Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 06:04 PM JST

PDB ID	:	7D1F / pdb_00007d1f
Title	:	Structure of the CYP102A1 Haem Domain with N-enanthyl-L-prolyl-L-phenylalanine in complex with Methylamine
Authors	:	Stanfield, J.K.; Sugimoto, H.; Shoji, O.
Deposited on	:	2020-09-14
Resolution	:	1.45 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 (i) 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 (i)) were used in the production of this report:

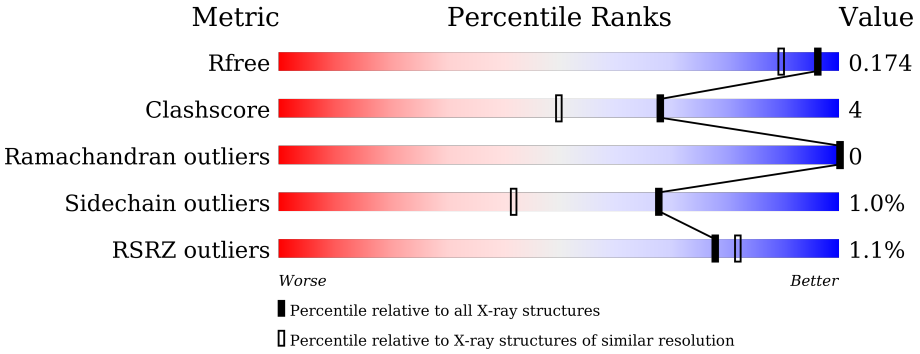
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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 <=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	2% 94% 6%
1	B	456	. % 92% 7%

2 Entry composition (i)

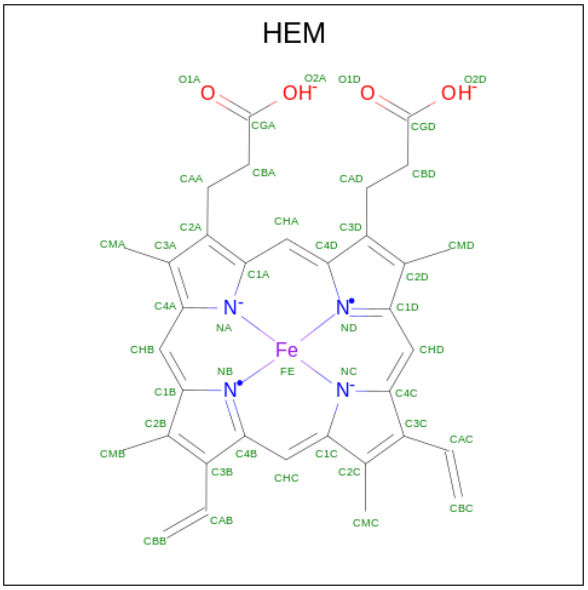
There are 6 unique types of molecules in this entry. The entry contains 8638 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

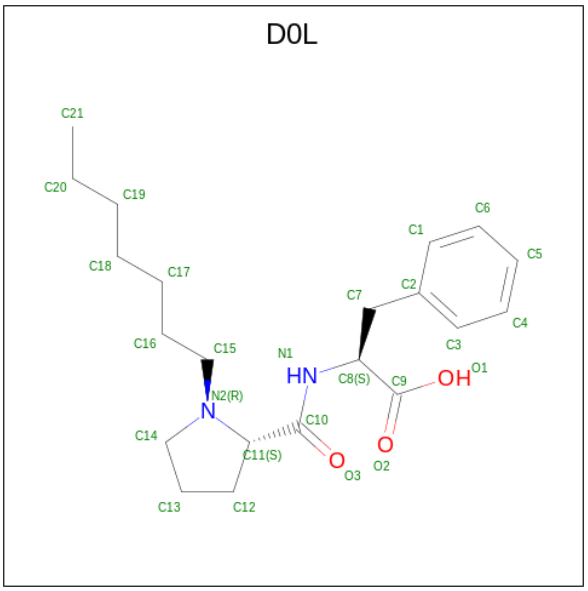
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	3834	2444	650	721	19	0	21	0
1	B	454	3839	2451	653	716	19	0	22	0

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



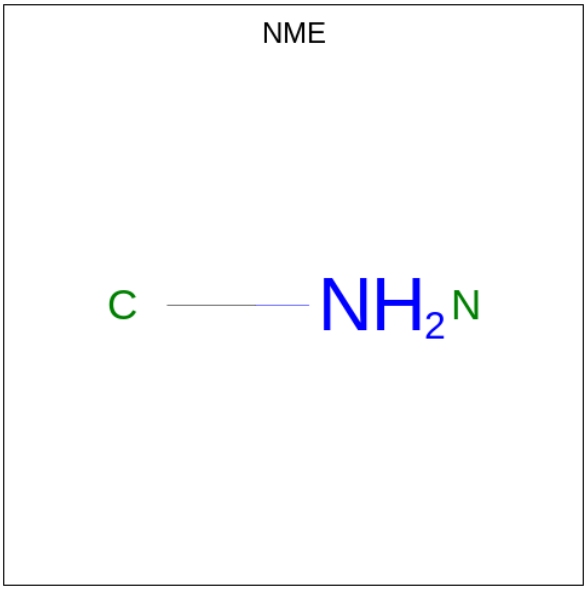
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	86	68	2	8	8	0	1
2	B	1	86	68	2	8	8	0	1

- Molecule 3 is (2S)-2-[[(2S)-1-heptylpyrrolidin-2-yl]carbonylamino]-3-phenyl-propanoic acid (CCD ID: D0L) (formula: $C_{21}H_{32}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



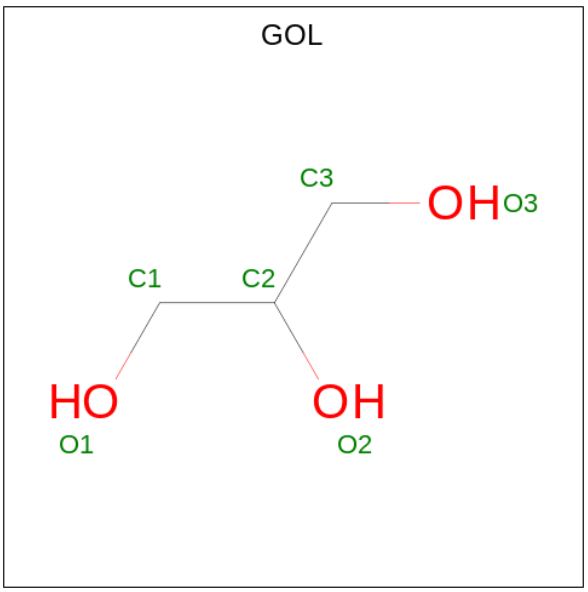
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	26	21	2	3	0	0
			Total	C	N	O		
3	B	1	26	21	2	3	0	0

- Molecule 4 is METHYLAMINE (CCD ID: NME) (formula: CH_5N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
4	A	1	4	2	2	0	1
			Total	C	N		
4	B	1	4	2	2	0	1

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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	A	1	Total	C	O		0	0
			6	3	3			
5	A	1	Total	C	O		0	0
			6	3	3			
5	A	1	Total	C	O		0	0
			6	3	3			
5	A	1	Total	C	O		0	0
			6	3	3			
5	A	1	Total	C	O		0	0
			6	3	3			
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	B	1	Total	C	O		0	0
			6	3	3			
5	B	1	Total	C	O		0	0
			6	3	3			
5	B	1	Total	C	O		0	0
			6	3	3			

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

- Molecule 6 is water.

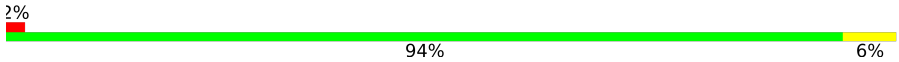
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	302	302	302	0	0
			Total	O		
6	B	311	311	311	0	0

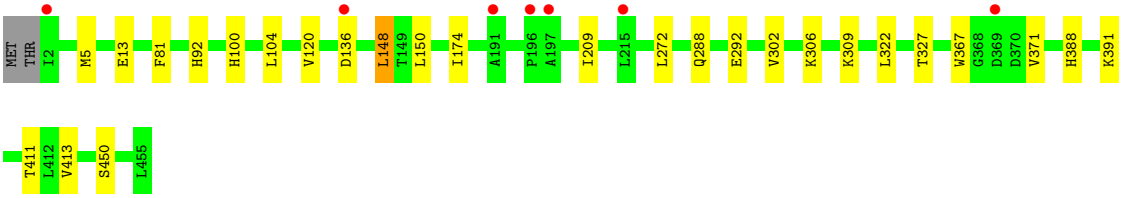
3 Residue-property plots (i)

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

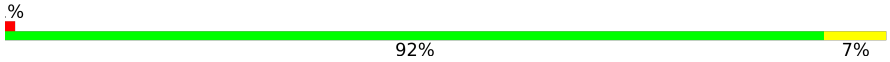
Chain A:

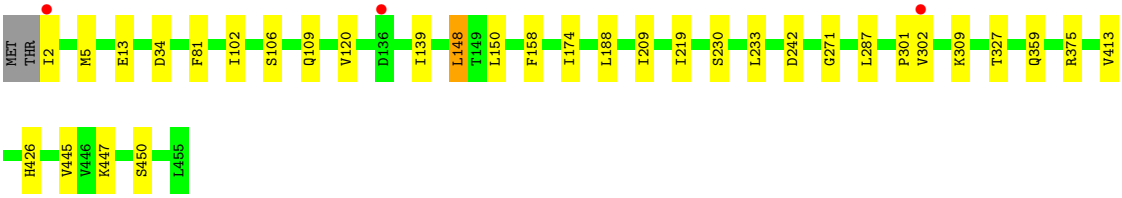




• Molecule 1: Bifunctional cytochrome P450/NADPH–P450 reductase

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.47Å 127.34Å 147.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.23 – 1.45 48.23 – 1.45	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.23-1.45) 99.2 (48.23-1.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
R, R_{free}	0.143 , 0.174 0.143 , 0.174	Depositor DCC
R_{free} test set	9666 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å^2)	17.4	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 36.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	8638	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9624e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NME, D0L, HEM, 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	0.94	0/3919	1.11	0/5297
1	B	0.92	0/3927	1.12	3/5305 (0.1%)
All	All	0.93	0/7846	1.11	3/10602 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	301	PRO	CA-C-N	5.21	127.86	123.33
1	B	301	PRO	C-N-CA	5.21	127.86	123.33
1	B	13	GLU	CB-CG-CD	5.10	121.27	112.60

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	3834	0	3789	19	0
1	B	3839	0	3813	24	0
2	A	86	0	60	7	0
2	B	86	0	60	8	0
3	A	26	0	0	0	0
3	B	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	54	0	72	6	0
5	B	66	0	88	4	0
6	A	302	0	0	0	0
6	B	311	0	0	1	0
All	All	8638	0	7882	57	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 (57) 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:102[B]:ILE:HD11	1:B:242:ASP:CA	2.03	0.89
1:B:102[B]:ILE:HD11	1:B:242:ASP:N	1.98	0.79
1:A:288[B]:GLN:O	1:A:292[B]:GLU:HG3	1.88	0.72
1:B:102[B]:ILE:HD11	1:B:242:ASP:HA	1.74	0.70
1:B:450:SER:H	5:B:512:GOL:C1	2.07	0.66
1:B:120:VAL:HG11	1:B:302:VAL:HG13	1.78	0.66
1:B:450:SER:H	5:B:512:GOL:H11	1.61	0.66
2:B:501[B]:HEM:HMC1	2:B:501[B]:HEM:HBC2	1.77	0.66
1:B:102[B]:ILE:CD1	1:B:242:ASP:HA	2.27	0.65
2:B:501[A]:HEM:HMC1	2:B:501[A]:HEM:HBC2	1.77	0.65
2:A:501[B]:HEM:CMB	2:A:501[B]:HEM:HBB2	2.29	0.63
1:A:411:THR:HG21	5:A:506:GOL:H2	1.82	0.60
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.83	0.60
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.83	0.59
1:A:367:TRP:HB2	1:A:371:VAL:HG12	1.86	0.57
2:B:501[A]:HEM:CMB	2:B:501[A]:HEM:HBB2	2.34	0.57
2:A:501[B]:HEM:HBB2	2:A:501[B]:HEM:HMB2	1.87	0.57
1:B:102[B]:ILE:N	1:B:102[B]:ILE:HD13	2.21	0.55
1:A:309:LYS:HA	5:A:506:GOL:H32	1.88	0.55
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.87	0.55
2:B:501[A]:HEM:HBB2	2:B:501[A]:HEM:HMB2	1.88	0.54
1:B:158:PHE:CE2	1:B:219[A]:ILE:HD13	2.42	0.54
1:B:309:LYS:HA	5:B:509:GOL:H32	1.91	0.52
2:B:501[B]:HEM:HBC2	2:B:501[B]:HEM:CMC	2.39	0.51
1:B:120:VAL:HG11	1:B:302:VAL:CG1	2.40	0.50
1:B:271:GLY:C	1:B:327[A]:THR:HG21	2.37	0.50
1:B:309:LYS:HA	5:B:509:GOL:C3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501[B]:HEM:HMC1	2:A:501[B]:HEM:HBC2	1.93	0.49
1:A:92:HIS:HB3	5:A:509:GOL:O1	2.13	0.47
1:A:120:VAL:HG11	1:A:302:VAL:HG13	1.95	0.47
2:B:501[B]:HEM:CMB	2:B:501[B]:HEM:HBB2	2.44	0.47
1:A:450:SER:CB	5:A:505:GOL:H32	2.45	0.46
2:A:501[B]:HEM:HBC2	2:A:501[B]:HEM:CMC	2.46	0.45
1:A:100:HIS:NE2	1:A:104[A]:LEU:HD11	2.31	0.45
1:A:450:SER:HB2	5:A:505:GOL:H32	1.98	0.45
1:A:13[A]:GLU:H	1:A:13[A]:GLU:CD	2.25	0.45
2:B:501[A]:HEM:HBC2	2:B:501[A]:HEM:CMC	2.47	0.45
2:A:501[A]:HEM:HMC1	2:A:501[A]:HEM:HBC2	1.99	0.44
1:B:106:SER:HB3	1:B:233:LEU:HD23	1.99	0.44
1:A:150:LEU:HD21	1:A:174:ILE:HG13	1.99	0.44
1:A:81:PHE:HB3	1:A:209:ILE:HG12	2.01	0.43
1:B:188[A]:LEU:C	1:B:188[A]:LEU:HD12	2.44	0.43
2:A:501[B]:HEM:HMB2	2:A:501[B]:HEM:CBB	2.49	0.43
1:A:309:LYS:HA	5:A:506:GOL:C3	2.49	0.42
1:A:322:LEU:HD22	2:A:501[B]:HEM:HBC1	2.01	0.42
2:B:501[B]:HEM:HBB2	2:B:501[B]:HEM:HMB2	2.01	0.42
1:A:272:LEU:N	1:A:327[A]:THR:HG21	2.35	0.42
1:B:139:ILE:O	1:B:445:VAL:HA	2.21	0.41
1:B:426:HIS:CD2	1:B:447:LYS:HE3	2.56	0.41
1:A:5[B]:MET:HE2	1:A:5[B]:MET:HB3	1.94	0.41
1:B:81:PHE:HB3	1:B:209:ILE:HG12	2.03	0.41
1:B:150:LEU:HD21	1:B:174:ILE:HG13	2.03	0.41
1:B:102[B]:ILE:HD11	1:B:242:ASP:CB	2.51	0.40
1:B:5[A]:MET:HE3	1:B:5[A]:MET:HB2	1.82	0.40
1:A:104[A]:LEU:HD23	1:A:104[A]:LEU:HA	1.95	0.40
1:B:34:ASP:OD1	1:B:359[B]:GLN:NE2	2.43	0.40
1:B:287[A]:LEU:HD23	6:B:889:HOH:O	2.21	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%)	459 (97%)	14 (3%)	0	100	100
1	B	474/456 (104%)	462 (98%)	12 (2%)	0	100	100
All	All	947/912 (104%)	921 (97%)	26 (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	418/400 (104%)	415 (99%)	3 (1%)	76	54
1	B	419/400 (105%)	414 (99%)	5 (1%)	63	33
All	All	837/800 (105%)	829 (99%)	8 (1%)	68	42

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	ASP
1	A	148	LEU
1	A	306	LYS
1	B	2	ILE
1	B	109	GLN
1	B	148	LEU
1	B	230	SER
1	B	375	ARG

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	73	GLN
1	A	192	ASN

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Mol	Chain	Res	Type
1	A	204	GLN
1	A	359	GLN
1	B	73	GLN
1	B	204	GLN
1	B	285	HIS

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)

30 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	$\#\|Z\| > 2$
5	GOL	B	512	-	5,5,5	0.10	0	5,5,5	0.66	0
2	HEM	A	501[B]	4,1	50,50,50	1.46	8 (16%)	66,82,82	1.64	10 (15%)
4	NME	B	503[B]	2	0,1,1	-	-	-		
5	GOL	A	510	-	5,5,5	0.11	0	5,5,5	0.31	0
5	GOL	B	506	-	5,5,5	0.10	0	5,5,5	0.27	0
5	GOL	A	507	-	5,5,5	0.24	0	5,5,5	0.61	0
5	GOL	A	512	-	5,5,5	0.10	0	5,5,5	0.27	0
5	GOL	A	504	-	5,5,5	0.09	0	5,5,5	0.24	0
5	GOL	B	507	-	5,5,5	0.08	0	5,5,5	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	D0L	A	502	-	27,27,27	0.68	0	34,34,34	1.41	4 (11%)
2	HEM	A	501[A]	4,1	50,50,50	1.32	6 (12%)	66,82,82	1.52	10 (15%)
4	NME	B	503[A]	2	0,1,1	-	-	-		
5	GOL	B	514	-	5,5,5	0.10	0	5,5,5	0.24	0
5	GOL	A	511	-	5,5,5	0.12	0	5,5,5	0.34	0
4	NME	A	503[B]	2	0,1,1	-	-	-		
5	GOL	A	506	-	5,5,5	0.16	0	5,5,5	0.34	0
3	D0L	B	502	-	27,27,27	0.82	0	34,34,34	1.07	3 (8%)
5	GOL	B	511	-	5,5,5	0.15	0	5,5,5	0.34	0
5	GOL	A	505	-	5,5,5	0.11	0	5,5,5	0.60	0
5	GOL	B	508	-	5,5,5	0.14	0	5,5,5	0.39	0
2	HEM	B	501[B]	4,1	50,50,50	1.35	6 (12%)	66,82,82	1.55	9 (13%)
5	GOL	B	509	-	5,5,5	0.10	0	5,5,5	0.28	0
5	GOL	B	510	-	5,5,5	0.12	0	5,5,5	0.33	0
4	NME	A	503[A]	2	0,1,1	-	-	-		
5	GOL	B	505	-	5,5,5	0.16	0	5,5,5	0.65	0
5	GOL	A	508	-	5,5,5	0.10	0	5,5,5	0.35	0
5	GOL	B	504	-	5,5,5	0.15	0	5,5,5	0.44	0
5	GOL	A	509	-	5,5,5	0.11	0	5,5,5	0.28	0
2	HEM	B	501[A]	4,1	50,50,50	1.29	7 (14%)	66,82,82	1.66	12 (18%)
5	GOL	B	513	-	5,5,5	0.09	0	5,5,5	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	512	-	-	2/4/4/4	-
2	HEM	A	501[B]	4,1	-	2/14/54/54	-
5	GOL	A	510	-	-	0/4/4/4	-
5	GOL	B	506	-	-	3/4/4/4	-
5	GOL	A	507	-	-	1/4/4/4	-
5	GOL	A	512	-	-	2/4/4/4	-
5	GOL	A	504	-	-	0/4/4/4	-
5	GOL	B	507	-	-	2/4/4/4	-
3	D0L	A	502	-	-	1/23/33/33	0/2/2/2
2	HEM	A	501[A]	4,1	-	2/14/54/54	-
5	GOL	B	514	-	-	1/4/4/4	-
5	GOL	A	511	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	506	-	-	2/4/4/4	-
3	D0L	B	502	-	-	1/23/33/33	0/2/2/2
5	GOL	B	511	-	-	2/4/4/4	-
5	GOL	A	505	-	-	3/4/4/4	-
5	GOL	B	508	-	-	2/4/4/4	-
2	HEM	B	501[B]	4,1	-	2/14/54/54	-
5	GOL	B	509	-	-	2/4/4/4	-
5	GOL	B	510	-	-	0/4/4/4	-
5	GOL	B	505	-	-	0/4/4/4	-
5	GOL	A	508	-	-	2/4/4/4	-
5	GOL	B	504	-	-	0/4/4/4	-
5	GOL	A	509	-	-	0/4/4/4	-
2	HEM	B	501[A]	4,1	-	2/14/54/54	-
5	GOL	B	513	-	-	2/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[B]	HEM	FE-NB	4.70	2.09	1.94
2	B	501[B]	HEM	FE-NB	4.44	2.08	1.94
2	A	501[A]	HEM	FE-NB	3.74	2.06	1.94
2	A	501[B]	HEM	C1B-NB	-3.33	1.34	1.40
2	B	501[A]	HEM	FE-NB	3.25	2.04	1.94
2	A	501[A]	HEM	FE-NC	3.23	2.06	1.95
2	B	501[A]	HEM	FE-NC	3.20	2.06	1.95
2	A	501[B]	HEM	FE-NC	3.17	2.05	1.95
2	A	501[A]	HEM	C1B-NB	-3.06	1.35	1.40
2	B	501[B]	HEM	C1B-NB	-2.83	1.35	1.40
2	B	501[B]	HEM	C4D-C3D	2.69	1.49	1.45
2	A	501[B]	HEM	C4D-ND	-2.64	1.35	1.40
2	B	501[A]	HEM	C4D-ND	-2.62	1.35	1.40
2	B	501[A]	HEM	C1B-NB	-2.61	1.35	1.40
2	B	501[B]	HEM	C4D-ND	-2.58	1.35	1.40
2	B	501[B]	HEM	FE-NC	2.48	2.03	1.95
2	B	501[A]	HEM	FE-NA	2.34	2.03	1.95
2	A	501[A]	HEM	C1C-C2C	-2.34	1.40	1.45
2	A	501[B]	HEM	C4D-C3D	2.28	1.49	1.45
2	A	501[A]	HEM	FE-NA	2.26	2.02	1.95
2	B	501[A]	HEM	C4B-NB	-2.25	1.34	1.38
2	B	501[A]	HEM	C1C-C2C	-2.21	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	HEM	C4D-ND	-2.17	1.36	1.40
2	A	501[B]	HEM	C1C-C2C	-2.11	1.41	1.45
2	A	501[B]	HEM	C3C-C4C	-2.09	1.42	1.46
2	A	501[B]	HEM	C1D-ND	-2.03	1.34	1.38
2	B	501[B]	HEM	C3C-C4C	-2.01	1.42	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	D0L	C7-C8-N1	-5.46	99.29	110.79
2	B	501[A]	HEM	CHC-C4B-NB	5.44	130.33	124.42
2	A	501[B]	HEM	CHC-C4B-NB	5.09	129.94	124.42
2	B	501[A]	HEM	C1B-NB-C4B	4.92	110.15	105.07
2	A	501[A]	HEM	C1B-NB-C4B	4.78	110.01	105.07
2	B	501[B]	HEM	C1B-NB-C4B	4.69	109.92	105.07
2	A	501[A]	HEM	CHC-C4B-NB	4.54	129.35	124.42
2	B	501[B]	HEM	CHD-C4C-NC	4.52	129.33	124.44
2	B	501[B]	HEM	CHC-C4B-NB	4.43	129.23	124.42
2	A	501[B]	HEM	C1B-NB-C4B	4.31	109.53	105.07
2	A	501[B]	HEM	CHD-C4C-NC	4.08	128.85	124.44
2	A	501[B]	HEM	C4C-NC-C1C	4.02	109.28	105.35
2	B	501[A]	HEM	C4C-NC-C1C	3.68	108.95	105.35
2	B	501[A]	HEM	CHB-C1B-NB	3.65	128.87	124.37
2	A	501[B]	HEM	CHB-C1B-NB	3.42	128.59	124.37
2	B	501[A]	HEM	CHD-C1D-ND	3.35	128.06	124.42
3	B	502	D0L	C7-C8-N1	-3.35	103.74	110.79
2	B	501[B]	HEM	C4C-NC-C1C	3.34	108.61	105.35
2	A	501[A]	HEM	CHD-C4C-NC	3.31	128.02	124.44
2	A	501[A]	HEM	C4C-NC-C1C	3.07	108.36	105.35
2	B	501[A]	HEM	CHD-C1D-C2D	-2.93	120.40	124.98
2	A	501[A]	HEM	O2A-CGA-CBA	2.83	123.14	114.03
2	B	501[A]	HEM	CHD-C4C-NC	2.80	127.47	124.44
2	A	501[A]	HEM	CHA-C4D-ND	2.78	127.81	124.37
2	A	501[B]	HEM	CHD-C1D-ND	2.69	127.34	124.42
2	A	501[A]	HEM	CHA-C4D-C3D	-2.68	120.29	125.33
2	B	501[A]	HEM	O2A-CGA-CBA	2.67	122.60	114.03
2	A	501[B]	HEM	CHD-C1D-C2D	-2.64	120.85	124.98
2	B	501[B]	HEM	CHA-C4D-ND	2.64	127.63	124.37
2	B	501[B]	HEM	CHD-C1D-C2D	-2.61	120.90	124.98
3	B	502	D0L	C13-C14-N2	2.52	108.26	104.15
2	A	501[A]	HEM	CHB-C1B-NB	2.49	127.45	124.37
3	A	502	D0L	C7-C8-C9	2.40	116.21	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501[B]	HEM	CHA-C4D-ND	2.40	127.33	124.37
2	A	501[A]	HEM	O1A-CGA-CBA	-2.39	115.39	123.08
2	B	501[B]	HEM	CHB-C1B-NB	2.25	127.15	124.37
2	B	501[B]	HEM	C2D-C1D-ND	2.22	112.54	109.88
2	B	501[A]	HEM	CHA-C4D-C3D	-2.21	121.17	125.33
2	A	501[B]	HEM	C1A-CHA-C4D	-2.16	121.20	126.34
2	A	501[A]	HEM	CHD-C1D-C2D	-2.16	121.60	124.98
3	B	502	D0L	C8-N1-C10	2.16	126.30	121.67
2	A	501[B]	HEM	CHA-C4D-C3D	-2.14	121.31	125.33
2	B	501[A]	HEM	CAD-C3D-C4D	2.13	128.38	124.66
2	B	501[A]	HEM	O1A-CGA-CBA	-2.12	116.28	123.08
2	B	501[B]	HEM	CHA-C4D-C3D	-2.08	121.43	125.33
2	B	501[A]	HEM	O2D-CGD-CBD	2.07	120.67	114.03
3	A	502	D0L	C13-C14-N2	2.06	107.50	104.15
3	A	502	D0L	C8-N1-C10	2.04	126.05	121.67

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	506	GOL	C1-C2-C3-O3
5	A	508	GOL	O1-C1-C2-C3
5	A	511	GOL	C1-C2-C3-O3
5	A	511	GOL	O2-C2-C3-O3
5	A	512	GOL	C1-C2-C3-O3
5	B	508	GOL	O1-C1-C2-C3
5	B	509	GOL	C1-C2-C3-O3
5	B	512	GOL	C1-C2-C3-O3
5	B	512	GOL	O2-C2-C3-O3
5	B	513	GOL	O1-C1-C2-O2
5	B	513	GOL	O1-C1-C2-C3
5	A	506	GOL	O2-C2-C3-O3
5	A	508	GOL	O1-C1-C2-O2
5	A	505	GOL	O1-C1-C2-C3
5	B	506	GOL	O1-C1-C2-C3
5	B	506	GOL	C1-C2-C3-O3
5	B	507	GOL	C1-C2-C3-O3
5	B	507	GOL	O2-C2-C3-O3
5	B	508	GOL	O1-C1-C2-O2
5	B	509	GOL	O2-C2-C3-O3
3	A	502	D0L	N2-C15-C16-C17
5	A	512	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	A	505	GOL	C1-C2-C3-O3
3	B	502	D0L	N2-C15-C16-C17
5	B	511	GOL	O2-C2-C3-O3
5	A	507	GOL	O1-C1-C2-O2
5	B	511	GOL	C1-C2-C3-O3
5	B	514	GOL	C1-C2-C3-O3
5	A	505	GOL	O1-C1-C2-O2
5	B	506	GOL	O2-C2-C3-O3
2	A	501[B]	HEM	CAA-CBA-CGA-O1A
2	B	501[B]	HEM	CAA-CBA-CGA-O1A
2	B	501[B]	HEM	CAA-CBA-CGA-O2A
2	A	501[B]	HEM	CAA-CBA-CGA-O2A
2	A	501[A]	HEM	CAD-CBD-CGD-O2D
2	B	501[A]	HEM	CAD-CBD-CGD-O2D
2	A	501[A]	HEM	CAD-CBD-CGD-O1D
2	B	501[A]	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

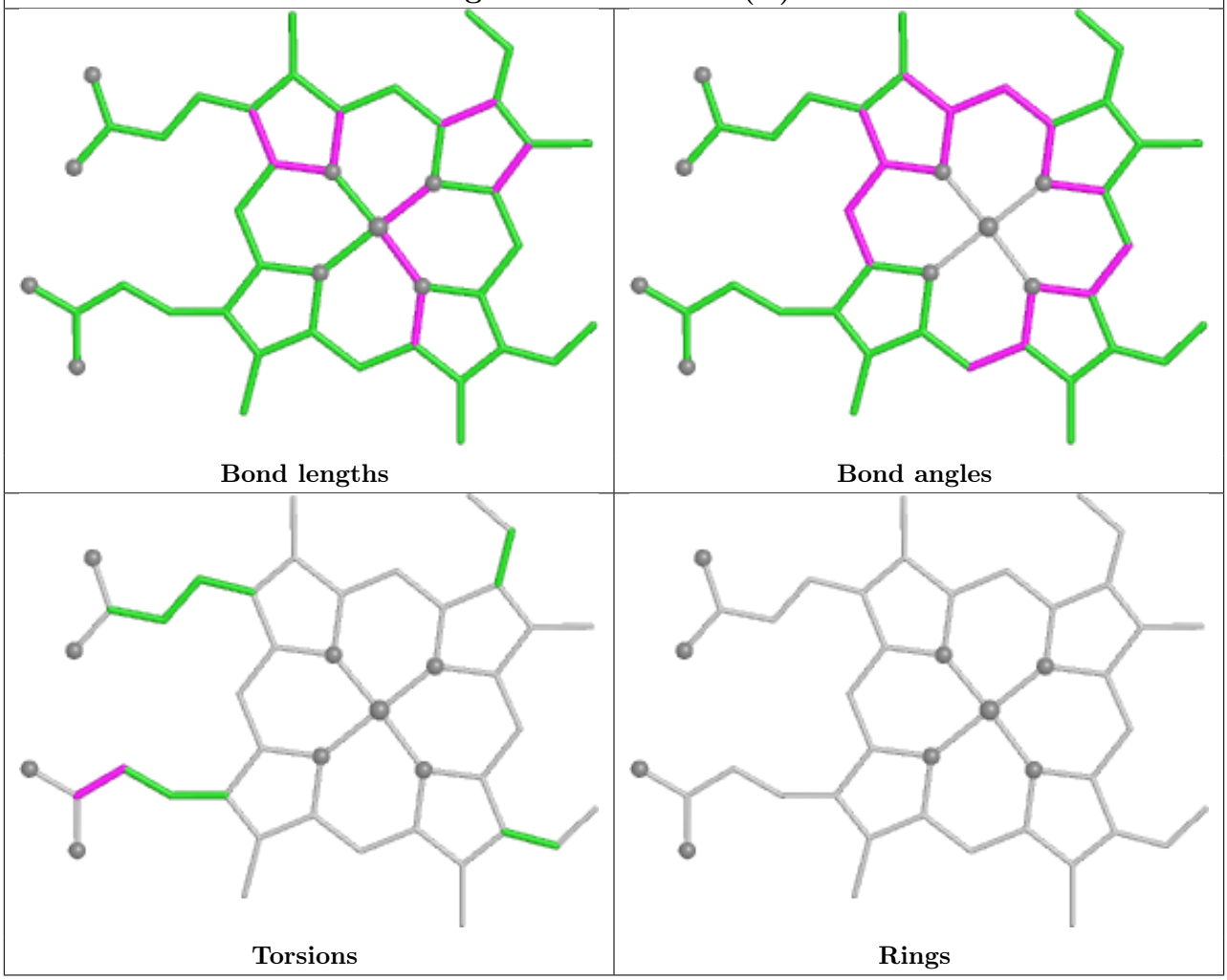
9 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	512	GOL	2	0
2	A	501[B]	HEM	6	0
2	A	501[A]	HEM	1	0
5	A	506	GOL	3	0
5	A	505	GOL	2	0
2	B	501[B]	HEM	4	0
5	B	509	GOL	2	0
5	A	509	GOL	1	0
2	B	501[A]	HEM	4	0

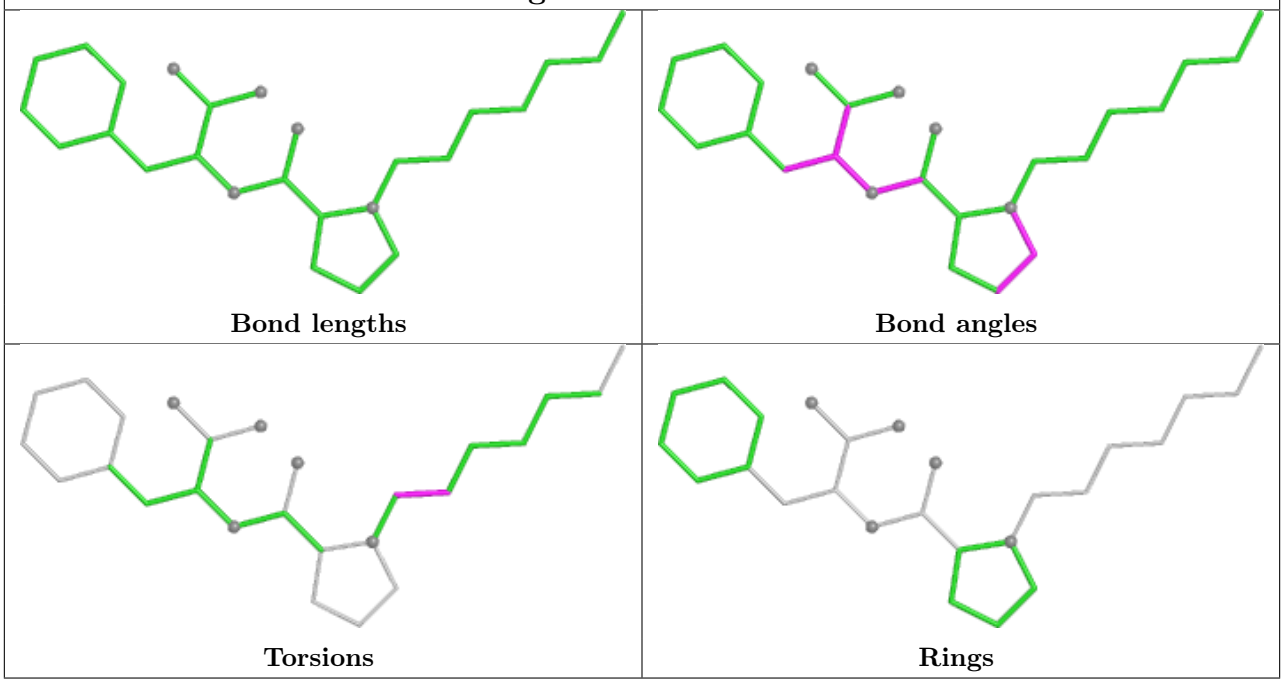
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

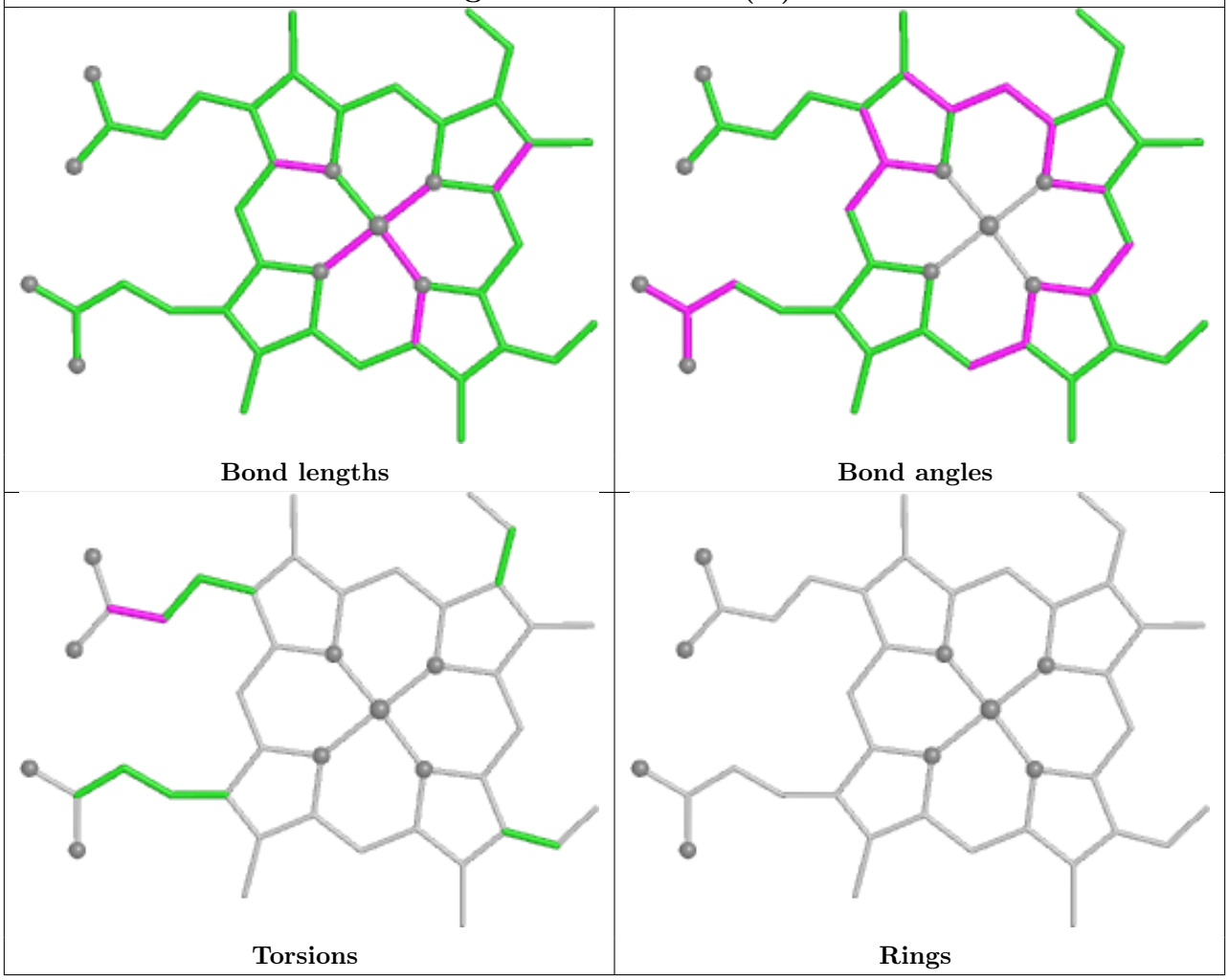
Ligand HEM A 501 (B)



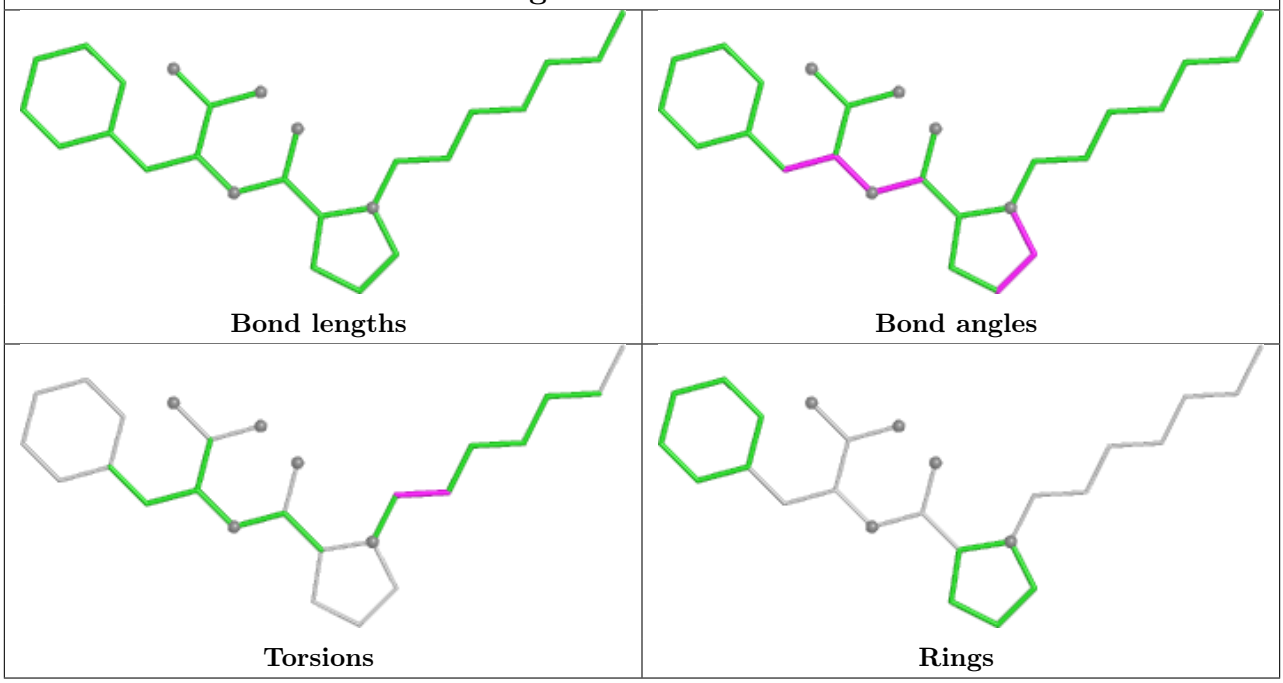
Ligand D0L A 502



Ligand HEM A 501 (A)



Ligand D0L B 502



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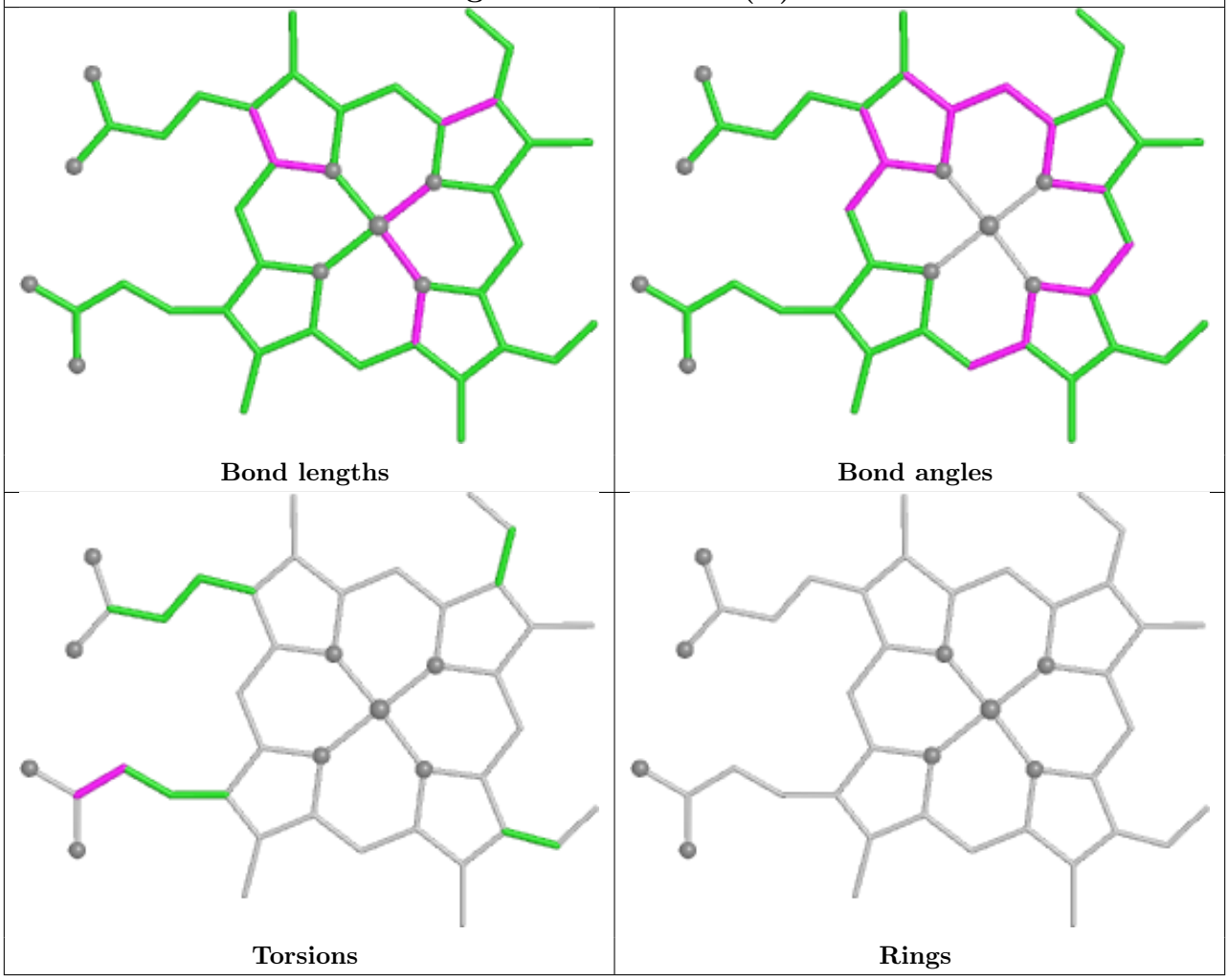
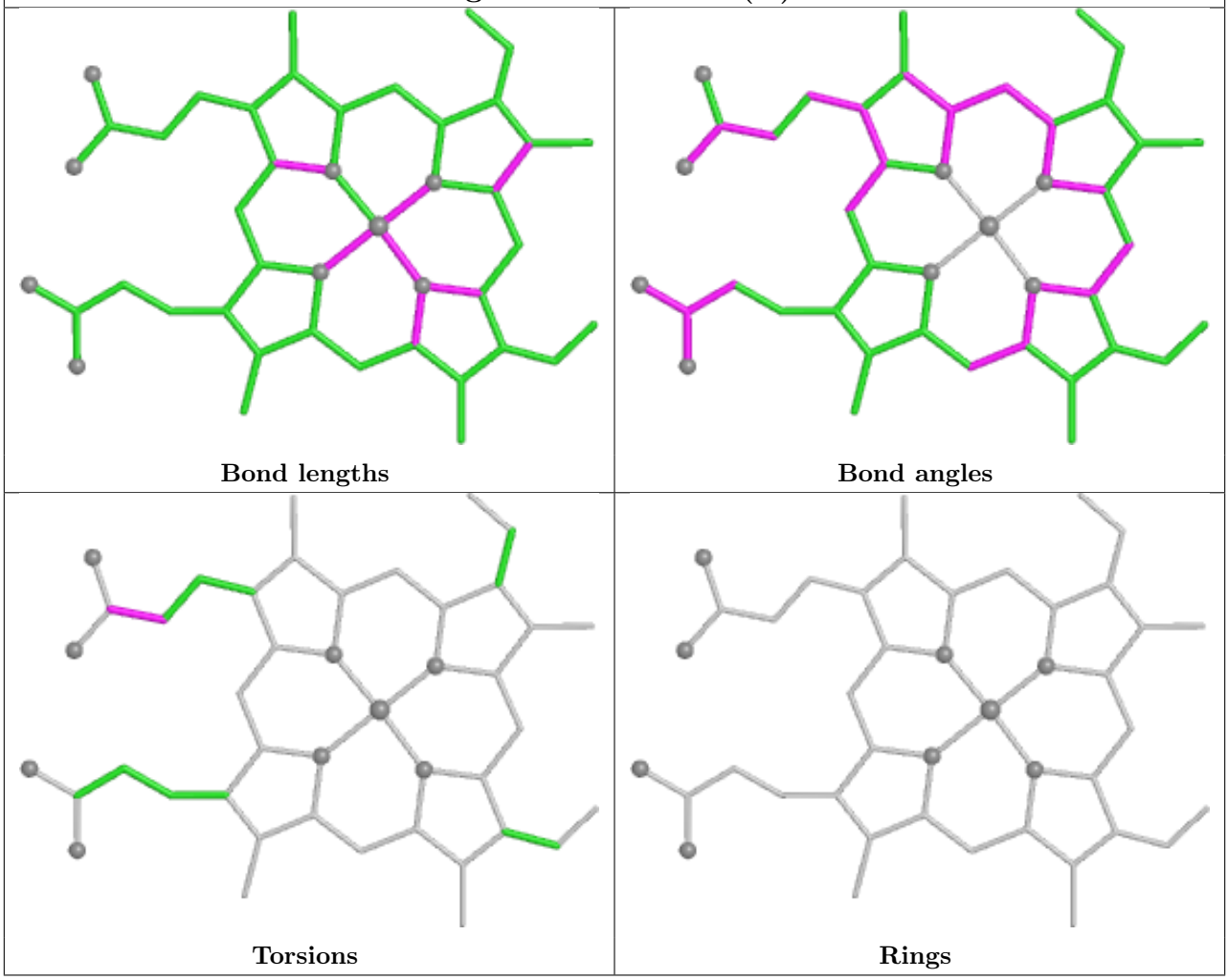


Ligand HEM B 501 (A)



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%)	-0.17	7 (1%)	72	75	8, 21, 48, 70	21 (4%)
1	B	454/456 (99%)	-0.30	3 (0%)	84	87	7, 20, 41, 60	22 (4%)
All	All	908/912 (99%)	-0.24	10 (1%)	78	82	7, 20, 43, 70	43 (4%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ILE	4.5
1	B	2	ILE	4.1
1	A	196	PRO	4.0
1	A	215	LEU	3.0
1	A	197	ALA	2.8
1	A	191	ALA	2.8
1	B	136	ASP	2.3
1	B	302	VAL	2.3
1	A	136	ASP	2.2
1	A	369	ASP	2.2

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)

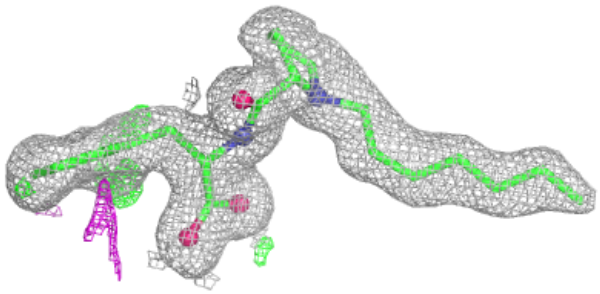
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

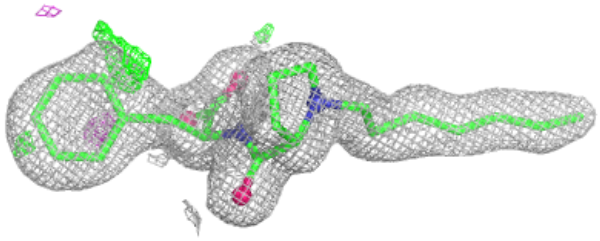
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	512	6/6	0.76	0.15	34,38,40,43	0
5	GOL	B	511	6/6	0.77	0.15	44,50,52,53	0
5	GOL	A	511	6/6	0.82	0.18	46,55,60,63	0
5	GOL	A	508	6/6	0.85	0.17	40,61,67,70	0
5	GOL	B	512	6/6	0.85	0.14	33,40,43,51	0
5	GOL	B	508	6/6	0.86	0.16	43,47,55,60	0
5	GOL	B	510	6/6	0.87	0.14	31,41,42,49	0
5	GOL	B	505	6/6	0.88	0.12	26,28,38,55	0
5	GOL	A	504	6/6	0.89	0.12	38,44,46,51	0
5	GOL	A	507	6/6	0.90	0.11	26,40,41,41	0
5	GOL	B	507	6/6	0.90	0.13	31,42,48,59	0
5	GOL	A	505	6/6	0.90	0.11	41,41,43,44	0
5	GOL	B	513	6/6	0.90	0.12	32,43,50,61	0
5	GOL	B	514	6/6	0.90	0.11	46,54,58,68	0
5	GOL	B	509	6/6	0.91	0.12	28,41,49,56	0
5	GOL	B	504	6/6	0.91	0.10	26,35,45,49	0
5	GOL	B	506	6/6	0.92	0.12	27,39,45,52	0
5	GOL	A	506	6/6	0.92	0.11	31,40,42,48	0
5	GOL	A	509	6/6	0.92	0.10	28,36,45,55	0
5	GOL	A	510	6/6	0.95	0.09	23,38,40,47	0
4	NME	B	503[B]	2/2	0.96	0.10	15,15,15,15	2
3	D0L	A	502	26/26	0.96	0.08	21,30,36,39	0
4	NME	B	503[A]	2/2	0.96	0.10	14,14,14,15	2
4	NME	A	503[A]	2/2	0.97	0.09	14,14,14,17	2
4	NME	A	503[B]	2/2	0.97	0.09	16,16,16,16	2
3	D0L	B	502	26/26	0.97	0.06	16,24,29,31	0
2	HEM	B	501[A]	43/43	0.99	0.04	10,13,15,18	43
2	HEM	B	501[B]	43/43	0.99	0.04	11,13,16,20	43
2	HEM	A	501[A]	43/43	0.99	0.04	13,14,17,23	43
2	HEM	A	501[B]	43/43	0.99	0.04	11,13,15,16	43

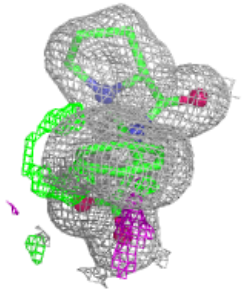
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around D0L A 502:

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

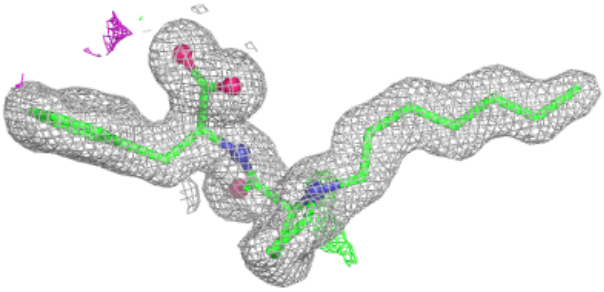


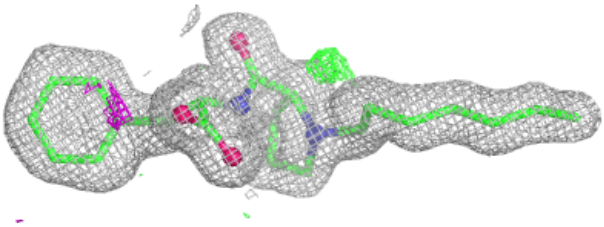


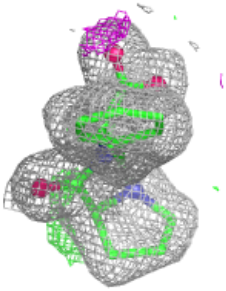


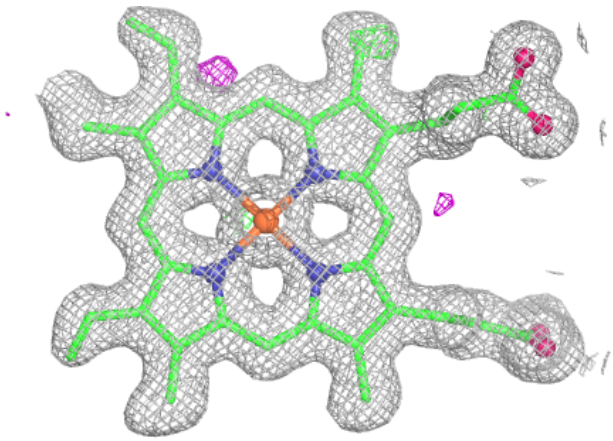
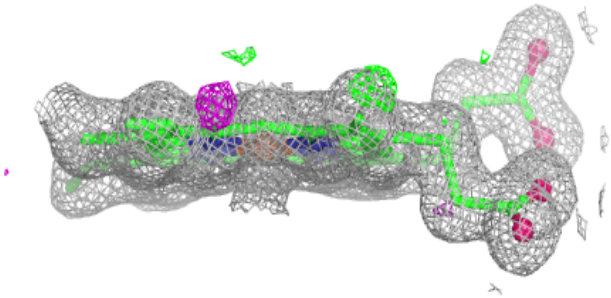
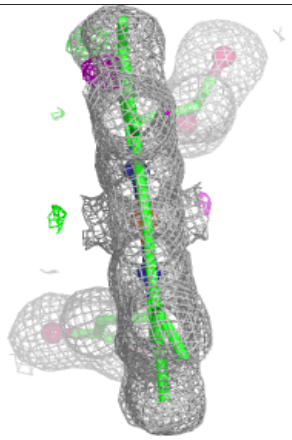
Electron density around D0L B 502:

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



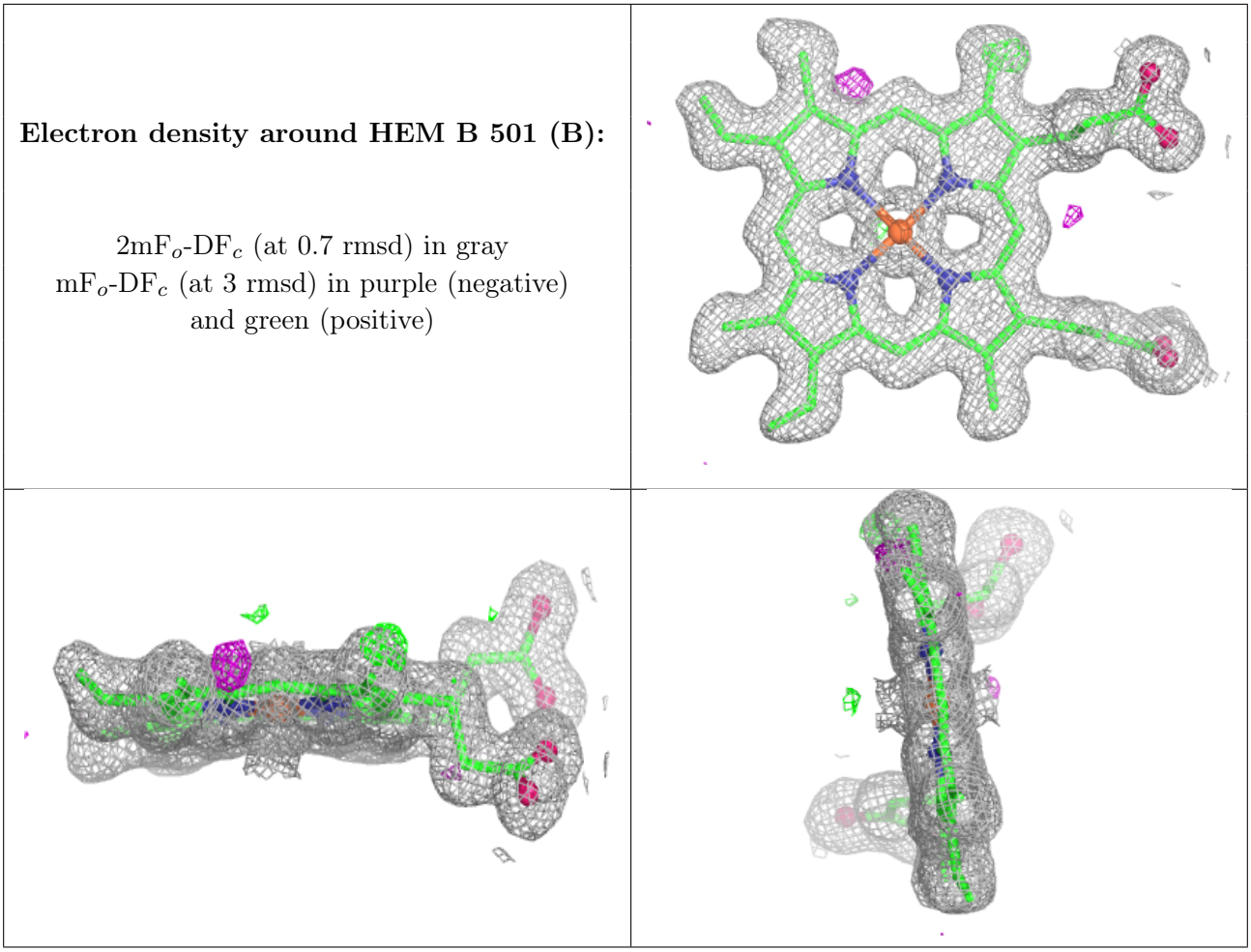




Electron density around HEM B 501 (A): $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

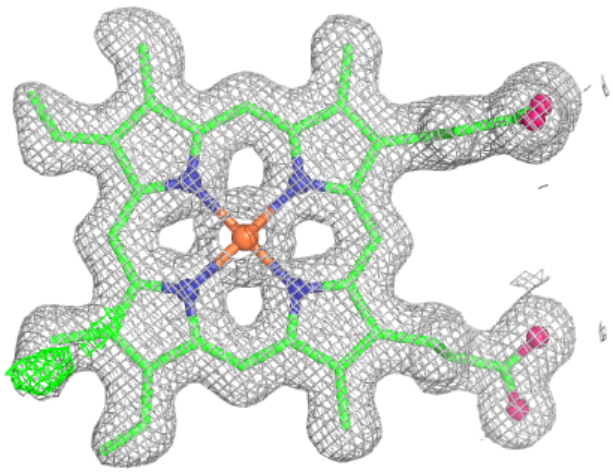
Electron density around HEM B 501 (B):

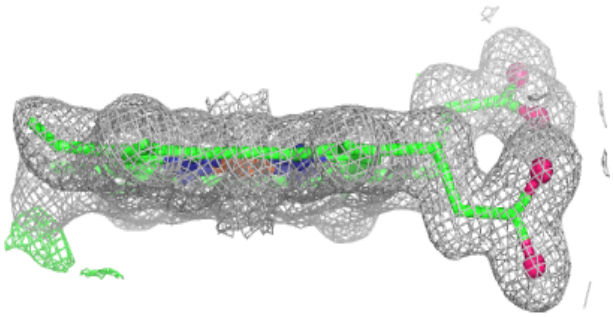
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

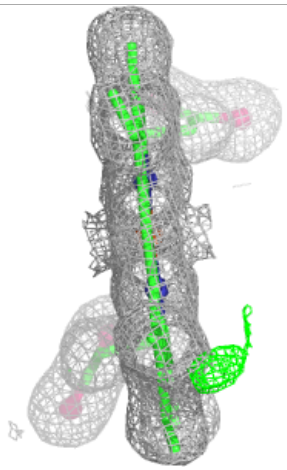


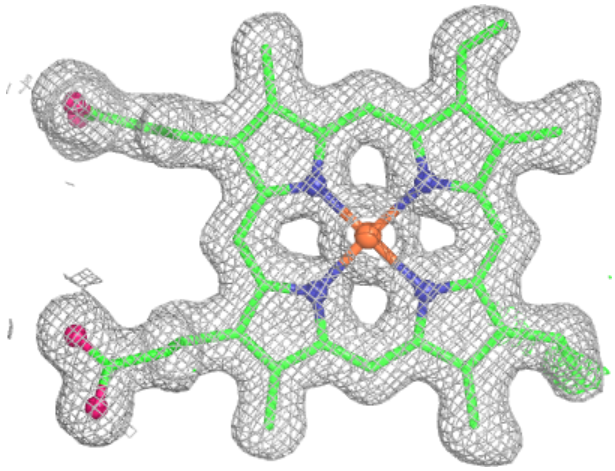
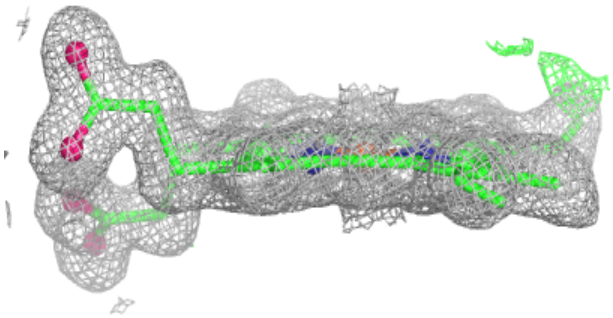
Electron density around HEM A 501 (A):

$2mF_o$-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.