wwPDB X-ray Structure Validation Summary Report (i)

May 21, 2020 – 11:20 pm BST

PDB ID	:	5MNV
Title	:	Structural and functional characterization of OleP in complex with 6DEB in PEG
Authors	:	Parisi, G.; Savino, C.; Montemiglio, L.C.
Deposited on	:	2016-12-13
Resolution	:	2.97 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 following versions of software and data (see references (1)) were used in the production of this report:

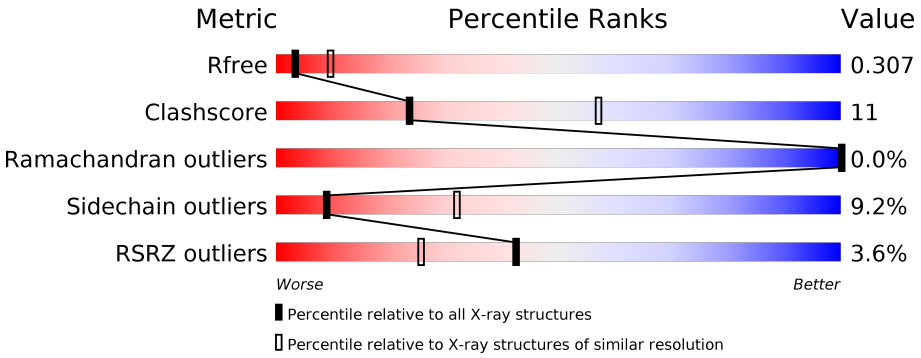
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.97 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}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 on 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	407	70% 25%
1	B	407	71% 23%
1	C	407	69% 27%
1	D	407	74% 20%
1	E	407	72% 21%
1	F	407	78% 18%

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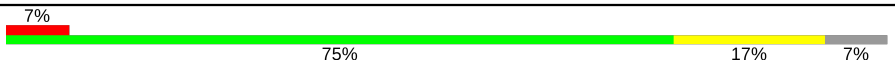
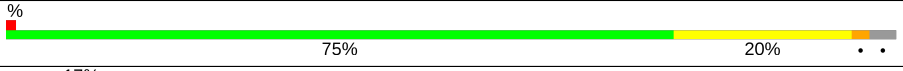
Mol	Chain	Length	Quality of chain
1	G	407	
1	H	407	
1	I	407	

2 Entry composition (i)

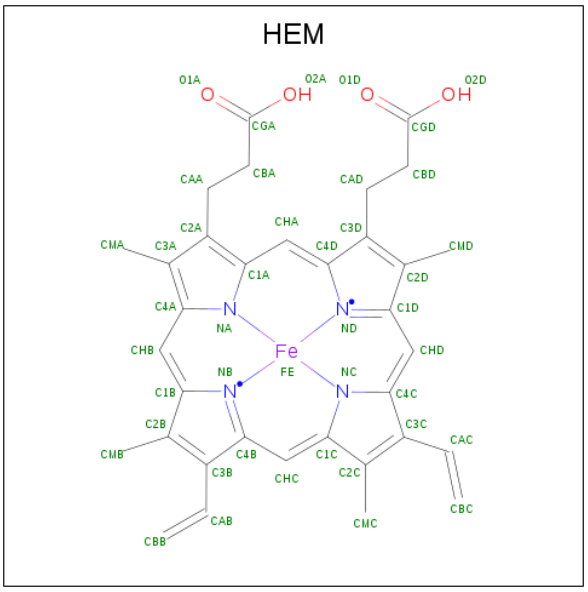
There are 4 unique types of molecules in this entry. The entry contains 27464 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

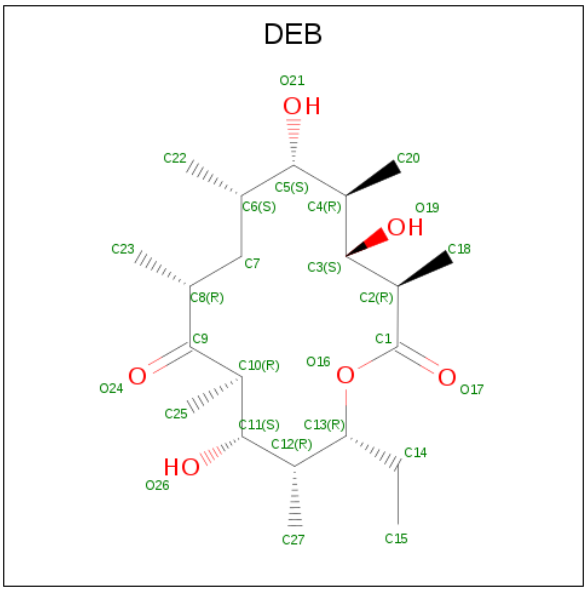
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	397	Total	C	N	O	S	0	0	0
			3091	1944	554	580	13			
1	B	394	Total	C	N	O	S	0	0	0
			3072	1934	551	574	13			
1	C	396	Total	C	N	O	S	0	0	0
			3086	1941	553	579	13			
1	D	394	Total	C	N	O	S	0	0	0
			3073	1934	551	575	13			
1	E	390	Total	C	N	O	S	0	0	0
			3034	1913	546	562	13			
1	F	395	Total	C	N	O	S	0	0	0
			3078	1937	552	576	13			
1	G	380	Total	C	N	O	S	0	0	0
			2961	1868	530	550	13			
1	H	395	Total	C	N	O	S	0	0	0
			3078	1937	552	576	13			
1	I	286	Total	C	N	O	S	0	0	0
			2250	1414	404	420	12			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: 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		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 6-DEOXYERYTHRONOLIDE B (three-letter code: 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
3	G	1	Total C O 27 21 6	0	0
3	H	1	Total C O 27 21 6	0	0
3	I	1	Total C O 27 21 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	26	Total O 26 26	0	0
4	B	7	Total O 7 7	0	0
4	C	13	Total O 13 13	0	0

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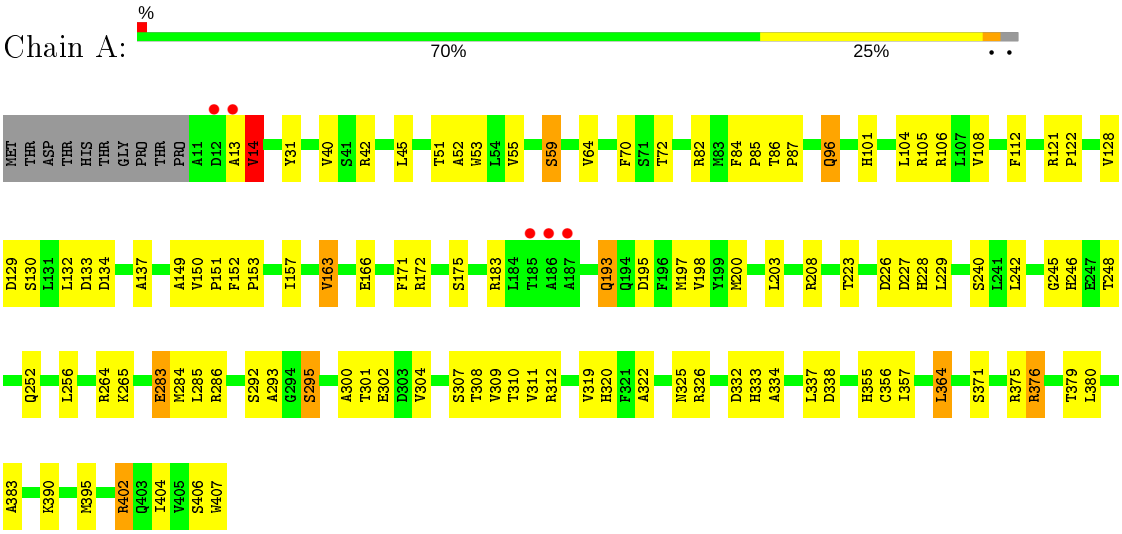
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	28	Total O 28 28	0	0
4	E	7	Total O 7 7	0	0
4	F	15	Total O 15 15	0	0
4	G	5	Total O 5 5	0	0
4	H	10	Total O 10 10	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

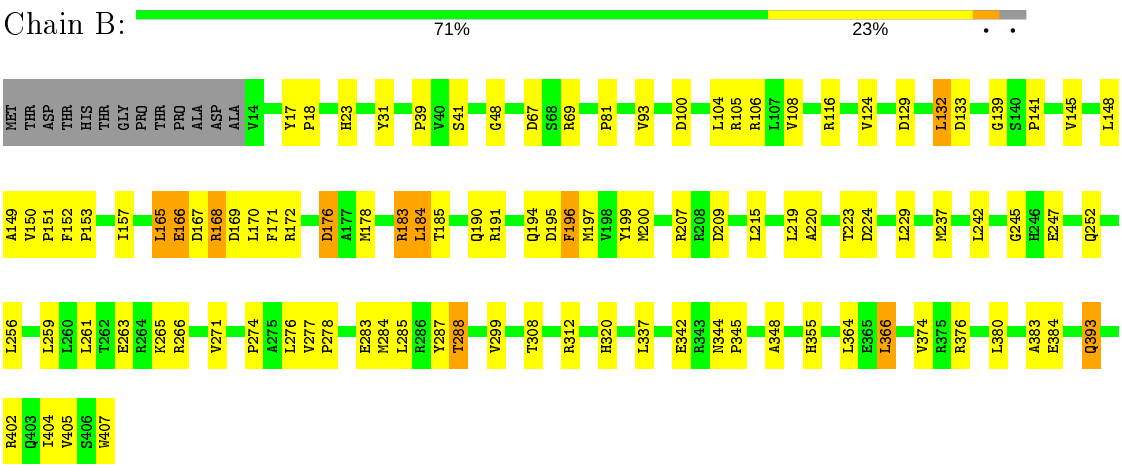
- Molecule 1: Cytochrome P-450

Chain A:



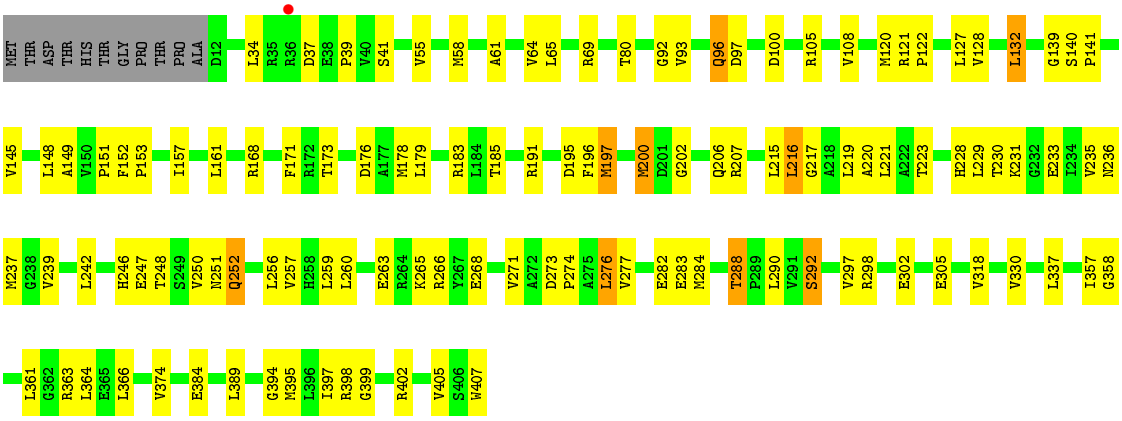
- Molecule 1: Cytochrome P-450

Chain B:



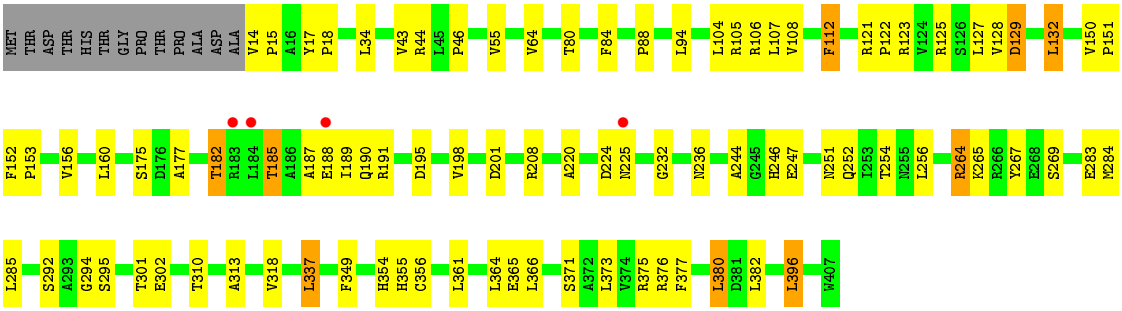
- Molecule 1: Cytochrome P-450

Chain C:



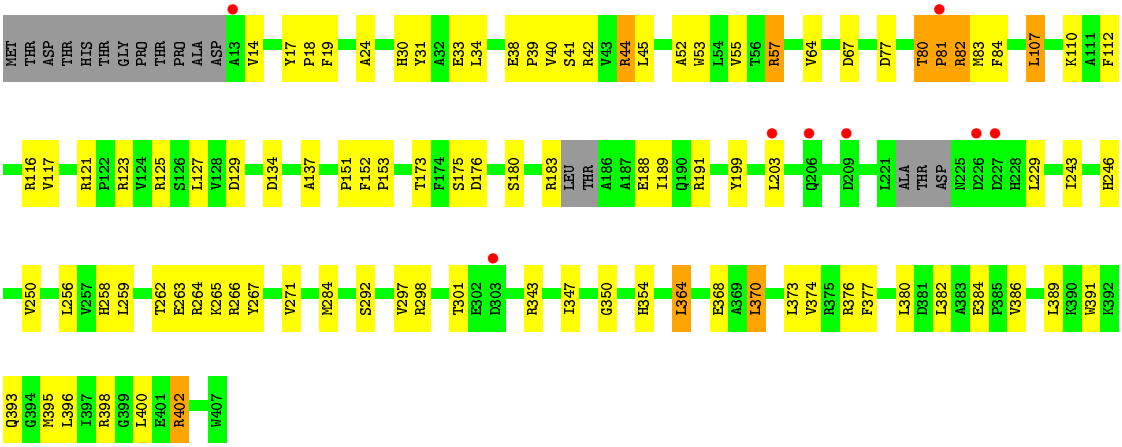
• Molecule 1: Cytochrome P-450

Chain D:



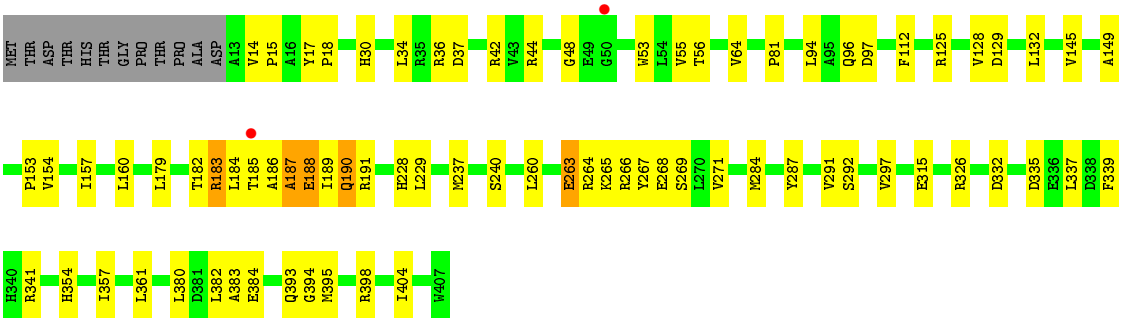
• Molecule 1: Cytochrome P-450

Chain E:



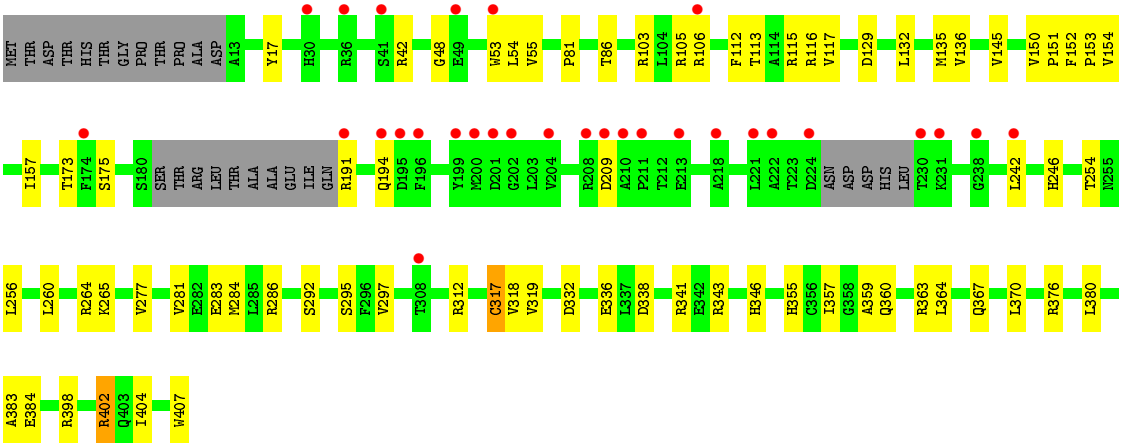
• Molecule 1: Cytochrome P-450

Chain F:



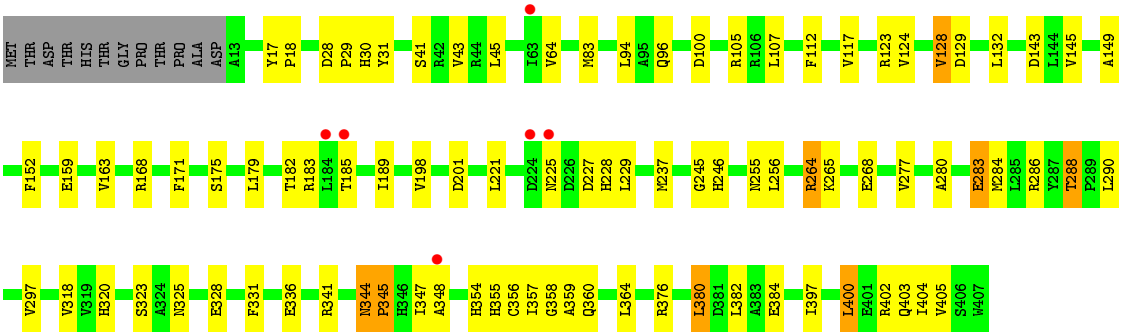
• Molecule 1: Cytochrome P-450

Chain G:



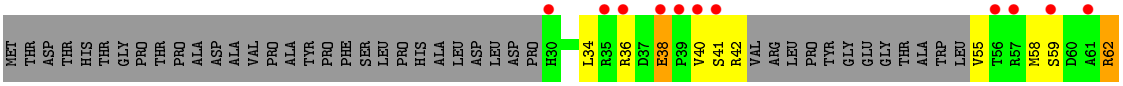
• Molecule 1: Cytochrome P-450

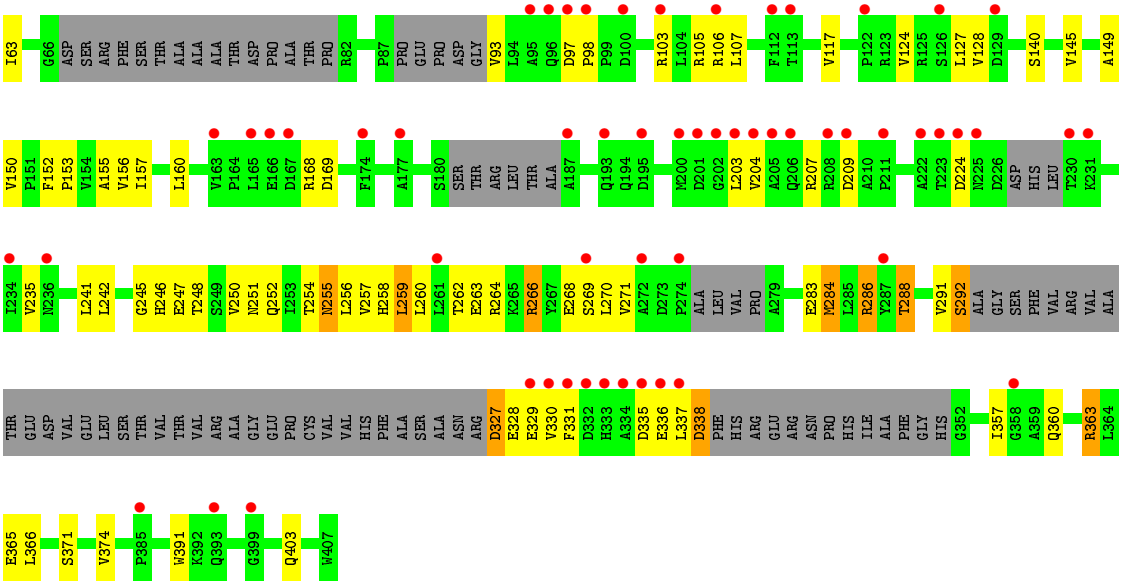
Chain H:



• Molecule 1: Cytochrome P-450

Chain I:




I63 G66 ASP SER ARG PHE SER THR ALA ALA ALA THR ASP PRO ALA THR PRO R82 P87 PRO GLU PRO ASP GLY V93 L94 A95 Q96 D97 P98 P99 D100 R103 L104 R105 R106 L107 F112 T113 V117 P122 R123 V124 R125 S126 L127 V128 D129 S140 V145 A149
V150 P151 F152 P153 V154 A155 V156 I157 L160 V163 P164 L165 E166 D167 R168 D169 F174 A177 S180 SER THR ARG LEU THR ALA A187 Q193 Q194 D196 M200 D201 G202 L203 V204 A205 Q206 R207 R208 D209 A210 P211 A222 T223 D224 N225 D226 ASP HIS LEU T230 K231
I234 V235 M236 L241 L242 G245 H246 E247 T248 S249 V250 N251 Q252 I253 T254 N255 L256 V257 H258 L259 L260 I261 T262 E263 R264 K265 R266 Y267 E268 S269 L270 V271 A272 D273 P274 ALA LEU VAL PRO A279 E283 M284 L285 R286 Y287 T288 V291 S292 ALA GLY SER PHE VAL ARG VAL ALA
THR GLU ASP VAL GLU LEU SER THR VAL THR VAL ARG ALA GLY GLU PRO CYS VAL VAL HIS PHE ALA SER ALA ASN ARG D327 E328 E329 V330 F331 D332 H333 A334 D335 E336 L337 D338 PHE HIS ARG GLU ARG ASN PRO HIS ILE ALA PHE GLY HIS G352 I357 G358 A359 Q360 R363 L364
E365 L366 S371 V374 P385 W391 K392 Q393 G399 Q403 W407

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	112.50Å 116.70Å 123.30Å 103.90° 104.30° 114.70°	Depositor
Resolution (Å)	39.97 – 2.97 39.97 – 2.97	Depositor EDS
% Data completeness (in resolution range)	97.1 (39.97-2.97) 97.1 (39.97-2.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.238 , 0.311 0.239 , 0.307	Depositor DCC
R_{free} test set	5097 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	54.4	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.010 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	27464	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

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	0.45	0/3158	0.69	2/4302 (0.0%)
1	B	0.37	0/3139	0.62	0/4276
1	C	0.47	0/3153	0.63	0/4295
1	D	0.38	0/3140	0.62	0/4277
1	E	0.37	0/3099	0.63	3/4217 (0.1%)
1	F	0.36	0/3145	0.62	3/4284 (0.1%)
1	G	0.38	0/3025	0.55	0/4117
1	H	0.38	0/3145	0.61	0/4284
1	I	0.39	0/2281	0.55	0/3081
All	All	0.40	0/27285	0.62	8/37133 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	187	ALA	N-CA-C	-7.33	91.20	111.00
1	E	81	PRO	CB-CA-C	-7.26	93.84	112.00
1	F	186	ALA	CB-CA-C	-7.10	99.45	110.10
1	F	186	ALA	N-CA-C	6.92	129.68	111.00
1	E	81	PRO	N-CA-C	6.27	128.41	112.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	293	ALA	Peptide
1	D	295	SER	Peptide

5.2 Too-close contacts

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	3091	0	3065	67	0
1	B	3072	0	3048	56	0
1	C	3086	0	3060	82	0
1	D	3073	0	3051	46	0
1	E	3034	0	3012	52	0
1	F	3078	0	3056	55	0
1	G	2961	0	2944	43	0
1	H	3078	0	3057	58	0
1	I	2250	0	2257	117	0
2	A	43	0	30	5	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	3	0
2	E	43	0	30	5	0
2	F	43	0	30	4	0
2	G	43	0	30	4	0
2	H	43	0	30	10	0
2	I	43	0	30	8	0
3	A	27	0	38	1	0
3	B	27	0	38	0	0
3	C	27	0	38	0	0
3	D	27	0	38	6	0
3	E	27	0	38	2	0
3	F	27	0	38	1	0
3	G	27	0	38	1	0
3	H	27	0	38	1	0
3	I	27	0	38	0	0
4	A	26	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	7	0	0	0	0
4	C	13	0	0	0	0
4	D	28	0	0	1	0
4	E	7	0	0	0	0
4	F	15	0	0	1	0
4	G	5	0	0	0	0
4	H	10	0	0	2	0
All	All	27464	0	27162	608	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 11.

The worst 5 of 608 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:I:263:GLU:HB3	1:I:266:ARG:CD	1.64	1.27
1:G:359:ALA:O	1:G:363:ARG:HG3	1.38	1.23
1:F:184:LEU:O	1:F:189:ILE:CG1	1.86	1.21
1:I:251:ASN:O	1:I:255:ASN:OD1	1.55	1.21
1:I:62:ARG:NH2	1:I:63:ILE:HG12	1.57	1.17

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	395/407 (97%)	374 (95%)	21 (5%)	0	100	100
1	B	392/407 (96%)	367 (94%)	25 (6%)	0	100	100
1	C	394/407 (97%)	358 (91%)	36 (9%)	0	100	100
1	D	392/407 (96%)	364 (93%)	28 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	384/407 (94%)	361 (94%)	23 (6%)	0	100	100
1	F	393/407 (97%)	360 (92%)	33 (8%)	0	100	100
1	G	374/407 (92%)	342 (91%)	32 (9%)	0	100	100
1	H	393/407 (97%)	354 (90%)	38 (10%)	1 (0%)	41	74
1	I	268/407 (66%)	255 (95%)	13 (5%)	0	100	100
All	All	3385/3663 (92%)	3135 (93%)	249 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	345	PRO

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	332/341 (97%)	299 (90%)	33 (10%)	8	28
1	B	330/341 (97%)	292 (88%)	38 (12%)	5	22
1	C	332/341 (97%)	301 (91%)	31 (9%)	9	31
1	D	331/341 (97%)	302 (91%)	29 (9%)	10	34
1	E	324/341 (95%)	290 (90%)	34 (10%)	7	25
1	F	331/341 (97%)	307 (93%)	24 (7%)	14	42
1	G	318/341 (93%)	298 (94%)	20 (6%)	18	49
1	H	331/341 (97%)	305 (92%)	26 (8%)	12	39
1	I	243/341 (71%)	214 (88%)	29 (12%)	5	21
All	All	2872/3069 (94%)	2608 (91%)	264 (9%)	9	32

5 of 264 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	264	ARG

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Mol	Chain	Res	Type
1	E	176	ASP
1	I	106	ARG
1	D	292	SER
1	E	57	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	194	GLN
1	D	354	HIS
1	H	320	HIS
1	D	228	HIS
1	D	236	ASN

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 carbohydrates 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	$\#\|Z\|>2$
3	DEB	H	502	-	27,27,27	1.07	1 (3%)	35,39,39	1.17	2 (5%)
2	HEM	H	501	1,4	27,50,50	0.82	1 (3%)	17,82,82	1.08	0
3	DEB	D	502	-	27,27,27	1.12	1 (3%)	35,39,39	1.32	7 (20%)
3	DEB	I	502	-	27,27,27	1.08	1 (3%)	35,39,39	1.19	4 (11%)
2	HEM	D	501	-	27,50,50	0.83	1 (3%)	17,82,82	1.30	3 (17%)
2	HEM	F	501	1,4	27,50,50	0.81	2 (7%)	17,82,82	1.18	1 (5%)
3	DEB	B	502	-	27,27,27	1.10	1 (3%)	35,39,39	1.19	3 (8%)
3	DEB	E	502	-	27,27,27	1.12	1 (3%)	35,39,39	1.36	3 (8%)
3	DEB	A	502	-	27,27,27	1.11	2 (7%)	35,39,39	1.02	2 (5%)
2	HEM	I	501	-	27,50,50	0.81	1 (3%)	17,82,82	1.30	1 (5%)
2	HEM	E	501	1	27,50,50	0.89	2 (7%)	17,82,82	0.85	0
3	DEB	F	502	-	27,27,27	1.10	1 (3%)	35,39,39	1.38	5 (14%)
2	HEM	G	501	1	27,50,50	0.78	0	17,82,82	0.99	0
2	HEM	A	501	1,4	27,50,50	0.88	2 (7%)	17,82,82	1.07	1 (5%)
2	HEM	C	501	1	27,50,50	0.82	1 (3%)	17,82,82	1.62	3 (17%)
3	DEB	C	502	-	27,27,27	1.12	1 (3%)	35,39,39	1.19	3 (8%)
3	DEB	G	502	-	27,27,27	1.12	1 (3%)	35,39,39	1.11	1 (2%)
2	HEM	B	501	1	27,50,50	0.78	1 (3%)	17,82,82	1.19	2 (11%)

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	H	502	-	-	8/50/50/50	0/1/1/1
2	HEM	H	501	1,4	-	0/6/54/54	-
3	DEB	D	502	-	-	9/50/50/50	0/1/1/1
3	DEB	I	502	-	-	8/50/50/50	0/1/1/1
2	HEM	D	501	-	-	0/6/54/54	-
2	HEM	F	501	1,4	-	0/6/54/54	-
3	DEB	B	502	-	-	12/50/50/50	0/1/1/1
3	DEB	E	502	-	-	15/50/50/50	0/1/1/1
3	DEB	A	502	-	-	1/50/50/50	0/1/1/1
2	HEM	I	501	-	-	2/6/54/54	-
2	HEM	E	501	1	-	0/6/54/54	-
3	DEB	F	502	-	-	13/50/50/50	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	G	501	1	-	0/6/54/54	-
2	HEM	A	501	1,4	-	0/6/54/54	-
2	HEM	C	501	1	-	2/6/54/54	-
3	DEB	C	502	-	-	8/50/50/50	0/1/1/1
3	DEB	G	502	-	-	4/50/50/50	0/1/1/1
2	HEM	B	501	1	-	0/6/54/54	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	DEB	O16-C1	5.52	1.47	1.34
3	G	502	DEB	O16-C1	5.38	1.46	1.34
3	B	502	DEB	O16-C1	5.21	1.46	1.34
3	I	502	DEB	O16-C1	5.15	1.46	1.34
3	C	502	DEB	O16-C1	5.12	1.46	1.34

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	DEB	O16-C1-C2	4.27	120.94	111.56
3	B	502	DEB	O16-C1-C2	4.10	120.55	111.56
3	E	502	DEB	O16-C1-C2	3.83	119.96	111.56
3	I	502	DEB	O16-C1-C2	3.78	119.86	111.56
3	E	502	DEB	C6-C5-C4	-3.78	110.41	116.27

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	502	DEB	C11-C12-C13-O16
3	H	502	DEB	C27-C12-C13-O16
3	D	502	DEB	C4-C5-C6-C7
3	D	502	DEB	O21-C5-C6-C7
3	D	502	DEB	O21-C5-C6-C22

There are no ring outliers.

15 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	502	DEB	1	0

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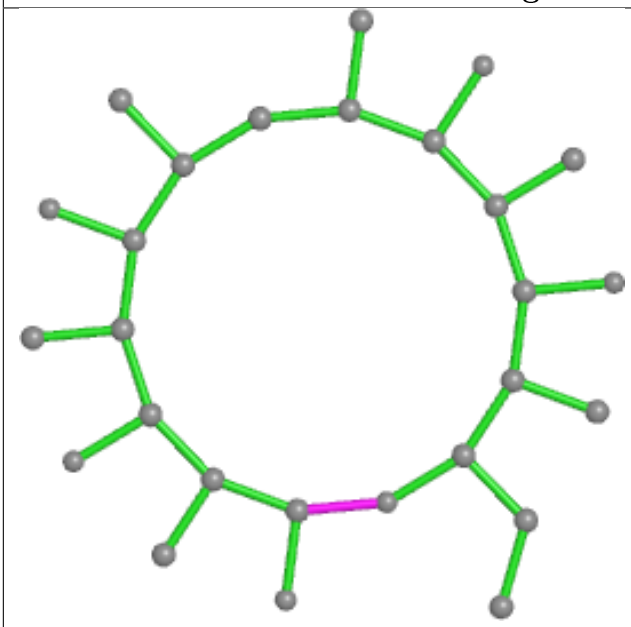
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	501	HEM	10	0
3	D	502	DEB	6	0
2	D	501	HEM	3	0
2	F	501	HEM	4	0
3	E	502	DEB	2	0
3	A	502	DEB	1	0
2	I	501	HEM	8	0
2	E	501	HEM	5	0
3	F	502	DEB	1	0
2	G	501	HEM	4	0
2	A	501	HEM	5	0
2	C	501	HEM	3	0
3	G	502	DEB	1	0
2	B	501	HEM	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 H 502



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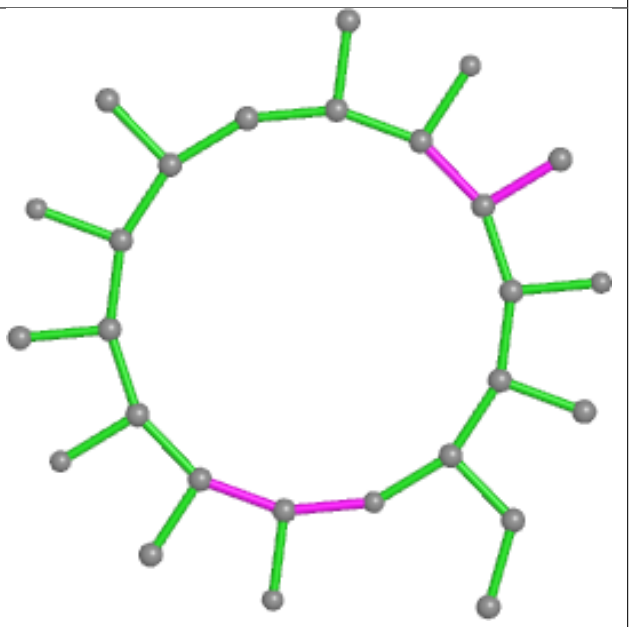

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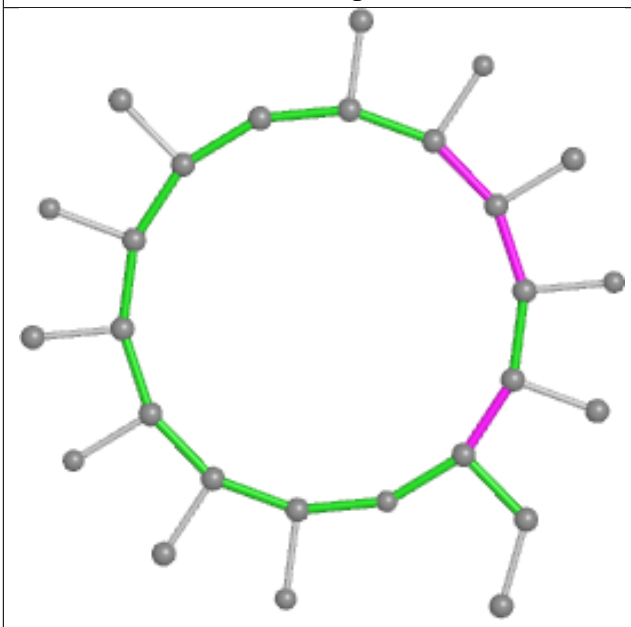

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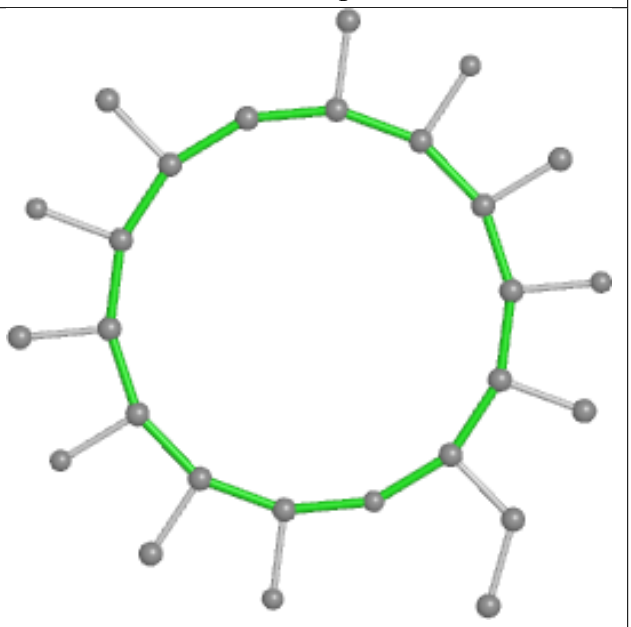
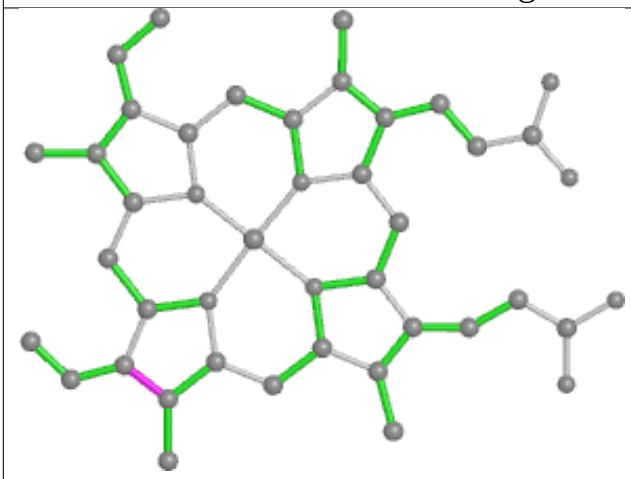


Rings

Ligand HEM H 501



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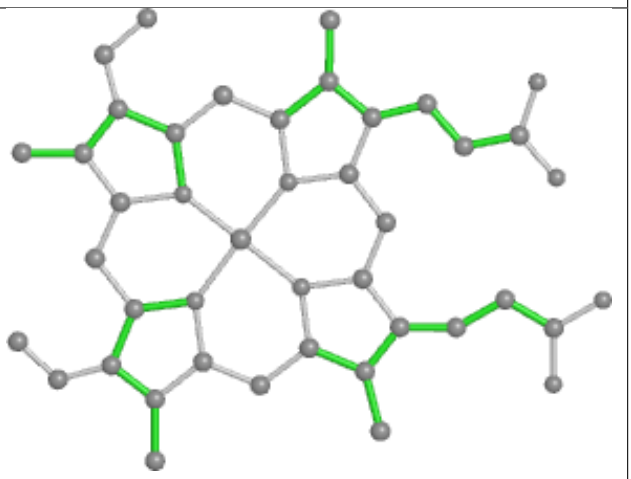

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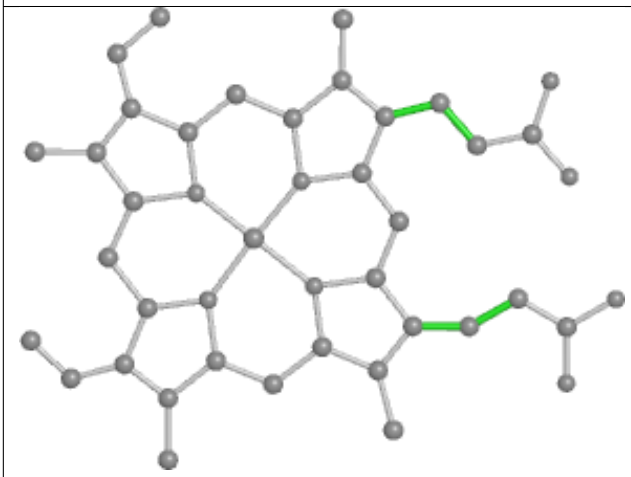

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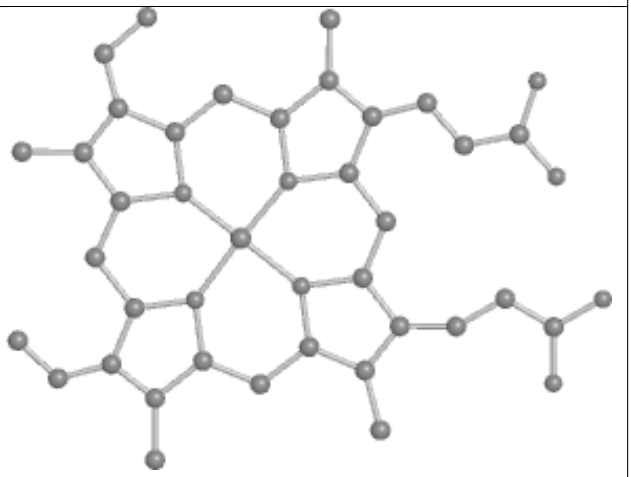
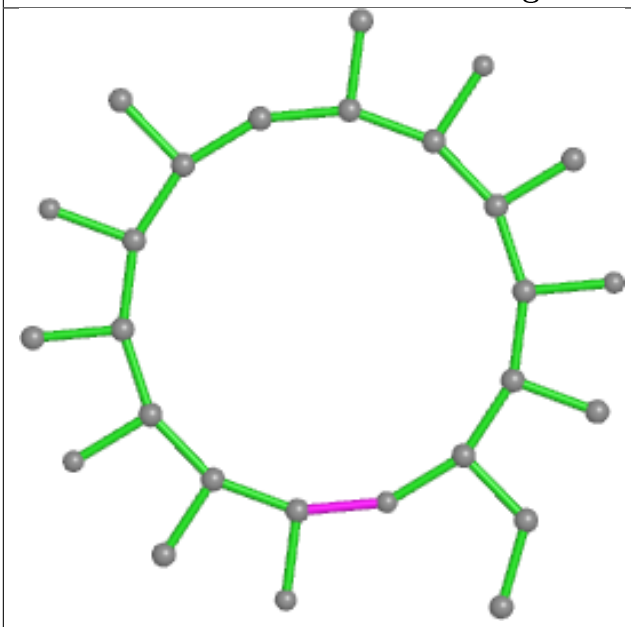


Rings

Ligand DEB D 502



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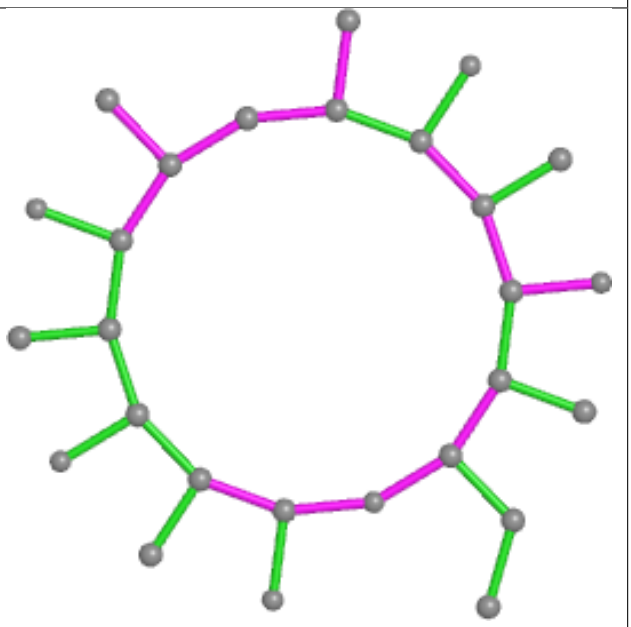

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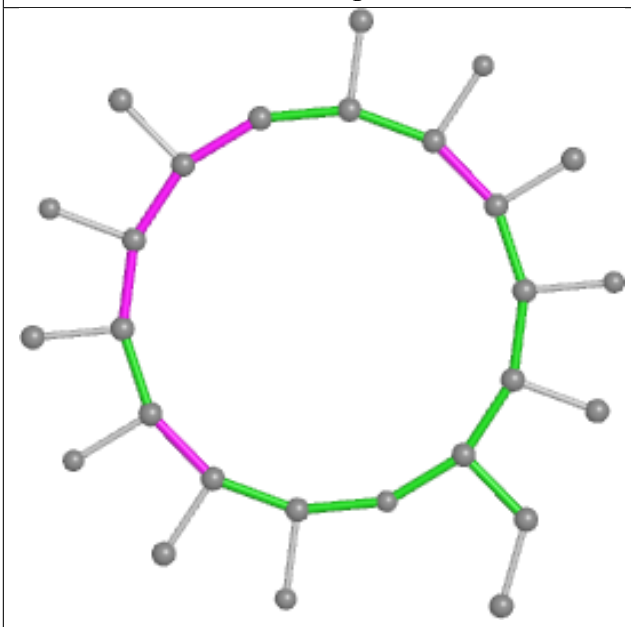

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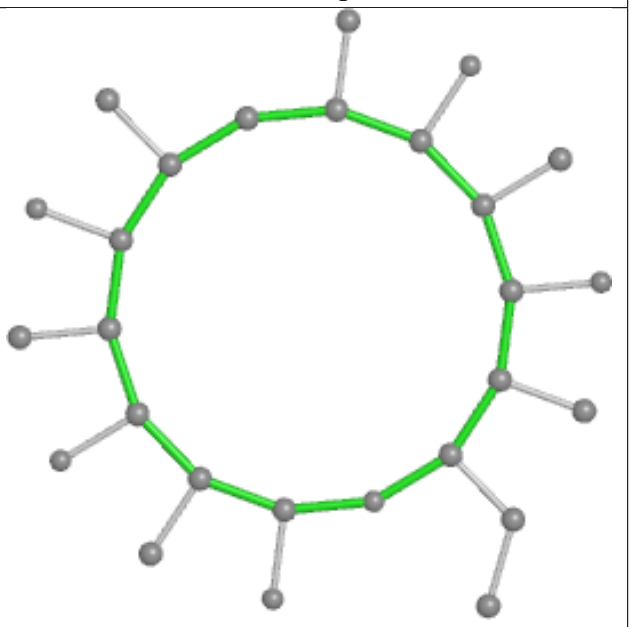
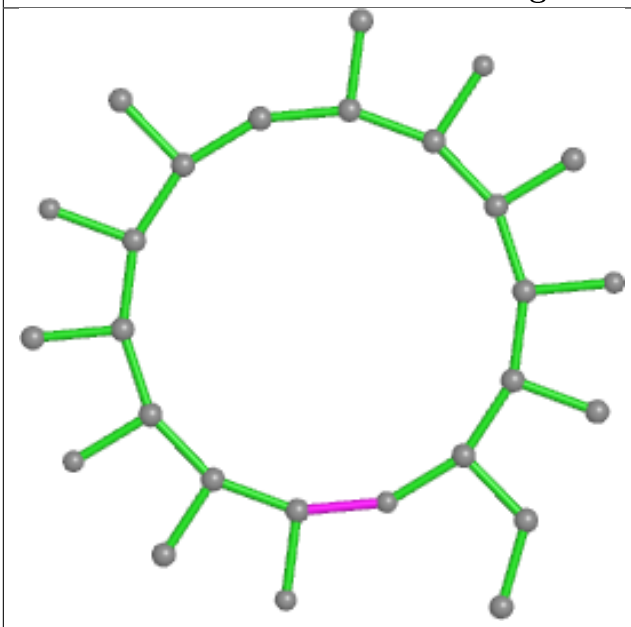


Rings

Ligand DEB I 502



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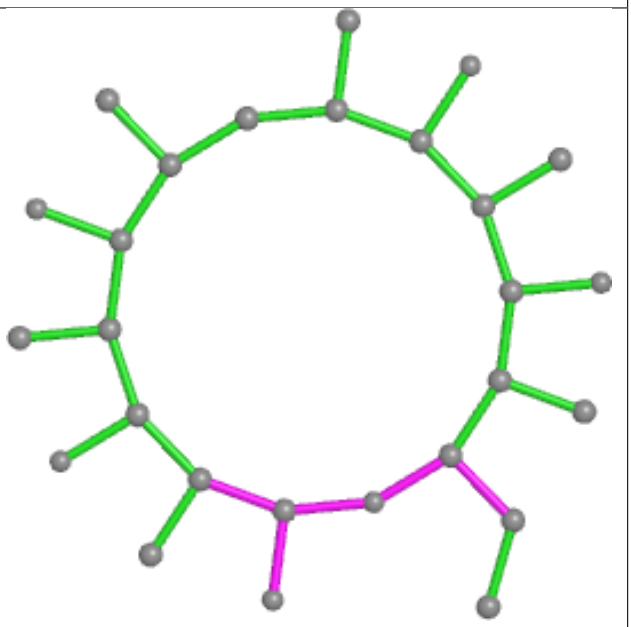

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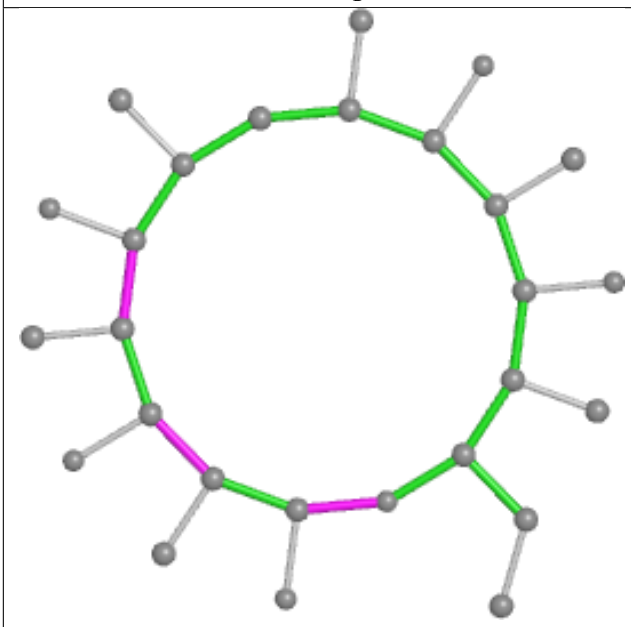

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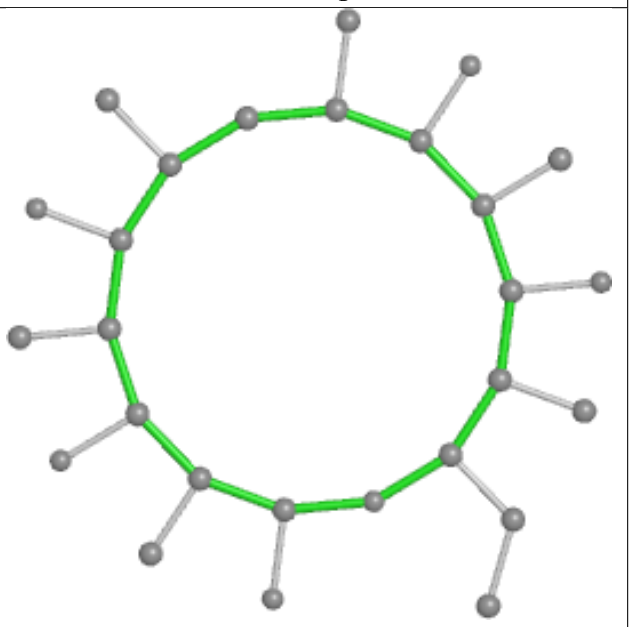
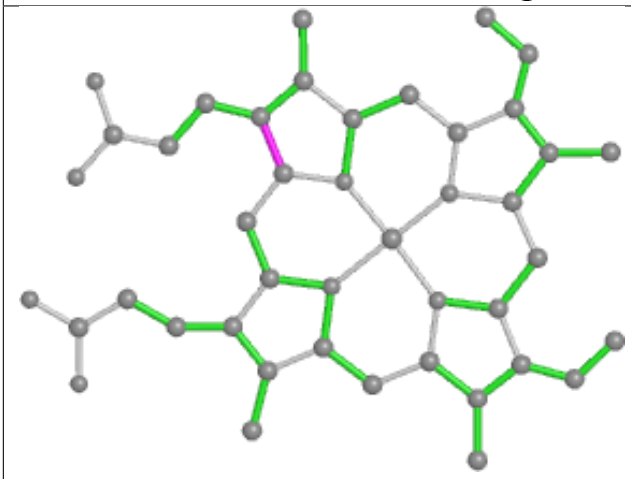


Rings

Ligand HEM D 501



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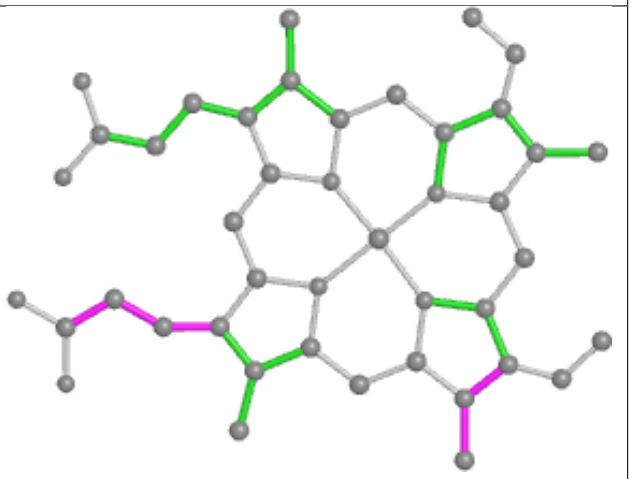

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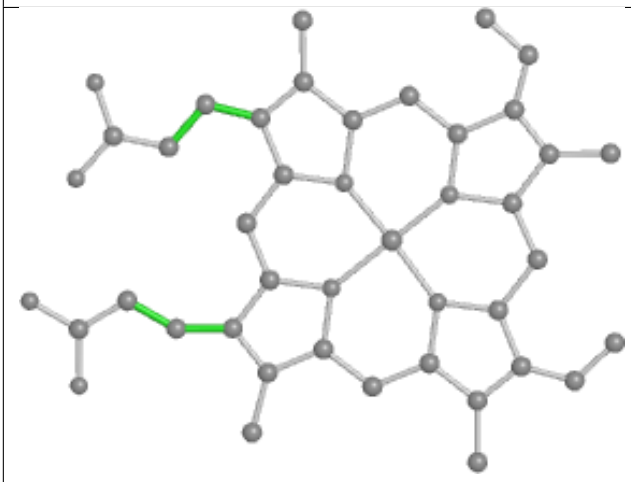

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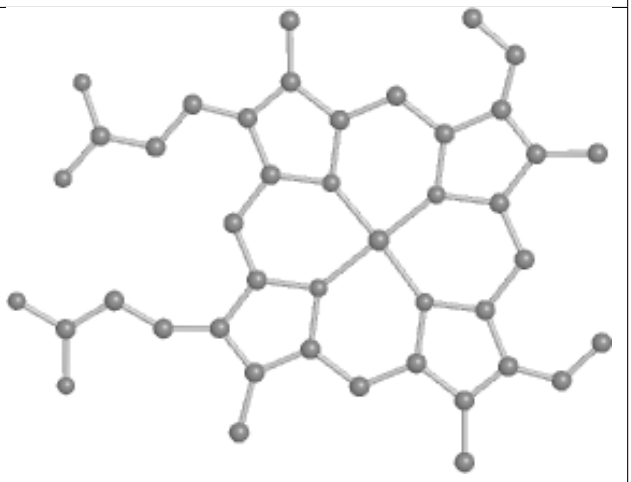

Rings

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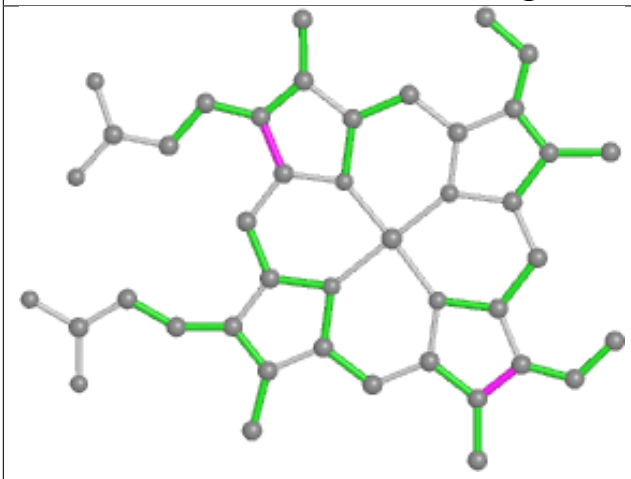

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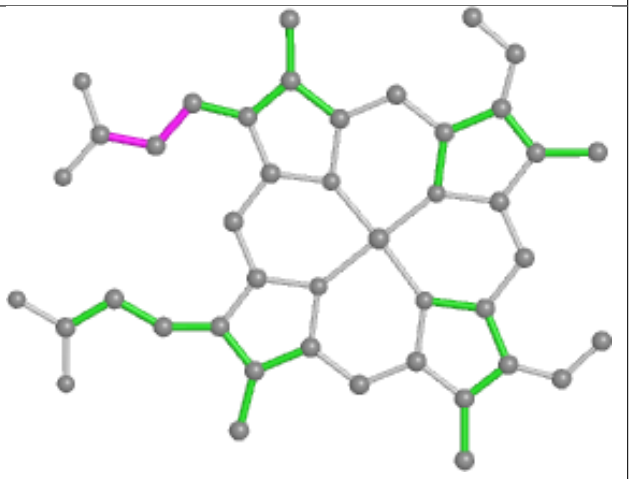

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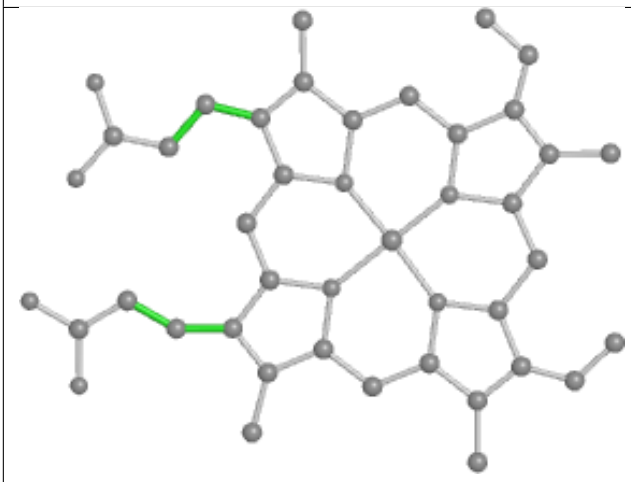

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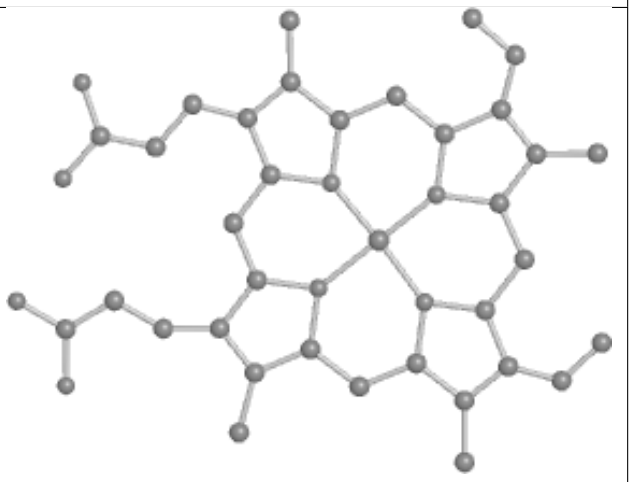
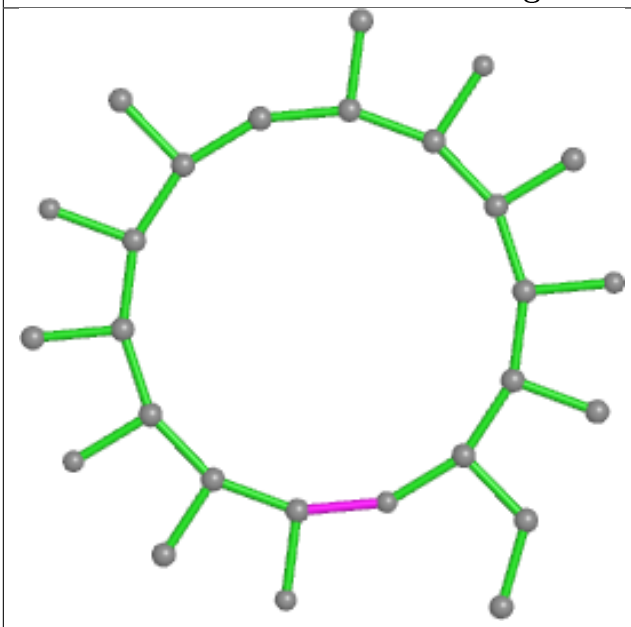


Rings

Ligand DEB B 502



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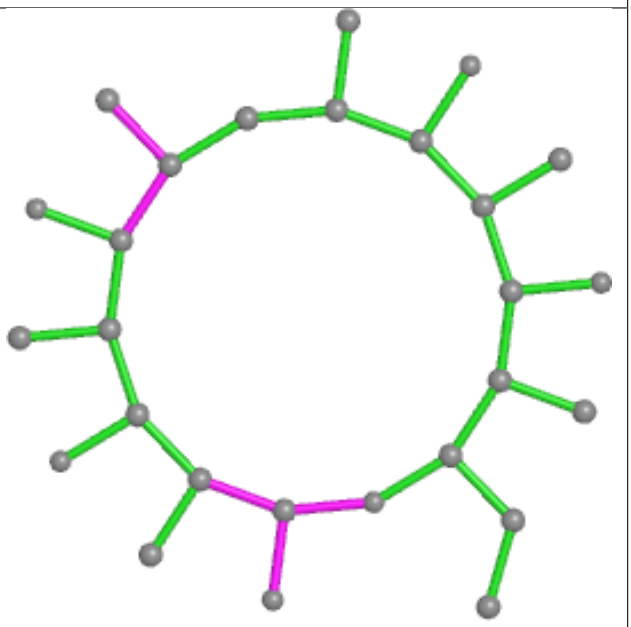

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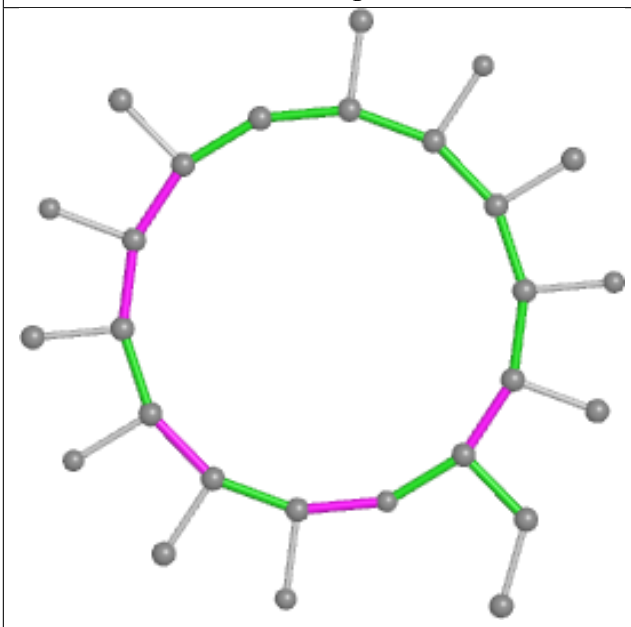

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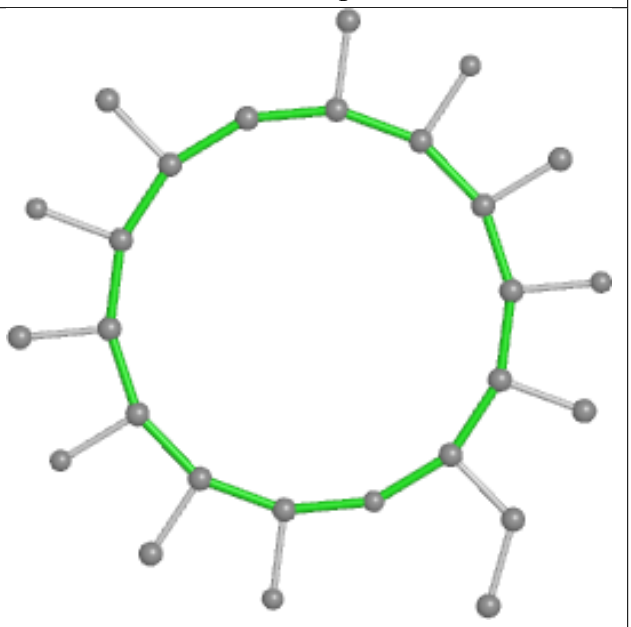

Rings

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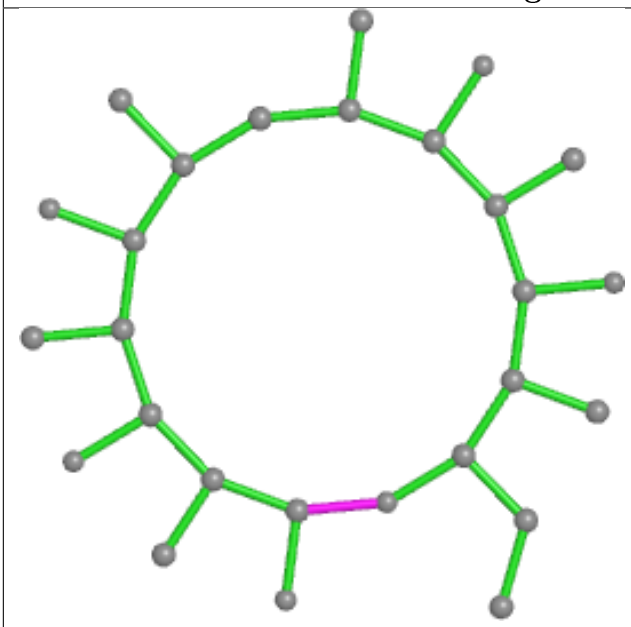

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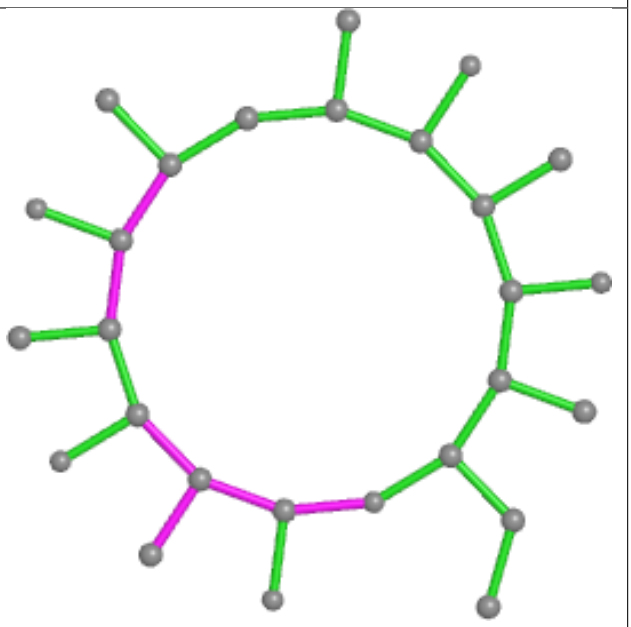

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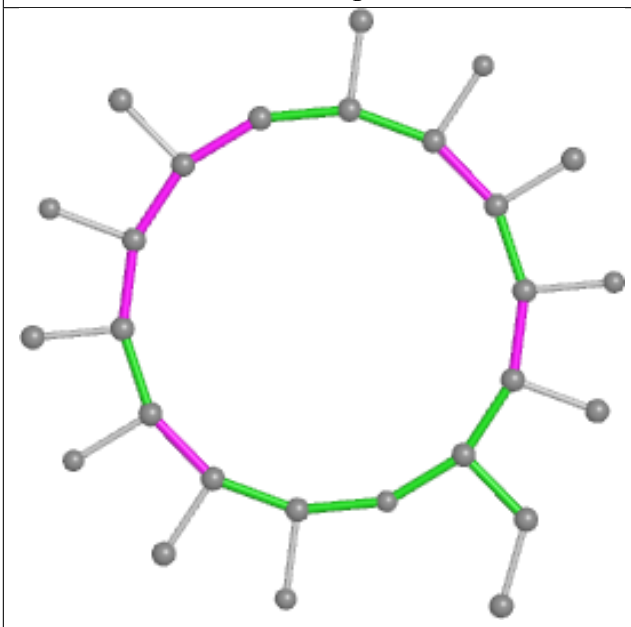

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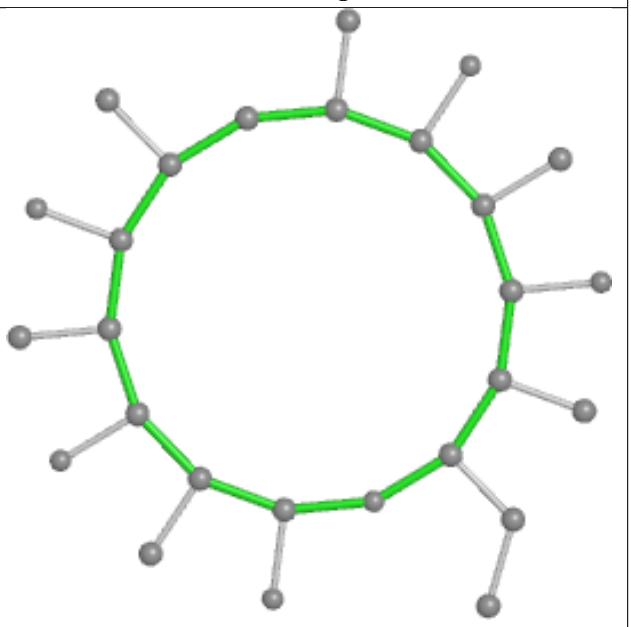
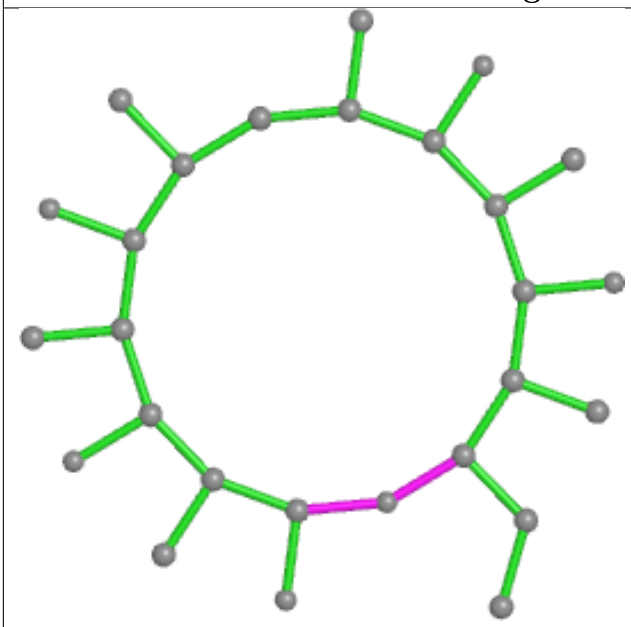


Rings

Ligand DEB A 502



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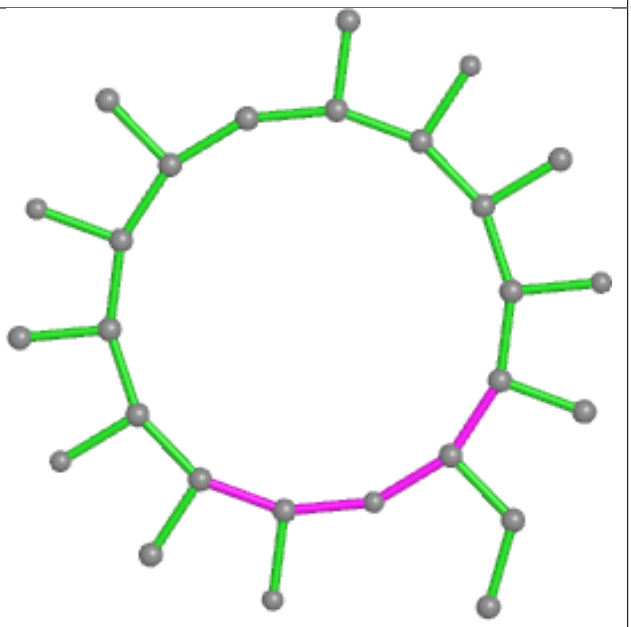
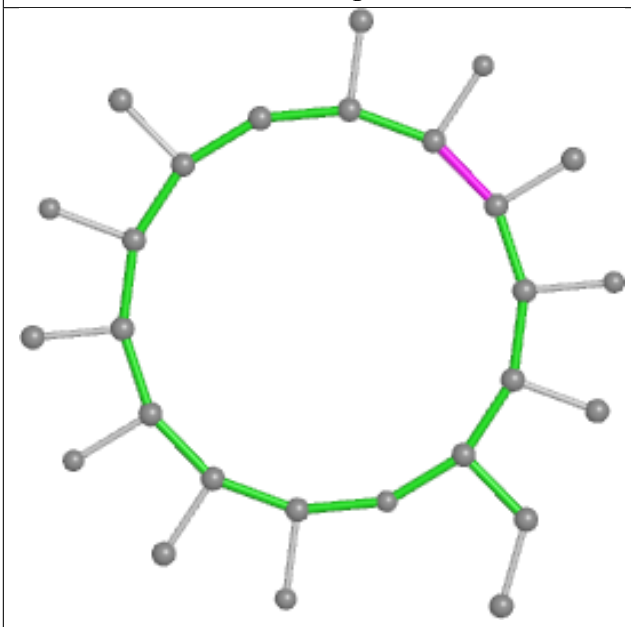


Bond angles



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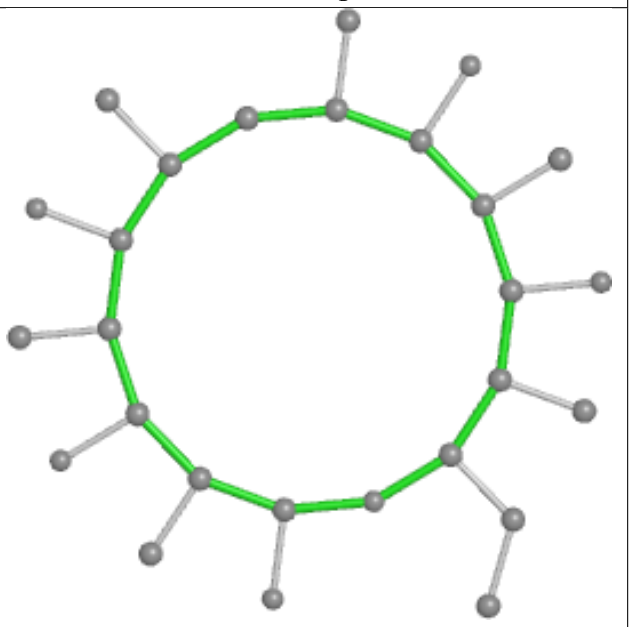
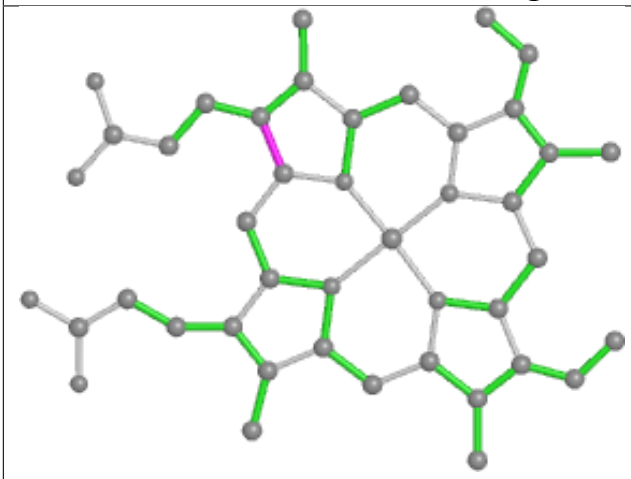


Rings

Ligand HEM I 501



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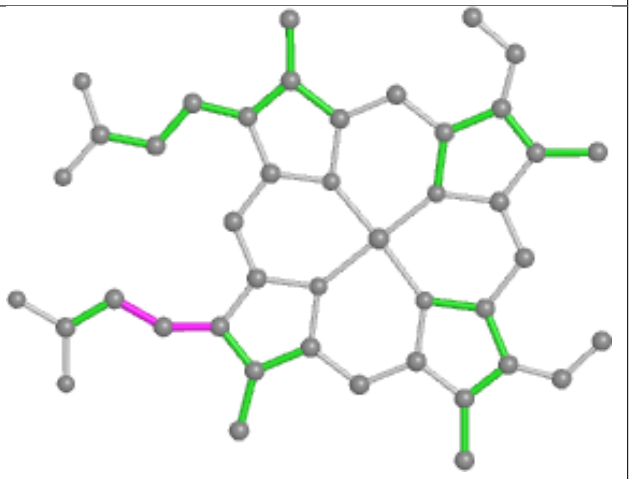
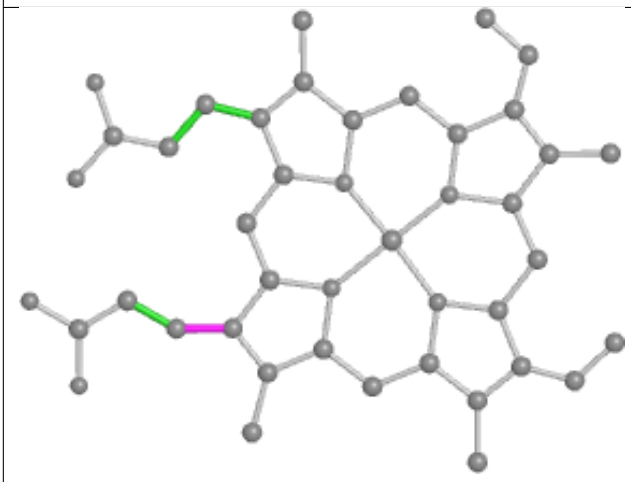
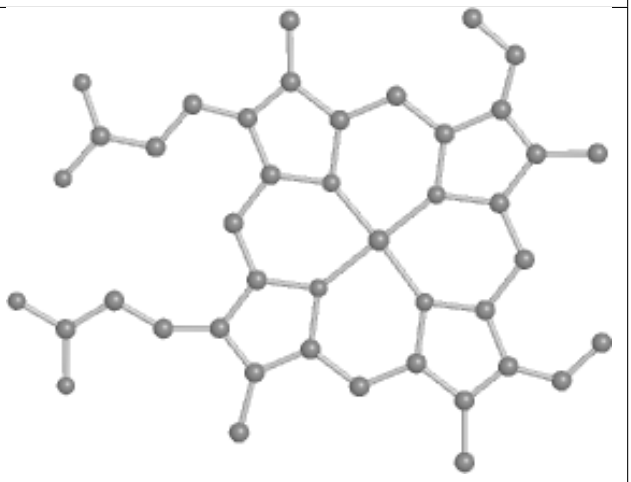


Bond angles

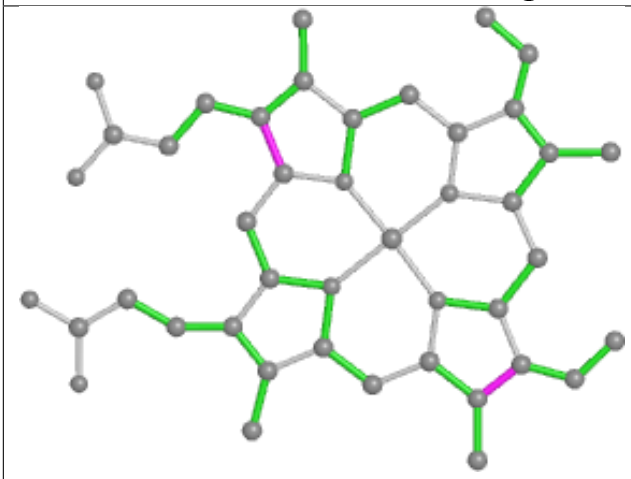


Torsions

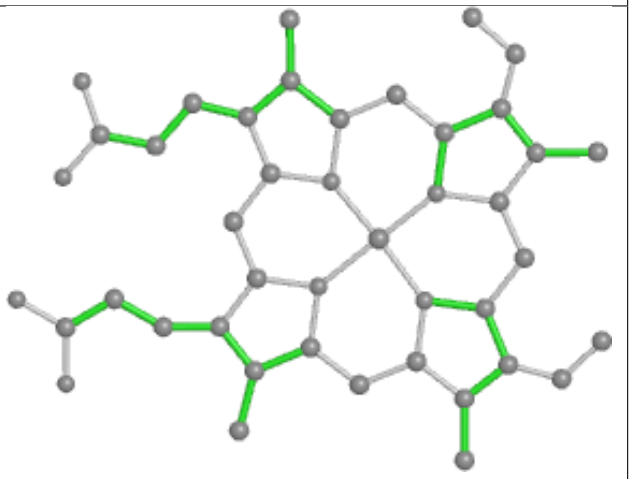


Rings

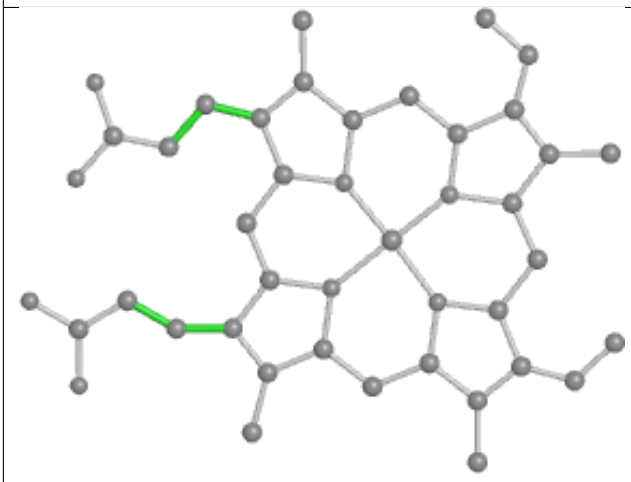
Ligand HEM E 501



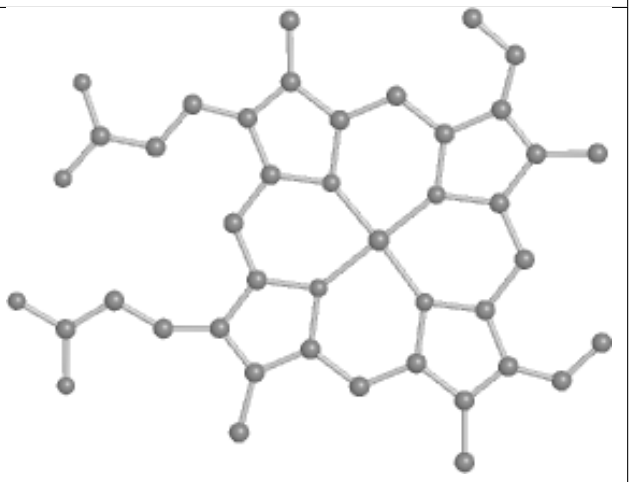
Bond lengths



Bond angles

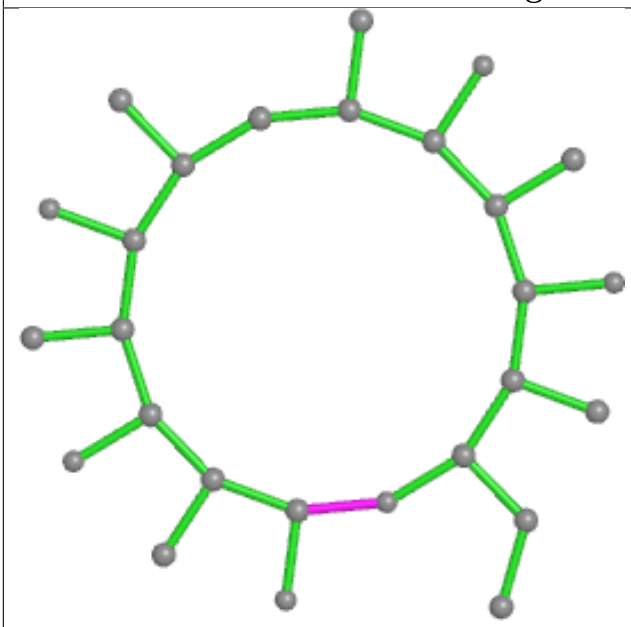


Torsions

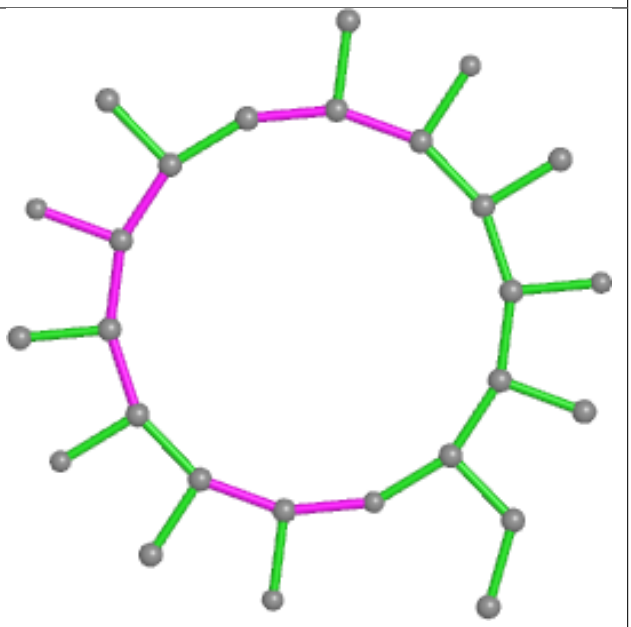


Rings

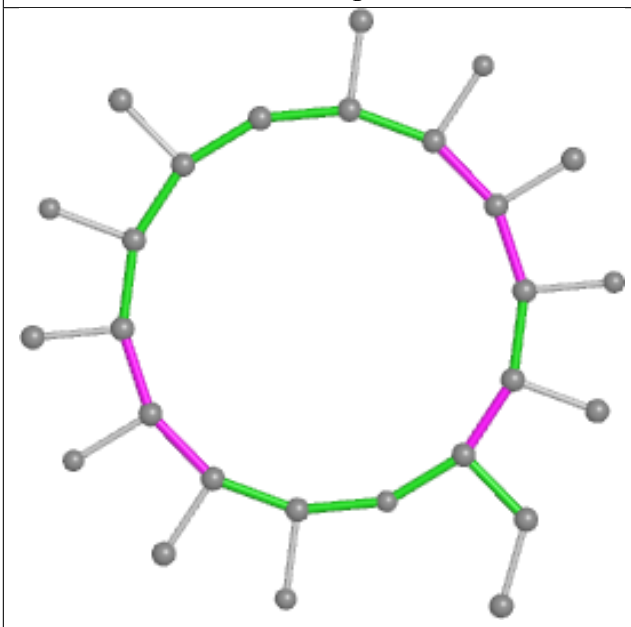
Ligand DEB F 502



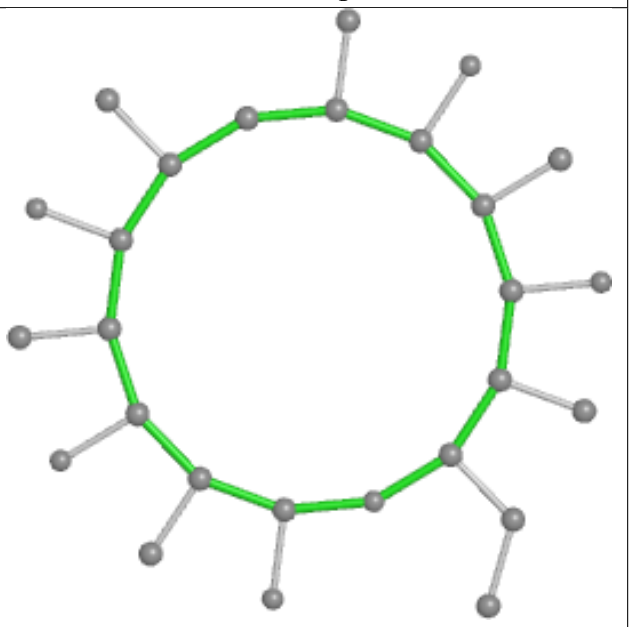
Bond lengths



Bond angles

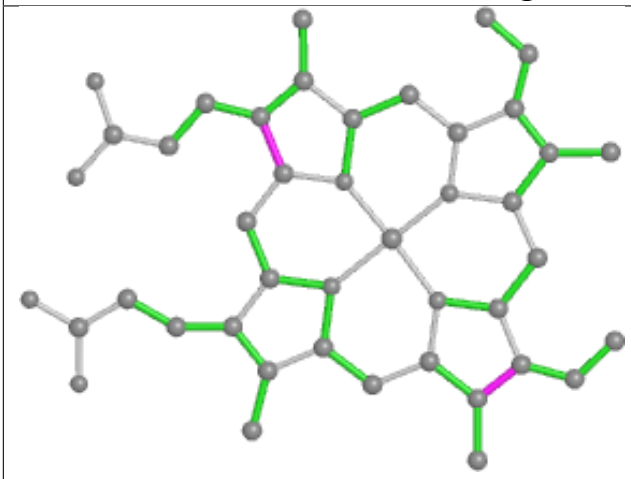


Torsions

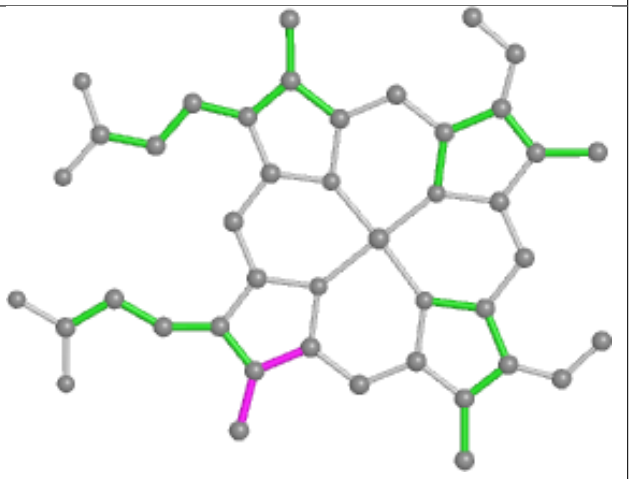


Rings

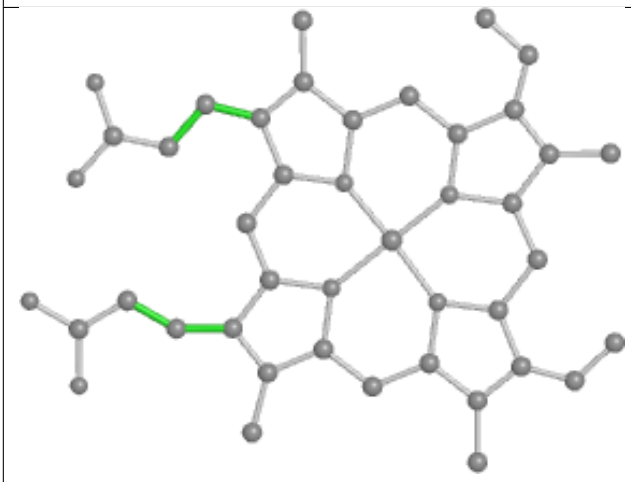
Ligand HEM A 501



Bond lengths



Bond angles



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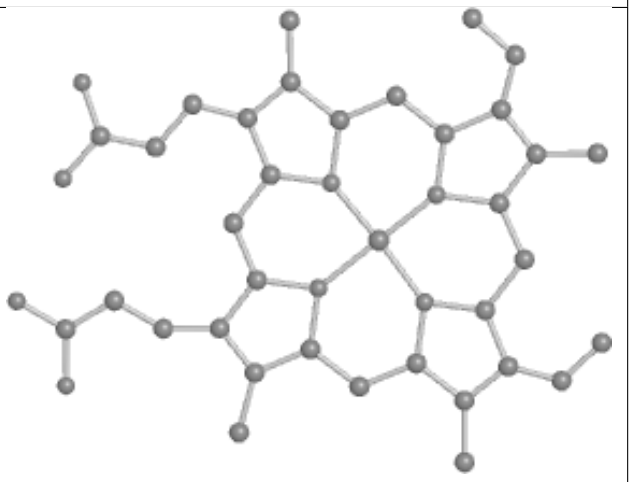
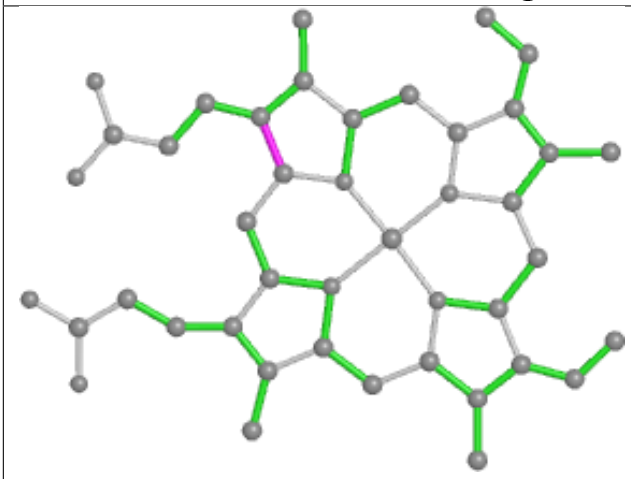
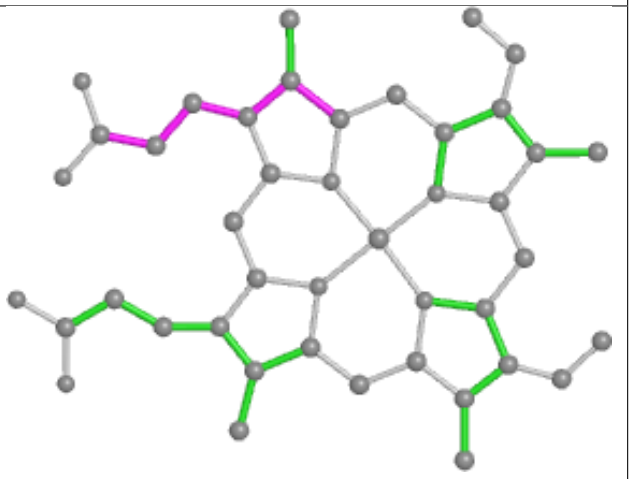


Rings

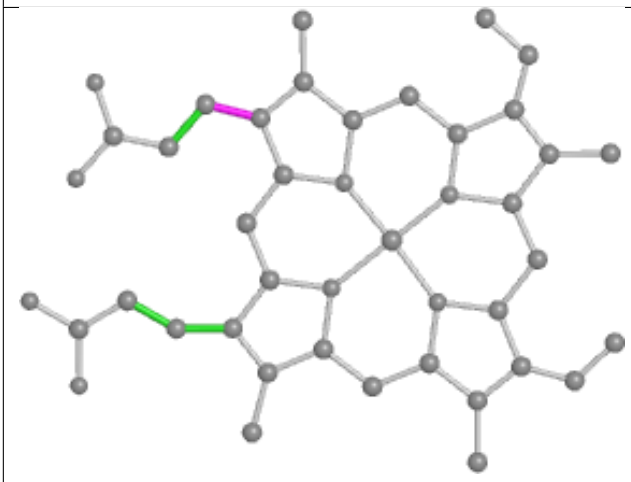
Ligand HEM C 501



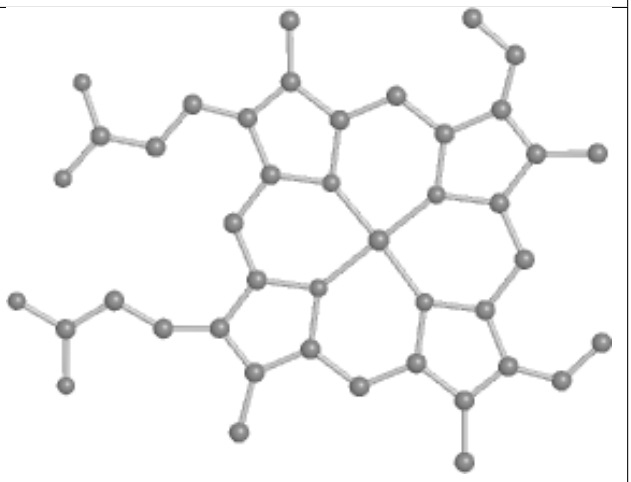
Bond lengths



Bond angles

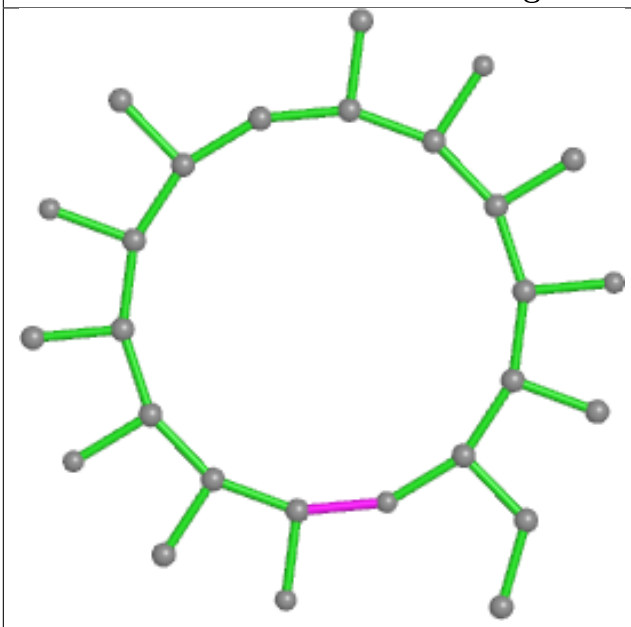


Torsions

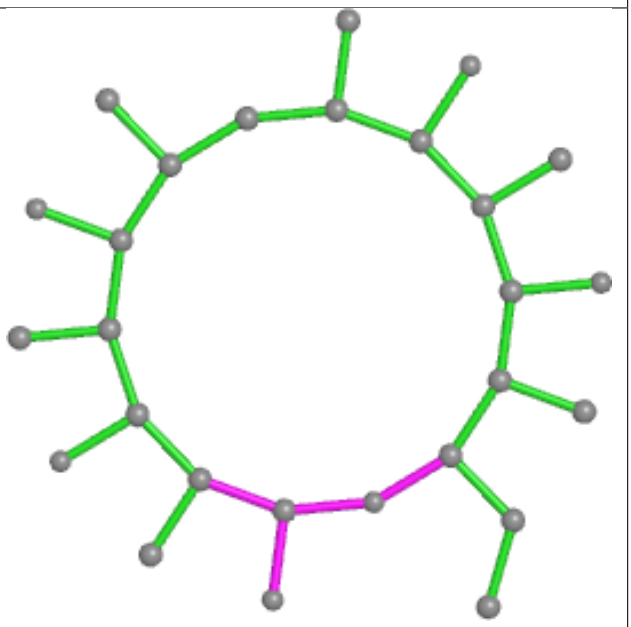


Rings

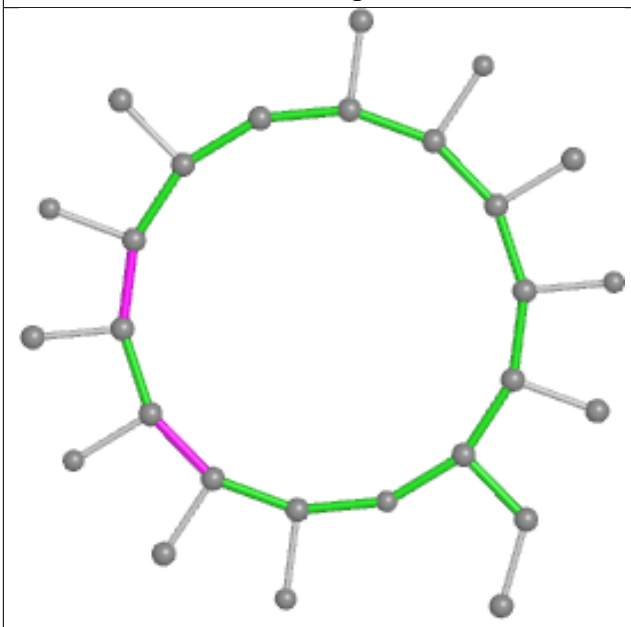
Ligand DEB C 502



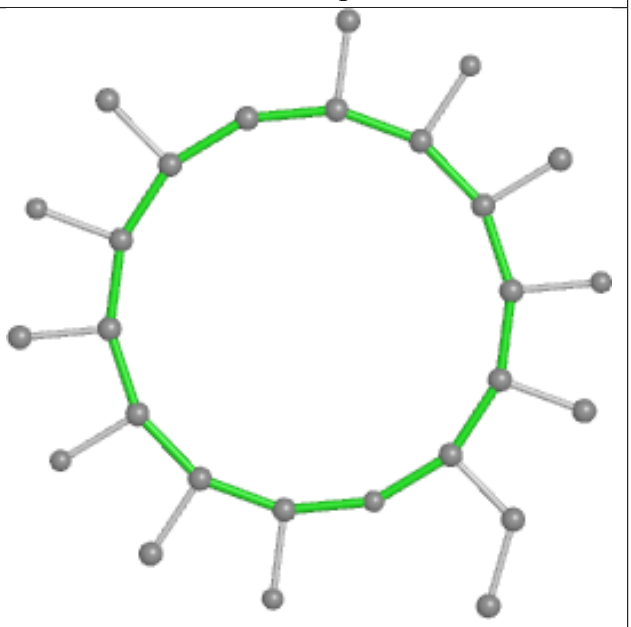
Bond lengths



Bond angles

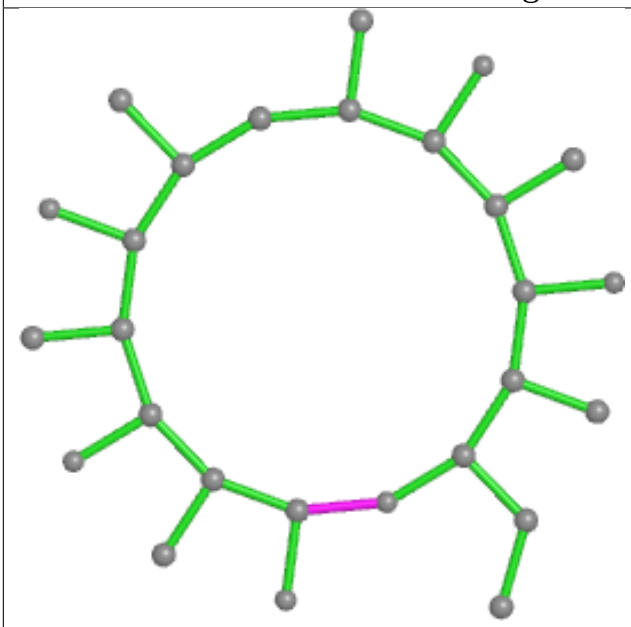


Torsions

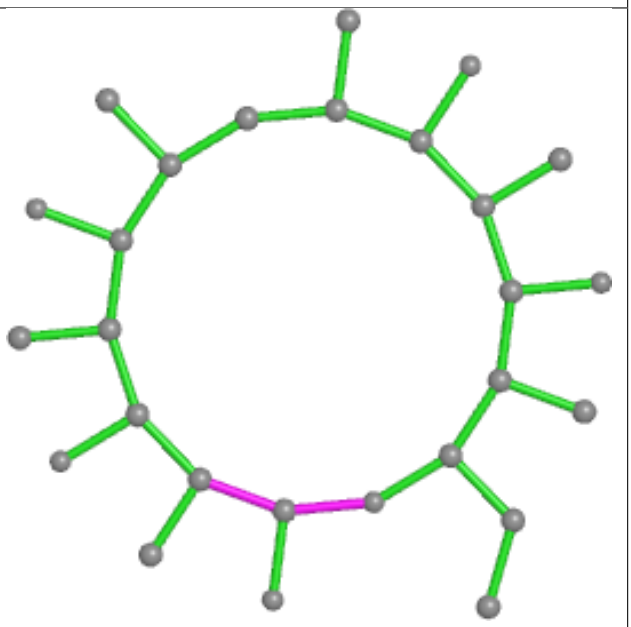


Rings

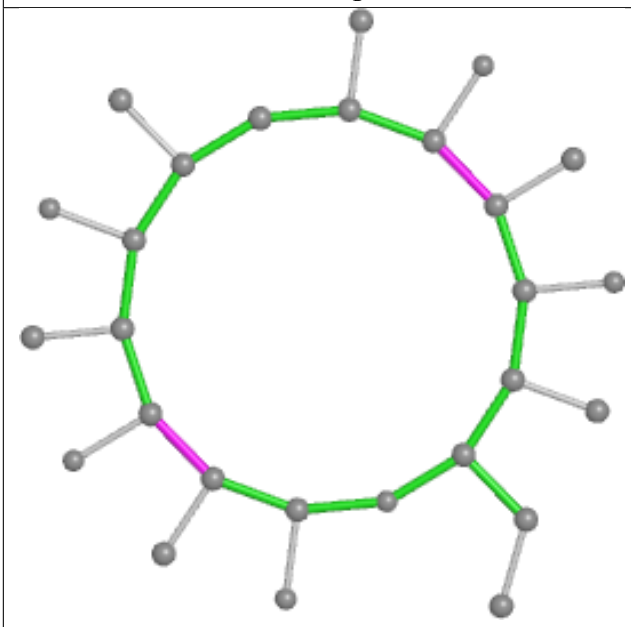
Ligand DEB G 502



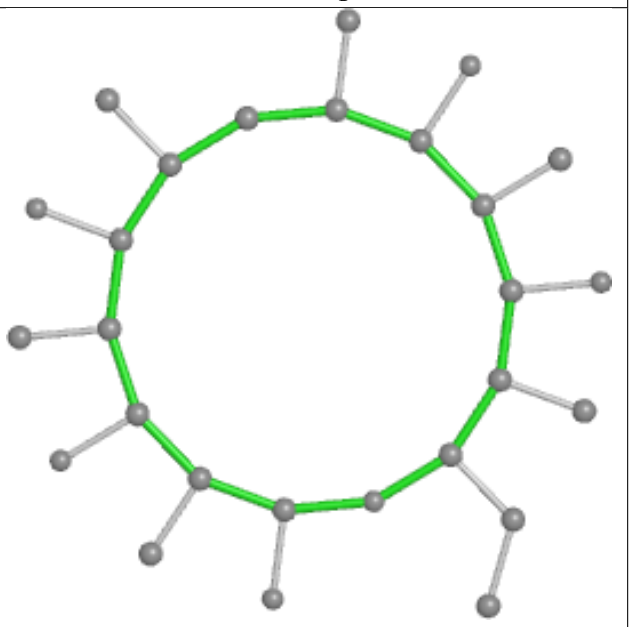
Bond lengths



Bond angles

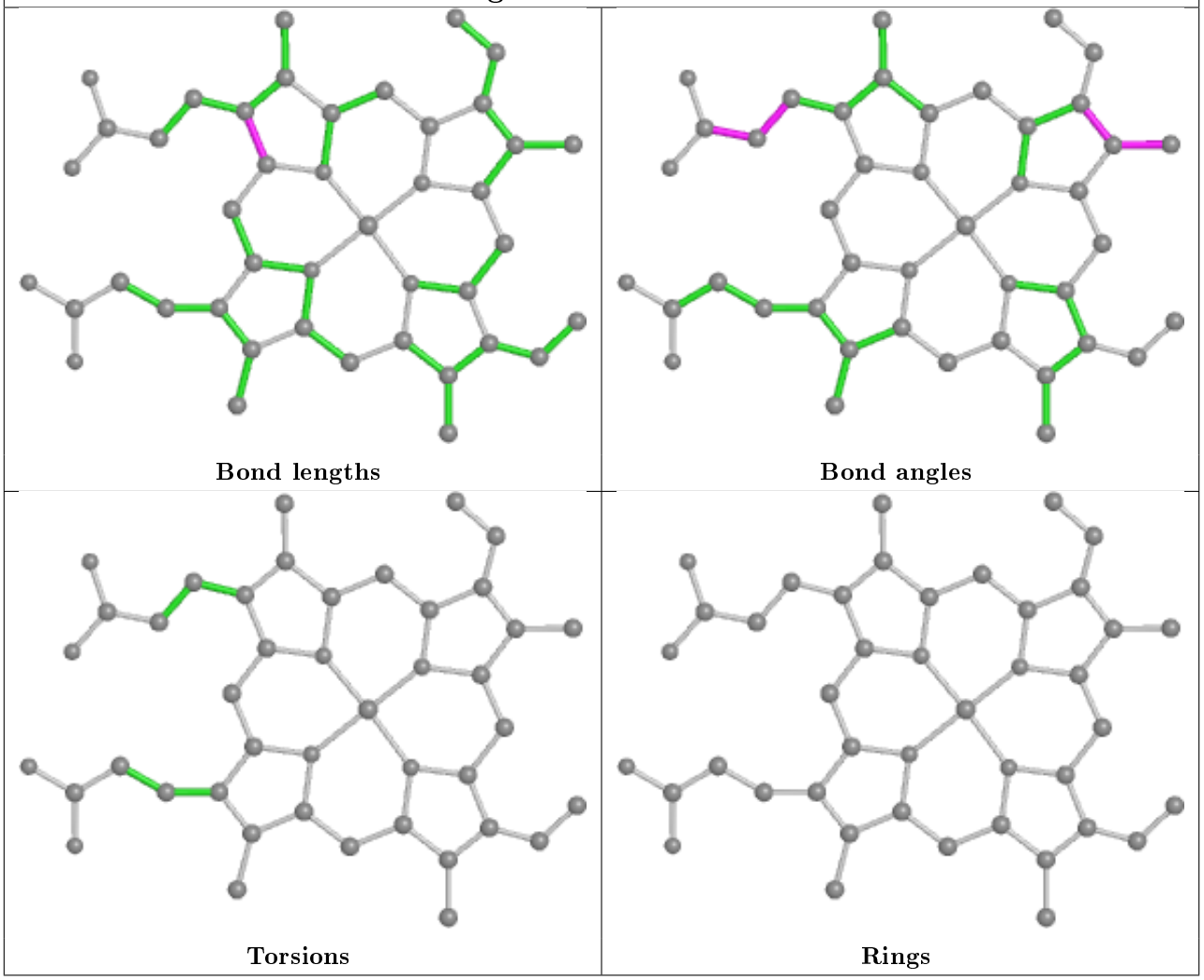


Torsions



Rings

Ligand HEM B 501



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, 95^{th} 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	397/407 (97%)	-0.48	5 (1%) 77 59	23, 43, 96, 128	0
1	B	394/407 (96%)	-0.36	0 100 100	33, 67, 97, 113	0
1	C	396/407 (97%)	-0.49	1 (0%) 94 87	19, 55, 82, 116	0
1	D	394/407 (96%)	-0.44	4 (1%) 82 66	28, 50, 96, 125	0
1	E	390/407 (95%)	-0.07	8 (2%) 63 43	34, 80, 117, 130	0
1	F	395/407 (97%)	-0.37	2 (0%) 91 80	30, 64, 98, 117	0
1	G	380/407 (93%)	0.26	30 (7%) 12 6	45, 96, 140, 168	0
1	H	395/407 (97%)	-0.15	6 (1%) 73 54	37, 71, 108, 148	0
1	I	286/407 (70%)	1.15	68 (23%) 0 0	88, 121, 148, 182	0
All	All	3427/3663 (93%)	-0.15	124 (3%) 42 26	19, 67, 126, 182	0

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	204	VAL	8.5
1	I	39	PRO	7.9
1	H	185	THR	6.7
1	I	177	ALA	6.5
1	I	59	SER	5.7

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 carbohydrates in this entry.

6.4 Ligands (i)

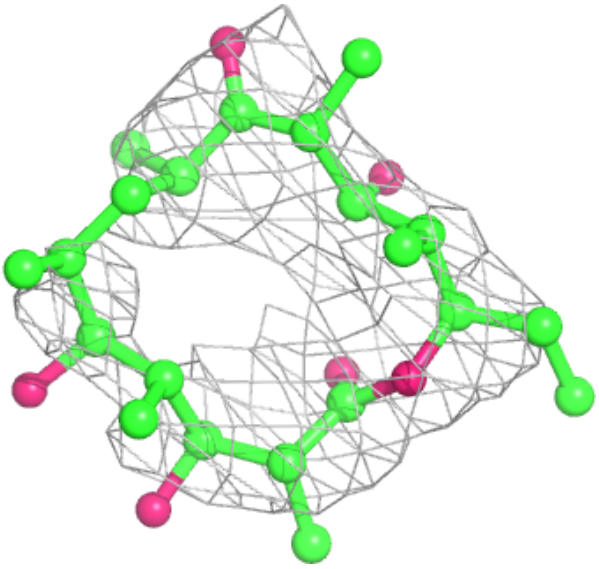
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

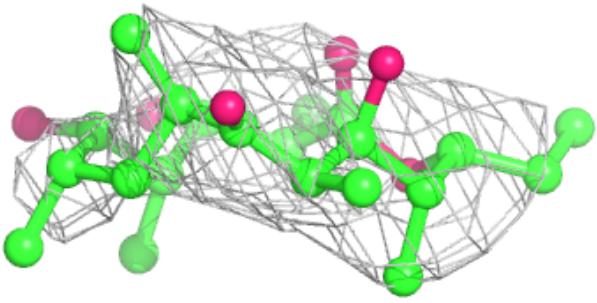
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DEB	G	502	27/27	0.84	0.33	101,112,116,118	0
3	DEB	F	502	27/27	0.88	0.25	55,58,62,64	0
3	DEB	I	502	27/27	0.88	0.31	116,128,135,139	0
3	DEB	H	502	27/27	0.89	0.22	60,65,68,71	0
2	HEM	I	501	43/43	0.89	0.21	107,135,141,146	0
3	DEB	A	502	27/27	0.93	0.19	41,46,53,56	0
2	HEM	F	501	43/43	0.94	0.22	65,81,84,89	0
3	DEB	E	502	27/27	0.94	0.23	72,77,82,85	0
3	DEB	D	502	27/27	0.94	0.20	41,44,51,52	0
3	DEB	B	502	27/27	0.96	0.18	51,53,56,62	0
2	HEM	E	501	43/43	0.96	0.27	61,68,81,86	0
2	HEM	D	501	43/43	0.96	0.18	31,35,41,44	0
2	HEM	G	501	43/43	0.96	0.24	77,84,97,98	0
2	HEM	H	501	43/43	0.96	0.22	63,84,89,94	0
2	HEM	B	501	43/43	0.96	0.21	54,60,71,80	0
2	HEM	C	501	43/43	0.97	0.20	43,46,52,57	0
3	DEB	C	502	27/27	0.97	0.17	42,45,47,50	0
2	HEM	A	501	43/43	0.98	0.16	26,35,38,41	0

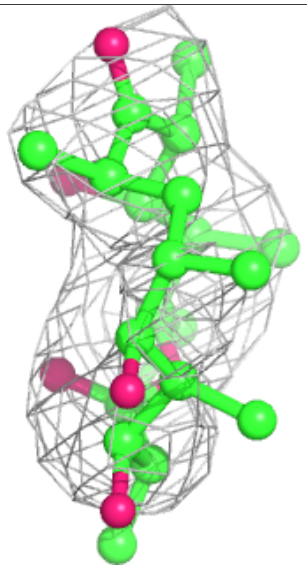
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DEB G 502:

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

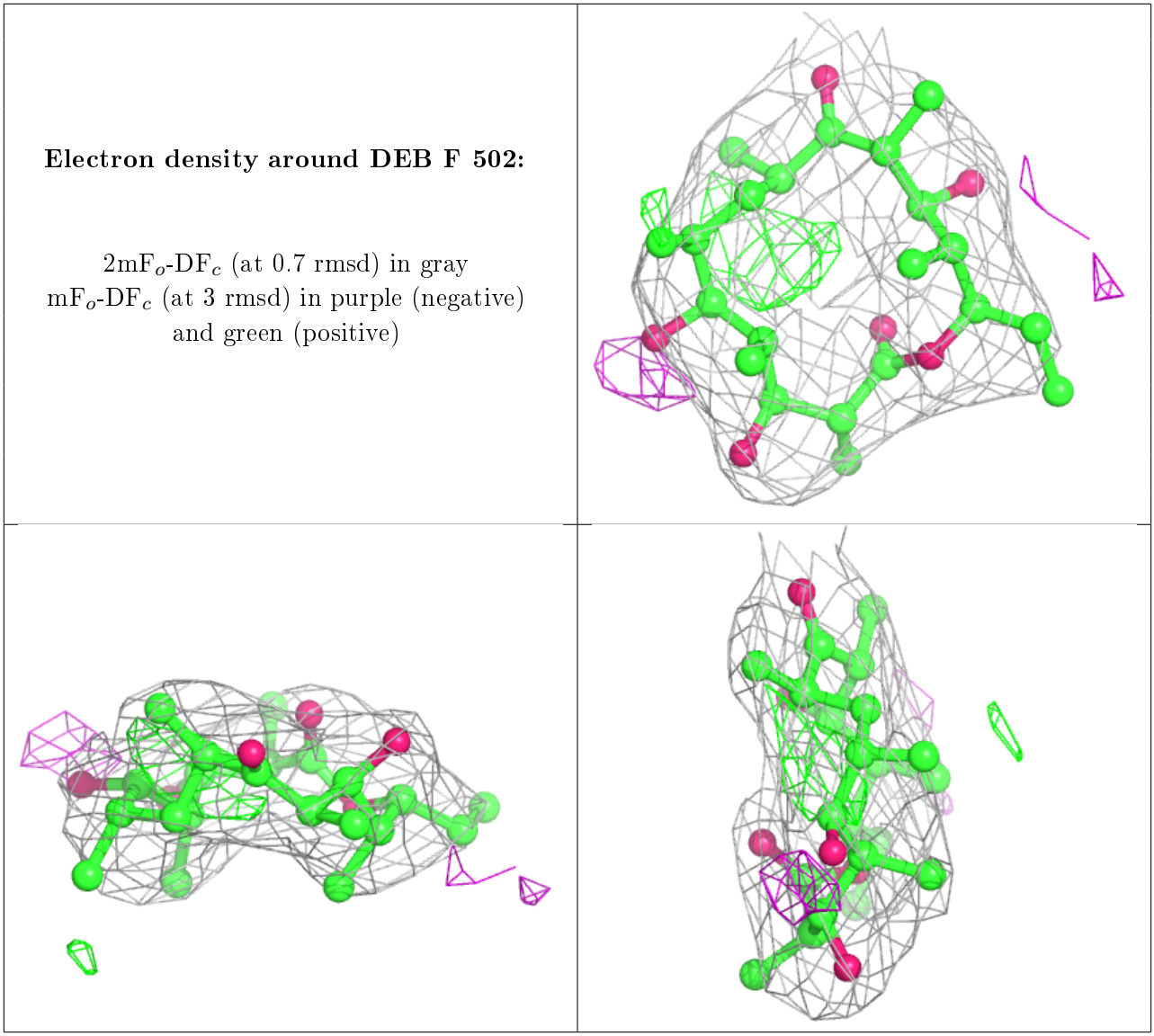






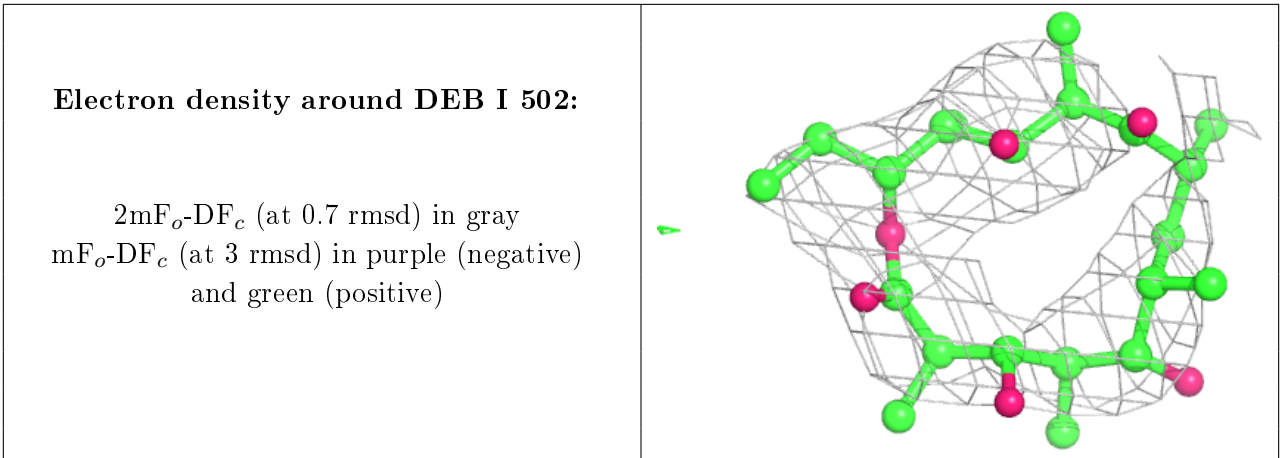
Electron density around DEB F 502:

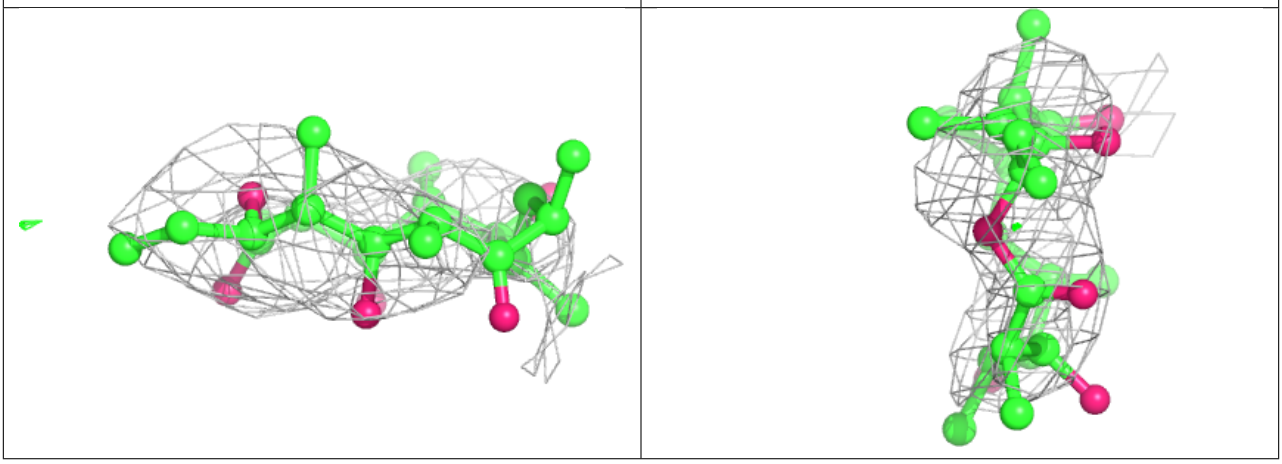
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DEB I 502:

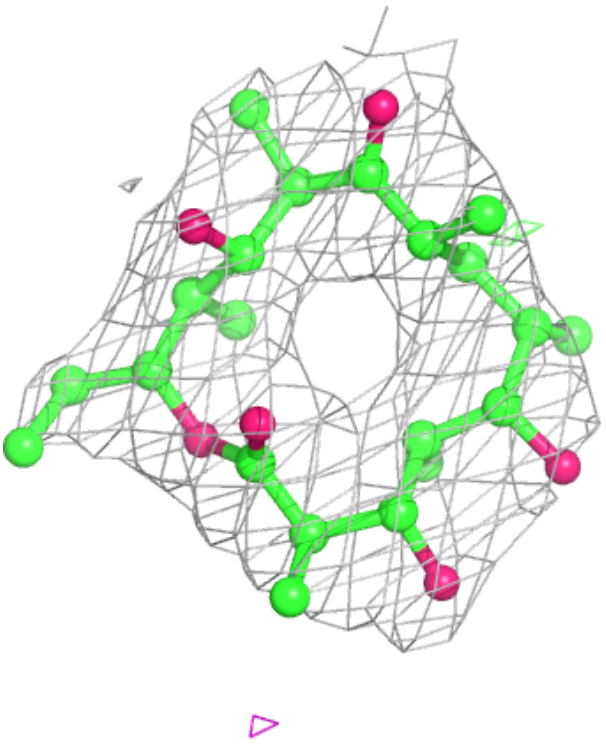
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

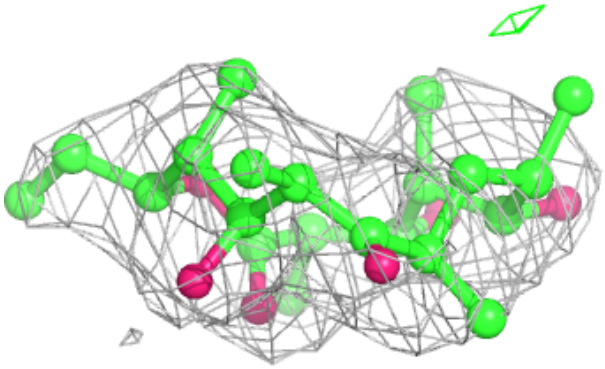


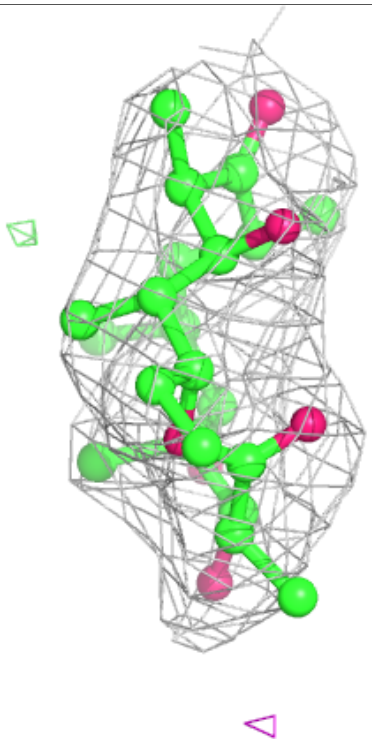


Electron density around DEB H 502:

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

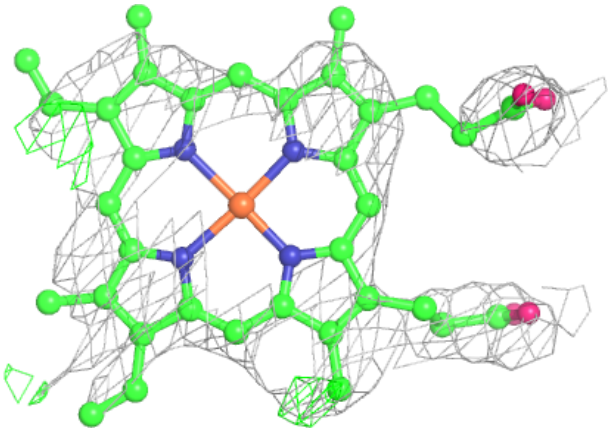


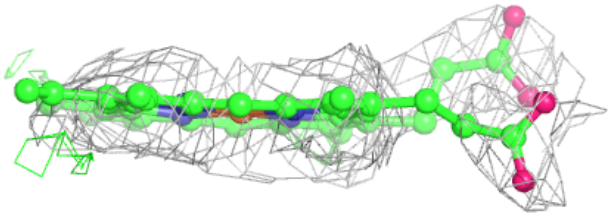


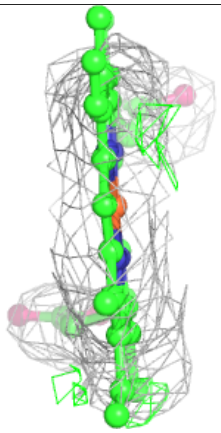


Electron density around HEM I 501:

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

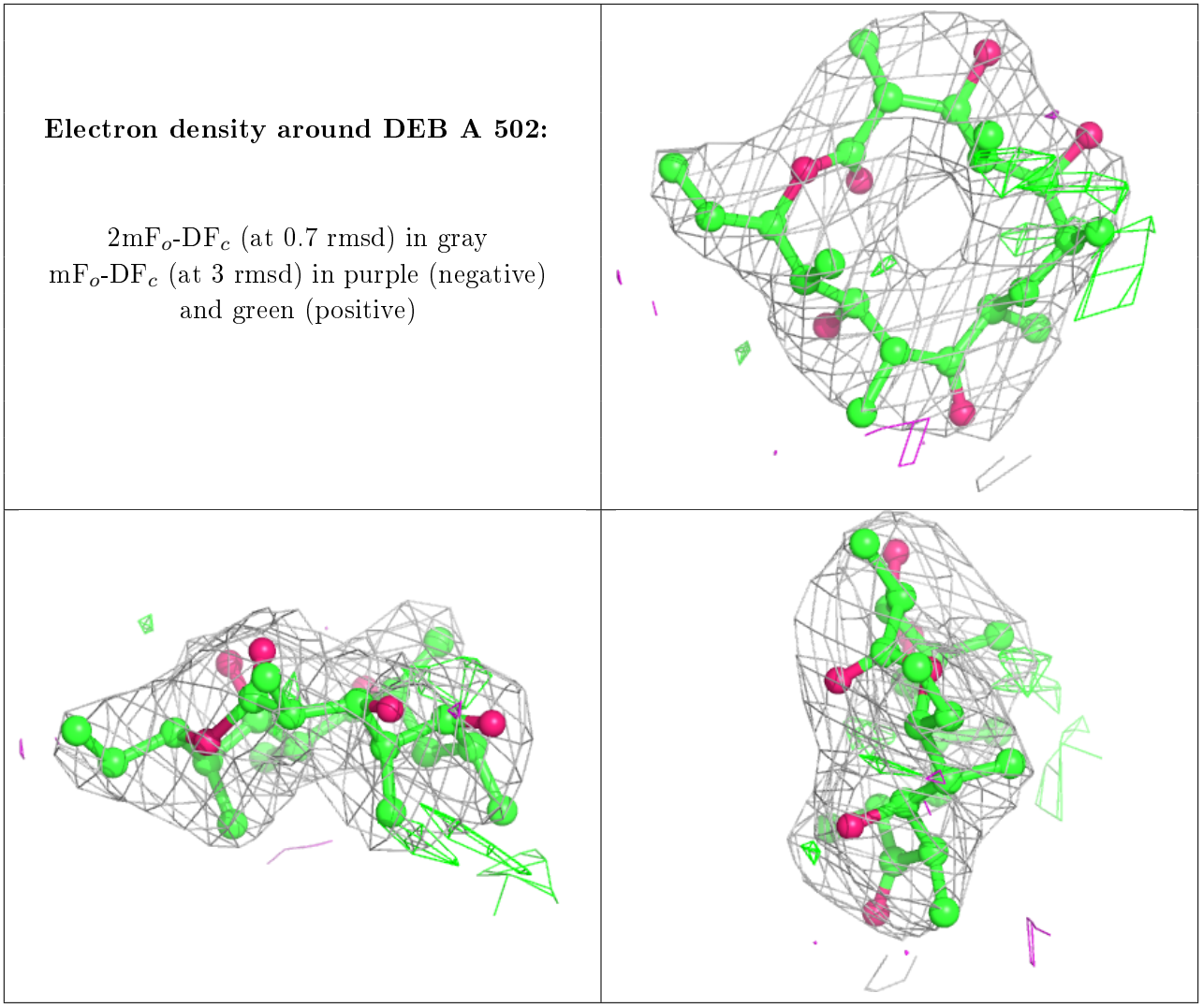






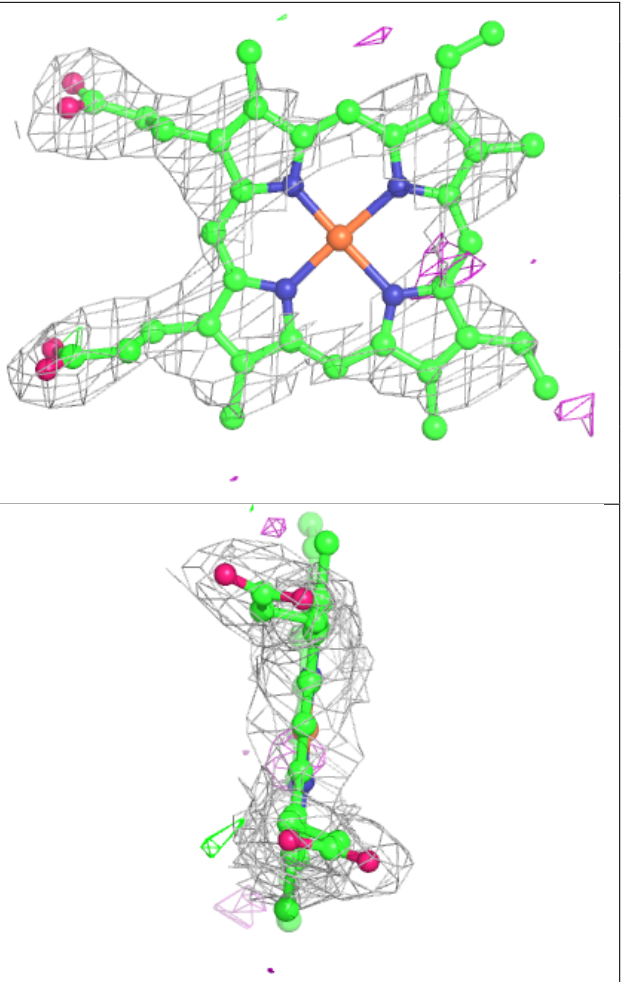
Electron density around DEB A 502:

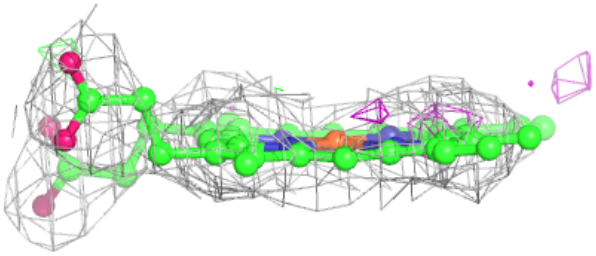
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEM F 501:

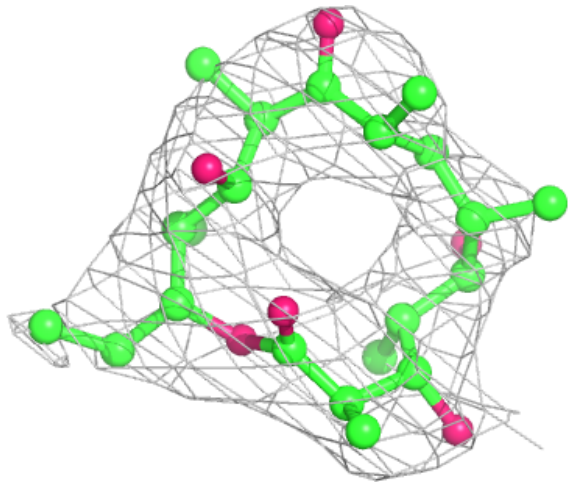
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

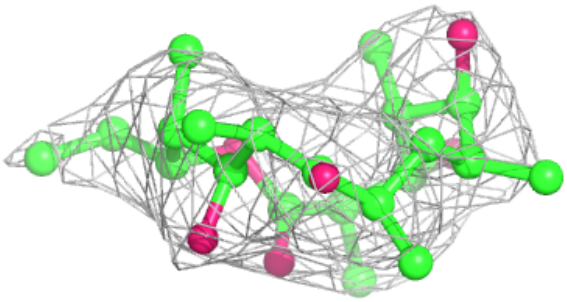


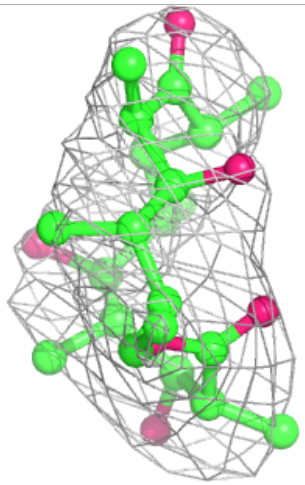


Electron density around DEB E 502:

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

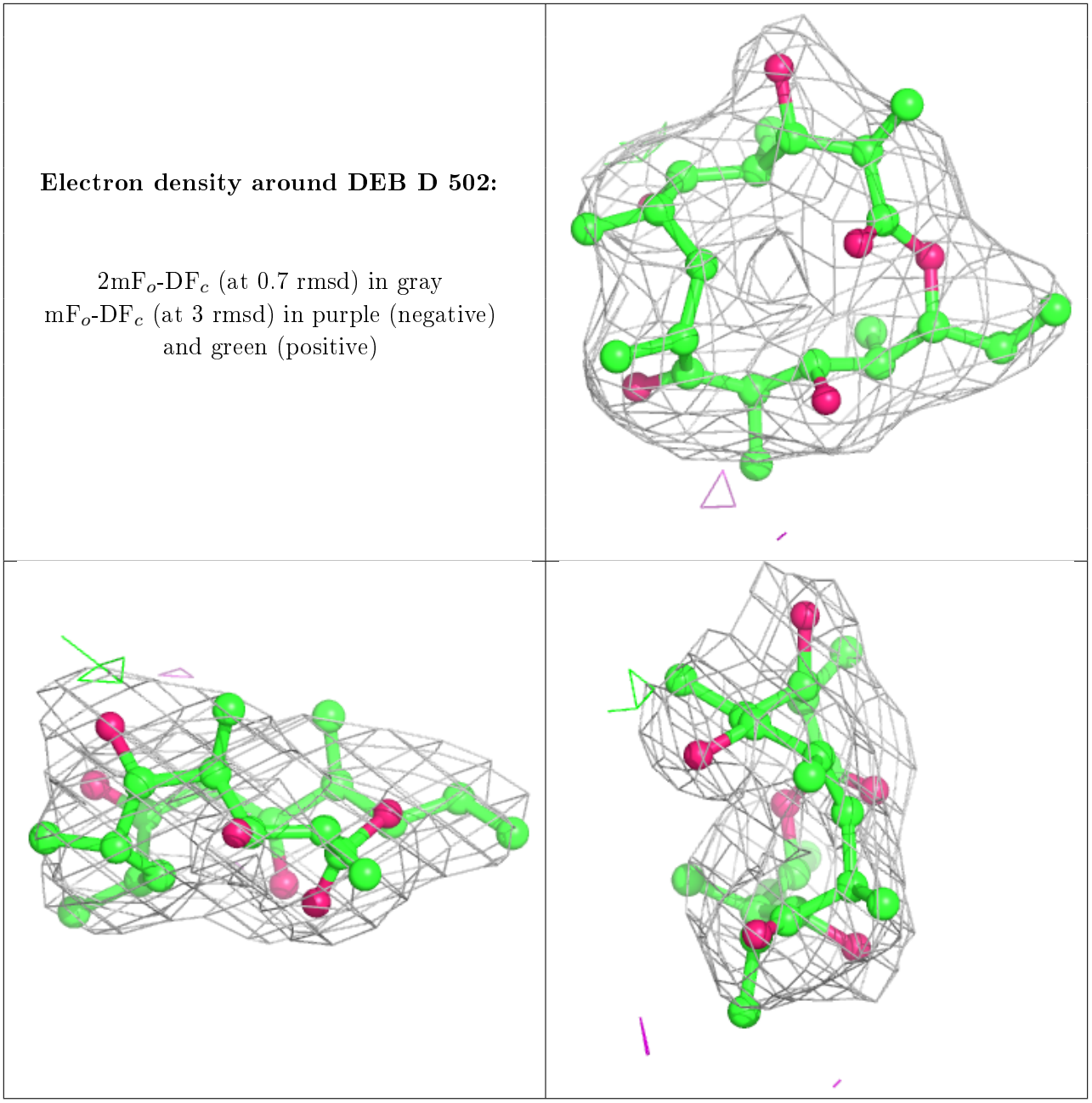






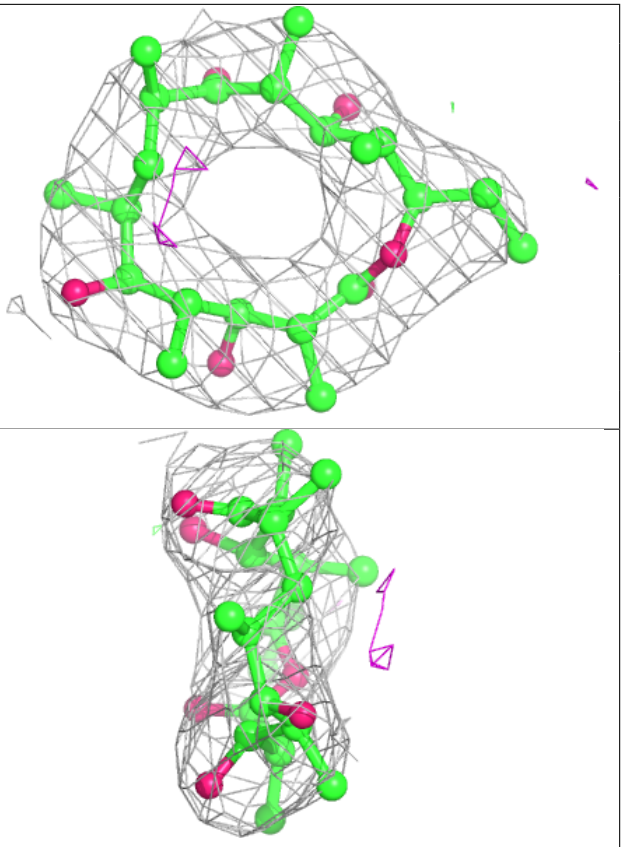
Electron density around DEB D 502:

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



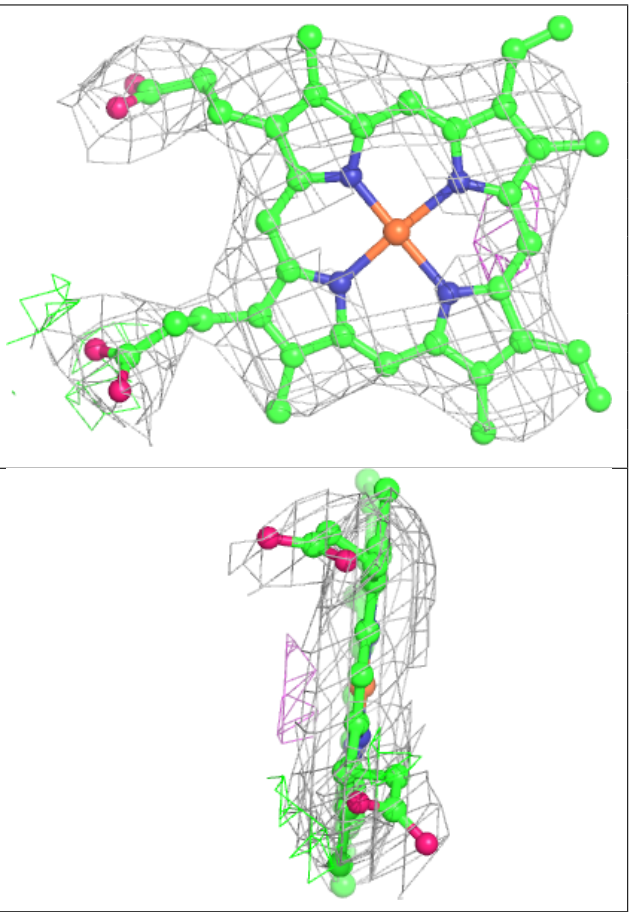
Electron density around DEB B 502:

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



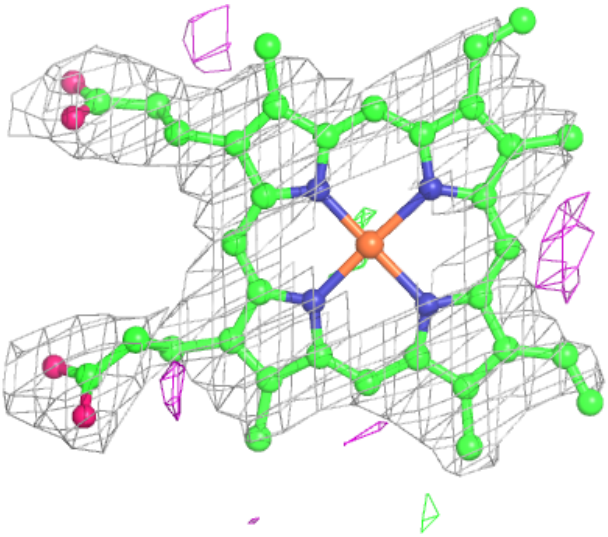
Electron density around HEM E 501:

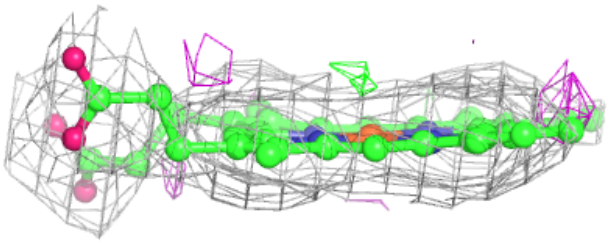
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

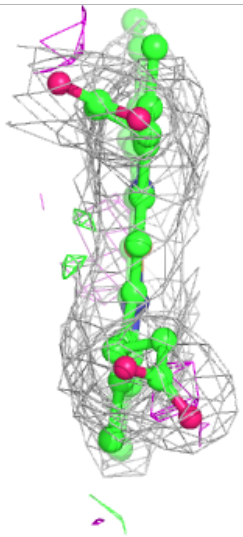


Electron density around HEM D 501:

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

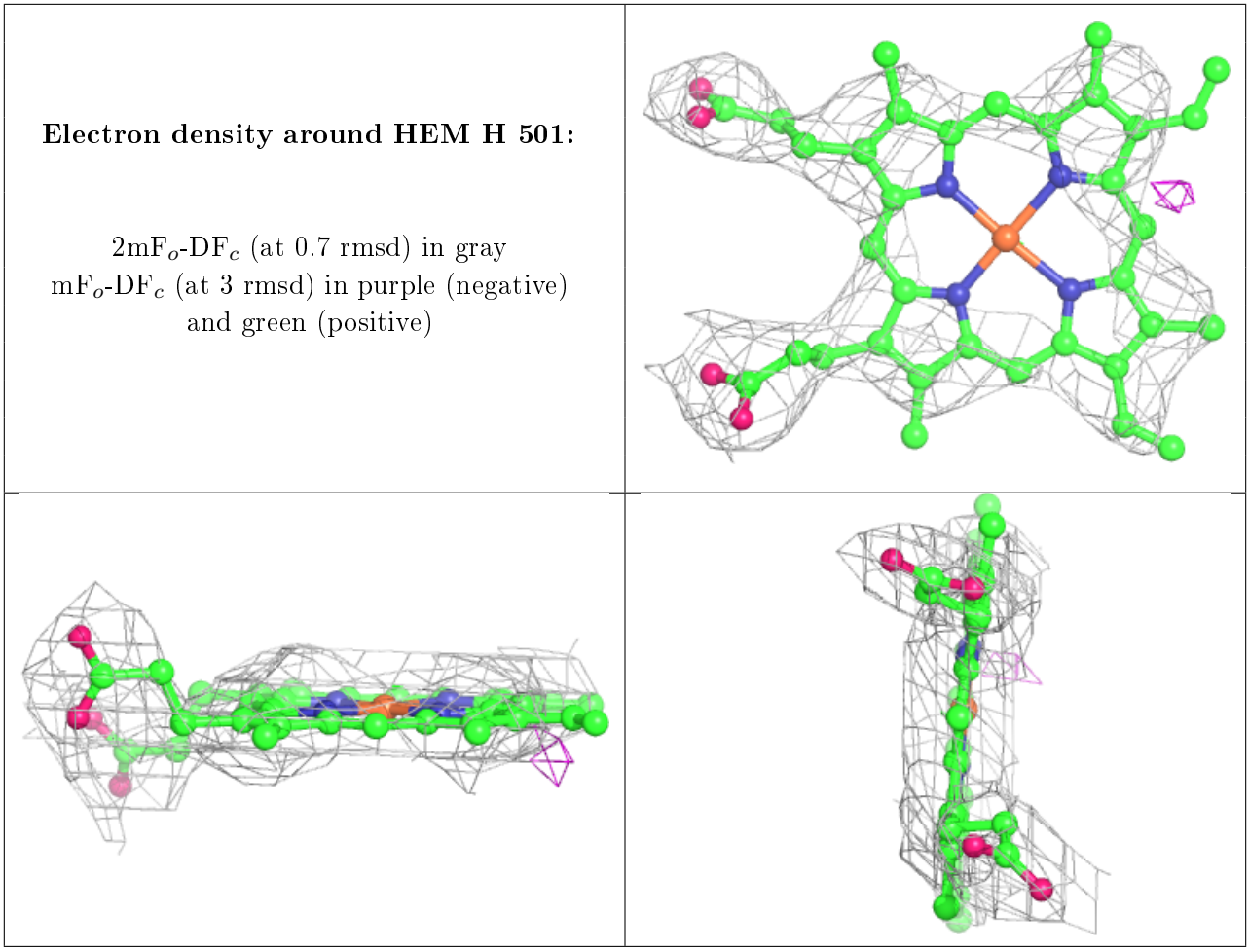






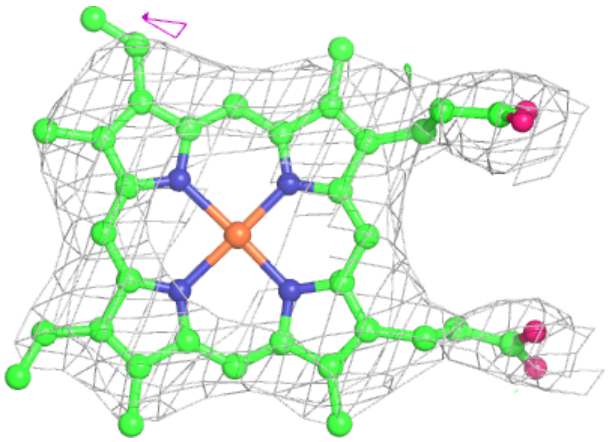
Electron density around HEM H 501:

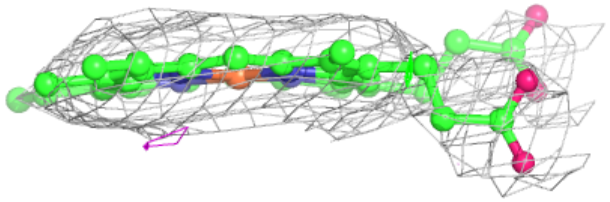
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

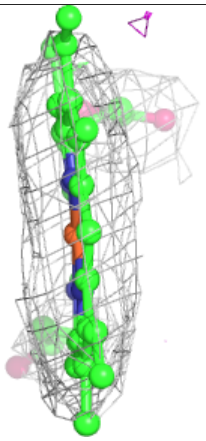


Electron density around HEM B 501:

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

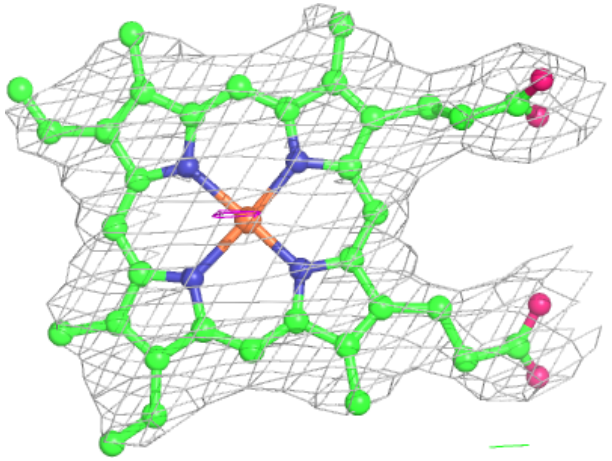


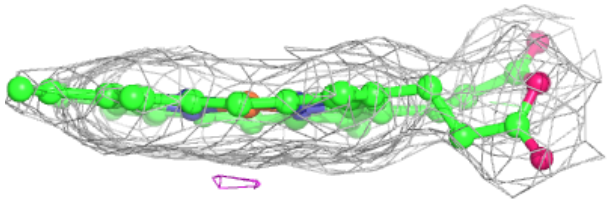


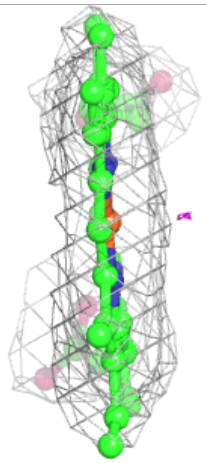


Electron density around HEM C 501:

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

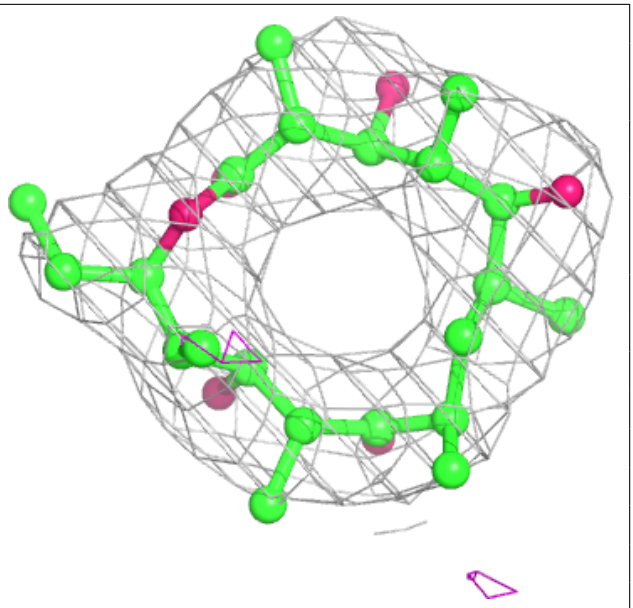


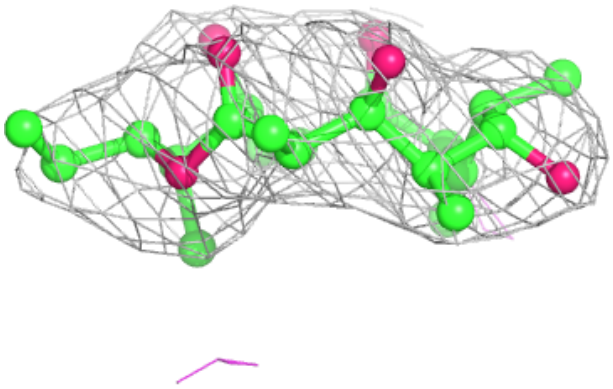


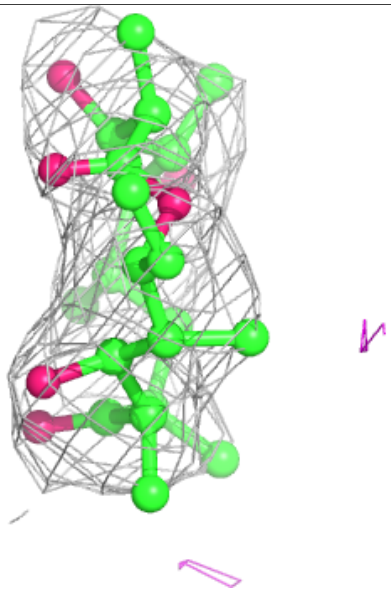


Electron density around DEB C 502:

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

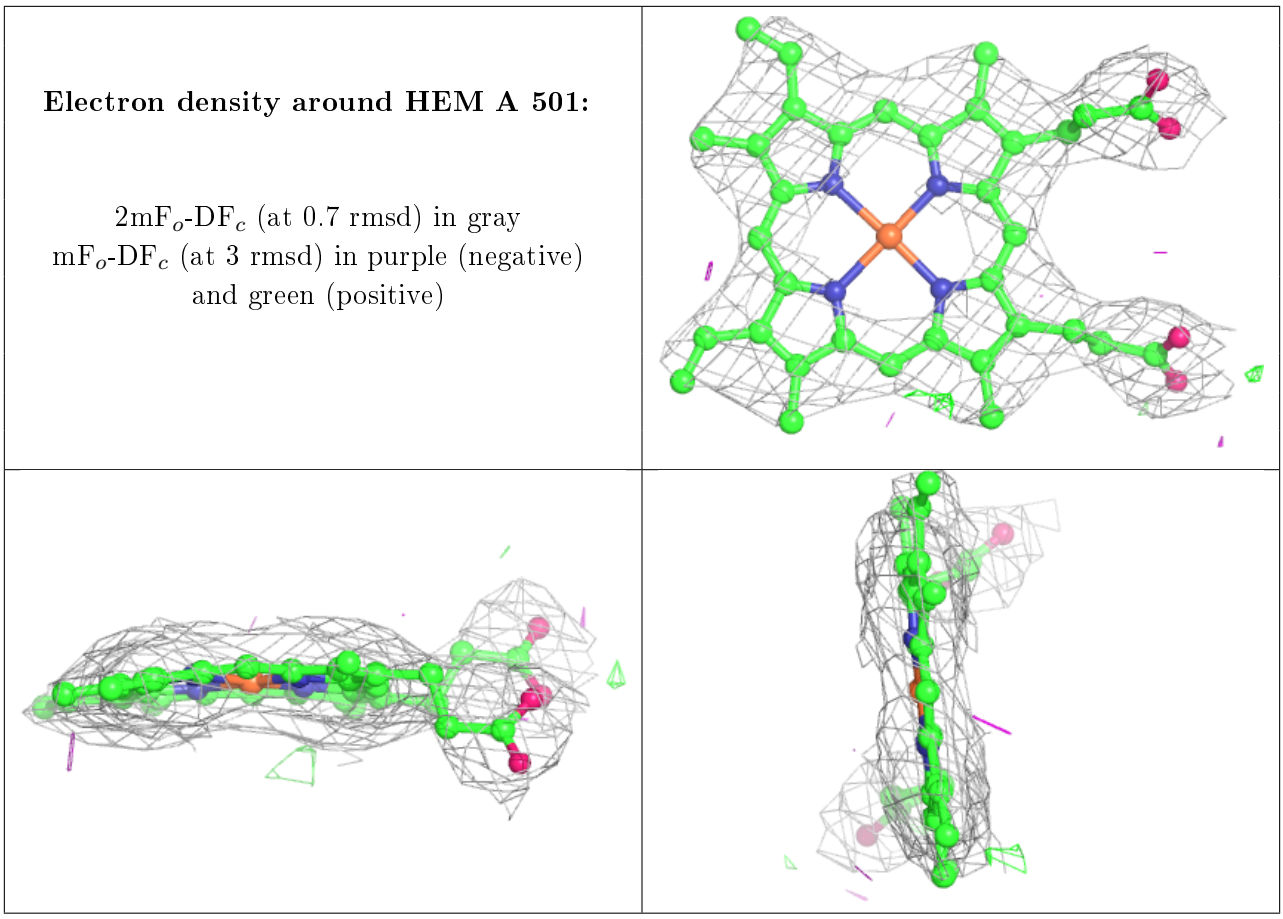






Electron density around HEM A 501:

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



6.5 Other polymers

There are no such residues in this entry.