



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:30 PM UTC

PDB ID : 6L1B / pdb_0000611b
Title : Crystal Structure of P450BM3 with N-(3-cyclopentylpropanoyl)-L-pipecolyl-L-phenylalanine
Authors : Shoji, O.; Yonemura, K.
Deposited on : 2019-09-28
Resolution : 1.74 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

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>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

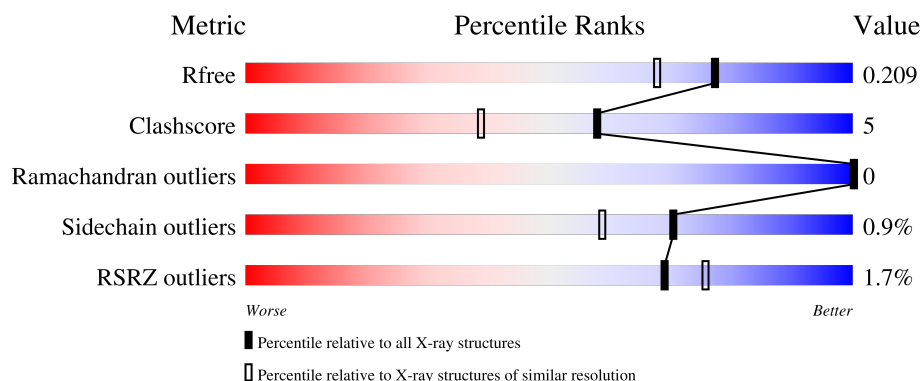
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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 ≥ 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	456	0% 92% 7%
1	B	456	2% 91% 8%

2 Entry composition [i](#)

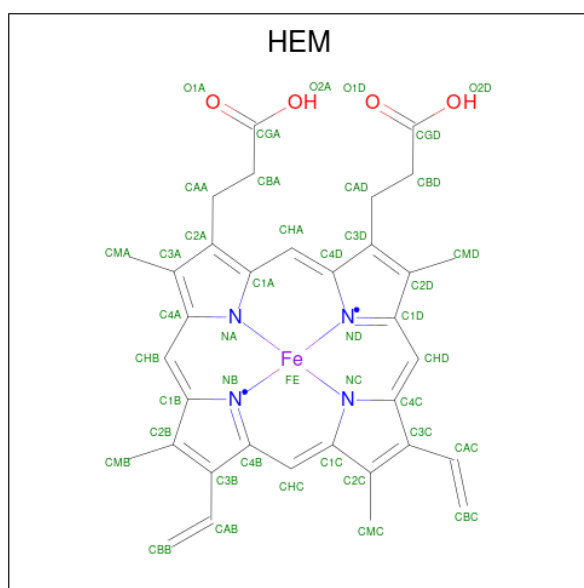
There are 6 unique types of molecules in this entry. The entry contains 8540 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	21	0
			3830	2445	648	718	19			
1	B	454	Total	C	N	O	S	0	25	0
			3867	2468	656	725	18			

- 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	C	Fe	N	O	0	1
			86	68	2	8	8		
2	B	1	Total	C	Fe	N	O	0	1
			86	68	2	8	8		

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



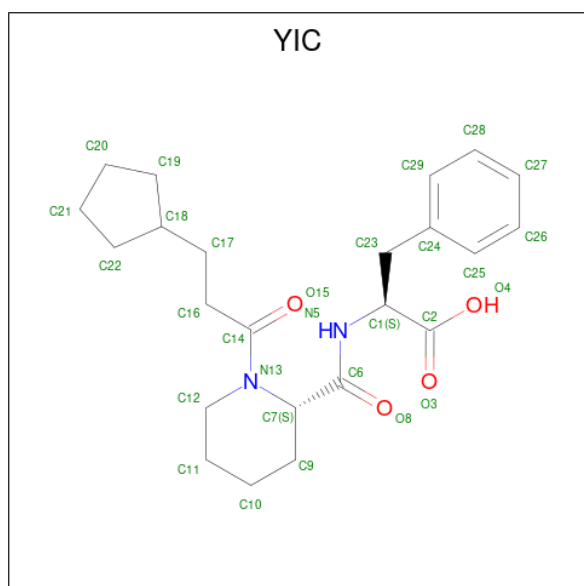
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	1
			12	6	6		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is (2S)-2-[[[(2S)-1-(3-cyclopentylpropanoyl)piperidin-2-yl]carbonylamino]-3-phenylpropanoic acid (CCD ID: YIC) (formula: C₂₃H₃₂N₂O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			29	23	2	4		
5	B	1	Total	C	N	O	0	0
			29	23	2	4		

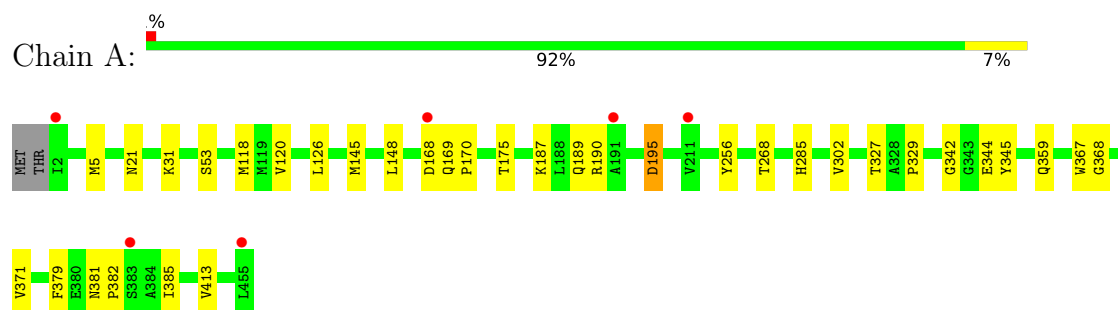
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	278	Total 278	O 278	0	0
6	B	267	Total 267	O 267	0	0

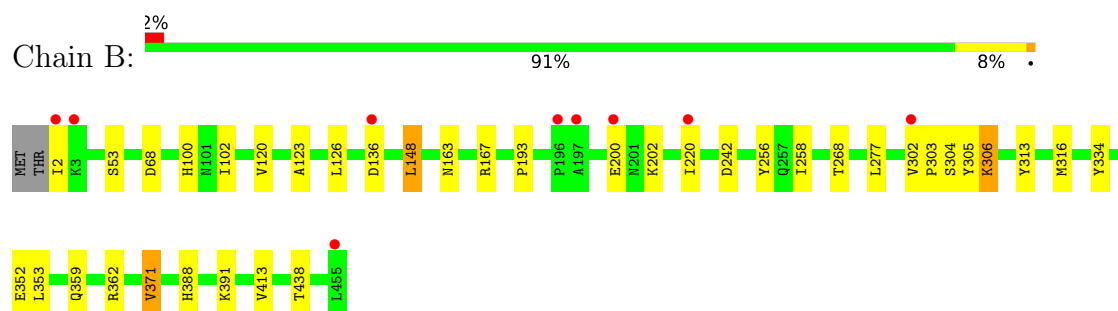
3 Residue-property plots [i](#)

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: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.85Å 148.30Å 63.69Å 90.00° 98.61° 90.00°	Depositor
Resolution (Å)	48.00 – 1.74 48.00 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.00-1.74) 99.0 (48.00-1.74)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.172 , 0.203 0.181 , 0.209	Depositor DCC
R_{free} test set	5450 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8540	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, YIC, DMS, 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	1.04	0/3915	1.22	2/5290 (0.0%)
1	B	1.06	0/3952	1.21	1/5342 (0.0%)
All	All	1.05	0/7867	1.21	3/10632 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	THR	CA-CB-OG1	-5.28	101.68	109.60
1	A	256	TYR	CA-C-O	-5.17	115.07	120.55
1	B	256	TYR	CA-C-O	-5.01	115.24	120.55

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	3830	0	3794	24	0
1	B	3867	0	3828	35	0
2	A	86	0	60	10	0
2	B	86	0	60	6	0
3	A	4	0	6	1	0
3	B	4	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	30	0	40	1	0
4	B	30	0	40	1	0
5	A	29	0	0	0	0
5	B	29	0	0	0	0
6	A	278	0	0	3	0
6	B	267	0	0	1	0
All	All	8540	0	7834	72	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 5.

All (72) 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:306[B]:LYS:H	1:B:306[B]:LYS:CE	1.72	1.01
1:A:327[B]:THR:HG22	2:A:501[B]:HEM:CBC	1.95	0.97
2:A:501[A]:HEM:HMC1	2:A:501[A]:HEM:HBC2	1.48	0.94
1:B:306[B]:LYS:H	1:B:306[B]:LYS:HE2	1.32	0.91
1:B:306[B]:LYS:HE2	1:B:306[B]:LYS:N	1.93	0.83
2:A:501[A]:HEM:HBC2	2:A:501[A]:HEM:CMC	2.14	0.78
2:B:501[B]:HEM:HMC2	2:B:501[B]:HEM:HBC2	1.73	0.71
1:B:306[B]:LYS:H	1:B:306[B]:LYS:HE3	1.53	0.71
1:A:285:HIS:HA	4:A:507:GOL:H31	1.72	0.70
2:B:501[A]:HEM:HMC1	2:B:501[A]:HEM:HBC2	1.73	0.69
1:B:306[B]:LYS:CE	1:B:306[B]:LYS:N	2.52	0.62
2:B:501[B]:HEM:CMB	2:B:501[B]:HEM:HBB2	2.29	0.62
2:B:501[B]:HEM:HBB2	2:B:501[B]:HEM:HMB2	1.80	0.62
1:A:268:THR:HG21	3:A:502:DMS:O	2.00	0.62
2:A:501[B]:HEM:HMC2	2:A:501[B]:HEM:HBC2	1.84	0.59
1:B:53[B]:SER:HB2	1:B:359:GLN:HB3	1.83	0.59
1:B:2:ILE:N	6:B:606:HOH:O	2.37	0.57
1:A:120:VAL:HG11	1:A:302:VAL:CG1	2.35	0.57
1:A:126[A]:LEU:HD21	1:A:145:MET:HE1	1.87	0.57
2:B:501[B]:HEM:HBC2	2:B:501[B]:HEM:CMC	2.34	0.57
1:B:268:THR:HG21	3:B:502:DMS:O	2.04	0.56
1:B:126[B]:LEU:C	1:B:126[B]:LEU:HD13	2.31	0.55
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.88	0.55
1:B:220[A]:ILE:HD11	1:B:258[A]:ILE:CD1	2.37	0.54
1:B:120:VAL:HG11	1:B:302[A]:VAL:HG13	1.91	0.53
1:A:327[B]:THR:CG2	2:A:501[B]:HEM:CBC	2.80	0.51
1:A:187:LYS:HG2	1:A:190:ARG:NH1	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501[A]:HEM:HMC1	2:A:501[A]:HEM:CBC	2.31	0.50
2:A:501[B]:HEM:HBC2	2:A:501[B]:HEM:CMC	2.41	0.50
1:B:148[A]:LEU:HD22	1:B:148[A]:LEU:O	2.12	0.49
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.94	0.49
1:A:327[B]:THR:O	1:A:329:PRO:HD3	2.13	0.49
2:A:501[A]:HEM:HMB2	2:A:501[A]:HEM:HBB2	1.95	0.48
1:B:268:THR:HG22	1:B:438[A]:THR:HG21	1.95	0.48
1:B:163:ASN:O	1:B:167[B]:ARG:HD3	2.14	0.48
1:A:195:ASP:OD1	1:A:195:ASP:C	2.56	0.48
1:B:123:ALA:HB2	1:B:413[B]:VAL:HG12	1.95	0.48
1:B:220[A]:ILE:HD11	1:B:258[A]:ILE:HD12	1.96	0.48
1:B:305:TYR:HB3	1:B:306[B]:LYS:HE2	1.96	0.48
1:A:21:ASN:OD1	1:A:189:GLN:OE1	2.33	0.47
1:A:118[A]:MET:HG3	6:A:690:HOH:O	2.14	0.47
1:B:313:TYR:HD1	1:B:316[A]:MET:HE3	1.80	0.47
1:A:148:LEU:HD21	1:A:413[A]:VAL:HG21	1.97	0.46
1:B:100:HIS:HE1	4:B:503:GOL:O2	1.98	0.46
1:B:362:ARG:HA	1:B:371[B]:VAL:CG2	2.46	0.45
1:A:53:SER:HB3	1:A:359:GLN:HB3	1.99	0.45
1:B:148[A]:LEU:C	1:B:148[A]:LEU:HD13	2.41	0.44
1:A:368:GLY:O	1:A:371:VAL:HG13	2.17	0.44
1:B:68:ASP:HB3	1:B:334:TYR:CE2	2.53	0.44
1:B:120:VAL:HG11	1:B:302[B]:VAL:HG13	1.98	0.44
1:B:313:TYR:CD1	1:B:316[A]:MET:HE3	2.52	0.43
1:A:379:PHE:CD1	1:A:385[A]:ILE:HD11	2.53	0.43
1:B:352[B]:GLU:HG2	1:B:353:LEU:N	2.34	0.42
1:A:169:GLN:HA	1:A:170:PRO:HD3	1.94	0.42
1:B:193:PRO:O	1:B:202[A]:LYS:NZ	2.53	0.42
2:B:501[B]:HEM:HMB2	2:B:501[B]:HEM:CBB	2.49	0.42
1:A:342:GLY:O	1:A:344:GLU:HG3	2.20	0.42
1:A:126[B]:LEU:HD11	1:A:145:MET:HE1	2.02	0.42
1:B:167[B]:ARG:HH11	1:B:167[B]:ARG:HB3	1.84	0.42
1:B:304:SER:HB2	1:B:306[B]:LYS:HE3	2.02	0.42
1:A:31[B]:LYS:NZ	6:A:611:HOH:O	2.47	0.41
1:A:327[B]:THR:HG22	2:A:501[B]:HEM:HBC1	1.95	0.41
1:A:345:TYR:OH	6:A:601:HOH:O	2.22	0.41
1:A:381:ASN:HA	1:A:382:PRO:HD2	1.83	0.41
1:B:163:ASN:O	1:B:167[B]:ARG:CD	2.68	0.41
1:A:5:MET:HE3	1:A:5:MET:HB2	1.95	0.41
1:B:302[B]:VAL:HA	1:B:303:PRO:HD3	1.89	0.41
1:B:362:ARG:HA	1:B:371[B]:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501[A]:HEM:HBB2	2:A:501[A]:HEM:CMB	2.50	0.41
1:B:102[B]:ILE:HD11	1:B:242:ASP:N	2.35	0.41
1:B:277:LEU:HD12	1:B:277:LEU:HA	1.91	0.41
1:B:120:VAL:HG11	1:B:302[B]:VAL:CG1	2.50	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	473/456 (104%)	461 (98%)	12 (2%)	0	100	100
1	B	477/456 (105%)	459 (96%)	18 (4%)	0	100	100
All	All	950/912 (104%)	920 (97%)	30 (3%)	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	419/400 (105%)	417 (100%)	2 (0%)	81	75
1	B	423/400 (106%)	414 (98%)	9 (2%)	47	24
All	All	842/800 (105%)	831 (99%)	11 (1%)	70	43

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	ASP
1	A	195	ASP
1	B	136	ASP
1	B	148[A]	LEU
1	B	148[B]	LEU
1	B	200[A]	GLU
1	B	200[B]	GLU
1	B	306[A]	LYS
1	B	306[B]	LYS
1	B	371[A]	VAL
1	B	371[B]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	204	GLN
1	A	310	GLN
1	A	319	ASN
1	A	359	GLN
1	B	27	GLN
1	B	73	GLN
1	B	100	HIS
1	B	204	GLN
1	B	285	HIS
1	B	359	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 ligands are modelled in this entry.

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
2	HEM	A	501[A]	1,3	50,50,50	1.44	6 (12%)	67,82,82	1.61	12 (17%)
2	HEM	B	501[B]	1,3	50,50,50	1.49	9 (18%)	67,82,82	1.83	16 (23%)
4	GOL	B	505[A]	-	5,5,5	0.10	0	5,5,5	0.26	0
4	GOL	A	507	-	5,5,5	0.08	0	5,5,5	0.37	0
4	GOL	B	506	-	5,5,5	0.08	0	5,5,5	0.30	0
4	GOL	A	506	-	5,5,5	0.15	0	5,5,5	0.34	0
2	HEM	A	501[B]	1,3	50,50,50	1.51	11 (22%)	67,82,82	1.45	10 (14%)
4	GOL	B	505[B]	-	5,5,5	0.12	0	5,5,5	0.26	0
4	GOL	B	504	-	5,5,5	0.16	0	5,5,5	0.35	0
3	DMS	A	502	2	3,3,3	0.50	0	3,3,3	0.31	0
4	GOL	B	503	-	5,5,5	0.13	0	5,5,5	0.43	0
4	GOL	A	505	-	5,5,5	0.23	0	5,5,5	0.51	0
3	DMS	B	502	2	3,3,3	0.21	0	3,3,3	0.41	0
4	GOL	A	504	-	5,5,5	0.18	0	5,5,5	0.43	0
5	YIC	A	508	-	31,31,31	0.94	1 (3%)	40,41,41	1.47	8 (20%)
4	GOL	A	503	-	5,5,5	0.07	0	5,5,5	0.10	0
2	HEM	B	501[A]	1,3	50,50,50	1.48	7 (14%)	67,82,82	1.61	13 (19%)
5	YIC	B	507	-	31,31,31	0.76	1 (3%)	40,41,41	0.99	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
2	HEM	A	501[A]	1,3	-	4/14/54/54	-
2	HEM	B	501[B]	1,3	-	2/14/54/54	-
4	GOL	B	505[A]	-	-	2/4/4/4	-
4	GOL	A	507	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	506	-	-	0/4/4/4	-
4	GOL	A	506	-	-	2/4/4/4	-
2	HEM	A	501[B]	1,3	-	2/14/54/54	-
4	GOL	B	505[B]	-	-	2/4/4/4	-
4	GOL	B	504	-	-	2/4/4/4	-
5	YIC	A	508	-	-	1/25/43/43	0/3/3/3
4	GOL	B	503	-	-	0/4/4/4	-
4	GOL	A	505	-	-	1/4/4/4	-
4	GOL	A	504	-	-	2/4/4/4	-
4	GOL	A	503	-	-	2/4/4/4	-
2	HEM	B	501[A]	1,3	-	2/14/54/54	-
5	YIC	B	507	-	-	1/25/43/43	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	HEM	FE-NB	4.59	2.09	1.94
2	A	501[B]	HEM	FE-NB	4.36	2.08	1.94
2	B	501[A]	HEM	FE-NB	4.17	2.07	1.94
2	B	501[B]	HEM	FE-NB	3.99	2.07	1.94
2	A	501[A]	HEM	FE-NC	3.69	2.07	1.95
2	A	501[A]	HEM	C1B-NB	-3.63	1.34	1.40
2	B	501[A]	HEM	C4B-NB	-3.61	1.31	1.38
2	B	501[A]	HEM	FE-NA	3.55	2.06	1.95
2	B	501[B]	HEM	C1B-NB	-3.49	1.34	1.40
2	B	501[B]	HEM	C4B-NB	-3.36	1.32	1.38
2	A	501[B]	HEM	C1B-NB	-3.23	1.34	1.40
2	B	501[A]	HEM	FE-NC	3.22	2.05	1.95
2	A	501[B]	HEM	C4D-ND	-3.21	1.34	1.40
2	B	501[B]	HEM	FE-NC	3.04	2.05	1.95
2	A	501[B]	HEM	C3B-C4B	3.01	1.50	1.44
2	A	501[B]	HEM	C3C-C4C	-2.99	1.40	1.46
2	B	501[A]	HEM	C1C-NC	-2.96	1.34	1.39
2	B	501[B]	HEM	C4D-ND	-2.93	1.35	1.40
2	B	501[B]	HEM	C4D-C3D	2.88	1.49	1.45
2	A	501[B]	HEM	FE-NC	2.81	2.04	1.95
2	B	501[B]	HEM	C1C-NC	-2.70	1.34	1.39
2	A	501[A]	HEM	C1D-ND	-2.57	1.33	1.38
2	B	501[A]	HEM	C1B-NB	-2.55	1.35	1.40
2	A	501[B]	HEM	C1C-C2C	-2.46	1.40	1.45
2	A	501[A]	HEM	C4D-ND	-2.40	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	HEM	FE-NA	2.36	2.02	1.95
5	A	508	YIC	C28-C29	2.34	1.42	1.38
2	A	501[B]	HEM	C4C-NC	-2.33	1.35	1.39
2	A	501[B]	HEM	FE-NA	2.28	2.02	1.95
2	A	501[B]	HEM	C4B-NB	-2.26	1.34	1.38
2	A	501[B]	HEM	C4D-C3D	2.24	1.48	1.45
2	B	501[A]	HEM	C3B-C4B	2.12	1.49	1.44
5	B	507	YIC	O3-C2	2.10	1.28	1.22
2	B	501[B]	HEM	FE-NA	2.06	2.02	1.95
2	B	501[B]	HEM	C1D-ND	-2.01	1.34	1.38

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501[B]	HEM	CHC-C4B-NB	6.29	131.19	124.42
2	B	501[B]	HEM	C1B-NB-C4B	5.82	112.10	105.21
2	A	501[A]	HEM	CHC-C4B-NB	5.62	130.47	124.42
2	B	501[A]	HEM	CHC-C4B-NB	4.59	129.36	124.42
2	B	501[B]	HEM	CHB-C1B-NB	4.25	129.63	124.37
2	B	501[A]	HEM	C1B-NB-C4B	4.11	110.07	105.21
2	A	501[A]	HEM	CHD-C1D-ND	4.00	128.73	124.42
2	A	501[A]	HEM	CHA-C4D-ND	3.92	129.22	124.37
2	A	501[B]	HEM	C1B-NB-C4B	3.85	109.76	105.21
2	B	501[A]	HEM	CHA-C4D-ND	3.76	129.02	124.37
2	B	501[A]	HEM	CHD-C4C-NC	3.75	128.53	124.45
2	A	501[B]	HEM	CHC-C4B-NB	3.61	128.31	124.42
2	A	501[A]	HEM	C1B-NB-C4B	3.53	109.39	105.21
2	B	501[B]	HEM	C3B-C4B-NB	-3.47	106.98	109.47
2	B	501[B]	HEM	CHD-C4C-NC	3.47	128.23	124.45
2	A	501[B]	HEM	CHD-C1D-C2D	-3.29	119.83	125.03
5	A	508	YIC	C25-C24-C29	3.16	122.93	118.23
2	B	501[A]	HEM	CAD-C3D-C4D	3.13	130.15	124.70
2	B	501[A]	HEM	CHD-C1D-ND	2.91	127.56	124.42
2	A	501[B]	HEM	C2D-C1D-ND	2.89	113.25	109.90
2	B	501[B]	HEM	CHA-C4D-ND	2.83	127.86	124.37
2	A	501[B]	HEM	CHD-C4C-NC	2.82	127.52	124.45
2	A	501[A]	HEM	CHD-C1D-C2D	-2.79	120.63	125.03
5	A	508	YIC	C23-C1-N5	-2.74	105.16	110.83
5	A	508	YIC	C1-N5-C6	2.73	127.52	121.65
2	B	501[A]	HEM	C4C-NC-C1C	2.72	110.26	105.82
2	B	501[B]	HEM	CHD-C1D-C2D	-2.69	120.78	125.03
2	A	501[A]	HEM	CHA-C4D-C3D	-2.63	120.38	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501[A]	HEM	CHA-C4D-C3D	-2.63	120.38	125.23
2	B	501[B]	HEM	CAD-C3D-C4D	2.61	129.25	124.70
5	A	508	YIC	C23-C24-C25	-2.57	116.12	120.90
5	A	508	YIC	C11-C10-C9	2.54	116.65	111.42
2	B	501[A]	HEM	CHD-C1D-C2D	-2.48	121.12	125.03
2	B	501[B]	HEM	C2B-C1B-NB	-2.46	107.02	109.84
2	A	501[B]	HEM	CHA-C1A-NA	2.43	128.27	123.86
2	B	501[B]	HEM	CHA-C4D-C3D	-2.42	120.76	125.23
2	B	501[B]	HEM	C1A-CHA-C4D	-2.42	120.56	126.25
2	B	501[A]	HEM	O2A-CGA-CBA	2.39	121.57	114.00
2	B	501[B]	HEM	CHA-C1A-NA	2.38	128.17	123.86
2	A	501[A]	HEM	CHD-C4C-NC	2.33	126.99	124.45
5	A	508	YIC	C28-C29-C24	-2.33	117.34	120.61
5	A	508	YIC	O3-C2-C1	-2.31	114.79	122.26
2	A	501[A]	HEM	O2A-CGA-CBA	2.30	121.26	114.00
2	B	501[A]	HEM	CHB-C1B-NB	2.28	127.19	124.37
5	A	508	YIC	O4-C2-C1	2.25	121.12	113.51
2	A	501[B]	HEM	CHD-C1D-ND	2.23	126.83	124.42
2	B	501[B]	HEM	C2D-C1D-ND	2.22	112.47	109.90
2	A	501[A]	HEM	CHB-C1B-NB	2.21	127.11	124.37
2	A	501[B]	HEM	O2A-CGA-CBA	2.21	120.99	114.00
2	A	501[A]	HEM	C4B-C3B-C2B	-2.20	105.26	107.28
2	B	501[A]	HEM	CAD-C3D-C2D	-2.20	123.75	127.87
2	B	501[A]	HEM	C1A-CHA-C4D	-2.17	121.15	126.25
2	B	501[B]	HEM	CHD-C1D-ND	2.16	126.75	124.42
2	A	501[A]	HEM	C1A-CHA-C4D	-2.10	121.30	126.25
2	A	501[B]	HEM	CHB-C1B-NB	2.07	126.93	124.37
2	A	501[B]	HEM	C1A-CHA-C4D	-2.05	121.42	126.25
2	B	501[B]	HEM	C3B-C2B-C1B	2.04	107.94	106.41
2	A	501[A]	HEM	O2D-CGD-CBD	2.03	120.41	114.00
2	B	501[B]	HEM	CAA-C2A-C1A	2.01	128.87	124.94

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	506	GOL	C1-C2-C3-O3
4	A	507	GOL	O1-C1-C2-C3
5	A	508	YIC	C14-C16-C17-C18
4	A	503	GOL	O1-C1-C2-C3
4	A	504	GOL	C1-C2-C3-O3
4	B	504	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	505[A]	GOL	C1-C2-C3-O3
4	B	505[B]	GOL	O1-C1-C2-C3
5	B	507	YIC	C14-C16-C17-C18
4	A	504	GOL	O2-C2-C3-O3
4	A	506	GOL	O2-C2-C3-O3
4	A	507	GOL	O1-C1-C2-O2
4	B	505[A]	GOL	O2-C2-C3-O3
4	B	505[B]	GOL	O1-C1-C2-O2
4	A	505	GOL	O2-C2-C3-O3
4	B	504	GOL	O2-C2-C3-O3
2	A	501[A]	HEM	CAD-CBD-CGD-O2D
2	A	501[B]	HEM	CAA-CBA-CGA-O2A
2	B	501[B]	HEM	CAA-CBA-CGA-O2A
2	B	501[A]	HEM	CAD-CBD-CGD-O2D
2	A	501[A]	HEM	CAD-CBD-CGD-O1D
2	B	501[B]	HEM	CAA-CBA-CGA-O1A
2	A	501[B]	HEM	CAA-CBA-CGA-O1A
2	B	501[A]	HEM	CAD-CBD-CGD-O1D
4	A	503	GOL	O1-C1-C2-O2
2	A	501[A]	HEM	CAA-CBA-CGA-O1A
2	A	501[A]	HEM	CAA-CBA-CGA-O2A

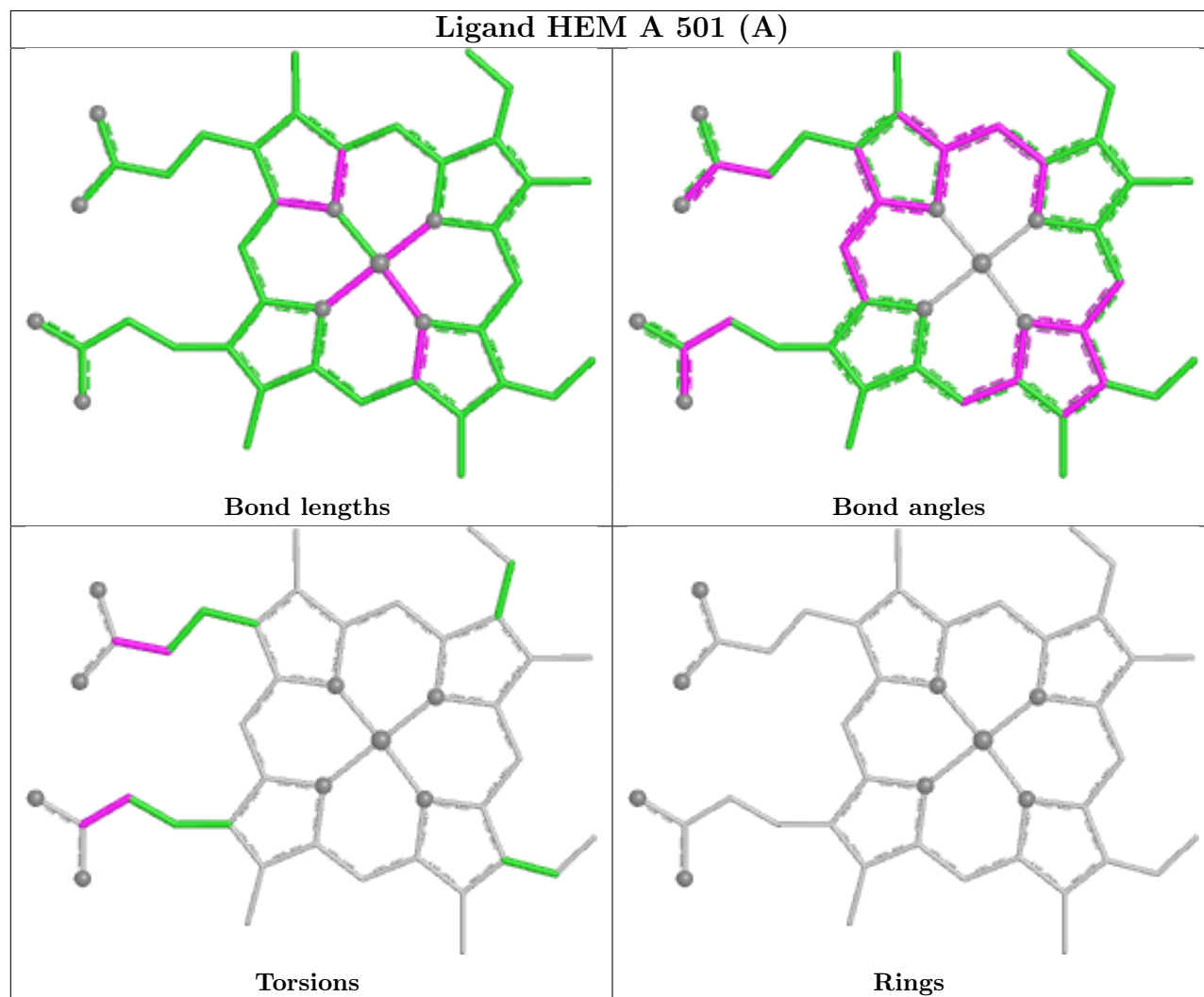
There are no ring outliers.

8 monomers are involved in 20 short contacts:

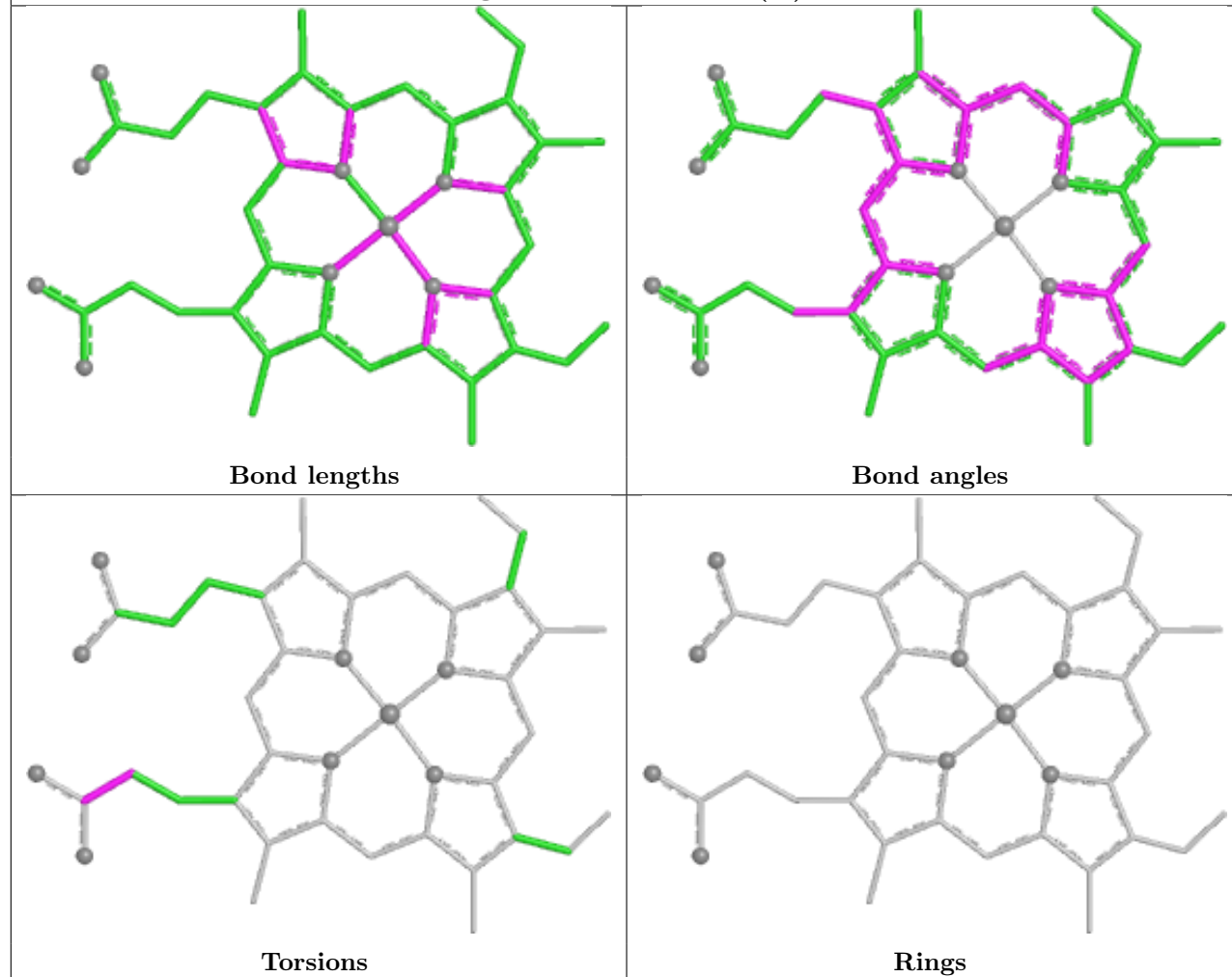
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501[A]	HEM	5	0
2	B	501[B]	HEM	5	0
4	A	507	GOL	1	0
2	A	501[B]	HEM	5	0
3	A	502	DMS	1	0
4	B	503	GOL	1	0
3	B	502	DMS	1	0
2	B	501[A]	HEM	1	0

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

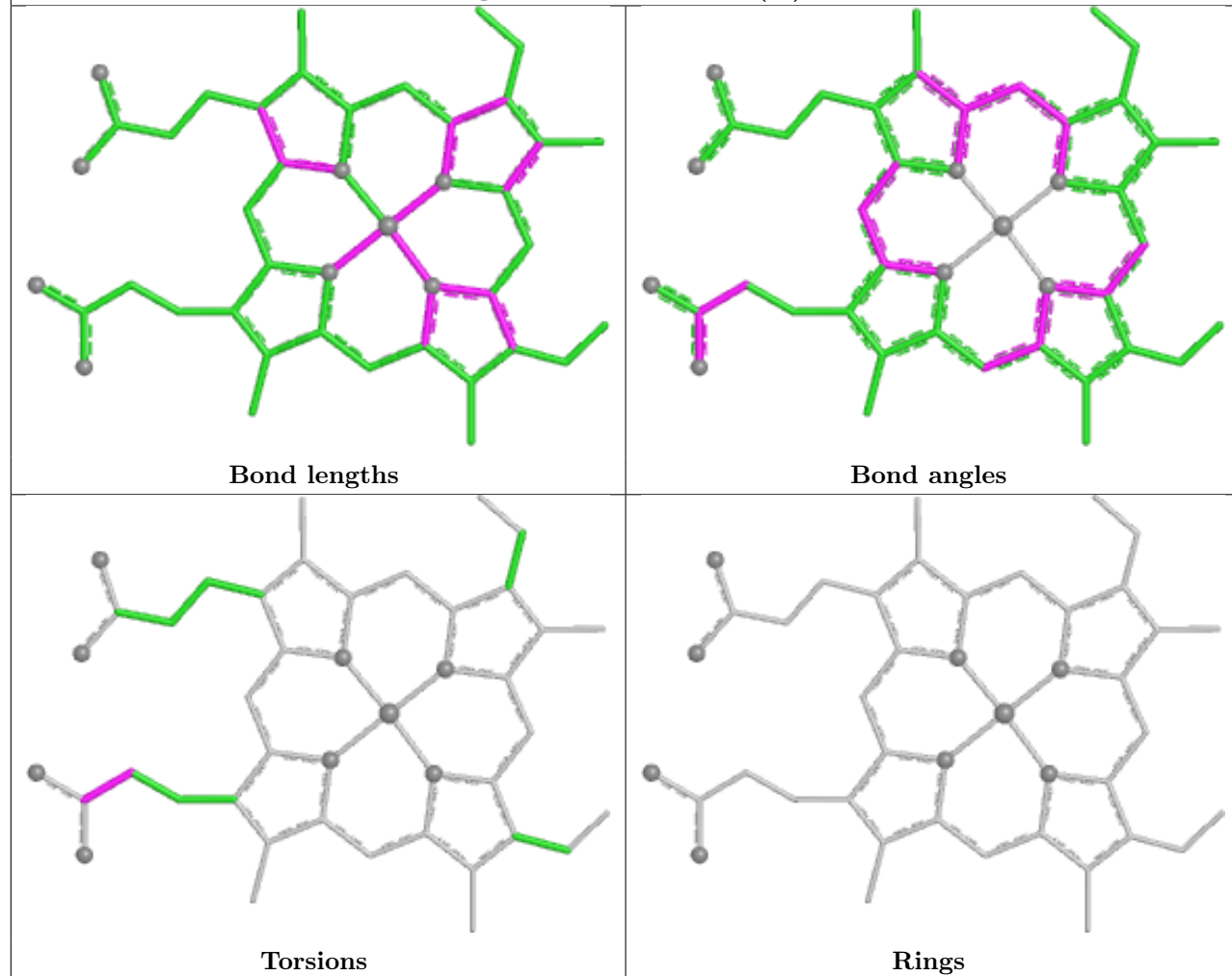
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

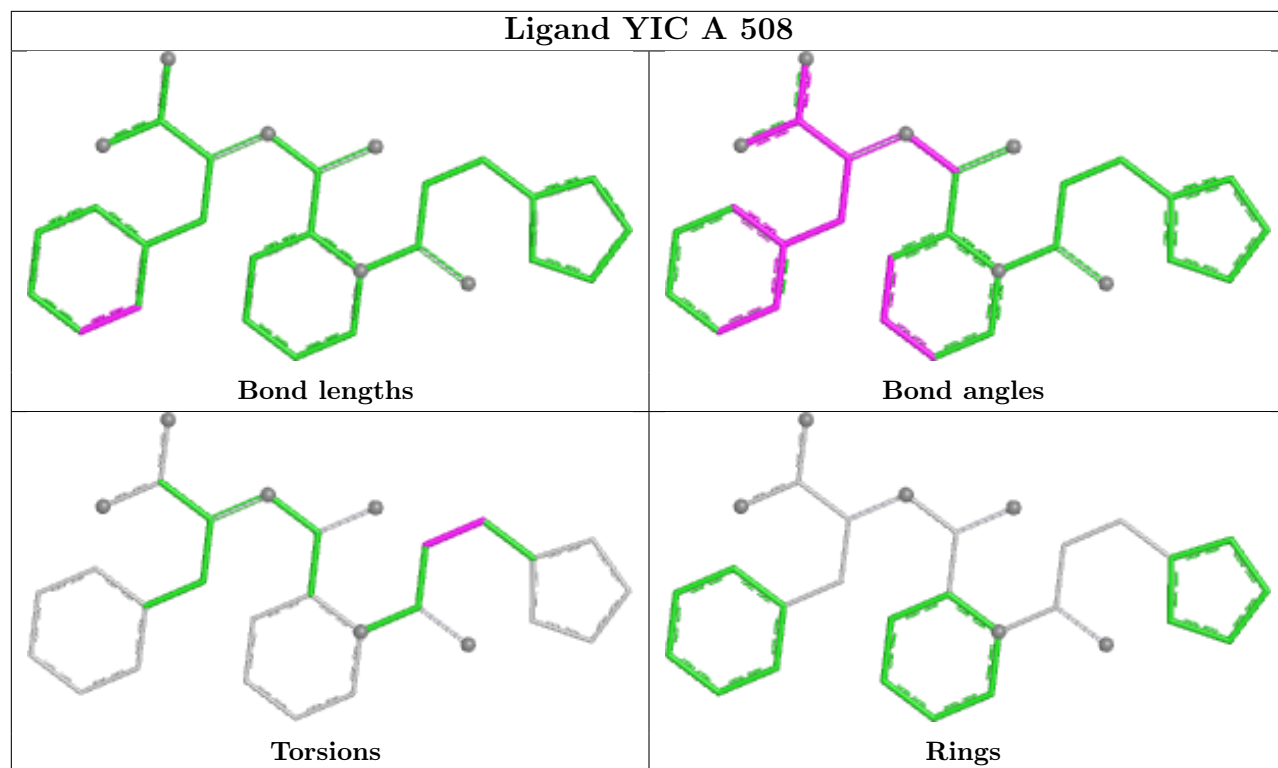


Ligand HEM B 501 (B)

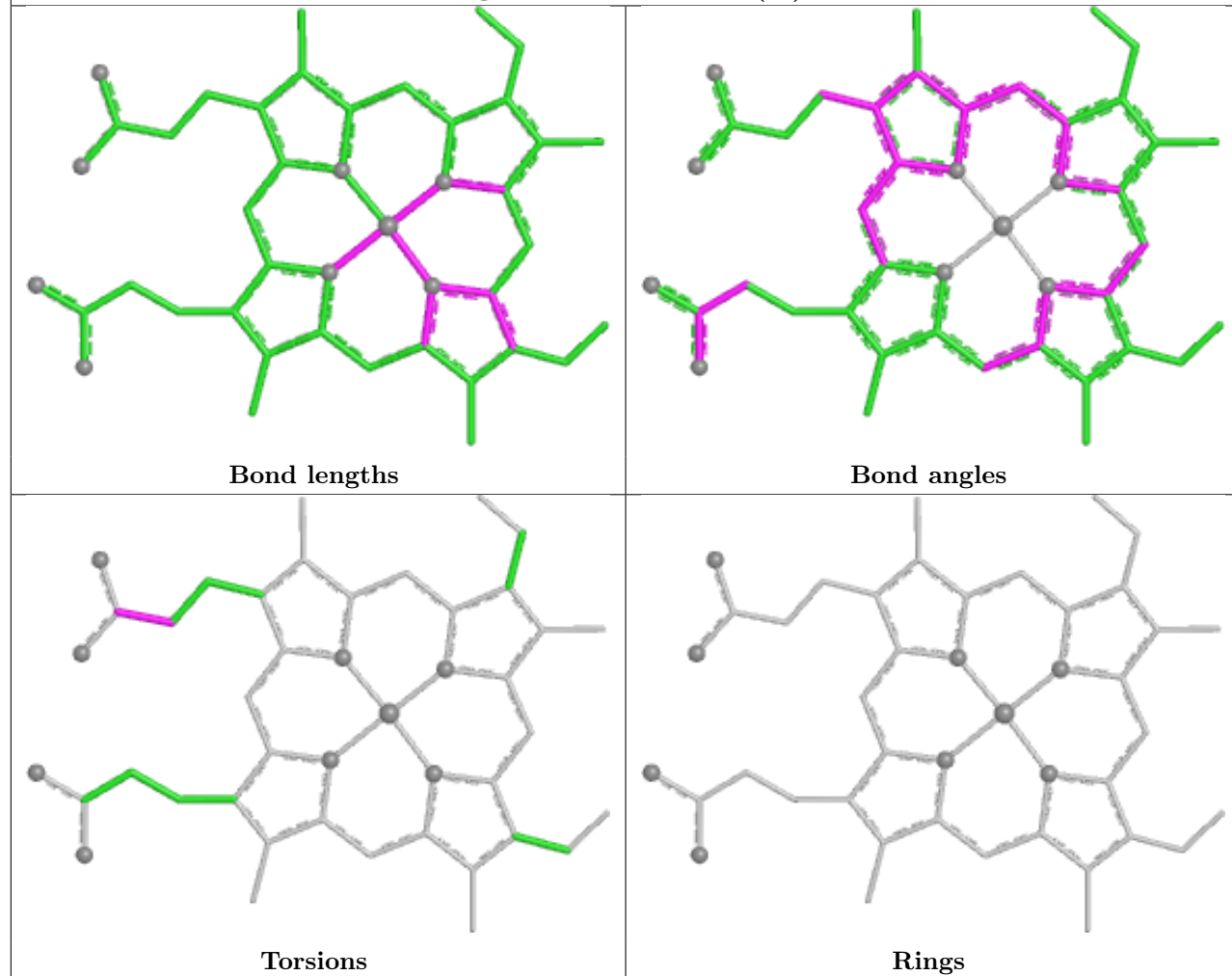


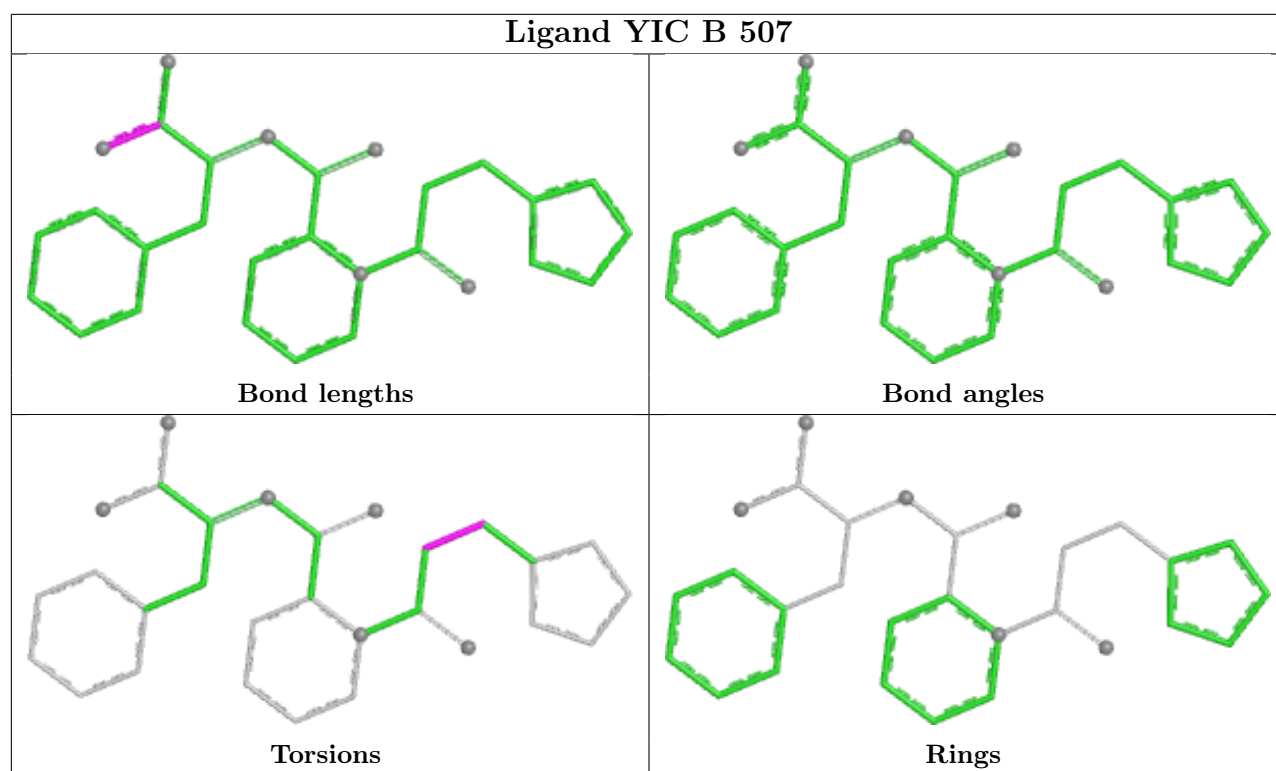
Ligand HEM A 501 (B)





Ligand HEM B 501 (A)





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th 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 ²)	Q<0.9
1	A	454/456 (99%)	-0.01	6 (1%) 75 82	8, 22, 41, 65	21 (4%)
1	B	454/456 (99%)	-0.05	9 (1%) 65 72	8, 21, 39, 61	25 (5%)
All	All	908/912 (99%)	-0.03	15 (1%) 69 76	8, 22, 41, 65	46 (5%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ILE	6.1
1	A	2	ILE	4.8
1	B	196	PRO	3.1
1	A	191	ALA	3.1
1	A	211	VAL	2.4
1	A	455	LEU	2.4
1	B	302[A]	VAL	2.3
1	B	455	LEU	2.2
1	A	383	SER	2.2
1	B	220[A]	ILE	2.2
1	B	197	ALA	2.1
1	B	136	ASP	2.1
1	B	3	LYS	2.1
1	B	200[A]	GLU	2.1
1	A	168	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

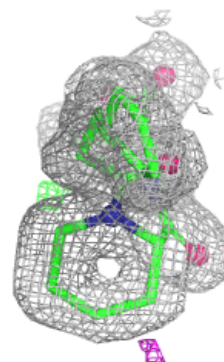
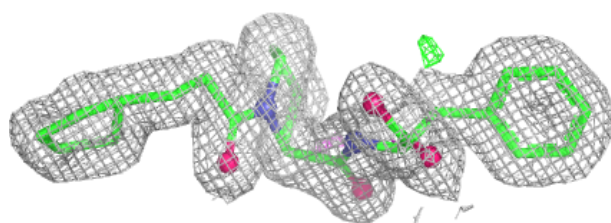
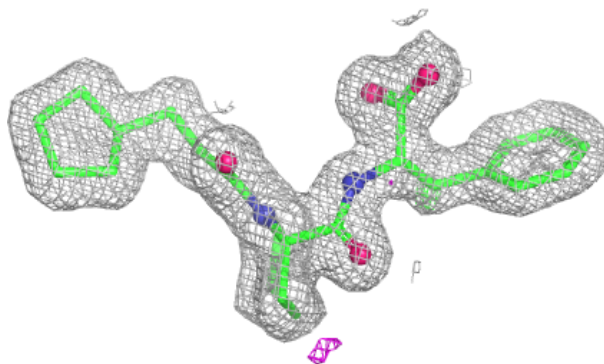
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	A	506	6/6	0.71	0.18	51,61,63,64	0
4	GOL	B	505[A]	6/6	0.81	0.16	37,39,43,46	6
4	GOL	B	505[B]	6/6	0.81	0.16	42,44,46,47	6
4	GOL	A	504	6/6	0.83	0.15	32,43,45,49	0
4	GOL	B	503	6/6	0.85	0.16	33,41,44,50	0
4	GOL	A	505	6/6	0.86	0.15	28,41,45,46	0
4	GOL	B	504	6/6	0.87	0.12	32,40,44,46	0
4	GOL	A	507	6/6	0.89	0.12	34,39,45,50	0
4	GOL	A	503	6/6	0.90	0.11	32,35,38,42	0
4	GOL	B	506	6/6	0.91	0.11	40,46,50,54	0
5	YIC	A	508	29/29	0.94	0.07	18,21,23,24	0
5	YIC	B	507	29/29	0.96	0.06	19,22,26,28	0
3	DMS	A	502	4/4	0.97	0.10	22,23,25,29	0
3	DMS	B	502	4/4	0.97	0.12	23,24,29,30	0
2	HEM	B	501[A]	43/43	0.98	0.06	14,15,18,22	43
2	HEM	B	501[B]	43/43	0.98	0.06	12,13,14,15	43
2	HEM	A	501[A]	43/43	0.98	0.06	13,15,17,18	43
2	HEM	A	501[B]	43/43	0.98	0.06	10,12,15,18	43

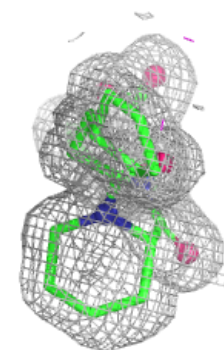
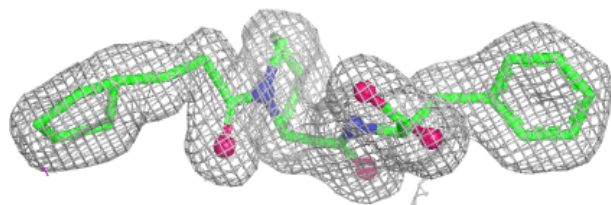
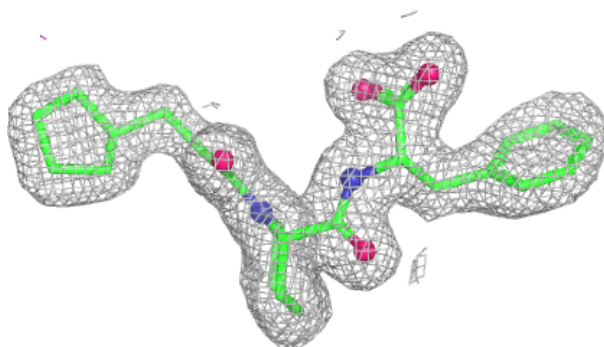
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YIC A 508:

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

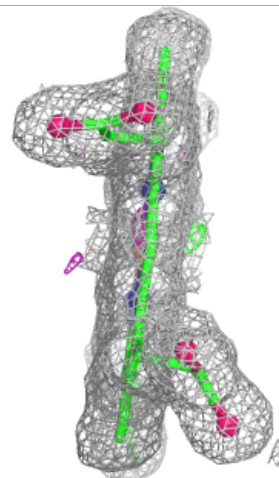
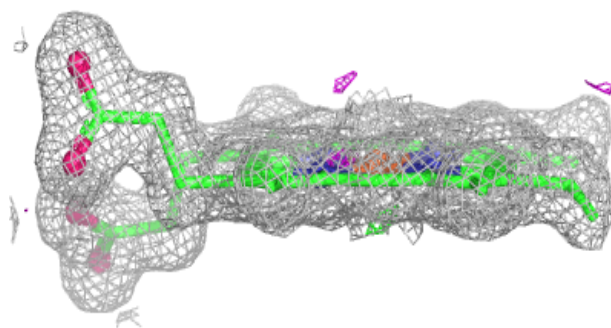
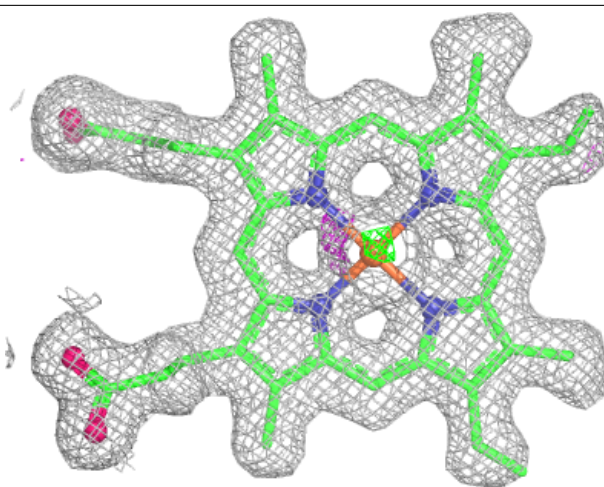
**Electron density around YIC B 507:**

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



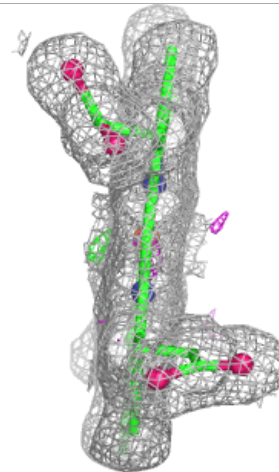
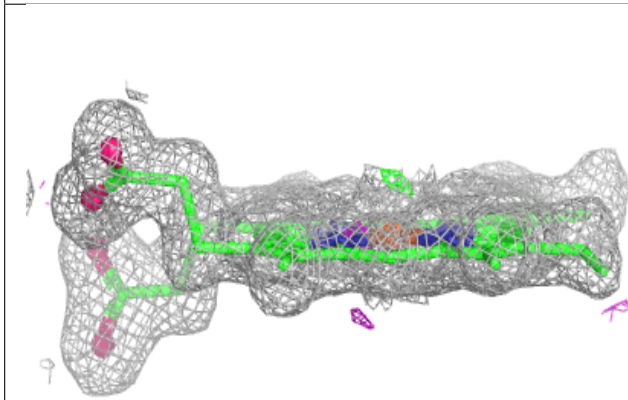
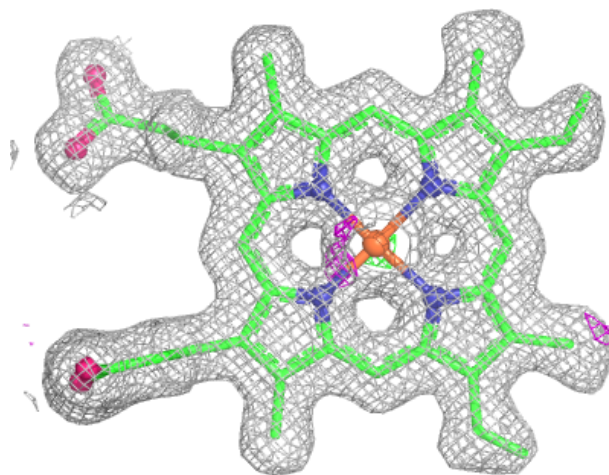
Electron density around HEM B 501 (A):

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



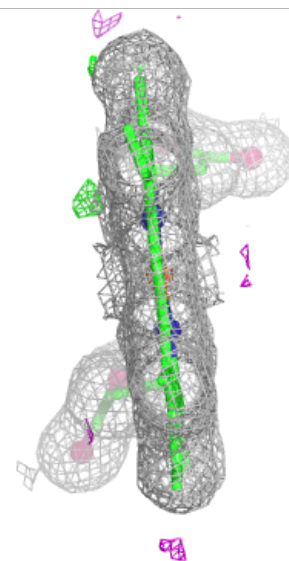
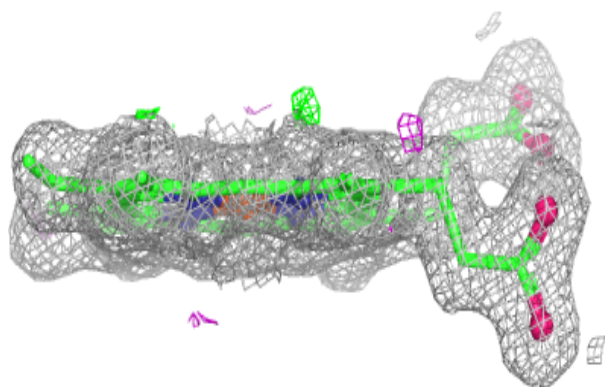
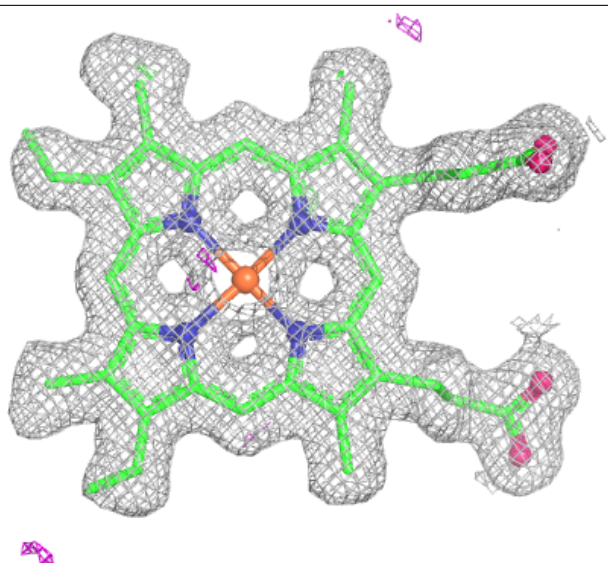
Electron density around HEM B 501 (B):

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



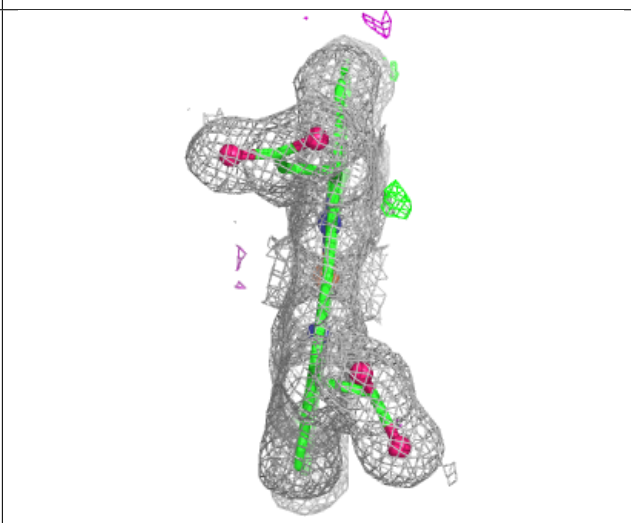
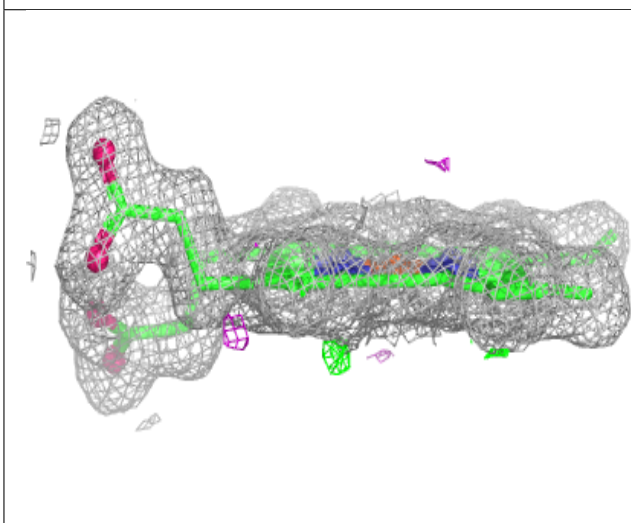
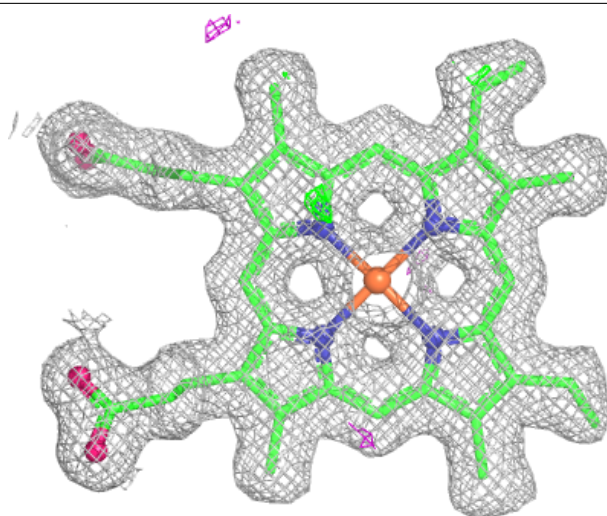
Electron density around HEM A 501 (A):

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



Electron density around HEM A 501 (B):

$2mF_o-DF_c$ (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.