



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2025 – 03:16 PM EDT

PDB ID : 9CW1 / pdb\_00009cw1  
Title : Structure of human neuronal nitric oxide synthase R354A/G357D mutant heme domain bound with 6-(2,3-difluoro-5-(2-(methylamino)ethyl)phenyl)-4-methylpyridin-2-amine dihydrochloride  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2024-07-29  
Resolution : 1.90 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.

The types of validation reports are described at

<http://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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

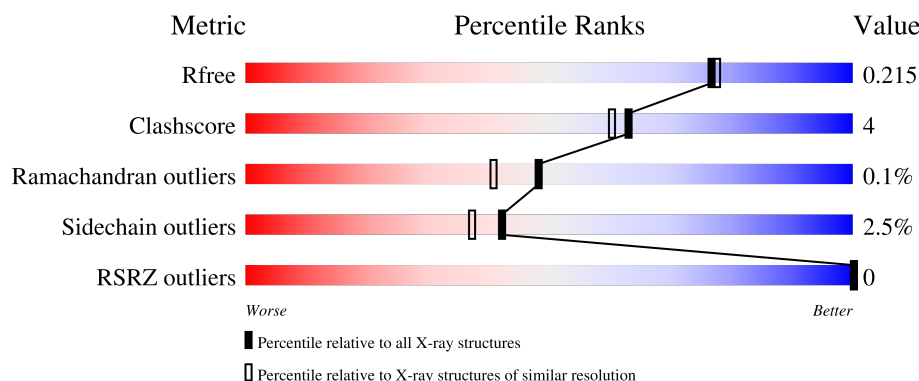
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 1.90 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))
$R_{free}$	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	423	
1	B	423	
1	C	423	
1	D	423	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15249 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.

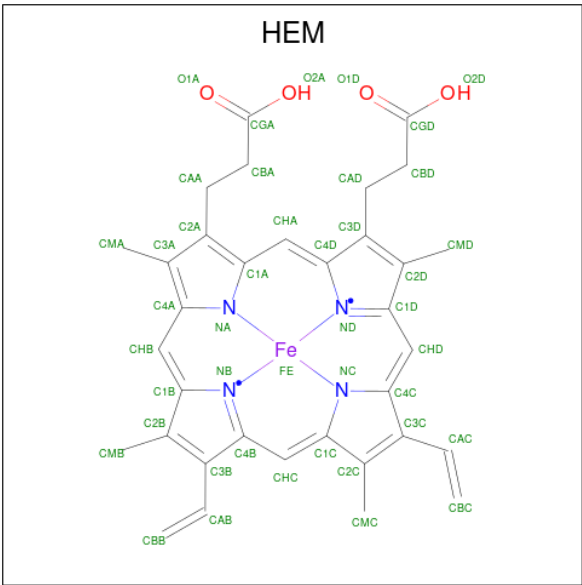
- Molecule 1 is a protein called Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	5	0
			3427	2193	587	625	22			
1	B	414	Total	C	N	O	S	0	2	0
			3379	2165	575	618	21			
1	C	413	Total	C	N	O	S	0	7	0
			3395	2177	577	619	22			
1	D	418	Total	C	N	O	S	0	4	0
			3427	2193	587	626	21			

There are 16 discrepancies between the modelled and reference sequences:

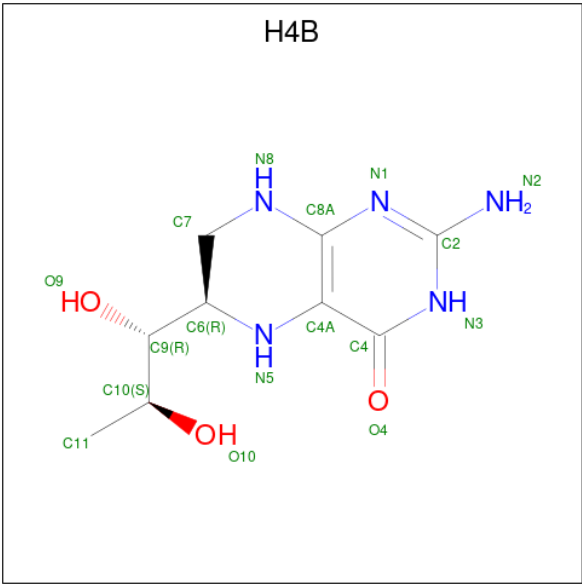
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	engineered mutation	UNP P29475
A	357	ASP	GLY	engineered mutation	UNP P29475
A	723	LEU	-	expression tag	UNP P29475
A	724	VAL	-	expression tag	UNP P29475
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475
B	723	LEU	-	expression tag	UNP P29475
B	724	VAL	-	expression tag	UNP P29475
C	354	ALA	ARG	engineered mutation	UNP P29475
C	357	ASP	GLY	engineered mutation	UNP P29475
C	723	LEU	-	expression tag	UNP P29475
C	724	VAL	-	expression tag	UNP P29475
D	354	ALA	ARG	engineered mutation	UNP P29475
D	357	ASP	GLY	engineered mutation	UNP P29475
D	723	LEU	-	expression tag	UNP P29475
D	724	VAL	-	expression tag	UNP P29475

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



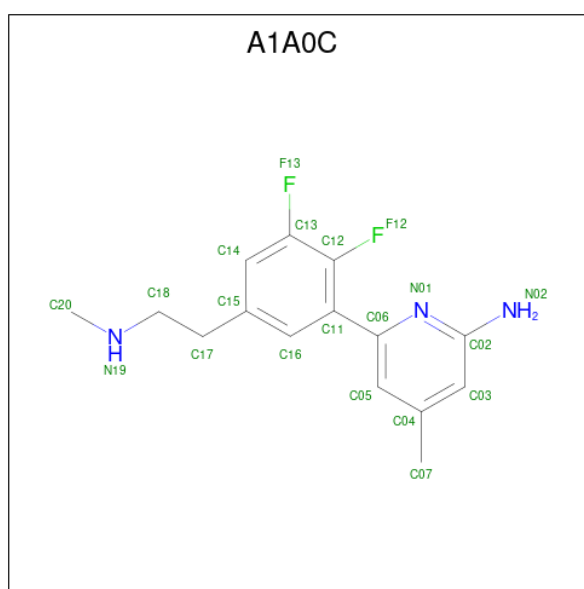
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (CCD ID: H4B) (formula: C<sub>9</sub>H<sub>15</sub>N<sub>5</sub>O<sub>3</sub>).



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		
3	C	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is (6M)-6-{2,3-difluoro-5-[2-(methylamino)ethyl]phenyl}-4-methylpyridin-2-amine (CCD ID: A1A0C) (formula: C<sub>15</sub>H<sub>17</sub>F<sub>2</sub>N<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	N	0	0
			20	15	2	3		
4	B	1	Total	C	F	N	0	0
			20	15	2	3		
4	C	1	Total	C	F	N	0	0
			20	15	2	3		
4	D	1	Total	C	F	N	0	0
			20	15	2	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	322	Total	O	0	0
			322	322		

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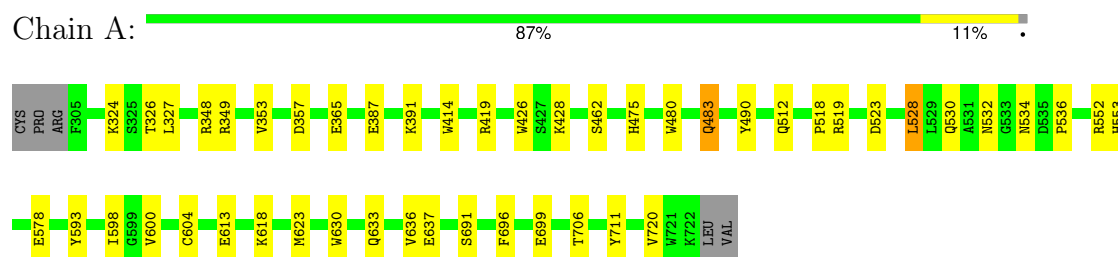
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	320	Total 320	O 320	0	0
7	C	327	Total 327	O 327	0	0
7	D	294	Total 294	O 294	0	0

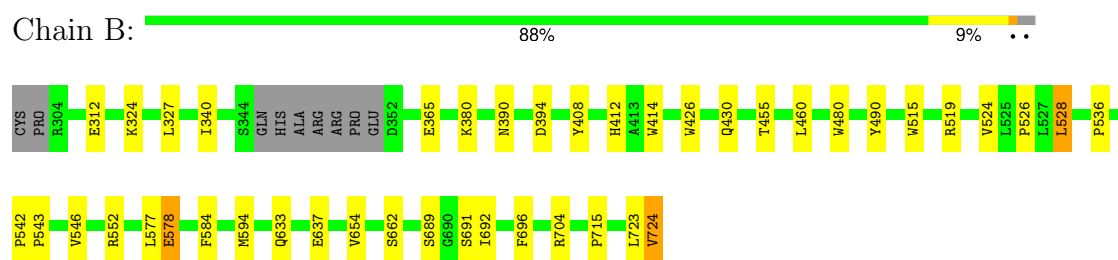
### 3 Residue-property plots

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.

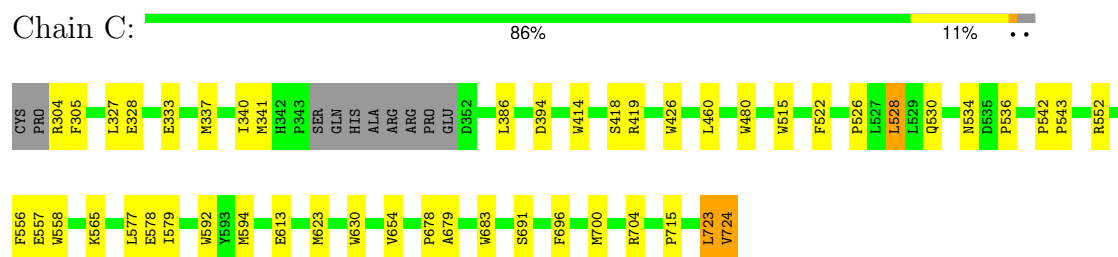
#### • Molecule 1: Nitric oxide synthase, brain



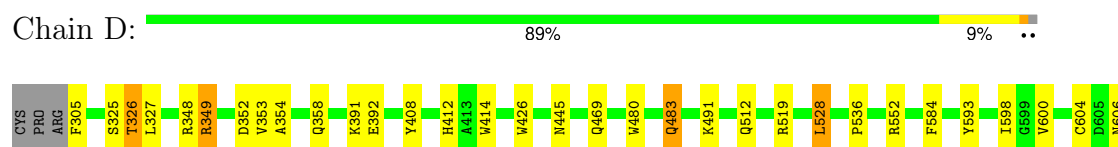
#### • Molecule 1: Nitric oxide synthase, brain



#### • Molecule 1: Nitric oxide synthase, brain



#### • Molecule 1: Nitric oxide synthase, brain





K625	I664	E668	C673	W681	V685	S689	G690	S691	I692	F696	E699	K722	LEU	VAL
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.56Å 116.07Å 163.03Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	49.15 – 1.90 49.15 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.5 (49.15-1.90) 98.9 (49.15-1.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.175 , 0.220 0.170 , 0.215	Depositor DCC
$R_{free}$ test set	7556 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 34.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	15249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: ZN, H4B, HEM, A1A0C, 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	0.37	0/3541	0.53	0/4807
1	B	0.39	0/3480	0.55	0/4721
1	C	0.39	0/3512	0.53	0/4767
1	D	0.37	0/3538	0.52	0/4803
All	All	0.38	0/14071	0.53	0/19098

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	3427	0	3339	26	0
1	B	3379	0	3295	23	0
1	C	3395	0	3320	29	0
1	D	3427	0	3335	24	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	17	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	17	0	15	0	0
3	C	17	0	15	0	0
3	D	17	0	15	0	0
4	A	20	0	0	1	0
4	B	20	0	0	0	0
4	C	20	0	0	1	0
4	D	20	0	0	1	0
5	A	12	0	16	0	0
5	B	6	0	8	0	0
5	C	12	0	16	0	0
5	D	6	0	8	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	322	0	0	5	0
7	B	320	0	0	3	1
7	C	327	0	0	1	0
7	D	294	0	0	5	1
All	All	15249	0	13517	107	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (107) 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:348:ARG:NH1	1:A:365:GLU:OE2	2.15	0.79
1:C:528:LEU:HD22	1:C:536:PRO:HB2	1.71	0.73
1:C:578:GLU:OE2	7:C:901:HOH:O	2.05	0.72
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.72	0.71
1:B:662[B]:SER:OG	7:B:901:HOH:O	2.07	0.71
1:C:327:LEU:HB3	1:C:704:ARG:HD3	1.71	0.71
1:D:528:LEU:HD22	1:D:536:PRO:HB2	1.73	0.70
1:D:664:ILE:O	1:D:668[B]:GLU:HG2	1.92	0.69
1:D:349:ARG:NH1	1:D:352:ASP:O	2.24	0.69
1:A:528:LEU:HD22	1:A:536:PRO:HB2	1.75	0.69
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.75	0.69
1:B:528:LEU:HD22	1:B:536:PRO:HB2	1.75	0.68
1:B:327:LEU:HB2	1:B:704:ARG:HD2	1.77	0.67
2:D:801:HEM:HBB2	2:D:801:HEM:HHC	1.78	0.66
2:B:801:HEM:HMC2	2:B:801:HEM:HBC2	1.78	0.65
2:D:801:HEM:HBC2	2:D:801:HEM:HMC2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:ASN:ND2	7:D:904:HOH:O	2.31	0.63
1:B:723:LEU:HD12	1:B:724:VAL:H	1.63	0.63
1:A:618:LYS:NZ	7:A:906:HOH:O	2.32	0.61
1:D:327:LEU:HD21	1:D:348:ARG:HG3	1.83	0.60
1:A:327:LEU:HD11	1:A:348:ARG:HG2	1.84	0.59
1:B:480:TRP:HB2	1:B:528:LEU:HB3	1.83	0.59
1:C:327:LEU:HG	1:C:328:GLU:H	1.68	0.58
1:C:304:ARG:HG2	1:C:305:PHE:CE1	2.40	0.56
1:A:480:TRP:HB2	1:A:528:LEU:HB3	1.86	0.56
1:C:480:TRP:HB2	1:C:528:LEU:HB3	1.88	0.56
1:C:414:TRP:CE3	1:C:426:TRP:HA	2.42	0.55
2:C:801:HEM:HHC	2:C:801:HEM:HBB2	1.88	0.55
2:A:801:HEM:O1D	4:A:803:A1A0C:N19	2.40	0.54
1:B:414:TRP:CE3	1:B:426:TRP:HA	2.44	0.53
1:D:325:SER:OG	7:D:901:HOH:O	2.15	0.53
1:A:483:GLN:NE2	7:A:901:HOH:O	2.17	0.53
1:C:340:ILE:HD13	1:D:699:GLU:HB3	1.91	0.51
1:A:699:GLU:HB3	1:B:340:ILE:HD13	1.91	0.51
2:D:801:HEM:O1D	4:D:803:A1A0C:N19	2.43	0.51
1:C:327:LEU:HG	1:C:328:GLU:N	2.26	0.51
1:B:480:TRP:CE2	1:B:715:PRO:HB2	2.45	0.51
1:C:522:PHE:HB2	1:C:565:LYS:HE3	1.93	0.50
1:A:348:ARG:NH1	1:A:706:THR:HG21	2.28	0.49
1:B:578:GLU:OE2	7:B:902:HOH:O	2.18	0.49
1:D:593:TYR:CD1	1:D:598:ILE:HD11	2.48	0.48
1:C:480:TRP:CE2	1:C:715:PRO:HB2	2.48	0.48
1:A:419:ARG:NH1	1:A:711:TYR:OH	2.47	0.48
1:A:365:GLU:OE2	7:A:902:HOH:O	2.20	0.47
1:B:430:GLN:OE1	7:B:903:HOH:O	2.20	0.47
1:A:518:PRO:HG2	1:A:523:ASP:CG	2.34	0.47
1:B:691:SER:HA	1:B:696:PHE:CG	2.49	0.47
1:D:349:ARG:NH2	7:D:915:HOH:O	2.48	0.47
1:A:691:SER:HA	1:A:696:PHE:CG	2.51	0.46
1:C:304:ARG:HG2	1:C:305:PHE:CD1	2.50	0.46
1:D:445:ASN:ND2	7:D:919:HOH:O	2.49	0.46
1:C:515:TRP:CE2	1:C:526:PRO:HD3	2.51	0.45
1:A:636:VAL:HG11	1:B:633:GLN:HG3	1.99	0.45
1:B:594:MET:HA	1:B:654:VAL:O	2.17	0.45
2:B:801:HEM:HBB2	2:B:801:HEM:HHC	1.97	0.45
1:A:414:TRP:CE3	1:A:426:TRP:HA	2.52	0.45
1:D:414:TRP:CE3	1:D:426:TRP:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:TRP:HB2	1:D:528:LEU:HB3	1.97	0.45
1:A:633:GLN:NE2	1:B:637:GLU:OE2	2.50	0.44
1:B:689:SER:HB3	1:B:692:ILE:HG12	1.99	0.44
1:C:556:PHE:HB3	1:C:558:TRP:CE2	2.52	0.44
1:D:408:TYR:CE1	1:D:412:HIS:CE1	3.05	0.44
1:A:387:GLU:O	1:A:391:LYS:HG2	2.18	0.44
1:A:490:TYR:CE1	1:A:519:ARG:HA	2.52	0.44
1:A:530:GLN:HG3	1:A:534:ASN:O	2.18	0.44
1:C:723:LEU:HD23	1:C:724:VAL:H	1.83	0.44
7:A:1094:HOH:O	1:B:312:GLU:HG3	2.17	0.43
1:C:419:ARG:HD3	1:C:683:TRP:CD2	2.53	0.43
1:D:681:TRP:CE2	1:D:685:VAL:HG21	2.53	0.43
1:D:691:SER:HA	1:D:696:PHE:CG	2.54	0.43
1:C:594:MET:HA	1:C:654:VAL:O	2.18	0.43
1:D:469:GLN:HB3	1:D:584:PHE:CE2	2.53	0.43
1:A:553:HIS:NE2	1:A:637:GLU:OE1	2.46	0.43
1:B:542:PRO:HA	1:B:543:PRO:HD3	1.93	0.43
1:C:337:MET:HB3	1:C:340:ILE:HG13	2.01	0.43
1:A:578:GLU:OE2	7:A:903:HOH:O	2.21	0.43
1:A:593:TYR:CD1	1:A:598:ILE:HD11	2.54	0.43
1:A:357:ASP:HB3	1:D:673:CYS:O	2.19	0.42
1:C:691:SER:HA	1:C:696:PHE:CG	2.53	0.42
1:B:577:LEU:HB3	1:B:584:PHE:HB2	2.02	0.42
1:C:577:LEU:HD21	1:C:579:ILE:HD11	2.00	0.42
1:C:460:LEU:HD12	1:C:592:TRP:HB3	2.01	0.42
1:C:530:GLN:HG3	1:C:534:ASN:O	2.20	0.42
1:D:689:SER:HB3	1:D:692:ILE:HD11	2.02	0.42
1:A:600:VAL:O	1:A:604:CYS:HB2	2.20	0.42
1:C:542:PRO:HA	1:C:543:PRO:HD3	1.93	0.42
1:D:391:LYS:HG3	1:D:392:GLU:N	2.34	0.42
1:D:354:ALA:HB1	1:D:358:GLN:HB2	2.00	0.42
1:D:681:TRP:CZ2	1:D:685:VAL:HG21	2.54	0.42
1:A:475:HIS:HB3	1:A:532:ASN:OD1	2.19	0.42
1:B:408:TYR:CE1	1:B:412:HIS:CE1	3.08	0.42
1:C:623:MET:HA	1:C:630:TRP:CD1	2.55	0.42
1:C:723:LEU:HD23	1:C:724:VAL:N	2.35	0.41
1:C:341:MET:HE2	1:C:341:MET:HB2	1.93	0.41
1:C:679:ALA:HB3	1:C:700:MET:HB3	2.00	0.41
1:B:490:TYR:CE1	1:B:519:ARG:HA	2.56	0.41
2:C:801:HEM:O1D	4:C:803:A1A0C:N19	2.53	0.41
1:D:326:THR:HG21	1:D:348:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LYS:O	1:A:462[A]:SER:OG	2.39	0.41
1:A:623:MET:HA	1:A:630:TRP:CD1	2.56	0.41
1:D:483:GLN:NE2	7:D:903:HOH:O	2.24	0.41
1:B:515:TRP:CE2	1:B:526:PRO:HD3	2.56	0.40
1:C:613:GLU:HG3	1:C:623:MET:HE3	2.03	0.40
1:D:600:VAL:O	1:D:604:CYS:HB2	2.22	0.40
1:B:455:THR:HA	1:B:460:LEU:HD22	2.01	0.40
1:B:524:VAL:HG21	1:B:546:VAL:HG11	2.03	0.40
1:C:418[B]:SER:OG	1:C:678:PRO:HB2	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:929:HOH:O	7:D:919:HOH:O[2_555]	2.13	0.07

## 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	421/423 (100%)	413 (98%)	7 (2%)	1 (0%)	44	36
1	B	412/423 (97%)	405 (98%)	7 (2%)	0	100	100
1	C	416/423 (98%)	407 (98%)	9 (2%)	0	100	100
1	D	420/423 (99%)	411 (98%)	9 (2%)	0	100	100
All	All	1669/1692 (99%)	1636 (98%)	32 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	353	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/378 (100%)	369 (98%)	9 (2%)	44	39
1	B	372/378 (98%)	363 (98%)	9 (2%)	44	39
1	C	376/378 (100%)	368 (98%)	8 (2%)	48	45
1	D	377/378 (100%)	366 (97%)	11 (3%)	37	31
All	All	1503/1512 (99%)	1466 (98%)	37 (2%)	42	37

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	LYS
1	A	326	THR
1	A	349	ARG
1	A	483	GLN
1	A	512	GLN
1	A	528	LEU
1	A	552	ARG
1	A	613	GLU
1	A	720	VAL
1	B	324	LYS
1	B	365	GLU
1	B	380	LYS
1	B	390	ASN
1	B	394	ASP
1	B	528	LEU
1	B	552	ARG
1	B	578	GLU
1	B	724	VAL
1	C	333	GLU
1	C	386	LEU
1	C	394	ASP
1	C	528	LEU
1	C	552	ARG
1	C	557	GLU

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Mol	Chain	Res	Type
1	C	723	LEU
1	C	724	VAL
1	D	305	PHE
1	D	326	THR
1	D	349	ARG
1	D	353	VAL
1	D	483	GLN
1	D	491	LYS
1	D	512	GLN
1	D	519	ARG
1	D	528	LEU
1	D	552	ARG
1	D	625	LYS

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

Mol	Chain	Res	Type
1	D	445	ASN
1	D	633	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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
4	A1A0C	A	803	-	21,21,21	0.41	0	28,29,29	1.66	4 (14%)
3	H4B	A	802	-	16,18,18	0.72	0	14,26,26	2.44	6 (42%)
3	H4B	C	802	-	16,18,18	0.79	0	14,26,26	2.44	7 (50%)
5	GOL	B	804	-	5,5,5	0.34	0	5,5,5	0.36	0
5	GOL	C	804	-	5,5,5	0.38	0	5,5,5	0.45	0
2	HEM	B	801	1	42,50,50	1.43	5 (11%)	46,82,82	1.62	5 (10%)
4	A1A0C	D	803	-	21,21,21	0.41	0	28,29,29	2.09	6 (21%)
5	GOL	C	805	-	5,5,5	0.38	0	5,5,5	0.19	0
4	A1A0C	C	803	-	21,21,21	0.39	0	28,29,29	2.03	7 (25%)
5	GOL	A	804	-	5,5,5	0.26	0	5,5,5	0.62	0
2	HEM	A	801	1	42,50,50	1.45	4 (9%)	46,82,82	1.77	9 (19%)
3	H4B	D	802	-	16,18,18	0.77	0	14,26,26	2.31	6 (42%)
2	HEM	C	801	1	42,50,50	1.47	4 (9%)	46,82,82	1.68	7 (15%)
5	GOL	A	806	-	5,5,5	0.42	0	5,5,5	0.07	0
5	GOL	D	804	-	5,5,5	0.34	0	5,5,5	0.43	0
4	A1A0C	B	803	-	21,21,21	0.59	0	28,29,29	2.06	7 (25%)
3	H4B	B	802	-	16,18,18	0.73	0	14,26,26	2.26	4 (28%)
2	HEM	D	801	1	42,50,50	1.44	4 (9%)	46,82,82	1.77	10 (21%)

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
4	A1A0C	A	803	-	-	3/8/8/8	0/2/2/2
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2
3	H4B	C	802	-	-	0/8/17/17	0/2/2/2
5	GOL	B	804	-	-	2/4/4/4	-
5	GOL	C	804	-	-	1/4/4/4	-
2	HEM	B	801	1	-	0/12/54/54	-
4	A1A0C	D	803	-	-	2/8/8/8	0/2/2/2
5	GOL	C	805	-	-	0/4/4/4	-
4	A1A0C	C	803	-	-	2/8/8/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	804	-	-	0/4/4/4	-
2	HEM	A	801	1	-	1/12/54/54	-
3	H4B	D	802	-	-	0/8/17/17	0/2/2/2
2	HEM	C	801	1	-	1/12/54/54	-
5	GOL	A	806	-	-	4/4/4/4	-
5	GOL	D	804	-	-	4/4/4/4	-
4	A1A0C	B	803	-	-	1/8/8/8	0/2/2/2
3	H4B	B	802	-	-	0/8/17/17	0/2/2/2
2	HEM	D	801	1	-	1/12/54/54	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	HEM	C3C-C2C	-4.33	1.34	1.40
2	A	801	HEM	C3C-C2C	-4.01	1.34	1.40
2	B	801	HEM	C3C-C2C	-3.63	1.35	1.40
2	D	801	HEM	C3C-C2C	-3.62	1.35	1.40
2	D	801	HEM	C3C-CAC	3.42	1.55	1.47
2	B	801	HEM	CAB-C3B	3.20	1.55	1.47
2	B	801	HEM	C3C-CAC	3.10	1.54	1.47
2	C	801	HEM	C3C-C4C	3.09	1.45	1.41
2	A	801	HEM	CAB-C3B	3.06	1.55	1.47
2	C	801	HEM	C3C-CAC	3.01	1.54	1.47
2	A	801	HEM	C3C-CAC	3.00	1.54	1.47
2	C	801	HEM	CAB-C3B	2.99	1.55	1.47
2	D	801	HEM	CAB-C3B	2.97	1.55	1.47
2	B	801	HEM	C3C-C4C	2.75	1.45	1.41
2	A	801	HEM	C3C-C4C	2.33	1.44	1.41
2	D	801	HEM	C3C-C4C	2.19	1.44	1.41
2	B	801	HEM	CMB-C2B	2.04	1.54	1.50

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	803	A1A0C	C06-C11-C12	-7.27	115.57	124.24
4	B	803	A1A0C	C06-C11-C12	-7.18	115.67	124.24
4	D	803	A1A0C	C06-C11-C12	-7.09	115.77	124.24
2	C	801	HEM	CBA-CAA-C2A	-6.26	102.02	112.54
2	A	801	HEM	CBA-CAA-C2A	-6.23	102.07	112.54
4	A	803	A1A0C	C06-C11-C12	-6.01	117.07	124.24
2	D	801	HEM	CBA-CAA-C2A	-5.87	102.68	112.54
2	B	801	HEM	CBA-CAA-C2A	-5.83	102.73	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	H4B	C8A-C4A-C4	5.13	119.16	114.50
3	D	802	H4B	C8A-C4A-C4	5.06	119.10	114.50
3	B	802	H4B	C8A-C4A-C4	5.05	119.09	114.50
4	D	803	A1A0C	C06-N01-C02	4.82	121.51	118.52
3	A	802	H4B	C8A-C4A-C4	4.59	118.68	114.50
2	D	801	HEM	C4B-CHC-C1C	4.50	128.49	122.56
2	A	801	HEM	C4B-CHC-C1C	4.26	128.18	122.56
2	B	801	HEM	C4B-CHC-C1C	4.26	128.18	122.56
3	A	802	H4B	C2-N3-C4	3.87	121.34	115.96
2	C	801	HEM	C4B-CHC-C1C	3.85	127.64	122.56
4	B	803	A1A0C	C16-C11-C12	3.70	121.37	117.44
3	D	802	H4B	C2-N3-C4	3.57	120.93	115.96
3	C	802	H4B	C2-N3-C4	3.57	120.93	115.96
3	A	802	H4B	N1-C2-N3	-3.50	120.12	125.48
4	C	803	A1A0C	C16-C11-C12	3.45	121.11	117.44
3	C	802	H4B	N1-C2-N3	-3.42	120.24	125.48
3	D	802	H4B	N1-C2-N3	-3.21	120.56	125.48
3	B	802	H4B	N1-C2-N3	-3.19	120.60	125.48
3	B	802	H4B	C2-N3-C4	3.17	120.37	115.96
3	C	802	H4B	C11-C10-C9	-2.93	108.52	112.11
4	B	803	A1A0C	C06-N01-C02	2.88	120.31	118.52
2	D	801	HEM	CMA-C3A-C4A	-2.86	124.27	128.46
4	C	803	A1A0C	C06-N01-C02	2.81	120.27	118.52
3	A	802	H4B	C11-C10-C9	-2.80	108.69	112.11
3	A	802	H4B	N2-C2-N1	2.75	121.34	117.22
4	B	803	A1A0C	C05-C06-C11	-2.74	116.79	121.98
4	A	803	A1A0C	C06-N01-C02	2.71	120.20	118.52
4	D	803	A1A0C	C16-C11-C12	2.71	120.32	117.44
3	D	802	H4B	N2-C2-N1	2.65	121.20	117.22
3	B	802	H4B	C2-N1-C8A	2.64	120.87	114.59
3	C	802	H4B	C2-N1-C8A	2.57	120.69	114.59
4	C	803	A1A0C	C05-C06-C11	-2.55	117.14	121.98
4	B	803	A1A0C	F13-C13-C14	2.52	123.67	118.64
3	A	802	H4B	C2-N1-C8A	2.46	120.43	114.59
4	A	803	A1A0C	C16-C11-C12	2.38	119.97	117.44
2	B	801	HEM	CMC-C2C-C3C	2.37	129.42	124.68
2	D	801	HEM	C3B-C4B-NB	-2.37	107.77	109.47
2	C	801	HEM	C3B-C2B-C1B	2.36	108.18	106.41
2	A	801	HEM	CMA-C3A-C4A	-2.35	125.01	128.46
4	C	803	A1A0C	F13-C13-C14	2.34	123.32	118.64
2	C	801	HEM	CMA-C3A-C4A	-2.32	125.05	128.46
4	D	803	A1A0C	C05-C06-C11	-2.27	117.68	121.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	802	H4B	N2-C2-N1	2.27	120.63	117.22
2	A	801	HEM	C3B-C2B-C1B	2.26	108.11	106.41
2	A	801	HEM	C4D-ND-C1D	2.26	107.88	105.21
3	D	802	H4B	C2-N1-C8A	2.23	119.90	114.59
2	D	801	HEM	C4D-ND-C1D	2.22	107.83	105.21
2	D	801	HEM	C3B-C2B-C1B	2.21	108.07	106.41
2	B	801	HEM	C3B-C2B-C1B	2.19	108.06	106.41
4	D	803	A1A0C	C11-C12-C13	-2.16	120.42	121.69
4	B	803	A1A0C	C11-C06-N01	2.12	121.73	116.69
2	A	801	HEM	C3D-C4D-ND	-2.11	107.85	110.17
4	A	803	A1A0C	C05-C06-C11	-2.11	117.99	121.98
3	C	802	H4B	C4A-N5-C6	-2.10	115.45	121.16
2	C	801	HEM	C3B-C4B-NB	-2.08	107.97	109.47
2	B	801	HEM	CMA-C3A-C4A	-2.08	125.41	128.46
4	C	803	A1A0C	C11-C06-N01	2.08	121.62	116.69
2	A	801	HEM	CAD-C3D-C2D	-2.07	123.98	127.87
2	A	801	HEM	C3B-C4B-NB	-2.07	107.98	109.47
4	C	803	A1A0C	C11-C12-C13	-2.05	120.49	121.69
2	A	801	HEM	CAD-C3D-C4D	2.05	128.27	124.70
4	B	803	A1A0C	C11-C16-C15	-2.04	118.41	121.81
2	D	801	HEM	C4C-CHD-C1D	2.03	125.23	122.56
2	C	801	HEM	C4D-ND-C1D	2.02	107.60	105.21
3	D	802	H4B	C11-C10-C9	-2.02	109.64	112.11
2	D	801	HEM	CMC-C2C-C3C	2.02	128.72	124.68
4	D	803	A1A0C	C11-C06-N01	2.02	121.48	116.69
2	D	801	HEM	CHC-C4B-C3B	2.01	127.65	124.57
2	D	801	HEM	C3D-C4D-ND	-2.01	107.97	110.17
2	C	801	HEM	CMC-C2C-C3C	2.00	128.69	124.68

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	A1A0C	C05-C06-C11-C12
4	A	803	A1A0C	C17-C18-N19-C20
4	B	803	A1A0C	C05-C06-C11-C12
4	C	803	A1A0C	C05-C06-C11-C12
4	D	803	A1A0C	C05-C06-C11-C12
5	A	806	GOL	O1-C1-C2-C3
5	A	806	GOL	C1-C2-C3-O3
5	B	804	GOL	O1-C1-C2-C3
5	D	804	GOL	O1-C1-C2-C3

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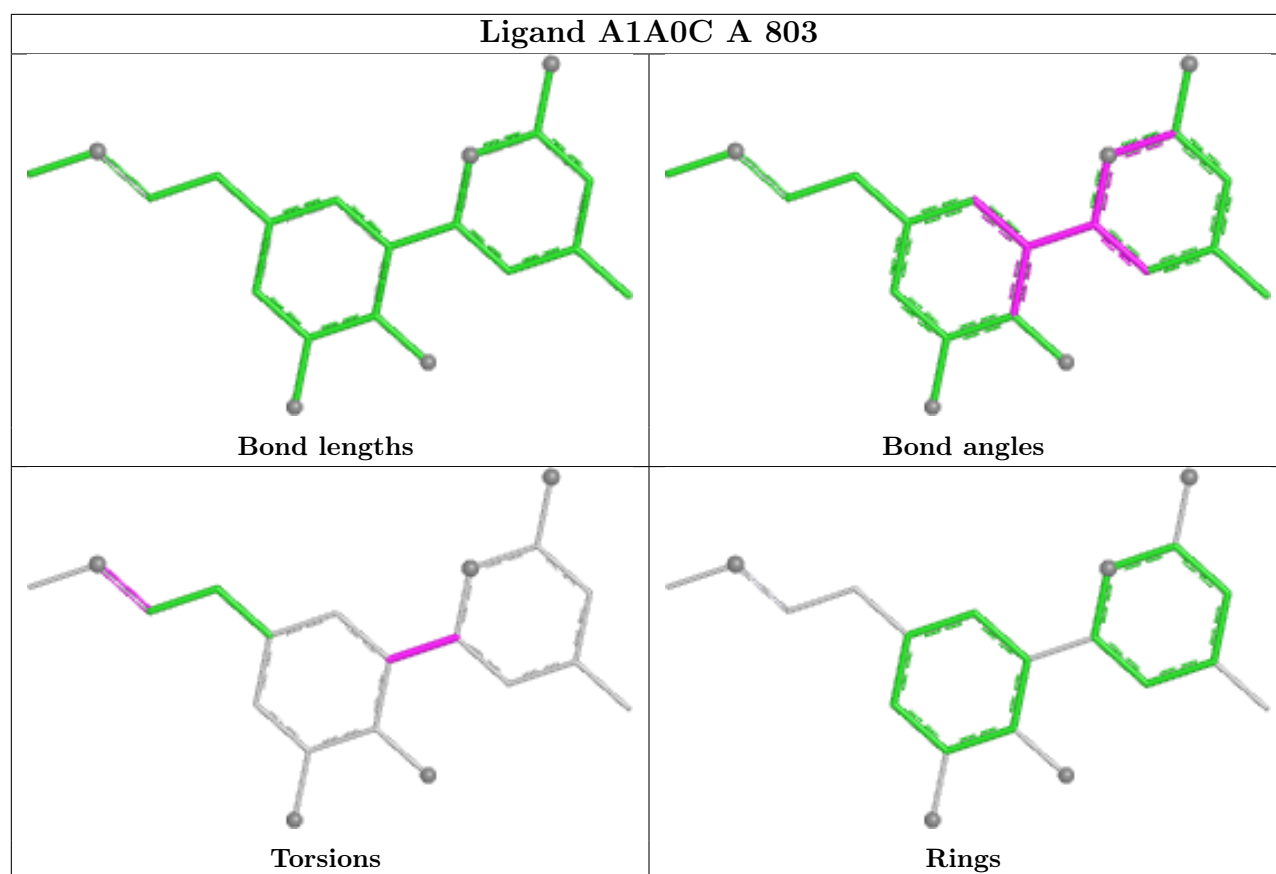
Mol	Chain	Res	Type	Atoms
5	A	806	GOL	O1-C1-C2-O2
5	A	806	GOL	O2-C2-C3-O3
5	B	804	GOL	O1-C1-C2-O2
5	C	804	GOL	O2-C2-C3-O3
2	A	801	HEM	C4B-C3B-CAB-CBB
2	D	801	HEM	C4B-C3B-CAB-CBB
5	D	804	GOL	C1-C2-C3-O3
4	A	803	A1A0C	N01-C06-C11-C12
4	C	803	A1A0C	N01-C06-C11-C12
5	D	804	GOL	O2-C2-C3-O3
2	C	801	HEM	C4B-C3B-CAB-CBB
5	D	804	GOL	O1-C1-C2-O2
4	D	803	A1A0C	N01-C06-C11-C12

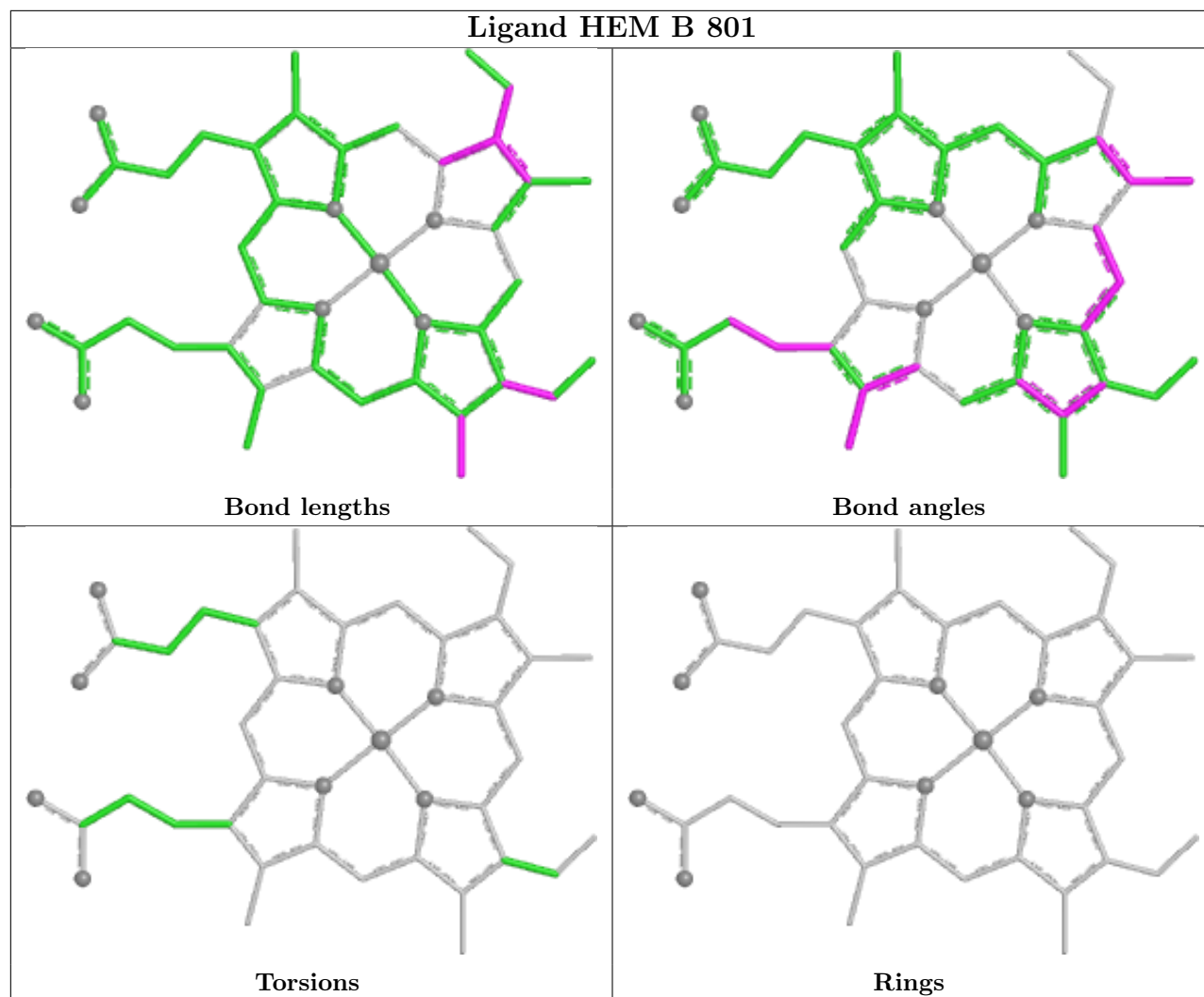
There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	803	A1A0C	1	0
2	B	801	HEM	2	0
4	D	803	A1A0C	1	0
4	C	803	A1A0C	1	0
2	A	801	HEM	3	0
2	C	801	HEM	2	0
2	D	801	HEM	3	0

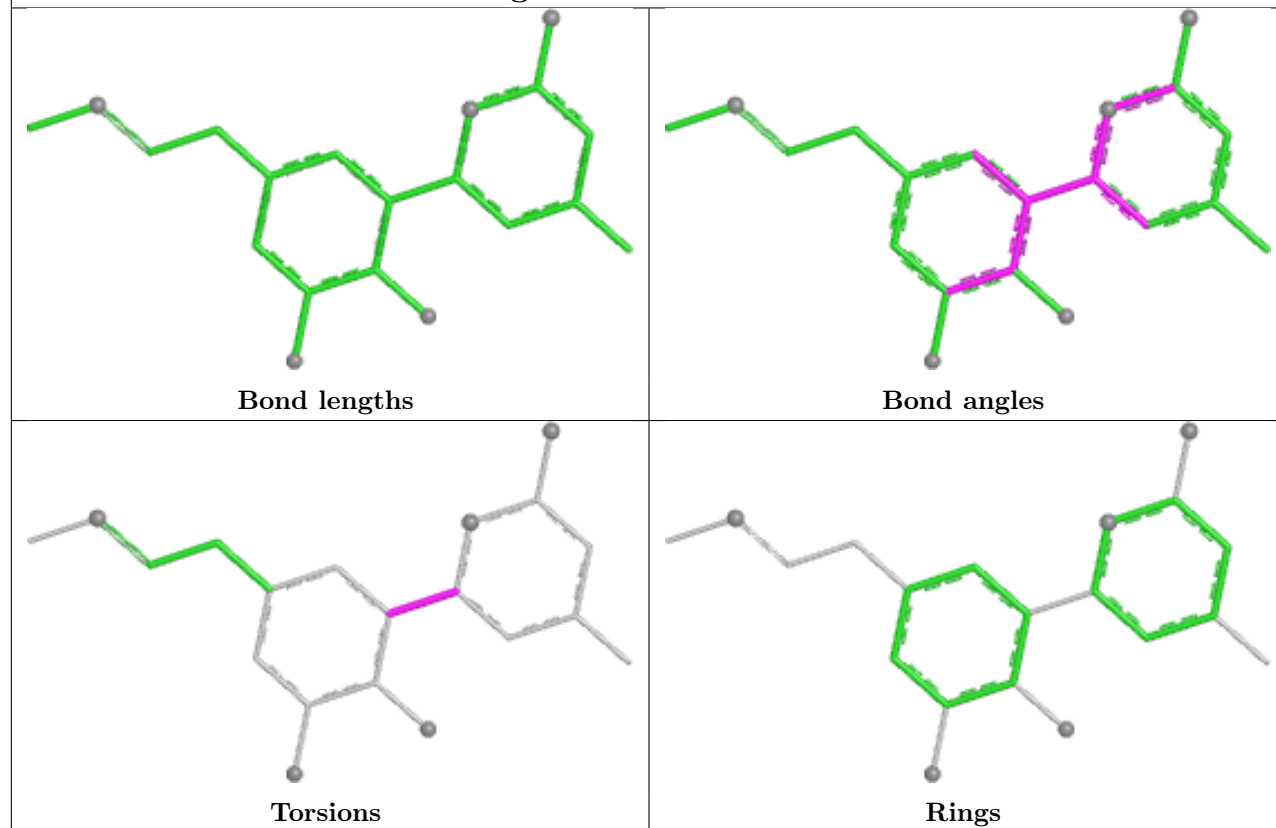
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



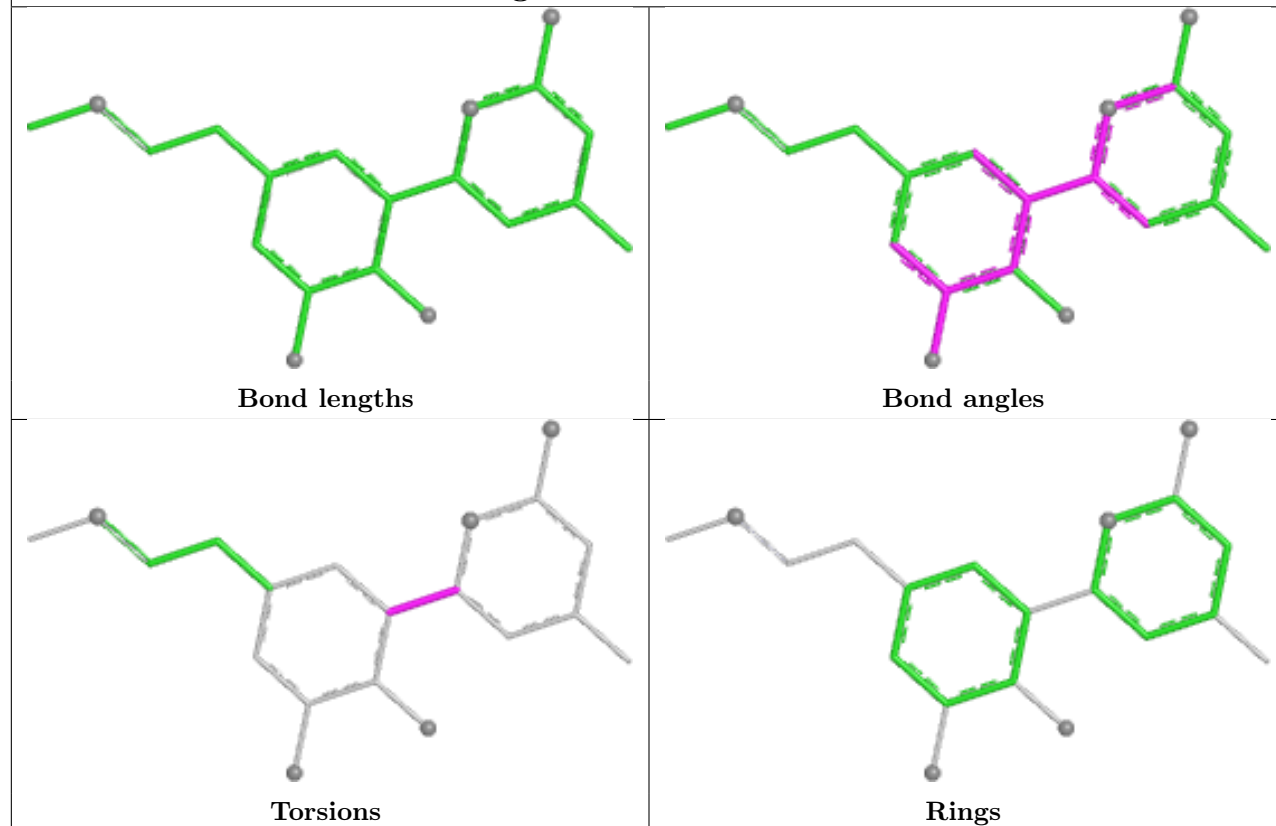


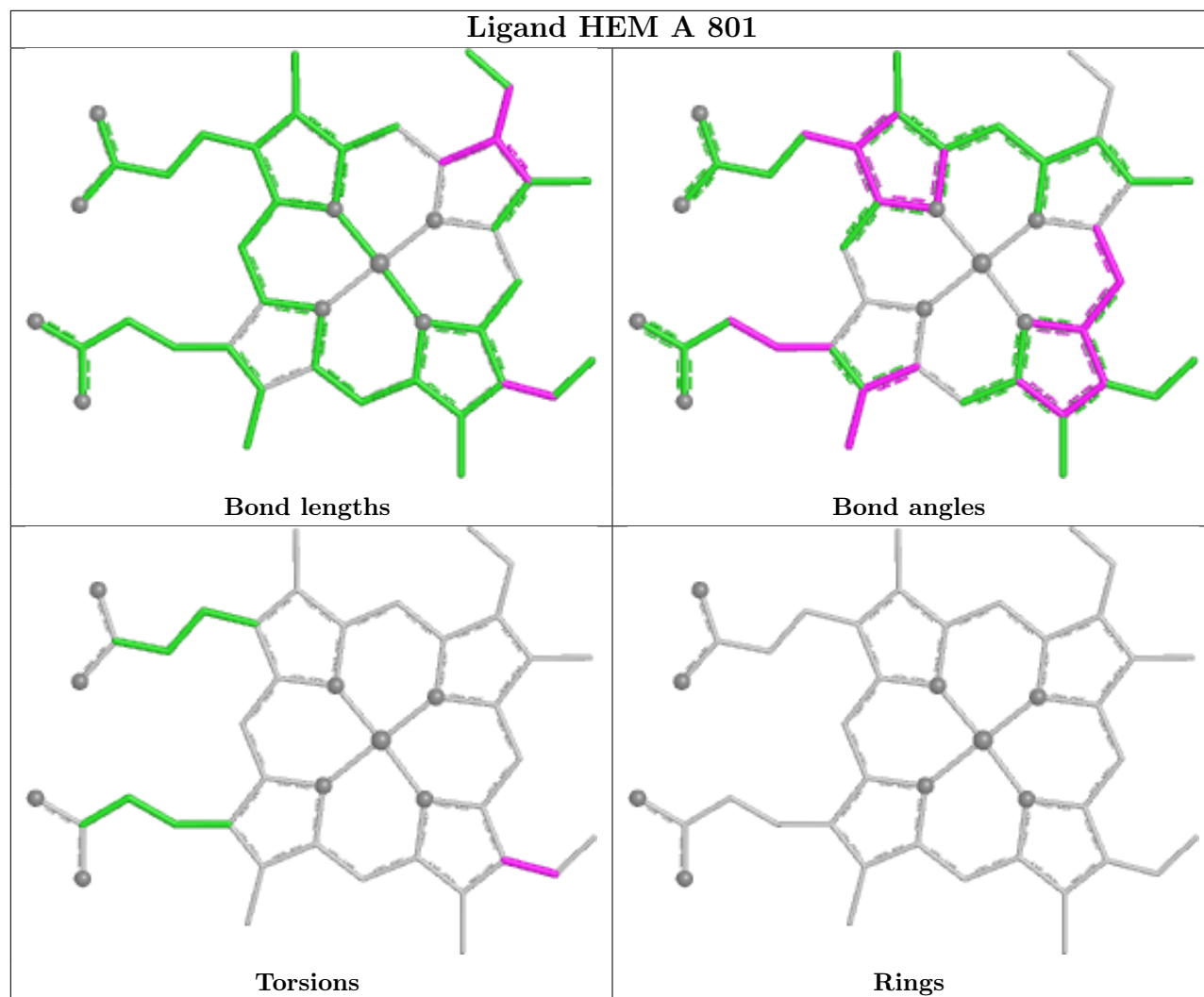


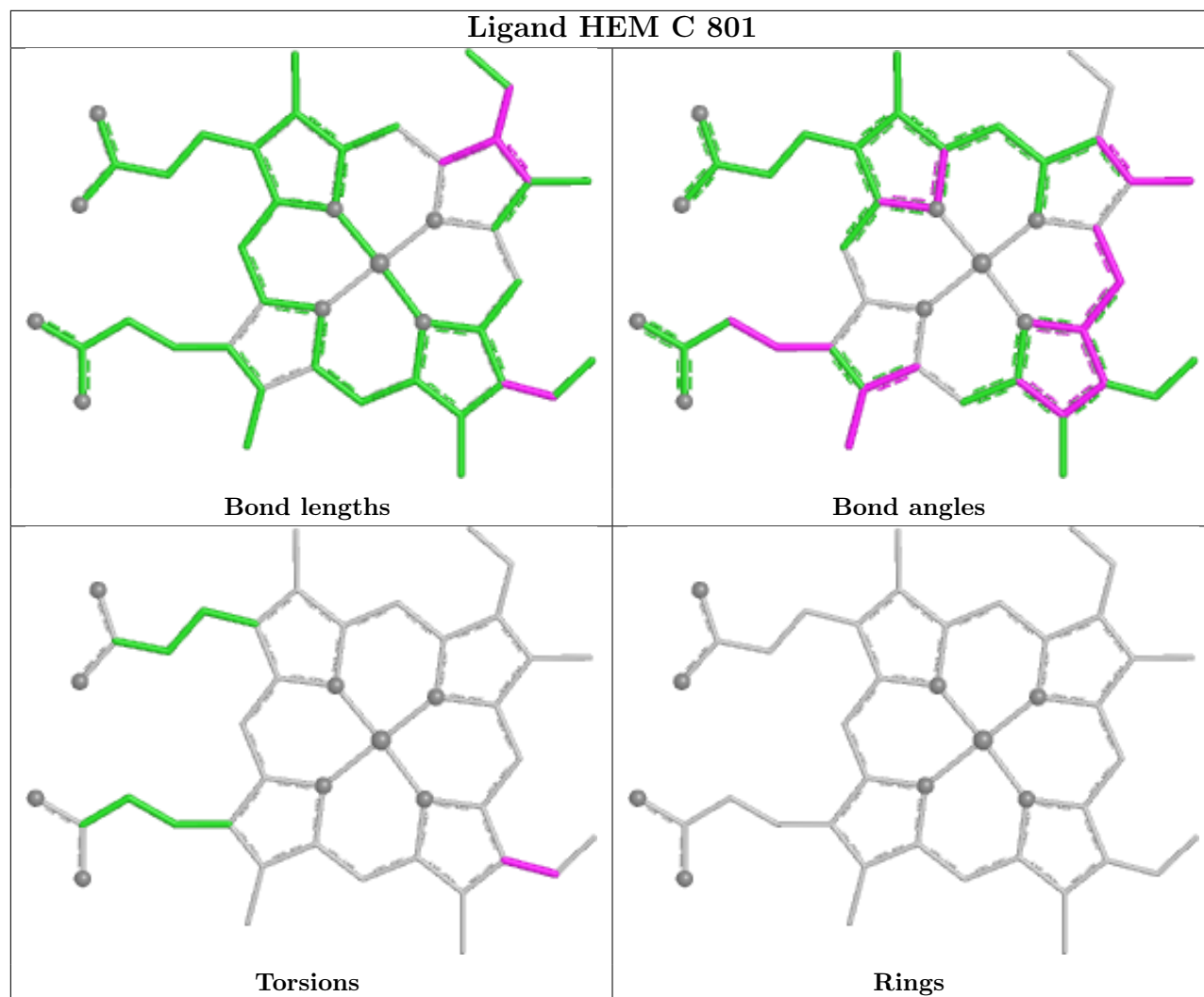
## Ligand A1A0C D 803

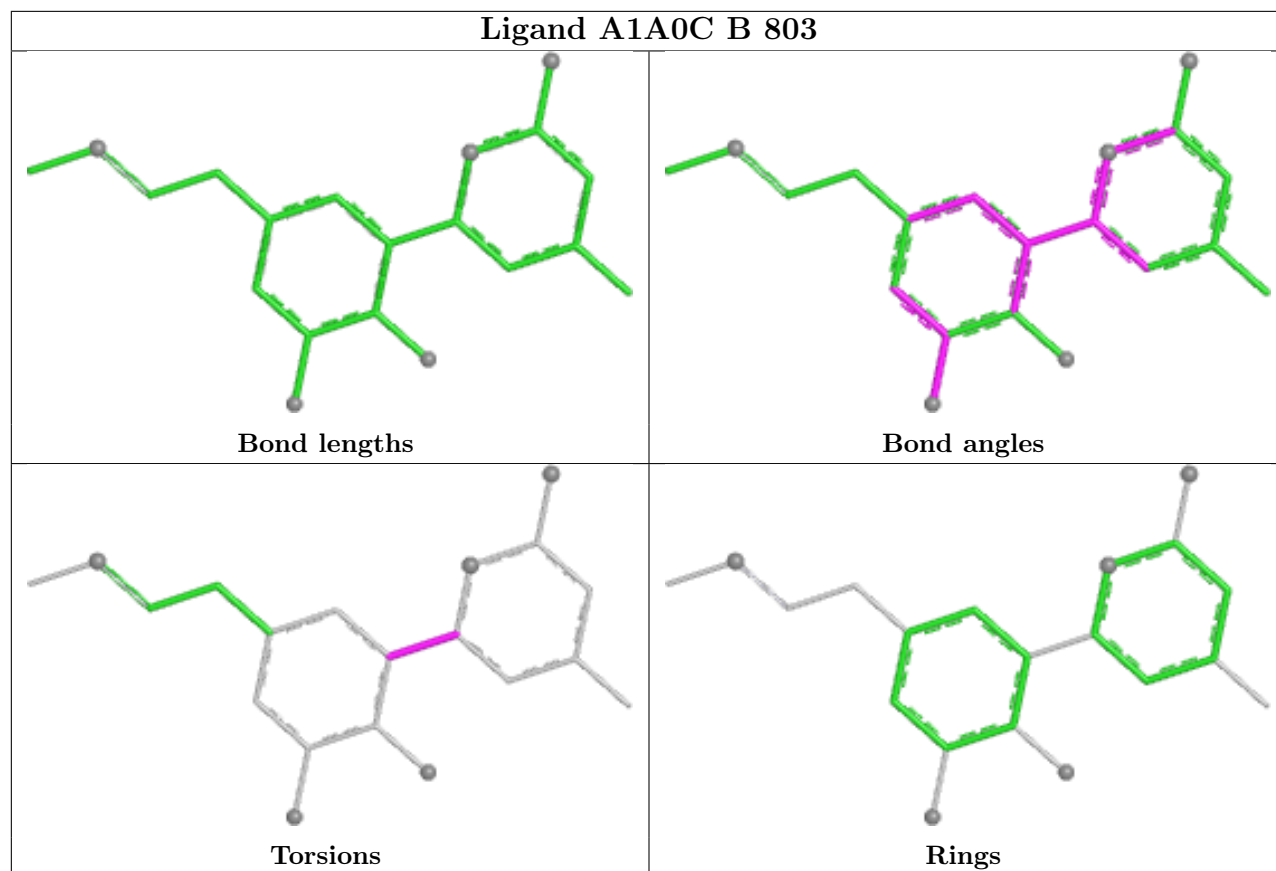


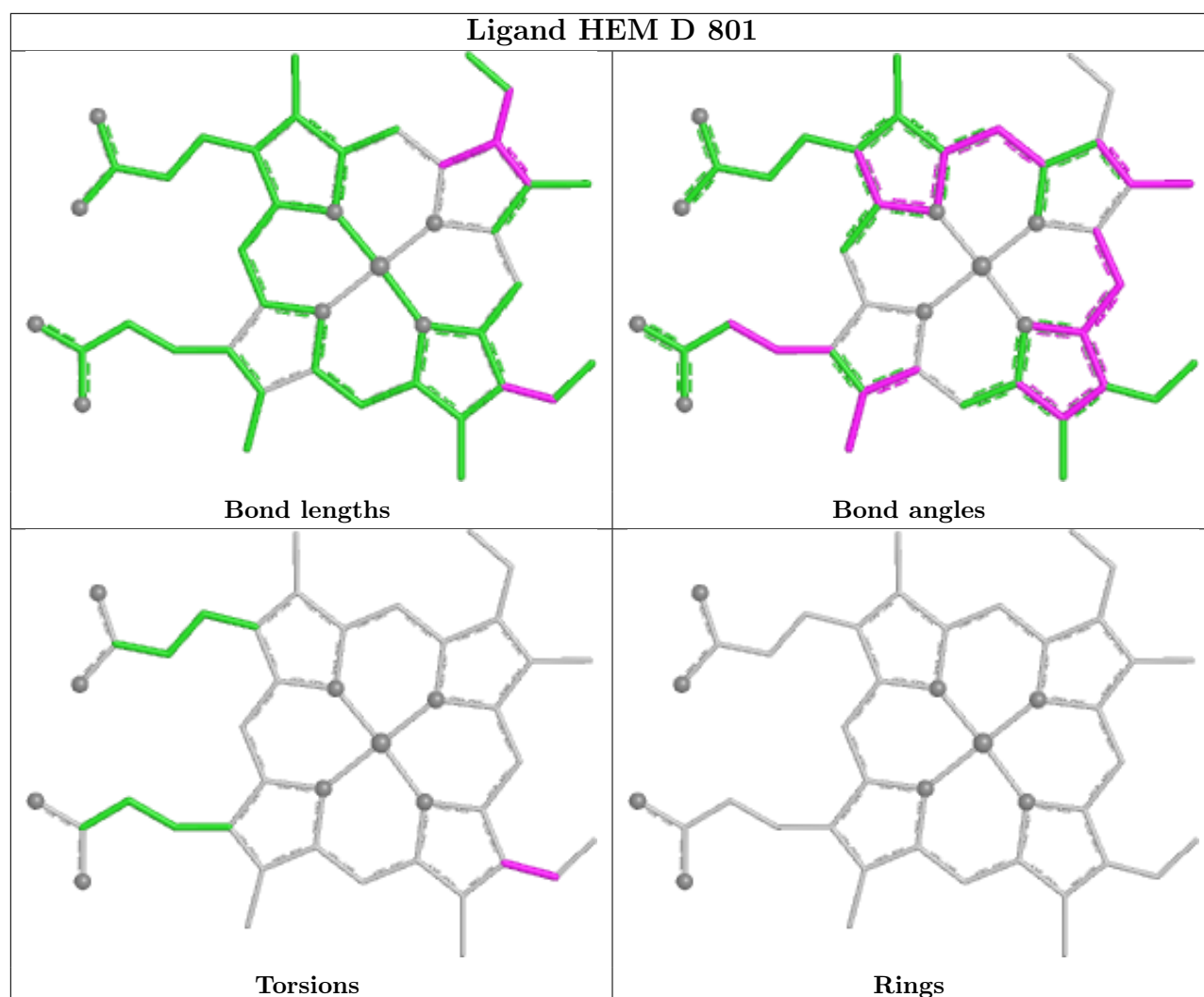
## Ligand A1A0C C 803











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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	418/423 (98%)	-1.51	0 100 100	14, 33, 63, 106	5 (1%)
1	B	414/423 (97%)	-1.53	0 100 100	15, 31, 59, 84	2 (0%)
1	C	413/423 (97%)	-1.55	0 100 100	15, 30, 60, 104	7 (1%)
1	D	418/423 (98%)	-1.51	0 100 100	15, 33, 64, 119	4 (0%)
All	All	1663/1692 (98%)	-1.53	0 100 100	14, 32, 62, 119	18 (1%)

There are no RSRZ outliers to report.

### 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.

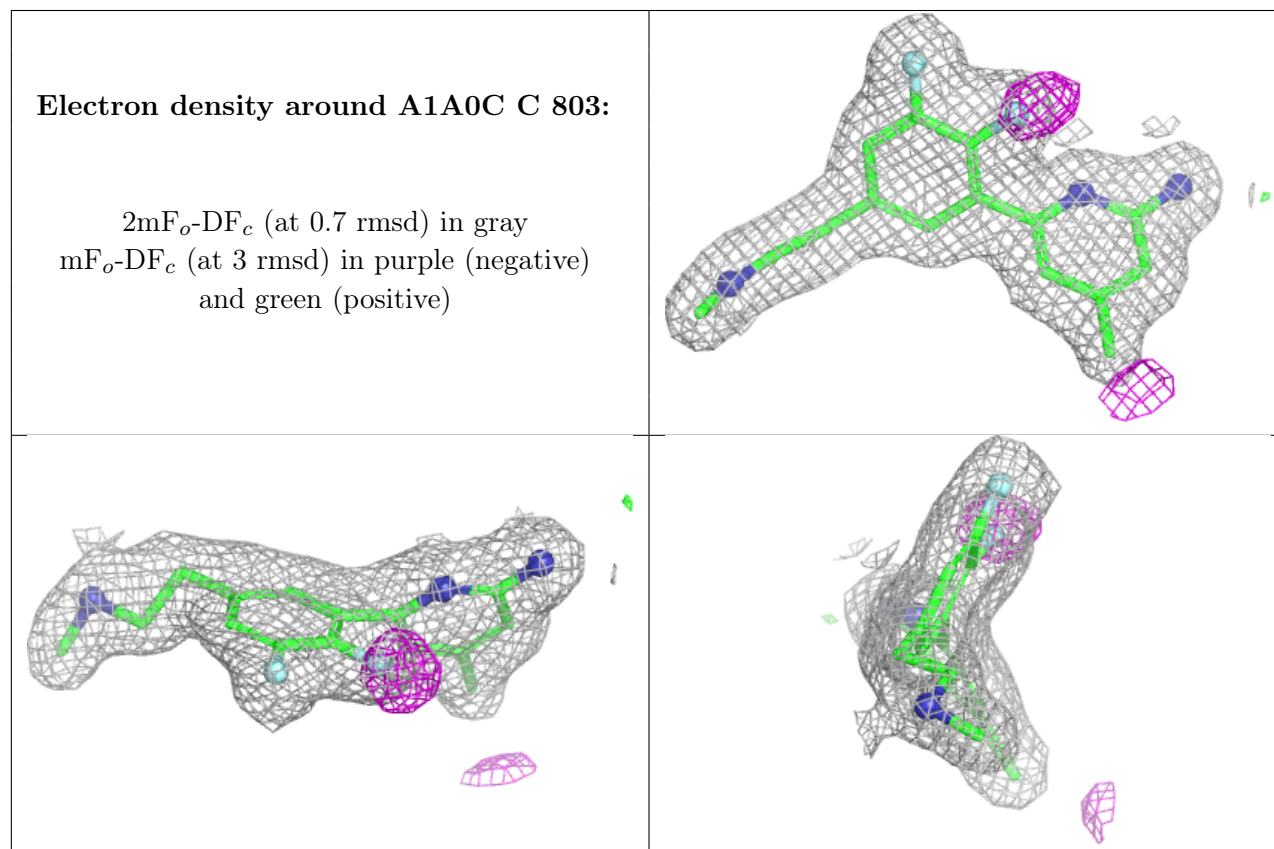
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	A	806	6/6	0.98	0.07	57,62,77,83	0
3	H4B	C	802	17/17	0.99	0.02	21,25,29,31	0
3	H4B	D	802	17/17	0.99	0.02	19,27,32,33	0
4	A1A0C	C	803	20/20	0.99	0.02	20,24,32,34	0

*Continued on next page...*

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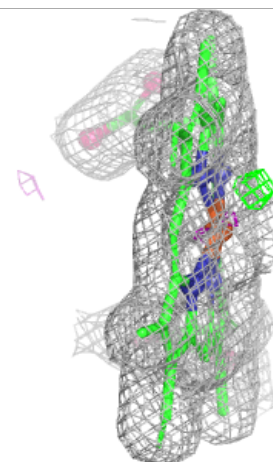
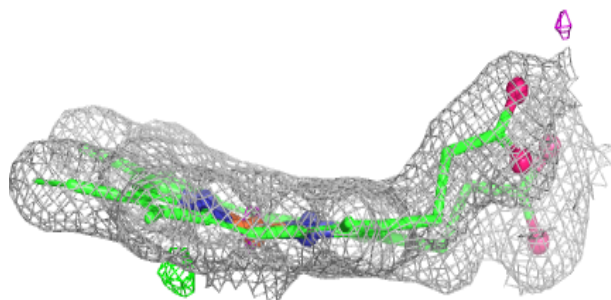
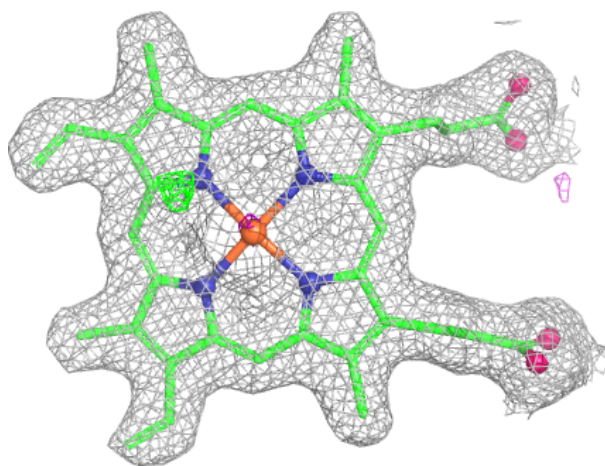
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	804	6/6	0.99	0.04	38,51,54,58	0
3	H4B	A	802	17/17	0.99	0.02	21,29,33,33	0
5	GOL	B	804	6/6	0.99	0.04	57,62,64,65	0
5	GOL	C	804	6/6	0.99	0.04	56,59,64,71	0
5	GOL	C	805	6/6	0.99	0.04	41,50,52,58	0
5	GOL	D	804	6/6	0.99	0.03	34,41,45,50	0
2	HEM	D	801	43/43	1.00	0.02	17,23,30,36	0
4	A1A0C	D	803	20/20	1.00	0.02	17,24,33,37	0
2	HEM	A	801	43/43	1.00	0.02	16,24,29,38	0
3	H4B	B	802	17/17	1.00	0.02	19,25,29,31	0
2	HEM	B	801	43/43	1.00	0.02	17,24,31,41	0
2	HEM	C	801	43/43	1.00	0.02	16,24,31,41	0
4	A1A0C	A	803	20/20	1.00	0.02	16,24,30,30	0
4	A1A0C	B	803	20/20	1.00	0.02	18,23,32,34	0
6	ZN	A	805	1/1	1.00	0.01	26,26,26,26	0
6	ZN	C	806	1/1	1.00	0.01	26,26,26,26	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 D 801:**

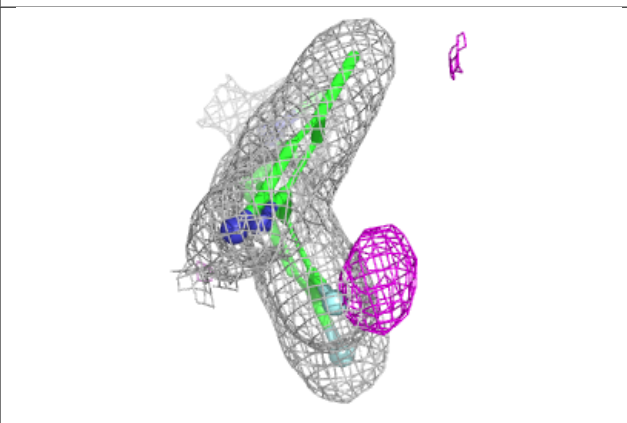
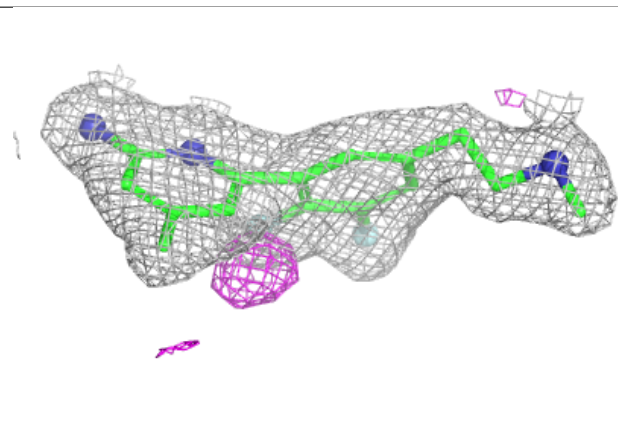
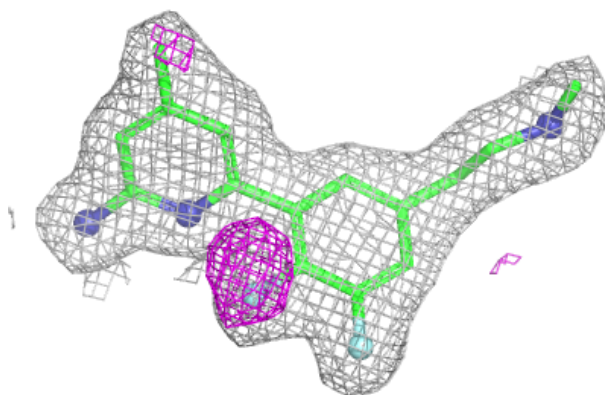
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





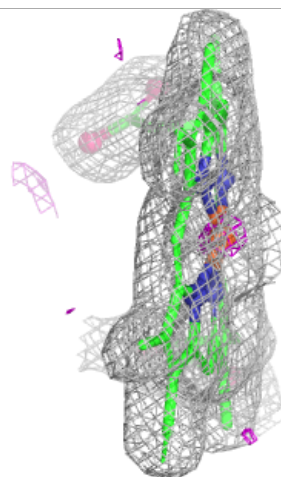
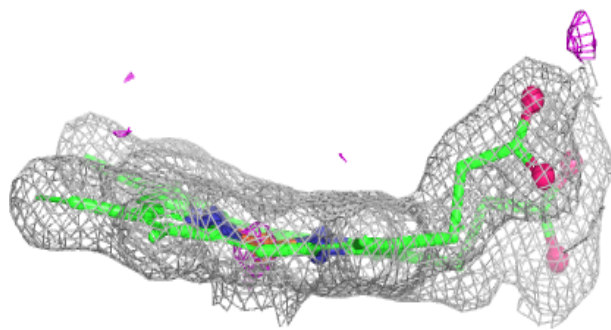
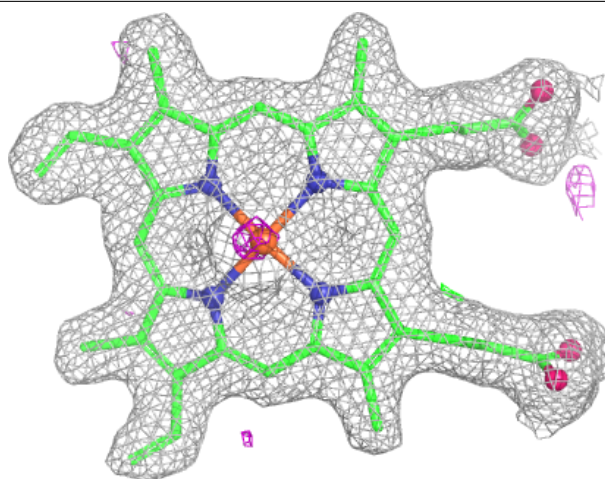
**Electron density around A1A0C D 803:**

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



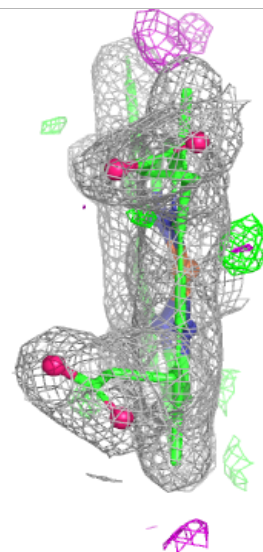
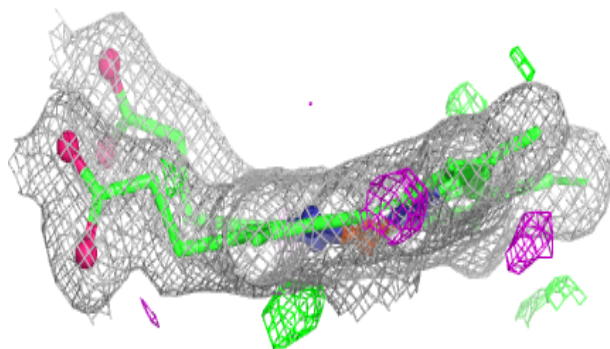
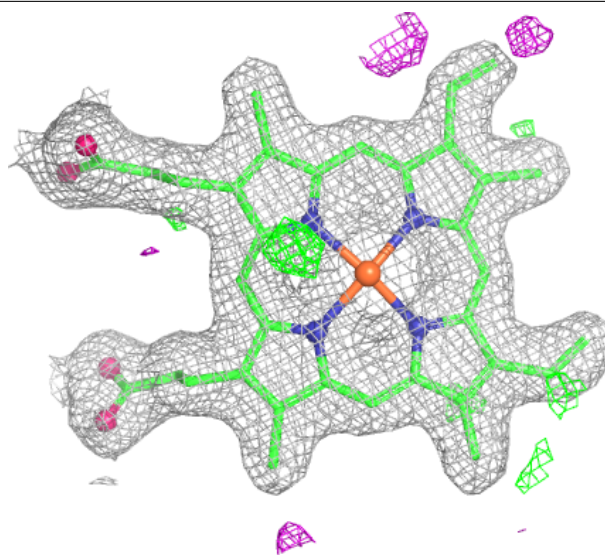
**Electron density around HEM A 801:**

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



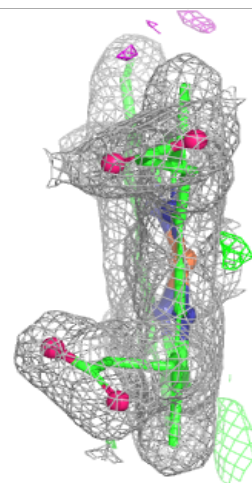
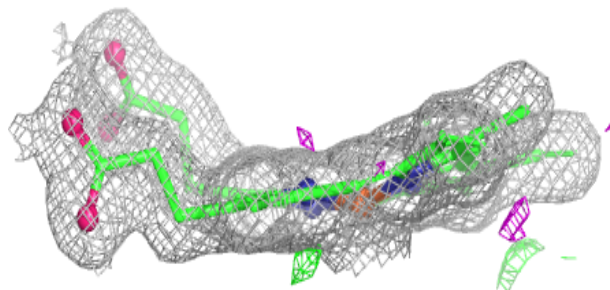
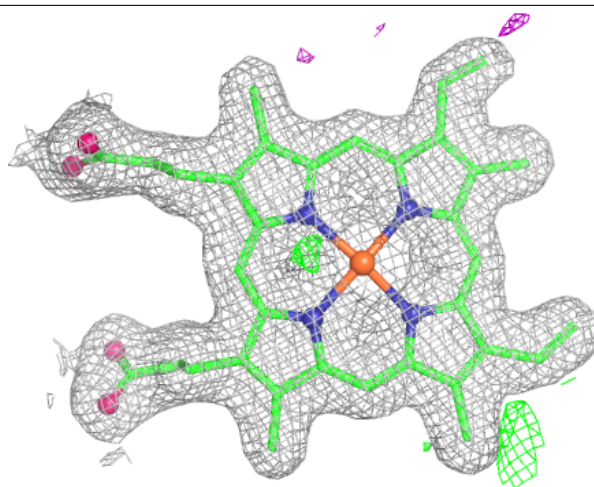
**Electron density around HEM B 801:**

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



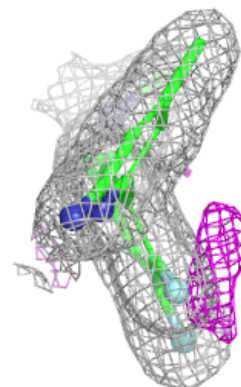
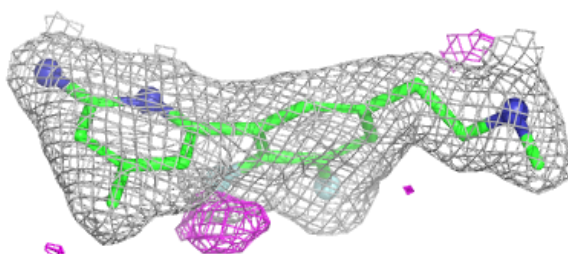
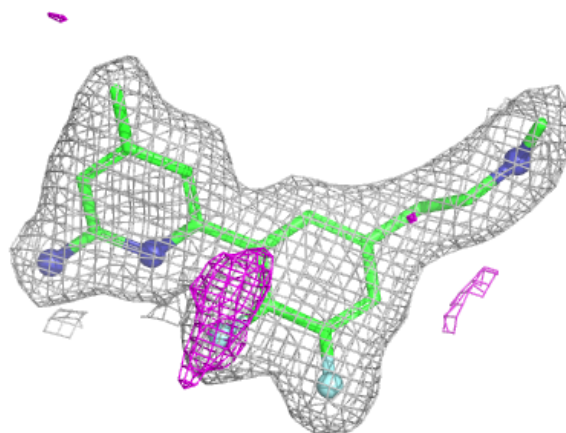
**Electron density around HEM C 801:**

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

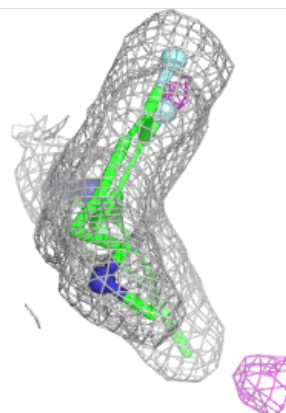
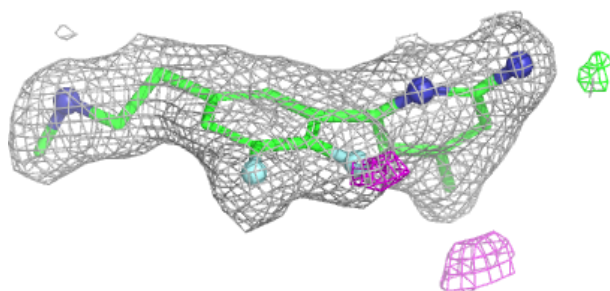
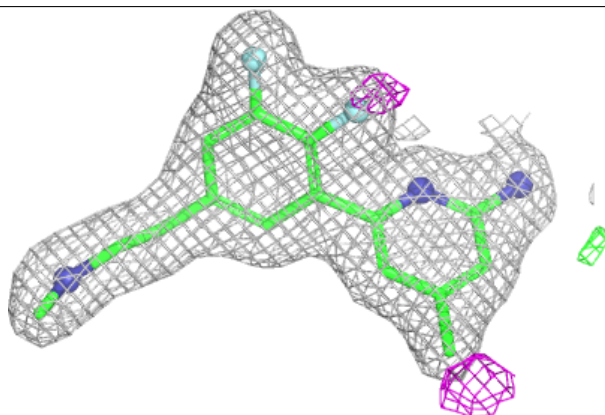


**Electron density around A1A0C A 803:**

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

**Electron density around A1A0C B 803:**

$2mF_o-DF_c$  (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.