 is 3-[(2-amino-4-methylquinolin-7-yl)methoxy]-5-[(2R)-2-(methylamino)propyl]benzonitrile (three-letter code: M4R) (formula: C<sub>22</sub>H<sub>24</sub>N<sub>4</sub>O).



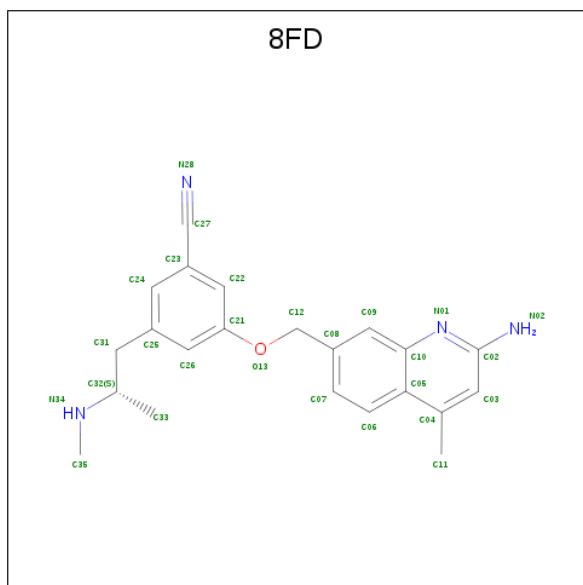
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			27	22	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	1
			27	22	4	1		

- Molecule 5 is 3-[(2-amino-4-methylquinolin-7-yl)methoxy]-5-[(2S)-2-(methylamino)propyl]benzonitrile (three-letter code: 8FD) (formula: C<sub>22</sub>H<sub>24</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			27	22	4	1		
5	B	1	Total	C	N	O	0	1
			27	22	4	1		

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

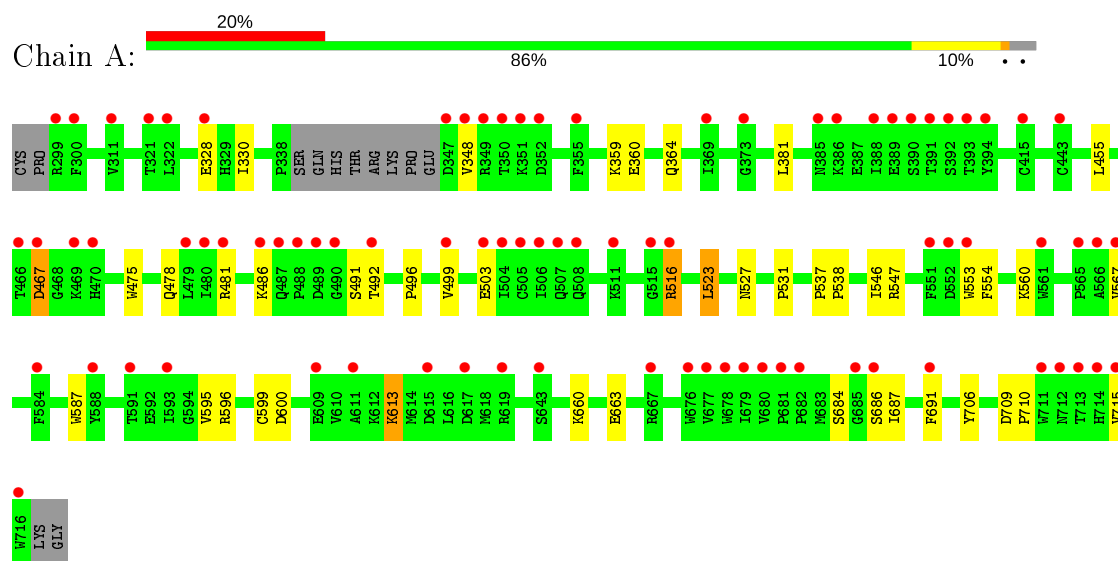
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	175	Total	O	0	0
			175	175		
8	B	231	Total	O	0	0
			231	231		

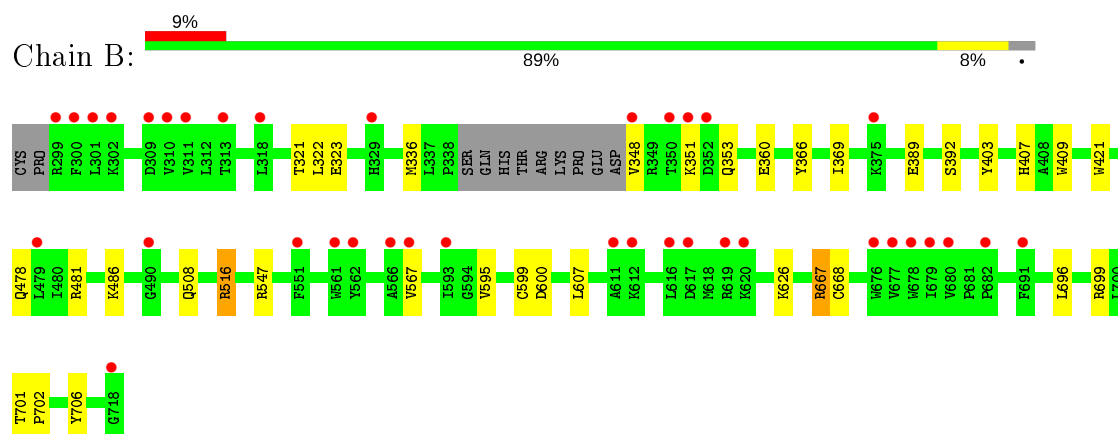
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitric oxide synthase, brain



- Molecule 1: Nitric oxide synthase, brain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.97Å 111.94Å 164.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.23 – 1.82 39.23 – 1.82	Depositor EDS
% Data completeness (in resolution range)	91.6 (39.23-1.82) 92.5 (39.23-1.82)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.34 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.193 , 0.238 0.195 , 0.236	Depositor DCC
$R_{free}$ test set	4013 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.3	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 61.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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: ZN, H4B, M4R, 8FD, ACT, HEM

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	0.38	0/3456	0.51	0/4688
1	B	0.40	0/3459	0.51	0/4689
All	All	0.39	0/6915	0.51	0/9377

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	3354	0	3264	27	0
1	B	3357	0	3275	18	0
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	27	0	0	1	0
4	B	27	0	0	1	0
5	A	27	0	0	1	0
5	B	27	0	0	1	0
6	A	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	4	0	3	0	0
7	A	1	0	0	0	0
8	A	175	0	0	1	0
8	B	231	0	0	3	0
All	All	7354	0	6635	47	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (47) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:801:HEM:HHC	2:A:801:HEM:HBB2	1.69	0.74
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.69	0.72
2:B:801:HEM:HBC2	2:B:801:HEM:HMC2	1.74	0.69
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.75	0.69
1:A:516:ARG:NH2	8:A:901:HOH:O	2.25	0.67
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.78	0.66
1:B:706:TYR:OH	2:B:801:HEM:O2D	2.11	0.65
1:A:467:ASP:OD1	1:A:467:ASP:N	2.28	0.64
1:A:706:TYR:OH	2:A:801:HEM:O2D	2.17	0.61
1:B:667:ARG:NH1	1:B:668:CYS:HB3	2.20	0.56
1:B:516:ARG:NH1	8:B:907:HOH:O	2.40	0.54
1:A:491:SER:OG	1:A:492:THR:N	2.39	0.54
1:A:660:LYS:O	1:A:663[B]:GLU:HG3	2.08	0.52
1:B:607:LEU:HD13	1:B:626:LYS:HG2	1.93	0.50
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.94	0.50
1:B:595:VAL:O	1:B:599:CYS:HB2	2.12	0.49
1:A:330:ILE:HD11	1:B:696:LEU:HD22	1.94	0.49
1:B:600:ASP:OD2	8:B:901:HOH:O	2.20	0.49
1:B:567:VAL:HG21	4:B:803[A]:M4R:C07	2.43	0.48
1:B:508:GLN:NE2	8:B:910:HOH:O	2.47	0.47
1:B:336:MET:HE2	1:B:336:MET:HB2	1.82	0.47
1:B:322:LEU:HD13	1:B:699:ARG:NH2	2.30	0.46
1:A:359:LYS:HE2	1:A:381:LEU:HD21	1.98	0.46
1:A:595:VAL:O	1:A:599:CYS:HB2	2.16	0.46
1:A:475:TRP:HB2	1:A:523:LEU:HB3	1.98	0.45
1:A:496:PRO:HA	1:A:499:VAL:HG23	1.97	0.45
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.99	0.45
1:B:567:VAL:HG21	5:B:804[B]:8FD:C07	2.46	0.45
1:B:323:GLU:O	1:B:699:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:TRP:HB2	1:A:613:LYS:NZ	2.33	0.44
1:A:546:ILE:HG22	1:A:554:PHE:HE2	1.83	0.44
1:A:567:VAL:HG21	4:A:803[A]:M4R:C07	2.48	0.44
1:A:567:VAL:HG21	5:A:804[B]:8FD:C07	2.48	0.43
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.53	0.43
1:A:360:GLU:O	1:A:364:GLN:HG2	2.18	0.43
1:A:475:TRP:CE2	1:A:710:PRO:HB2	2.53	0.43
1:A:684:SER:HB3	1:A:687:ILE:HD11	2.00	0.43
1:B:366:TYR:HA	1:B:369:ILE:HG12	2.01	0.42
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.54	0.42
1:A:596:ARG:NH2	1:A:600:ASP:OD2	2.51	0.42
1:B:403:TYR:CE1	1:B:407:HIS:CE1	3.08	0.41
1:A:546:ILE:HG12	1:A:560:LYS:HA	2.03	0.41
1:A:709:ASP:HA	1:A:710:PRO:HD3	1.87	0.41
1:A:328:GLU:H	1:A:328:GLU:HG3	1.62	0.41
1:A:537:PRO:HA	1:A:538:PRO:HD3	1.93	0.41
1:B:701:THR:HA	1:B:702:PRO:C	2.41	0.40
1:A:686:SER:HA	1:A:691:PHE:CG	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/422 (97%)	391 (96%)	18 (4%)	0	100	100
1	B	410/422 (97%)	399 (97%)	11 (3%)	0	100	100
All	All	819/844 (97%)	790 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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%)	359 (97%)	10 (3%)	44	30
1	B	369/377 (98%)	358 (97%)	11 (3%)	41	26
All	All	738/754 (98%)	717 (97%)	21 (3%)	42	29

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	348	VAL
1	A	467	ASP
1	A	486	LYS
1	A	503	GLU
1	A	516	ARG
1	A	523	LEU
1	A	527	ASN
1	A	547	ARG
1	A	613	LYS
1	A	715	VAL
1	B	321	THR
1	B	348	VAL
1	B	351	LYS
1	B	353	GLN
1	B	360	GLU
1	B	389	GLU
1	B	392	SER
1	B	486	LYS
1	B	516	ARG
1	B	547	ARG
1	B	667	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 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	H4B	B	802	-	16,18,18	0.88	0	11,26,26	2.50	5 (45%)
3	H4B	A	802	-	16,18,18	0.88	0	11,26,26	2.60	5 (45%)
6	ACT	A	805	-	1,3,3	1.35	0	0,3,3	0.00	-
5	8FD	B	804[B]	-	29,29,29	1.58	1 (3%)	38,40,40	1.04	2 (5%)
5	8FD	A	804[B]	-	29,29,29	1.54	1 (3%)	38,40,40	1.14	3 (7%)
2	HEM	A	801	1	27,50,50	2.24	7 (25%)	17,82,82	1.31	2 (11%)
2	HEM	B	801	1	27,50,50	2.25	8 (29%)	17,82,82	1.69	3 (17%)
4	M4R	A	803[A]	-	29,29,29	1.55	1 (3%)	38,40,40	1.04	2 (5%)
6	ACT	B	805	-	1,3,3	1.18	0	0,3,3	0.00	-
4	M4R	B	803[A]	-	29,29,29	1.58	2 (6%)	38,40,40	0.97	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	H4B	B	802	-	-	1/8/17/17	0/2/2/2
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
5	8FD	B	804[B]	-	-	2/13/13/13	0/3/3/3
5	8FD	A	804[B]	-	-	1/13/13/13	0/3/3/3
2	HEM	A	801	1	-	5/6/54/54	-
2	HEM	B	801	1	-	1/6/54/54	-
4	M4R	A	803[A]	-	-	2/13/13/13	0/3/3/3
4	M4R	B	803[A]	-	-	1/13/13/13	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	804[B]	8FD	C23-C27	-7.04	1.28	1.44
4	B	803[A]	M4R	C23-C27	-7.04	1.28	1.44
5	A	804[B]	8FD	C23-C27	-6.99	1.29	1.44
4	A	803[A]	M4R	C23-C27	-6.91	1.29	1.44
2	B	801	HEM	C3D-C2D	5.37	1.53	1.37
2	A	801	HEM	C3D-C2D	5.31	1.53	1.37
2	A	801	HEM	C3B-C2B	-5.09	1.33	1.40
2	B	801	HEM	C3B-C2B	-4.75	1.33	1.40
2	A	801	HEM	C3B-CAB	3.88	1.55	1.47
2	B	801	HEM	C3C-C2C	-3.75	1.35	1.40
2	A	801	HEM	C3C-C2C	-3.69	1.35	1.40
2	B	801	HEM	C3C-CAC	3.64	1.55	1.47
2	B	801	HEM	C3B-CAB	3.59	1.55	1.47
2	A	801	HEM	C3C-CAC	3.58	1.55	1.47
2	A	801	HEM	C1D-ND	2.53	1.41	1.36
2	B	801	HEM	C4B-NB	2.17	1.40	1.36
2	B	801	HEM	C1D-ND	2.14	1.40	1.36
2	B	801	HEM	CMD-C2D	2.04	1.55	1.51
2	A	801	HEM	CMD-C2D	2.01	1.55	1.51
4	B	803[A]	M4R	C09-C10	-2.01	1.38	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	H4B	C4-C4A-C8A	5.74	119.67	114.57
3	B	802	H4B	C4-C4A-C8A	5.42	119.39	114.57
5	A	804[B]	8FD	C04-C05-C10	3.29	119.79	118.01
3	A	802	H4B	N3-C2-N1	-3.11	120.54	125.42
4	A	803[A]	M4R	C04-C05-C10	3.10	119.69	118.01
2	B	801	HEM	CBA-CAA-C2A	-3.02	106.92	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	H4B	C2-N1-C8A	3.01	121.28	114.54
2	B	801	HEM	C1D-C2D-C3D	-2.99	104.92	107.00
3	B	802	H4B	N3-C2-N1	-2.92	120.84	125.42
3	B	802	H4B	C2-N1-C8A	2.87	120.97	114.54
5	B	804[B]	8FD	C04-C05-C10	2.84	119.55	118.01
2	B	801	HEM	CAD-CBD-CGD	-2.80	107.97	112.67
3	A	802	H4B	C4-N3-C2	2.78	120.35	115.93
5	A	804[B]	8FD	C05-C10-N01	-2.72	119.92	122.81
4	B	803[A]	M4R	C04-C05-C10	2.69	119.47	118.01
3	B	802	H4B	C4-N3-C2	2.67	120.17	115.93
2	A	801	HEM	CAD-CBD-CGD	-2.62	108.28	112.67
3	B	802	H4B	C4-C4A-N5	2.48	121.20	119.12
5	A	804[B]	8FD	C12-O13-C21	2.38	123.54	117.65
4	A	803[A]	M4R	C05-C10-N01	-2.34	120.33	122.81
5	B	804[B]	8FD	C05-C10-N01	-2.23	120.44	122.81
3	A	802	H4B	N2-C2-N3	2.18	120.64	117.25
4	B	803[A]	M4R	C05-C10-N01	-2.10	120.59	122.81
2	A	801	HEM	CBA-CAA-C2A	-2.00	108.79	112.49

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C1A-C2A-CAA-CBA
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	A	803[A]	M4R	C25-C29-C30-C31
4	B	803[A]	M4R	C25-C29-C30-C31
2	A	801	HEM	C3A-C2A-CAA-CBA
3	B	802	H4B	C7-C6-C9-C10
4	A	803[A]	M4R	C25-C29-C30-N32
2	B	801	HEM	C2A-CAA-CBA-CGA
5	B	804[B]	8FD	C22-C23-C27-N28
5	A	804[B]	8FD	C24-C23-C27-N28
5	B	804[B]	8FD	C25-C31-C32-N34

There are no ring outliers.

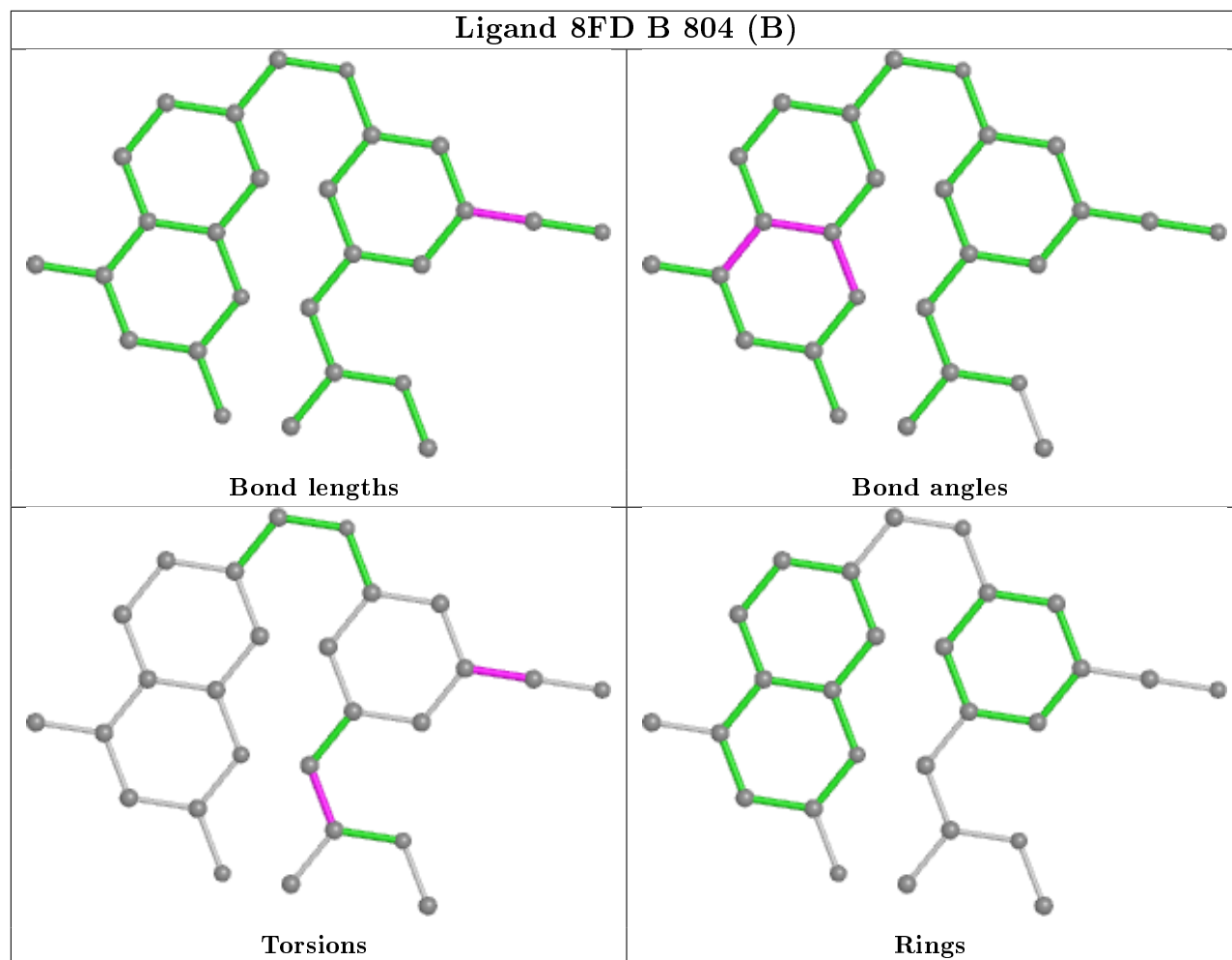
6 monomers are involved in 9 short contacts:

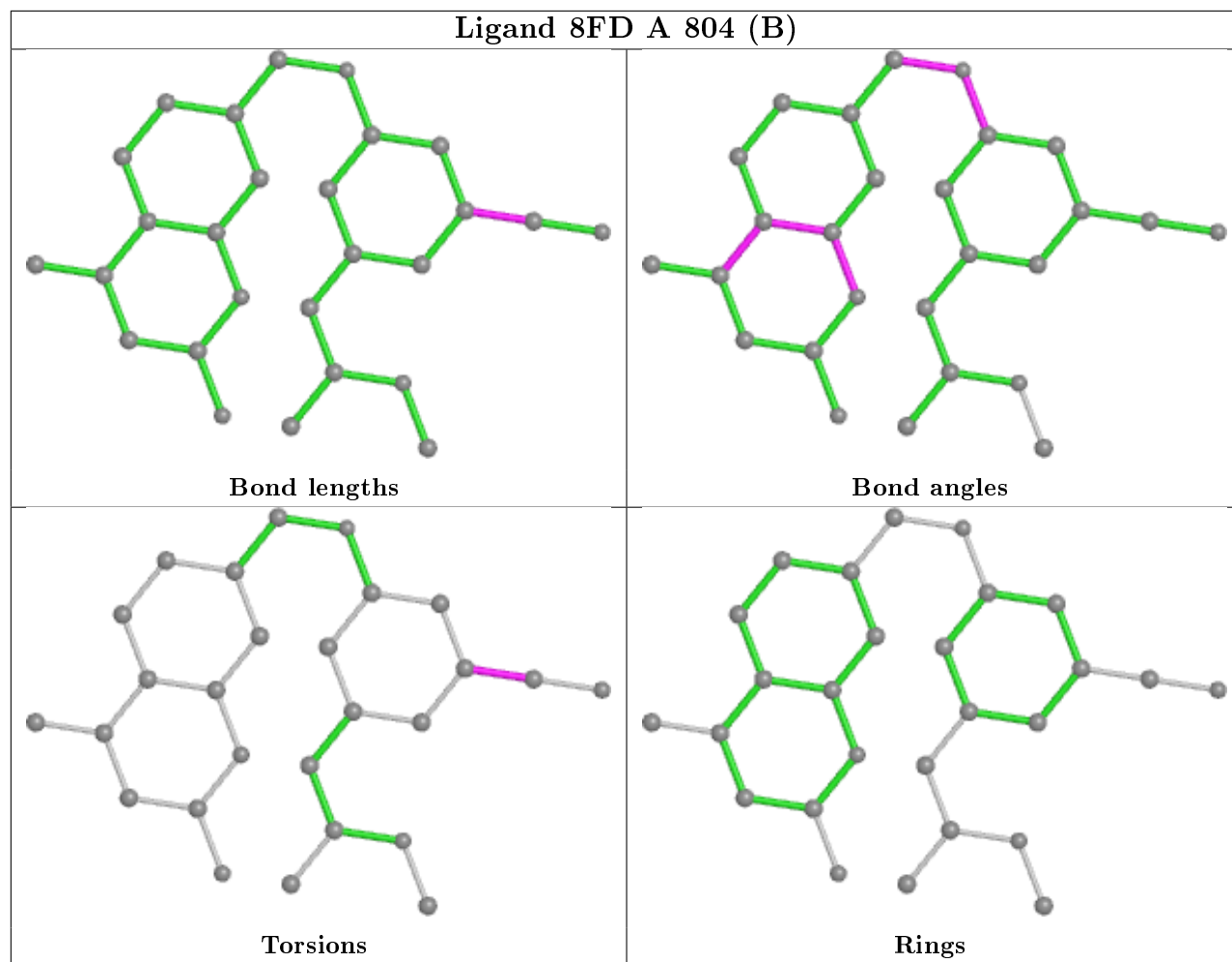
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	804[B]	8FD	1	0
5	A	804[B]	8FD	1	0
2	A	801	HEM	2	0
2	B	801	HEM	3	0
4	A	803[A]	M4R	1	0
4	B	803[A]	M4R	1	0

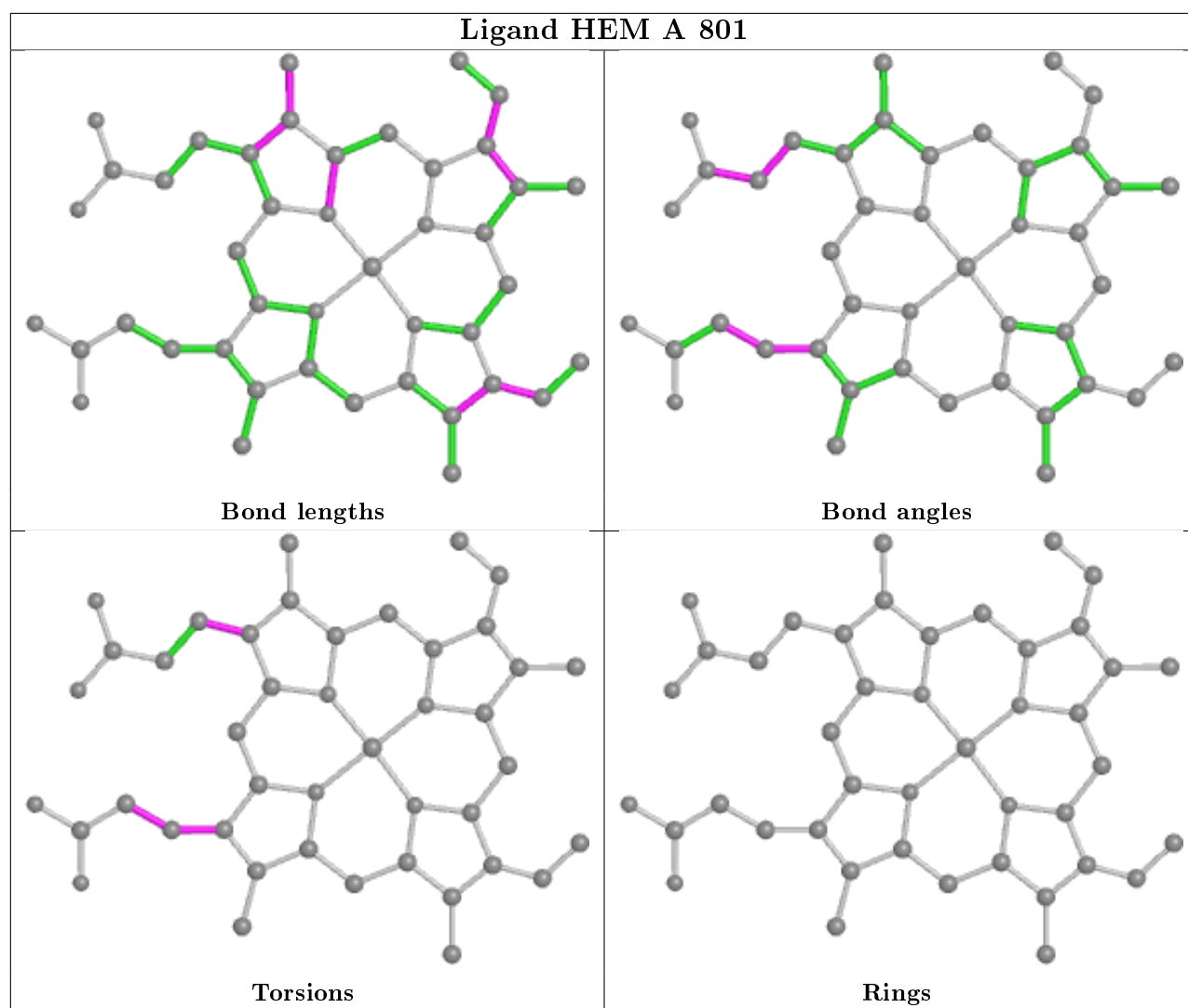
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

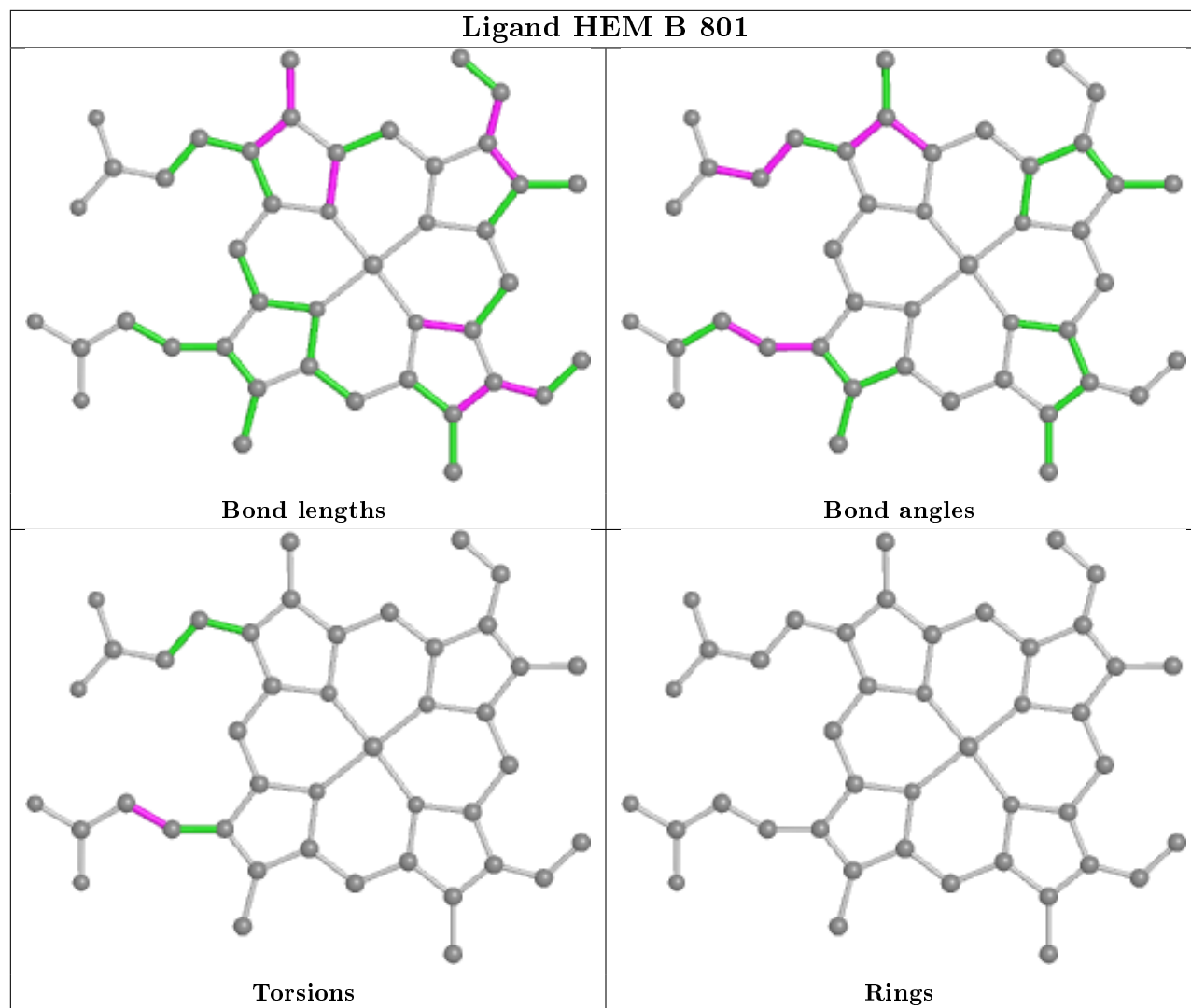


## Ligand 8FD B 804 (B)

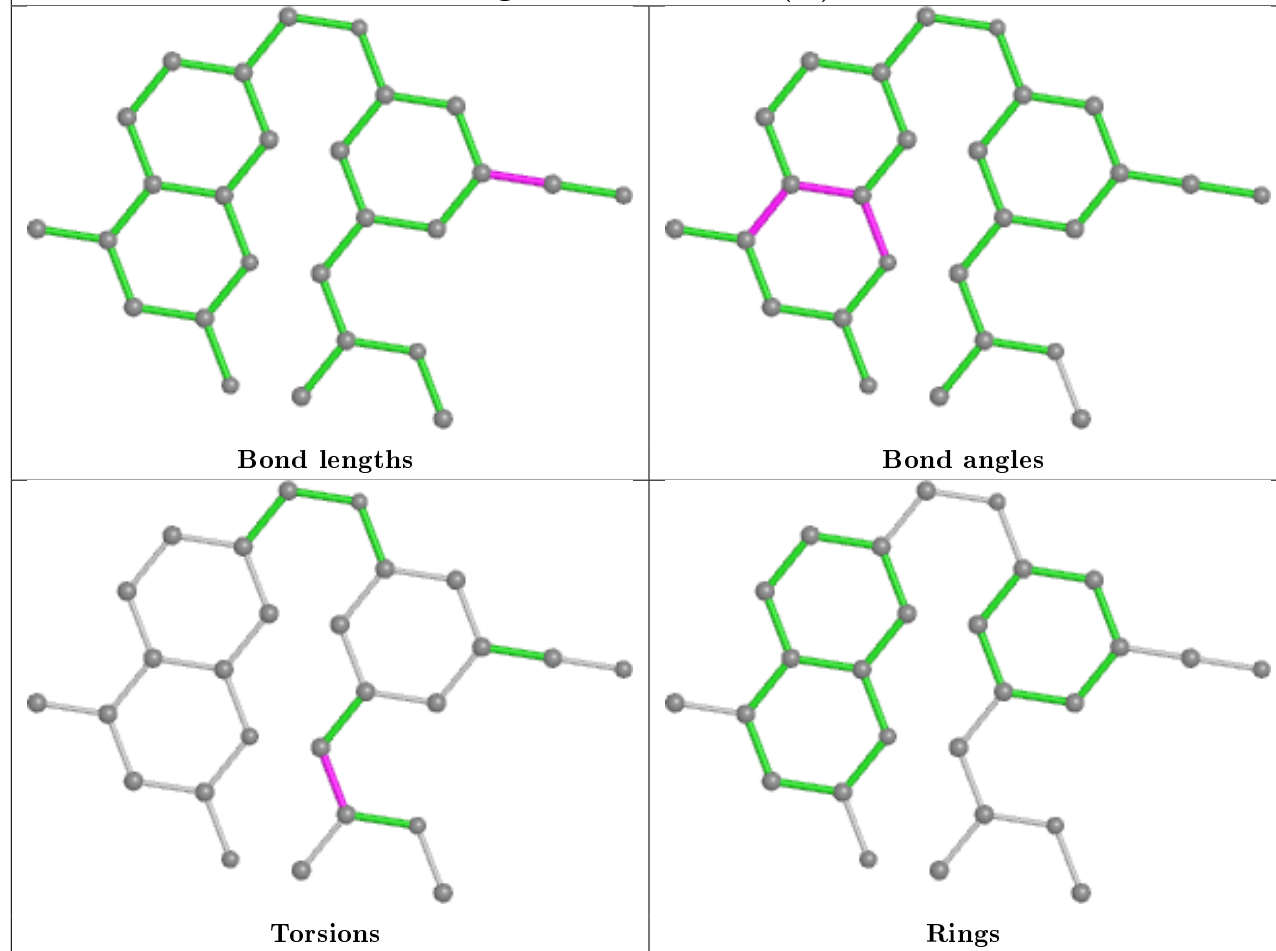


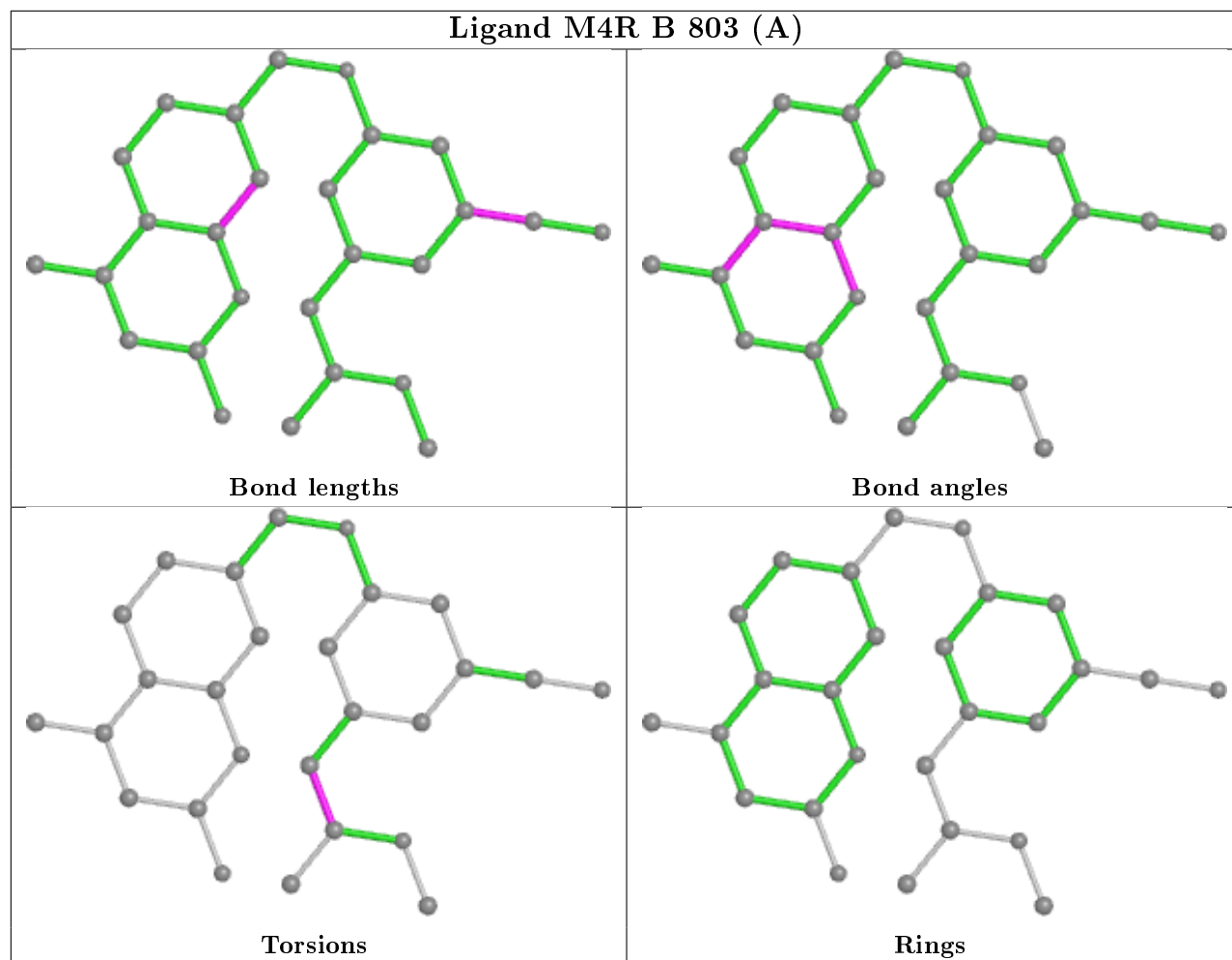






## Ligand M4R A 803 (A)





## 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%)	1.06	83 (20%) <b>1</b> <b>0</b>	30, 62, 115, 162	0
1	B	411/422 (97%)	0.44	37 (9%) <b>9</b> <b>7</b>	30, 51, 87, 117	0
All	All	821/844 (97%)	0.75	120 (14%) <b>2</b> <b>1</b>	30, 56, 108, 162	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	715	VAL	9.4
1	A	716	TRP	8.5
1	A	486	LYS	7.9
1	A	488	PRO	7.2
1	A	348	VAL	7.0
1	A	347	ASP	7.0
1	B	300	PHE	6.6
1	A	355	PHE	5.9
1	A	507	GLN	5.7
1	A	388	ILE	5.3
1	A	489	ASP	5.2
1	B	350	THR	4.9
1	A	352	ASP	4.9
1	A	351	LYS	4.9
1	A	506	ILE	4.8
1	A	551	PHE	4.8
1	A	713	THR	4.7
1	A	711	TRP	4.7
1	A	299	ARG	4.6
1	A	349	ARG	4.6
1	A	391	THR	4.5
1	A	712	ASN	4.4
1	B	677	VAL	4.3
1	A	508	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	718	GLY	4.2
1	A	678	TRP	4.2
1	B	619	ARG	4.1
1	A	503	GLU	4.1
1	A	389	GLU	4.1
1	A	714	HIS	4.0
1	A	677	VAL	3.9
1	B	351	LYS	3.9
1	B	348	VAL	3.9
1	A	679	ILE	3.8
1	A	643	SER	3.8
1	A	386	LYS	3.8
1	B	680	VAL	3.7
1	B	678	TRP	3.6
1	A	470	HIS	3.6
1	A	467	ASP	3.5
1	A	567	VAL	3.5
1	A	390	SER	3.5
1	A	322	LEU	3.5
1	A	681	PRO	3.4
1	A	511	LYS	3.4
1	A	676	TRP	3.3
1	A	393	THR	3.3
1	A	499	VAL	3.3
1	B	301	LEU	3.3
1	A	553	TRP	3.3
1	B	299	ARG	3.3
1	B	352	ASP	3.2
1	B	617	ASP	3.2
1	A	392	SER	3.2
1	A	504	ILE	3.1
1	A	480	ILE	3.1
1	A	667	ARG	3.0
1	A	373	GLY	3.0
1	A	619	ARG	2.9
1	B	329	HIS	2.9
1	A	505	CYS	2.9
1	A	321	THR	2.8
1	B	676	TRP	2.8
1	A	350	THR	2.8
1	A	516	ARG	2.8
1	A	487	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	369	ILE	2.8
1	A	682	PRO	2.8
1	B	593	ILE	2.8
1	A	300	PHE	2.8
1	A	588	TYR	2.8
1	A	685	GLY	2.7
1	A	566	ALA	2.7
1	A	691	PHE	2.7
1	A	492	THR	2.7
1	B	682	PRO	2.7
1	B	611	ALA	2.6
1	B	311	VAL	2.6
1	B	561	TRP	2.6
1	A	584	PHE	2.6
1	B	479	LEU	2.6
1	B	616	LEU	2.6
1	A	479	LEU	2.5
1	A	311	VAL	2.5
1	B	490	GLY	2.5
1	B	567	VAL	2.5
1	A	481	ARG	2.5
1	A	385	ASN	2.4
1	B	620	LYS	2.4
1	A	490	GLY	2.4
1	A	609	GLU	2.4
1	B	302	LYS	2.4
1	B	679	ILE	2.4
1	A	611	ALA	2.3
1	B	309	ASP	2.3
1	B	551	PHE	2.3
1	A	686	SER	2.3
1	B	691	PHE	2.3
1	B	310	VAL	2.3
1	A	565	PRO	2.3
1	A	469	LYS	2.2
1	A	415	CYS	2.2
1	B	375	LYS	2.2
1	B	612	LYS	2.2
1	B	313	THR	2.2
1	B	318	LEU	2.2
1	A	617	ASP	2.1
1	B	566	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	561	TRP	2.1
1	A	552	ASP	2.1
1	A	466	THR	2.1
1	A	591	THR	2.1
1	A	515	GLY	2.1
1	B	562	TYR	2.0
1	A	443	CYS	2.0
1	A	394	TYR	2.0
1	A	680	VAL	2.0
1	A	328	GLU	2.0
1	A	615	ASP	2.0
1	A	593	ILE	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 ⓘ

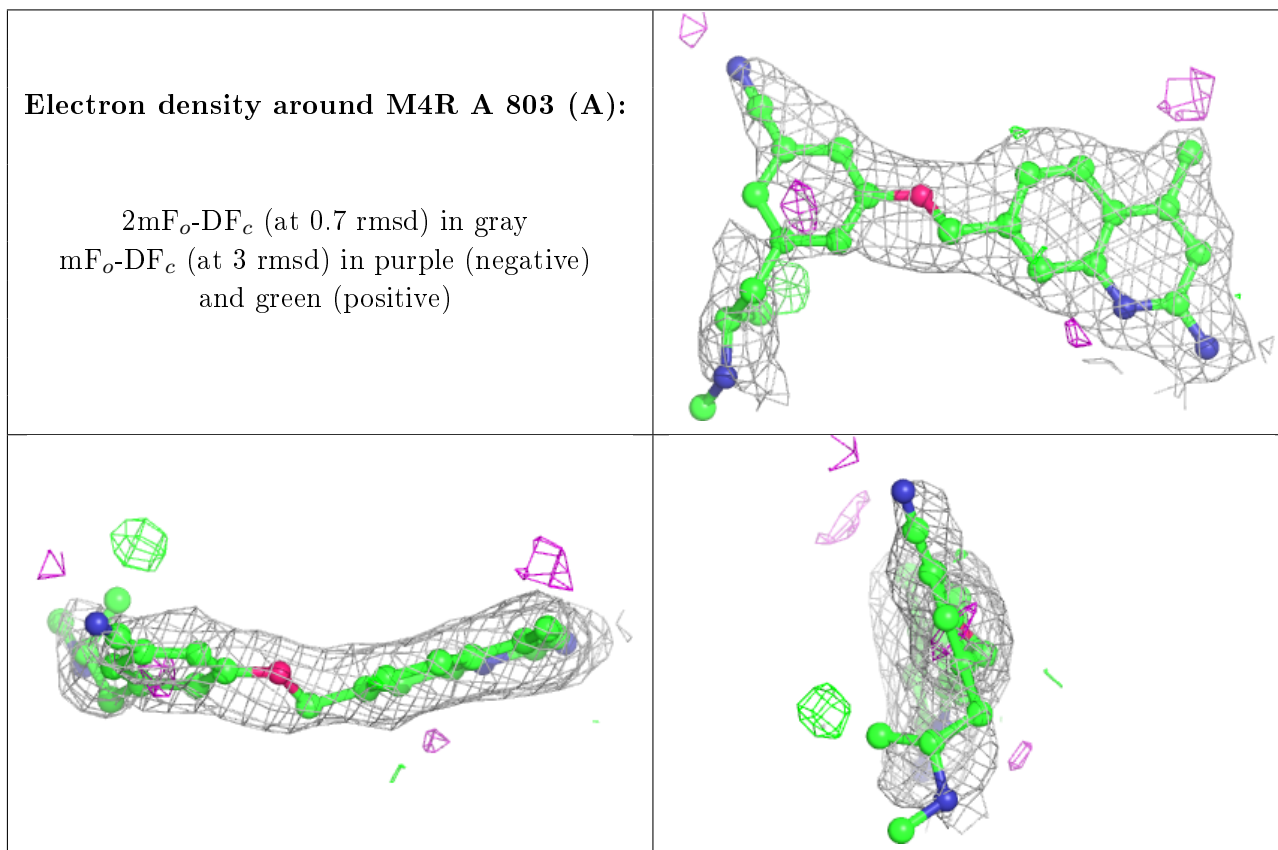
There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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.

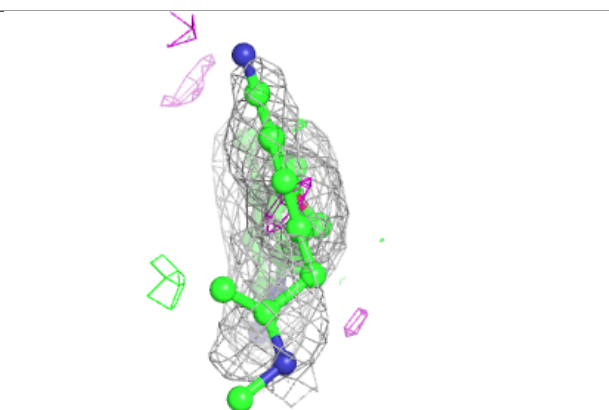
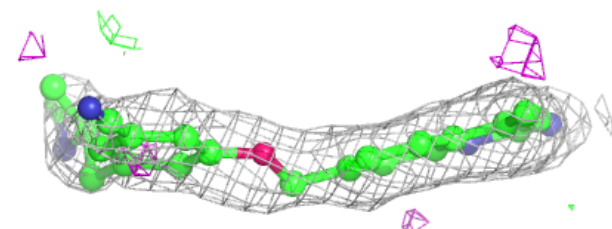
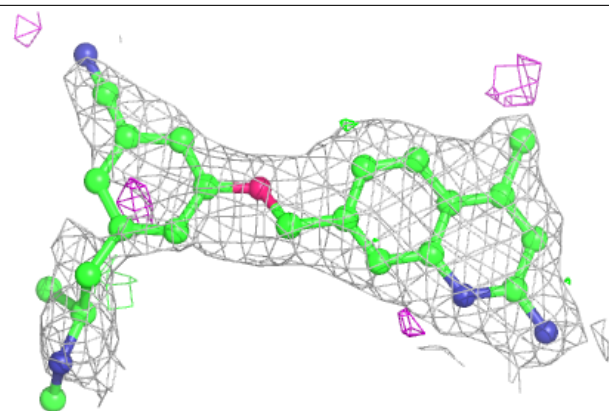
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	ACT	A	805	4/4	0.80	0.22	56,62,63,63	0
4	M4R	A	803[A]	27/27	0.88	0.35	32,56,84,88	27
5	8FD	A	804[B]	27/27	0.89	0.34	33,54,84,87	27
3	H4B	B	802	17/17	0.89	0.19	36,45,52,53	0
5	8FD	B	804[B]	27/27	0.90	0.33	32,52,82,84	27
4	M4R	B	803[A]	27/27	0.91	0.33	32,52,83,85	27
3	H4B	A	802	17/17	0.92	0.18	32,47,59,65	0
6	ACT	B	805	4/4	0.95	0.19	49,56,57,58	0
2	HEM	B	801	43/43	0.97	0.18	28,40,62,65	0
2	HEM	A	801	43/43	0.97	0.22	26,40,71,74	0
7	ZN	A	806	1/1	0.99	0.08	42,42,42,42	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.

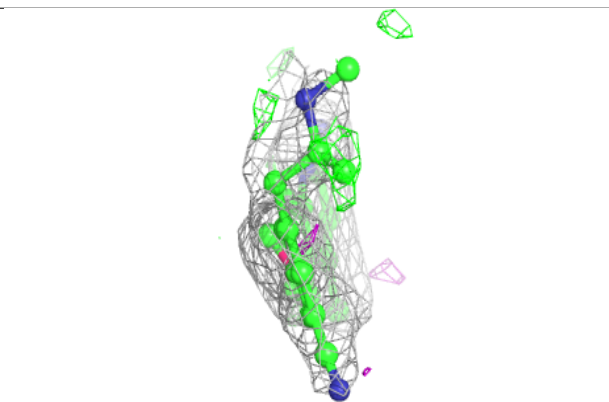
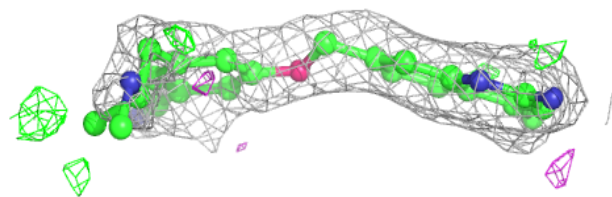
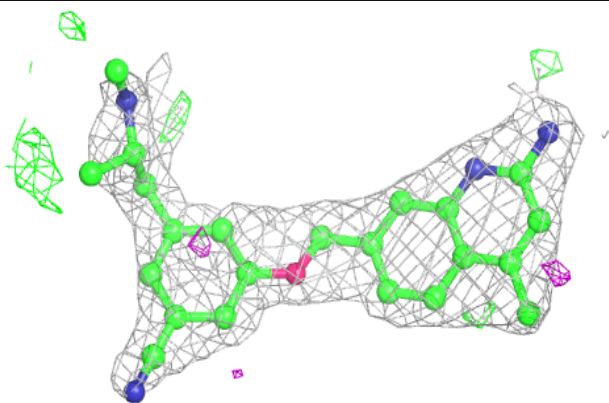


**Electron density around 8FD A 804 (B):**

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

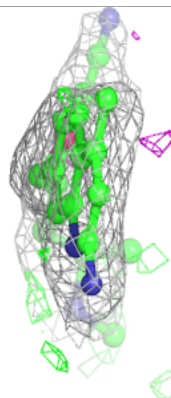
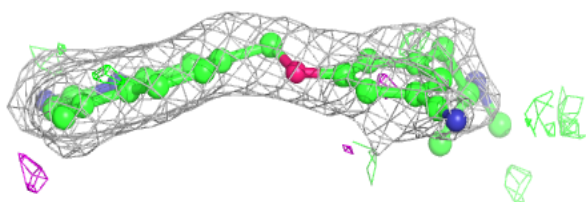
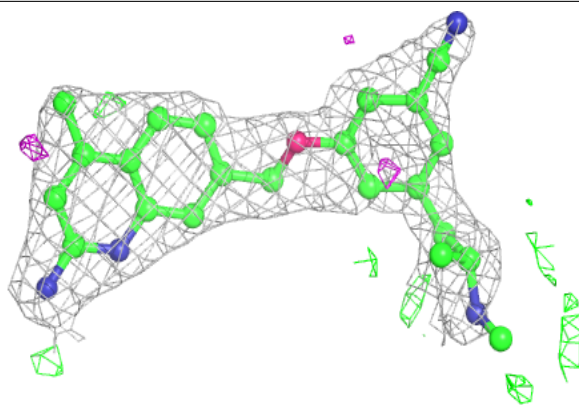
**Electron density around 8FD B 804 (B):**

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



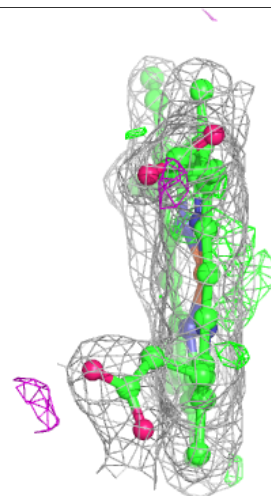
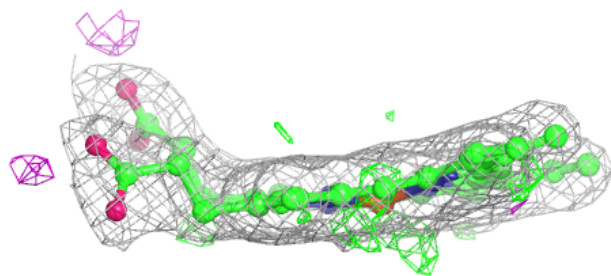
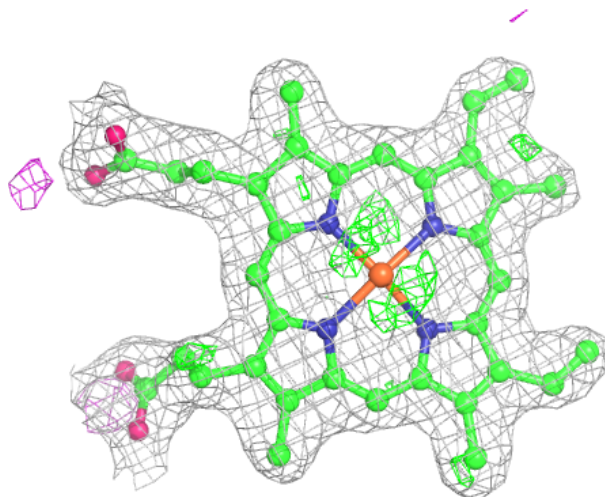
**Electron density around M4R B 803 (A):**

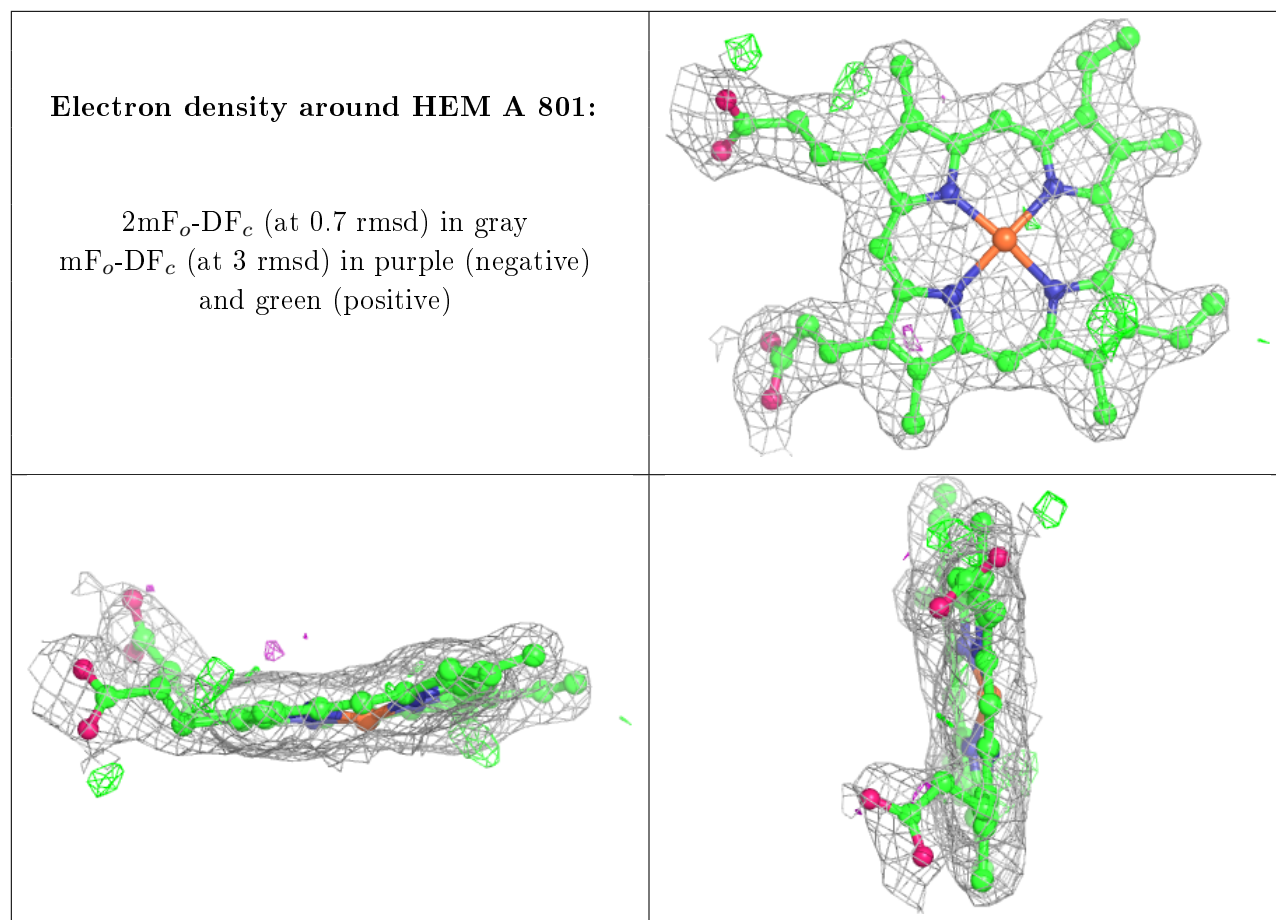
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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 ⓘ

There are no such residues in this entry.