



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 08:38 AM BST

PDB ID : 5UO5  
Title : Structure of human 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 : 2.00 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

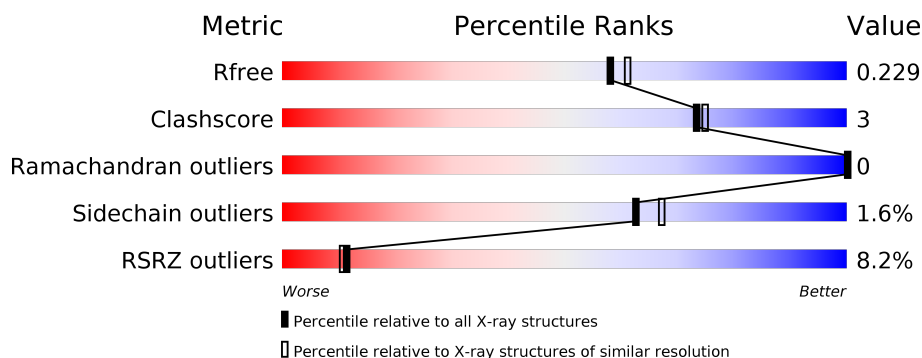
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	421	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div></div> </div> </div>
1	B	421	<div> <div>10%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div></div> </div> </div>



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.

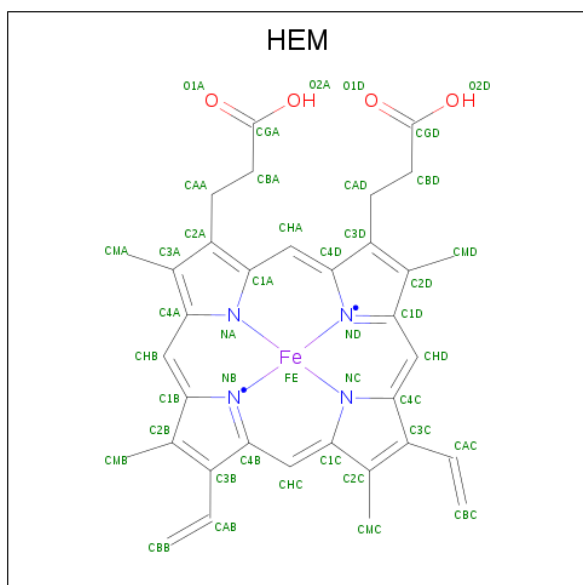
- Molecule 1 is a protein called Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	415	Total 3387	C 2169	N 576	O 620	S 22	0	2	0
1	B	410	Total 3349	C 2145	N 571	O 612	S 21	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	engineered mutation	UNP P29475
A	357	ASP	GLY	engineered mutation	UNP P29475
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475

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



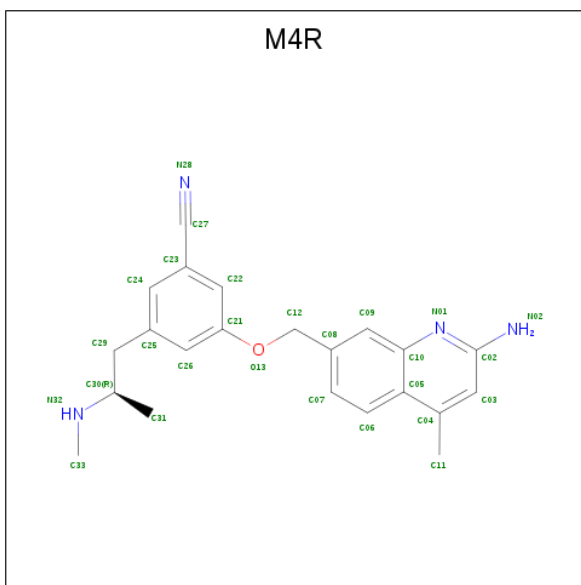
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



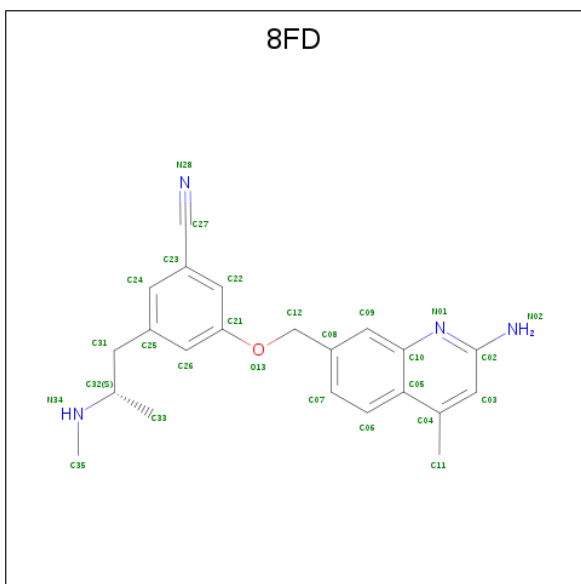
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 3-[(2-amino-4-methylquinolin-7-yl)methoxy]-5-[(2R)-2-(methylamino)propyl]benzonitrile (three-letter code: M4R) (formula:  $C_{22}H_{24}N_4O$ ).



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

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

- 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		

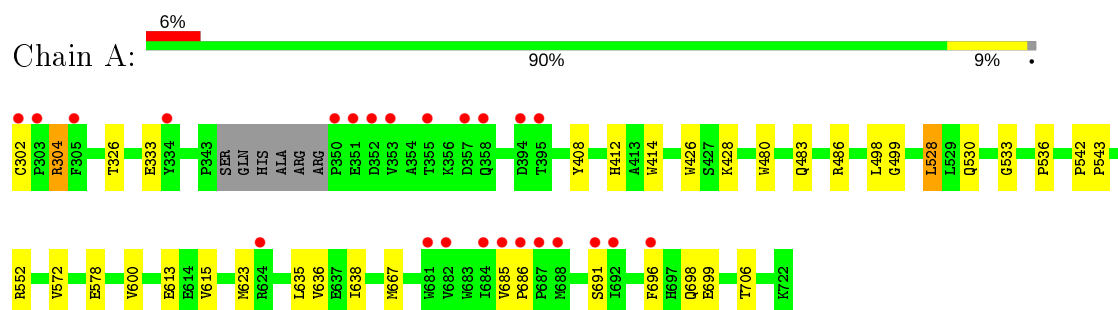
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	291	Total	O	0	0
			291	291		
7	B	228	Total	O	0	0
			228	228		

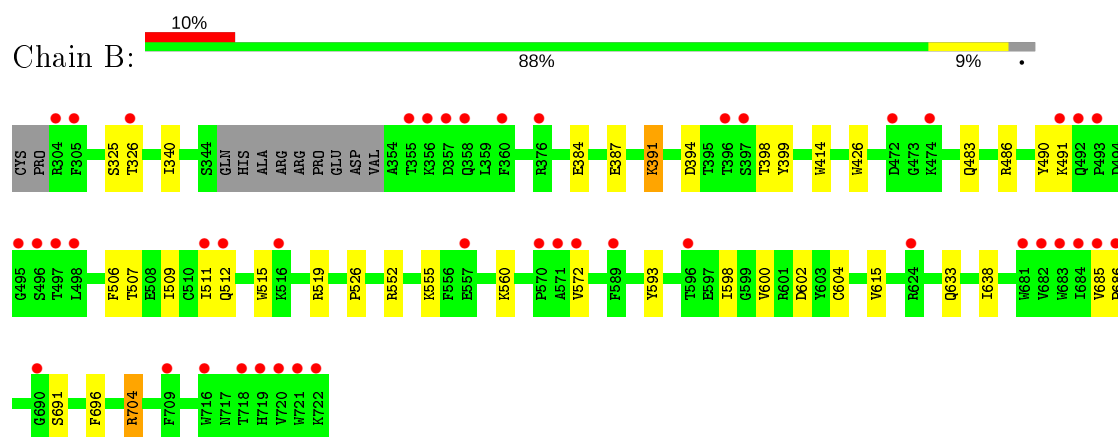
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	52.39Å 122.71Å 165.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.71 – 2.00 39.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 (39.71-2.00) 96.9 (39.71-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.179 , 0.227 0.181 , 0.229	Depositor DCC
$R_{free}$ test set	3484 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.6	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	7484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: M4R, HEM, ZN, H4B, 8FD

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	0/3490	0.50	0/4735
1	B	0.36	0/3450	0.48	0/4679
All	All	0.37	0/6940	0.49	0/9414

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	3387	0	3296	23	0
1	B	3349	0	3262	21	0
2	A	43	0	30	2	0
2	B	43	0	30	1	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	0	0
5	B	27	0	0	1	0
6	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	291	0	0	3	0
7	B	228	0	0	1	0
All	All	7484	0	6648	45	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 (45) 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:326:THR:HG21	1:A:706:THR:HG22	1.69	0.74
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.74	0.70
1:A:528:LEU:HD22	1:A:536:PRO:HB2	1.73	0.69
1:A:483:GLN:HB2	1:A:486:ARG:HG3	1.82	0.60
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.83	0.59
1:A:667:MET:HE1	1:A:698:GLN:HG2	1.86	0.56
2:A:801:HEM:HHC	2:A:801:HEM:HBB2	1.87	0.56
1:A:480:TRP:HB2	1:A:528:LEU:HB3	1.88	0.56
1:A:428:LYS:NZ	7:A:903:HOH:O	2.32	0.52
1:A:486:ARG:NE	7:A:907:HOH:O	2.37	0.52
1:A:304:ARG:HB2	1:A:304:ARG:HH11	1.76	0.51
1:A:530:GLN:HE21	1:A:533:GLY:HA2	1.77	0.49
1:A:613:GLU:HG3	1:A:623:MET:HE3	1.96	0.48
1:A:691:SER:HA	1:A:696:PHE:CG	2.49	0.48
1:B:414:TRP:CE3	1:B:426:TRP:HA	2.49	0.48
1:A:615:VAL:HG21	1:A:638:ILE:HD11	1.98	0.46
1:B:598:ILE:HA	1:B:602:ASP:HB2	1.97	0.46
1:A:333:GLU:HB2	7:B:1002:HOH:O	2.17	0.45
1:B:593:TYR:CD1	1:B:598:ILE:HD11	2.52	0.45
1:A:578:GLU:OE1	7:A:901:HOH:O	2.21	0.44
1:A:636:VAL:HG11	1:B:633:GLN:HG3	1.99	0.44
1:B:491:LYS:HB3	1:B:491:LYS:HE2	1.85	0.44
1:A:498:LEU:HD12	1:A:499:GLY:H	1.83	0.44
1:B:600:VAL:O	1:B:604:CYS:HB2	2.18	0.44
1:B:506:PHE:HA	1:B:509:ILE:HD12	2.00	0.43
1:A:414:TRP:CE3	1:A:426:TRP:HA	2.53	0.43
1:B:685:VAL:HA	1:B:686:PRO:HD3	1.87	0.43
1:B:615:VAL:HG21	1:B:638:ILE:HD11	2.00	0.43
1:B:555:LYS:HA	1:B:555:LYS:HD2	1.75	0.42
1:B:572:VAL:HG21	5:B:804[B]:8FD:C07	2.49	0.42
1:B:490:TYR:CE1	1:B:519:ARG:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:507:THR:O	1:B:511:ILE:HG13	2.20	0.42
1:B:398:THR:OG1	1:B:399:TYR:N	2.51	0.42
1:A:685:VAL:HA	1:A:686:PRO:HD3	1.94	0.42
1:B:572:VAL:HG21	4:B:803[A]:M4R:C07	2.50	0.42
1:A:699:GLU:HB3	1:B:340:ILE:HD13	2.01	0.41
1:B:387:GLU:O	1:B:391:LYS:HD2	2.21	0.41
1:B:515:TRP:CE2	1:B:526:PRO:HD3	2.56	0.41
1:B:325:SER:HB2	1:B:704:ARG:O	2.21	0.41
1:B:483:GLN:HB2	1:B:486:ARG:HG2	2.03	0.41
1:B:691:SER:HA	1:B:696:PHE:CG	2.56	0.41
1:A:408:TYR:CE1	1:A:412:HIS:CE1	3.09	0.40
1:A:600:VAL:HG22	1:A:635:LEU:HD11	2.03	0.40
1:A:542:PRO:HA	1:A:543:PRO:HD3	1.90	0.40
1:A:572:VAL:HG21	4:A:803[A]:M4R:C07	2.52	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	413/421 (98%)	409 (99%)	4 (1%)	0	100	100
1	B	408/421 (97%)	396 (97%)	12 (3%)	0	100	100
All	All	821/842 (98%)	805 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/376 (99%)	369 (99%)	4 (1%)	73	78
1	B	368/376 (98%)	360 (98%)	8 (2%)	52	55
All	All	741/752 (98%)	729 (98%)	12 (2%)	62	67

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	CYS
1	A	304	ARG
1	A	528	LEU
1	A	552	ARG
1	B	326	THR
1	B	384	GLU
1	B	391	LYS
1	B	394	ASP
1	B	512	GLN
1	B	552	ARG
1	B	560	LYS
1	B	704	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	8FD	A	804[B]	-	29,29,29	1.60	2 (6%)	38,40,40	1.02	3 (7%)
5	8FD	B	804[B]	-	29,29,29	1.61	2 (6%)	38,40,40	1.01	2 (5%)
4	M4R	B	803[A]	-	29,29,29	1.58	2 (6%)	38,40,40	1.05	3 (7%)
4	M4R	A	803[A]	-	29,29,29	1.59	2 (6%)	38,40,40	1.02	2 (5%)
2	HEM	B	801	1	27,50,50	2.18	6 (22%)	17,82,82	2.08	4 (23%)
2	HEM	A	801	1	27,50,50	2.13	6 (22%)	17,82,82	2.03	5 (29%)
3	H4B	A	802	-	16,18,18	0.76	0	11,26,26	2.58	5 (45%)
3	H4B	B	802	-	16,18,18	0.88	0	11,26,26	2.61	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
5	8FD	A	804[B]	-	-	0/13/13/13	0/3/3/3
5	8FD	B	804[B]	-	-	0/13/13/13	0/3/3/3
4	M4R	B	803[A]	-	-	2/13/13/13	0/3/3/3
4	M4R	A	803[A]	-	-	3/13/13/13	0/3/3/3
2	HEM	B	801	1	-	0/6/54/54	-
2	HEM	A	801	1	-	0/6/54/54	-
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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	804[B]	8FD	C23-C27	-7.13	1.28	1.44
4	A	803[A]	M4R	C23-C27	-7.06	1.28	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803[A]	M4R	C23-C27	-6.99	1.29	1.44
5	B	804[B]	8FD	C23-C27	-6.98	1.29	1.44
2	B	801	HEM	C3D-C2D	5.14	1.52	1.37
2	A	801	HEM	C3D-C2D	5.07	1.52	1.37
2	A	801	HEM	C3B-C2B	-4.89	1.33	1.40
2	B	801	HEM	C3B-C2B	-4.78	1.33	1.40
2	B	801	HEM	C3C-C2C	-4.22	1.34	1.40
2	A	801	HEM	C3C-C2C	-3.93	1.34	1.40
2	A	801	HEM	C3B-CAB	3.83	1.55	1.47
2	B	801	HEM	C3C-CAC	3.60	1.55	1.47
2	B	801	HEM	C3B-CAB	3.56	1.55	1.47
2	A	801	HEM	C3C-CAC	3.32	1.54	1.47
5	B	804[B]	8FD	C05-C10	-2.36	1.38	1.42
5	A	804[B]	8FD	C05-C10	-2.29	1.38	1.42
4	B	803[A]	M4R	C05-C10	-2.26	1.38	1.42
4	A	803[A]	M4R	C05-C10	-2.26	1.38	1.42
2	B	801	HEM	CMC-C2C	2.10	1.56	1.51
2	A	801	HEM	C1D-ND	2.03	1.40	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CBA-CAA-C2A	-5.21	102.88	112.49
3	B	802	H4B	C4-C4A-C8A	5.17	119.17	114.57
3	A	802	H4B	C4-C4A-C8A	4.92	118.94	114.57
2	B	801	HEM	CBA-CAA-C2A	-4.91	103.43	112.49
2	B	801	HEM	CAD-CBD-CGD	-4.00	105.95	112.67
3	B	802	H4B	C4-N3-C2	3.42	121.36	115.93
3	A	802	H4B	C4-N3-C2	3.37	121.29	115.93
2	A	801	HEM	C1D-C2D-C3D	-3.32	104.69	107.00
3	A	802	H4B	N3-C2-N1	-3.21	120.39	125.42
3	B	802	H4B	N3-C2-N1	-3.20	120.41	125.42
2	B	801	HEM	CMA-C3A-C4A	-3.09	123.72	128.46
3	A	802	H4B	C4-C4A-N5	2.99	121.63	119.12
3	B	802	H4B	C4-C4A-N5	2.92	121.57	119.12
2	B	801	HEM	C1D-C2D-C3D	-2.90	104.98	107.00
5	A	804[B]	8FD	C04-C05-C10	2.74	119.49	118.01
4	B	803[A]	M4R	C04-C05-C10	2.73	119.49	118.01
4	A	803[A]	M4R	C04-C05-C10	2.71	119.48	118.01
2	A	801	HEM	CMC-C2C-C3C	2.70	129.73	124.68
5	B	804[B]	8FD	C05-C10-N01	-2.54	120.12	122.81
3	B	802	H4B	C2-N1-C8A	2.50	120.14	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	H4B	C2-N1-C8A	2.50	120.14	114.54
5	A	804[B]	8FD	C05-C10-N01	-2.48	120.18	122.81
4	A	803[A]	M4R	C05-C10-N01	-2.47	120.19	122.81
5	B	804[B]	8FD	C04-C05-C10	2.47	119.35	118.01
2	A	801	HEM	CAD-CBD-CGD	-2.36	108.71	112.67
4	B	803[A]	M4R	C05-C10-N01	-2.24	120.44	122.81
5	A	804[B]	8FD	C12-O13-C21	2.15	122.97	117.65
4	B	803[A]	M4R	C12-O13-C21	2.05	122.72	117.65
2	A	801	HEM	CMA-C3A-C4A	-2.05	125.31	128.46

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	803[A]	M4R	C25-C29-C30-C31
4	B	803[A]	M4R	C25-C29-C30-N32
4	A	803[A]	M4R	C25-C29-C30-C31
4	A	803[A]	M4R	C25-C29-C30-N32
4	A	803[A]	M4R	C24-C23-C27-N28

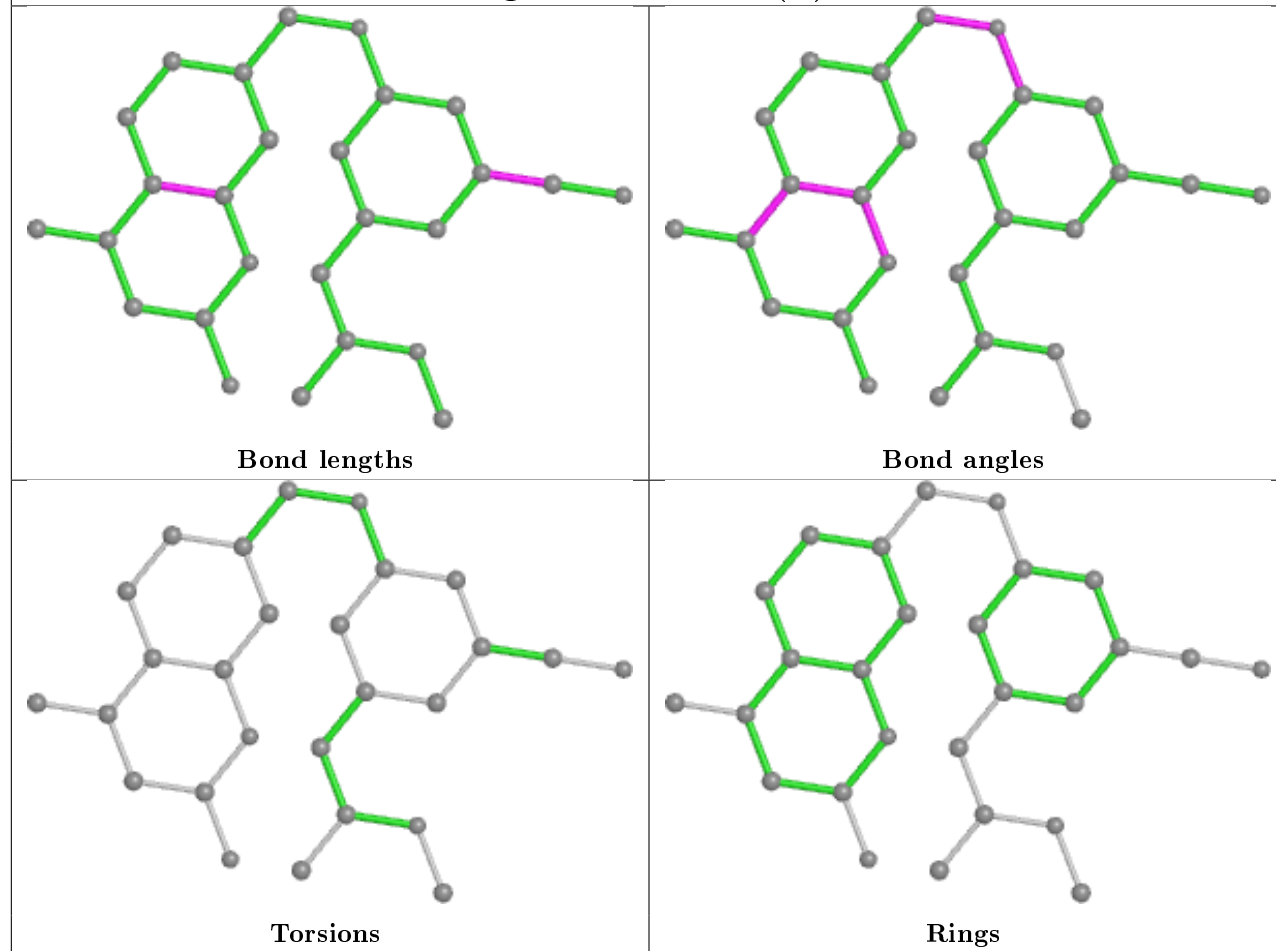
There are no ring outliers.

5 monomers are involved in 6 short contacts:

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

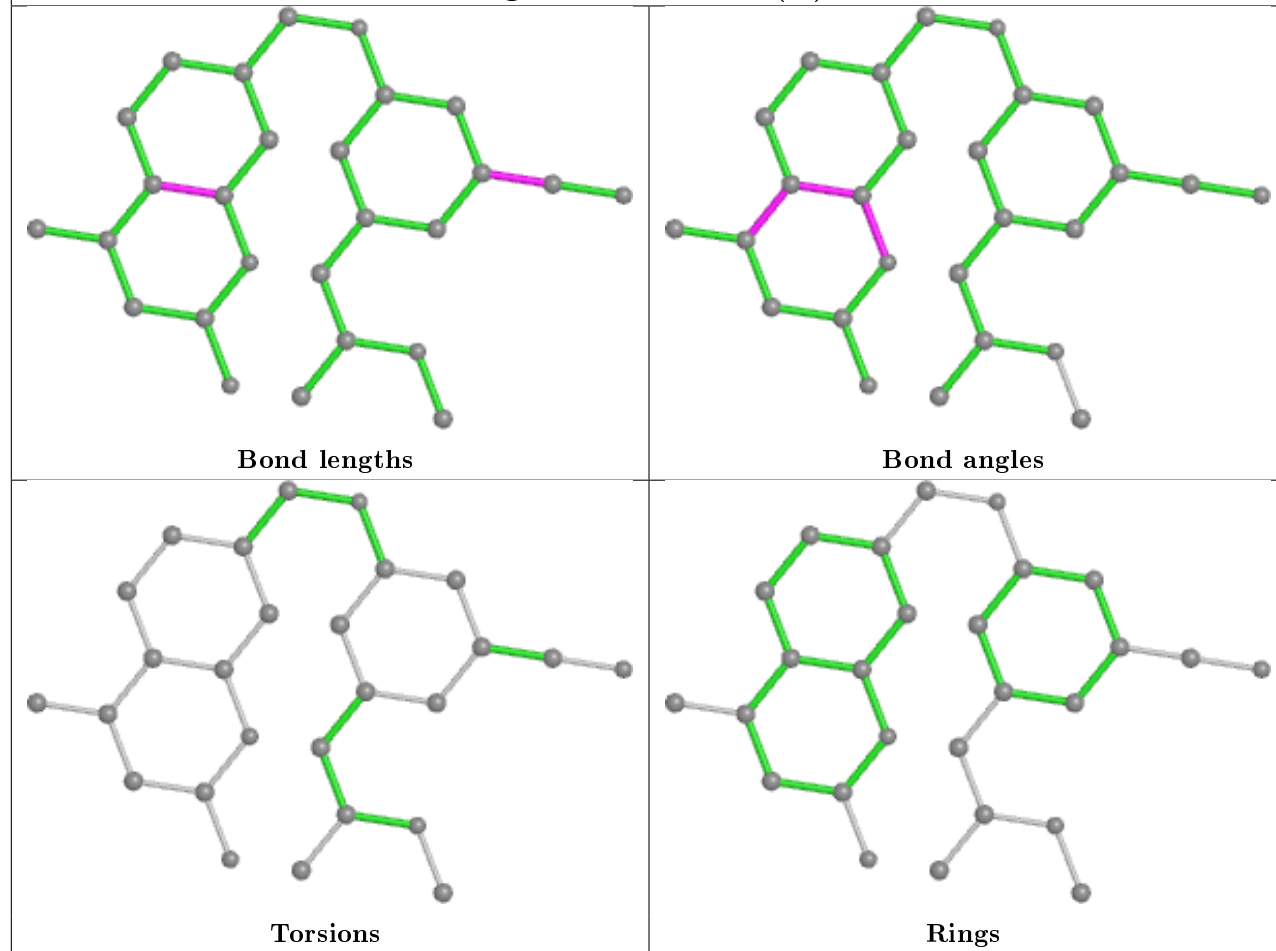
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 8FD A 804 (B)

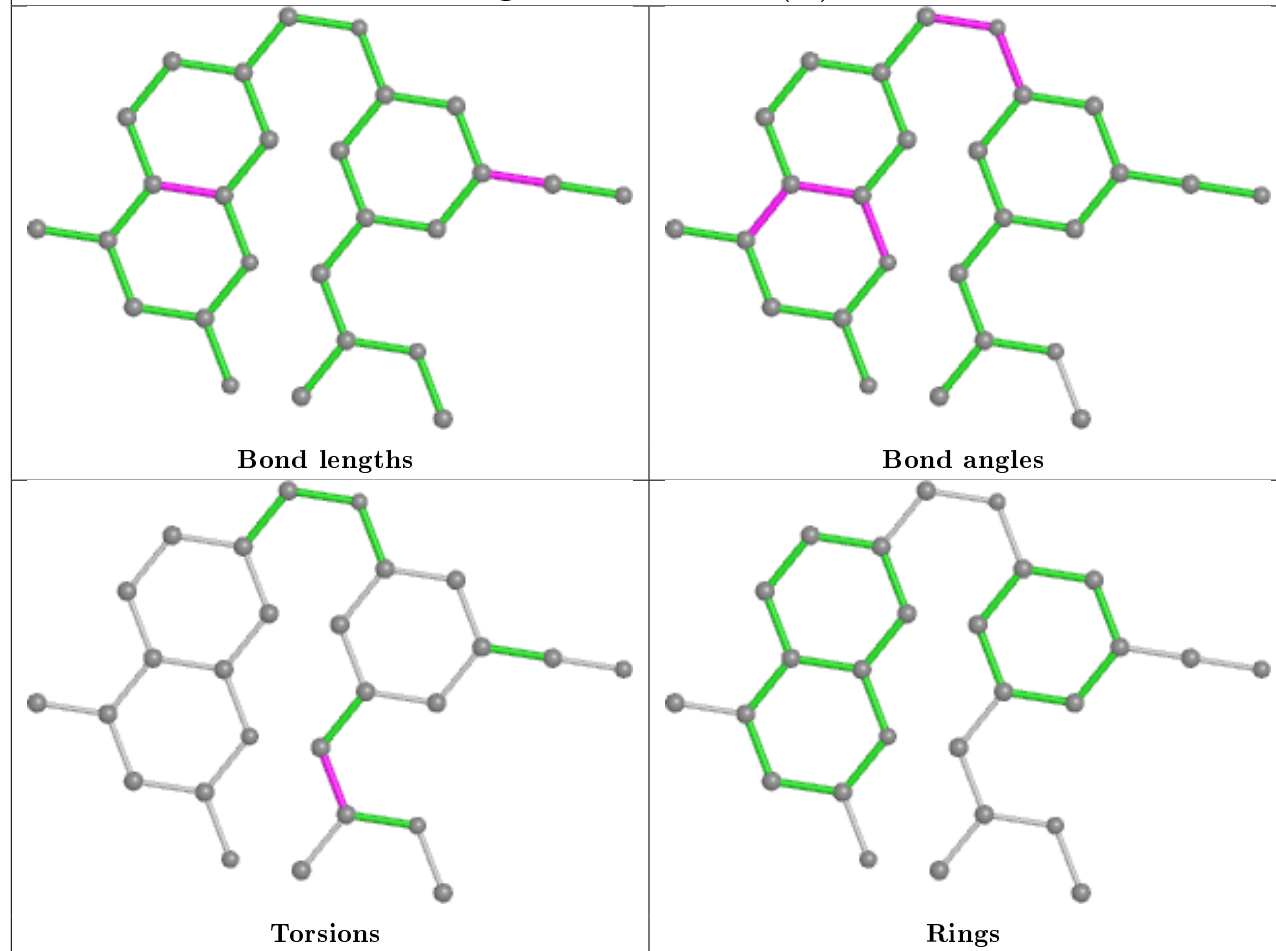




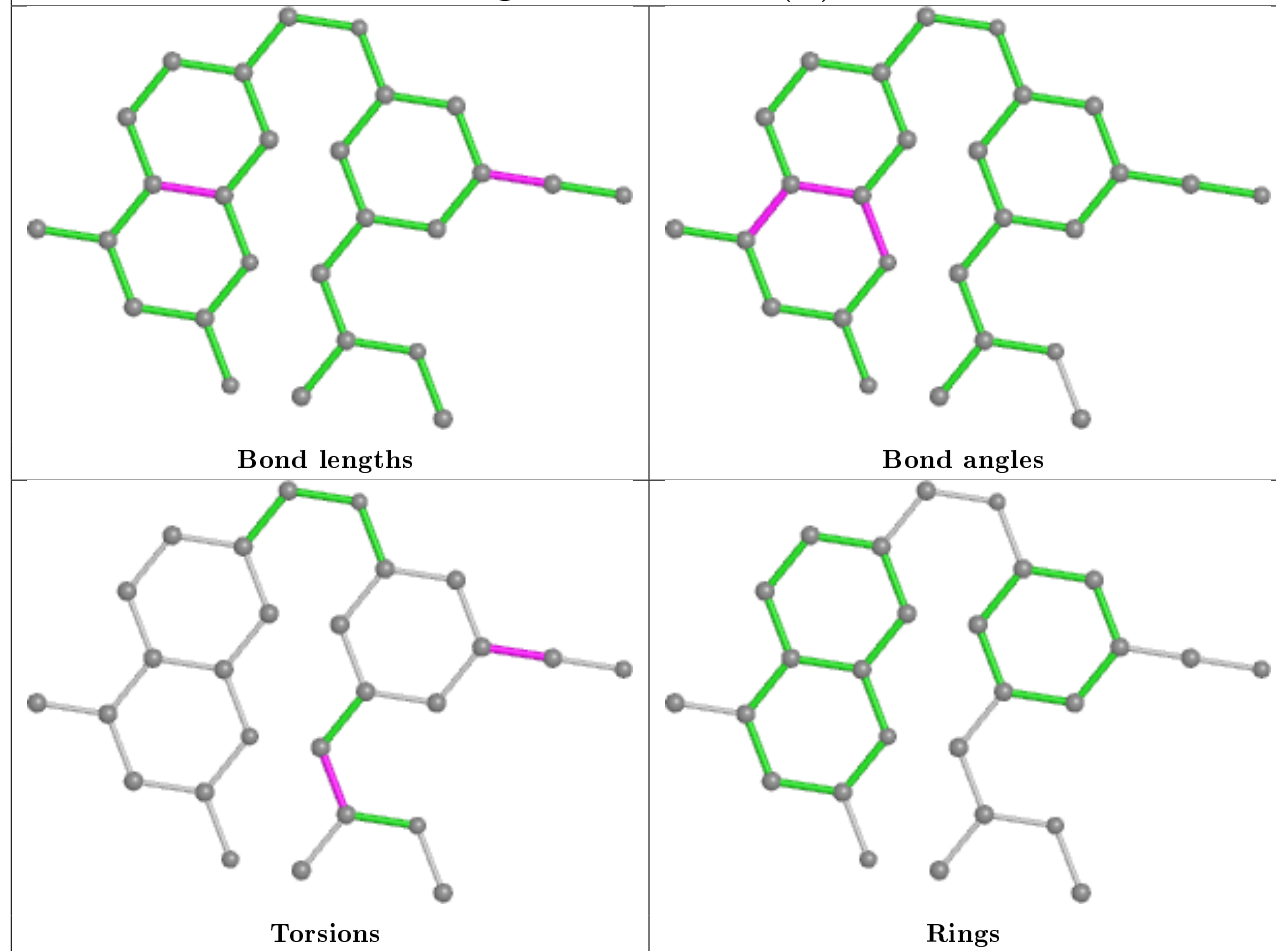
## Ligand 8FD B 804 (B)

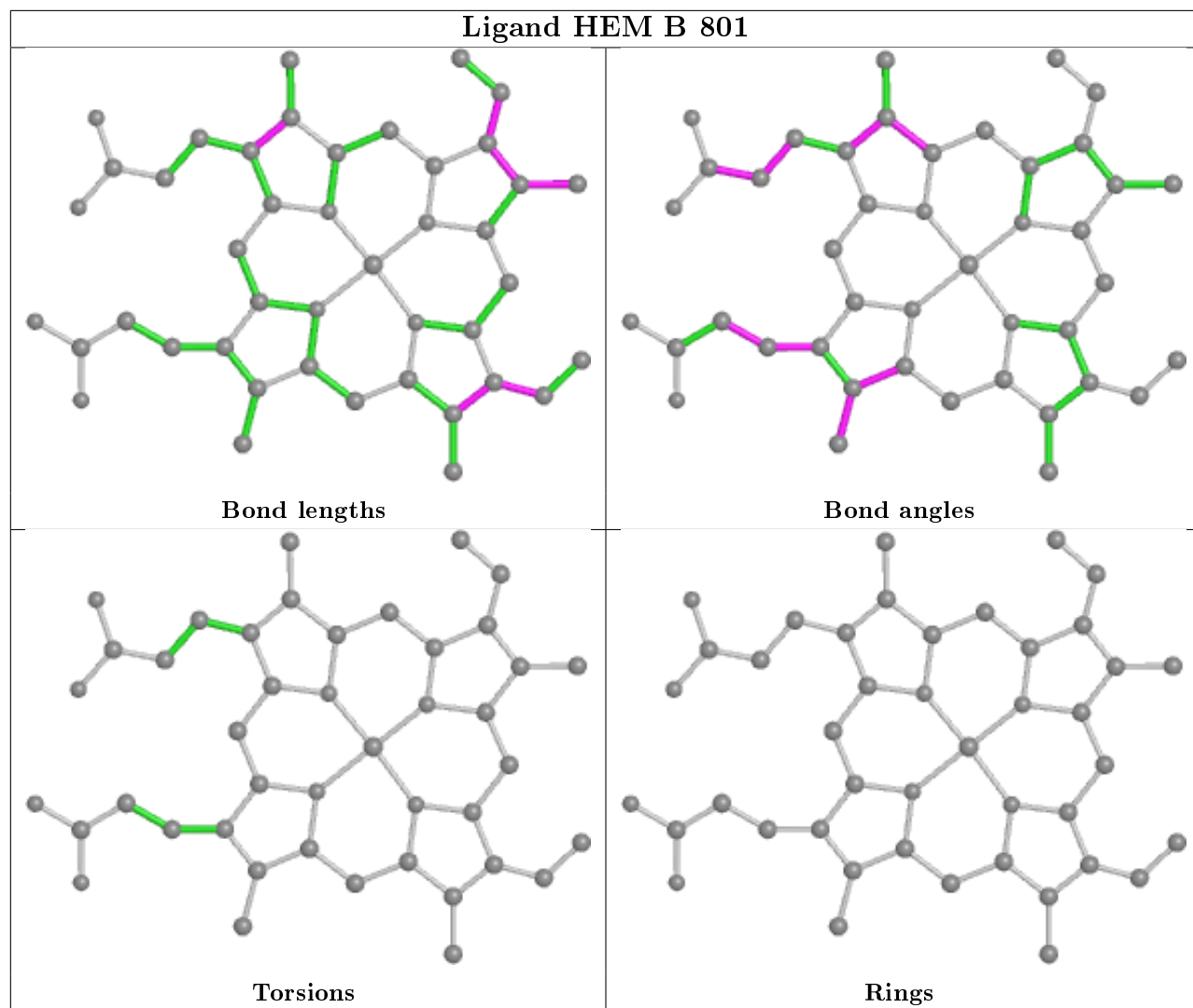


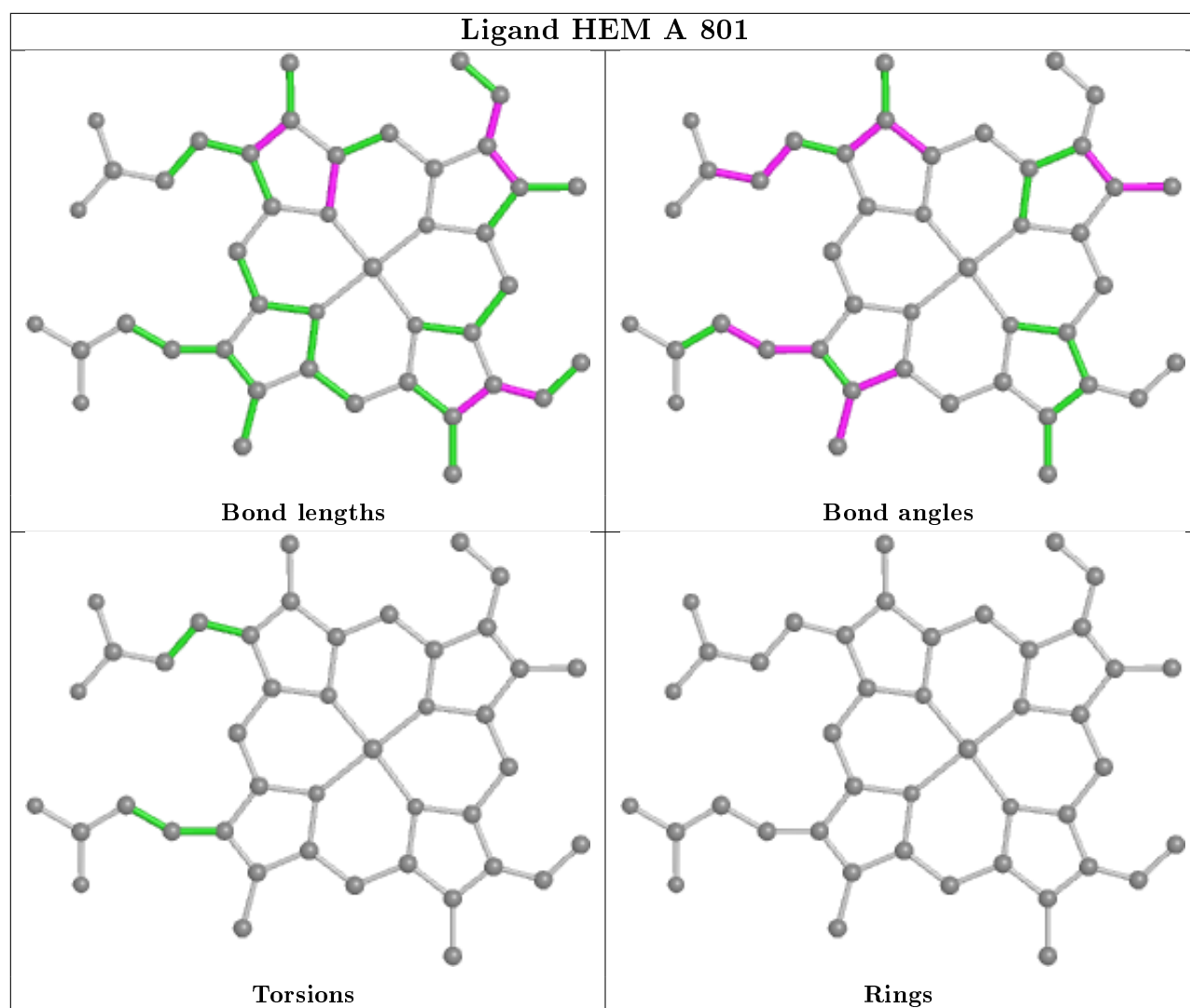
## Ligand M4R B 803 (A)



## 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	415/421 (98%)	0.16	24 (5%) 23 22	31, 46, 76, 115	0
1	B	410/421 (97%)	0.49	44 (10%) 6 5	34, 52, 90, 116	0
All	All	825/842 (97%)	0.32	68 (8%) 11 11	31, 48, 85, 116	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	357	ASP	6.9
1	B	721	TRP	5.9
1	B	720	VAL	5.4
1	B	493	PRO	5.1
1	B	718	THR	4.4
1	B	722	LYS	4.4
1	B	683	TRP	3.9
1	B	305	PHE	3.9
1	A	351	GLU	3.8
1	B	360	PHE	3.7
1	A	353	VAL	3.6
1	B	685	VAL	3.6
1	A	305	PHE	3.5
1	A	685	VAL	3.4
1	B	716	TRP	3.3
1	A	696	PHE	3.3
1	B	304	ARG	3.3
1	B	624	ARG	3.2
1	B	682	VAL	3.1
1	B	719	HIS	3.1
1	B	589	PHE	3.0
1	B	326	THR	3.0
1	B	690	GLY	2.9
1	A	624	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	687	PRO	2.8
1	A	682	VAL	2.8
1	A	681	TRP	2.8
1	B	686	PRO	2.8
1	A	686	PRO	2.8
1	B	684	ILE	2.7
1	A	302	CYS	2.7
1	B	596	THR	2.7
1	A	352	ASP	2.7
1	B	498	LEU	2.7
1	B	396	THR	2.6
1	B	572	VAL	2.6
1	B	495	GLY	2.5
1	B	571	ALA	2.5
1	A	334	TYR	2.5
1	A	355	THR	2.5
1	A	357	ASP	2.5
1	B	557	GLU	2.5
1	B	492	GLN	2.4
1	A	684	ILE	2.4
1	B	570	PRO	2.4
1	B	358	GLN	2.4
1	B	474	LYS	2.3
1	A	358	GLN	2.3
1	B	496	SER	2.3
1	A	303	PRO	2.2
1	B	355	THR	2.2
1	B	512	GLN	2.2
1	B	356	LYS	2.2
1	B	511	ILE	2.1
1	A	394	ASP	2.1
1	B	491	LYS	2.1
1	A	691	SER	2.1
1	B	516	LYS	2.1
1	B	397	SER	2.1
1	A	395	THR	2.1
1	A	688	MET	2.1
1	B	497	THR	2.1
1	B	376	ARG	2.1
1	A	692	ILE	2.1
1	B	709	PHE	2.1
1	B	681	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	350	PRO	2.0
1	B	472	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

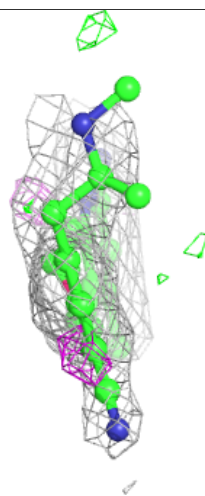
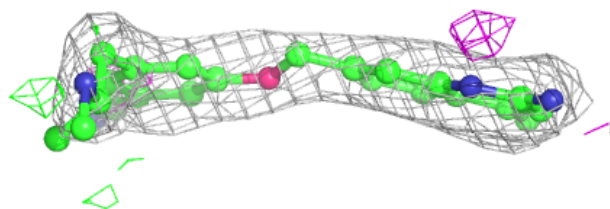
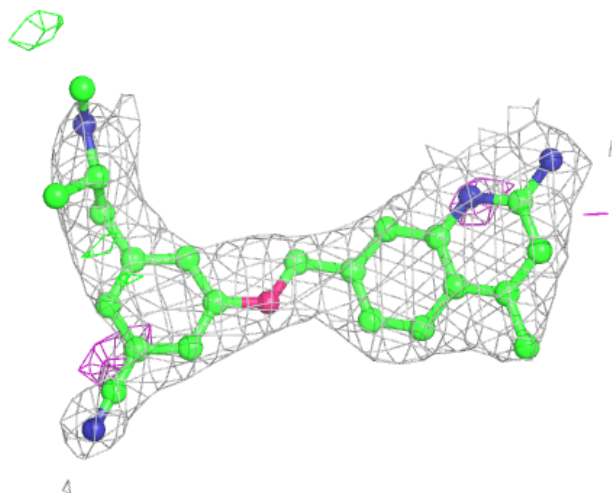
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	8FD	B	804[B]	27/27	0.92	0.29	31,58,79,79	27
3	H4B	B	802	17/17	0.92	0.24	38,53,65,69	0
4	M4R	B	803[A]	27/27	0.93	0.28	36,60,79,81	27
4	M4R	A	803[A]	27/27	0.94	0.23	33,55,75,77	27
5	8FD	A	804[B]	27/27	0.94	0.22	33,53,74,77	27
3	H4B	A	802	17/17	0.96	0.16	34,45,52,57	0
2	HEM	B	801	43/43	0.98	0.20	29,39,52,65	0
2	HEM	A	801	43/43	0.98	0.19	27,36,51,61	0
6	ZN	A	805	1/1	0.99	0.11	43,43,43,43	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.



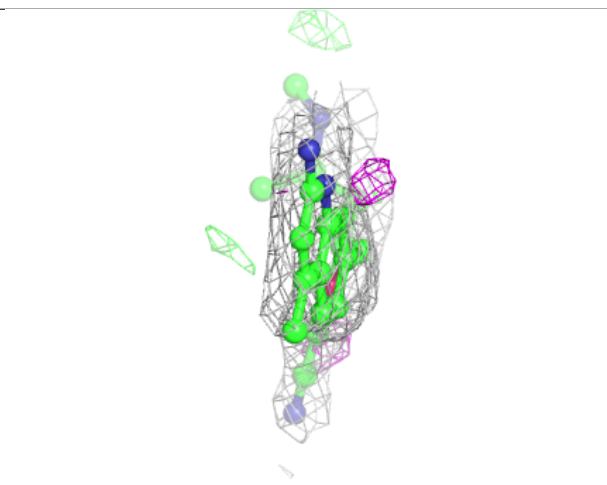
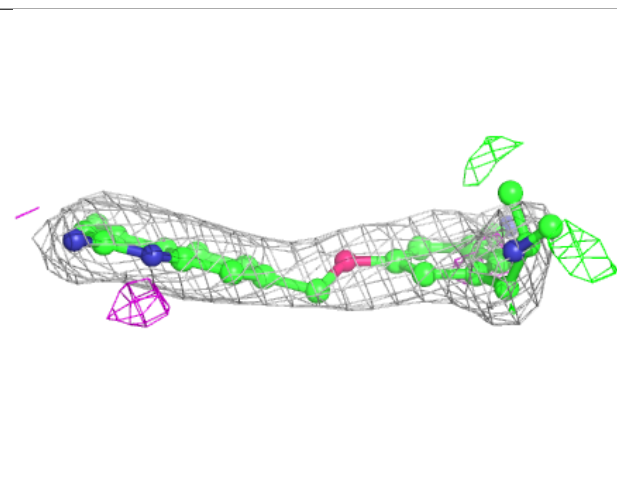
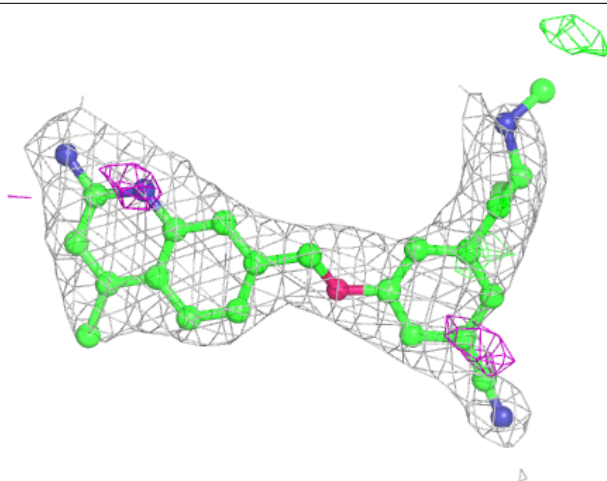
**Electron density around 8FD B 804 (B):**

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



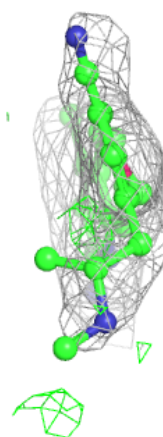
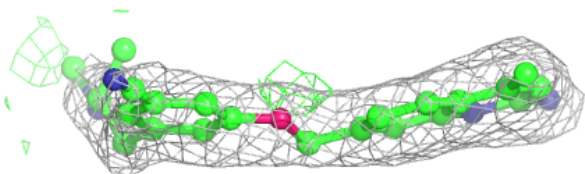
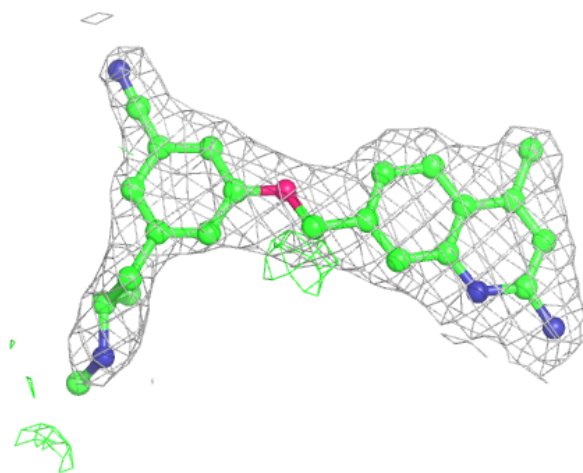
**Electron density around M4R B 803 (A):**

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



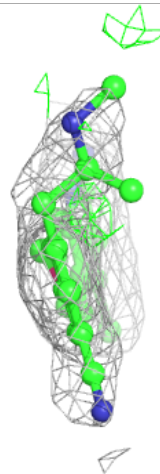
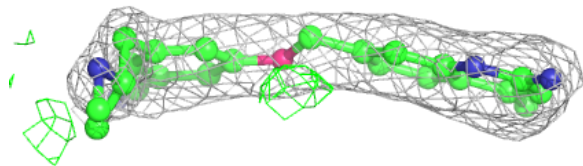
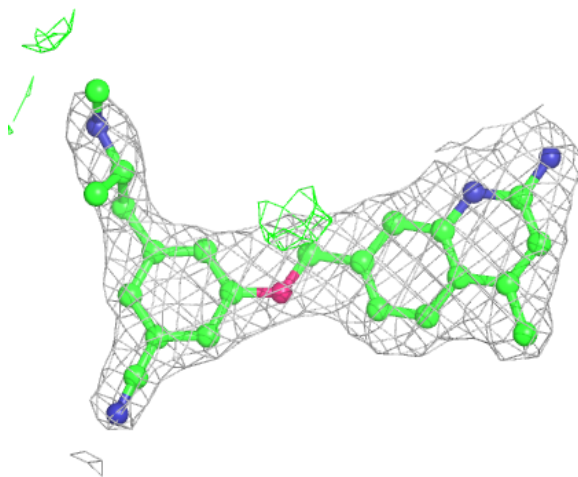
**Electron density around M4R A 803 (A):**

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



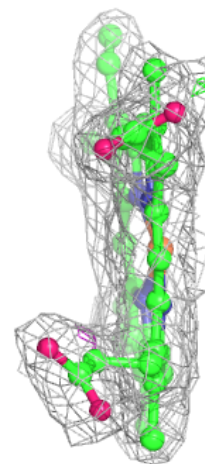
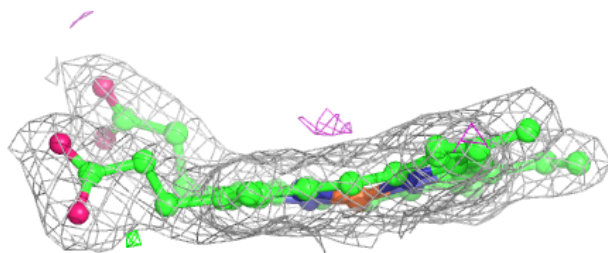
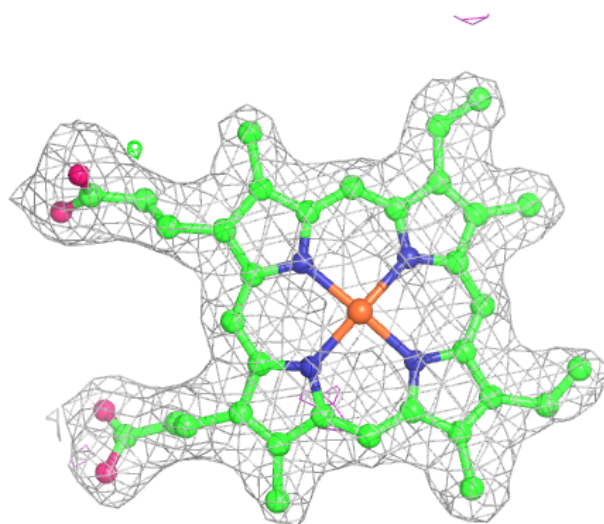
**Electron density around 8FD A 804 (B):**

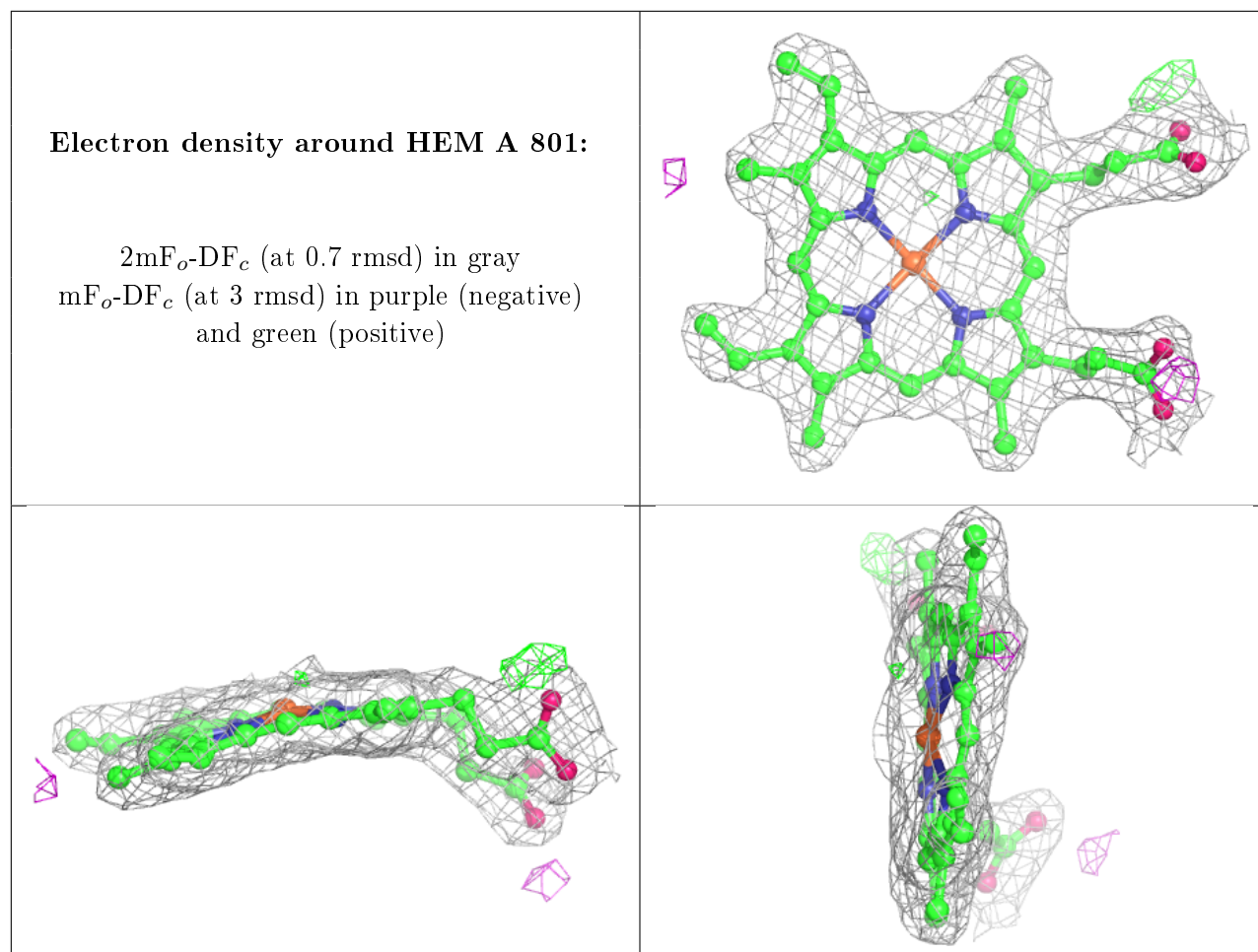
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 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.