



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 12, 2023 – 10:36 am GMT

PDB ID : 4D1N  
Title : Structure of human nNOS heme domain with L-Arg bound  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2014-05-02  
Resolution : 2.03 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

<https://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

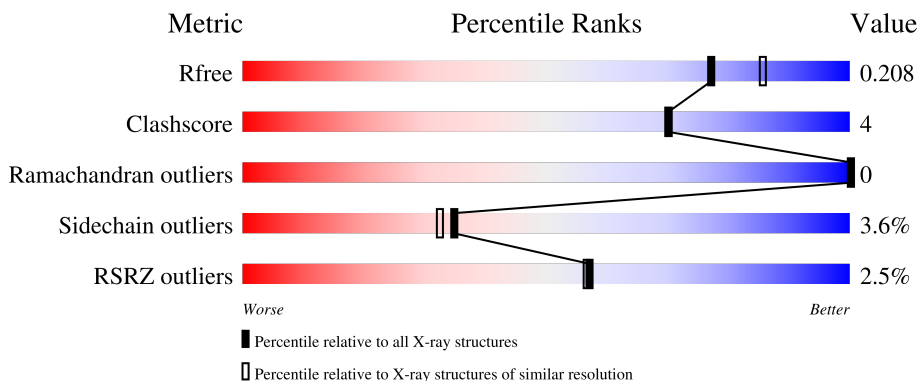
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 of 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	420	 2% 90% 9%
1	B	420	 2% 86% 11%
1	C	420	 % 91% 8%
1	D	420	 4% 87% 10%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14747 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.

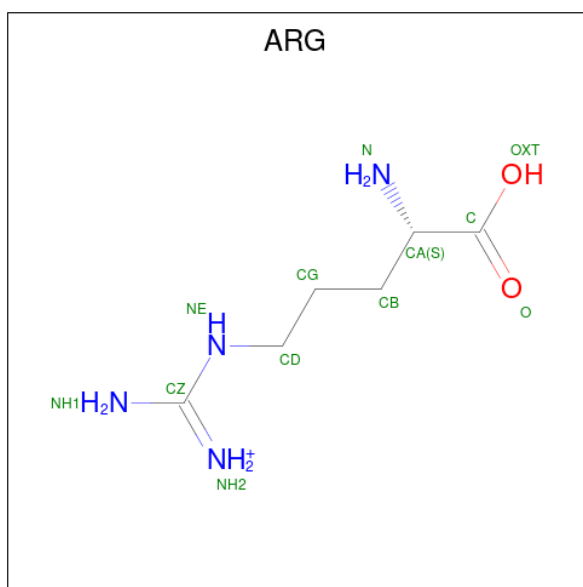
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, BRAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	420	3430	2192	590	626	22	0	1	0
1	B	411	3351	2147	571	611	22	0	1	0
1	C	420	3430	2192	589	627	22	0	1	0
1	D	411	3348	2145	571	610	22	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

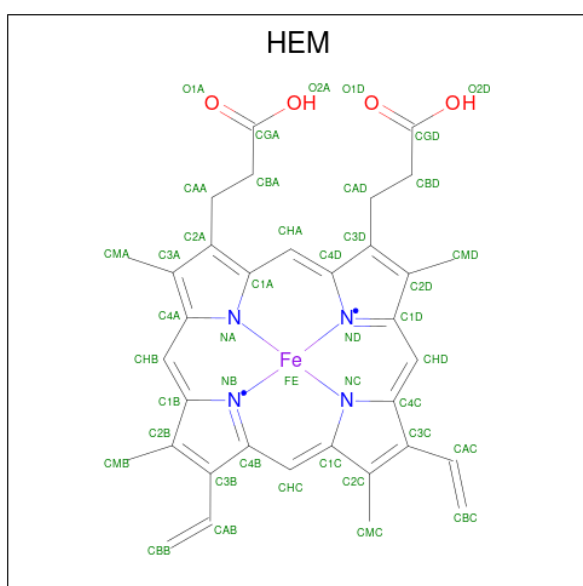
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	engineered mutation	UNP P29475
A	357	ASP	GLY	engineered mutation	UNP P29475
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475
C	354	ALA	ARG	engineered mutation	UNP P29475
C	357	ASP	GLY	engineered mutation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

- Molecule 2 is ARGININE (three-letter code: ARG) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>4</sub>O<sub>2</sub>).



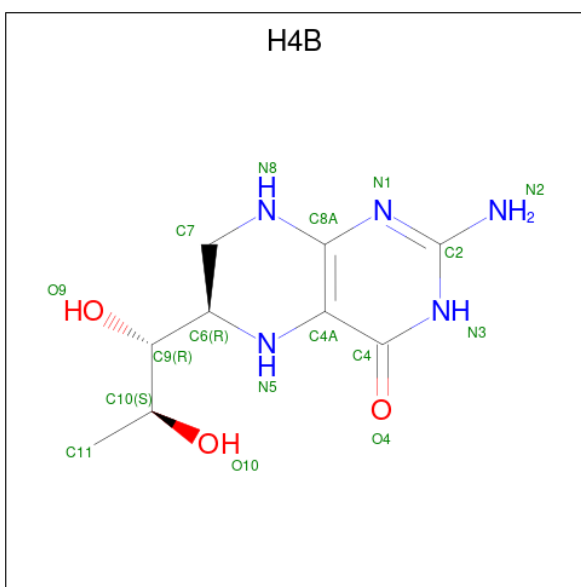
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	4	2		
2	B	1	Total	C	N	O	0	0
			12	6	4	2		
2	C	1	Total	C	N	O	0	0
			12	6	4	2		
2	D	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

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

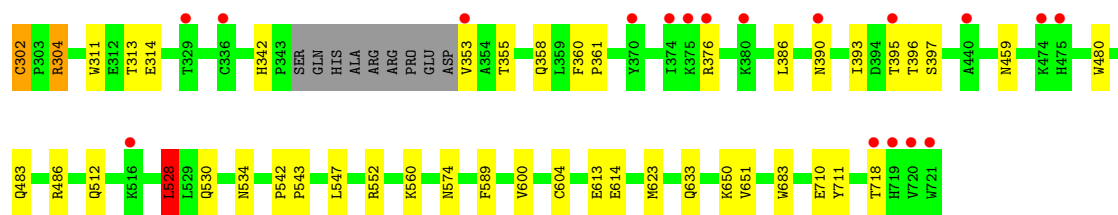
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Zn 1 1	0	0
6	C	1	Total Zn 1 1	0	0

- Molecule 7 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	A	214	Total 214	O 214	0	0
7	B	206	Total 206	O 206	0	0
7	C	265	Total 265	O 265	0	0
7	D	171	Total 171	O 171	0	0







## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.92Å 84.66Å 166.75Å 90.00° 90.94° 90.00°	Depositor
Resolution (Å)	46.60 – 2.03 46.56 – 2.03	Depositor EDS
% Data completeness (in resolution range)	94.5 (46.60-2.03) 94.5 (46.56-2.03)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.03Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.177 , 0.209 0.176 , 0.208	Depositor DCC
$R_{free}$ test set	7549 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.9	Xtrriage
Anisotropy	0.342	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 46.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14747	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2984e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: HEM, H4B, ZN, GOL

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	0.52	0/3532	0.63	0/4794
1	B	0.55	0/3450	0.65	1/4682 (0.0%)
1	C	0.58	0/3532	0.67	1/4794 (0.0%)
1	D	0.56	0/3444	0.67	2/4674 (0.0%)
All	All	0.55	0/13958	0.65	4/18944 (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	B	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	CYS	CA-CB-SG	-5.85	103.48	114.00
1	D	302	CYS	CA-CB-SG	-5.50	104.09	114.00
1	C	494	ASP	CB-CA-C	-5.18	100.04	110.40
1	D	528	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	379	SER	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	3430	0	3332	26	0
1	B	3351	0	3260	29	0
1	C	3430	0	3330	22	0
1	D	3348	0	3255	25	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	43	0	30	0	0
3	B	43	0	30	2	0
3	C	43	0	30	1	0
3	D	43	0	30	2	0
4	A	17	0	15	0	0
4	B	17	0	15	0	0
4	C	17	0	15	1	0
4	D	17	0	15	1	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
5	C	18	0	24	0	0
5	D	12	0	16	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	214	0	0	1	0
7	B	206	0	0	0	0
7	C	265	0	0	5	0
7	D	171	0	0	1	0
All	All	14747	0	13461	99	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.

The worst 5 of 99 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:B:379:SER:HB2	1:B:380:LYS:HB2	1.31	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ARG:HD2	7:C:2167:HOH:O	1.64	0.97
1:D:355:THR:H	1:D:358:GLN:HE21	1.27	0.83
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.64	0.78
1:C:494:ASP:HB3	1:C:496:SER:H	1.52	0.74

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	419/420 (100%)	411 (98%)	8 (2%)	0	100	100
1	B	408/420 (97%)	396 (97%)	12 (3%)	0	100	100
1	C	419/420 (100%)	411 (98%)	8 (2%)	0	100	100
1	D	407/420 (97%)	396 (97%)	11 (3%)	0	100	100
All	All	1653/1680 (98%)	1614 (98%)	39 (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	376/375 (100%)	363 (96%)	13 (4%)	36	34
1	B	368/375 (98%)	356 (97%)	12 (3%)	38	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	376/375 (100%)	362 (96%)	14 (4%)	34	31
1	D	367/375 (98%)	352 (96%)	15 (4%)	30	27
All	All	1487/1500 (99%)	1433 (96%)	54 (4%)	35	32

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	380	LYS
1	C	614	GLU
1	D	560	LYS
1	C	494	ASP
1	C	552	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	532	ASN
1	D	459	ASN
1	C	574	ASN
1	C	702	ASN
1	D	513	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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	GOL	C	880	-	5,5,5	0.30	0	5,5,5	0.25	0
3	HEM	A	750	1	41,50,50	1.25	4 (9%)	45,82,82	1.78	12 (26%)
5	GOL	D	881	-	5,5,5	0.36	0	5,5,5	0.42	0
3	HEM	D	750	1	41,50,50	1.27	4 (9%)	45,82,82	1.79	12 (26%)
2	ARG	A	770	-	10,11,11	0.70	0	11,13,13	1.09	1 (9%)
2	ARG	D	770	-	10,11,11	0.91	0	11,13,13	1.01	0
3	HEM	B	750	1	41,50,50	1.27	3 (7%)	45,82,82	1.77	12 (26%)
5	GOL	D	880	-	5,5,5	0.33	0	5,5,5	0.27	0
2	ARG	B	770	-	10,11,11	0.81	0	11,13,13	0.96	0
5	GOL	B	880	-	5,5,5	0.49	0	5,5,5	0.59	0
5	GOL	A	880	-	5,5,5	0.30	0	5,5,5	0.33	0
4	H4B	B	760	-	16,18,18	1.02	0	11,26,26	2.57	7 (63%)
4	H4B	C	760	-	16,18,18	1.24	2 (12%)	11,26,26	2.45	6 (54%)
4	H4B	A	760	-	16,18,18	1.24	1 (6%)	11,26,26	2.55	7 (63%)
4	H4B	D	760	-	16,18,18	1.12	2 (12%)	11,26,26	2.22	5 (45%)
3	HEM	C	750	1	41,50,50	1.29	4 (9%)	45,82,82	1.80	7 (15%)
5	GOL	C	881	-	5,5,5	0.24	0	5,5,5	0.33	0
5	GOL	C	882	-	5,5,5	0.29	0	5,5,5	0.46	0
2	ARG	C	770	-	10,11,11	0.99	1 (10%)	11,13,13	0.91	0

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	GOL	C	880	-	-	0/4/4/4	-
3	HEM	A	750	1	-	4/12/54/54	-
5	GOL	D	881	-	-	4/4/4/4	-
3	HEM	D	750	1	-	2/12/54/54	-
2	ARG	A	770	-	-	0/11/11/11	-
2	ARG	D	770	-	-	0/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	750	1	-	0/12/54/54	-
5	GOL	D	880	-	-	2/4/4/4	-
2	ARG	B	770	-	-	0/11/11/11	-
5	GOL	B	880	-	-	4/4/4/4	-
5	GOL	A	880	-	-	4/4/4/4	-
4	H4B	B	760	-	-	0/8/17/17	0/2/2/2
4	H4B	C	760	-	-	0/8/17/17	0/2/2/2
4	H4B	A	760	-	-	0/8/17/17	0/2/2/2
4	H4B	D	760	-	-	0/8/17/17	0/2/2/2
3	HEM	C	750	1	-	0/12/54/54	-
5	GOL	C	881	-	-	2/4/4/4	-
5	GOL	C	882	-	-	2/4/4/4	-
2	ARG	C	770	-	-	0/11/11/11	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	750	HEM	C1B-NB	-4.28	1.32	1.40
4	C	760	H4B	C7-C6	3.60	1.55	1.52
3	C	750	HEM	C1B-NB	-3.46	1.34	1.40
3	D	750	HEM	C1B-NB	-3.18	1.34	1.40
4	A	760	H4B	C7-C6	3.06	1.55	1.52

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	760	H4B	C8A-C4A-C4	4.83	118.86	114.57
4	D	760	H4B	C8A-C4A-C4	4.79	118.83	114.57
3	C	750	HEM	C1B-NB-C4B	4.75	109.98	105.07
4	C	760	H4B	C8A-C4A-C4	4.62	118.67	114.57
4	B	760	H4B	C8A-C4A-C4	4.42	118.50	114.57

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	880	GOL	C1-C2-C3-O3
5	B	880	GOL	C1-C2-C3-O3
5	C	882	GOL	C1-C2-C3-O3
5	D	881	GOL	O1-C1-C2-C3

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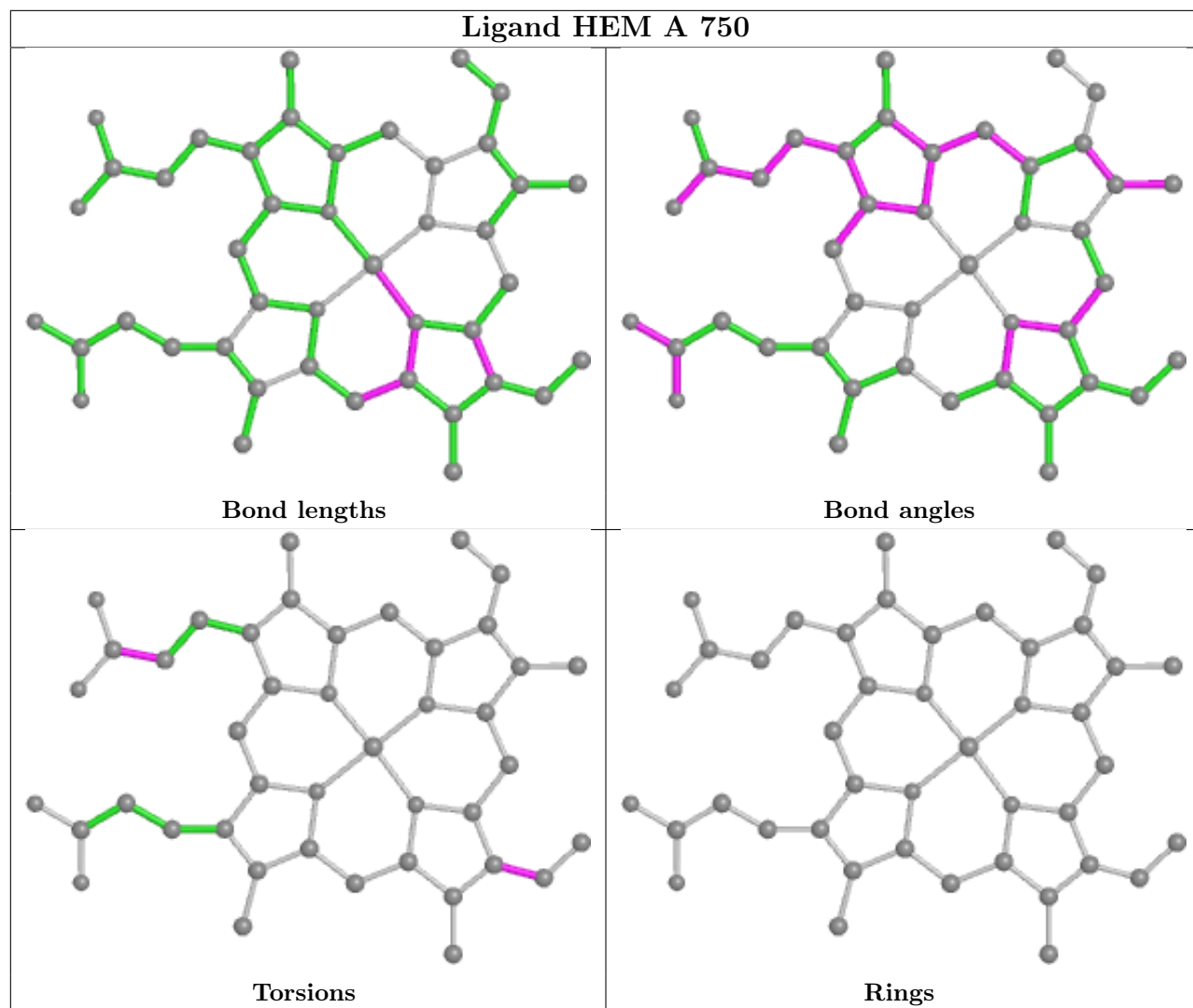
Mol	Chain	Res	Type	Atoms
5	B	880	GOL	O2-C2-C3-O3

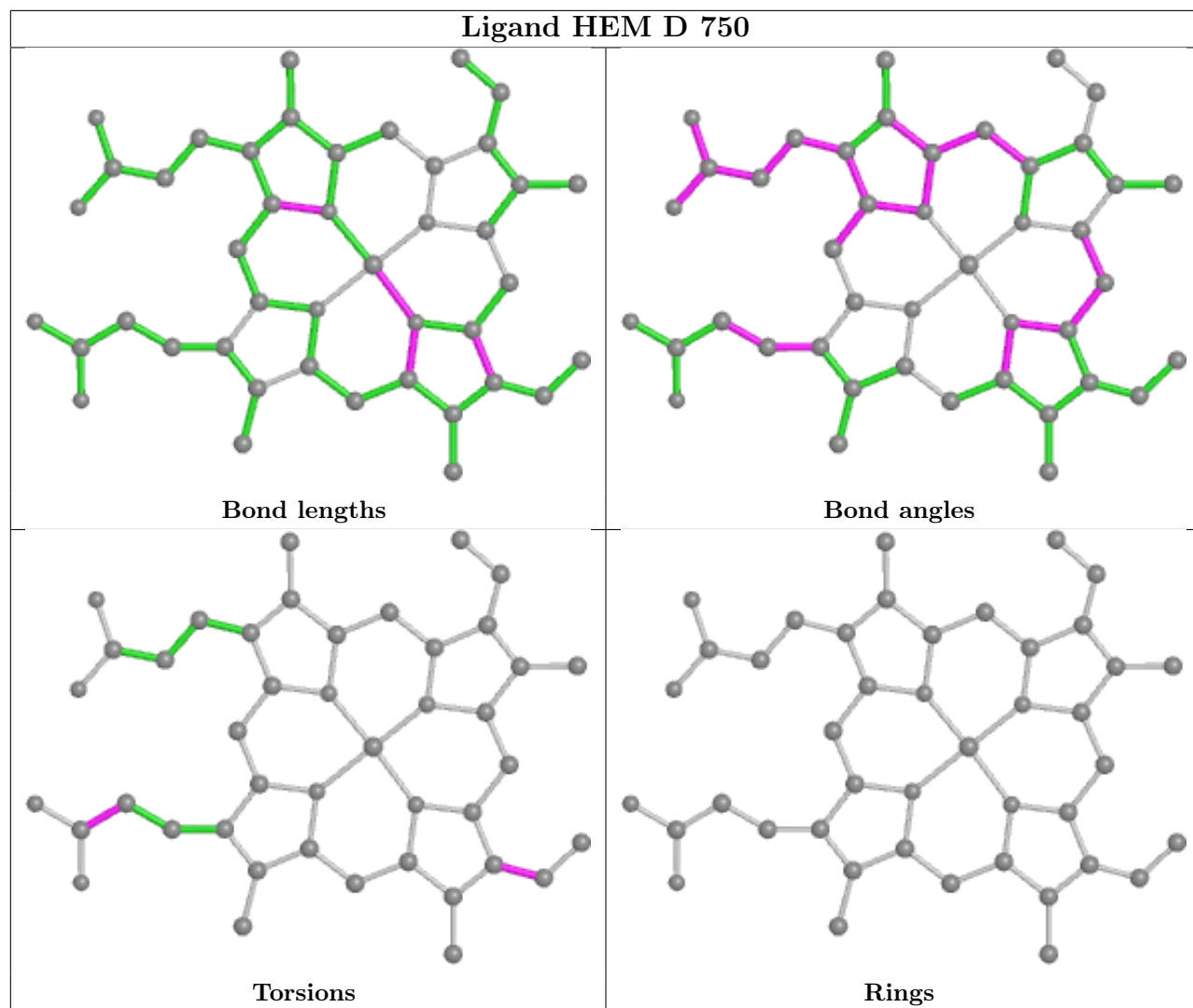
There are no ring outliers.

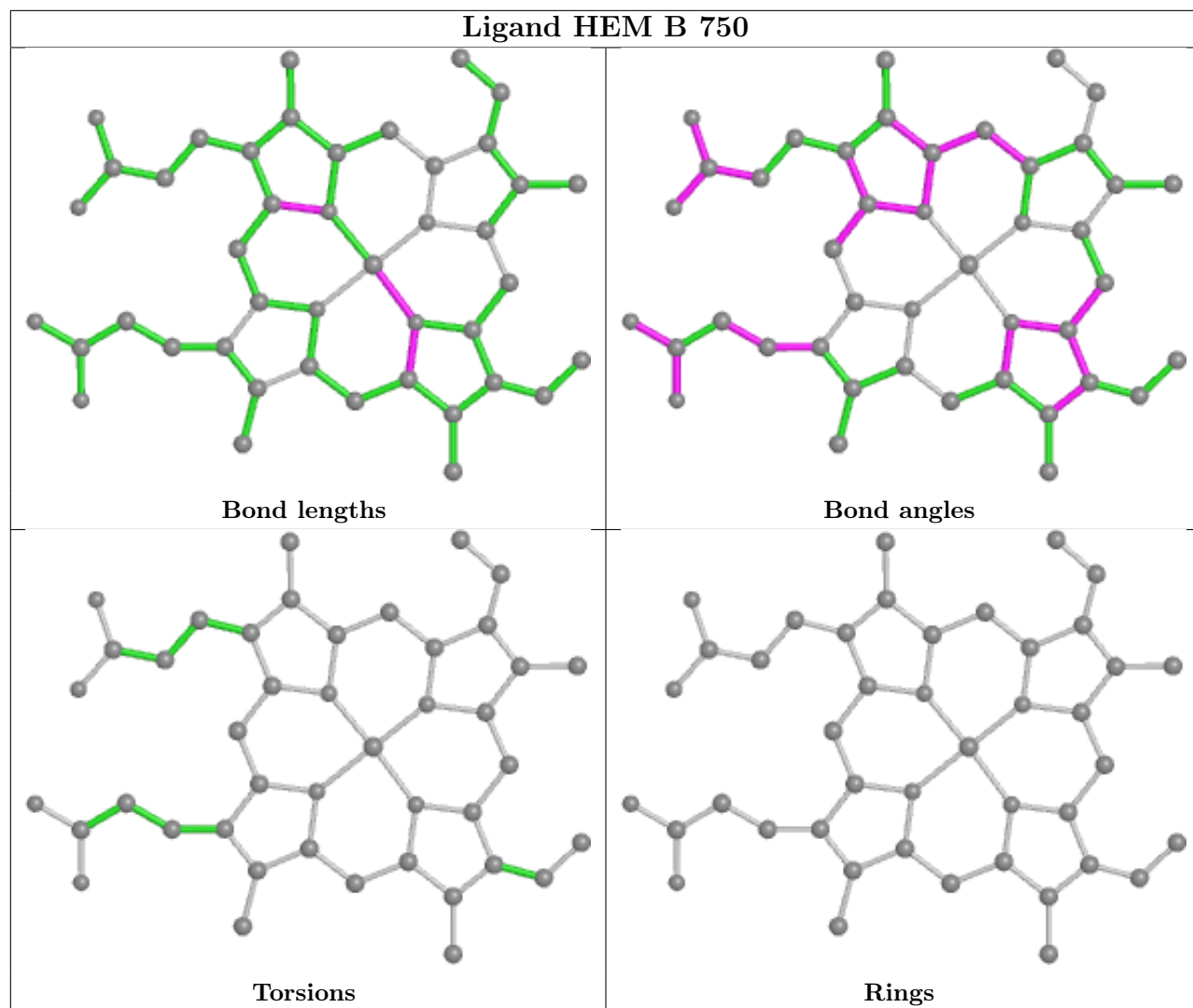
6 monomers are involved in 8 short contacts:

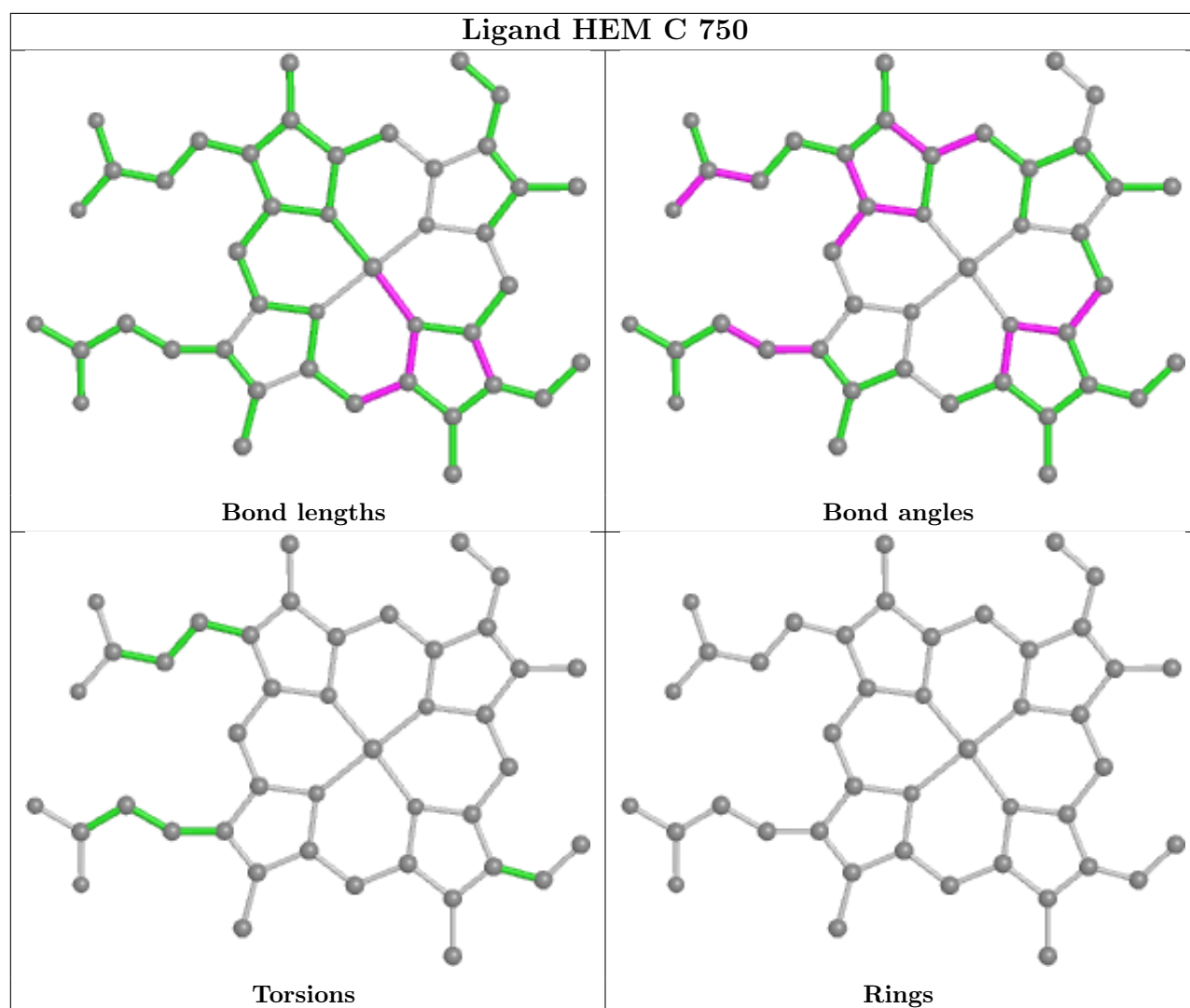
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	750	HEM	2	0
3	B	750	HEM	2	0
5	A	880	GOL	1	0
4	C	760	H4B	1	0
4	D	760	H4B	1	0
3	C	750	HEM	1	0

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.









## 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](#)

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	420/420 (100%)	0.16	9 (2%) 63 63	27, 45, 66, 83	0
1	B	411/420 (97%)	0.14	10 (2%) 59 58	26, 42, 68, 87	0
1	C	420/420 (100%)	0.05	5 (1%) 79 78	24, 39, 61, 78	0
1	D	411/420 (97%)	0.22	18 (4%) 34 33	24, 43, 71, 96	0
All	All	1662/1680 (98%)	0.14	42 (2%) 57 57	24, 42, 67, 96	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	720	VAL	8.3
1	B	720	VAL	7.9
1	D	721	TRP	6.5
1	A	720	VAL	5.4
1	B	721	TRP	4.9

### 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](#)

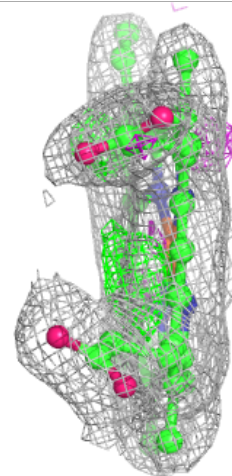
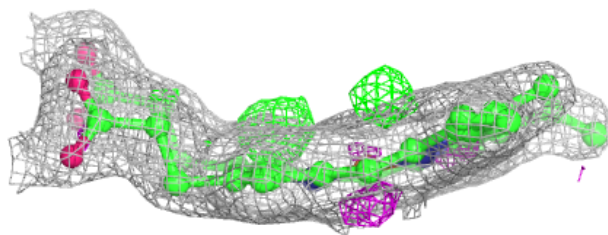
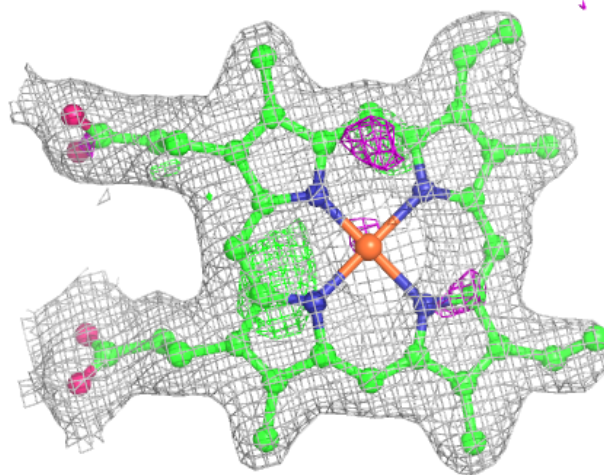
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	D	881	6/6	0.82	0.14	66,74,74,74	0
5	GOL	C	881	6/6	0.84	0.20	67,71,73,73	0
5	GOL	B	880	6/6	0.86	0.17	53,58,61,62	0
5	GOL	D	880	6/6	0.92	0.15	48,55,58,58	0
5	GOL	C	882	6/6	0.93	0.18	43,53,55,57	0
2	ARG	A	770	12/12	0.93	0.14	42,45,48,48	0
2	ARG	D	770	12/12	0.93	0.13	40,43,45,46	0
5	GOL	A	880	6/6	0.94	0.14	51,57,60,63	0
2	ARG	B	770	12/12	0.94	0.11	39,43,48,49	0
3	HEM	A	750	43/43	0.96	0.15	33,37,42,46	0
5	GOL	C	880	6/6	0.96	0.13	43,51,54,54	0
2	ARG	C	770	12/12	0.96	0.16	35,39,42,42	0
3	HEM	D	750	43/43	0.97	0.12	31,34,42,45	0
4	H4B	D	760	17/17	0.97	0.18	27,29,31,32	0
3	HEM	B	750	43/43	0.97	0.13	32,35,39,44	0
3	HEM	C	750	43/43	0.98	0.13	27,32,36,38	0
4	H4B	A	760	17/17	0.98	0.16	28,31,32,32	0
4	H4B	B	760	17/17	0.99	0.17	29,31,32,33	0
4	H4B	C	760	17/17	0.99	0.17	23,26,30,30	0
6	ZN	A	900	1/1	1.00	0.17	28,28,28,28	0
6	ZN	C	900	1/1	1.00	0.14	27,27,27,27	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 HEM A 750:**

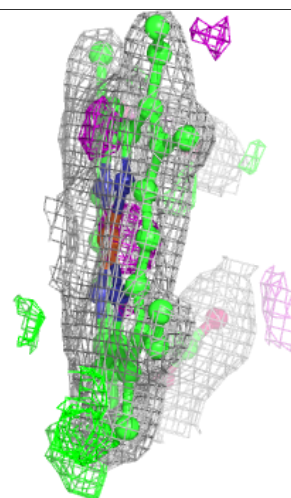
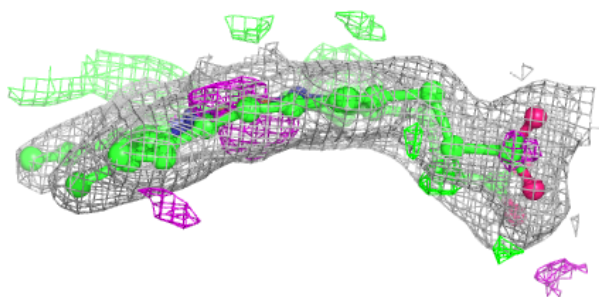
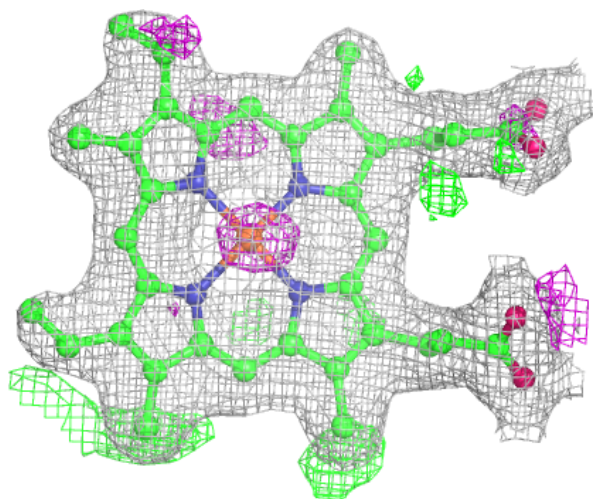
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





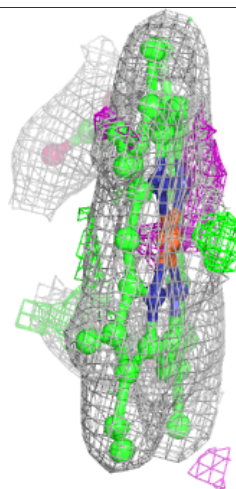
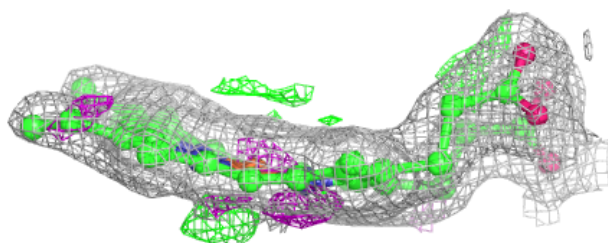
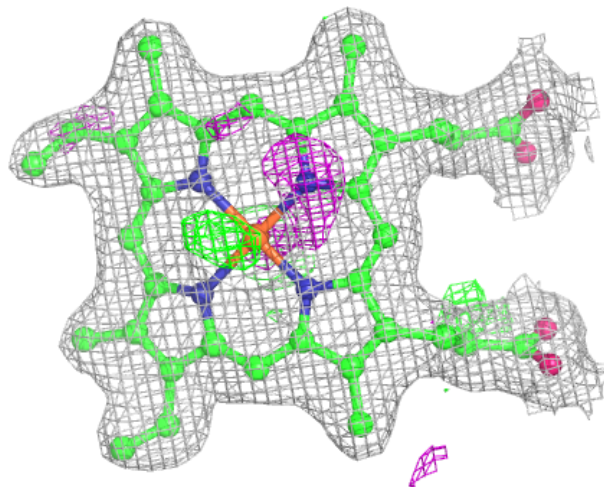
**Electron density around HEM D 750:**

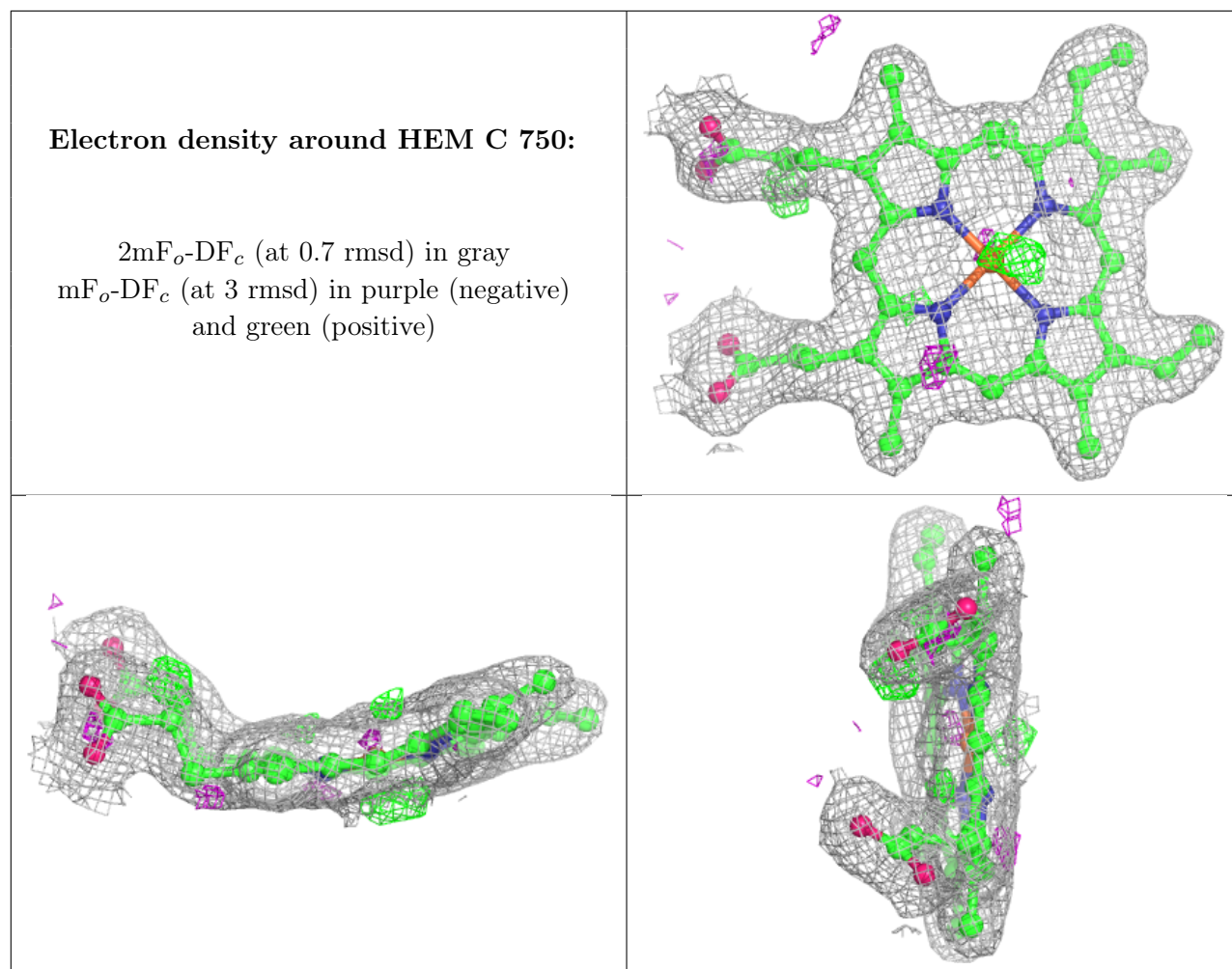
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM B 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](#)

There are no such residues in this entry.