



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:46 pm BST

PDB ID : 5AGL  
Title : Structure of rat neuronal nitric oxide synthase heme domain in complex with (S)-2-Amino-5-(2-(methylsulfonyl)acetimidamido)pentanoic acid  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2015-02-02  
Resolution : 1.94 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

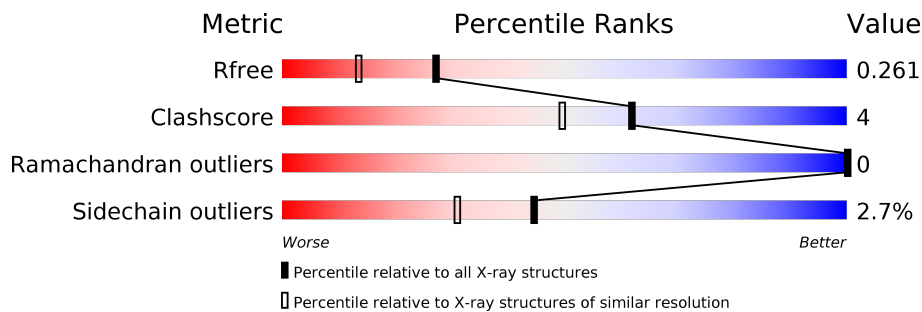
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)

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  $\leq 5\%$

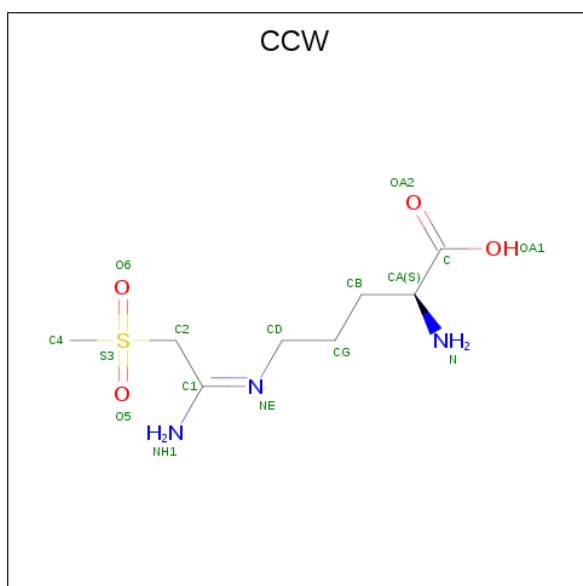
Mol	Chain	Length	Quality of chain
1	A	422	
1	B	422	





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

- Molecule 4 is (S)-2-Amino-5-(2-(methylsulfonyl)acetimidamido)pentanoic acid (three-letter code: CCW) (formula: C<sub>8</sub>H<sub>17</sub>N<sub>3</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	16	8	3	4	1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	16	8	3	4	1	0	0

- Molecule 5 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
			Total	C	O		
5	A	1	4	2	2	0	0
5	B	1	4	2	2	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	B	1	1	1	0	0

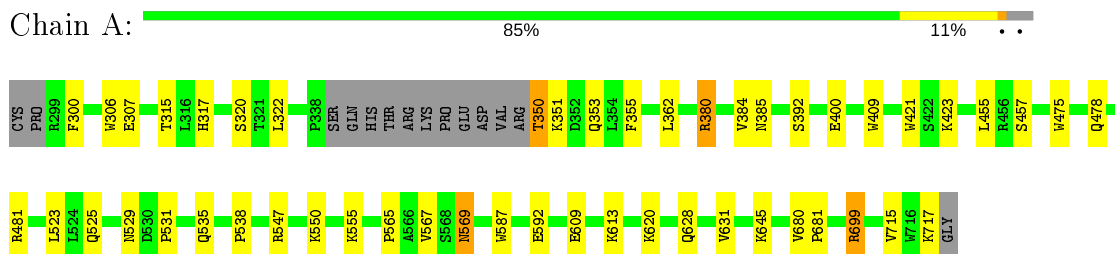
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	154	154	154	0	0
7	B	206	206	206	0	0

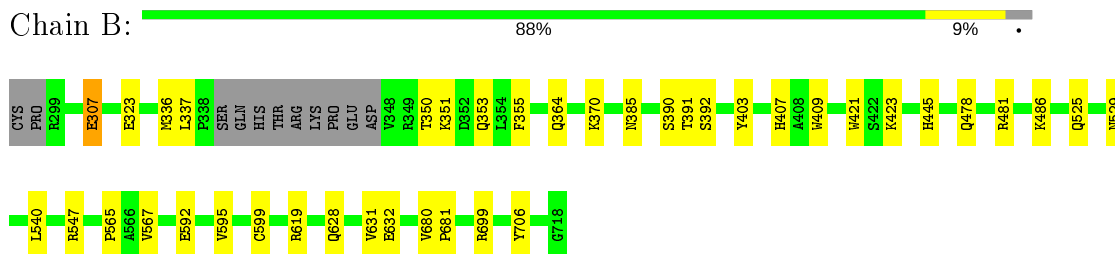
### 3 Residue-property plots [i](#)

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. 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. 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, $\alpha$ , $\beta$ , $\gamma$	52.01Å 111.34Å 164.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.59 – 1.94 38.59 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.59-1.94) 99.6 (38.59-1.94)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 1.94Å)	Xtrriage
Refinement program	REFMAC 5.5.0089	Depositor
R, $R_{free}$	0.179 , 0.210 0.236 , 0.261	Depositor DCC
$R_{free}$ test set	3533 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtrriage
Anisotropy	0.677	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7220	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CCW, 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	0.61	0/3444	0.64	0/4672
1	B	0.64	0/3465	0.65	0/4697
All	All	0.62	0/6909	0.65	0/9369

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3339	0	3256	33	0
1	B	3360	0	3280	24	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
3	A	17	0	15	0	0
3	B	17	0	15	0	0
4	A	16	0	16	4	0
4	B	16	0	16	5	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	154	0	0	2	0
7	B	206	0	0	2	0
All	All	7220	0	6664	60	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 (60) 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:565:PRO:HB2	4:A:800:CCW:H42C	1.37	1.06
1:B:565:PRO:HB2	4:B:800:CCW:H42C	1.52	0.89
1:A:350:THR:N	1:A:353:GLN:HE21	1.79	0.80
1:B:706:TYR:OH	2:B:750:HEM:O1D	2.09	0.71
1:A:350:THR:N	1:A:353:GLN:NE2	2.41	0.67
4:A:800:CCW:HD2C	4:A:800:CCW:H41C	1.77	0.64
1:B:567:VAL:HG23	4:B:800:CCW:H41C	1.80	0.63
1:A:628:GLN:HG2	1:B:631:VAL:HG11	1.80	0.62
1:A:322:LEU:HD13	1:A:699:ARG:HH21	1.66	0.61
4:B:800:CCW:H41C	4:B:800:CCW:HD2C	1.83	0.60
1:A:478:GLN:HB2	1:A:481:ARG:HG3	1.85	0.59
2:B:750:HEM:HHC	2:B:750:HEM:HBB2	1.85	0.58
1:A:380:ARG:HD3	1:A:400:GLU:OE2	2.07	0.55
1:A:300:PHE:HD1	1:A:315:THR:HG22	1.72	0.54
2:A:750:HEM:HBB2	2:A:750:HEM:HHC	1.91	0.53
1:A:355:PHE:CE1	1:A:385:ASN:HB2	2.45	0.52
2:B:750:HEM:HBC2	2:B:750:HEM:CMC	2.40	0.52
1:A:306:TRP:CE2	1:B:336:MET:HE3	2.45	0.52
1:B:478:GLN:HB2	1:B:481:ARG:HG3	1.91	0.52
1:A:609:GLU:HG3	7:A:2119:HOH:O	2.10	0.51
1:B:403:TYR:CE1	1:B:407:HIS:CE1	2.98	0.51
1:A:362:LEU:HD11	1:A:384:VAL:HG21	1.91	0.51
1:B:351:LYS:HE3	1:B:392:SER:OG	2.11	0.51
1:A:306:TRP:CD2	1:B:336:MET:HE3	2.46	0.50
1:A:567:VAL:HG23	4:A:800:CCW:H41C	1.92	0.50
1:B:355:PHE:CE1	1:B:385:ASN:HB2	2.46	0.50
1:A:592:GLU:OE1	4:A:800:CCW:NE	2.45	0.50
1:A:475:TRP:CZ2	1:A:531:PRO:HG3	2.47	0.49
2:A:750:HEM:CMC	2:A:750:HEM:HBC2	2.42	0.49
1:B:323:GLU:O	1:B:699:ARG:HD3	2.14	0.48
1:A:317:HIS:O	1:A:320:SER:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:VAL:O	1:B:599:CYS:HB2	2.16	0.46
1:A:455:LEU:HD12	1:A:587:TRP:HB3	1.98	0.46
1:A:523:LEU:HD22	1:A:531:PRO:HB2	1.98	0.45
1:A:569:ASN:H	1:A:569:ASN:HD22	1.64	0.45
1:A:717:LYS:N	7:A:2096:HOH:O	2.48	0.45
1:A:628:GLN:NE2	1:B:632:GLU:OE2	2.50	0.45
2:A:750:HEM:HMC1	2:A:750:HEM:HBC2	1.99	0.45
1:A:535:GLN:HE21	1:A:538:PRO:HD3	1.82	0.45
1:B:364:GLN:NE2	7:B:2018:HOH:O	2.47	0.45
1:B:619:ARG:HB2	1:B:619:ARG:HE	1.49	0.44
1:B:307[B]:GLU:OE1	7:B:2003:HOH:O	2.21	0.44
1:A:423[B]:LYS:O	1:A:457[B]:SER:OG	2.35	0.44
1:B:680:VAL:HA	1:B:681:PRO:HD3	1.88	0.44
1:A:525:GLN:HG3	1:A:529:ASN:O	2.18	0.44
1:A:351:LYS:HE2	1:A:392:SER:HB3	2.00	0.43
1:A:409:TRP:CE3	1:A:421:TRP:HA	2.53	0.43
1:A:550:LYS:HB2	1:A:550:LYS:HE3	1.73	0.43
1:A:306:TRP:CD1	1:B:336:MET:HE2	2.54	0.43
1:A:609:GLU:O	1:A:613:LYS:HG2	2.19	0.42
1:B:409:TRP:CE3	1:B:421:TRP:HA	2.54	0.42
1:B:525:GLN:HG3	1:B:529:ASN:O	2.19	0.42
1:B:445:HIS:C	1:B:445:HIS:CD2	2.93	0.42
1:A:475:TRP:CE2	1:A:531:PRO:HG3	2.55	0.41
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.89	0.41
1:B:391:THR:O	1:B:392:SER:HB2	2.20	0.41
2:B:750:HEM:HBC2	2:B:750:HEM:HMC1	2.02	0.41
4:B:800:CCW:HD2C	4:B:800:CCW:C4	2.49	0.41
1:A:631:VAL:HG11	1:B:628:GLN:CG	2.51	0.40
1:B:592:GLU:OE1	4:B:800:CCW:NE	2.55	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%)	398 (97%)	11 (3%)	0	100	100
1	B	411/422 (97%)	405 (98%)	6 (2%)	0	100	100
All	All	820/844 (97%)	803 (98%)	17 (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	368/377 (98%)	357 (97%)	11 (3%)	41	27
1	B	370/377 (98%)	359 (97%)	11 (3%)	41	27
All	All	738/754 (98%)	716 (97%)	22 (3%)	44	27

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307[A]	GLU
1	A	307[B]	GLU
1	A	350	THR
1	A	380	ARG
1	A	547	ARG
1	A	555	LYS
1	A	569	ASN
1	A	620	LYS
1	A	645	LYS
1	A	699	ARG
1	A	715	VAL
1	B	307[A]	GLU
1	B	307[B]	GLU
1	B	337	LEU
1	B	350	THR
1	B	353	GLN
1	B	370	LYS
1	B	390	SER

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Mol	Chain	Res	Type
1	B	423	LYS
1	B	486	LYS
1	B	540	LEU
1	B	547	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	GLN
1	A	454	ASN
1	A	508	GLN
1	A	535	GLN
1	A	569	ASN
1	A	605	ASN
1	A	628	GLN
1	A	697	ASN
1	B	364	GLN
1	B	454	ASN
1	B	507	GLN
1	B	529	ASN
1	B	535	GLN
1	B	601	ASN
1	B	605	ASN
1	B	628	GLN
1	B	697	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 carbohydrates 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
3	H4B	A	760	-	16,18,18	1.04	1 (6%)	11,26,26	2.92	7 (63%)
4	CCW	A	800	-	10,15,15	2.39	4 (40%)	8,20,20	3.56	5 (62%)
4	CCW	B	800	-	10,15,15	2.44	4 (40%)	8,20,20	2.91	4 (50%)
3	H4B	B	760	-	16,18,18	1.46	3 (18%)	11,26,26	2.43	5 (45%)
5	ACT	A	860	-	1,3,3	1.38	0	0,3,3	0.00	-
2	HEM	B	750	1	27,50,50	2.09	8 (29%)	17,82,82	2.50	5 (29%)
2	HEM	A	750	1	27,50,50	2.18	8 (29%)	17,82,82	2.34	6 (35%)
5	ACT	B	860	-	1,3,3	1.44	0	0,3,3	0.00	-

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	A	760	-	-	0/8/17/17	0/2/2/2
4	CCW	A	800	-	-	2/8/16/16	-
4	CCW	B	800	-	-	2/8/16/16	-
3	H4B	B	760	-	-	0/8/17/17	0/2/2/2
2	HEM	B	750	1	-	0/6/54/54	-
2	HEM	A	750	1	-	0/6/54/54	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	800	CCW	C2-S3	-5.78	1.69	1.79
4	A	800	CCW	C2-S3	-5.76	1.69	1.79
2	A	750	HEM	C3B-C2B	-5.71	1.32	1.40
2	B	750	HEM	C3B-C2B	-4.82	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	750	HEM	C3D-C2D	4.75	1.51	1.37
2	B	750	HEM	C3C-C2C	-4.58	1.34	1.40
2	B	750	HEM	C3D-C2D	4.42	1.50	1.37
2	A	750	HEM	C3B-CAB	3.55	1.55	1.47
3	B	760	H4B	C7-C6	3.33	1.55	1.52
2	B	750	HEM	C3B-CAB	3.26	1.54	1.47
2	A	750	HEM	C3C-C2C	-3.25	1.35	1.40
2	A	750	HEM	C3C-CAC	3.20	1.54	1.47
4	A	800	CCW	C1-NE	3.18	1.35	1.28
4	B	800	CCW	C1-NH1	-2.98	1.28	1.33
2	B	750	HEM	C3C-CAC	2.94	1.53	1.47
4	B	800	CCW	C1-NE	2.73	1.34	1.28
4	B	800	CCW	C4-S3	-2.70	1.65	1.75
4	A	800	CCW	C1-NH1	-2.67	1.28	1.33
3	B	760	H4B	C4-C4A	-2.38	1.38	1.41
3	B	760	H4B	C7-N8	2.33	1.48	1.44
4	A	800	CCW	C4-S3	-2.30	1.66	1.75
2	B	750	HEM	CAD-C3D	2.26	1.56	1.52
2	A	750	HEM	CMD-C2D	2.23	1.56	1.51
2	B	750	HEM	CMD-C2D	2.14	1.56	1.51
2	A	750	HEM	CMC-C2C	2.11	1.56	1.51
2	A	750	HEM	CAA-C2A	2.09	1.55	1.52
3	A	760	H4B	C4-C4A	-2.07	1.38	1.41
2	B	750	HEM	CMC-C2C	2.04	1.56	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	CCW	O6-S3-C4	7.19	116.14	108.91
2	B	750	HEM	CBA-CAA-C2A	-7.05	99.48	112.49
2	A	750	HEM	CBA-CAA-C2A	-6.66	100.21	112.49
4	B	800	CCW	O6-S3-C4	5.83	114.77	108.91
3	A	760	H4B	C4-C4A-C8A	4.45	118.53	114.57
3	B	760	H4B	C4-C4A-C8A	4.29	118.38	114.57
2	B	750	HEM	CBD-CAD-C3D	-4.14	104.84	112.48
3	A	760	H4B	N3-C2-N1	-4.11	118.97	125.42
2	A	750	HEM	CBD-CAD-C3D	-4.01	105.08	112.48
4	A	800	CCW	O5-S3-C4	-3.98	104.91	108.91
3	A	760	H4B	C4-N3-C2	3.93	122.17	115.93
3	B	760	H4B	C4-N3-C2	3.87	122.08	115.93
4	A	800	CCW	CG-CD-NE	3.61	117.22	110.66
2	B	750	HEM	C4C-C3C-C2C	3.48	109.33	106.90

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	760	H4B	C4-C4A-N5	3.32	121.91	119.12
3	B	760	H4B	N3-C2-N1	-3.31	120.23	125.42
4	A	800	CCW	O5-S3-O6	-3.27	110.11	117.09
2	B	750	HEM	C1D-C2D-C3D	-3.26	104.73	107.00
4	B	800	CCW	O5-S3-C4	-3.21	105.68	108.91
3	A	760	H4B	C2-N1-C8A	3.07	121.42	114.54
2	A	750	HEM	C4C-C3C-C2C	3.05	109.03	106.90
4	B	800	CCW	CG-CD-NE	2.86	115.87	110.66
3	A	760	H4B	N2-C2-N3	2.84	121.67	117.25
2	A	750	HEM	CMC-C2C-C3C	2.72	129.76	124.68
4	B	800	CCW	C2-C1-NH1	2.49	120.69	117.24
3	A	760	H4B	C4A-N5-C6	-2.45	114.48	121.16
4	A	800	CCW	C2-C1-NH1	2.37	120.53	117.24
2	A	750	HEM	C1D-C2D-C3D	-2.27	105.41	107.00
3	B	760	H4B	C4-C4A-N5	2.22	120.98	119.12
2	B	750	HEM	CMC-C2C-C3C	2.13	128.66	124.68
3	B	760	H4B	C2-N1-C8A	2.04	119.10	114.54
2	A	750	HEM	C3C-C4C-NC	-2.01	107.15	110.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	800	CCW	NE-CD-CG-CB
4	B	800	CCW	NE-CD-CG-CB
4	A	800	CCW	CA-CB-CG-CD
4	B	800	CCW	CA-CB-CG-CD

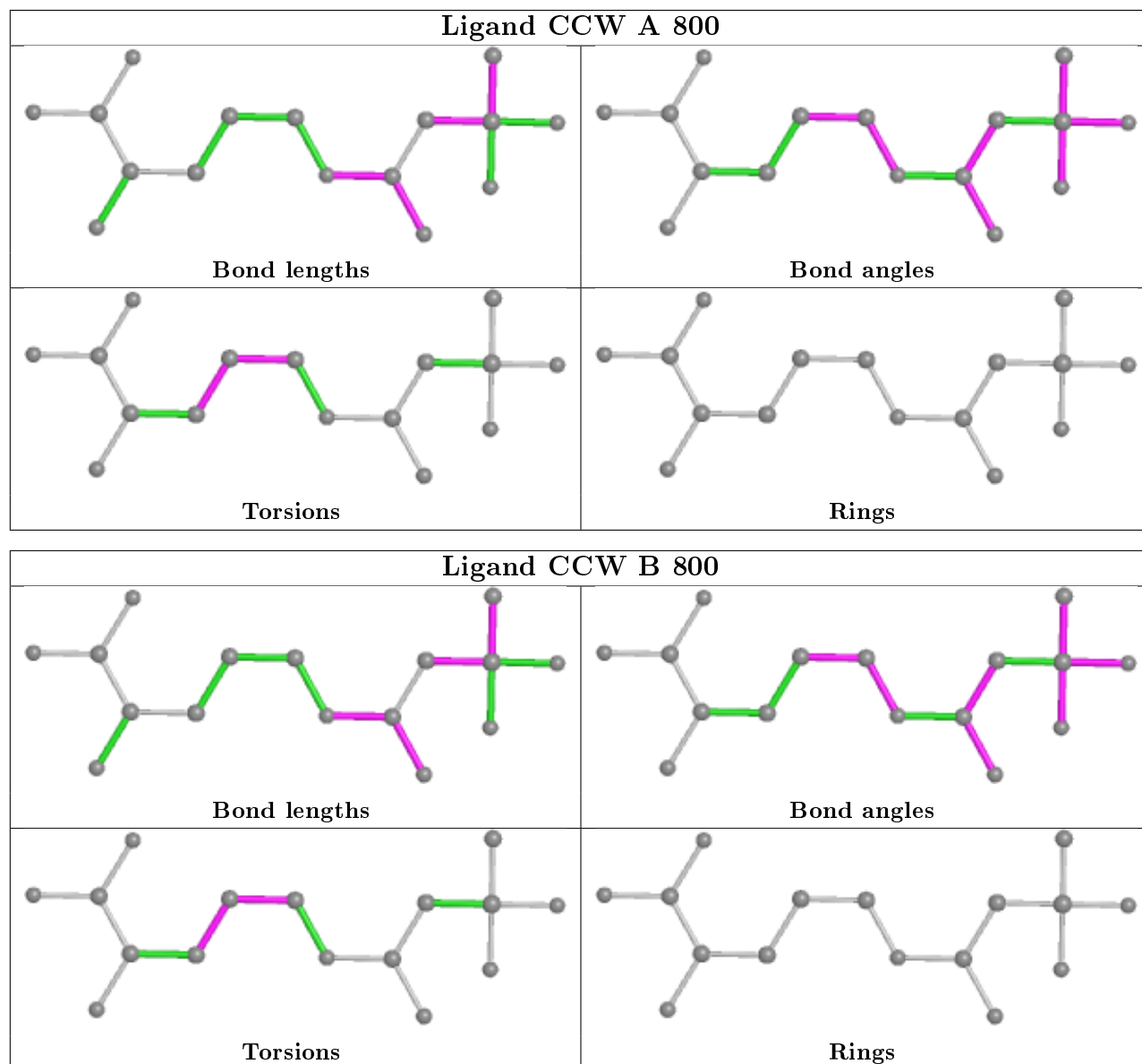
There are no ring outliers.

4 monomers are involved in 16 short contacts:

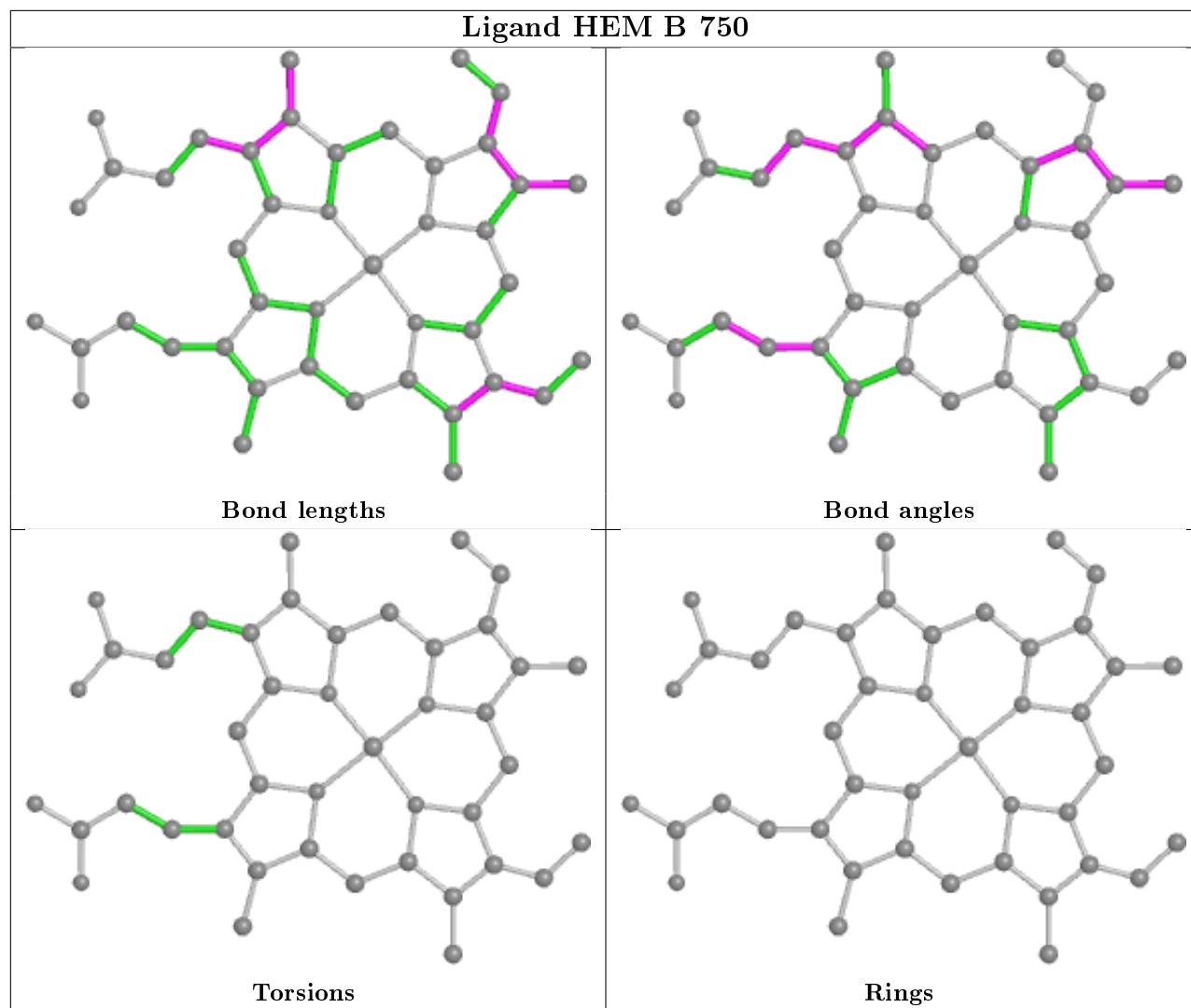
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	CCW	4	0
4	B	800	CCW	5	0
2	B	750	HEM	4	0
2	A	750	HEM	3	0

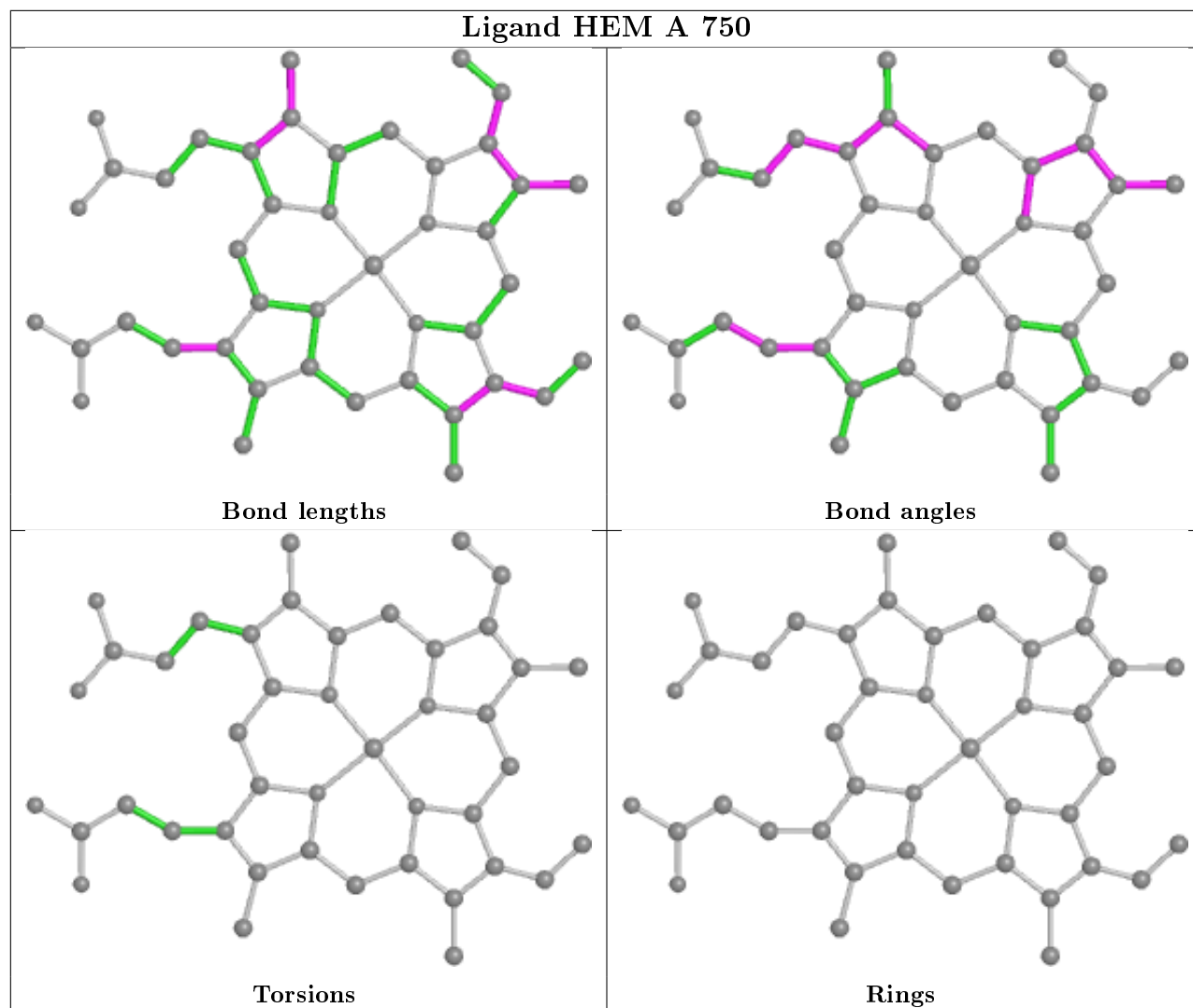
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [\(i\)](#)

### 6.1 Protein, DNA and RNA chains [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

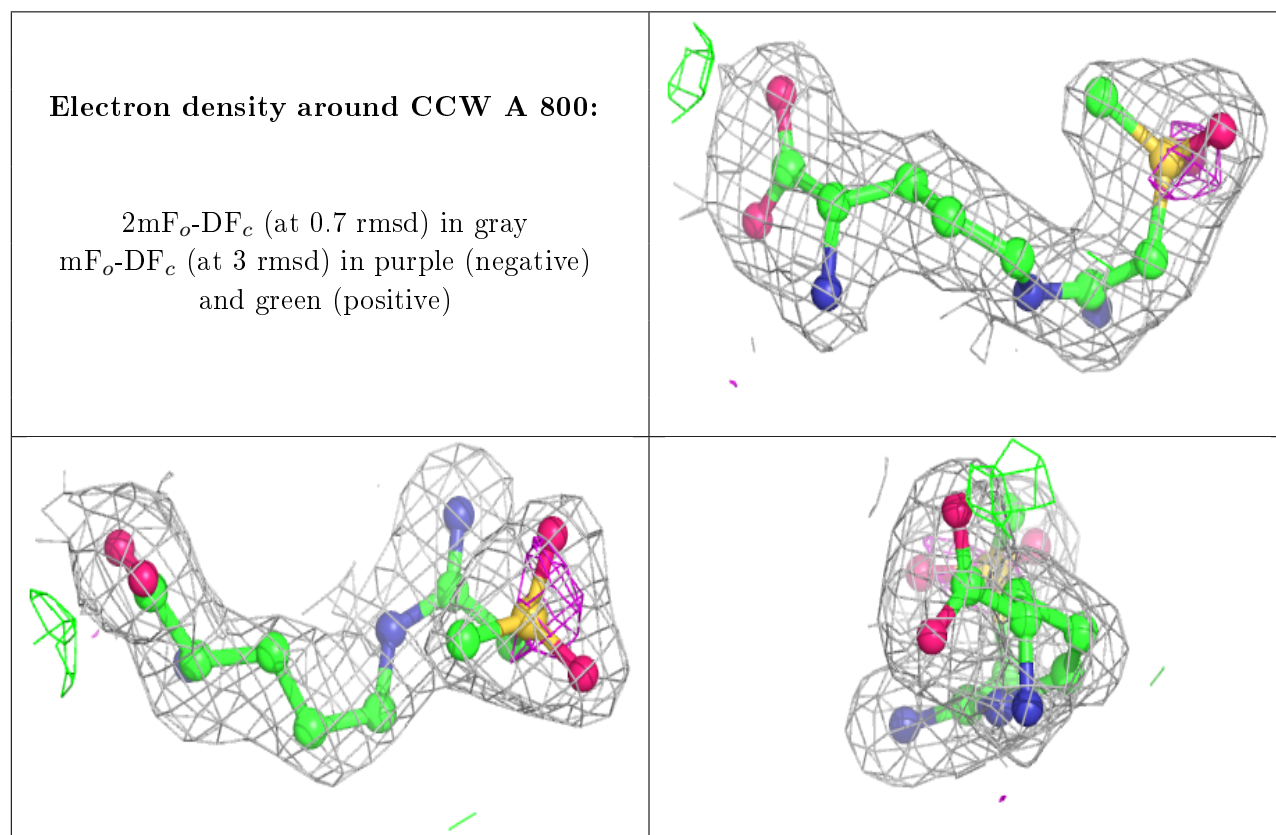
### 6.3 Carbohydrates [\(i\)](#)

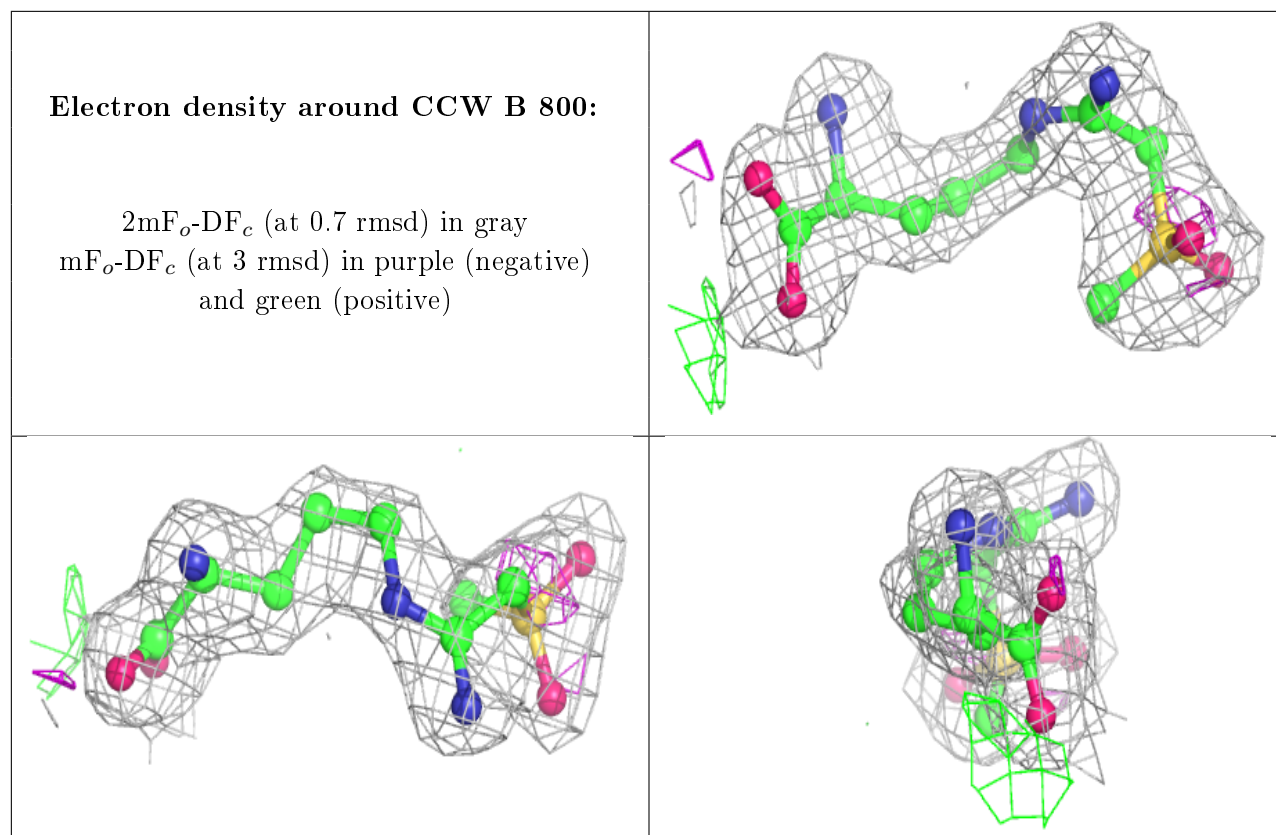
Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

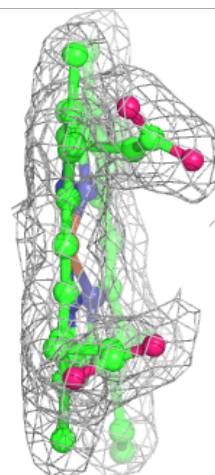
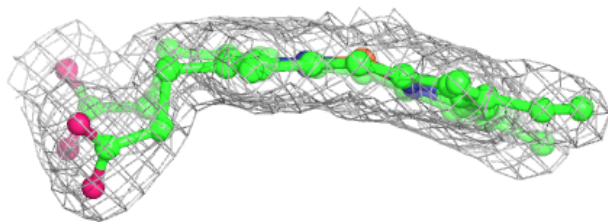
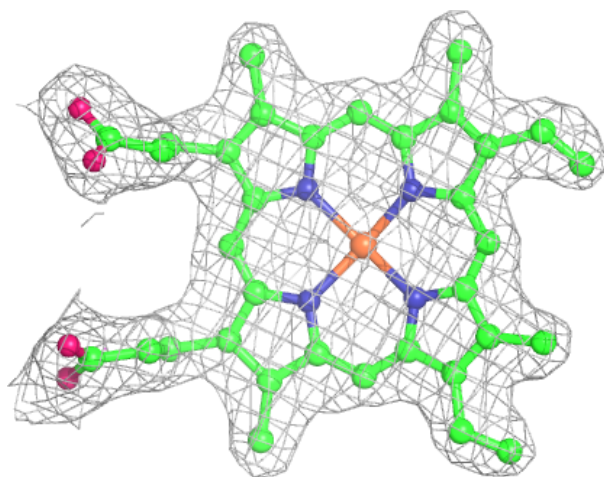
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

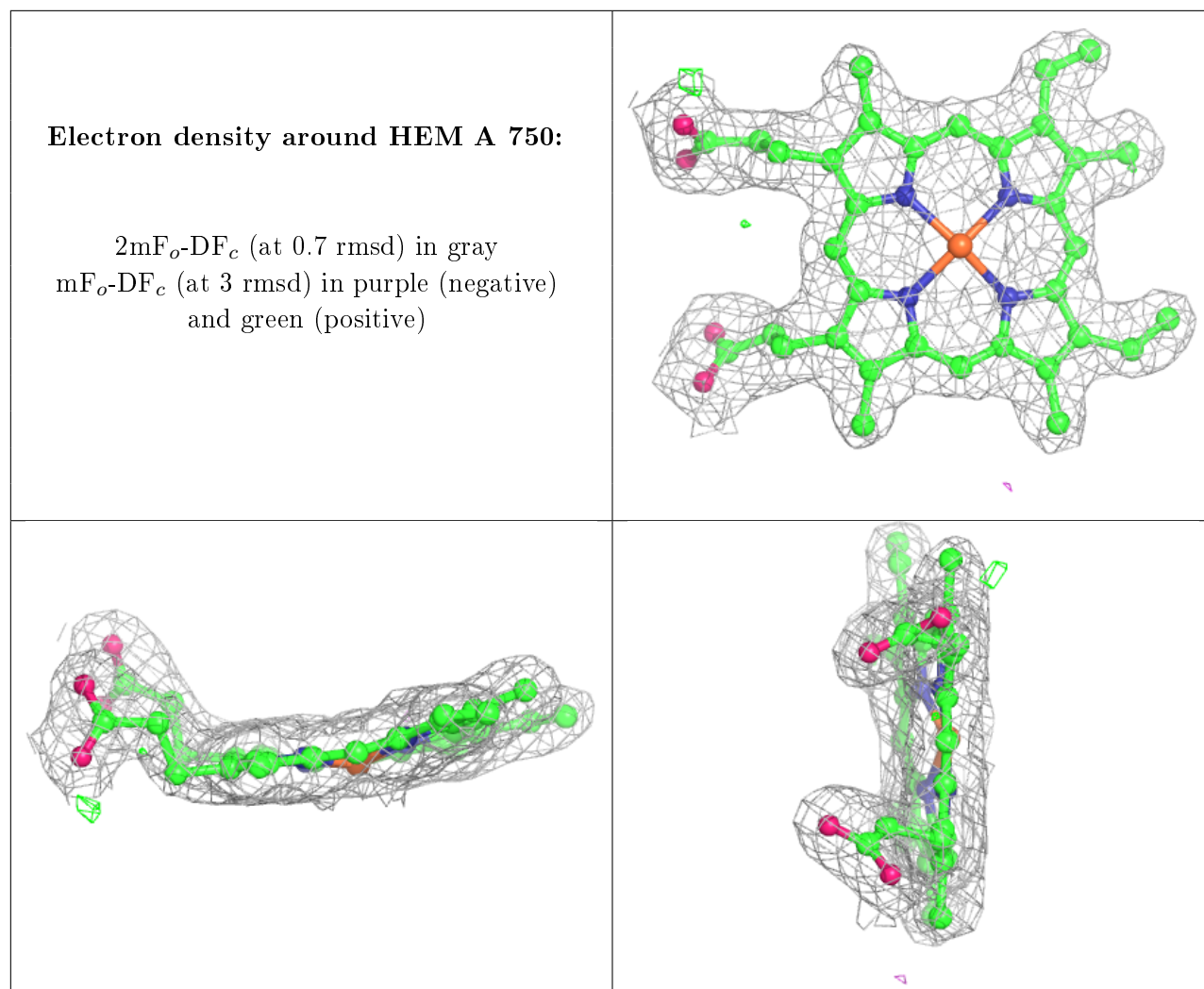




**Electron density around HEM B 750:**

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





## 6.5 Other polymers [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.