wwPDB X-ray Structure Validation Summary Report (i)

Aug 25, 2026 – 12:17 pm BST

PDB ID	:	7Q6X / pdb_00007q6x
Title	:	OleP mutant S240Y in complex with 6DEB
Authors	:	Savino, C.; Montemiglio, L.C.; Vallone, B.; Exertier, C.; Freda, I.; Gugole, E.
Deposited on	:	2021-11-09
Resolution	:	2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
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:

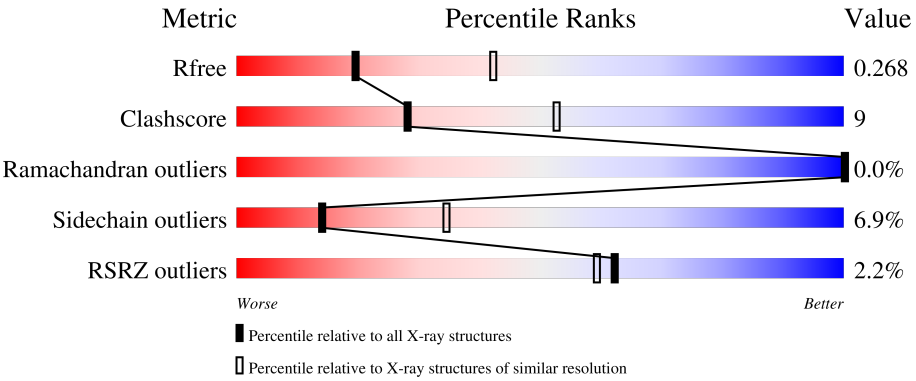
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	406	73% 23%
1	B	406	78% 21%
1	C	406	80% 17%
1	D	406	70% 26%
1	E	406	74% 21%

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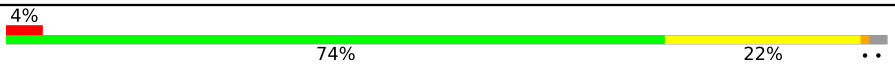
Mol	Chain	Length	Quality of chain
1	F	406	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20720 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 Cytochrome P-450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	41	0
			3355	2126	598	616	15			
1	B	406	Total	C	N	O	S	0	32	0
			3361	2128	603	617	13			
1	C	399	Total	C	N	O	S	0	24	0
			3262	2060	585	604	13			
1	D	396	Total	C	N	O	S	0	48	0
			3396	2161	606	616	13			
1	E	395	Total	C	N	O	S	0	31	0
			3282	2082	587	599	14			
1	F	397	Total	C	N	O	S	0	50	0
			3402	2161	601	626	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	-	expression tag	UNP Q59819
A	3	ALA	-	expression tag	UNP Q59819
A	240	TYR	SER	engineered mutation	UNP Q59819
B	2	ALA	-	expression tag	UNP Q59819
B	3	ALA	-	expression tag	UNP Q59819
B	240	TYR	SER	engineered mutation	UNP Q59819
C	2	ALA	-	expression tag	UNP Q59819
C	3	ALA	-	expression tag	UNP Q59819
C	240	TYR	SER	engineered mutation	UNP Q59819
D	2	ALA	-	expression tag	UNP Q59819
D	3	ALA	-	expression tag	UNP Q59819
D	240	TYR	SER	engineered mutation	UNP Q59819
E	2	ALA	-	expression tag	UNP Q59819
E	3	ALA	-	expression tag	UNP Q59819
E	240	TYR	SER	engineered mutation	UNP Q59819
F	2	ALA	-	expression tag	UNP Q59819
F	3	ALA	-	expression tag	UNP Q59819

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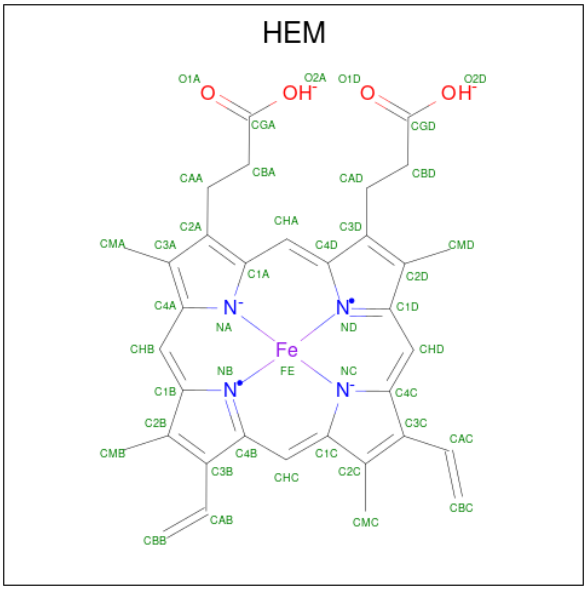
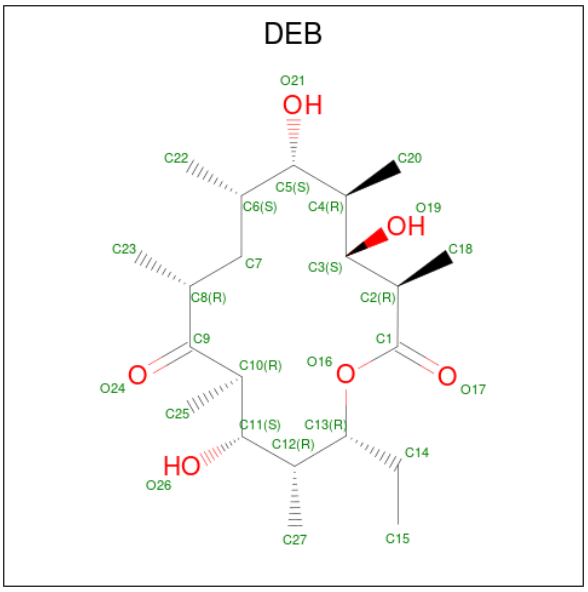
Chain	Residue	Modelled	Actual	Comment	Reference
F	240	TYR	SER	engineered mutation	UNP Q59819

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



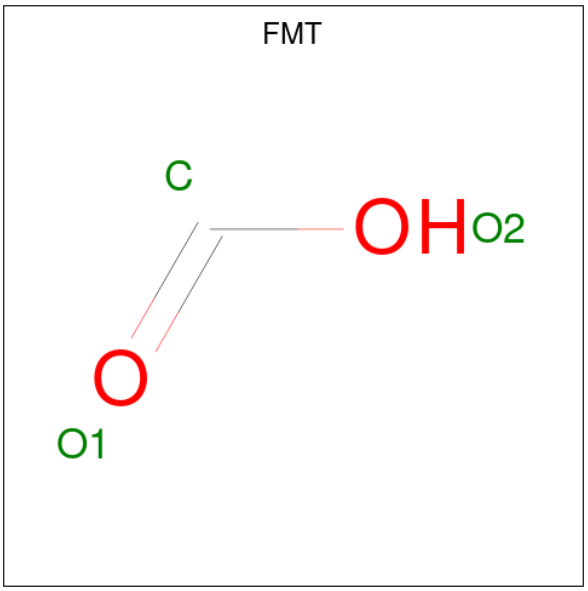
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 6-DEOXYERYTHRONOLIDE B (CCD ID: DEB) (formula: $C_{21}H_{38}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 27 21 6	0	0
3	B	1	Total C O 27 21 6	0	0
3	C	1	Total C O 27 21 6	0	0
3	D	1	Total C O 27 21 6	0	0
3	E	1	Total C O 27 21 6	0	0
3	F	1	Total C O 27 21 6	0	0

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	A	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0
4	D	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	38	Total O 38 38	0	0
5	B	48	Total O 48 48	0	0
5	C	55	Total O 55 55	0	3
5	D	19	Total O 19 19	0	2
5	E	28	Total O 28 28	0	0
5	F	36	Total O 36 36	0	2

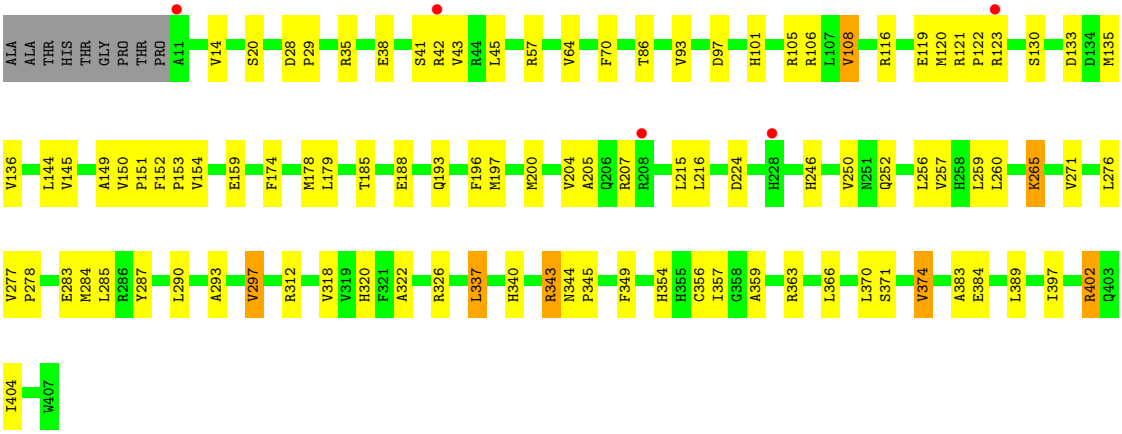
3 Residue-property plots (i)

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: Cytochrome P-450

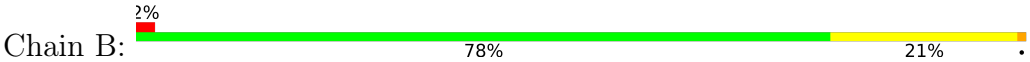
Chain A:

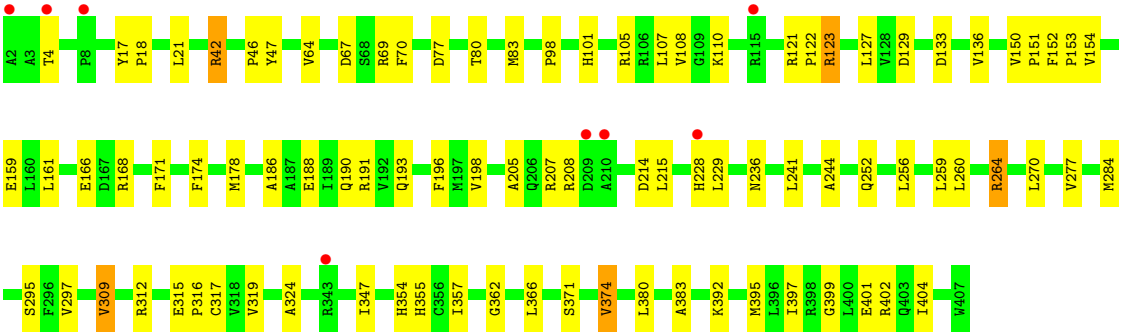




• Molecule 1: Cytochrome P-450

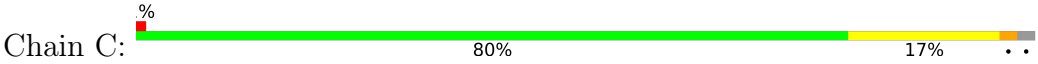
Chain B:



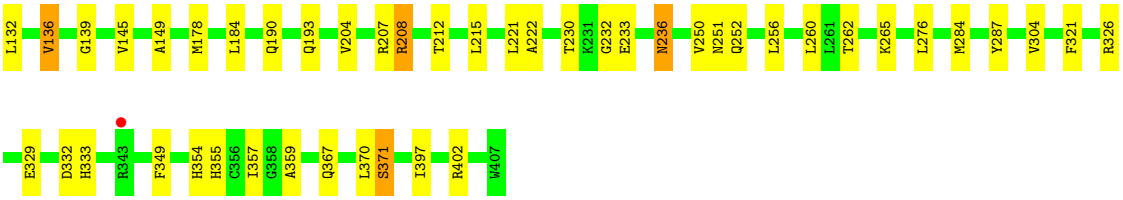


• Molecule 1: Cytochrome P-450

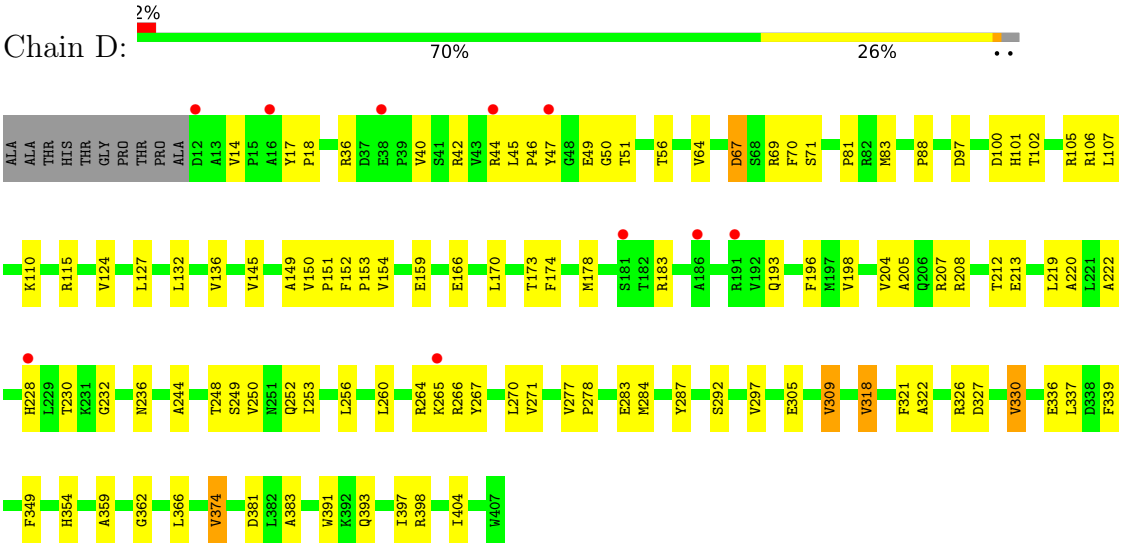
Chain C:



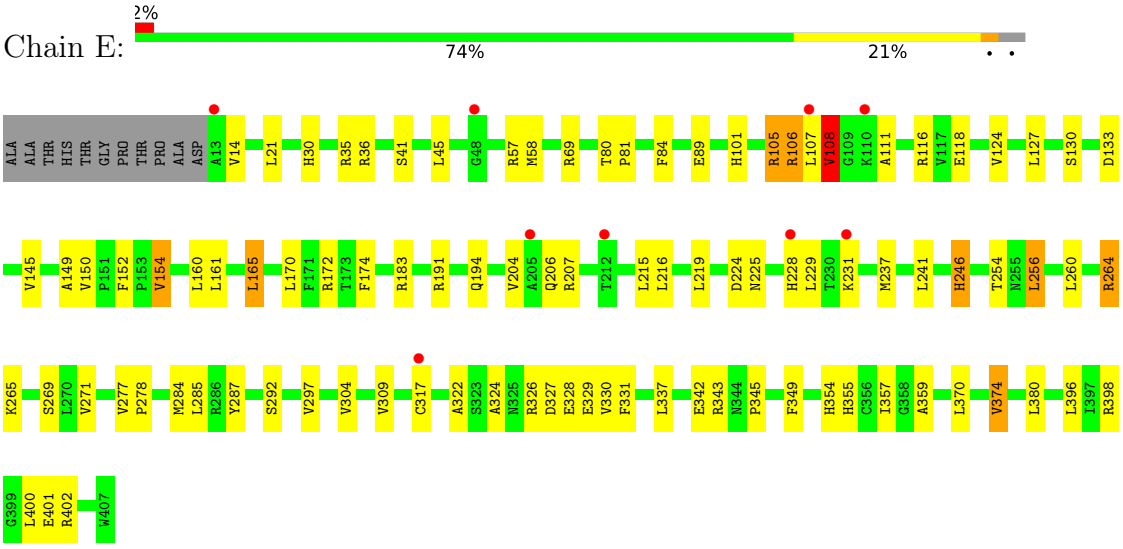




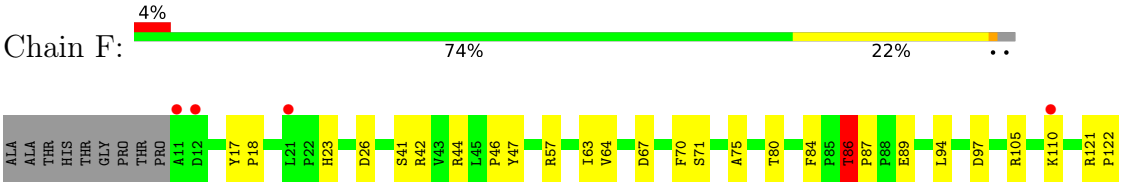
• Molecule 1: Cytochrome P-450

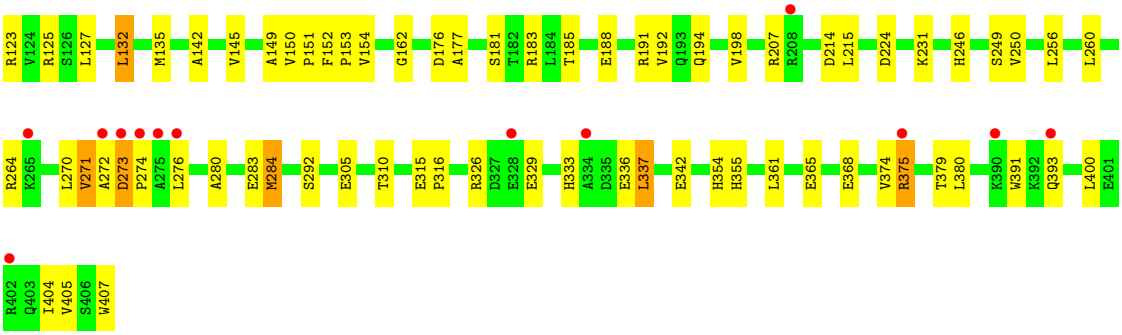


• Molecule 1: Cytochrome P-450



• Molecule 1: Cytochrome P-450




R123 V124 R125 S126 L127 L132 M135 A142 V145 A149 V150 P151 F152 P153 V154 G162 D176 A177 S181 T182 R183 L184 T185 E188 R191 V192 Q193 Q194 V198 R207 R208 D214 L215 D224 K231 H246 S249 V250 L256 L260
R264 K265 L270 V271 A272 D273 P274 A275 L276 A280 E283 M284 S292 E305 T310 E315 P316 R326 D327 E328 E329 H333 A334 D335 E336 L337 E342 H354 H355 L361 E365 E368 V374 R375 T379 L380 K390 W391 K392 Q393 L400 E401
R402 Q403 I404 V405 S406 W407

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	248.62Å 110.36Å 160.05Å 90.00° 129.63° 90.00°	Depositor
Resolution (Å)	51.34 – 2.70 51.34 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (51.34-2.70) 99.9 (51.34-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.204 , 0.268 0.206 , 0.268	Depositor DCC
R_{free} test set	5565 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	75.4	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20720	wwPDB-VP
Average B, all atoms (Å^2)	70.0	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 40.21 % 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 2.8308e-04. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, DEB, FMT

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	1.02	0/3543	1.44	6/4812 (0.1%)
1	B	1.03	3/3531 (0.1%)	1.49	4/4801 (0.1%)
1	C	1.00	2/3395 (0.1%)	1.43	5/4620 (0.1%)
1	D	1.06	4/3617 (0.1%)	1.47	2/4912 (0.0%)
1	E	1.05	4/3446 (0.1%)	1.50	8/4679 (0.2%)
1	F	1.10	10/3622 (0.3%)	1.47	7/4917 (0.1%)
All	All	1.04	23/21154 (0.1%)	1.46	32/28741 (0.1%)

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110[A]	LYS	C-O	7.03	1.32	1.24
1	B	110[B]	LYS	C-O	7.03	1.32	1.24
1	B	110[C]	LYS	C-O	7.03	1.32	1.24
1	E	343[A]	ARG	C-O	6.94	1.32	1.23
1	E	343[B]	ARG	C-O	6.94	1.32	1.23

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	272	ALA	N-CA-C	-7.01	104.85	113.19
1	F	274	PRO	N-CA-CB	6.83	109.70	103.34
1	C	276	LEU	CA-C-N	6.79	125.77	120.33
1	C	276	LEU	C-N-CA	6.79	125.77	120.33
1	A	356	CYS	N-CA-CB	6.23	119.14	109.48

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	3355	0	3408	66	0
1	B	3361	0	3417	55	0
1	C	3262	0	3270	51	0
1	D	3396	0	3492	80	0
1	E	3282	0	3347	59	0
1	F	3402	0	3487	45	0
2	A	43	0	30	4	0
2	B	43	0	30	5	0
2	C	43	0	30	7	0
2	D	43	0	30	7	0
2	E	43	0	30	2	0
2	F	43	0	30	3	0
3	A	27	0	38	0	0
3	B	27	0	38	0	0
3	C	27	0	38	0	0
3	D	27	0	38	1	0
3	E	27	0	38	0	0
3	F	27	0	38	1	0
4	A	9	0	3	1	0
4	C	3	0	1	0	0
4	D	3	0	1	0	0
4	E	3	0	1	0	0
5	A	38	0	0	2	0
5	B	48	0	0	0	0
5	C	55	0	0	3	0
5	D	19	0	0	4	0
5	E	28	0	0	1	0
5	F	36	0	0	1	0
All	All	20720	0	20835	367	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 9.

The worst 5 of 367 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:D:42[A]:ARG:NE	5:D:601[A]:HOH:O	1.80	1.15
1:E:106[A]:ARG:CG	1:E:106[A]:ARG:HH21	1.61	1.14
1:E:106[B]:ARG:HH11	1:E:106[B]:ARG:HG2	0.95	1.09
1:E:106[A]:ARG:HH21	1:E:106[A]:ARG:HG2	1.13	1.08
1:A:106[B]:ARG:HG2	1:A:106[B]:ARG:HH11	1.14	1.06

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	436/406 (107%)	410 (94%)	26 (6%)	0	100	100
1	B	437/406 (108%)	417 (95%)	20 (5%)	0	100	100
1	C	420/406 (103%)	403 (96%)	17 (4%)	0	100	100
1	D	443/406 (109%)	410 (93%)	33 (7%)	0	100	100
1	E	424/406 (104%)	398 (94%)	26 (6%)	0	100	100
1	F	445/406 (110%)	423 (95%)	21 (5%)	1 (0%)	43	68
All	All	2605/2436 (107%)	2461 (94%)	143 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	273	ASP

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	373/338 (110%)	352 (94%)	21 (6%)	19 44
1	B	371/338 (110%)	346 (93%)	25 (7%)	15 36
1	C	355/338 (105%)	330 (93%)	25 (7%)	14 34
1	D	380/338 (112%)	356 (94%)	24 (6%)	16 39
1	E	362/338 (107%)	326 (90%)	36 (10%)	7 19
1	F	380/338 (112%)	348 (92%)	32 (8%)	10 26
All	All	2221/2028 (110%)	2058 (93%)	163 (7%)	14 32

5 of 163 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	206	GLN
1	F	215	LEU
1	E	264	ARG
1	E	402	ARG
1	F	256	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	355	HIS
1	F	193	GLN
1	E	320	HIS
1	E	206	GLN
1	E	340	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)

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	$\#\|Z\| > 2$
3	DEB	E	502	-	27,27,27	0.37	0	35,39,39	0.73	1 (2%)
2	HEM	C	501	1	50,50,50	1.66	10 (20%)	66,82,82	1.98	14 (21%)
2	HEM	F	501	1	50,50,50	1.51	6 (12%)	66,82,82	1.58	9 (13%)
3	DEB	B	502	-	27,27,27	0.47	0	35,39,39	0.89	1 (2%)
2	HEM	B	501	1	50,50,50	1.68	10 (20%)	66,82,82	1.81	16 (24%)
4	FMT	A	504	-	2,2,2	0.29	0	1,1,1	0.20	0
2	HEM	E	501	1	50,50,50	1.58	7 (14%)	66,82,82	1.60	17 (25%)
4	FMT	A	505	-	2,2,2	0.47	0	1,1,1	0.00	0
3	DEB	C	502	-	27,27,27	0.39	0	35,39,39	0.90	1 (2%)
2	HEM	A	501	1	50,50,50	1.80	11 (22%)	66,82,82	2.95	27 (40%)
3	DEB	F	502	-	27,27,27	0.29	0	35,39,39	0.67	0
4	FMT	C	503	-	2,2,2	0.27	0	1,1,1	0.19	0
3	DEB	D	502	-	27,27,27	0.56	1 (3%)	35,39,39	0.90	1 (2%)
2	HEM	D	501	1	50,50,50	1.66	10 (20%)	66,82,82	1.76	14 (21%)
4	FMT	D	503	-	2,2,2	0.26	0	1,1,1	0.18	0
3	DEB	A	502	-	27,27,27	0.48	0	35,39,39	0.97	2 (5%)
4	FMT	E	503	-	2,2,2	0.46	0	1,1,1	0.04	0
4	FMT	A	503	-	2,2,2	0.28	0	1,1,1	0.18	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
3	DEB	E	502	-	-	12/50/50/50	0/1/1/1
2	HEM	C	501	1	-	2/14/54/54	-
2	HEM	F	501	1	-	0/14/54/54	-
3	DEB	B	502	-	-	8/50/50/50	0/1/1/1
2	HEM	B	501	1	-	4/14/54/54	-
2	HEM	E	501	1	-	3/14/54/54	-
3	DEB	C	502	-	-	8/50/50/50	0/1/1/1
2	HEM	A	501	1	-	0/14/54/54	-
3	DEB	F	502	-	-	10/50/50/50	0/1/1/1
3	DEB	D	502	-	-	10/50/50/50	0/1/1/1
2	HEM	D	501	1	-	2/14/54/54	-
3	DEB	A	502	-	-	10/50/50/50	0/1/1/1

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	HEM	FE-NB	5.05	2.10	1.94
2	F	501	HEM	FE-NB	4.97	2.10	1.94
2	A	501	HEM	C1B-NB	-4.84	1.32	1.40
2	B	501	HEM	C1B-NB	-4.46	1.32	1.40
2	F	501	HEM	FE-NC	4.35	2.09	1.95

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	HEM	C1B-NB-C4B	10.26	115.67	105.07
2	A	501	HEM	C4D-ND-C1D	-8.48	96.31	105.07
2	C	501	HEM	CHC-C4B-NB	7.35	132.41	124.42
2	A	501	HEM	CHD-C1D-C2D	-7.31	113.56	124.98
2	A	501	HEM	CHC-C4B-NB	7.22	132.26	124.42

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	HEM	C1A-C2A-CAA-CBA
3	A	502	DEB	C12-C13-C14-C15
3	A	502	DEB	O16-C13-C14-C15
3	B	502	DEB	C12-C13-C14-C15
3	B	502	DEB	O16-C13-C14-C15

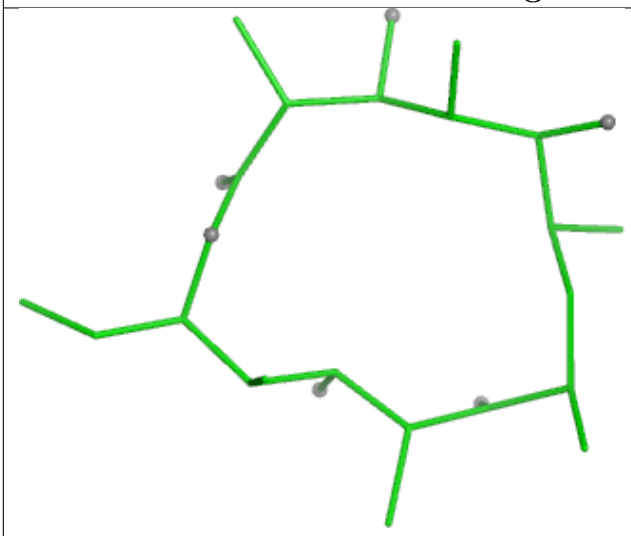
There are no ring outliers.

9 monomers are involved in 30 short contacts:

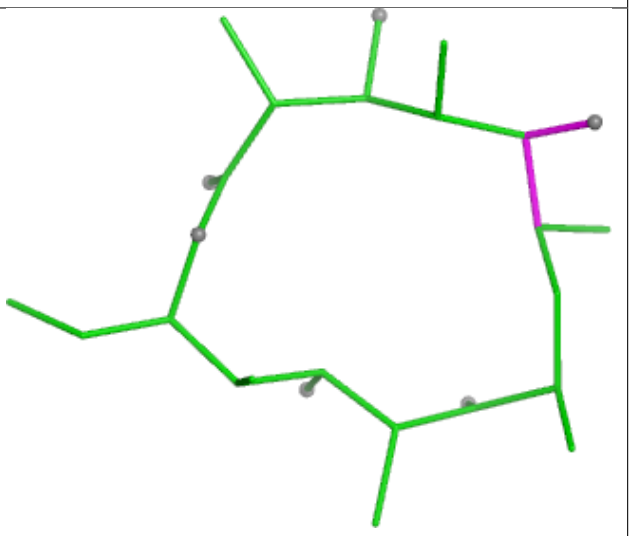
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	HEM	7	0
2	F	501	HEM	3	0
2	B	501	HEM	5	0
4	A	504	FMT	1	0
2	E	501	HEM	2	0
2	A	501	HEM	4	0
3	F	502	DEB	1	0
3	D	502	DEB	1	0
2	D	501	HEM	7	0

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.

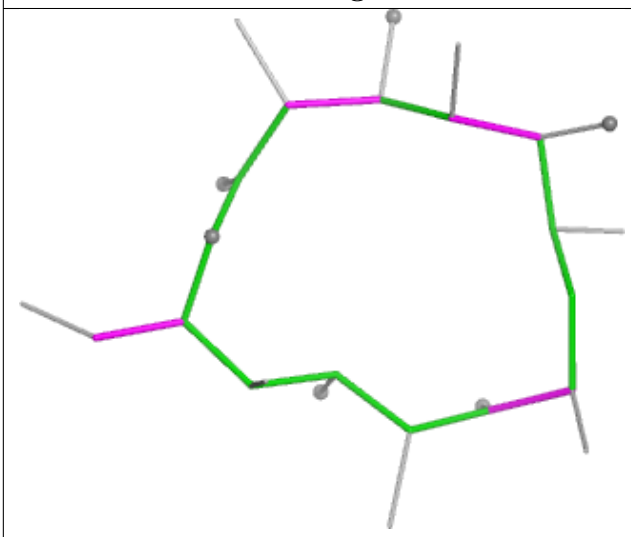
Ligand DEB E 502



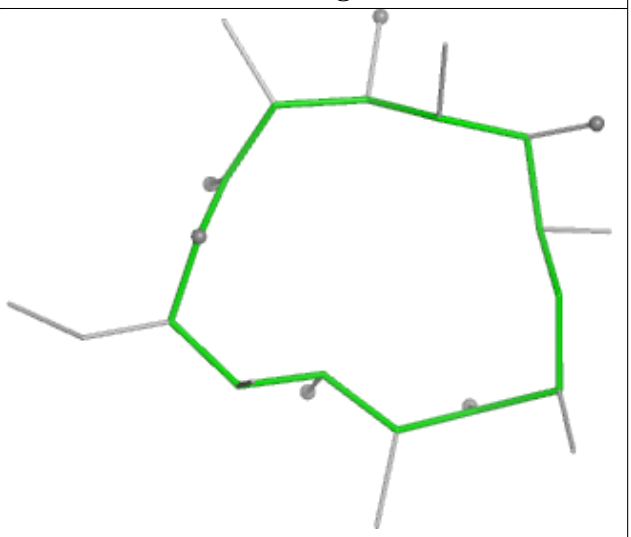
Bond lengths



Bond angles

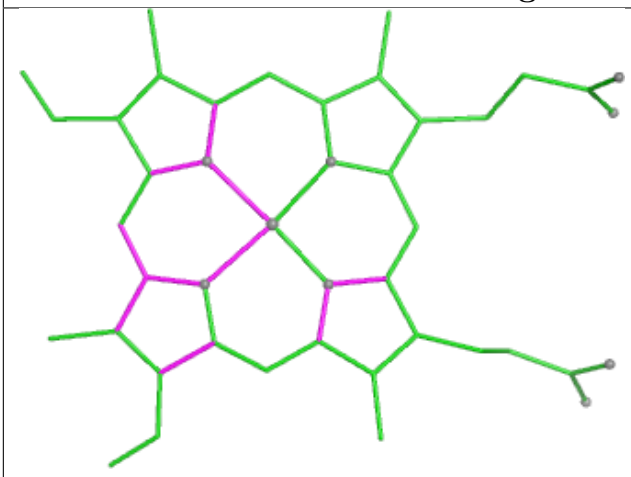


Torsions



Rings

Ligand HEM C 501



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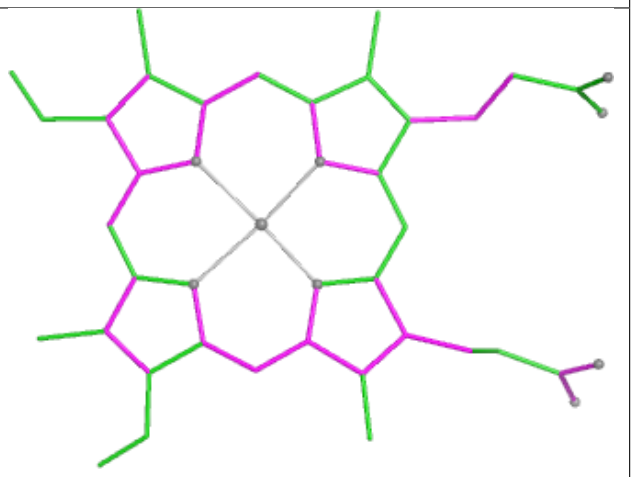

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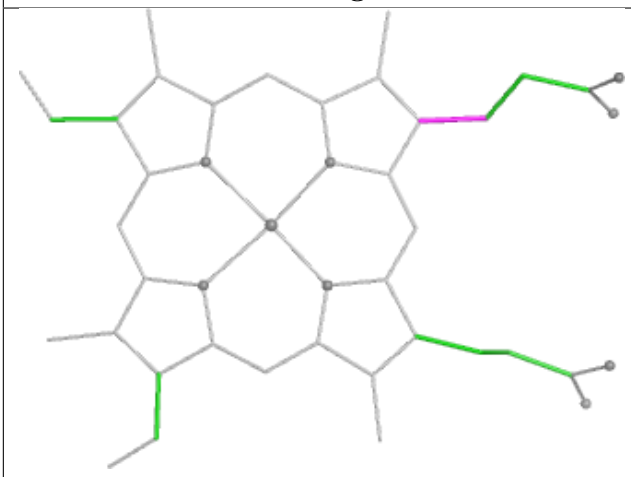

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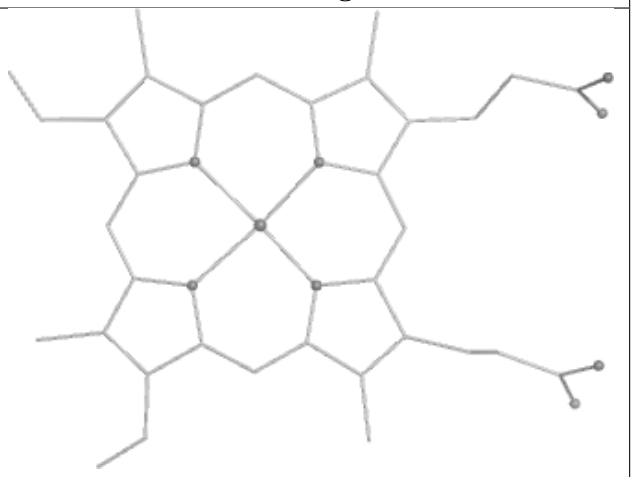

Rings

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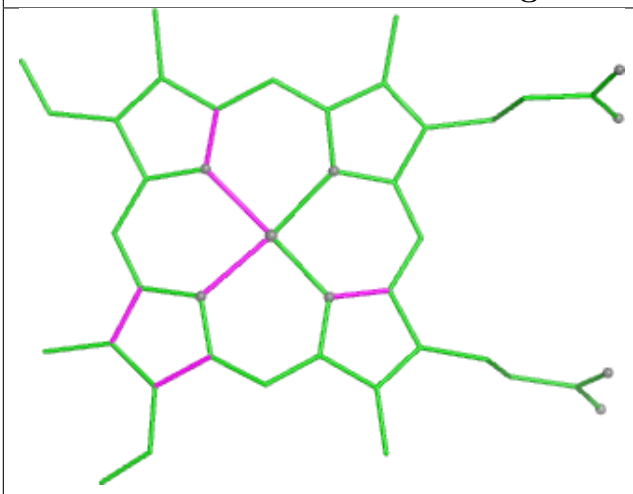

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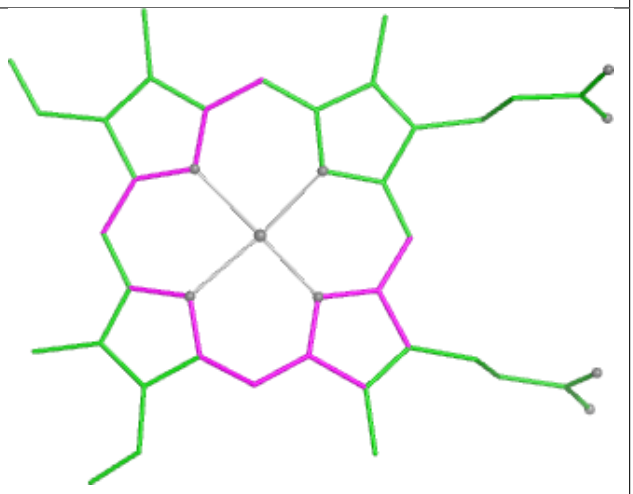

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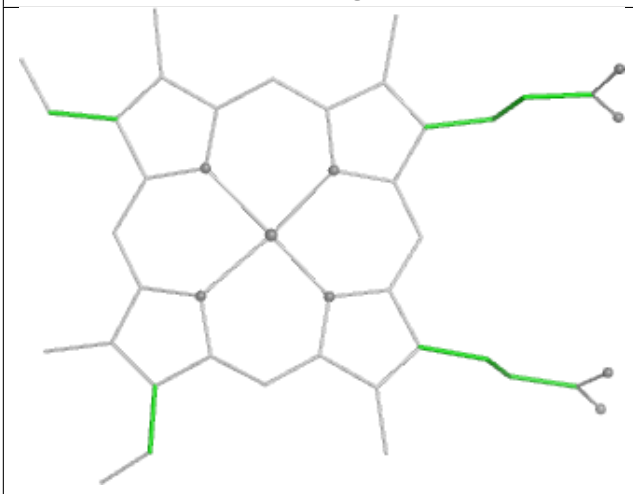

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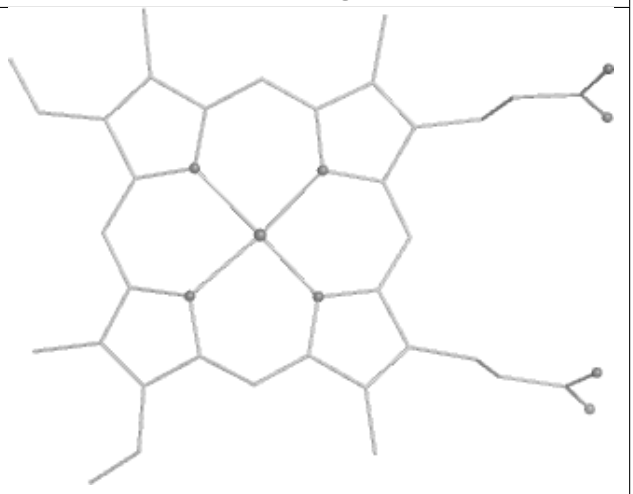
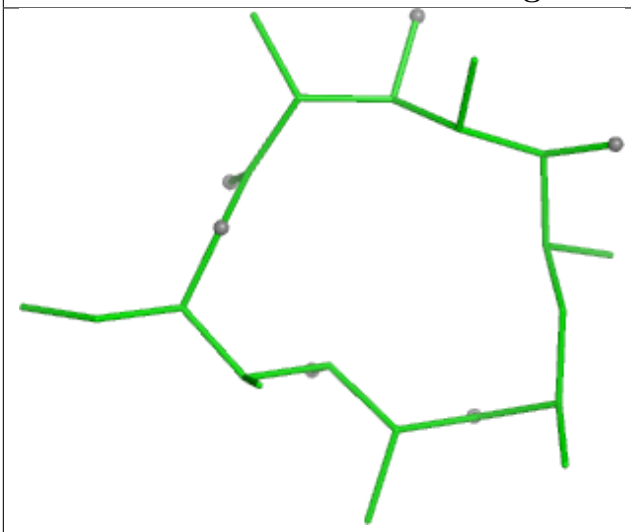


Rings

Ligand DEB B 502



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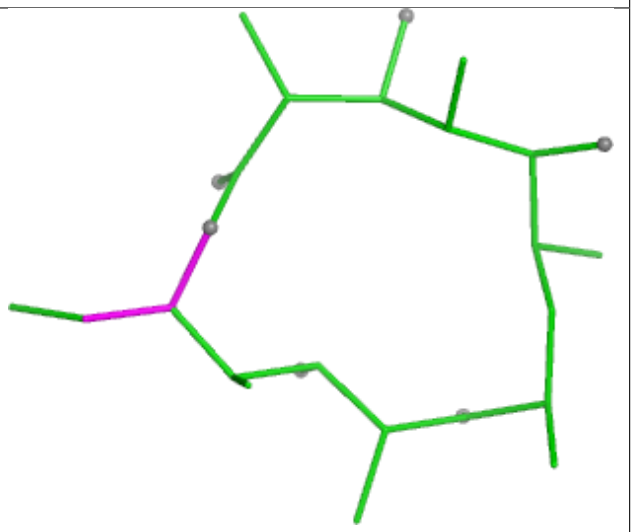

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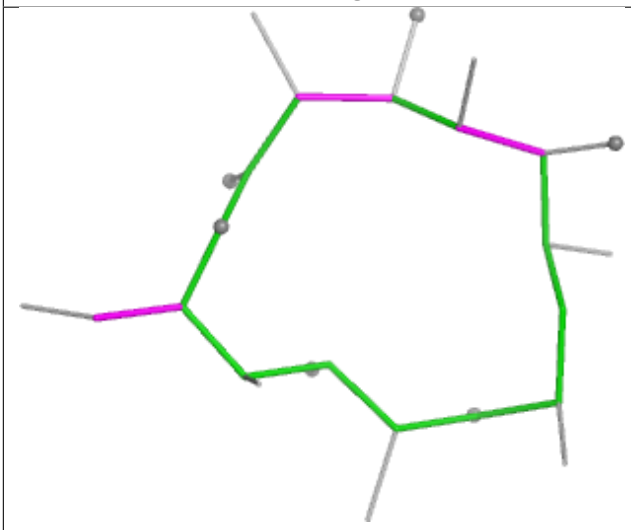

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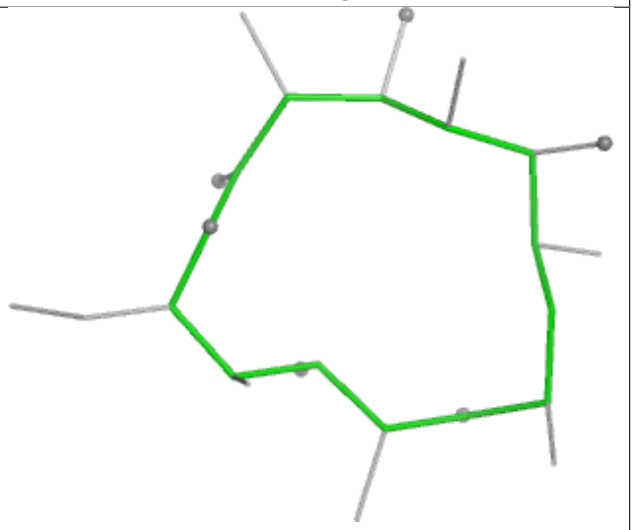
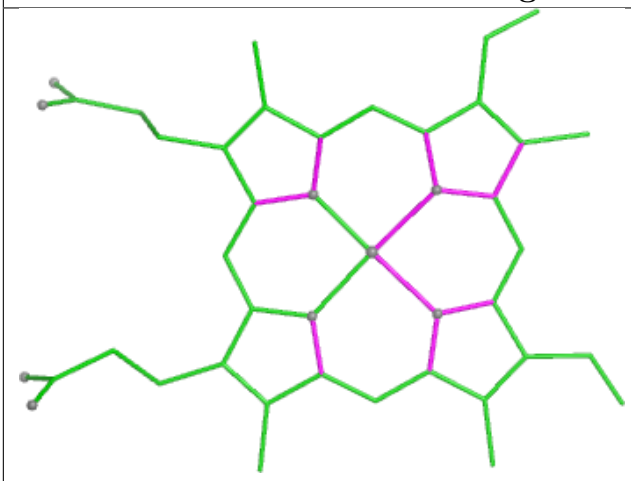


Rings

Ligand HEM B 501



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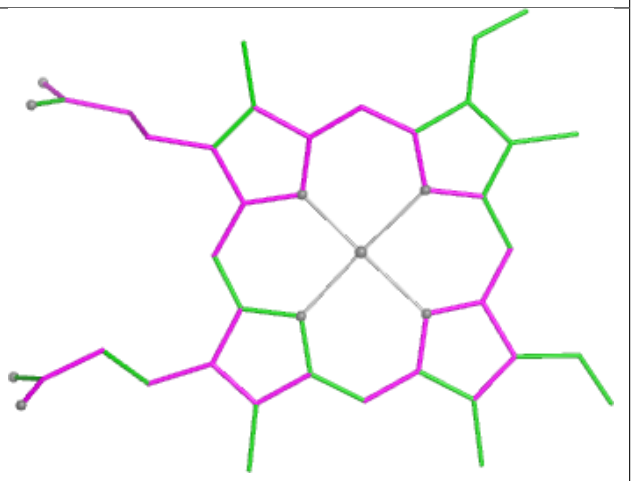

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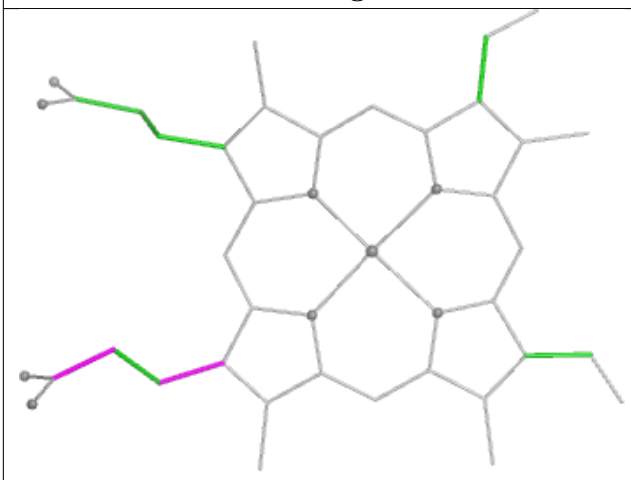

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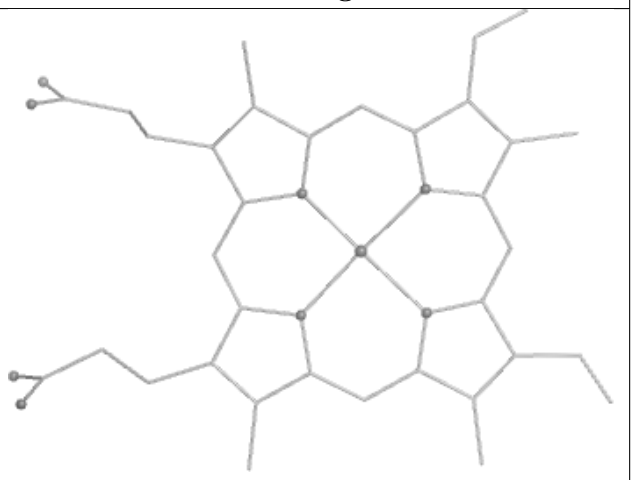
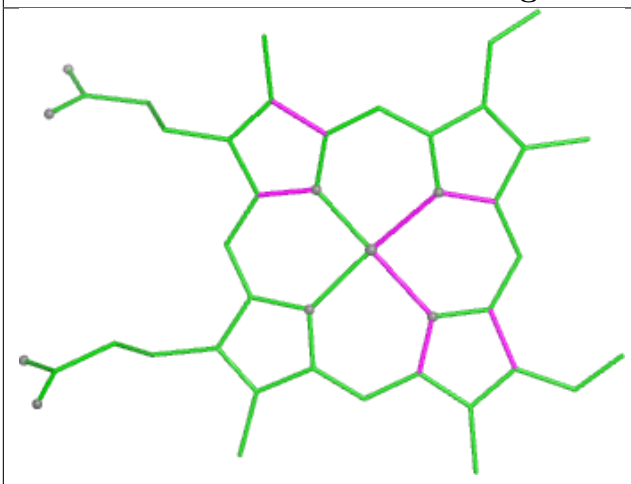


Rings

Ligand HEM E 501



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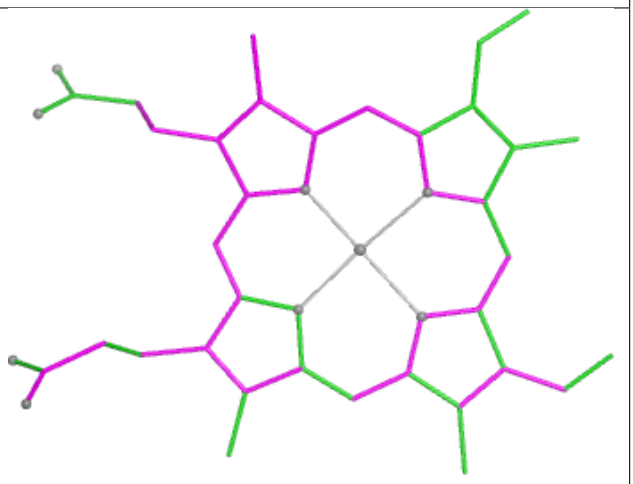

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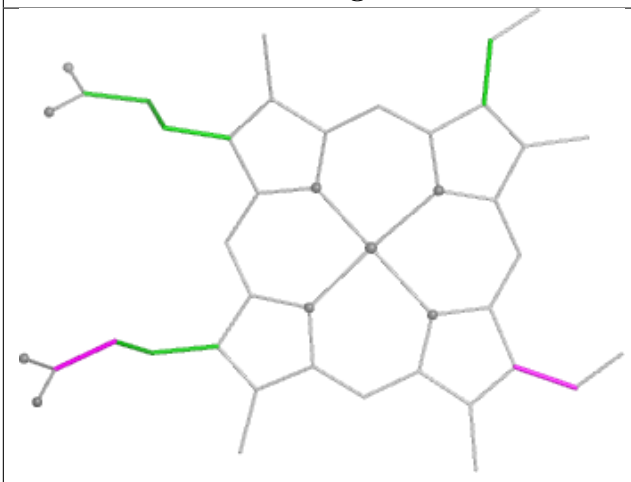

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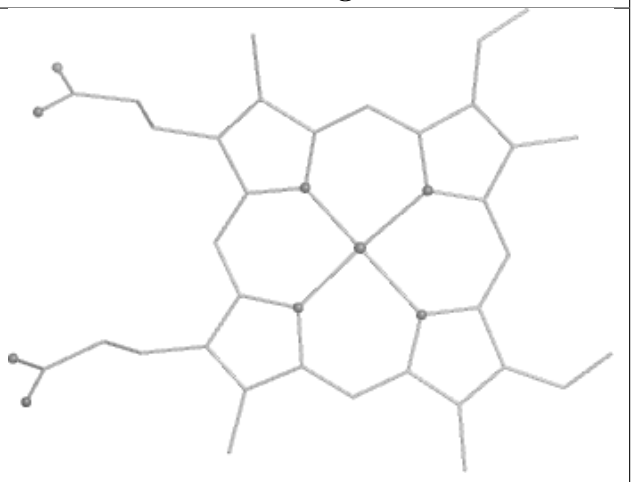


Rings

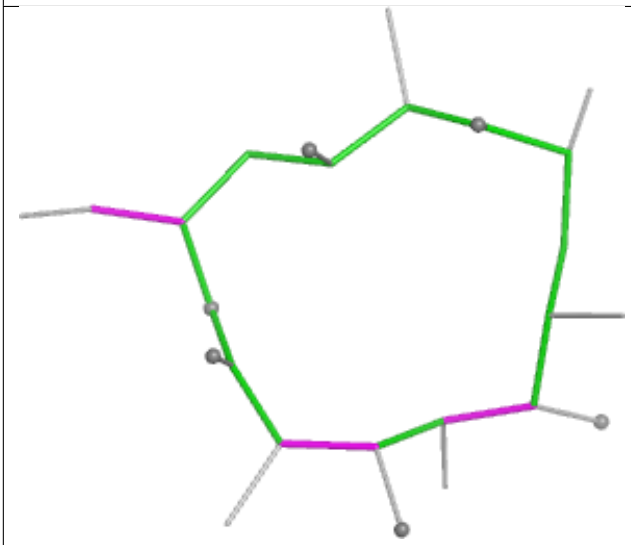
Ligand DEB C 502



Bond lengths



Bond angles



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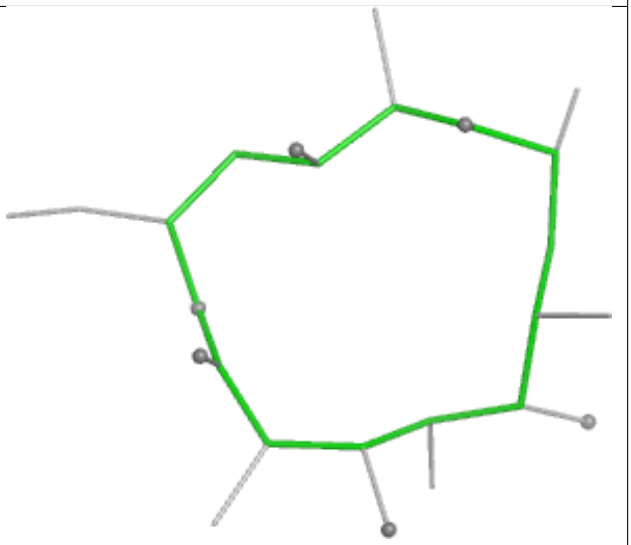
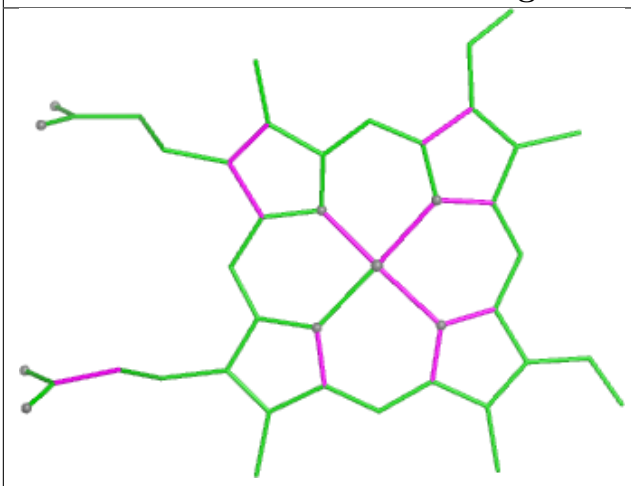


Rings

Ligand HEM A 501



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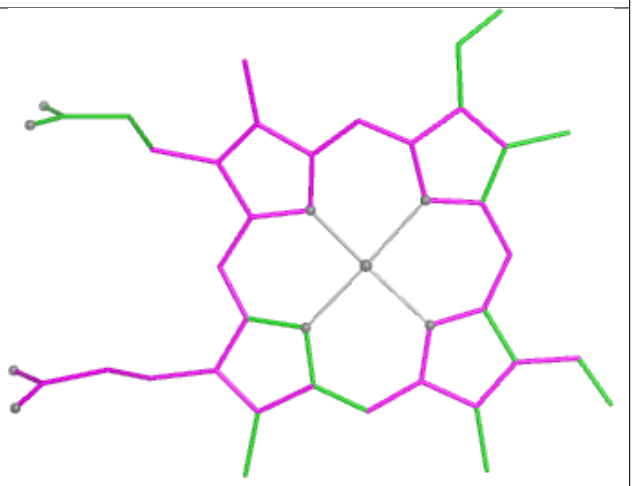

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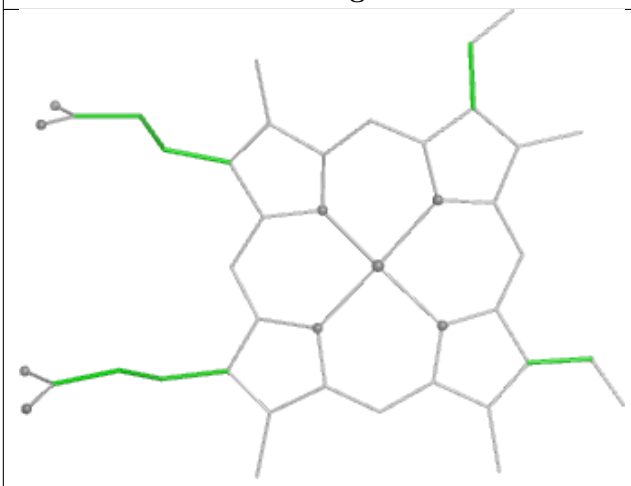

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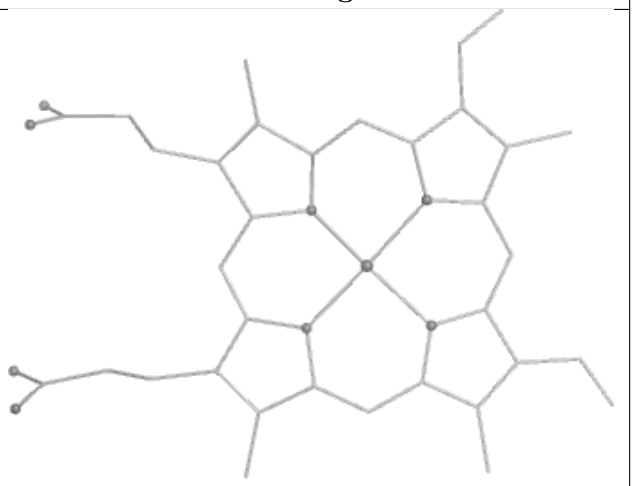
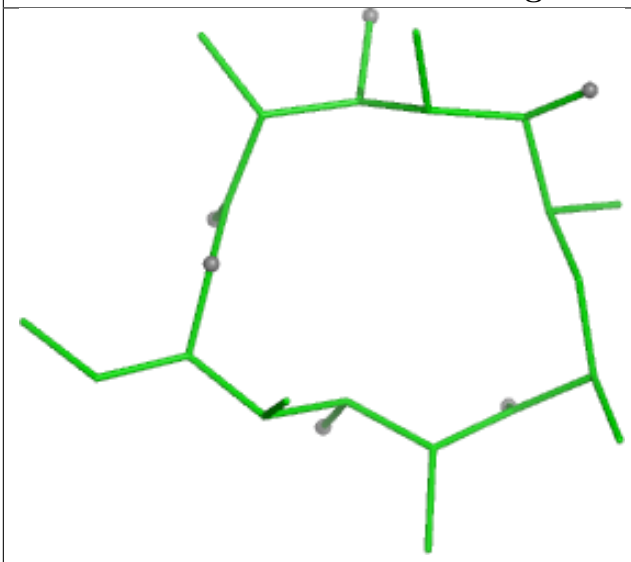


Rings

Ligand DEB F 502



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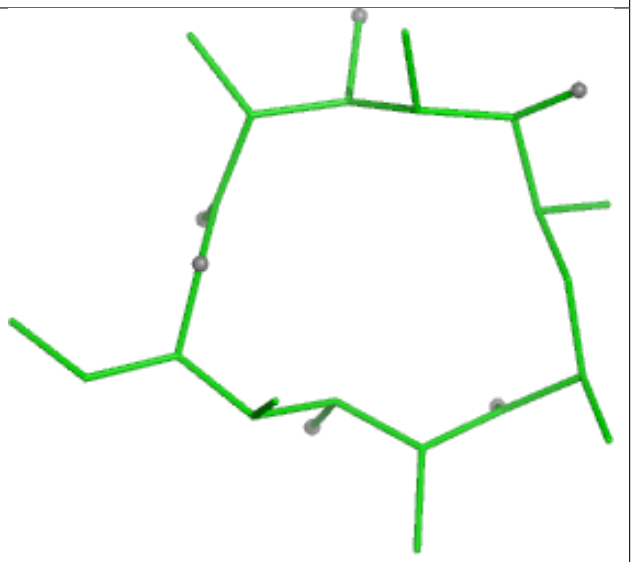
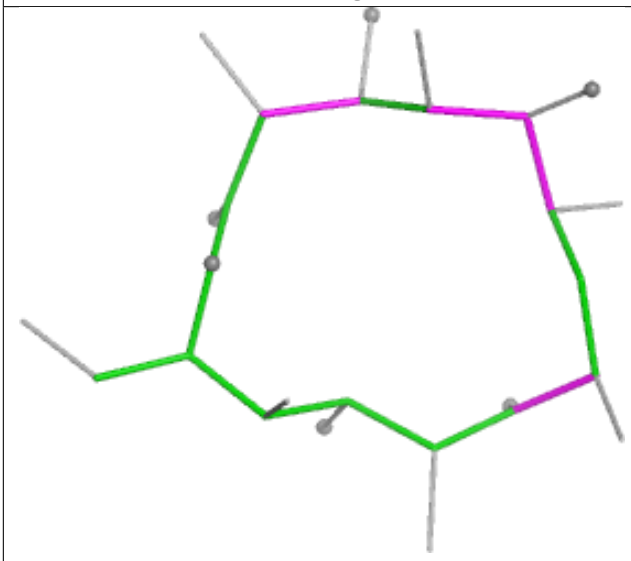


Bond angles



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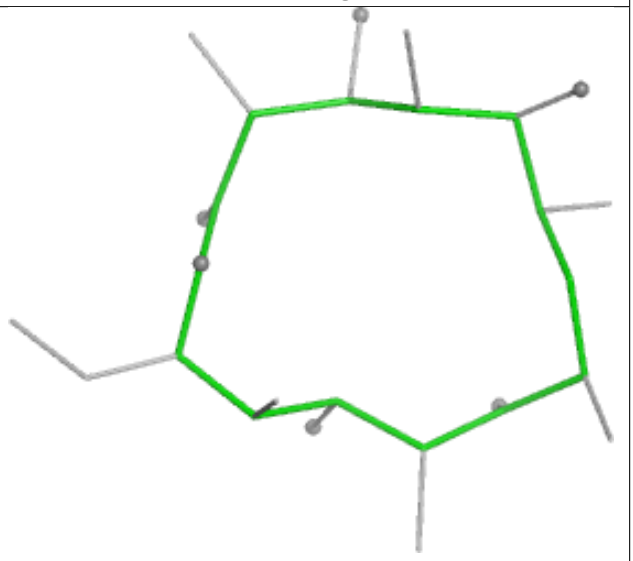
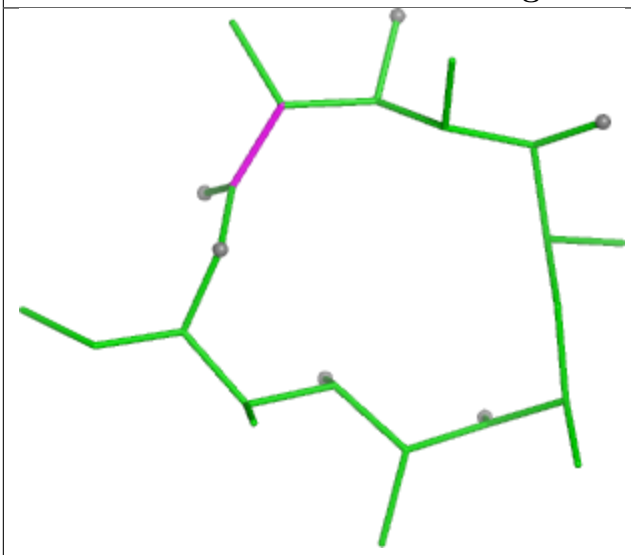


Rings

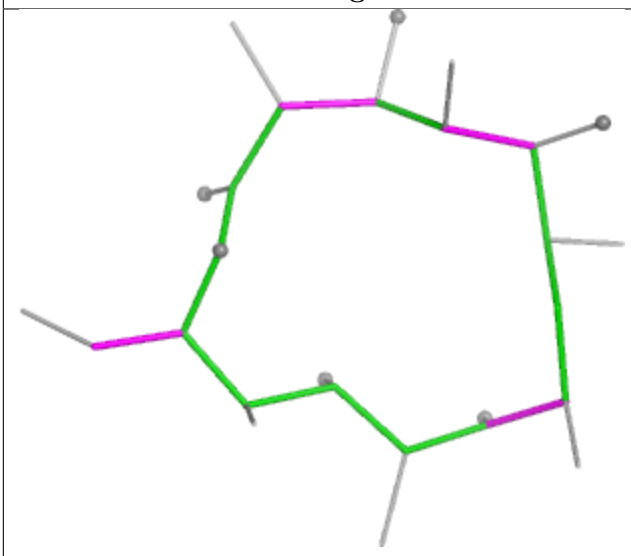
Ligand DEB D 502



Bond lengths



Bond angles



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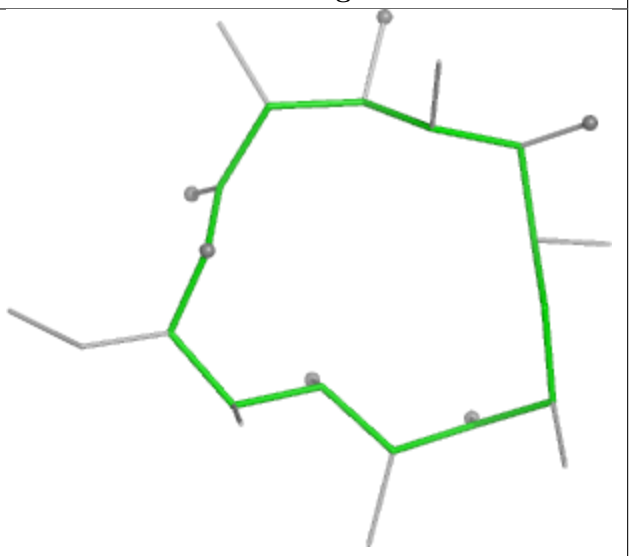
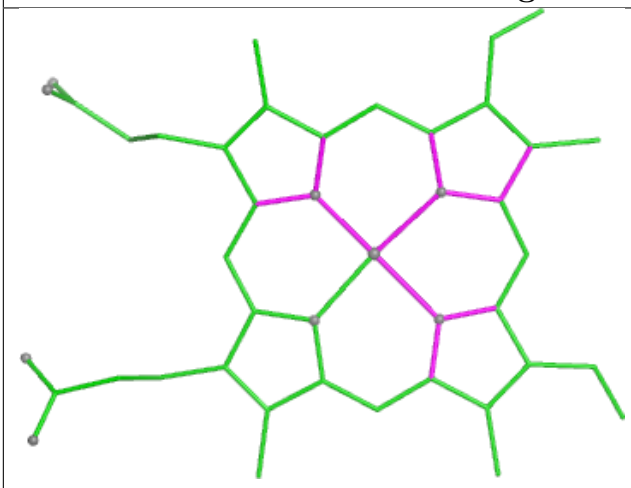


Rings

Ligand HEM D 501



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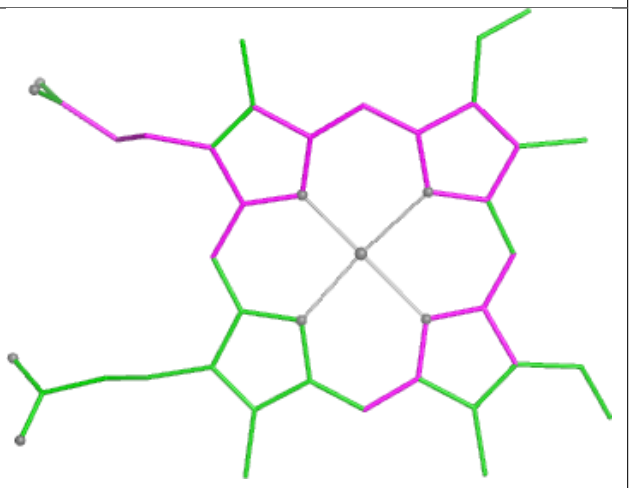

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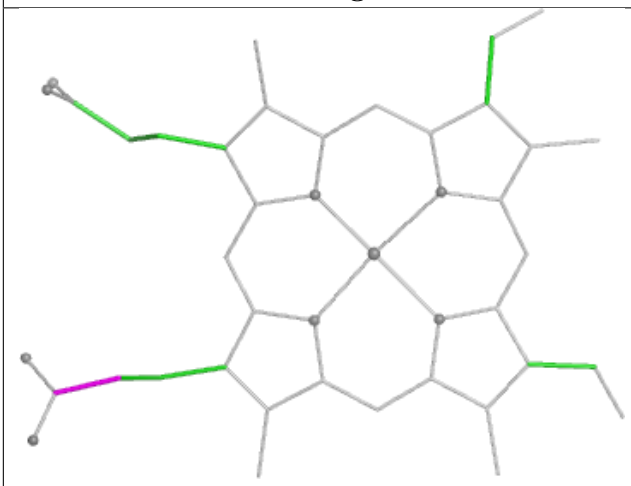

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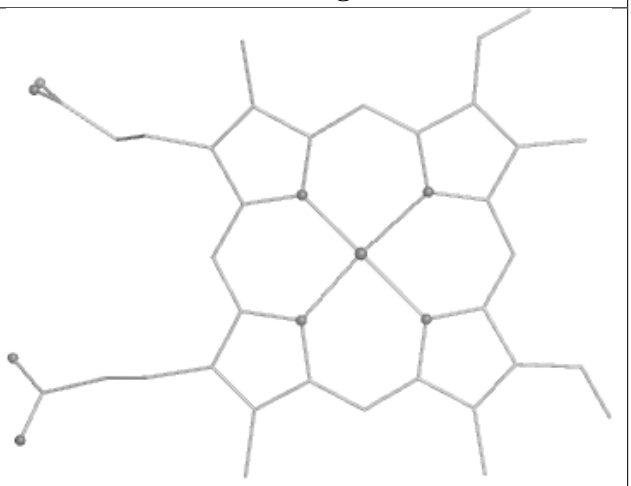
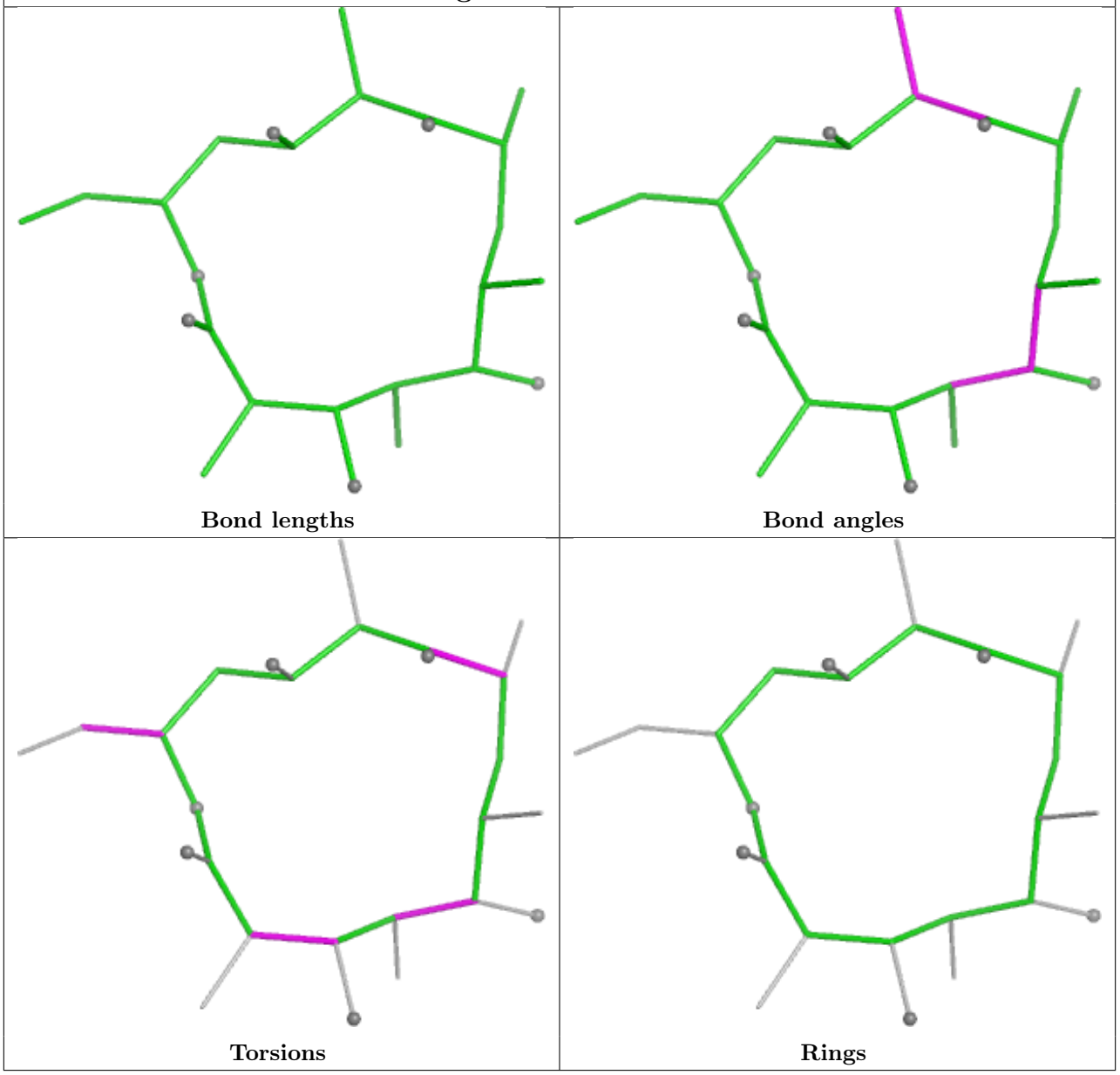


Rings

Ligand DEB A 502



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

6.1 Protein, DNA and RNA chains

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	397/406 (97%)	-0.17	5 (1%)	75	73	22, 58, 83, 129	41 (10%)
1	B	406/406 (100%)	-0.18	8 (1%)	65	62	25, 58, 82, 168	32 (7%)
1	C	399/406 (98%)	-0.27	4 (1%)	79	78	28, 54, 72, 96	24 (6%)
1	D	396/406 (97%)	0.24	10 (2%)	58	55	31, 70, 95, 115	48 (12%)
1	E	395/406 (97%)	0.09	9 (2%)	61	58	35, 73, 101, 150	31 (7%)
1	F	397/406 (97%)	0.32	17 (4%)	40	36	37, 74, 115, 135	50 (12%)
All	All	2390/2436 (98%)	0.00	53 (2%)	62	59	22, 64, 98, 168	226 (9%)

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	10[A]	PRO	11.5
1	C	9[A]	THR	10.4
1	C	11[A]	ALA	7.4
1	B	228[A]	HIS	4.9
1	A	228[A]	HIS	4.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

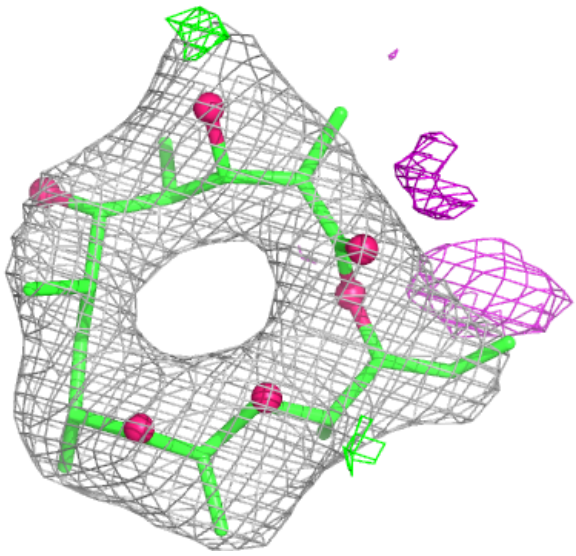
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

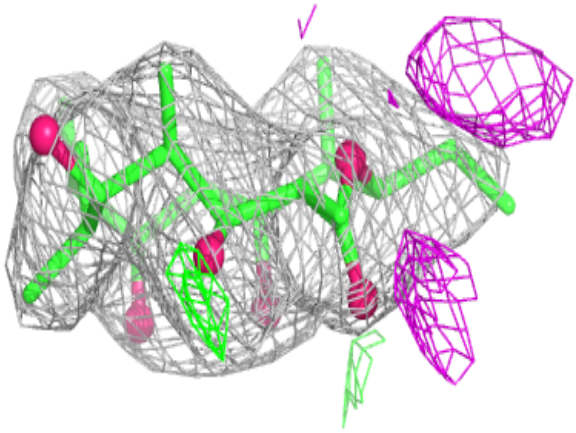
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FMT	A	504	3/3	0.67	0.18	91,91,94,98	0
4	FMT	C	503	3/3	0.69	0.11	96,96,97,100	0
4	FMT	A	503	3/3	0.71	0.10	87,87,92,93	0
4	FMT	D	503	3/3	0.77	0.11	98,98,101,102	0
4	FMT	E	503	3/3	0.84	0.23	81,81,93,93	0
4	FMT	A	505	3/3	0.94	0.09	59,59,62,66	0
3	DEB	D	502	27/27	0.94	0.11	58,64,68,78	0
3	DEB	F	502	27/27	0.95	0.11	66,74,81,87	0
3	DEB	A	502	27/27	0.96	0.08	45,49,52,54	0
3	DEB	E	502	27/27	0.96	0.09	58,63,67,68	0
3	DEB	C	502	27/27	0.96	0.09	46,52,56,57	0
2	HEM	E	501	43/43	0.97	0.07	44,51,57,58	0
3	DEB	B	502	27/27	0.97	0.09	47,50,55,57	0
2	HEM	F	501	43/43	0.97	0.08	55,62,69,75	0
2	HEM	D	501	43/43	0.98	0.06	40,43,55,61	0
2	HEM	A	501	43/43	0.98	0.07	38,42,47,48	0
2	HEM	B	501	43/43	0.98	0.06	36,40,49,52	0
2	HEM	C	501	43/43	0.99	0.06	39,43,48,54	0

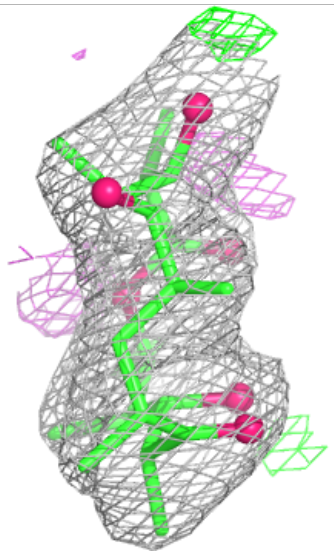
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DEB D 502:

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

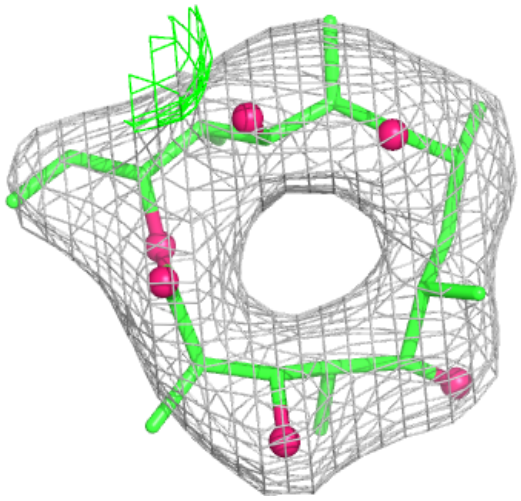


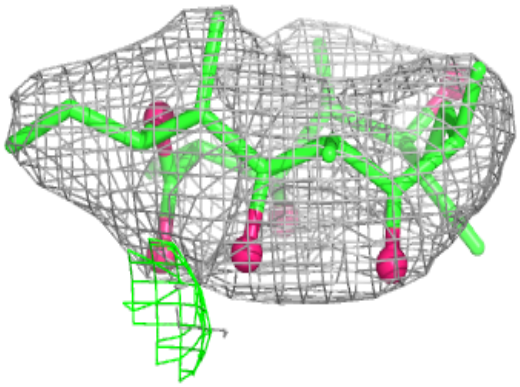


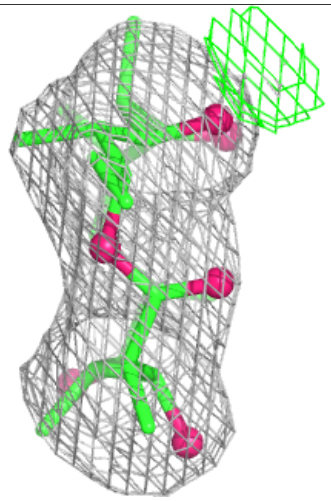


Electron density around DEB F 502:

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

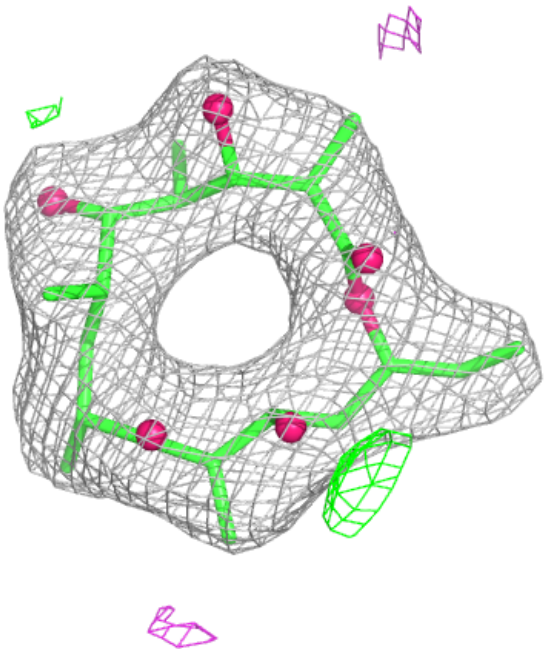


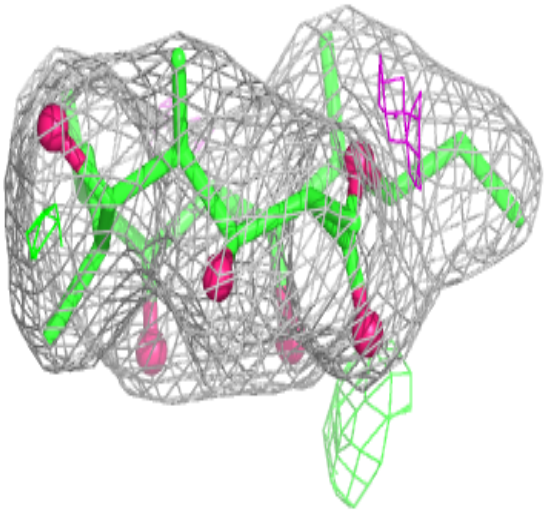


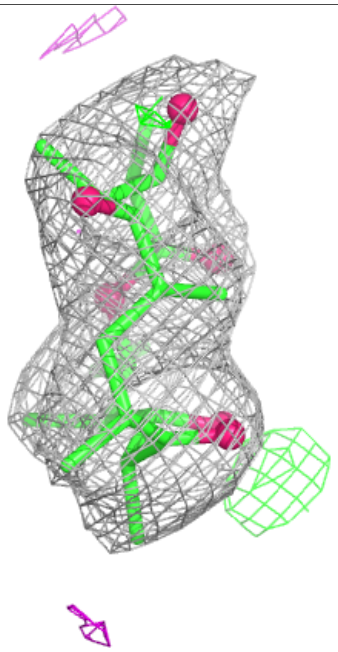


Electron density around DEB A 502:

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

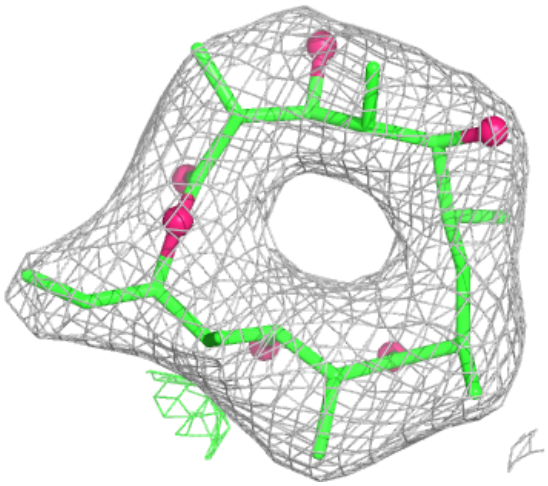


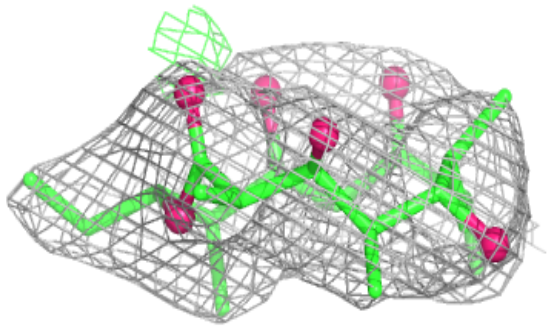


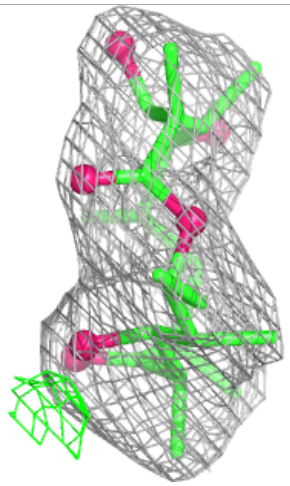


Electron density around DEB E 502:

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

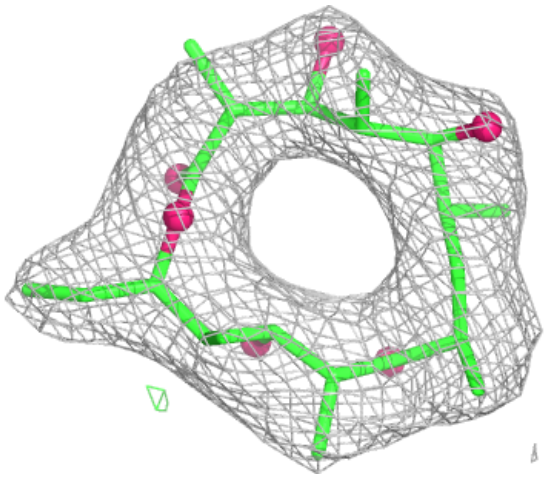


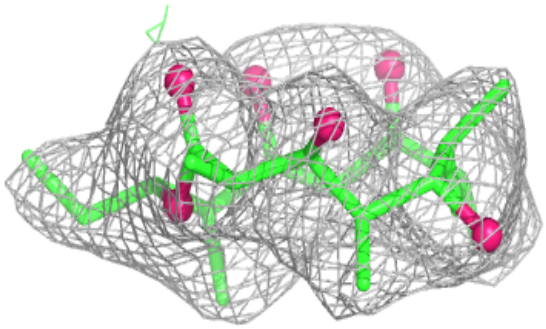


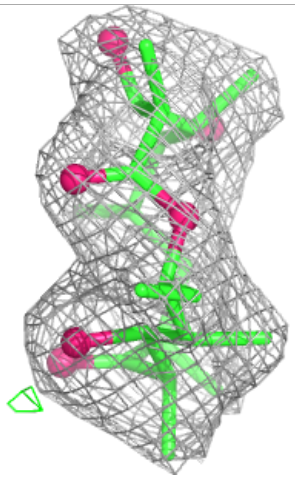


Electron density around DEB C 502:

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

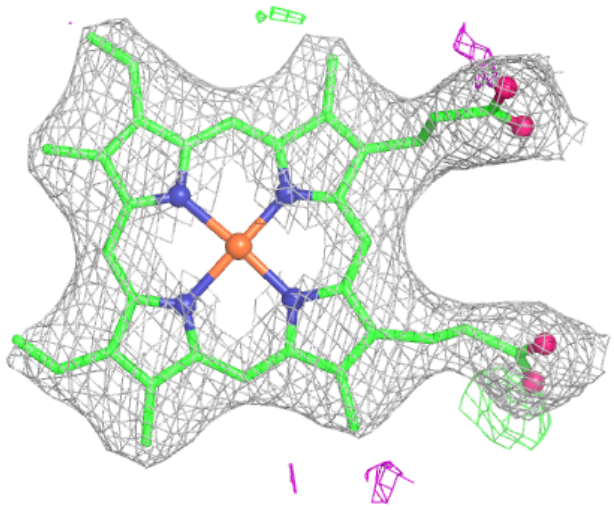


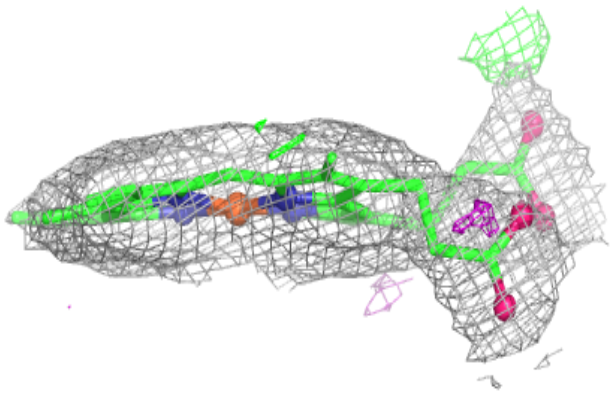


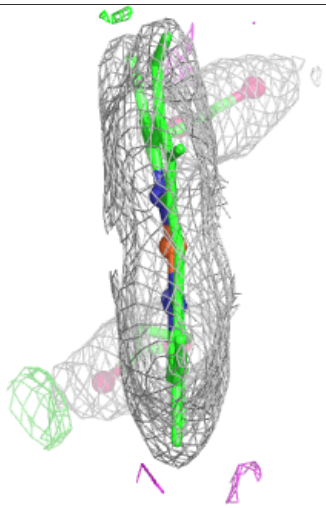


Electron density around HEM E 501:

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

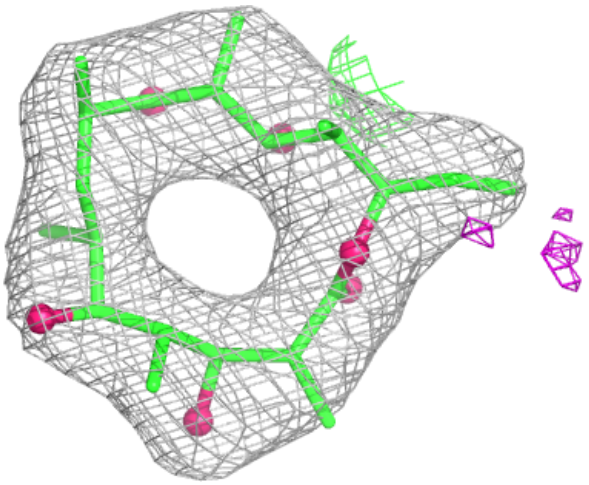


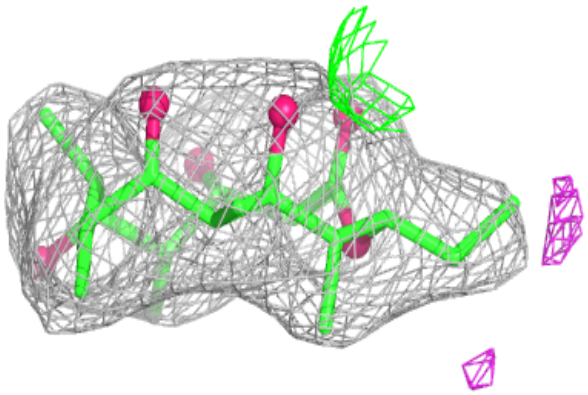


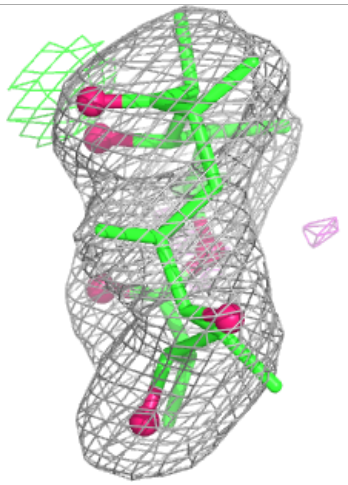


Electron density around DEB B 502:

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

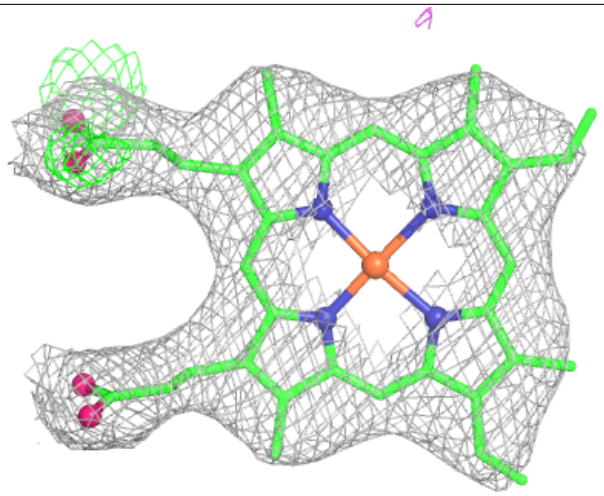


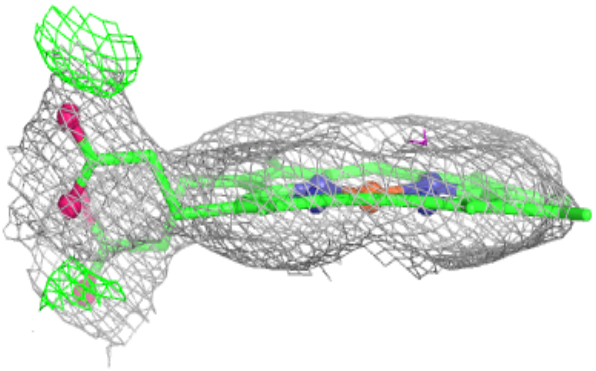


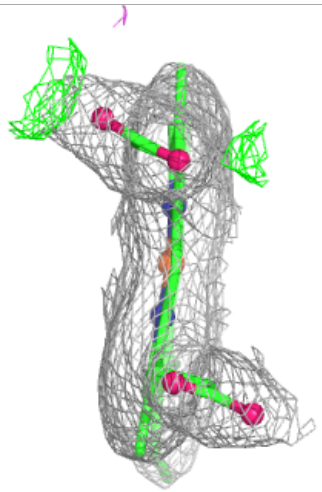


Electron density around HEM F 501:

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

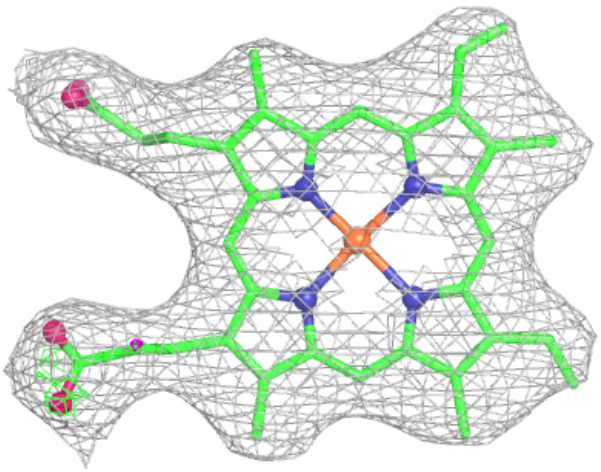


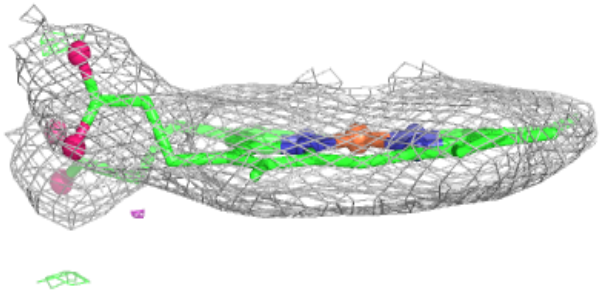




Electron density around HEM D 501:

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

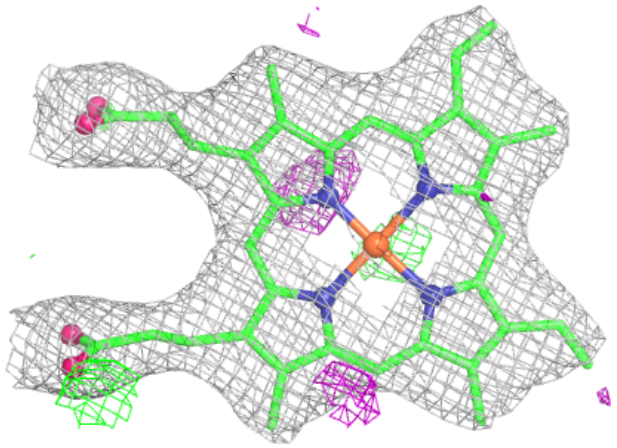


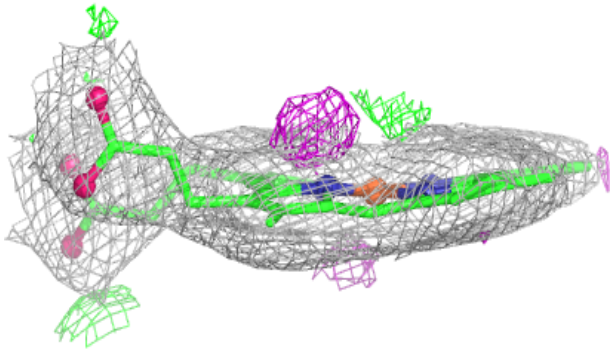


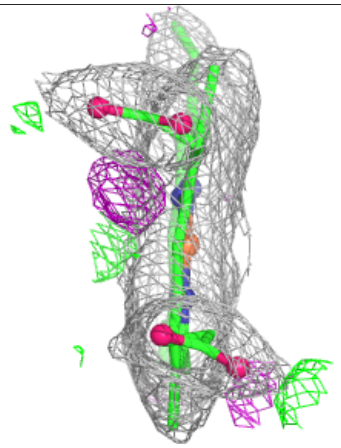


Electron density around HEM A 501:

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

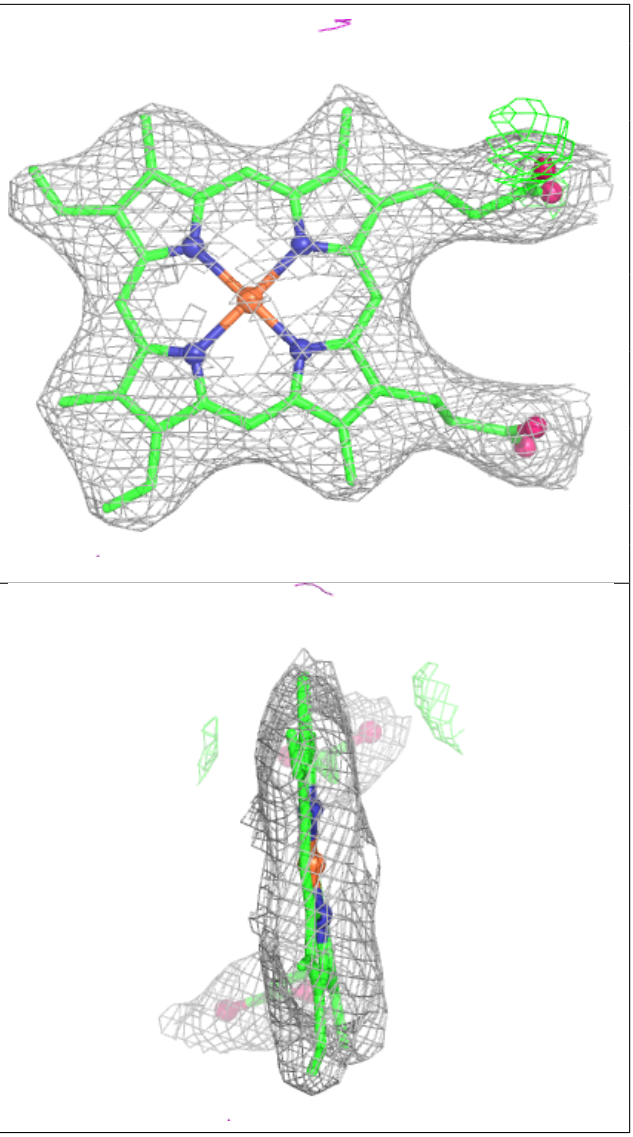






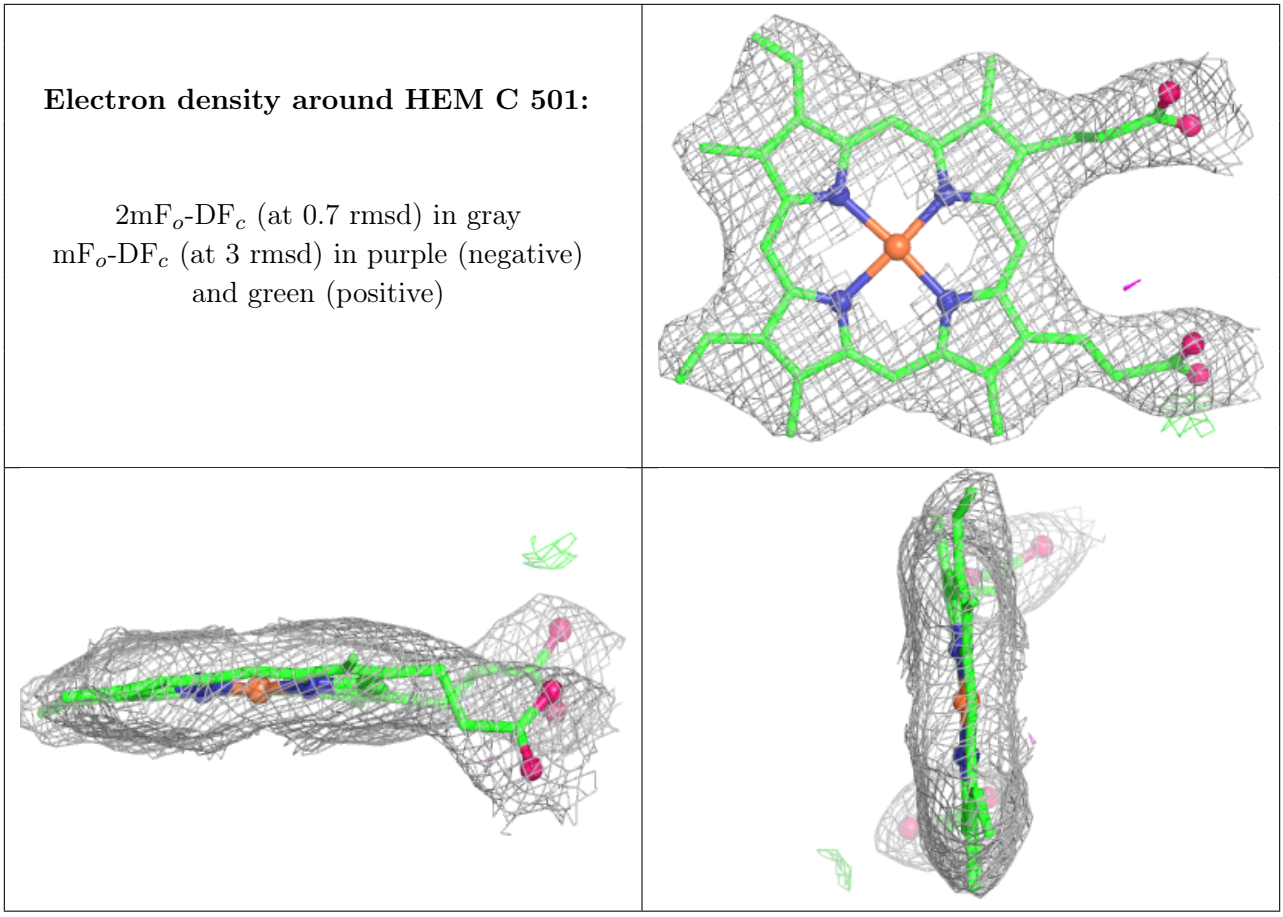
Electron density around HEM B 501:

$2mF_o$-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 501:

$2mF_o$-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.