



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2025 – 12:32 PM EDT

PDB ID : 9Q4H / pdb\_00009q4h  
Title : Structure of human neuronal nitric oxide synthase R354A/G357D mutant heme domain bound with 6-((2,3-difluoro-5-(2-(methylamino)ethyl)phenoxy)methyl)-4-methylpyridin-2-amine  
Authors : Li, H.; Poulos, T.L.  
Deposited on : 2025-08-20  
Resolution : 1.99 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	:	4-5-2 with Phenix2.0rc1
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)	:	2.45.1

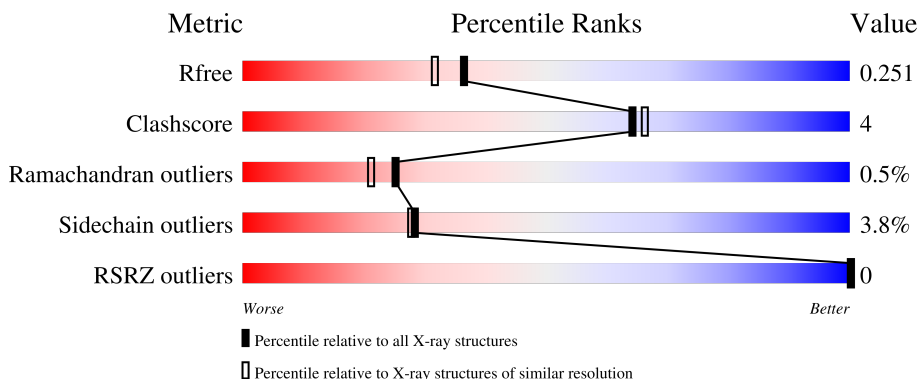
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.99 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	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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 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 14650 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.

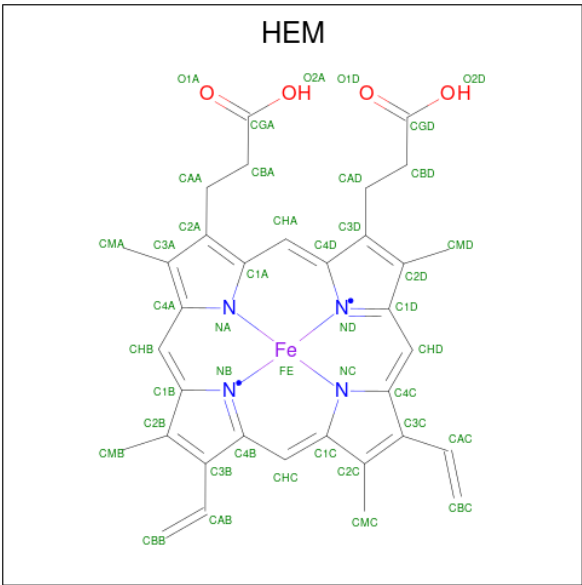
- Molecule 1 is a protein called Nitric oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	3	0
			3388	2170	578	619	21			
1	B	419	Total	C	N	O	S	0	3	0
			3431	2194	589	627	21			
1	C	420	Total	C	N	O	S	0	2	0
			3432	2195	590	626	21			
1	D	412	Total	C	N	O	S	0	2	0
			3362	2155	573	613	21			

There are 16 discrepancies between the modelled and reference sequences:

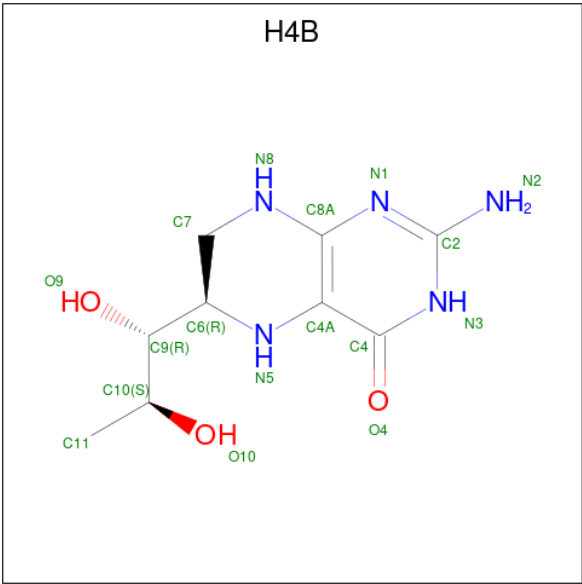
Chain	Residue	Modelled	Actual	Comment	Reference
A	354	ALA	ARG	engineered mutation	UNP P29475
A	357	ASP	GLY	engineered mutation	UNP P29475
A	723	LEU	-	expression tag	UNP P29475
A	724	VAL	-	expression tag	UNP P29475
B	354	ALA	ARG	engineered mutation	UNP P29475
B	357	ASP	GLY	engineered mutation	UNP P29475
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:  $C_{34}H_{32}FeN_4O_4$ ).



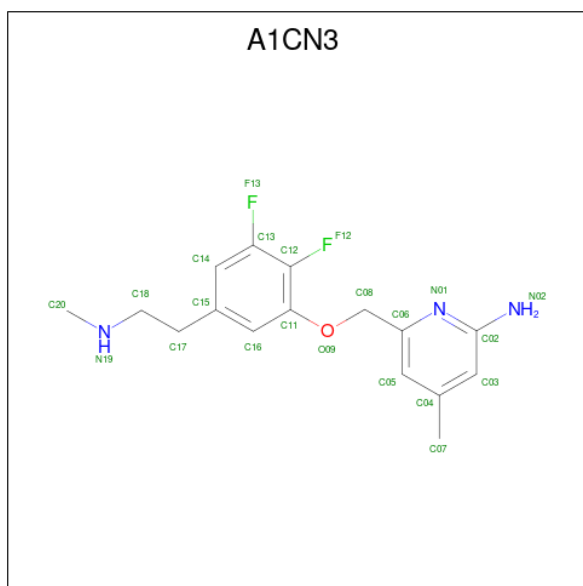
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- 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	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	D	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 6-(2,3-difluoro-5-[2-(methylamino)ethyl]phenoxy)methyl)-4-methylpyridine-2-amine (CCD ID: A1CN3) (formula: C<sub>16</sub>H<sub>19</sub>F<sub>2</sub>N<sub>3</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			22	16	2	3	1		
4	B	1	Total	C	F	N	O	0	0
			22	16	2	3	1		
4	C	1	Total	C	F	N	O	0	0
			22	16	2	3	1		
4	D	1	Total	C	F	N	O	0	0
			22	16	2	3	1		

- 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	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	B	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	181	Total	O	0	0
			181	181		
7	B	153	Total	O	0	0
			153	153		
7	C	164	Total	O	0	0
			164	164		

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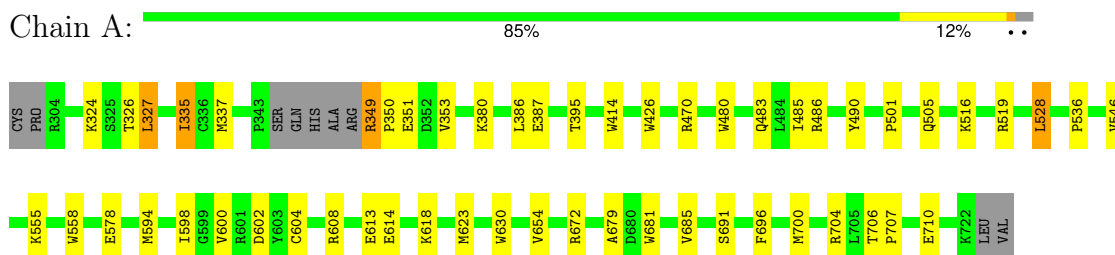
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	185	Total 185	O 185	0	0

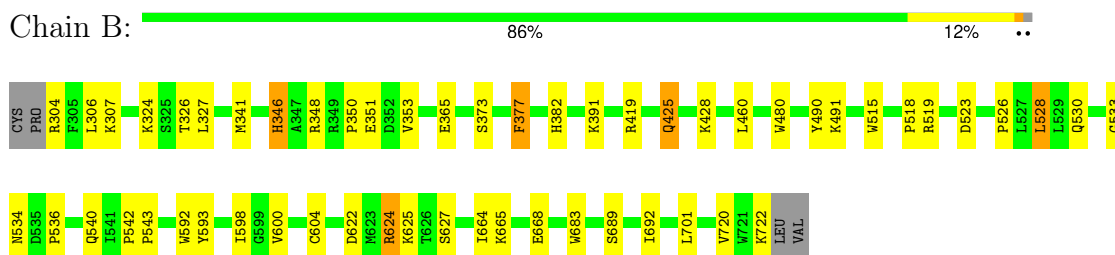
### 3 Residue-property plots [i](#)

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.

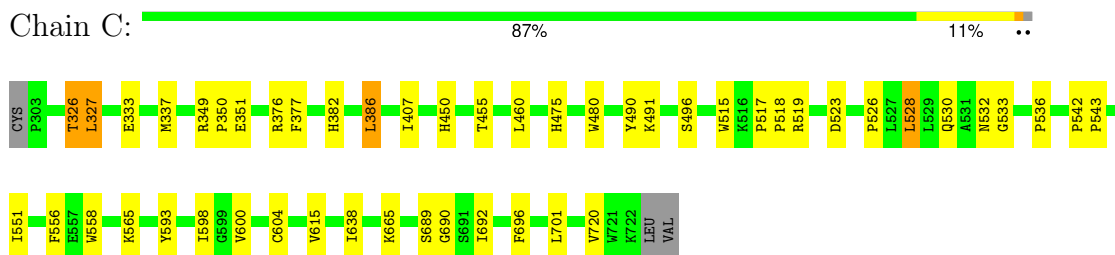
- Molecule 1: Nitric oxide synthase, brain



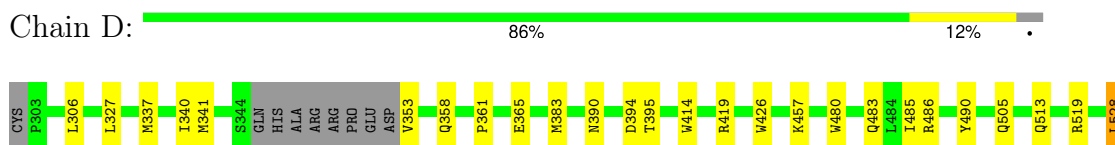
- Molecule 1: Nitric oxide synthase, brain



- Molecule 1: Nitric oxide synthase, brain



- Molecule 1: Nitric oxide synthase, brain







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.34Å 52.18Å 164.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.28 – 1.99 39.28 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.28-1.99) 98.5 (39.28-1.99)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, $R_{free}$	0.209 , 0.253 0.205 , 0.251	Depositor DCC
$R_{free}$ test set	6856 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.829	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14650	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: A1CN3, HEM, H4B, GOL, ZN

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	0.31	0/3493	0.49	0/4741
1	B	0.29	0/3538	0.46	0/4801
1	C	0.29	0/3537	0.46	0/4800
1	D	0.32	0/3464	0.49	0/4700
All	All	0.30	0/14032	0.47	0/19042

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	3388	0	3303	26	0
1	B	3431	0	3341	23	0
1	C	3432	0	3343	26	0
1	D	3362	0	3279	24	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	2	0
3	A	34	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	34	0	30	1	0
4	A	22	0	0	1	0
4	B	22	0	0	1	0
4	C	22	0	0	0	0
4	D	22	0	0	0	0
5	A	12	0	16	0	0
5	C	6	0	8	1	0
5	D	6	0	8	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	181	0	0	0	0
7	B	153	0	0	1	0
7	C	164	0	0	2	0
7	D	185	0	0	0	0
All	All	14650	0	13478	105	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 (105) 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:528:LEU:HD22	1:B:536:PRO:HB2	1.58	0.85
1:C:528:LEU:HD22	1:C:536:PRO:HB2	1.59	0.83
1:A:528:LEU:HD22	1:A:536:PRO:HB2	1.69	0.74
1:A:349:ARG:HG2	1:A:350:PRO:HD2	1.72	0.71
1:D:528:LEU:HD22	1:D:536:PRO:HB2	1.72	0.71
1:A:335:ILE:HD11	1:B:701:LEU:HD22	1.73	0.70
1:D:337:MET:HE2	1:D:340:ILE:HG13	1.73	0.69
2:C:801:HEM:HBC2	2:C:801:HEM:HMC2	1.75	0.68
2:C:801:HEM:HHC	2:C:801:HEM:HBB2	1.75	0.68
2:B:802:HEM:HHC	2:B:802:HEM:HBB2	1.76	0.66
1:B:327:LEU:HD11	1:B:348:ARG:HD2	1.79	0.65
2:A:801:HEM:HMC2	2:A:801:HEM:HBC2	1.78	0.64
2:A:801:HEM:HBB2	2:A:801:HEM:HHC	1.80	0.64
2:D:802:HEM:HMC2	2:D:802:HEM:HBC2	1.79	0.63
1:B:664:ILE:O	1:B:668[B]:GLU:HG2	1.99	0.63
2:B:802:HEM:HMC2	2:B:802:HEM:HBC2	1.80	0.62
1:C:701:LEU:HD21	1:D:337:MET:HE3	1.81	0.62
1:A:613:GLU:HG3	1:A:623:MET:HE1	1.83	0.60
1:A:480:TRP:HB2	1:A:528:LEU:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ILE:HD13	1:A:546:VAL:HG13	1.86	0.56
1:D:480:TRP:HB2	1:D:528:LEU:HB3	1.86	0.56
1:C:600:VAL:O	1:C:604:CYS:HB2	2.06	0.56
1:D:341:MET:HE2	3:D:803:H4B:H9	1.87	0.56
1:C:530:GLN:HE21	1:C:533:GLY:HA2	1.71	0.55
1:B:600:VAL:O	1:B:604:CYS:HB2	2.07	0.54
1:B:593:TYR:CD2	1:B:598:ILE:HD11	2.42	0.54
1:C:556:PHE:HB3	1:C:558:TRP:CE2	2.44	0.53
1:C:480:TRP:HB2	1:C:528:LEU:HB3	1.91	0.52
1:B:518:PRO:HG2	1:B:523:ASP:CG	2.35	0.52
1:C:376:ARG:HB3	7:C:904:HOH:O	2.10	0.52
2:B:802:HEM:HBD1	4:B:803:A1CN3:F12	2.02	0.50
1:B:480:TRP:HB2	1:B:528:LEU:HB3	1.94	0.50
1:C:475:HIS:HB3	1:C:532:ASN:OD1	2.13	0.49
1:B:490:TYR:CE2	1:B:519:ARG:HA	2.49	0.48
1:D:594:MET:HA	1:D:654:VAL:O	2.13	0.48
1:B:377:PHE:HA	1:B:382:HIS:ND1	2.28	0.48
1:D:598:ILE:HA	1:D:602:ASP:HB2	1.95	0.48
1:A:327:LEU:H	1:A:327:LEU:HD23	1.78	0.47
1:B:530:GLN:HG3	1:B:534:ASN:O	2.14	0.47
1:C:382:HIS:HB2	7:C:904:HOH:O	2.13	0.47
1:C:490:TYR:CE2	1:C:519:ARG:HA	2.49	0.47
1:A:598:ILE:HA	1:A:602:ASP:HB2	1.95	0.47
1:B:460:LEU:HD12	1:B:592:TRP:HB3	1.97	0.47
1:D:691:SER:HA	1:D:696:PHE:CG	2.50	0.47
1:A:414:TRP:CE3	1:A:426:TRP:HA	2.51	0.46
1:C:615:VAL:HG21	1:C:638:ILE:HD11	1.98	0.46
1:D:327:LEU:HD12	1:D:704:ARG:HG2	1.98	0.46
1:B:341:MET:HE2	1:B:341:MET:HB2	1.81	0.45
1:D:556:PHE:HB3	1:D:558:TRP:CE2	2.51	0.45
1:B:689:SER:HB3	1:B:692:ILE:HD11	1.99	0.45
1:C:407:ILE:HG21	5:C:803:GOL:H31	1.99	0.45
1:C:689:SER:HB3	1:C:692:ILE:HD11	1.99	0.45
1:D:358:GLN:O	1:D:361:PRO:HD2	2.16	0.44
1:A:704:ARG:NH2	1:A:710:GLU:OE2	2.50	0.44
1:A:337:MET:HE1	1:B:306:LEU:HD22	1.98	0.44
1:B:530:GLN:HE21	1:B:533:GLY:HA2	1.81	0.44
1:C:337:MET:HE2	1:D:306:LEU:HD13	1.99	0.44
1:D:706:THR:HA	1:D:707:PRO:C	2.42	0.44
1:A:706[A]:THR:HA	1:A:707:PRO:C	2.42	0.44
1:B:419:ARG:HD3	1:B:683:TRP:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:TRP:CE2	1:C:526:PRO:HD3	2.53	0.44
1:C:690:GLY:O	1:C:696:PHE:HB2	2.18	0.44
1:D:513:GLN:HB2	1:D:538:LEU:HD11	2.00	0.43
1:C:326:THR:HB	1:C:327:LEU:HD23	2.00	0.43
1:C:518:PRO:HG2	1:C:523:ASP:CG	2.43	0.43
1:B:515:TRP:CE2	1:B:526:PRO:HD3	2.53	0.43
1:C:551:ILE:HG12	1:C:565:LYS:HA	2.01	0.43
1:A:501:PRO:HG2	1:A:608:ARG:O	2.18	0.43
1:A:704:ARG:CZ	1:A:704:ARG:HB3	2.43	0.43
1:C:542:PRO:HA	1:C:543:PRO:HD3	1.92	0.43
1:D:480:TRP:CE2	1:D:715:PRO:HB2	2.54	0.43
1:A:483:GLN:HB2	1:A:486:ARG:HG2	2.01	0.43
1:B:425:GLN:H	1:B:425:GLN:HG2	1.67	0.43
1:D:664:ILE:O	1:D:668:GLU:HG3	2.20	0.42
2:A:801:HEM:HBD1	4:A:803:A1CN3:F12	2.10	0.42
1:B:327:LEU:HD23	1:B:346:HIS:O	2.20	0.42
1:A:691:SER:HA	1:A:696:PHE:CG	2.54	0.42
1:C:593:TYR:CD2	1:C:598:ILE:HD11	2.54	0.42
1:D:337:MET:HB3	1:D:340:ILE:HG13	2.02	0.42
2:D:802:HEM:HBB2	2:D:802:HEM:HHC	2.02	0.41
1:A:681:TRP:CE2	1:A:685:VAL:HG21	2.55	0.41
1:A:558:TRP:CZ3	1:A:618:LYS:HB2	2.55	0.41
1:B:542:PRO:HA	1:B:543:PRO:HD3	1.93	0.41
1:B:622:ASP:OD1	1:B:624:ARG:HG3	2.20	0.41
1:C:515:TRP:O	1:C:517:PRO:HD3	2.21	0.41
1:A:558:TRP:CD1	1:A:558:TRP:H	2.39	0.41
1:A:679:ALA:HB3	1:A:700:MET:HB3	2.01	0.41
1:B:491:LYS:HD3	7:B:922:HOH:O	2.20	0.41
1:A:353:VAL:HG12	1:A:470:ARG:HD3	2.03	0.41
1:C:327:LEU:HD23	1:C:327:LEU:N	2.35	0.41
1:D:558:TRP:CE3	1:D:618:LYS:HE3	2.56	0.41
1:A:594:MET:HA	1:A:654:VAL:O	2.21	0.41
1:D:679:ALA:HB3	1:D:700:MET:HB3	2.02	0.41
1:A:623:MET:HA	1:A:630:TRP:CD1	2.56	0.40
1:D:419:ARG:HD3	1:D:683:TRP:CD2	2.55	0.40
1:D:483:GLN:HB2	1:D:486:ARG:HG2	2.02	0.40
1:A:600:VAL:O	1:A:604:CYS:HB2	2.22	0.40
1:D:490:TYR:CE2	1:D:519:ARG:HA	2.56	0.40
1:A:490:TYR:CE2	1:A:519:ARG:HA	2.57	0.40
1:C:386:LEU:HD12	1:C:386:LEU:HA	1.93	0.40
1:D:414:TRP:CE3	1:D:426:TRP:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:ILE:HD13	1:D:546:VAL:HG13	2.03	0.40
1:A:706[B]:THR:HA	1:A:707:PRO:C	2.46	0.40
1:C:450:HIS:CD2	1:C:450:HIS:C	3.00	0.40
1:C:455:THR:HA	1:C:460:LEU:HD22	2.03	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	413/423 (98%)	401 (97%)	12 (3%)	0	100	100
1	B	420/423 (99%)	401 (96%)	15 (4%)	4 (1%)	13	8
1	C	420/423 (99%)	403 (96%)	13 (3%)	4 (1%)	13	8
1	D	410/423 (97%)	399 (97%)	11 (3%)	0	100	100
All	All	1663/1692 (98%)	1604 (96%)	51 (3%)	8 (0%)	25	21

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	351	GLU
1	C	377	PHE
1	B	377	PHE
1	B	351	GLU
1	B	346	HIS
1	C	496	SER
1	C	350	PRO
1	B	350	PRO

### 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	373/378 (99%)	356 (95%)	17 (5%)	23	21
1	B	377/378 (100%)	359 (95%)	18 (5%)	21	19
1	C	377/378 (100%)	368 (98%)	9 (2%)	44	47
1	D	370/378 (98%)	358 (97%)	12 (3%)	34	35
All	All	1497/1512 (99%)	1441 (96%)	56 (4%)	28	29

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	LYS
1	A	326	THR
1	A	327	LEU
1	A	335	ILE
1	A	349	ARG
1	A	351	GLU
1	A	380	LYS
1	A	386	LEU
1	A	387	GLU
1	A	395	THR
1	A	505	GLN
1	A	516	LYS
1	A	528	LEU
1	A	555	LYS
1	A	578	GLU
1	A	614	GLU
1	A	672	ARG
1	B	304	ARG
1	B	307	LYS
1	B	324	LYS
1	B	326	THR
1	B	353	VAL
1	B	365	GLU
1	B	373	SER

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Mol	Chain	Res	Type
1	B	391	LYS
1	B	425	GLN
1	B	428	LYS
1	B	528	LEU
1	B	540	GLN
1	B	624	ARG
1	B	625	LYS
1	B	627	SER
1	B	665	LYS
1	B	720	VAL
1	B	722	LYS
1	C	326	THR
1	C	327	LEU
1	C	333	GLU
1	C	349	ARG
1	C	386	LEU
1	C	491	LYS
1	C	528	LEU
1	C	665	LYS
1	C	720	VAL
1	D	353	VAL
1	D	365	GLU
1	D	383	MET
1	D	390	ASN
1	D	394	ASP
1	D	395	THR
1	D	457	LYS
1	D	505	GLN
1	D	528	LEU
1	D	578	GLU
1	D	620	ASN
1	D	720	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	430	GLN
1	A	503	ASN
1	B	369	GLN
1	B	540	GLN
1	C	369	GLN
1	C	441	HIS

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Mol	Chain	Res	Type
1	D	540	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 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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	D	803	-	16,18,18	0.76	0	14,26,26	2.31	5 (35%)
3	H4B	D	801	-	16,18,18	0.85	0	14,26,26	2.26	5 (35%)
3	H4B	A	806	-	16,18,18	0.85	0	14,26,26	2.26	5 (35%)
4	A1CN3	A	803	-	23,23,23	0.47	0	28,31,31	1.51	3 (10%)
2	HEM	A	801	1	42,50,50	1.52	5 (11%)	46,82,82	1.77	7 (15%)
4	A1CN3	B	803	-	23,23,23	0.44	0	28,31,31	1.56	3 (10%)
4	A1CN3	D	804	-	23,23,23	0.45	0	28,31,31	1.31	2 (7%)
5	GOL	A	804	-	5,5,5	0.39	0	5,5,5	0.65	0
5	GOL	A	805	-	5,5,5	0.12	0	5,5,5	0.96	0
5	GOL	C	803	-	5,5,5	0.15	0	5,5,5	0.70	0
5	GOL	D	805	-	5,5,5	0.35	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	D	802	1	42,50,50	1.48	4 (9%)	46,82,82	1.61	5 (10%)
2	HEM	B	802	1	42,50,50	1.55	7 (16%)	46,82,82	1.72	10 (21%)
4	A1CN3	C	802	-	23,23,23	0.49	0	28,31,31	1.44	4 (14%)
2	HEM	C	801	1	42,50,50	1.56	7 (16%)	46,82,82	1.58	6 (13%)
3	H4B	A	802	-	16,18,18	0.68	0	14,26,26	2.25	6 (42%)

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	D	803	-	-	0/8/17/17	0/2/2/2
3	H4B	D	801	-	-	0/8/17/17	0/2/2/2
3	H4B	A	806	-	-	0/8/17/17	0/2/2/2
4	A1CN3	A	803	-	-	3/9/9/9	0/2/2/2
2	HEM	A	801	1	-	7/12/54/54	-
4	A1CN3	B	803	-	-	2/9/9/9	0/2/2/2
4	A1CN3	D	804	-	-	3/9/9/9	0/2/2/2
5	GOL	A	804	-	-	2/4/4/4	-
5	GOL	A	805	-	-	2/4/4/4	-
5	GOL	C	803	-	-	3/4/4/4	-
5	GOL	D	805	-	-	2/4/4/4	-
2	HEM	D	802	1	-	5/12/54/54	-
2	HEM	B	802	1	-	7/12/54/54	-
4	A1CN3	C	802	-	-	1/9/9/9	0/2/2/2
2	HEM	C	801	1	-	6/12/54/54	-
3	H4B	A	802	-	-	0/8/17/17	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	802	HEM	C3C-C2C	-4.40	1.34	1.40
2	A	801	HEM	C3C-C2C	-3.72	1.35	1.40
2	A	801	HEM	C3C-CAC	3.67	1.55	1.47
2	B	802	HEM	C3C-CAC	3.66	1.55	1.47
2	C	801	HEM	C3C-C2C	-3.60	1.35	1.40
2	B	802	HEM	C3C-C2C	-3.57	1.35	1.40
2	D	802	HEM	C3C-CAC	3.34	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	HEM	CAB-C3B	3.33	1.56	1.47
2	C	801	HEM	CAB-C3B	3.27	1.56	1.47
2	C	801	HEM	C3C-CAC	3.14	1.54	1.47
2	A	801	HEM	C3C-C4C	3.10	1.45	1.41
2	A	801	HEM	CAB-C3B	3.01	1.55	1.47
2	B	802	HEM	C3C-C4C	2.95	1.45	1.41
2	C	801	HEM	C3C-C4C	2.95	1.45	1.41
2	D	802	HEM	CAB-C3B	2.90	1.55	1.47
2	B	802	HEM	CMD-C2D	2.40	1.55	1.50
2	C	801	HEM	CMD-C2D	2.33	1.55	1.50
2	D	802	HEM	C3C-C4C	2.31	1.44	1.41
2	B	802	HEM	CMB-C2B	2.21	1.55	1.50
2	C	801	HEM	FE-NB	2.20	2.10	1.98
2	A	801	HEM	C3B-C2B	-2.15	1.32	1.37
2	C	801	HEM	CMB-C2B	2.10	1.55	1.50
2	B	802	HEM	CHB-C1B	2.00	1.39	1.34

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CBA-CAA-C2A	-6.39	101.80	112.54
4	A	803	A1CN3	C02-N01-C06	6.15	122.67	118.07
2	D	802	HEM	CBA-CAA-C2A	-6.11	102.27	112.54
2	B	802	HEM	CBA-CAA-C2A	-5.84	102.72	112.54
4	B	803	A1CN3	C02-N01-C06	5.41	122.12	118.07
3	D	803	H4B	C8A-C4A-C4	5.40	119.41	114.50
4	C	802	A1CN3	C02-N01-C06	5.38	122.09	118.07
3	D	801	H4B	C8A-C4A-C4	5.06	119.10	114.50
3	A	802	H4B	C8A-C4A-C4	4.88	118.94	114.50
2	A	801	HEM	C4B-CHC-C1C	4.76	128.84	122.56
4	D	804	A1CN3	C02-N01-C06	4.63	121.53	118.07
3	A	806	H4B	C8A-C4A-C4	4.62	118.70	114.50
2	C	801	HEM	CBA-CAA-C2A	-4.41	105.13	112.54
2	C	801	HEM	C4B-CHC-C1C	3.88	127.68	122.56
2	D	802	HEM	C4B-CHC-C1C	3.82	127.59	122.56
2	B	802	HEM	C4B-CHC-C1C	3.69	127.43	122.56
3	D	803	H4B	C2-N3-C4	3.65	121.04	115.96
3	D	801	H4B	C2-N3-C4	3.64	121.02	115.96
3	A	806	H4B	C2-N3-C4	3.60	120.97	115.96
3	A	802	H4B	C2-N3-C4	3.58	120.94	115.96
3	A	806	H4B	N1-C2-N3	-3.54	120.05	125.48
4	B	803	A1CN3	O09-C11-C12	3.47	121.16	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	HEM	C3B-C2B-C1B	3.45	109.00	106.41
2	B	802	HEM	C3B-C2B-C1B	3.45	109.00	106.41
3	D	801	H4B	N1-C2-N3	-3.38	120.30	125.48
2	A	801	HEM	CAD-CBD-CGD	-3.10	105.43	113.67
3	D	803	H4B	N1-C2-N3	-3.09	120.75	125.48
3	A	802	H4B	N1-C2-N3	-3.05	120.80	125.48
2	D	802	HEM	C3B-C2B-C1B	2.84	108.55	106.41
2	D	802	HEM	CAD-CBD-CGD	-2.75	106.36	113.67
2	C	801	HEM	C4C-CHD-C1D	2.73	126.16	122.56
4	C	802	A1CN3	O09-C11-C12	2.69	119.99	115.92
2	C	801	HEM	C4D-ND-C1D	2.53	108.20	105.21
3	A	802	H4B	C4-C4A-N5	2.52	122.17	118.57
3	A	806	H4B	C2-N1-C8A	2.50	120.52	114.59
2	B	802	HEM	C3D-C4D-ND	-2.50	107.43	110.17
2	B	802	HEM	C4C-CHD-C1D	2.48	125.83	122.56
2	A	801	HEM	CMA-C3A-C4A	-2.47	124.83	128.46
2	A	801	HEM	C3B-C4B-NB	-2.45	107.71	109.47
2	B	802	HEM	C4D-ND-C1D	2.43	108.09	105.21
2	C	801	HEM	C3D-C4D-ND	-2.40	107.54	110.17
2	B	802	HEM	C1B-NB-C4B	2.39	108.03	105.21
4	D	804	A1CN3	C05-C06-N01	-2.35	120.06	122.73
3	D	803	H4B	C4-C4A-N5	2.35	121.92	118.57
2	A	801	HEM	CHA-C4D-ND	2.31	127.24	124.37
3	D	801	H4B	C2-N1-C8A	2.31	120.08	114.59
4	A	803	A1CN3	C05-C06-N01	-2.30	120.11	122.73
3	D	803	H4B	C2-N1-C8A	2.30	120.06	114.59
3	A	802	H4B	C2-N1-C8A	2.28	120.00	114.59
4	A	803	A1CN3	O09-C11-C12	2.26	119.33	115.92
2	A	801	HEM	C3B-C2B-C1B	2.21	108.07	106.41
4	C	802	A1CN3	O09-C08-C06	2.20	115.64	109.56
3	A	802	H4B	N2-C2-N1	2.19	120.51	117.22
4	C	802	A1CN3	C05-C06-N01	-2.19	120.24	122.73
3	D	801	H4B	N2-C2-N1	2.17	120.47	117.22
4	B	803	A1CN3	C05-C06-N01	-2.15	120.28	122.73
3	A	806	H4B	N2-C2-N1	2.12	120.40	117.22
2	B	802	HEM	C2B-C1B-NB	-2.11	107.41	109.84
2	B	802	HEM	CMA-C3A-C4A	-2.04	125.46	128.46
2	D	802	HEM	C3D-C4D-ND	-2.04	107.94	110.17
2	B	802	HEM	C3B-C4B-NB	-2.03	108.01	109.47

There are no chirality outliers.

All (43) torsion outliers are listed below:

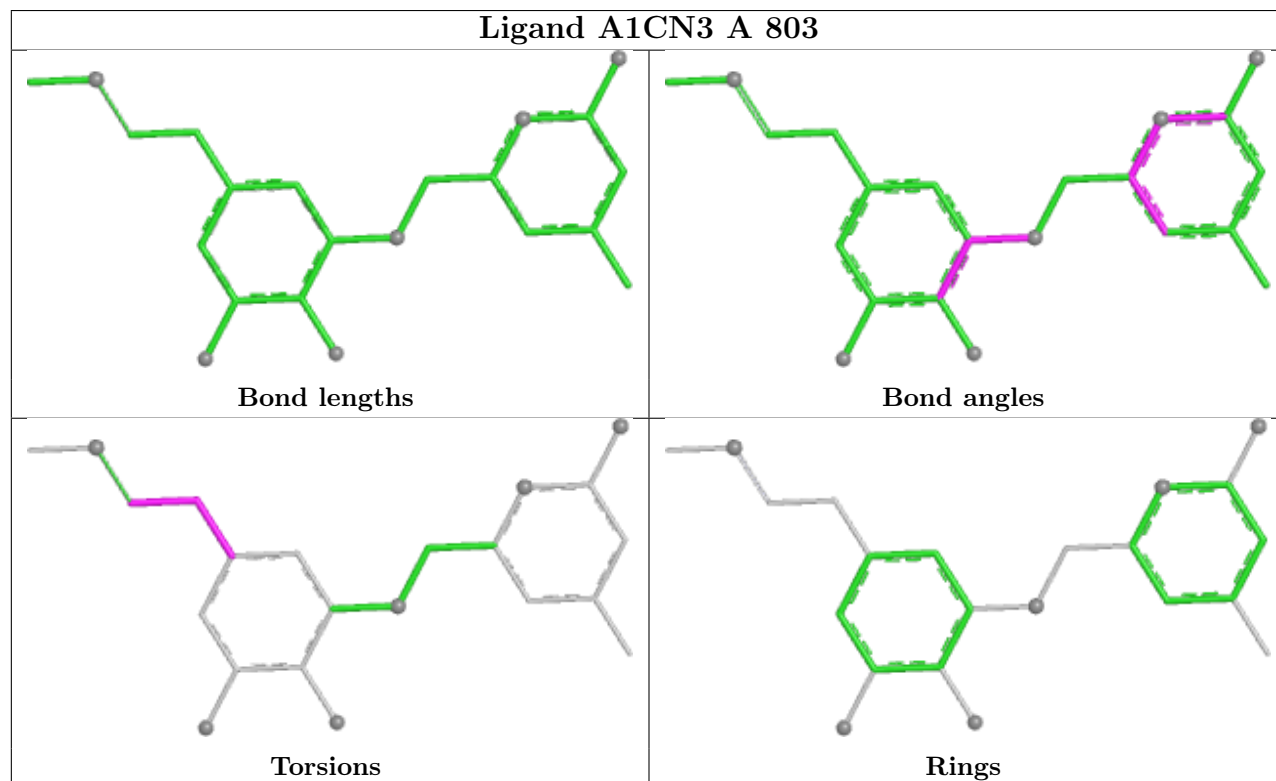
Mol	Chain	Res	Type	Atoms
2	A	801	HEM	C2D-C3D-CAD-CBD
2	A	801	HEM	C4D-C3D-CAD-CBD
2	D	802	HEM	C2D-C3D-CAD-CBD
2	D	802	HEM	C4D-C3D-CAD-CBD
4	A	803	A1CN3	C15-C17-C18-N19
4	B	803	A1CN3	C15-C17-C18-N19
4	B	803	A1CN3	C17-C18-N19-C20
4	C	802	A1CN3	C15-C17-C18-N19
4	D	804	A1CN3	C15-C17-C18-N19
5	A	804	GOL	O1-C1-C2-C3
5	A	805	GOL	O1-C1-C2-O2
5	A	805	GOL	O1-C1-C2-C3
5	C	803	GOL	O1-C1-C2-O2
2	C	801	HEM	C2A-CAA-CBA-CGA
5	C	803	GOL	O1-C1-C2-C3
5	C	803	GOL	C1-C2-C3-O3
5	D	805	GOL	O1-C1-C2-C3
5	A	804	GOL	O1-C1-C2-O2
2	C	801	HEM	C4D-C3D-CAD-CBD
5	D	805	GOL	O1-C1-C2-O2
2	C	801	HEM	C2D-C3D-CAD-CBD
2	B	802	HEM	C4D-C3D-CAD-CBD
2	B	802	HEM	C2D-C3D-CAD-CBD
2	A	801	HEM	C4B-C3B-CAB-CBB
2	B	802	HEM	C4B-C3B-CAB-CBB
2	C	801	HEM	C4B-C3B-CAB-CBB
2	D	802	HEM	C2A-CAA-CBA-CGA
2	C	801	HEM	CAD-CBD-CGD-O2D
2	B	802	HEM	CAD-CBD-CGD-O2D
2	C	801	HEM	CAD-CBD-CGD-O1D
2	B	802	HEM	CAD-CBD-CGD-O1D
2	B	802	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	D	802	HEM	CAD-CBD-CGD-O1D
2	A	801	HEM	CAD-CBD-CGD-O2D
2	B	802	HEM	CAA-CBA-CGA-O1A
2	D	802	HEM	CAD-CBD-CGD-O2D
4	A	803	A1CN3	C14-C15-C17-C18
2	A	801	HEM	CAD-CBD-CGD-O1D
4	D	804	A1CN3	C14-C15-C17-C18
4	A	803	A1CN3	C16-C15-C17-C18
4	D	804	A1CN3	C16-C15-C17-C18

There are no ring outliers.

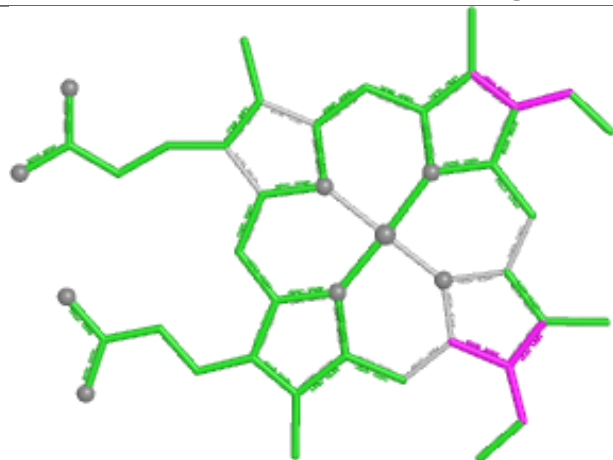
8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	803	H4B	1	0
4	A	803	A1CN3	1	0
2	A	801	HEM	3	0
4	B	803	A1CN3	1	0
5	C	803	GOL	1	0
2	D	802	HEM	2	0
2	B	802	HEM	3	0
2	C	801	HEM	2	0

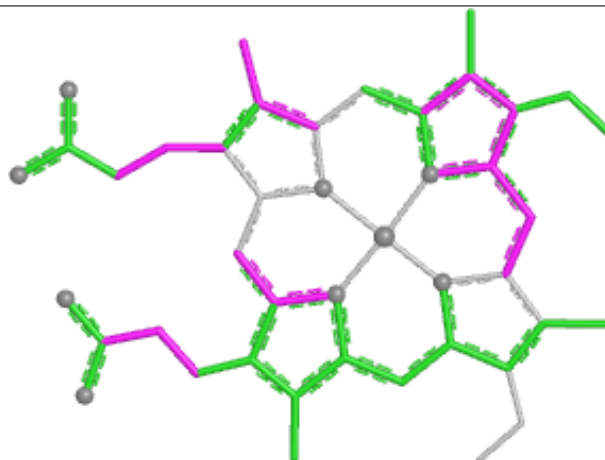
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



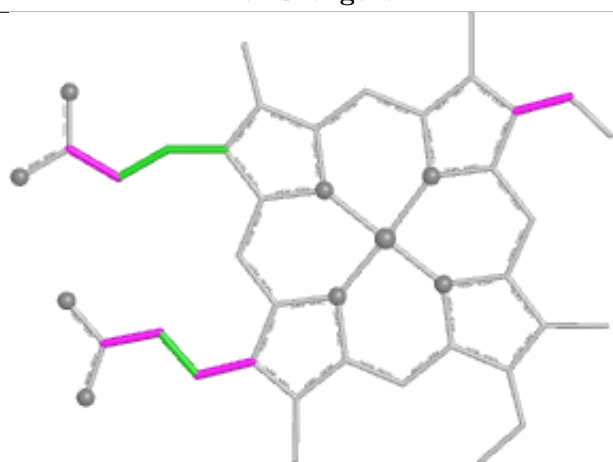
## Ligand HEM A 801



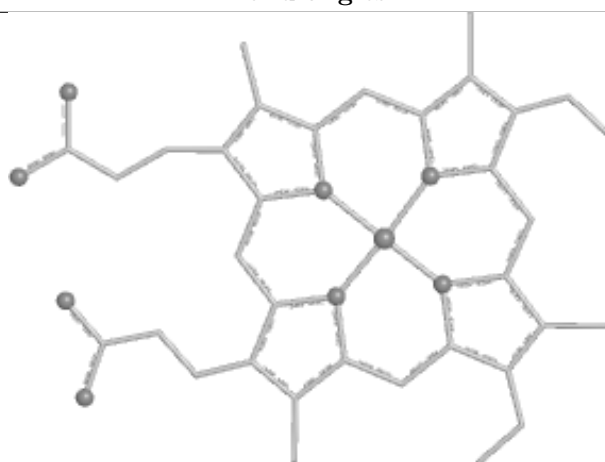
Bond lengths



Bond angles



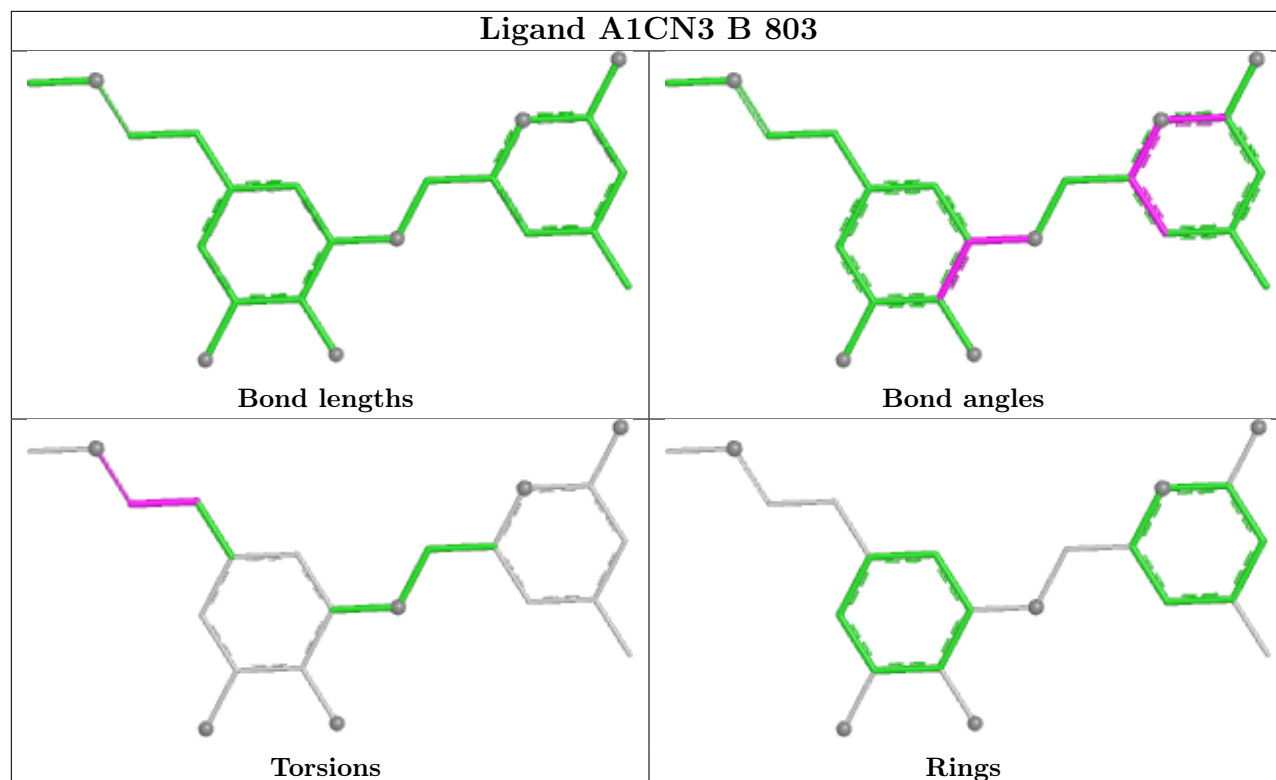
Torsions



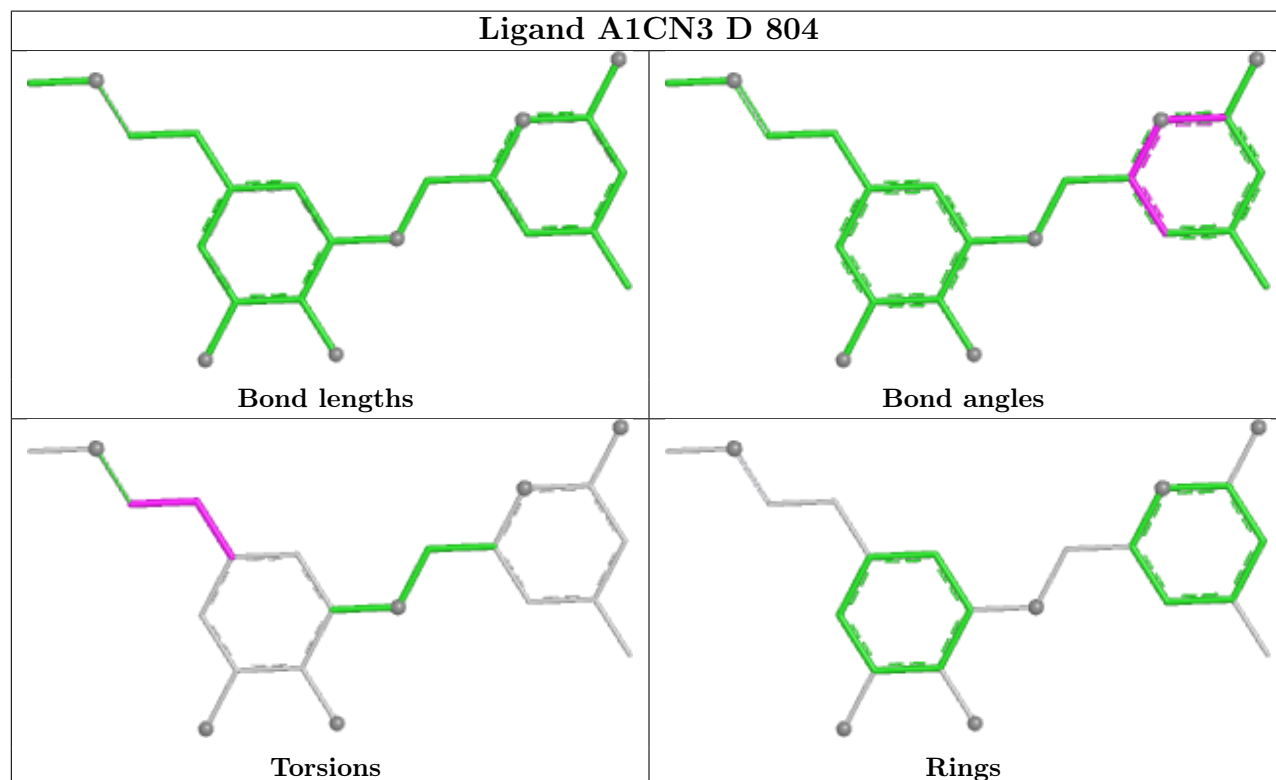
Rings

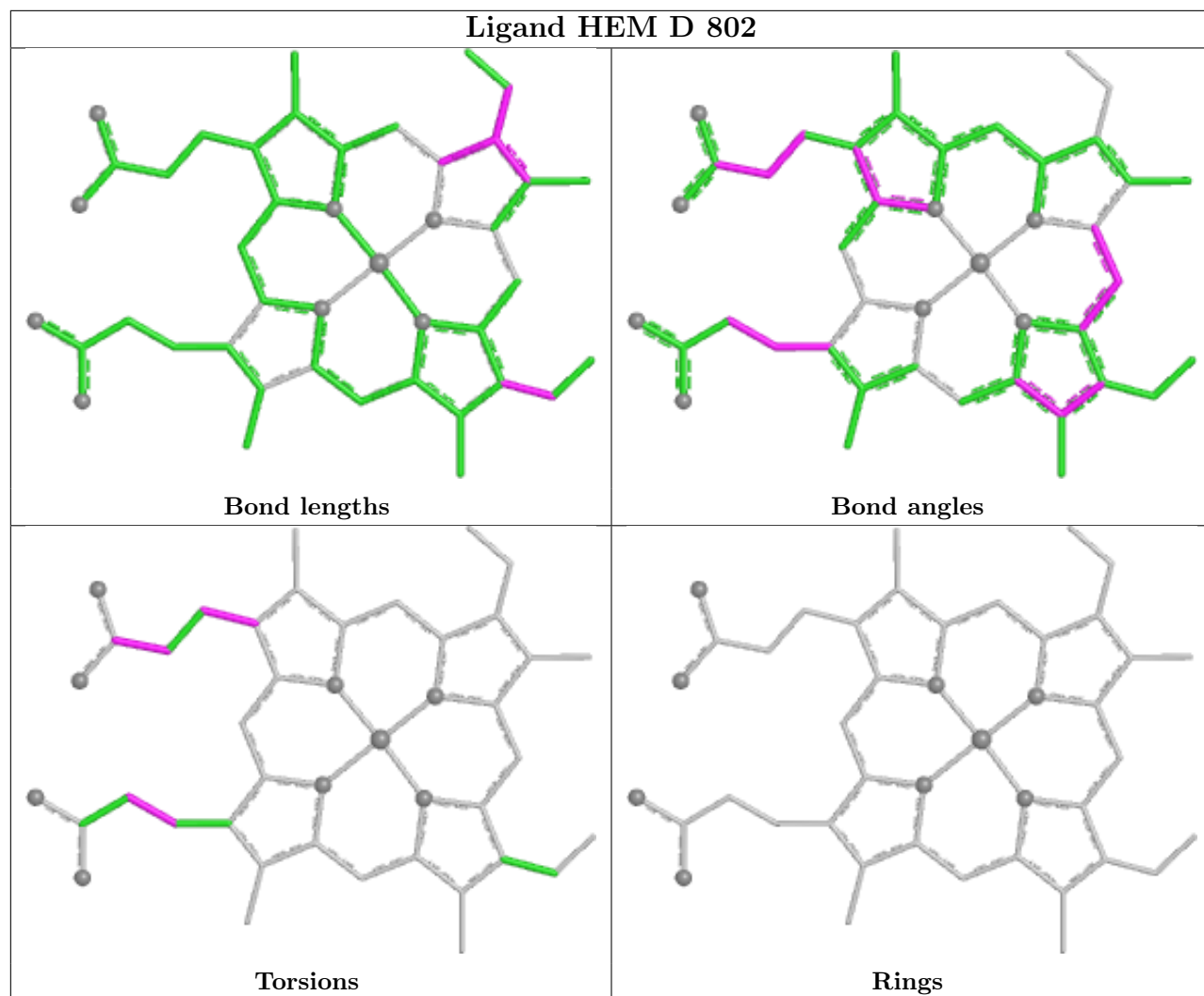


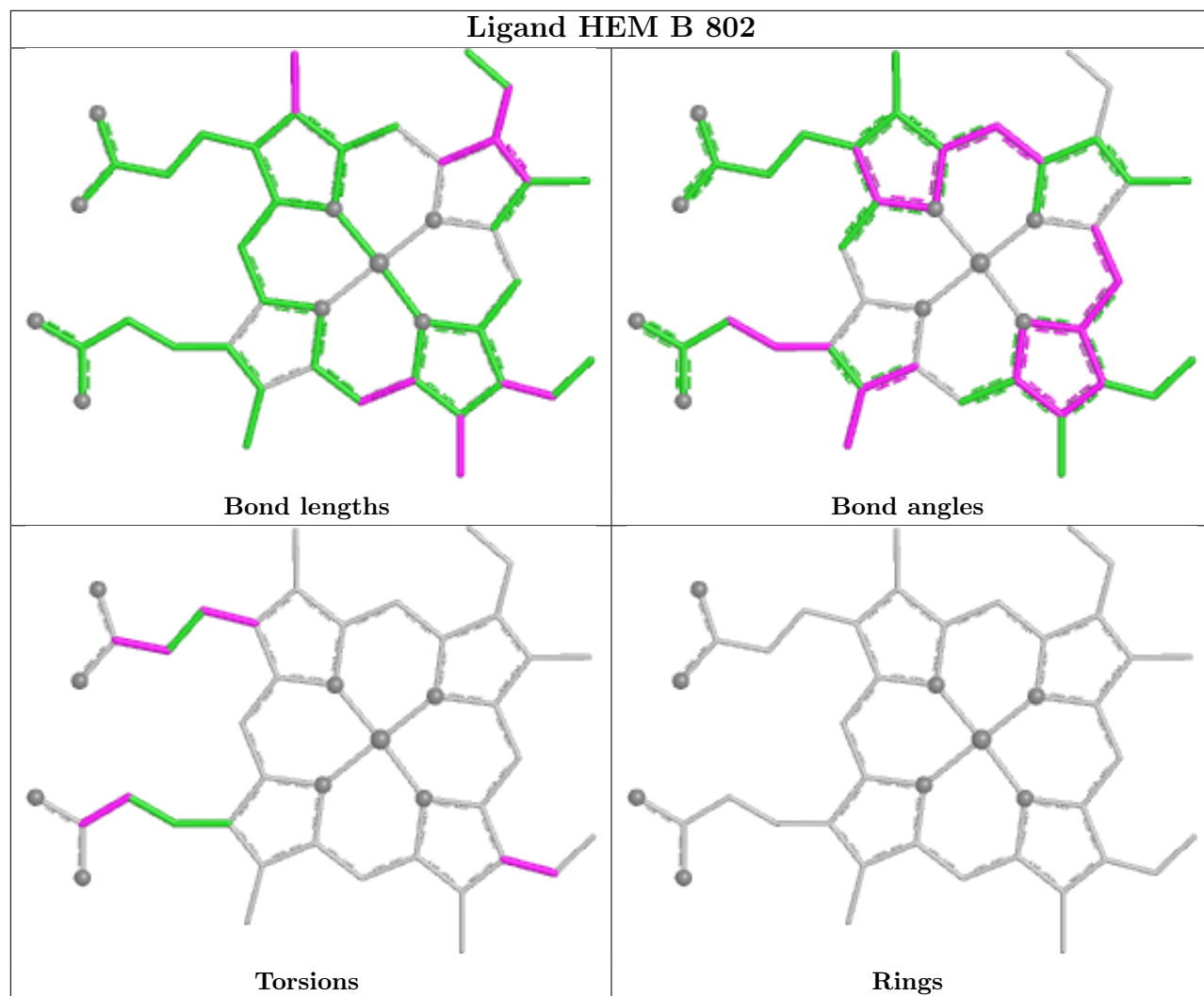
## Ligand A1CN3 B 803

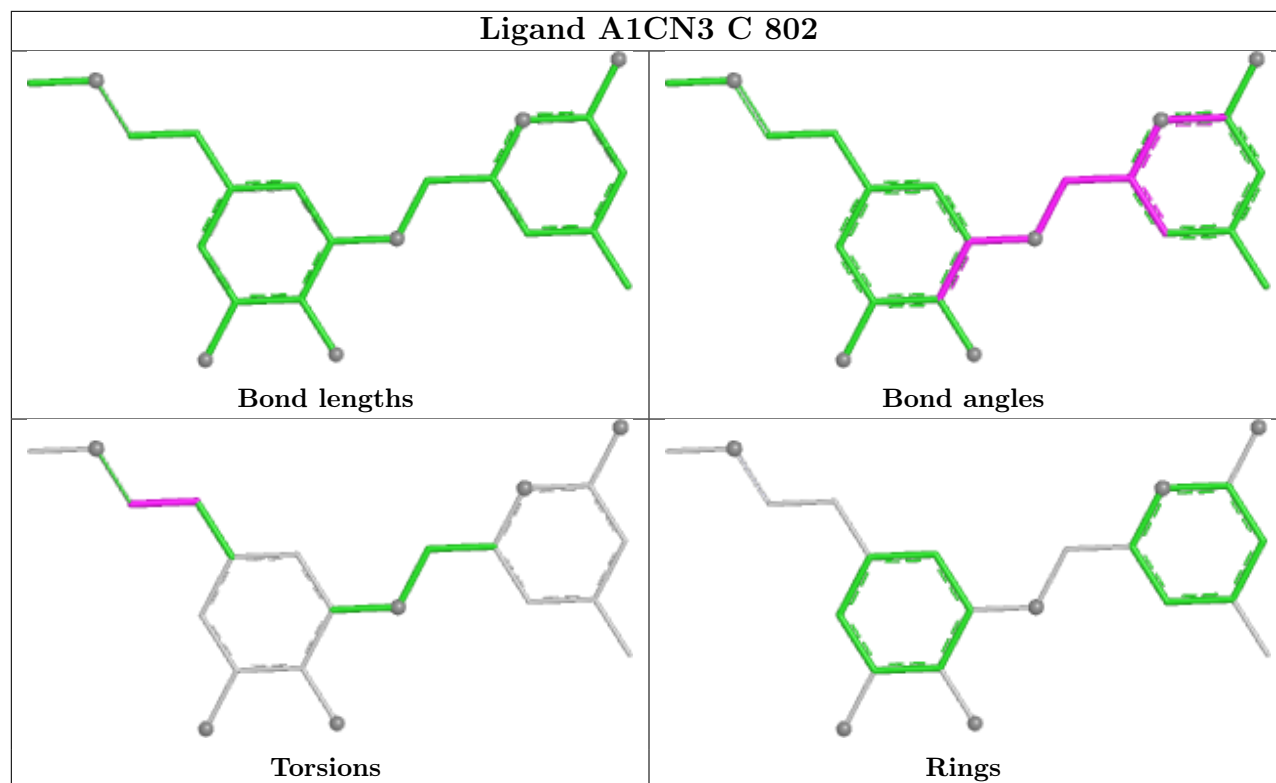


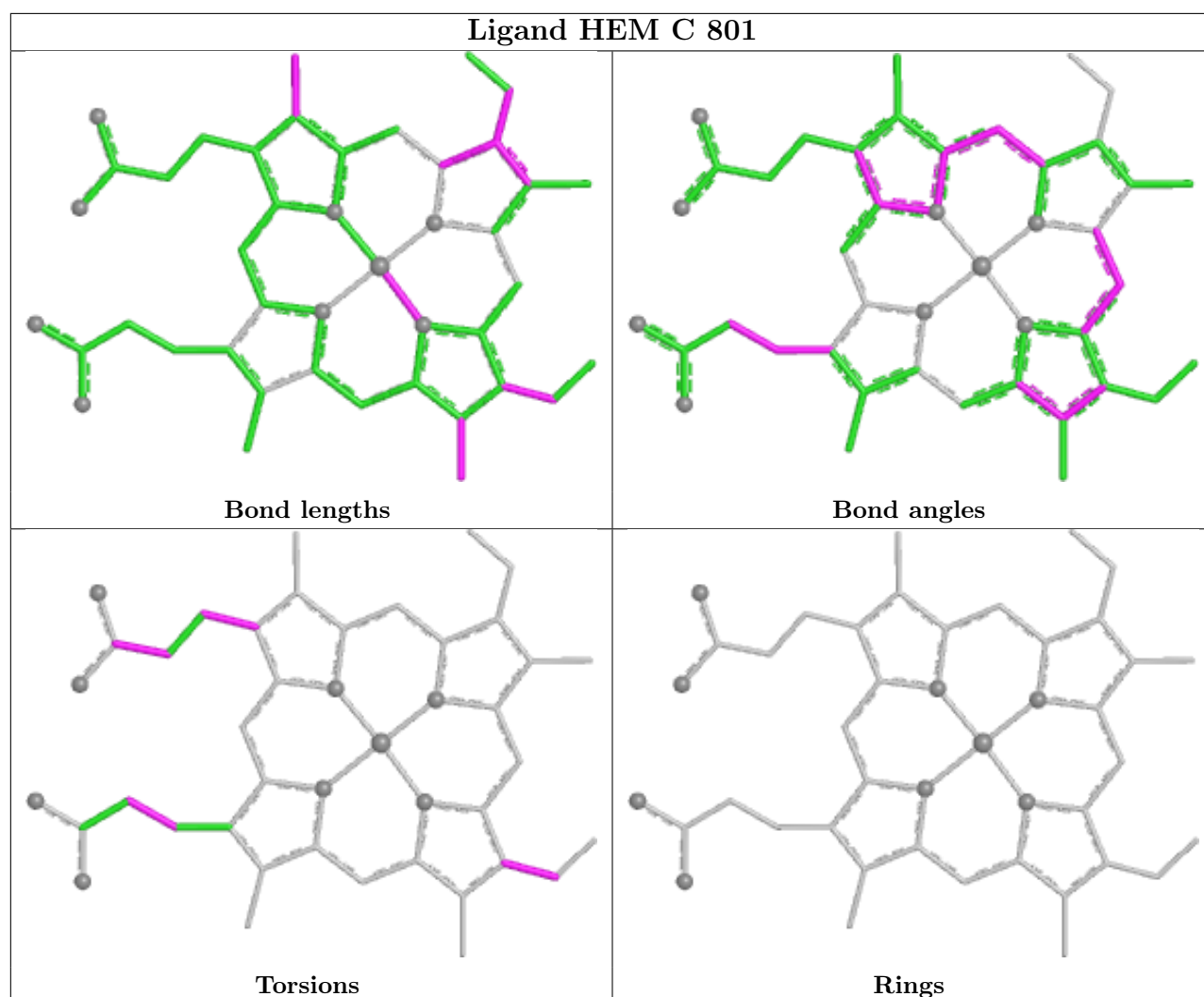
## Ligand A1CN3 D 804











## 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	414/423 (97%)	-1.20	0 100 100	24, 51, 75, 122	3 (0%)
1	B	419/423 (99%)	-1.11	0 100 100	29, 55, 85, 122	3 (0%)
1	C	420/423 (99%)	-1.08	0 100 100	28, 56, 86, 120	2 (0%)
1	D	412/423 (97%)	-1.18	0 100 100	26, 51, 75, 95	2 (0%)
All	All	1665/1692 (98%)	-1.14	0 100 100	24, 53, 80, 122	10 (0%)

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 oligosaccharides 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.

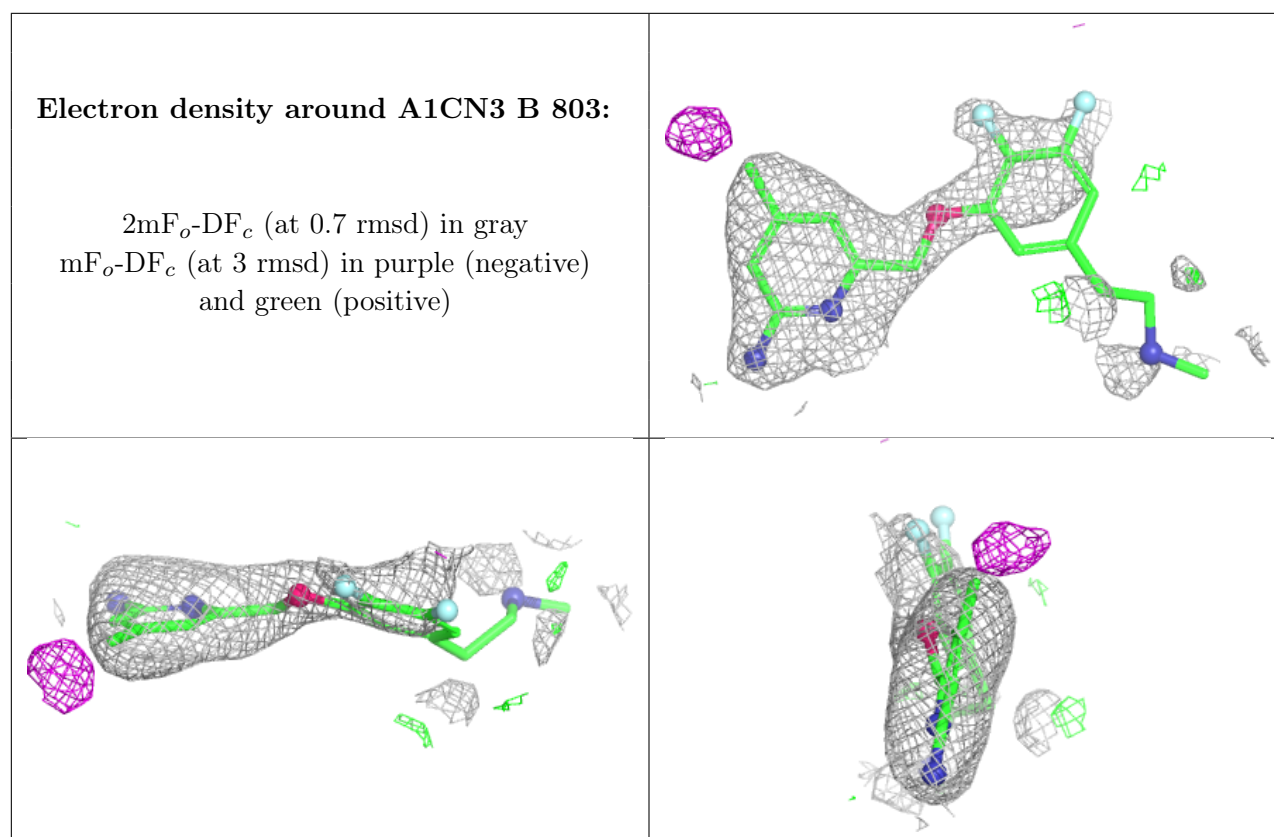
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	C	803	6/6	0.97	0.05	57,58,66,67	0
4	A1CN3	B	803	22/22	0.98	0.07	43,80,94,96	0
4	A1CN3	D	804	22/22	0.98	0.06	42,73,93,96	0
5	GOL	A	804	6/6	0.98	0.05	53,62,63,69	0

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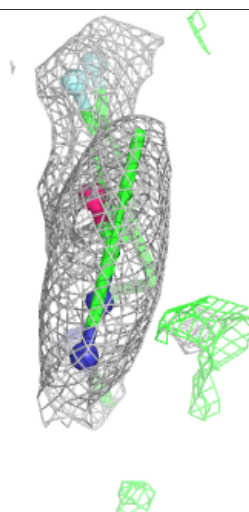
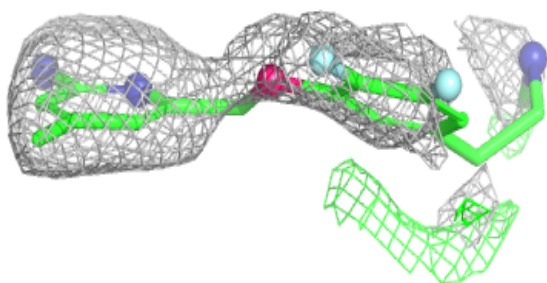
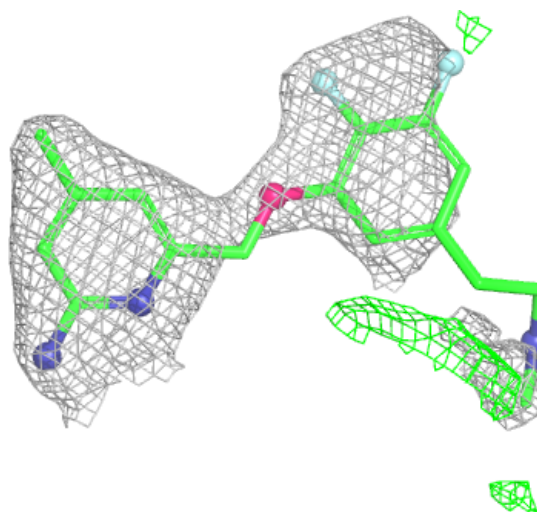
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	A	805	6/6	0.98	0.06	50,56,62,63	0
3	H4B	D	801	17/17	0.98	0.06	50,55,60,65	0
5	GOL	D	805	6/6	0.98	0.05	58,62,67,72	0
4	A1CN3	C	802	22/22	0.99	0.06	44,75,86,87	0
3	H4B	A	806	17/17	0.99	0.04	49,54,60,62	0
2	HEM	C	801	43/43	0.99	0.04	41,46,67,74	0
3	H4B	D	803	17/17	0.99	0.04	43,52,55,57	0
4	A1CN3	A	803	22/22	0.99	0.06	40,70,87,88	0
3	H4B	A	802	17/17	0.99	0.04	47,52,56,58	0
2	HEM	B	802	43/43	1.00	0.04	39,47,66,77	0
2	HEM	A	801	43/43	1.00	0.04	35,42,57,70	0
2	HEM	D	802	43/43	1.00	0.04	39,45,60,69	0
6	ZN	B	801	1/1	1.00	0.01	43,43,43,43	0
6	ZN	C	804	1/1	1.00	0.01	44,44,44,44	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 A1CN3 D 804:**

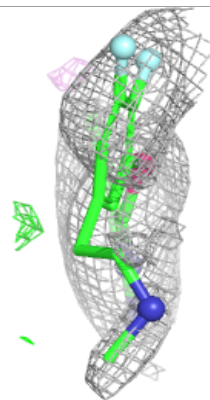
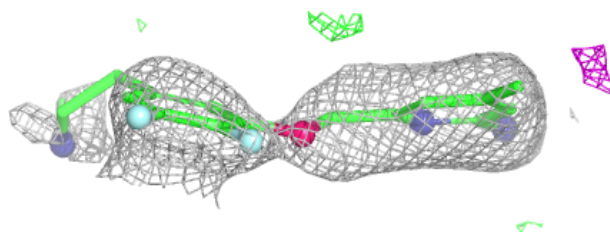
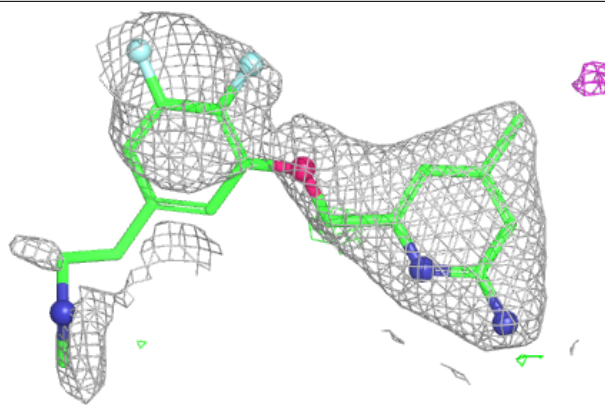
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





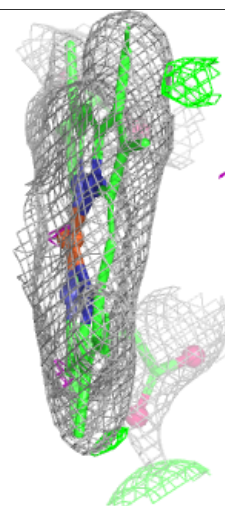
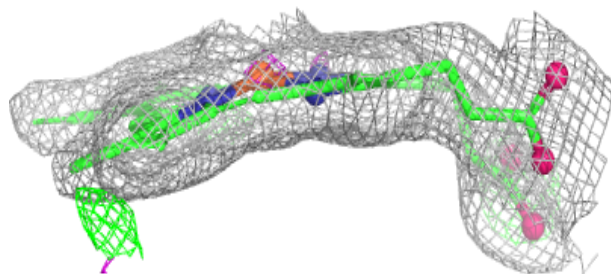
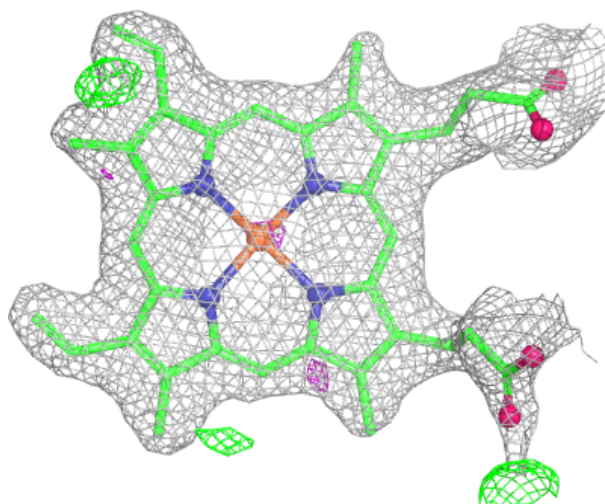
**Electron density around A1CN3 C 802:**

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



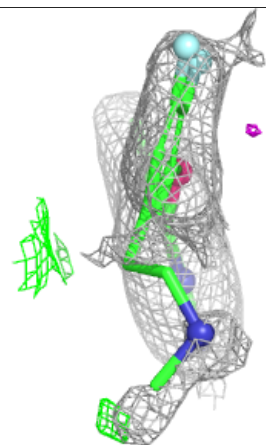
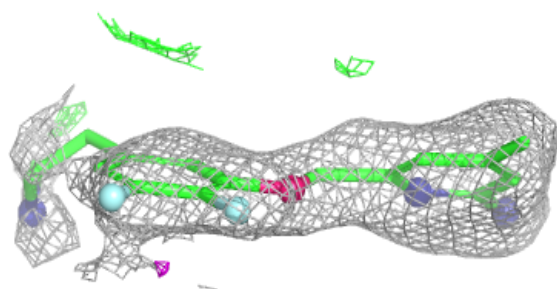
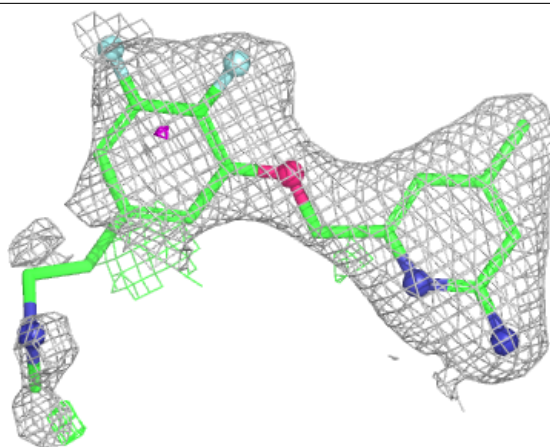
**Electron density around HEM C 801:**

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



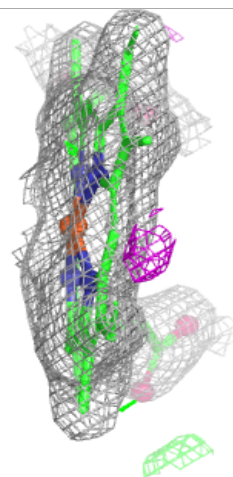
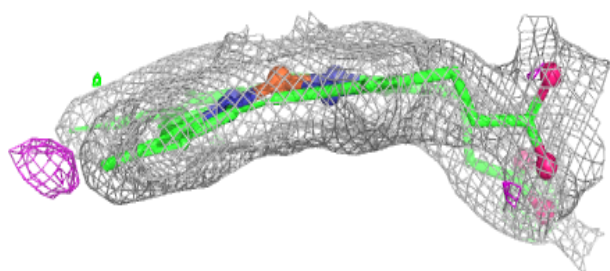
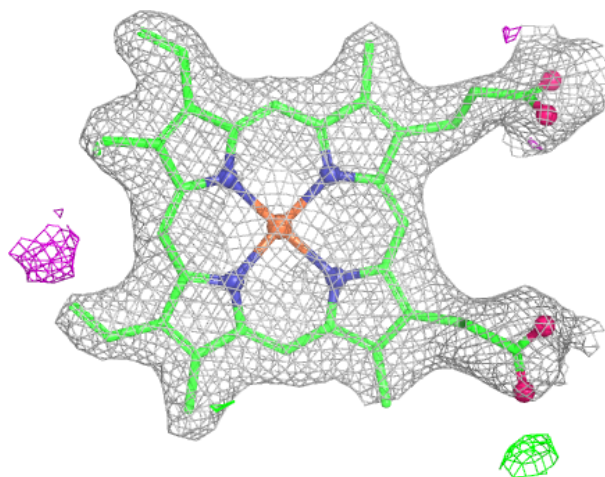
**Electron density around A1CN3 A 803:**

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



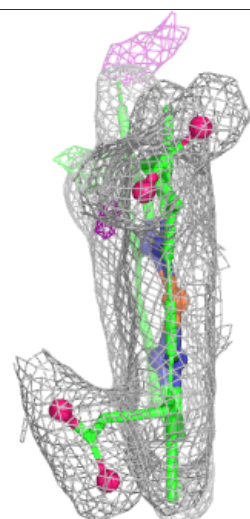
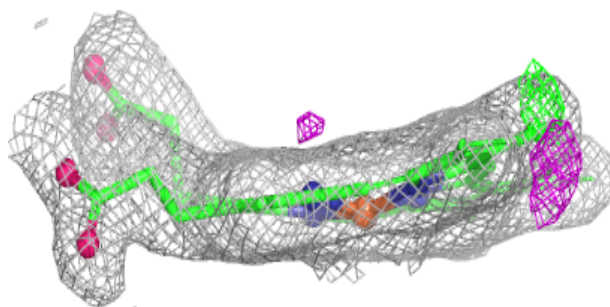
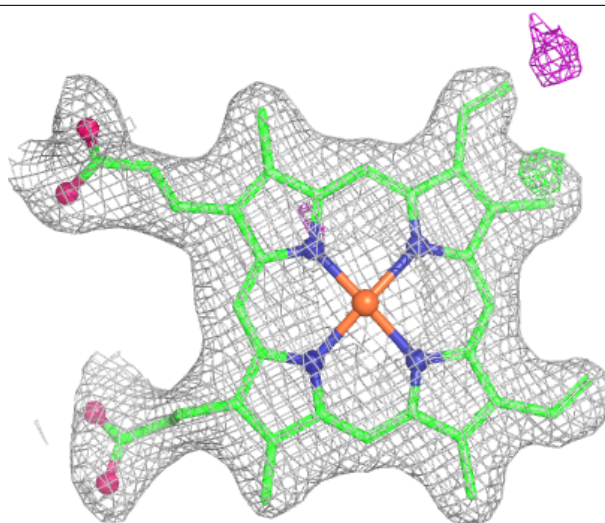
**Electron density around HEM B 802:**

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



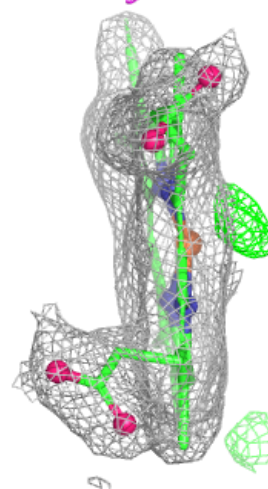
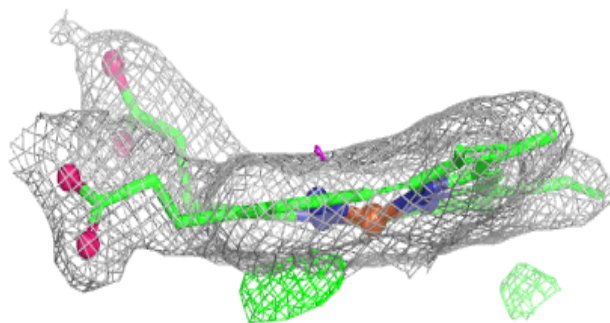
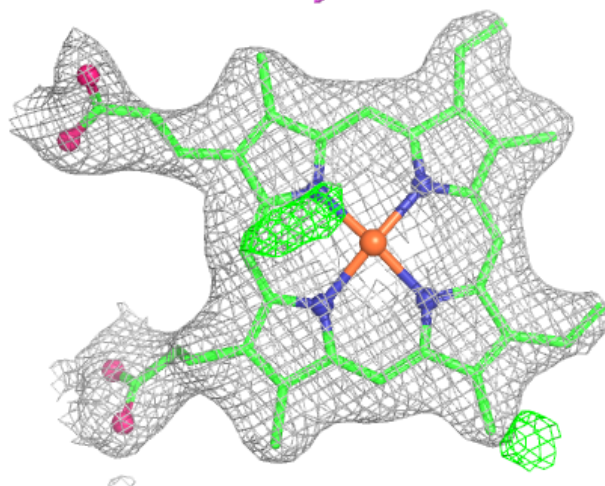
**Electron density around HEM A 801:**

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



**Electron density around HEM D 802:**

$2mF_o-DF_c$  (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.