wwPDB X-ray Structure Validation Summary Report (i)

Oct 12, 2020 – 09:25 PM BST

PDB ID	:	6ZI2
Title	:	OleP-oleandolide(DEO) in low salt crystallization conditions
Authors	:	Savino, C.; Montemiglio, L.C.; Vallone, B.; Parisi, G.; Cecchetti, C.
Deposited on	:	2020-06-24
Resolution	:	2.93 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 (i)) were used in the production of this report:

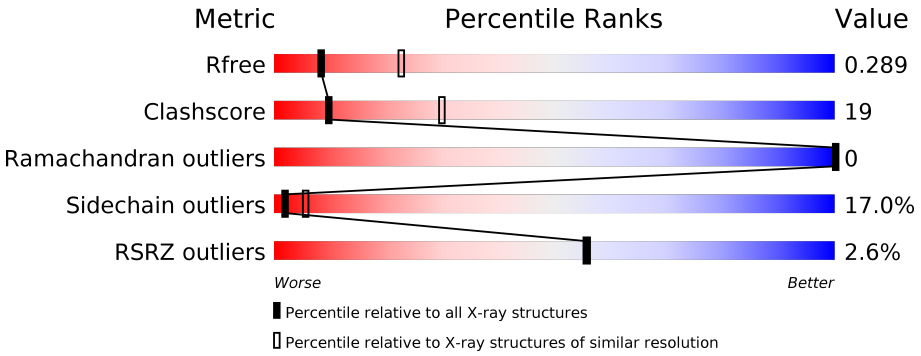
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 2.93 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	61% 32%
1	B	407	55% 32% 11%
1	C	407	57% 33% 7%
1	D	407	63% 30%
1	E	407	% 60% 29% 6% 5%
1	F	407	% 64% 27% 6%

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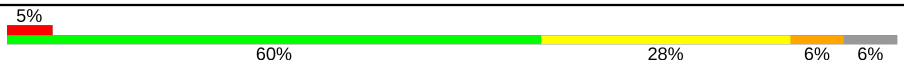
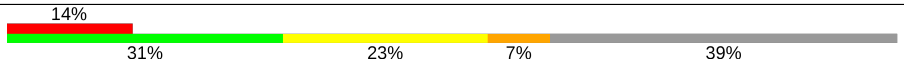
Mol	Chain	Length	Quality of chain
1	G	407	
1	H	407	
1	I	407	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	QR8	E	502	X	X	-	-

2 Entry composition (i)

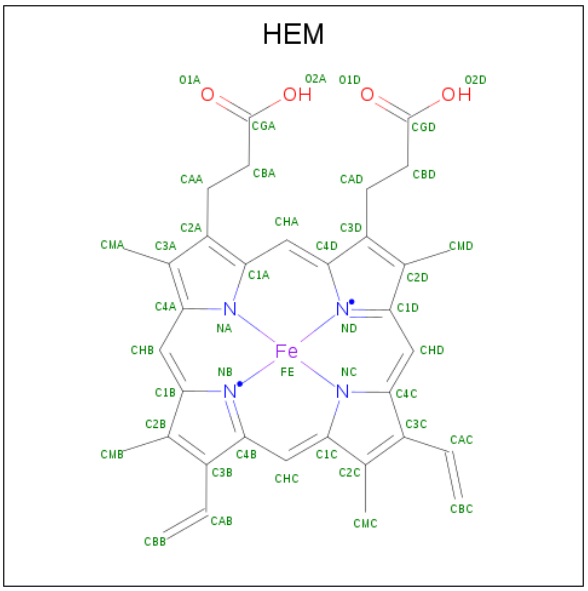
There are 4 unique types of molecules in this entry. The entry contains 27067 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

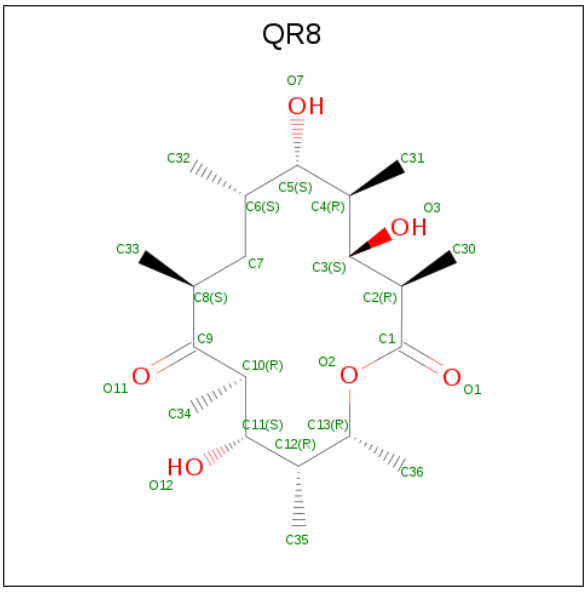
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	0	0	0
			3073	1934	551	575	13			
1	B	395	Total	C	N	O	S	0	0	0
			3078	1937	552	576	13			
1	C	395	Total	C	N	O	S	0	0	0
			3078	1937	552	576	13			
1	D	394	Total	C	N	O	S	0	0	0
			3067	1931	548	575	13			
1	E	386	Total	C	N	O	S	0	0	0
			3012	1897	540	563	12			
1	F	394	Total	C	N	O	S	0	0	0
			3073	1934	551	575	13			
1	G	381	Total	C	N	O	S	0	0	0
			2976	1879	534	550	13			
1	H	395	Total	C	N	O	S	0	0	0
			3078	1937	552	576	13			
1	I	248	Total	C	N	O	S	0	0	0
			1915	1214	344	346	11			

- 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 (3 {R},4 {S},5 {R},6 {S},7 {S},9 {S},11 {R},12 {S},13 {R},14 {R})-3,5,7,9 ,11,13,14-heptamethyl-4,6,12-tris(oxidanyl)-1-oxacyclotetradecane-2,10-dione (three-letter code: QR8) (formula: $C_{20}H_{36}O_6$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 26 20 6	0	0
3	B	1	Total C O 26 20 6	0	0
3	C	1	Total C O 26 20 6	0	0
3	D	1	Total C O 26 20 6	0	0
3	E	1	Total C O 26 20 6	0	0
3	F	1	Total C O 26 20 6	0	0
3	G	1	Total C O 26 20 6	0	0
3	H	1	Total C O 26 20 6	0	0
3	I	1	Total C O 26 20 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	19	Total O 19 19	0	0
4	B	7	Total O 7 7	0	0
4	C	14	Total O 14 14	0	0

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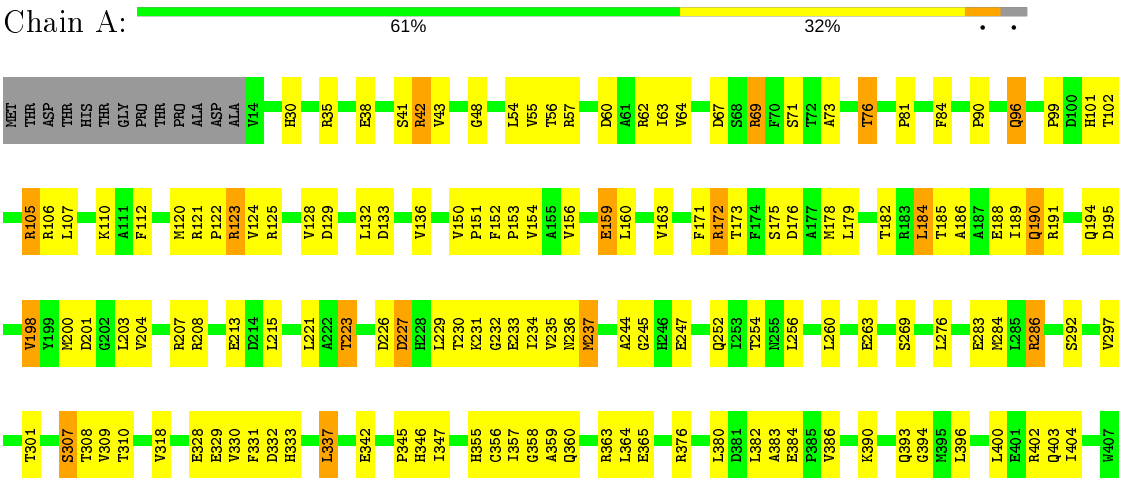
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	25	Total O 25 25	0	0
4	E	6	Total O 6 6	0	0
4	F	7	Total O 7 7	0	0
4	G	9	Total O 9 9	0	0
4	H	4	Total O 4 4	0	0
4	I	5	Total O 5 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

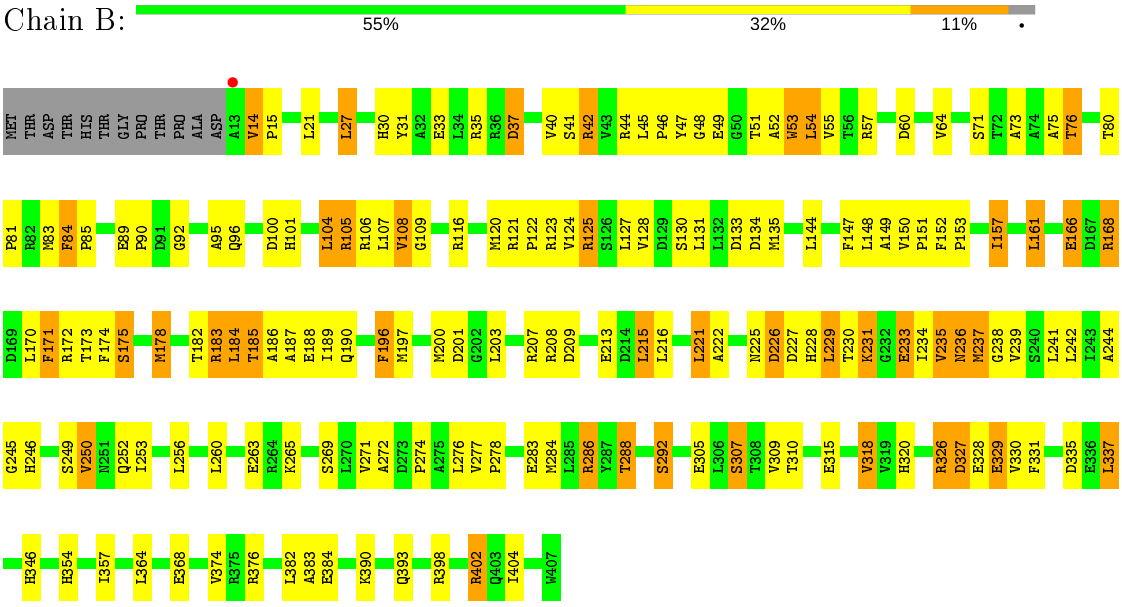
- Molecule 1: Cytochrome P-450

Chain A:



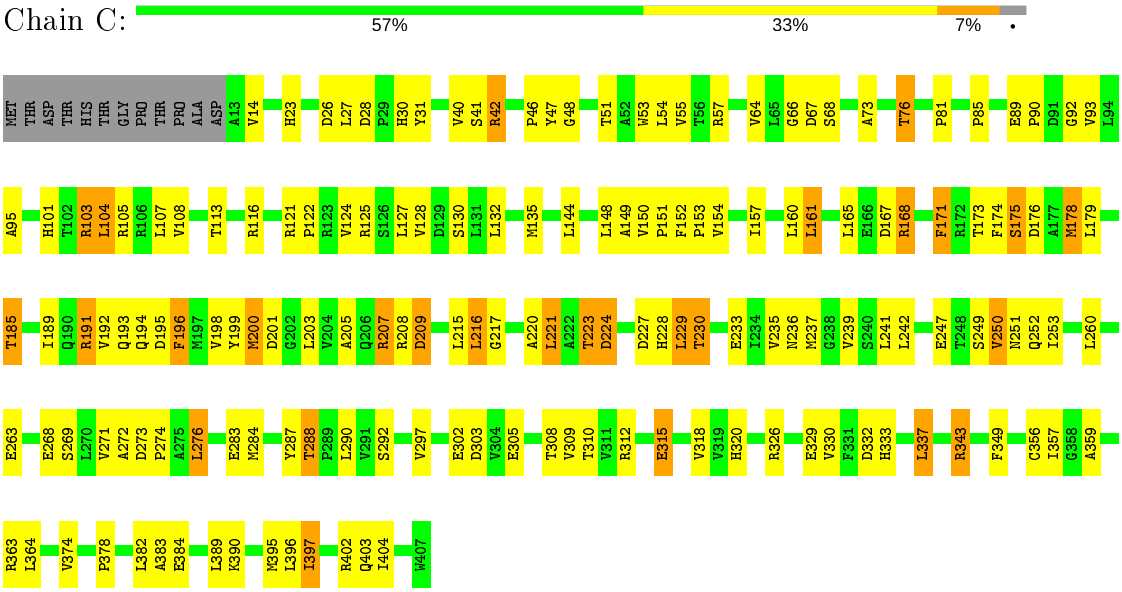
- Molecule 1: Cytochrome P-450

Chain B:



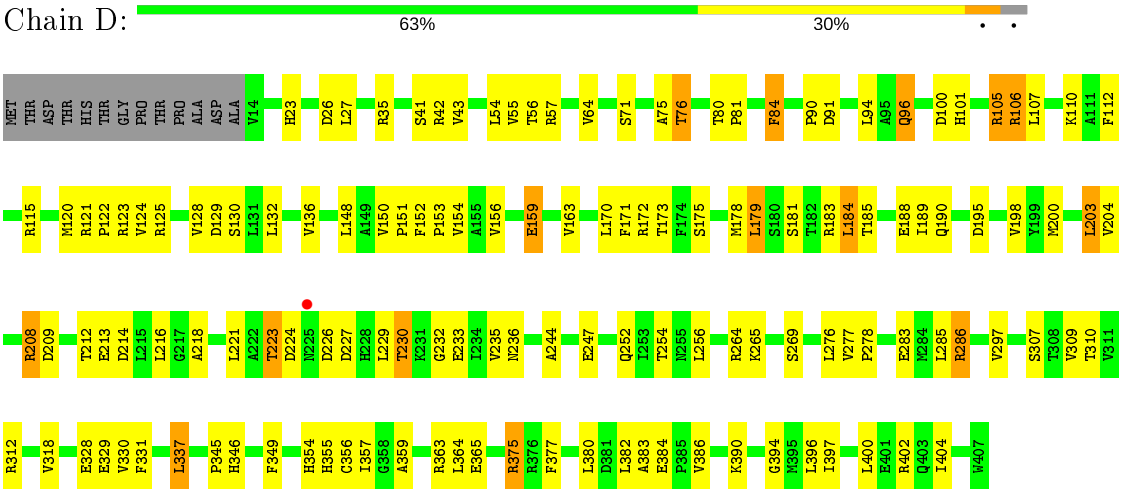
- Molecule 1: Cytochrome P-450

Chain C:



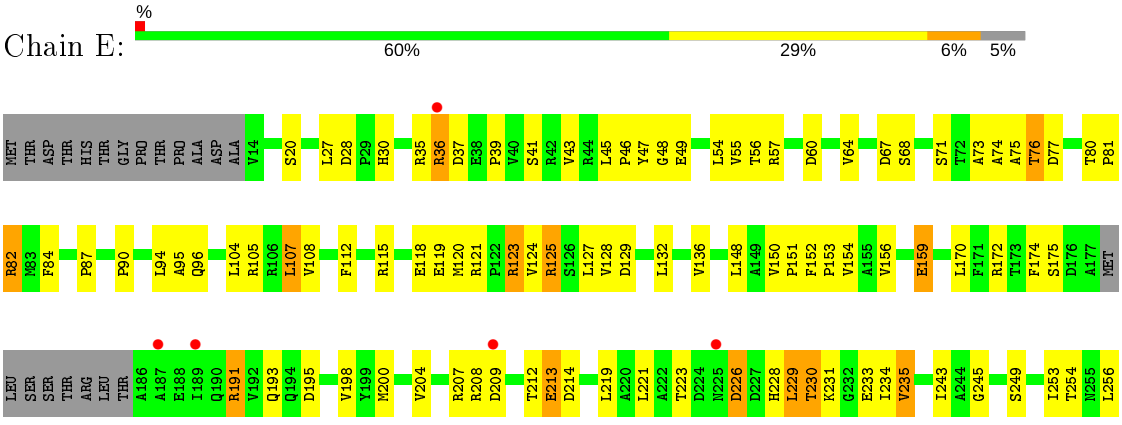
• Molecule 1: Cytochrome P-450

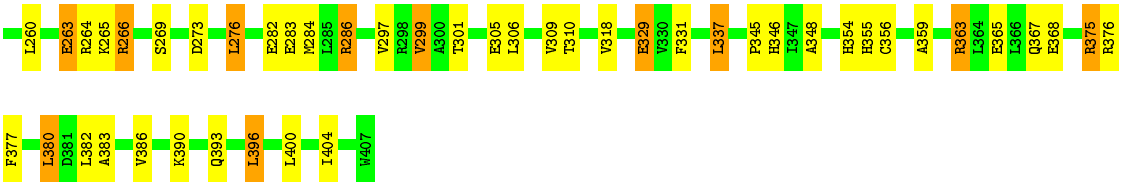
Chain D:



• Molecule 1: Cytochrome P-450

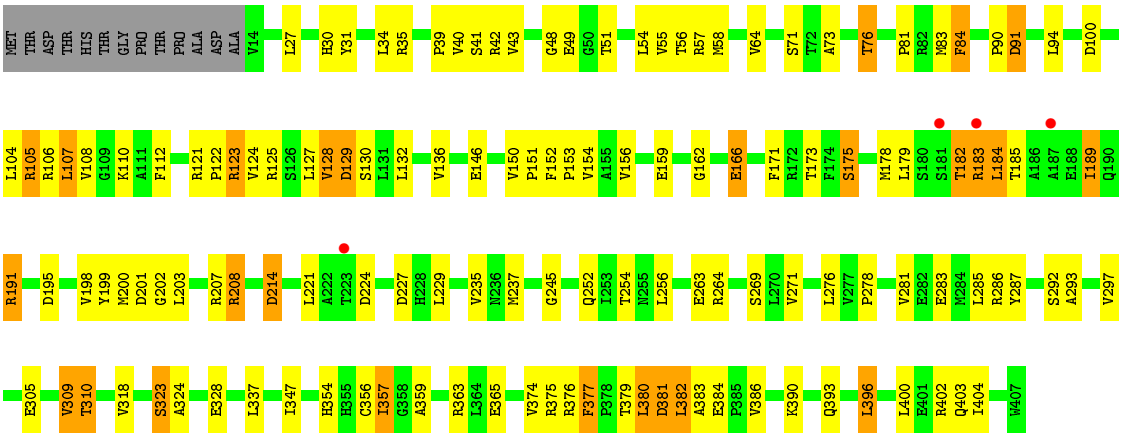
Chain E:





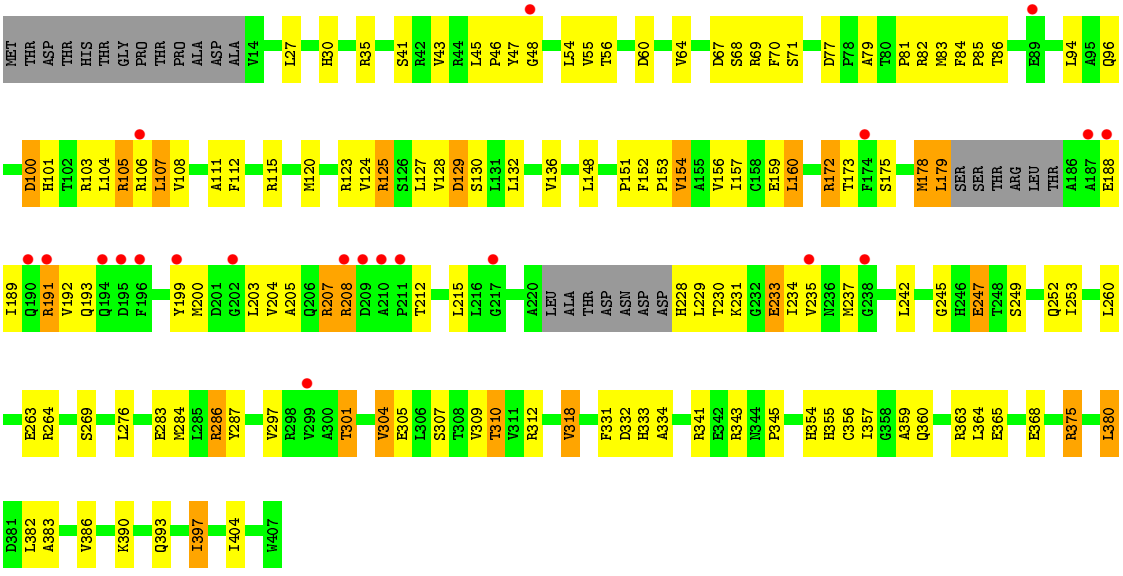
• Molecule 1: Cytochrome P-450

Chain F:



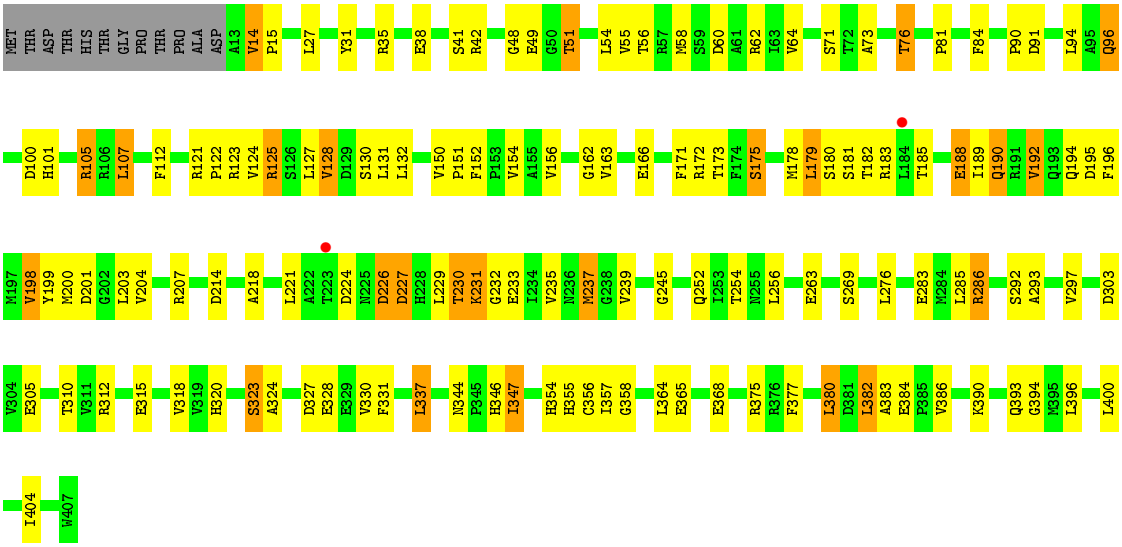
• Molecule 1: Cytochrome P-450

Chain G:



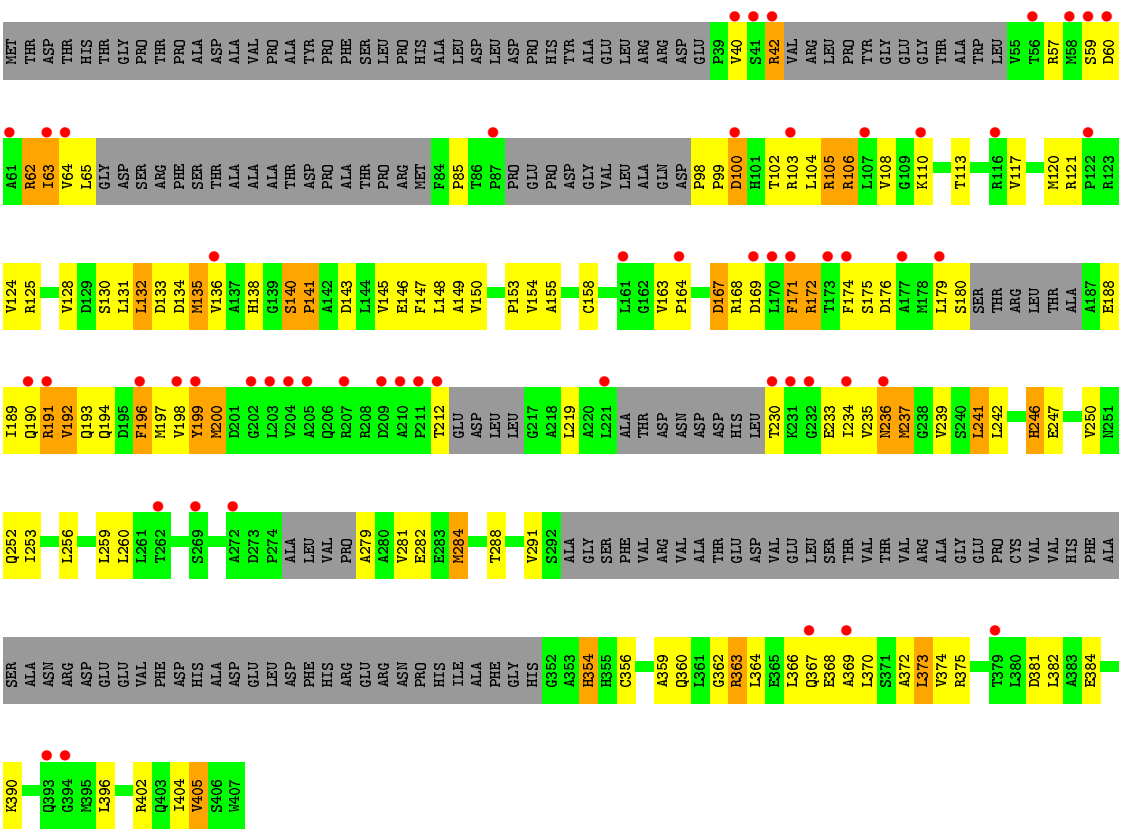
• Molecule 1: Cytochrome P-450

Chain H:



- Molecule 1: Cytochrome P-450

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	112.07Å 116.64Å 125.17Å 104.43° 104.25° 113.91°	Depositor
Resolution (Å)	39.89 – 2.93 39.89 – 2.93	Depositor EDS
% Data completeness (in resolution range)	84.2 (39.89-2.93) 84.2 (39.89-2.93)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.57 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.239 , 0.291 0.240 , 0.289	Depositor DCC
R_{free} test set	4684 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 40.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.015 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	27067	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: QR8, HEM

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	0.74	0/3140	0.93	1/4277 (0.0%)
1	B	0.70	0/3145	0.93	1/4284 (0.0%)
1	C	0.72	1/3145 (0.0%)	0.91	1/4284 (0.0%)
1	D	0.73	0/3134	0.90	2/4270 (0.0%)
1	E	0.68	0/3078	0.87	2/4192 (0.0%)
1	F	0.67	0/3140	0.87	0/4277
1	G	0.67	0/3041	0.85	1/4138 (0.0%)
1	H	0.67	0/3145	0.87	1/4284 (0.0%)
1	I	0.84	2/1942 (0.1%)	0.92	2/2622 (0.1%)
All	All	0.71	3/26910 (0.0%)	0.89	11/36628 (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	B	0	1
1	D	0	1
1	H	0	1
1	I	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	141	PRO	C-O	-17.84	0.87	1.23
1	I	212	THR	C-O	5.61	1.34	1.23
1	C	268	GLU	CD-OE2	5.09	1.31	1.25

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	141	PRO	O-C-N	15.29	147.17	122.70
1	I	141	PRO	CA-C-O	-9.18	98.17	120.20
1	E	363	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	E	363	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	A	57	ARG	NE-CZ-NH1	6.90	123.75	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	394	GLY	Peptide
1	B	402	ARG	Sidechain
1	D	394	GLY	Peptide
1	H	394	GLY	Peptide
1	I	140	SER	Peptide

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	3073	0	3051	103	0
1	B	3078	0	3056	159	0
1	C	3078	0	3057	115	0
1	D	3067	0	3041	79	0
1	E	3012	0	2983	114	0
1	F	3073	0	3052	95	0
1	G	2976	0	2961	94	0
1	H	3078	0	3057	120	0
1	I	1915	0	1945	123	0
2	A	43	0	30	12	0
2	B	43	0	30	5	0
2	C	43	0	30	3	0
2	D	43	0	30	9	0
2	E	43	0	30	15	0
2	F	43	0	30	11	0
2	G	43	0	30	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	43	0	30	13	0
2	I	43	0	30	6	0
3	A	26	0	0	10	0
3	B	26	0	0	2	0
3	C	26	0	0	1	0
3	D	26	0	0	4	0
3	E	26	0	0	5	0
3	F	26	0	0	4	0
3	G	26	0	0	4	0
3	H	26	0	0	4	0
3	I	26	0	0	5	0
4	A	19	0	0	2	0
4	B	7	0	0	1	0
4	C	14	0	0	1	0
4	D	25	0	0	1	0
4	E	6	0	0	1	0
4	F	7	0	0	2	0
4	G	9	0	0	0	0
4	H	4	0	0	0	0
4	I	5	0	0	1	0
All	All	27067	0	26473	1030	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 19.

The worst 5 of 1030 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:135:MET:CE	1:I:147:PHE:HB2	1.71	1.20
1:B:185:THR:HG21	1:H:166:GLU:OE1	0.99	1.16
1:F:185:THR:O	1:F:189:ILE:HG22	1.45	1.16
1:D:185:THR:HB	1:D:188:GLU:HB2	1.18	1.14
1:B:185:THR:CG2	1:H:166:GLU:OE1	1.94	1.14

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	392/407 (96%)	380 (97%)	12 (3%)	0	100	100
1	B	393/407 (97%)	374 (95%)	19 (5%)	0	100	100
1	C	393/407 (97%)	382 (97%)	11 (3%)	0	100	100
1	D	392/407 (96%)	381 (97%)	11 (3%)	0	100	100
1	E	382/407 (94%)	370 (97%)	12 (3%)	0	100	100
1	F	392/407 (96%)	374 (95%)	18 (5%)	0	100	100
1	G	375/407 (92%)	365 (97%)	10 (3%)	0	100	100
1	H	393/407 (97%)	379 (96%)	14 (4%)	0	100	100
1	I	230/407 (56%)	219 (95%)	11 (5%)	0	100	100
All	All	3342/3663 (91%)	3224 (96%)	118 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/341 (97%)	281 (85%)	50 (15%)	3	8
1	B	331/341 (97%)	255 (77%)	76 (23%)	1	2
1	C	331/341 (97%)	279 (84%)	52 (16%)	2	7
1	D	330/341 (97%)	276 (84%)	54 (16%)	2	6
1	E	323/341 (95%)	268 (83%)	55 (17%)	2	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	331/341 (97%)	278 (84%)	53 (16%)	2 7
1	G	319/341 (94%)	268 (84%)	51 (16%)	2 7
1	H	331/341 (97%)	281 (85%)	50 (15%)	3 8
1	I	205/341 (60%)	165 (80%)	40 (20%)	1 3
All	All	2832/3069 (92%)	2351 (83%)	481 (17%)	2 5

5 of 481 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	269	SER
1	E	276	LEU
1	I	62	ARG
1	D	318	VAL
1	E	112	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	194	GLN
1	F	236	ASN
1	H	344	ASN
1	F	228	HIS
1	F	354	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 monosaccharides 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	$\#\|Z\| > 2$
2	HEM	D	501	4	27,50,50	1.11	1 (3%)	17,82,82	1.36	3 (17%)
3	QR8	G	502	-	26,26,26	1.59	5 (19%)	35,38,38	1.77	9 (25%)
2	HEM	B	501	1	27,50,50	1.26	4 (14%)	17,82,82	1.72	5 (29%)
3	QR8	A	502	-	26,26,26	1.79	7 (26%)	35,38,38	2.22	12 (34%)
3	QR8	C	502	-	26,26,26	1.71	6 (23%)	35,38,38	2.23	9 (25%)
3	QR8	B	502	-	26,26,26	2.01	7 (26%)	35,38,38	1.82	6 (17%)
2	HEM	A	501	1,4	27,50,50	1.36	4 (14%)	17,82,82	1.20	1 (5%)
3	QR8	I	502	1	26,26,26	1.32	3 (11%)	35,38,38	2.12	9 (25%)
2	HEM	H	501	4	27,50,50	1.11	2 (7%)	17,82,82	1.22	1 (5%)
2	HEM	I	501	1	27,50,50	0.98	2 (7%)	17,82,82	1.58	2 (11%)
3	QR8	D	502	-	26,26,26	1.70	5 (19%)	35,38,38	2.45	11 (31%)
2	HEM	G	501	-	27,50,50	0.98	1 (3%)	17,82,82	1.31	3 (17%)
3	QR8	F	502	-	26,26,26	1.59	5 (19%)	35,38,38	1.94	12 (34%)
2	HEM	E	501	-	27,50,50	1.47	3 (11%)	17,82,82	1.19	1 (5%)
2	HEM	C	501	1	27,50,50	1.05	2 (7%)	17,82,82	2.39	5 (29%)
3	QR8	H	502	-	26,26,26	1.60	4 (15%)	35,38,38	2.40	12 (34%)
2	HEM	F	501	4	27,50,50	1.03	2 (7%)	17,82,82	1.38	2 (11%)
3	QR8	E	502	-	26,26,26	1.51	2 (7%)	35,38,38	2.52	15 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	501	4	-	0/6/54/54	-
3	QR8	G	502	-	-	19/48/48/48	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	501	1	-	0/6/54/54	-
3	QR8	A	502	-	-	18/48/48/48	0/1/1/1
3	QR8	C	502	-	-	23/48/48/48	0/1/1/1
3	QR8	B	502	-	-	24/48/48/48	0/1/1/1
2	HEM	A	501	1,4	-	0/6/54/54	-
3	QR8	I	502	1	-	16/48/48/48	0/1/1/1
2	HEM	H	501	4	-	0/6/54/54	-
2	HEM	I	501	1	-	2/6/54/54	-
3	QR8	D	502	-	-	25/48/48/48	0/1/1/1
2	HEM	G	501	-	-	0/6/54/54	-
3	QR8	F	502	-	-	27/48/48/48	0/1/1/1
2	HEM	E	501	-	-	0/6/54/54	-
2	HEM	C	501	1	-	2/6/54/54	-
3	QR8	H	502	-	-	20/48/48/48	0/1/1/1
2	HEM	F	501	4	-	0/6/54/54	-
3	QR8	E	502	-	2/2/12/12	29/48/48/48	1/1/1/1

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	HEM	C3B-C2B	-5.36	1.32	1.40
3	E	502	QR8	O2-C1	-5.26	1.22	1.34
3	B	502	QR8	O2-C13	-4.84	1.38	1.46
3	G	502	QR8	O2-C1	4.68	1.45	1.34
3	A	502	QR8	C10-C9	-4.57	1.45	1.52

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	502	QR8	C13-O2-C1	-8.04	105.86	117.51
3	H	502	QR8	C35-C12-C13	-6.25	104.10	112.18
2	C	501	HEM	CAA-CBA-CGA	-6.16	102.33	112.67
3	H	502	QR8	C6-C5-C4	-5.97	107.02	116.27
3	E	502	QR8	O2-C1-C2	5.70	124.08	111.56

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	E	502	QR8	C8
3	E	502	QR8	C11

5 of 205 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	QR8	C10-C11-C12-C35
3	A	502	QR8	C10-C11-C12-C13
3	A	502	QR8	O12-C11-C12-C13
3	A	502	QR8	C11-C12-C13-O2
3	A	502	QR8	C35-C12-C13-O2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	502	QR8	C1-C10-C11-C12-C13-C2-C3-C4-C5-C6-C7-C8-C9-O2

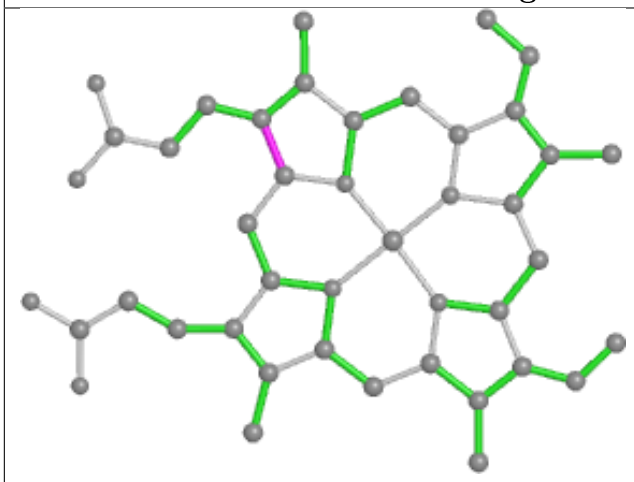
18 monomers are involved in 116 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	HEM	9	0
3	G	502	QR8	4	0
2	B	501	HEM	5	0
3	A	502	QR8	10	0
3	C	502	QR8	1	0
3	B	502	QR8	2	0
2	A	501	HEM	12	0
3	I	502	QR8	5	0
2	H	501	HEM	13	0
2	I	501	HEM	6	0
3	D	502	QR8	4	0
2	G	501	HEM	9	0
3	F	502	QR8	4	0
2	E	501	HEM	15	0
2	C	501	HEM	3	0
3	H	502	QR8	4	0
2	F	501	HEM	11	0
3	E	502	QR8	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEM D 501



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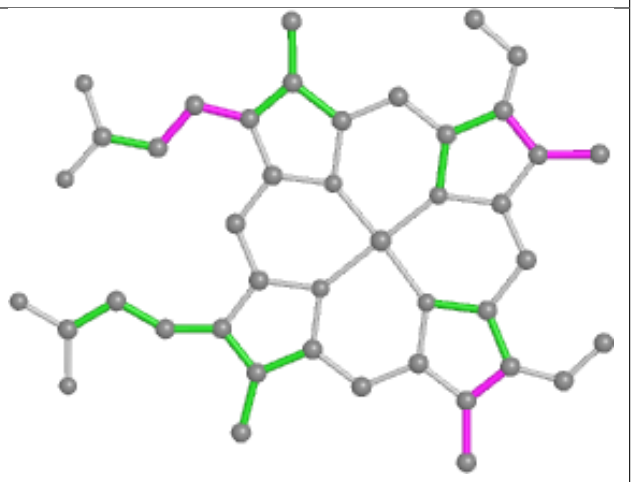

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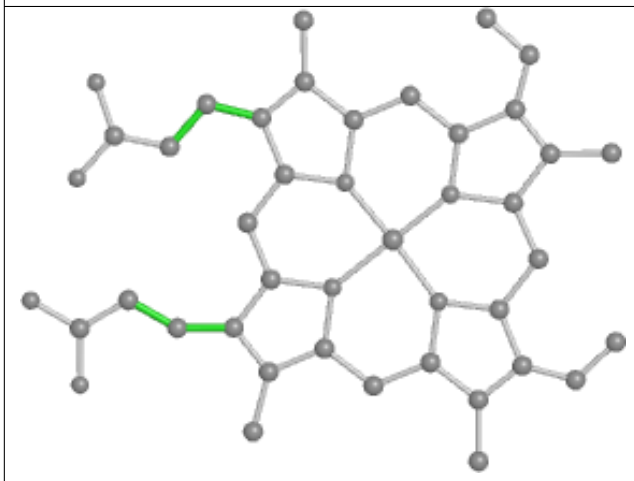

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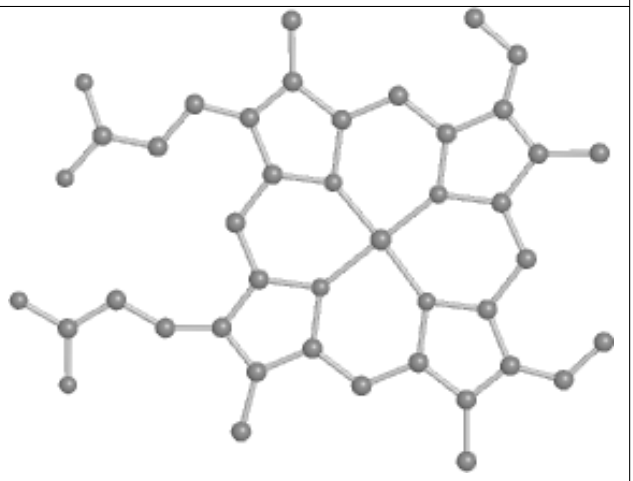
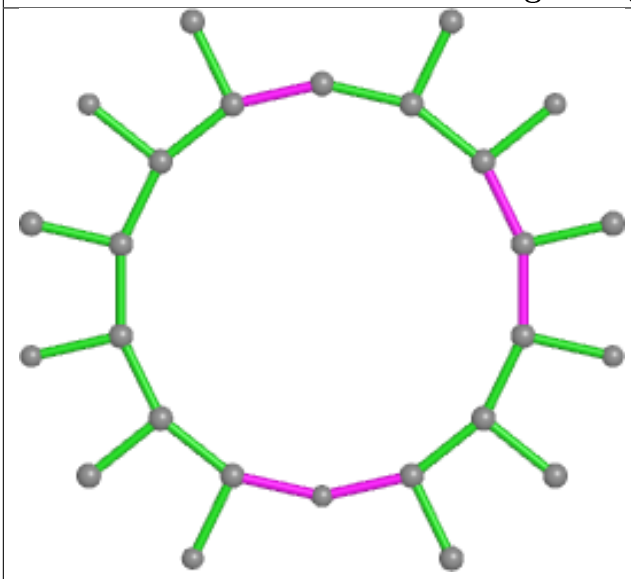


Rings

Ligand QR8 G 502



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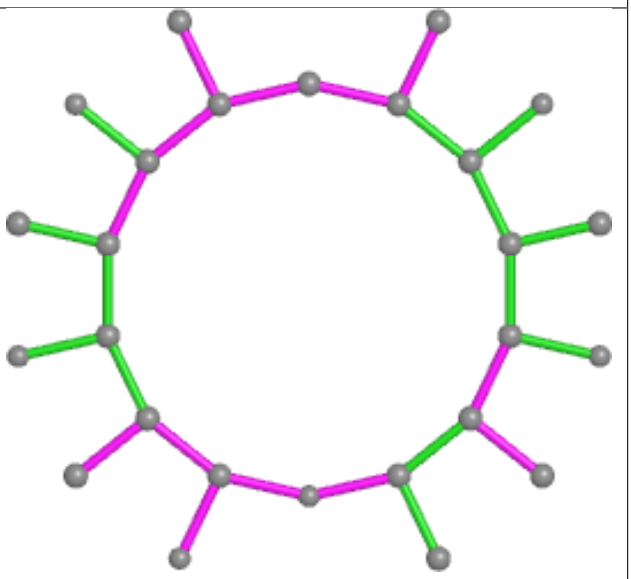

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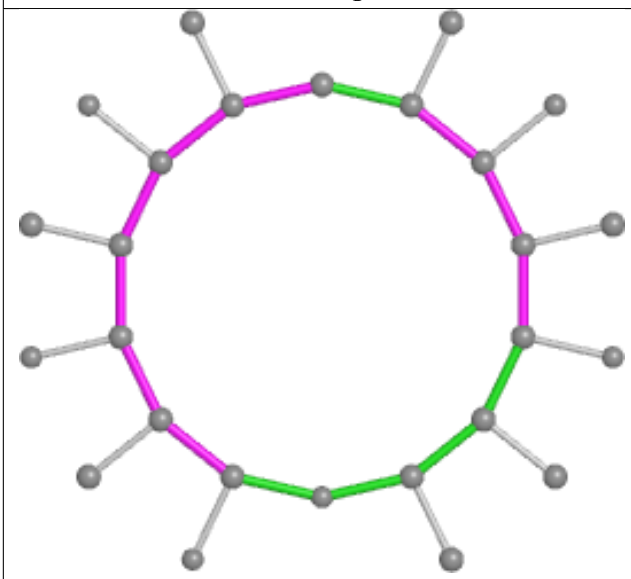

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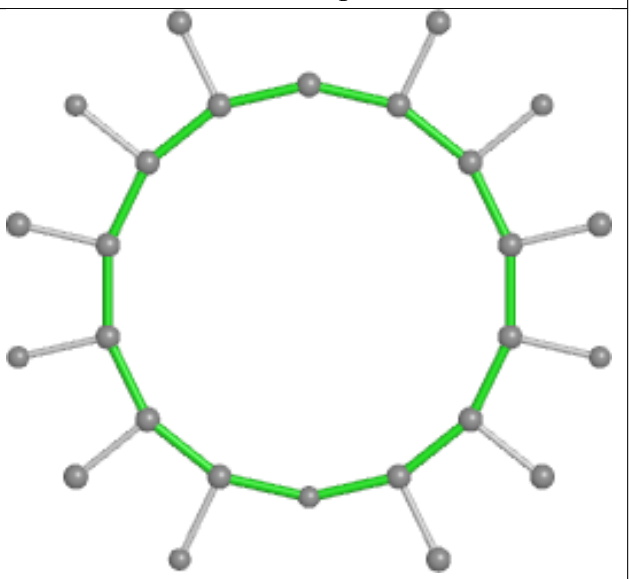
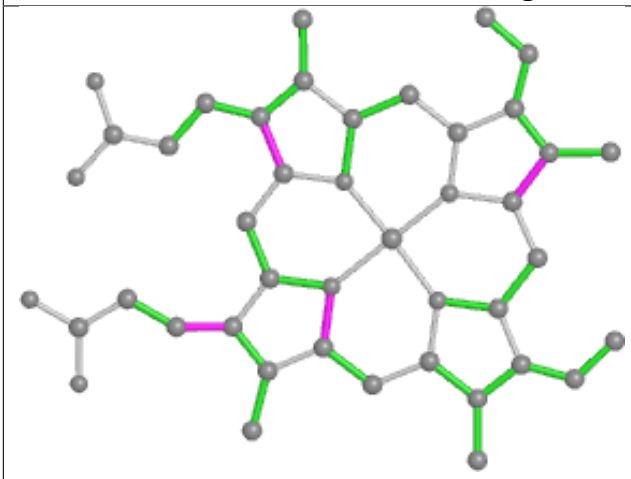


Rings

Ligand HEM B 501



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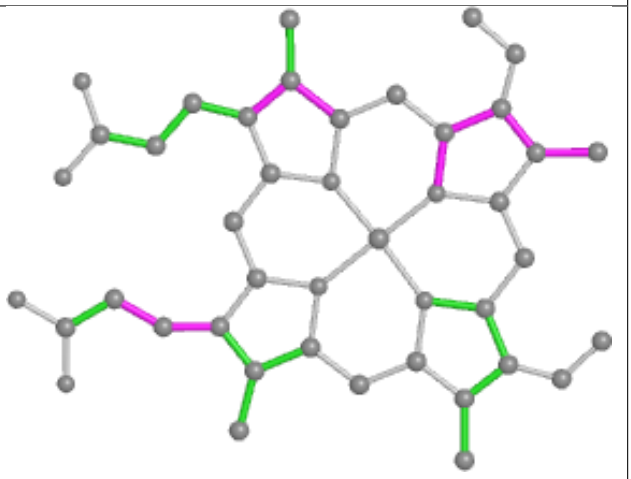

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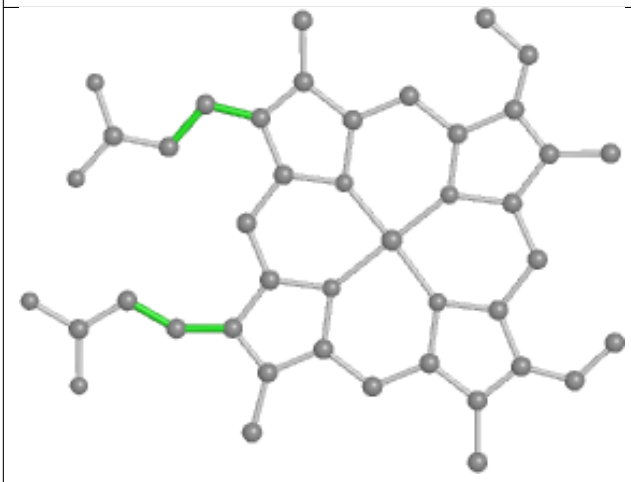

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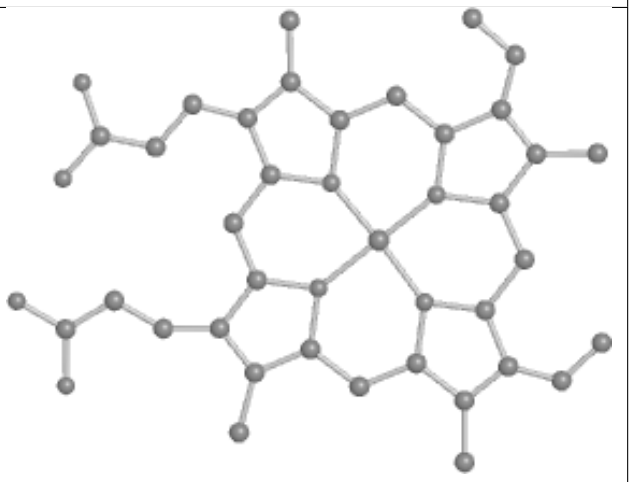
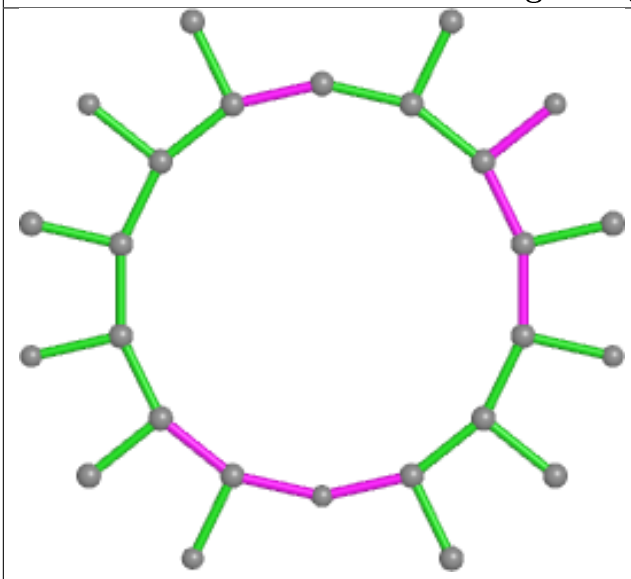


Rings

Ligand QR8 A 502



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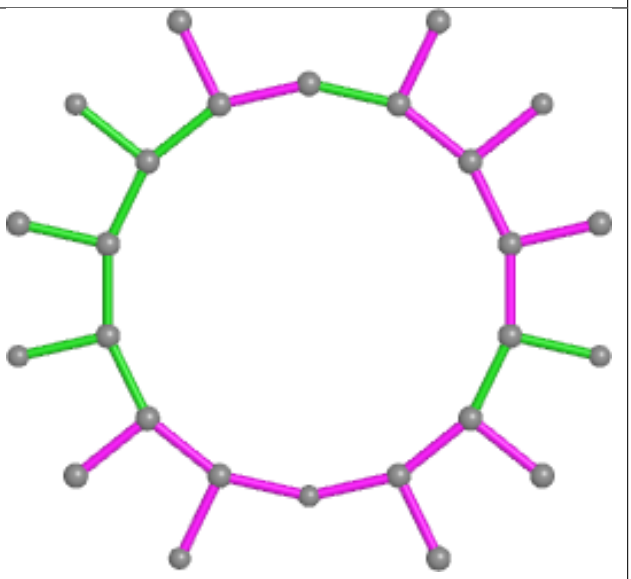

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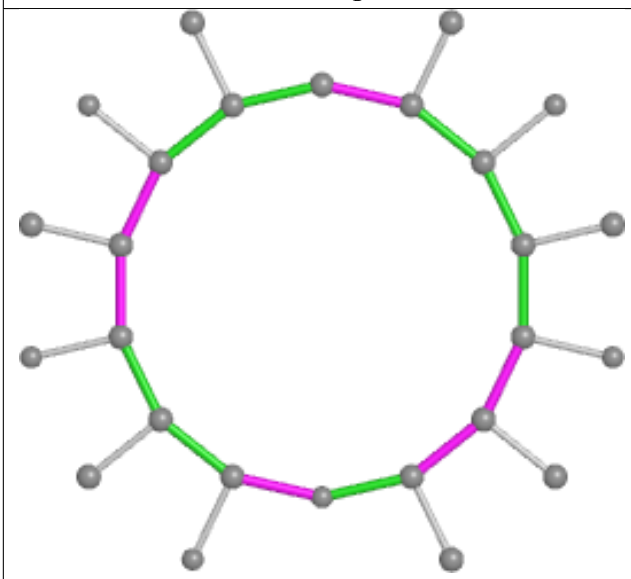

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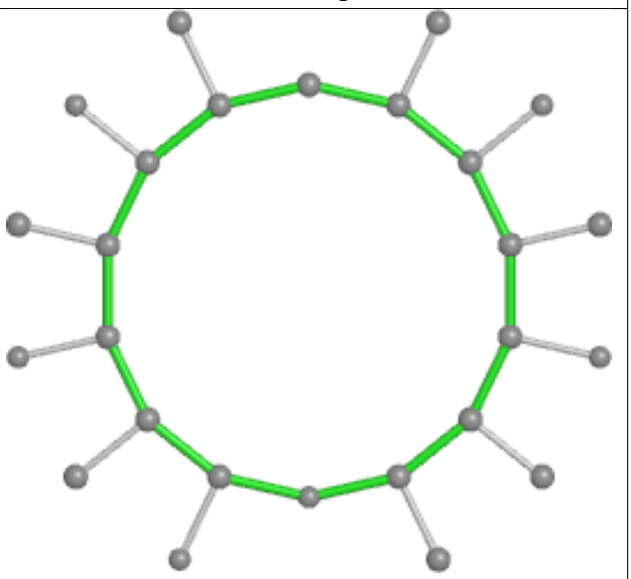
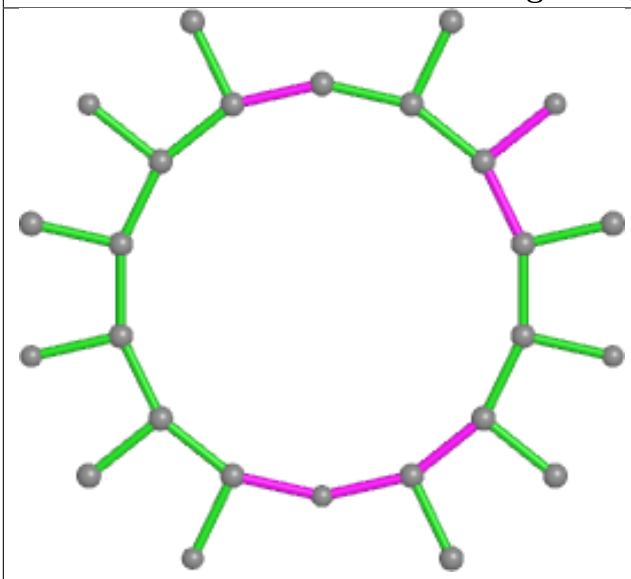


Rings

Ligand QR8 C 502



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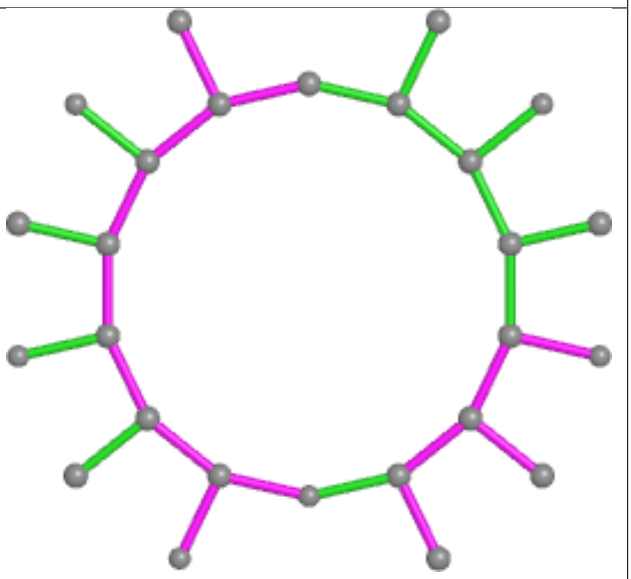

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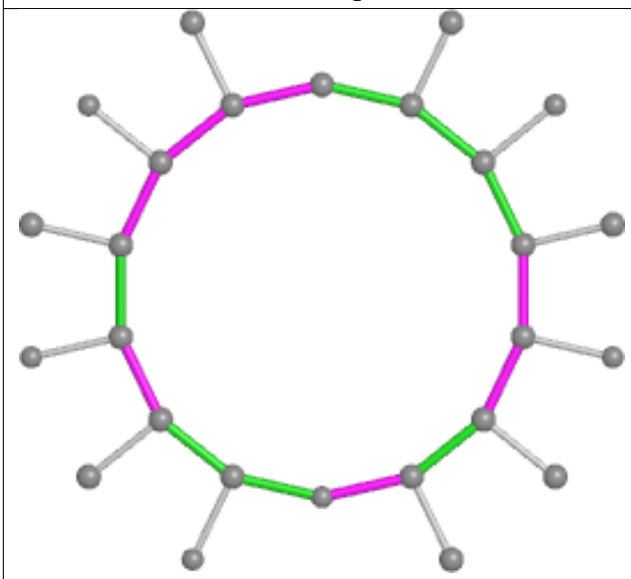

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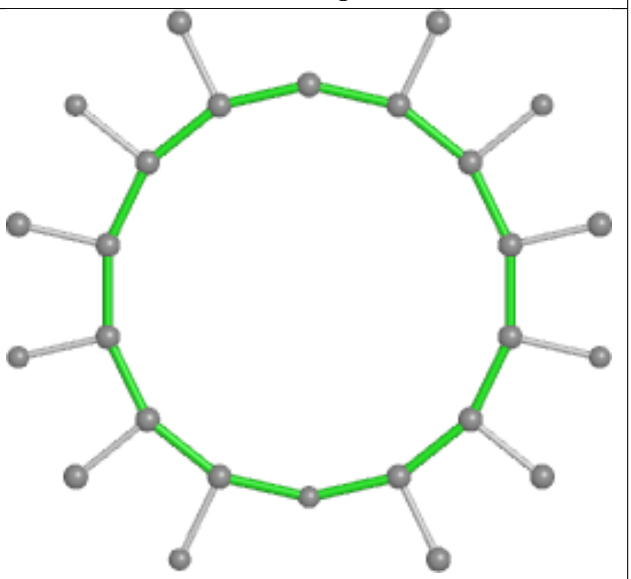
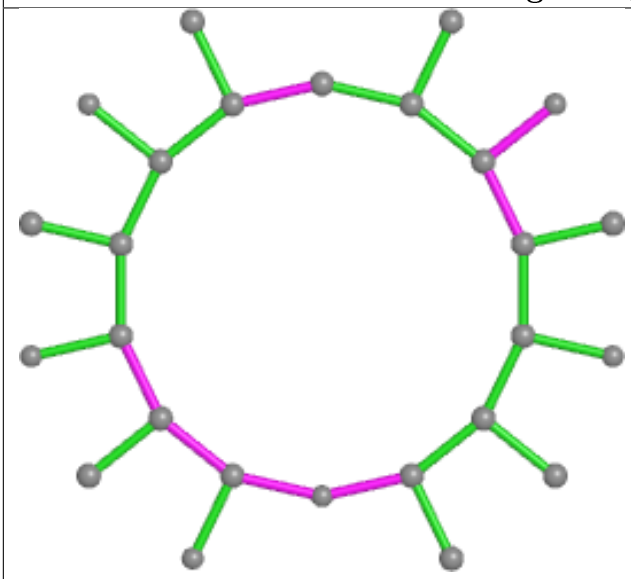


Rings

Ligand QR8 B 502



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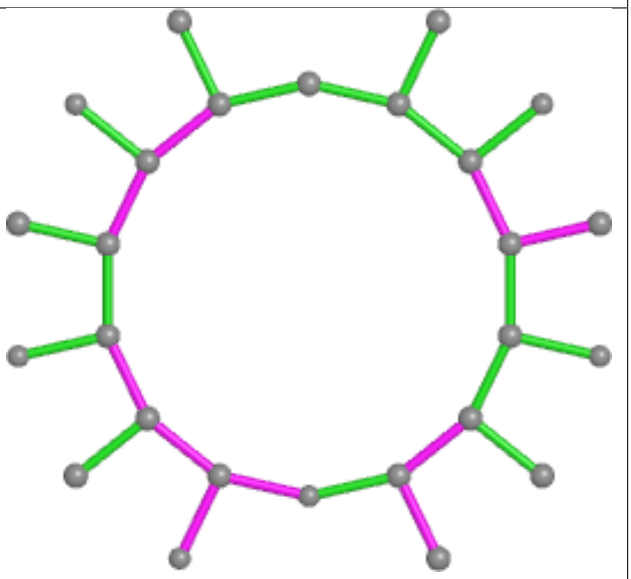

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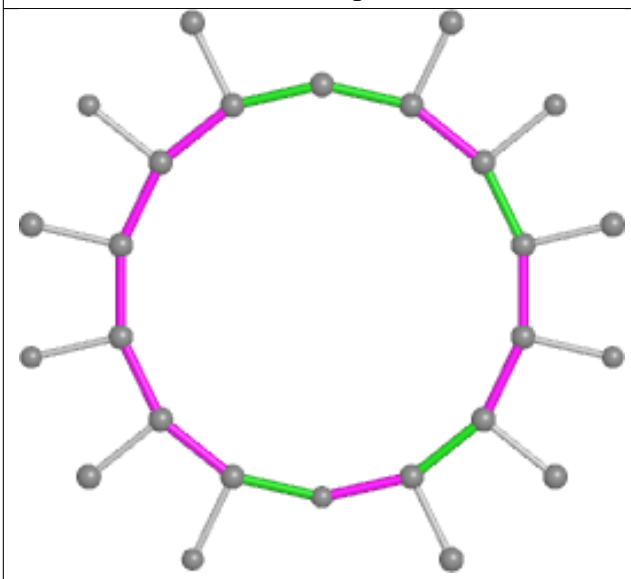

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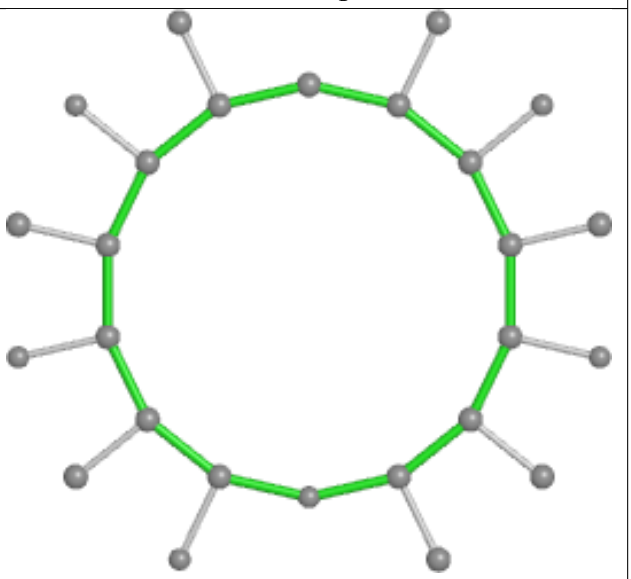
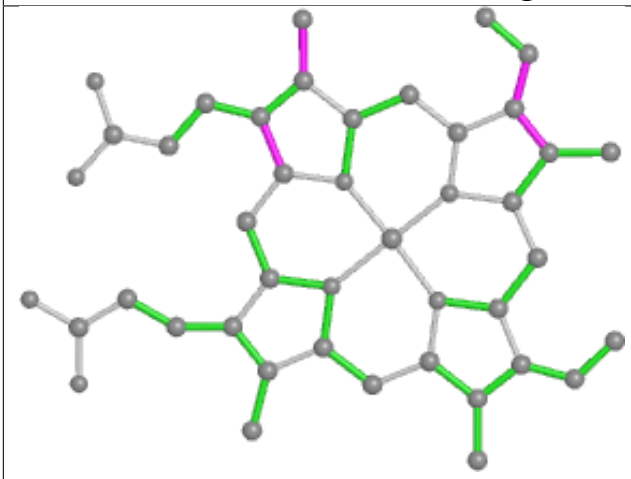


Rings

Ligand HEM A 501



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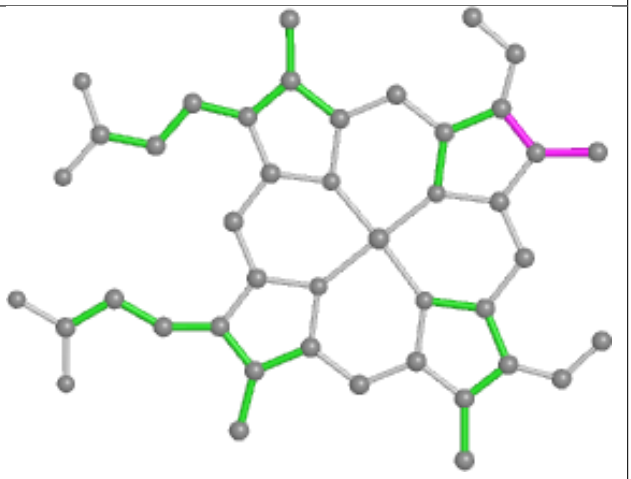

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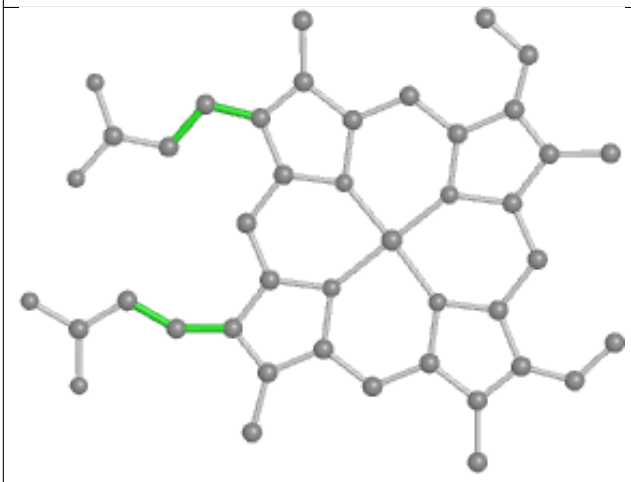

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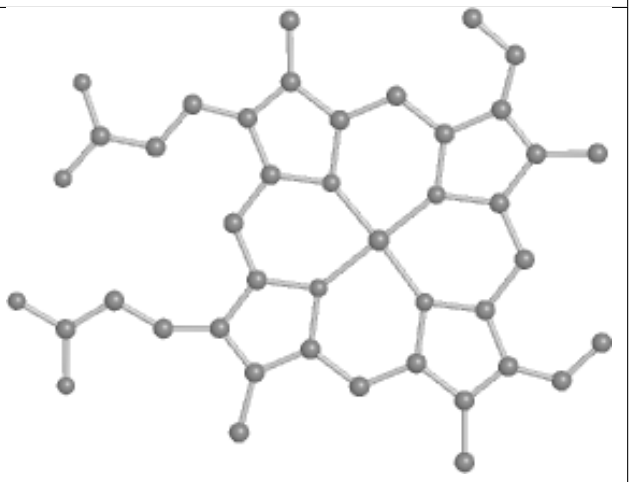
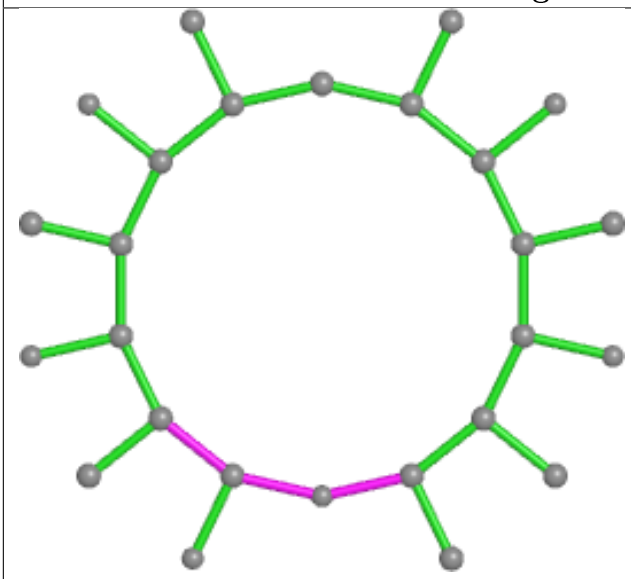


Rings

Ligand QR8 I 502



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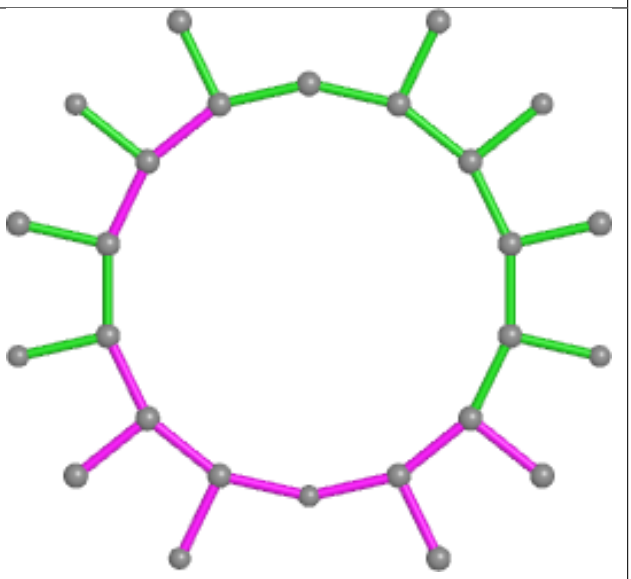

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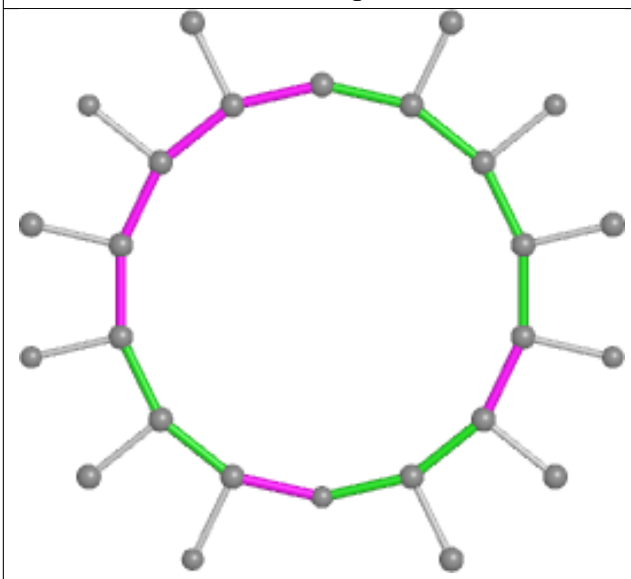

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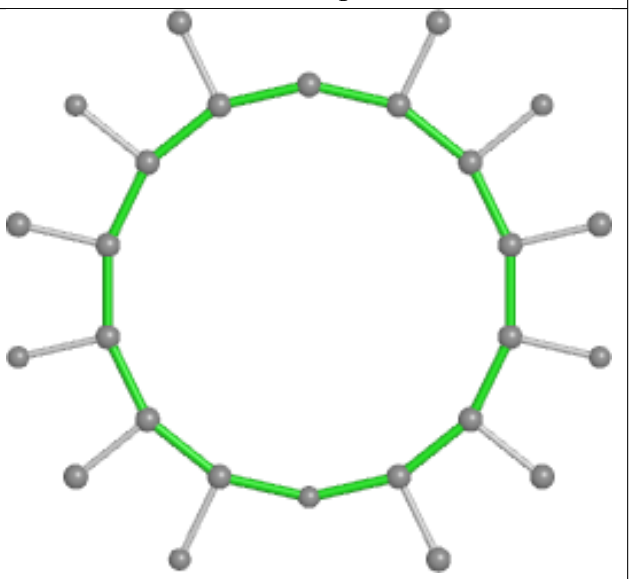
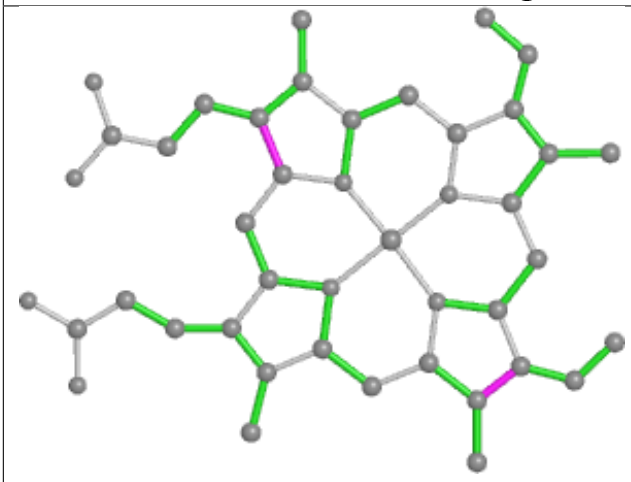


Rings

Ligand HEM H 501



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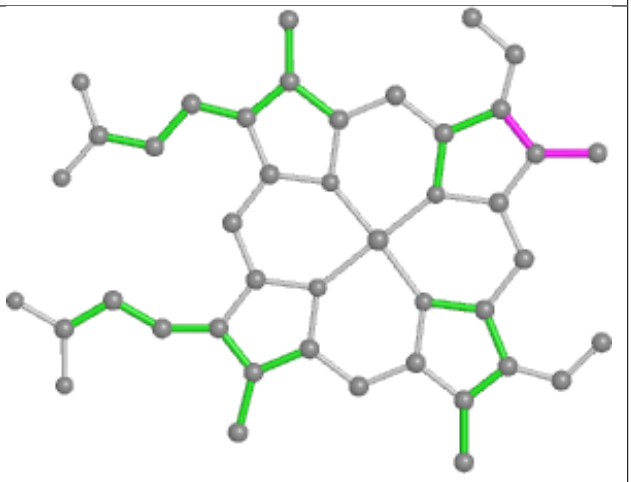

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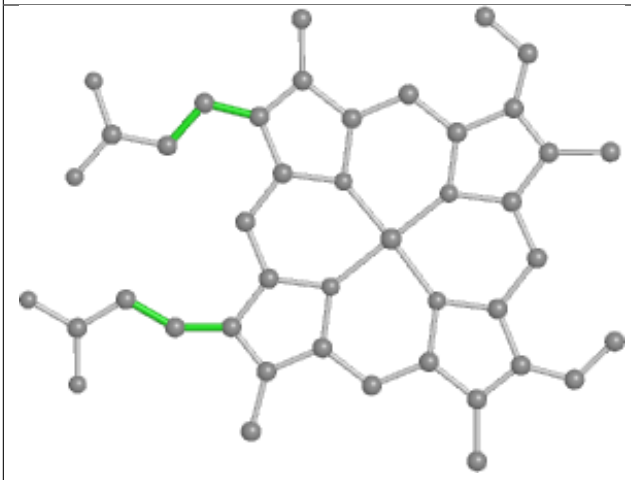

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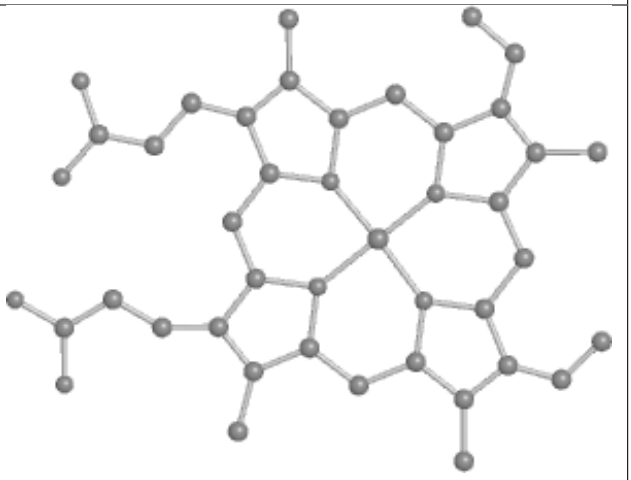
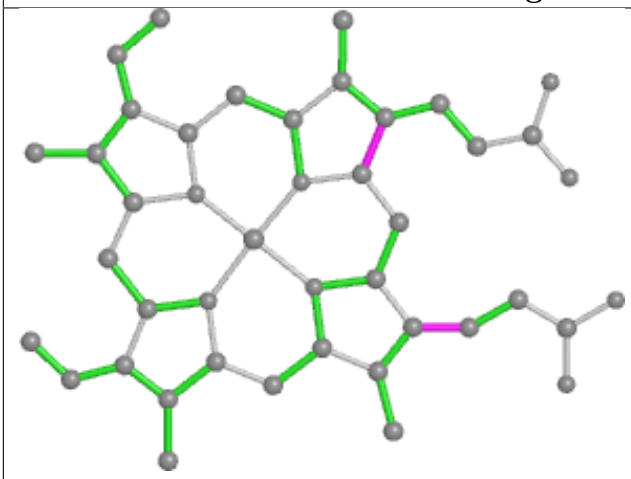


Rings

Ligand HEM I 501



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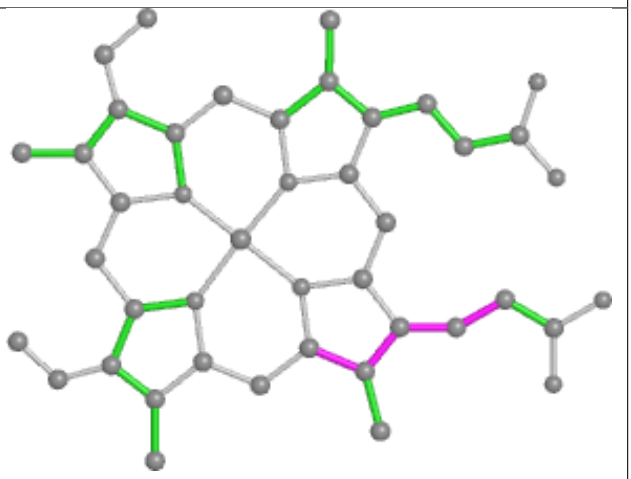
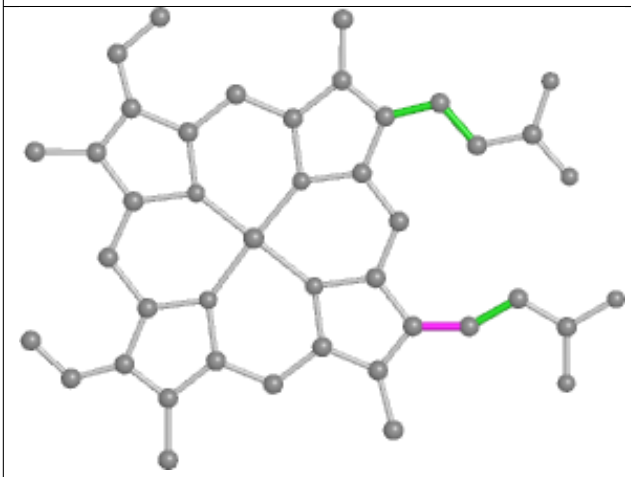
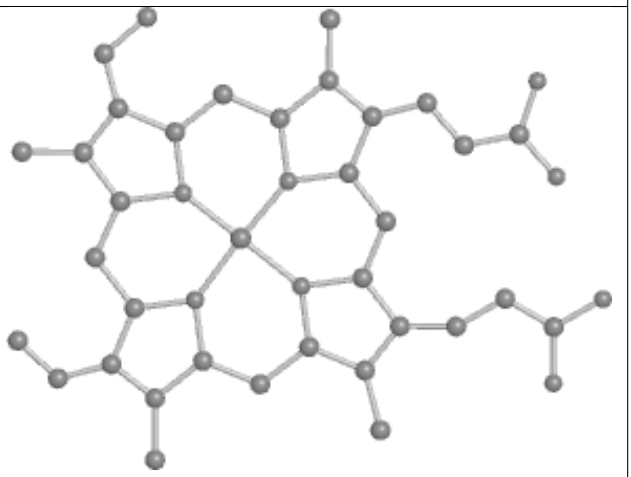


Bond angles

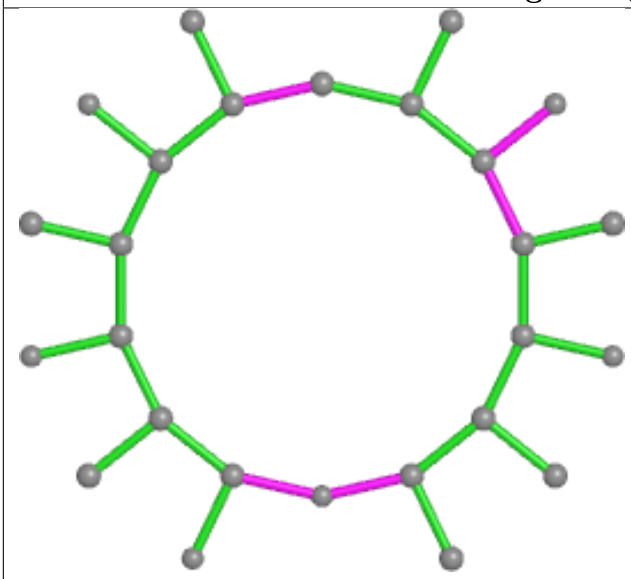


Torsions

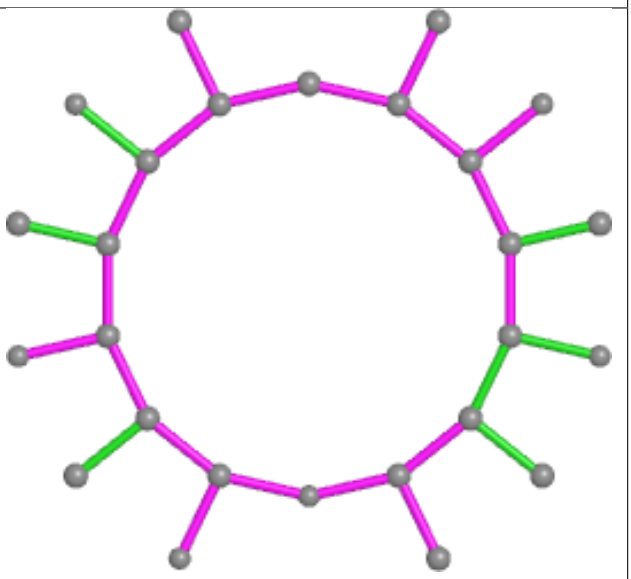


Rings

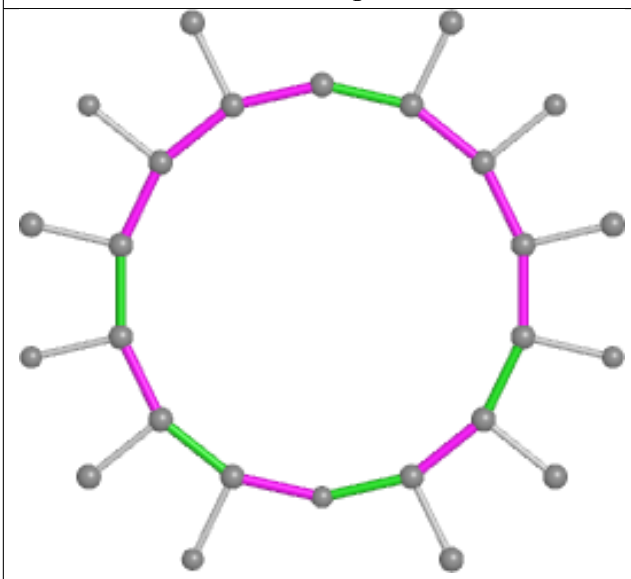
Ligand QR8 D 502



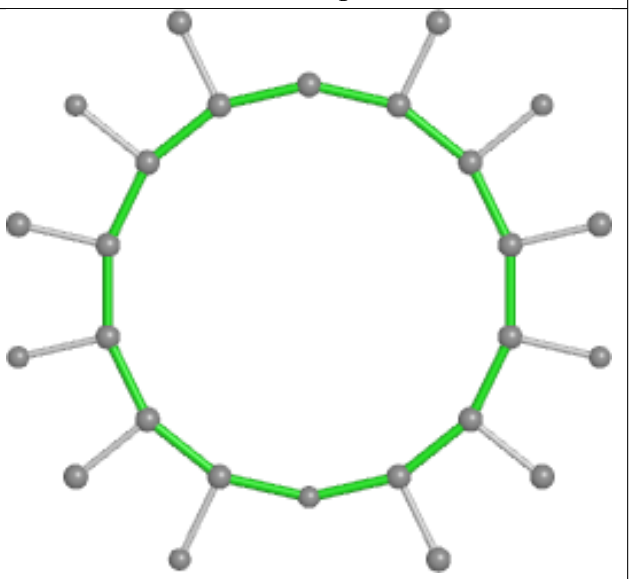
Bond lengths



Bond angles

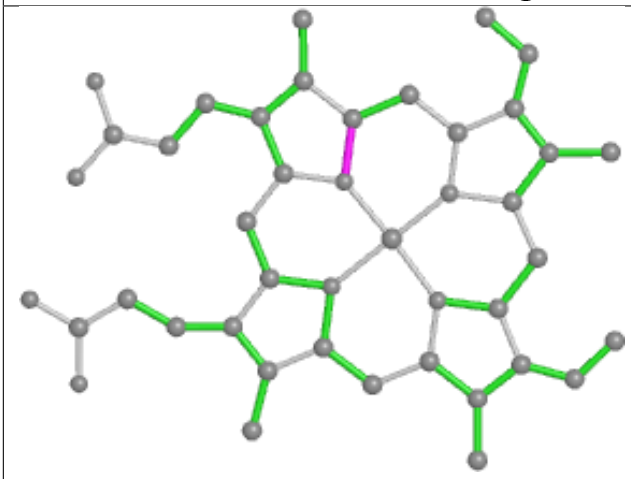


Torsions

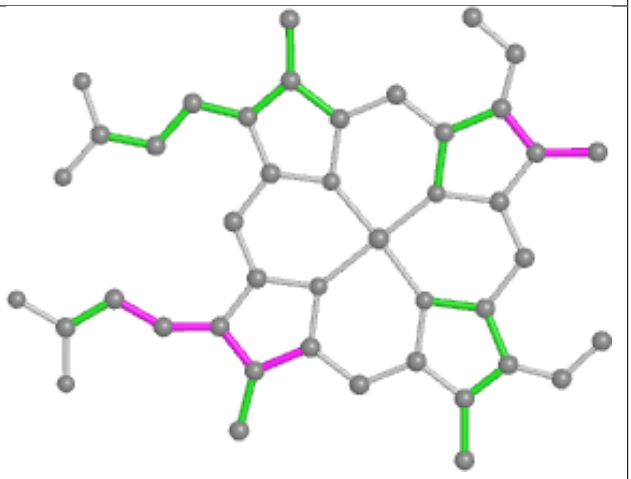


Rings

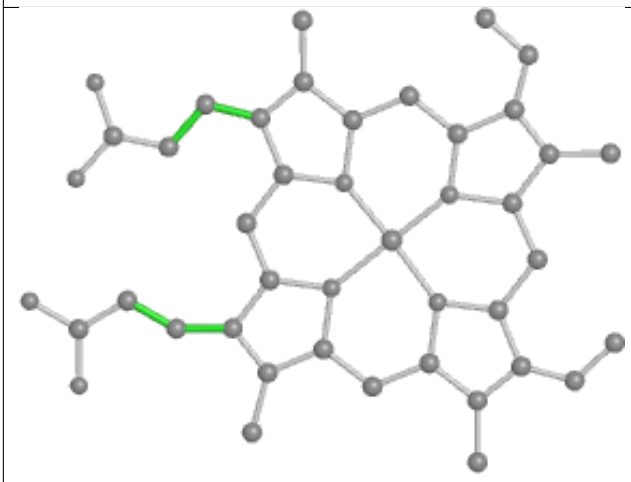
Ligand HEM G 501



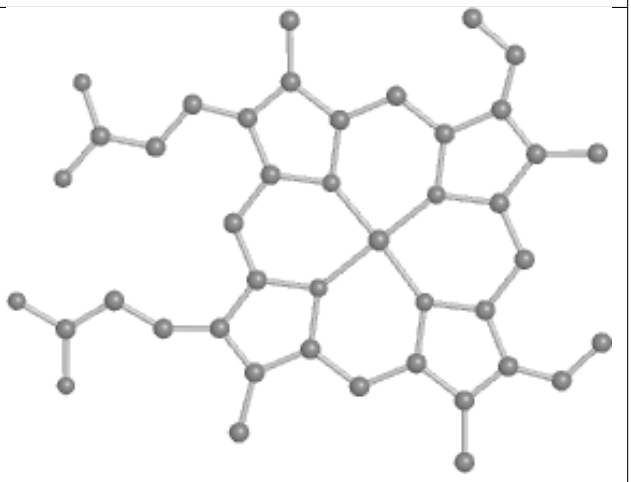
Bond lengths



Bond angles

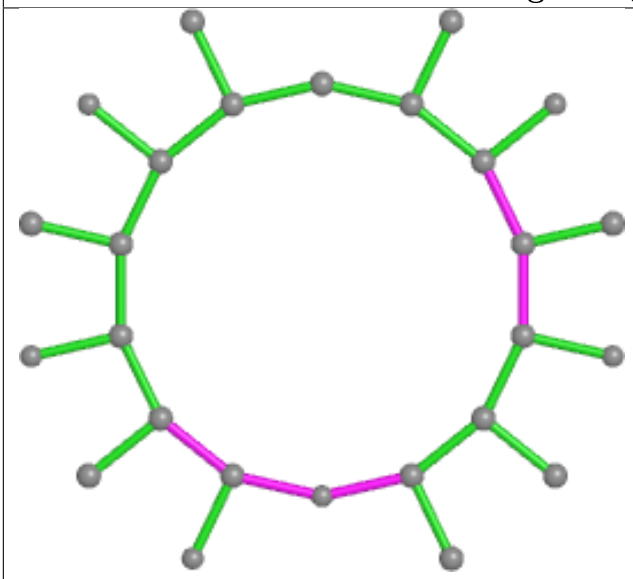


Torsions

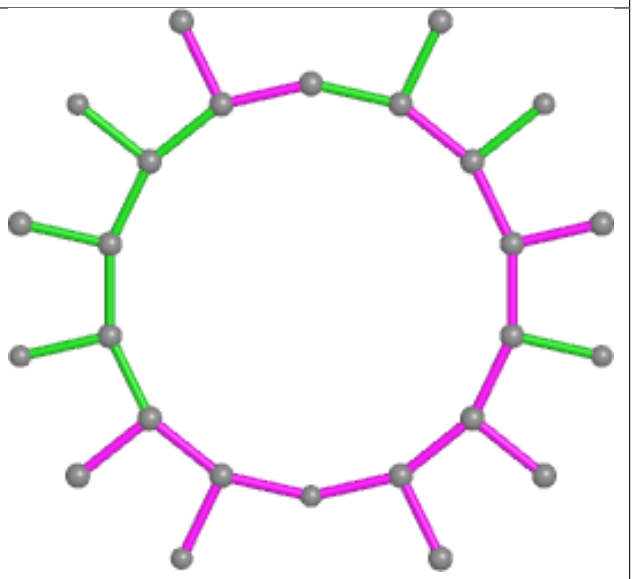


Rings

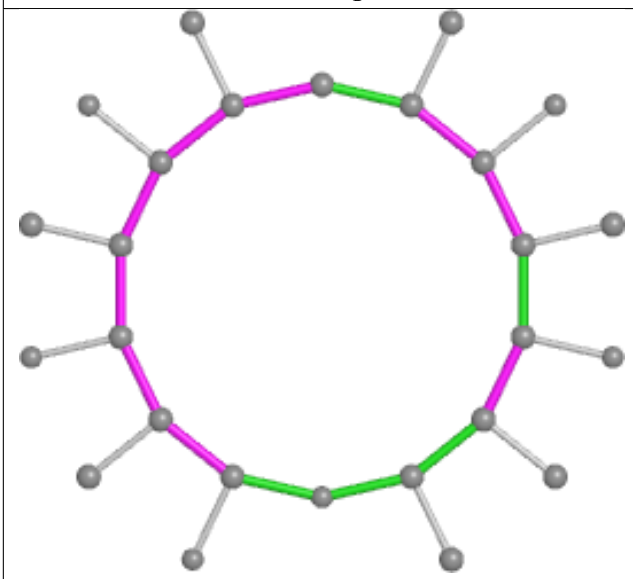
Ligand QR8 F 502



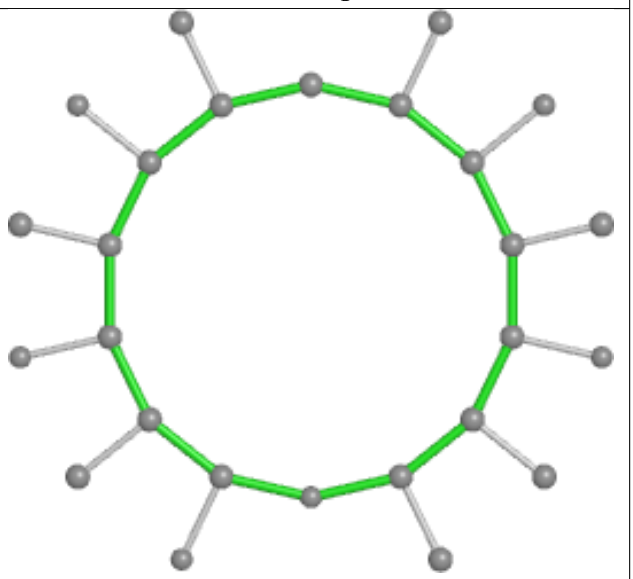
Bond lengths



Bond angles

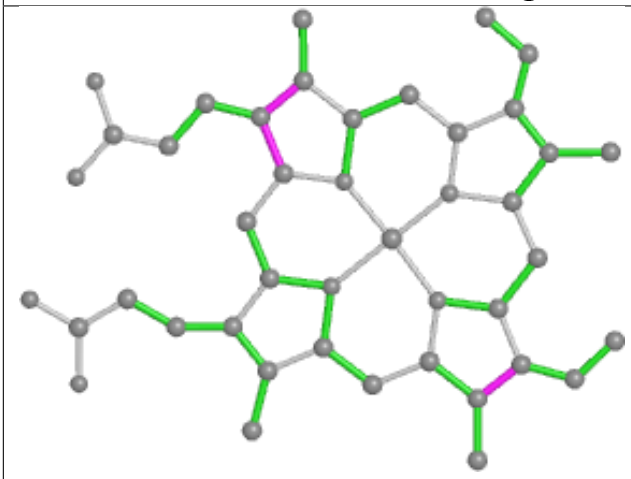


Torsions



Rings

Ligand HEM E 501



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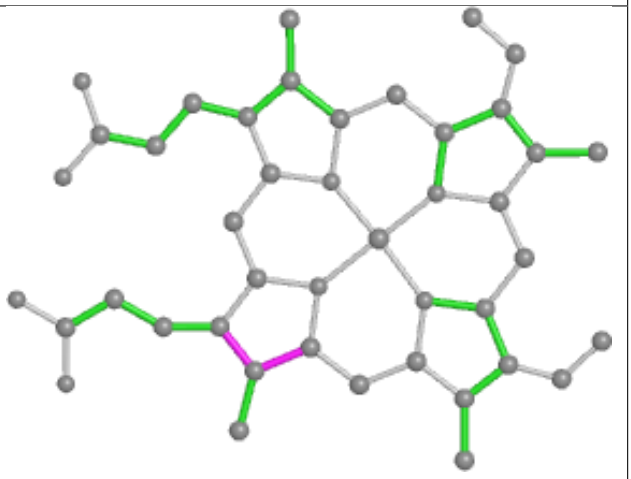
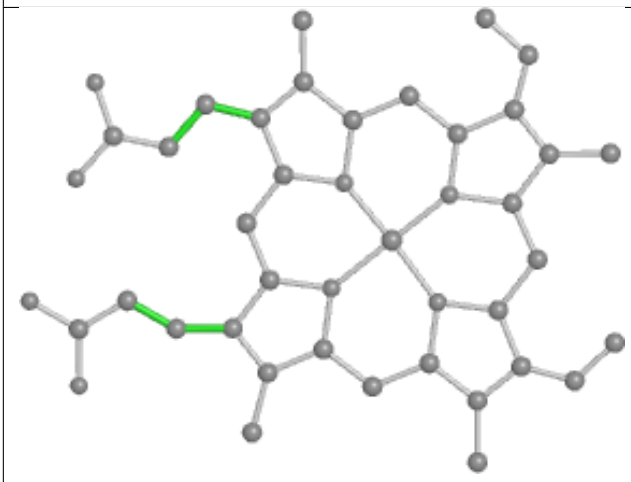
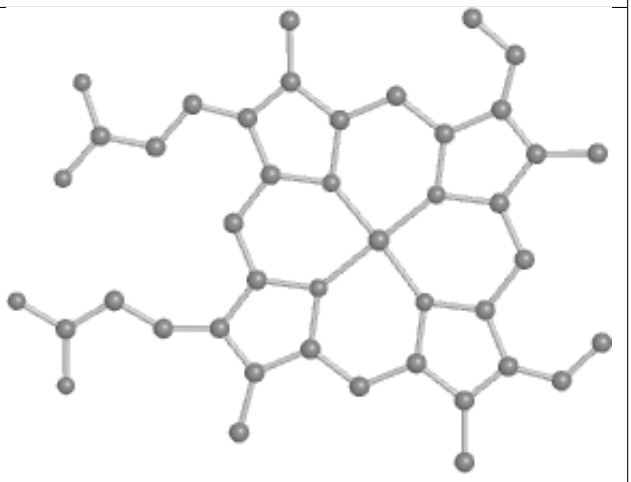


Bond angles

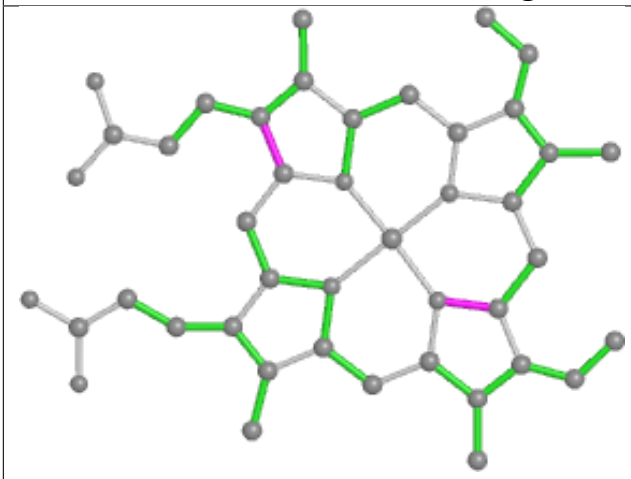


Torsions

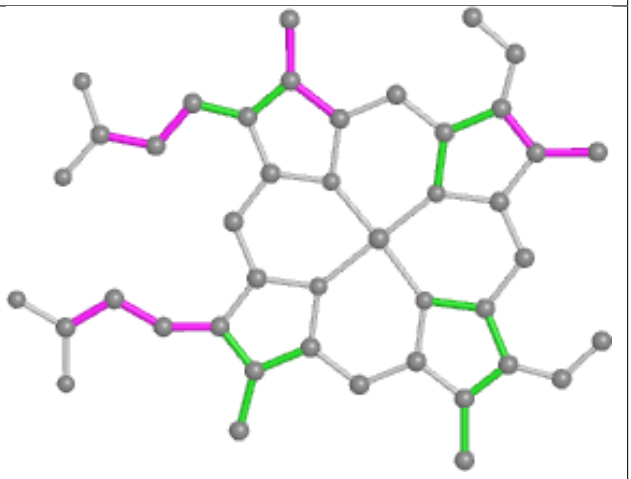


Rings

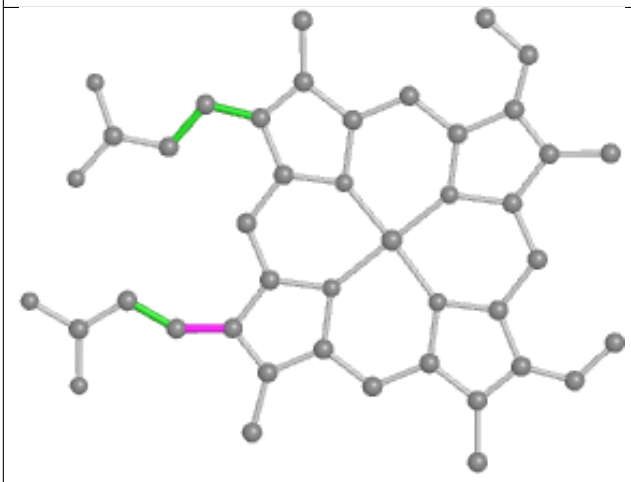
Ligand HEM C 501



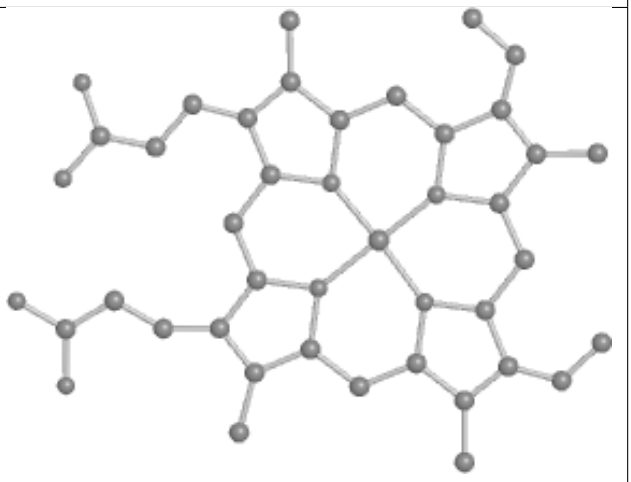
Bond lengths



Bond angles

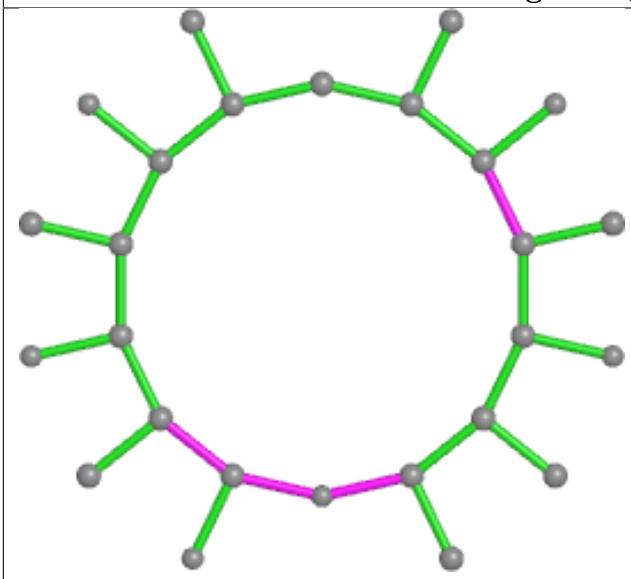


Torsions

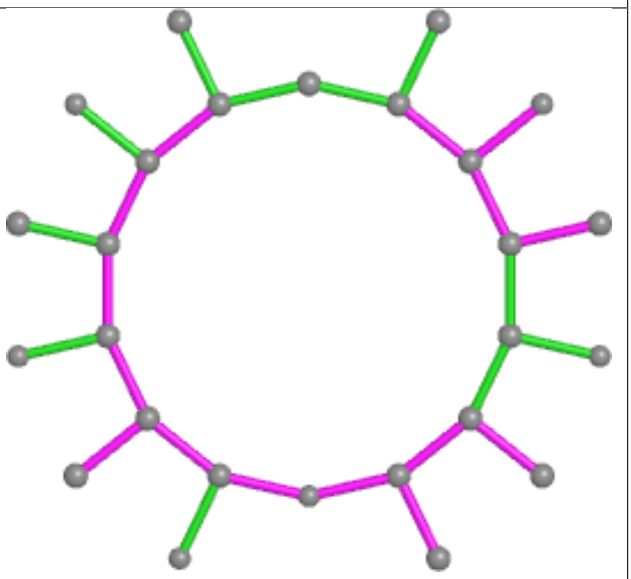


Rings

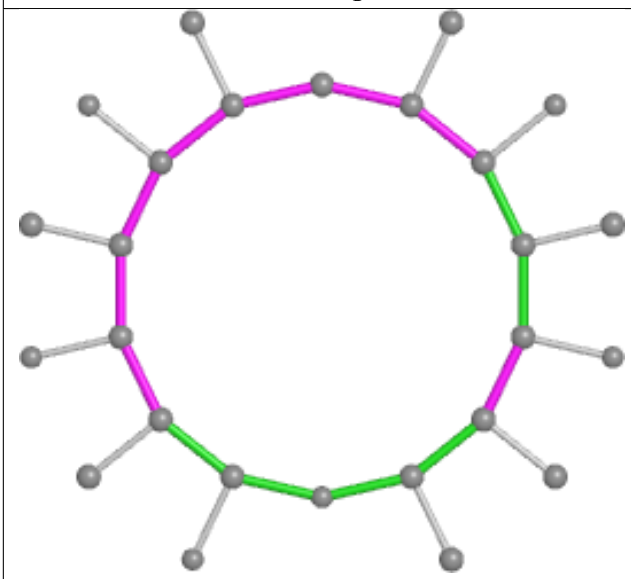
Ligand QR8 H 502



Bond lengths



Bond angles



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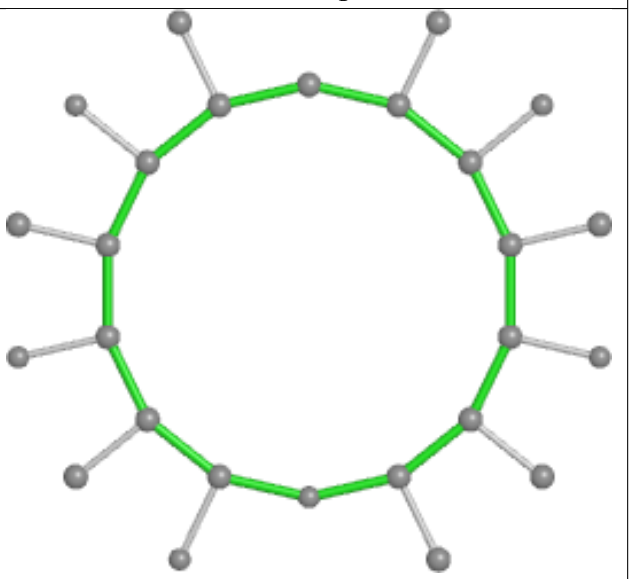
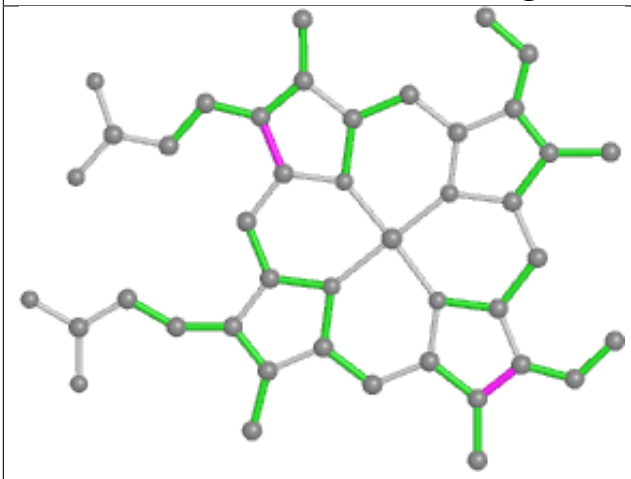
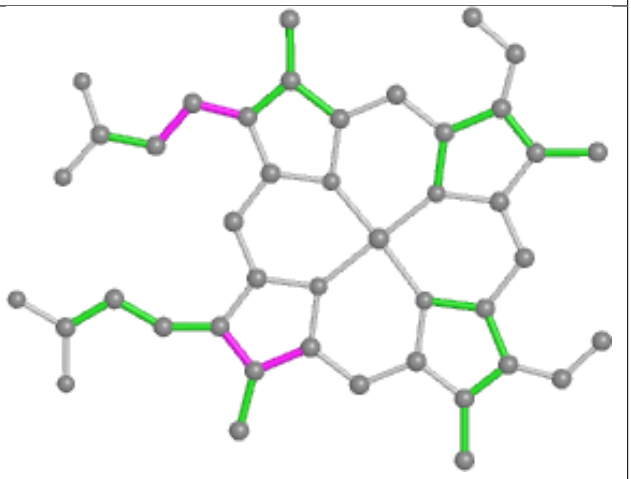


Rings

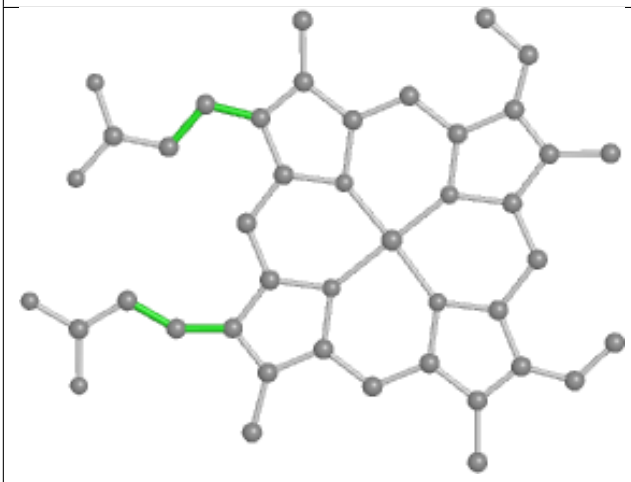
Ligand HEM F 501



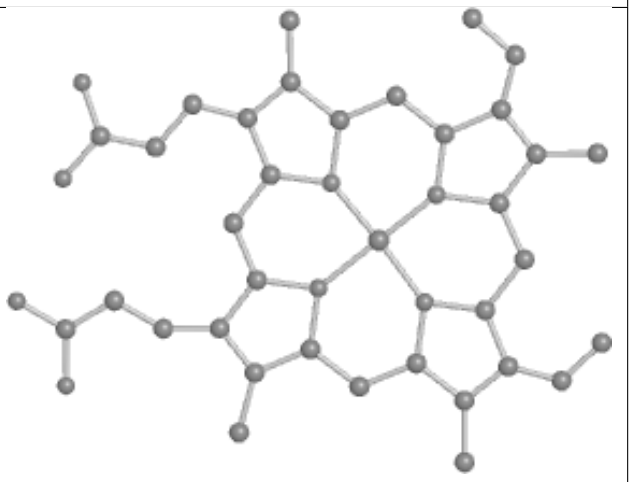
Bond lengths



Bond angles

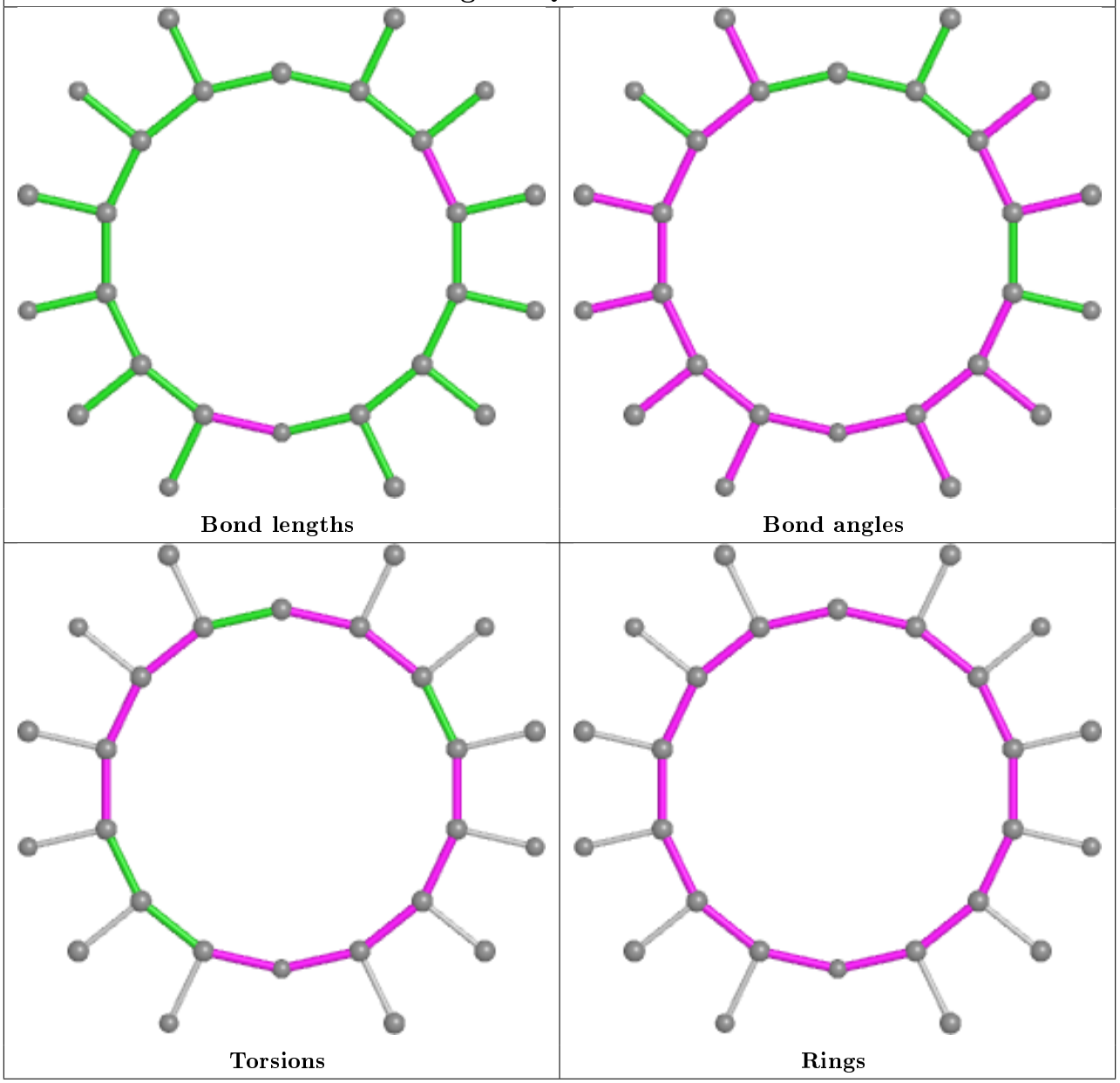


Torsions



Rings

Ligand QR8 E 502



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	394/407 (96%)	-0.69	0 100 100	9, 28, 77, 129	0
1	B	395/407 (97%)	-0.50	1 (0%) 94 94	16, 46, 84, 116	0
1	C	395/407 (97%)	-0.64	0 100 100	13, 40, 69, 107	0
1	D	394/407 (96%)	-0.61	1 (0%) 94 94	15, 33, 80, 128	0
1	E	386/407 (94%)	-0.24	5 (1%) 77 78	18, 58, 101, 167	0
1	F	394/407 (96%)	-0.47	4 (1%) 82 83	16, 49, 85, 147	0
1	G	381/407 (93%)	-0.01	21 (5%) 25 23	22, 65, 129, 172	0
1	H	395/407 (97%)	-0.39	2 (0%) 91 91	21, 50, 86, 126	0
1	I	248/407 (60%)	1.17	55 (22%) 0 0	69, 109, 148, 182	0
All	All	3382/3663 (92%)	-0.33	89 (2%) 56 56	9, 48, 112, 182	0

The worst 5 of 89 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	394	GLY	7.0
1	G	211	PRO	6.2
1	G	238	GLY	6.1
1	I	209	ASP	6.1
1	I	177	ALA	5.6

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 monosaccharides in this entry.

6.4 Ligands (i)

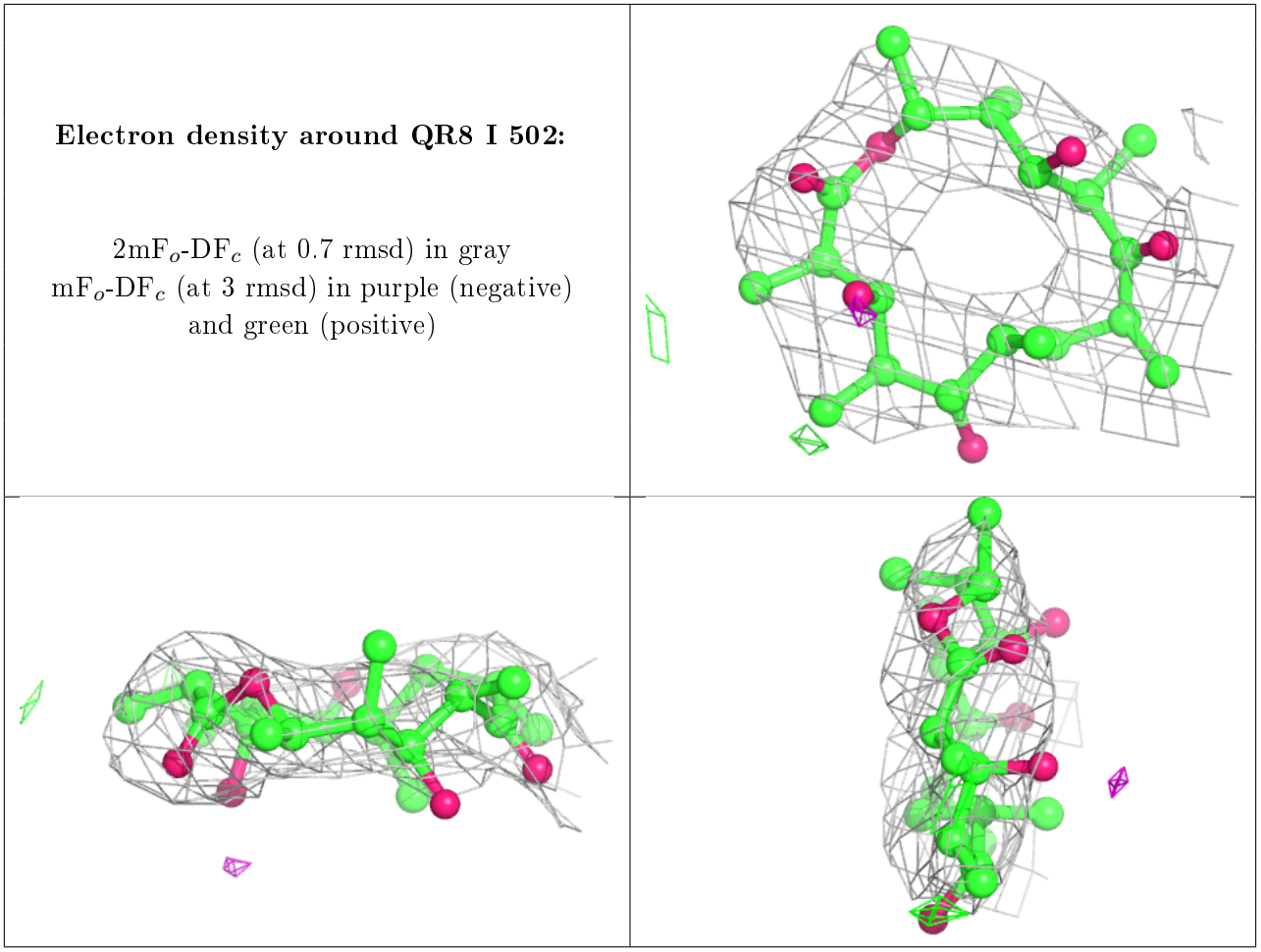
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	QR8	I	502	26/26	0.86	0.26	82,110,131,138	0
2	HEM	I	501	43/43	0.86	0.24	88,152,169,172	0
3	QR8	G	502	26/26	0.87	0.25	46,57,78,85	0
3	QR8	H	502	26/26	0.87	0.20	38,45,52,56	0
3	QR8	F	502	26/26	0.88	0.23	49,53,61,67	0
3	QR8	E	502	26/26	0.89	0.21	44,74,99,102	0
3	QR8	A	502	26/26	0.90	0.20	27,33,39,44	0
3	QR8	D	502	26/26	0.93	0.16	36,46,52,52	0
2	HEM	F	501	43/43	0.95	0.20	35,68,79,81	0
3	QR8	B	502	26/26	0.95	0.16	28,31,36,42	0
2	HEM	B	501	43/43	0.96	0.19	28,33,42,46	0
3	QR8	C	502	26/26	0.96	0.14	16,18,19,21	0
2	HEM	H	501	43/43	0.96	0.19	26,57,69,75	0
2	HEM	E	501	43/43	0.97	0.22	34,39,48,54	0
2	HEM	G	501	43/43	0.97	0.20	47,53,67,70	0
2	HEM	A	501	43/43	0.98	0.11	7,8,9,10	0
2	HEM	D	501	43/43	0.98	0.13	19,24,40,48	0
2	HEM	C	501	43/43	0.98	0.17	21,23,28,33	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.

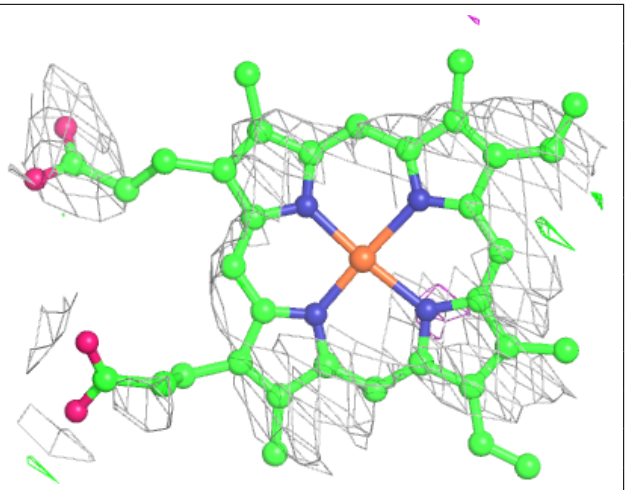
Electron density around QR8 I 502:

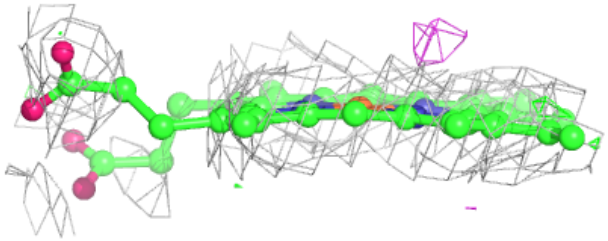
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

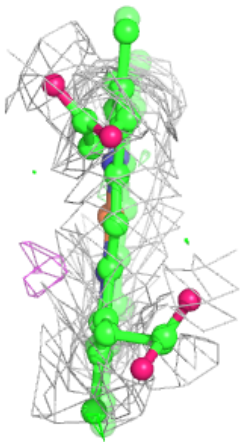


Electron density around HEM I 501:

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

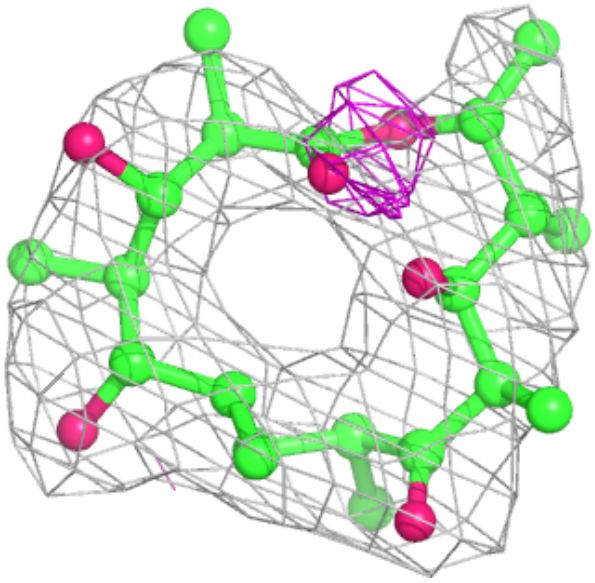


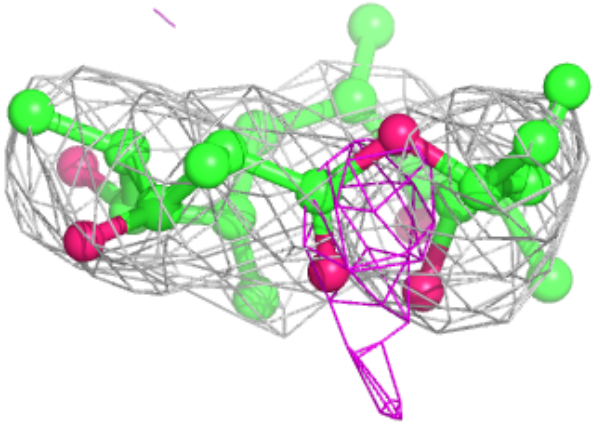


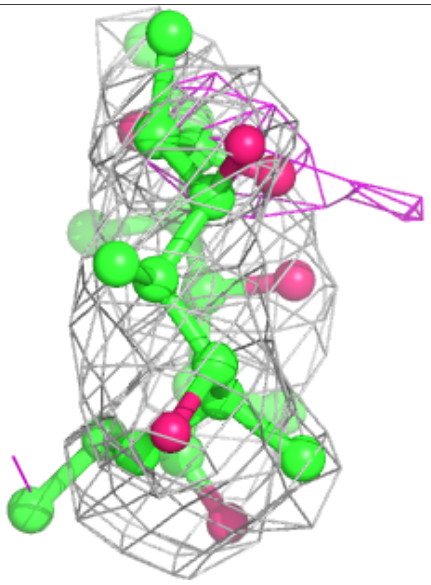


Electron density around QR8 G 502:

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

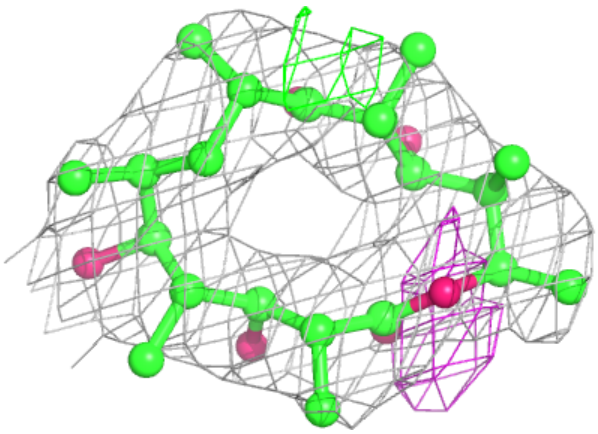


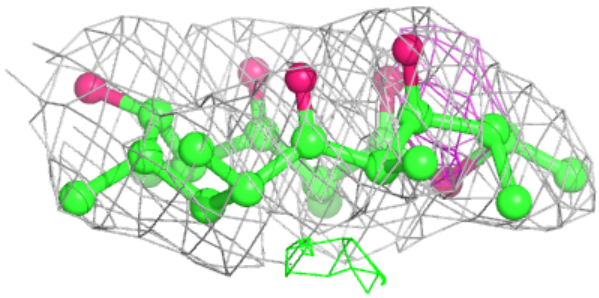


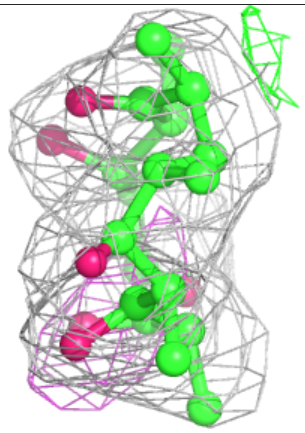


Electron density around QR8 H 502:

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

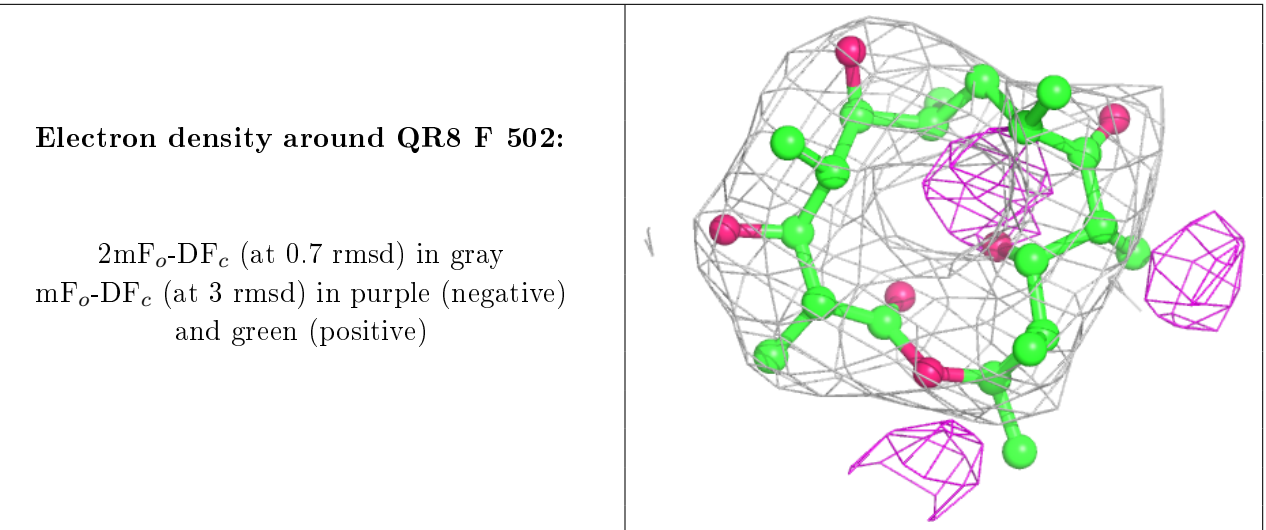


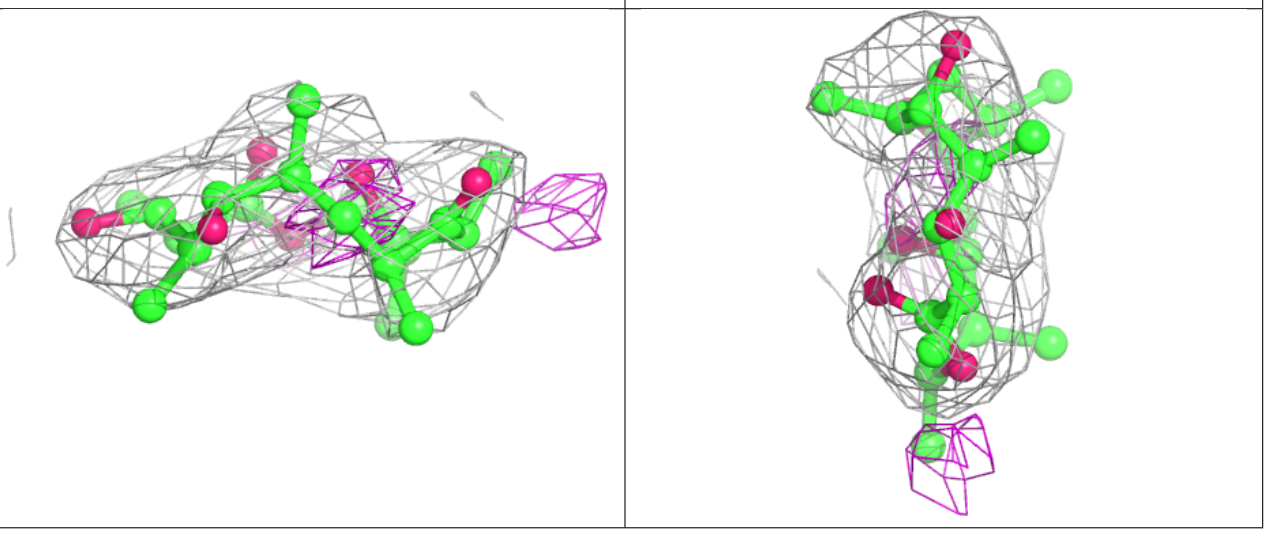




Electron density around QR8 F 502:

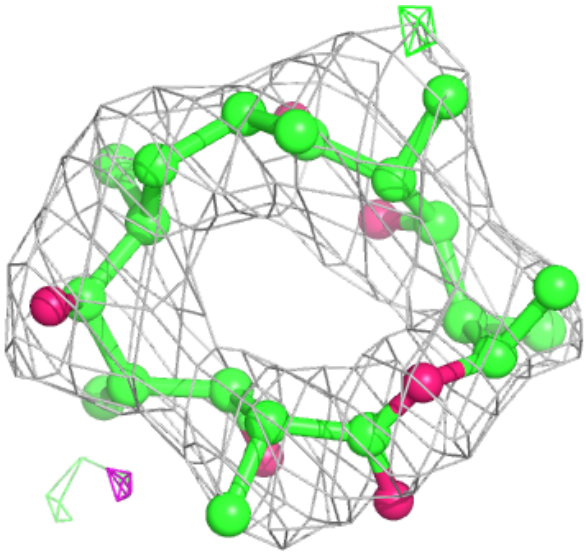
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

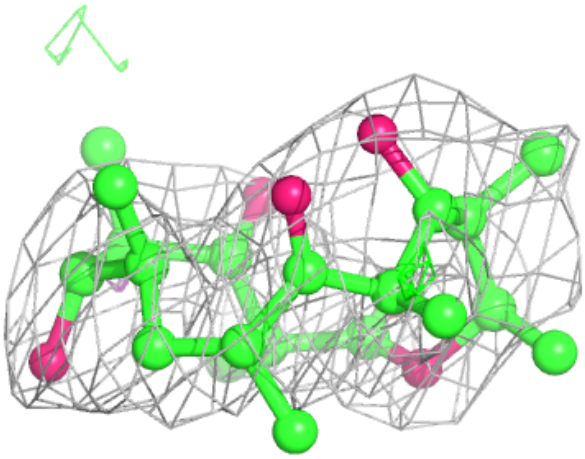


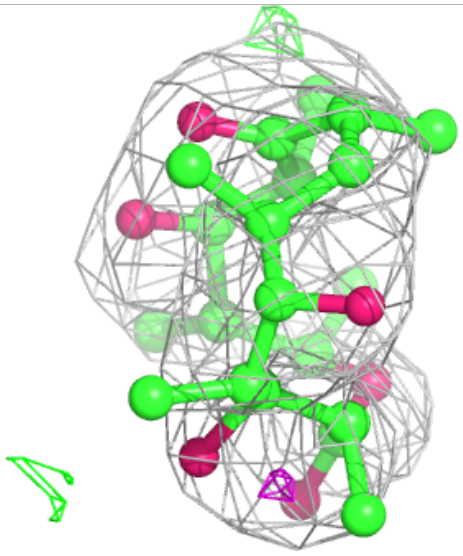


Electron density around QR8 E 502:

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

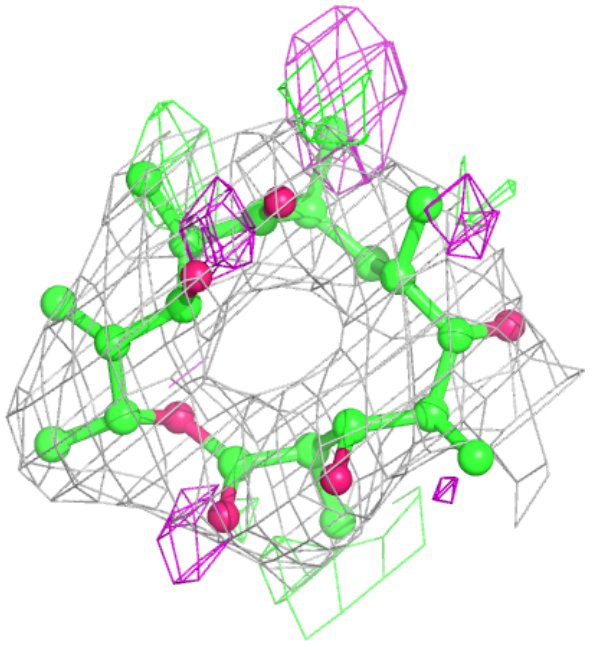


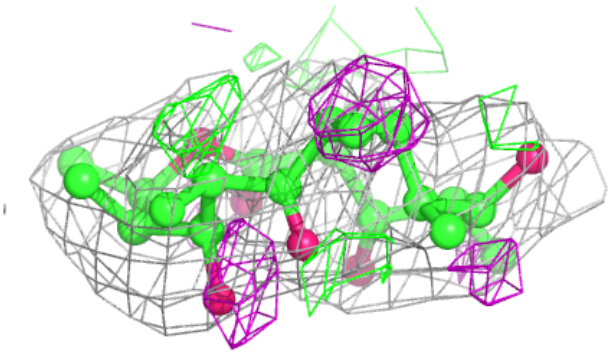


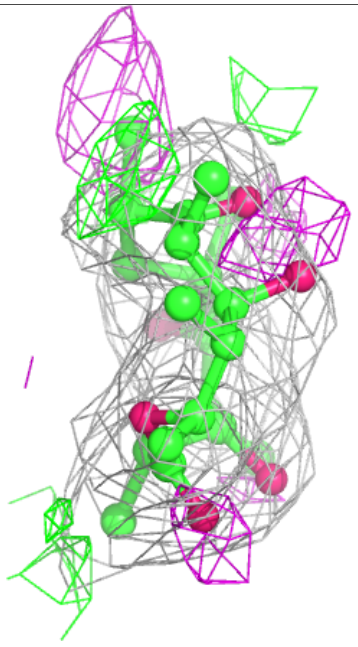


Electron density around QR8 A 502:

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

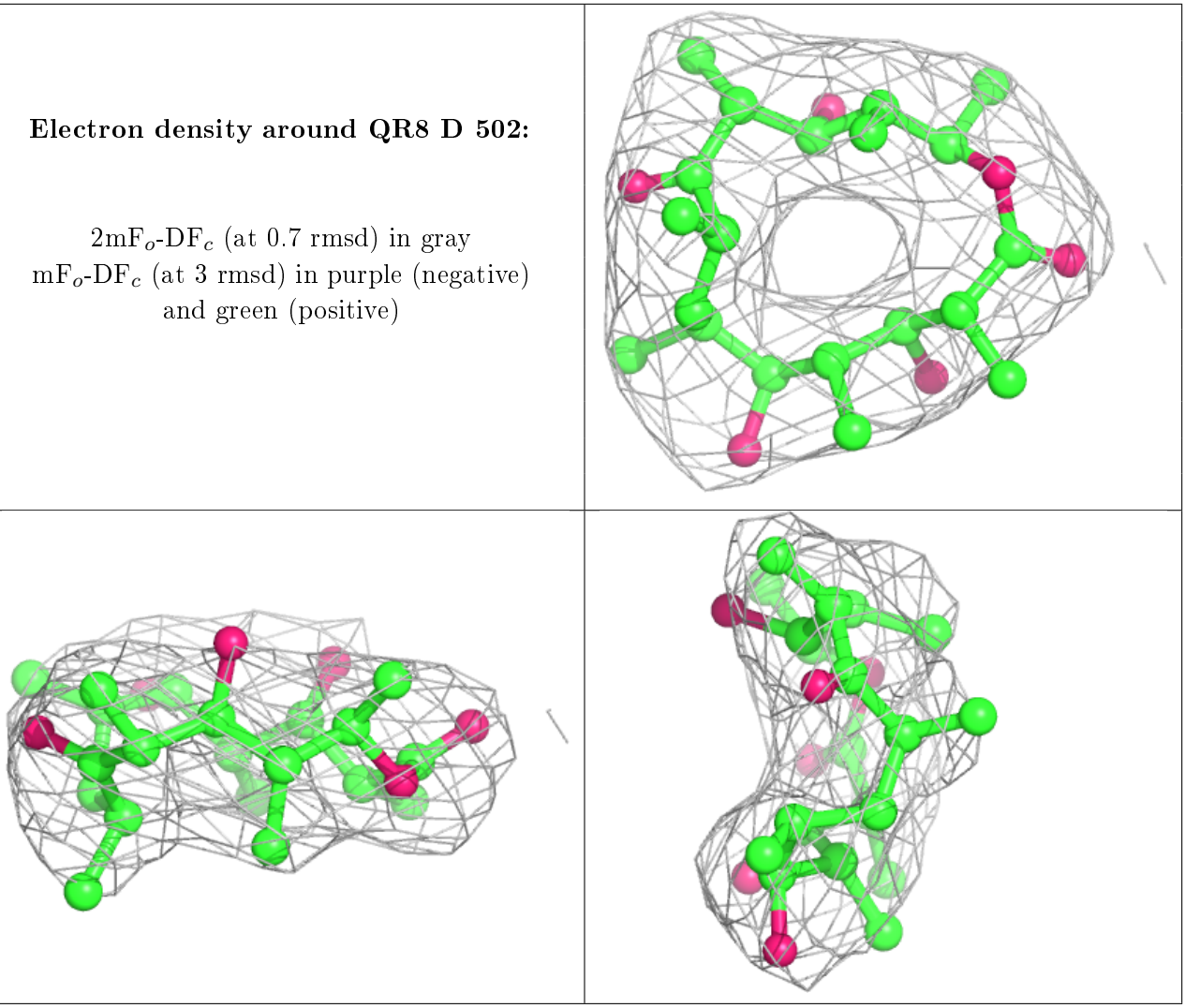






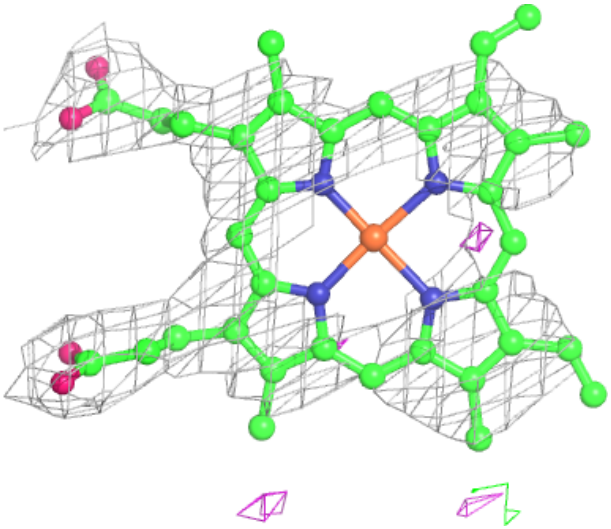
Electron density around QR8 D 502:

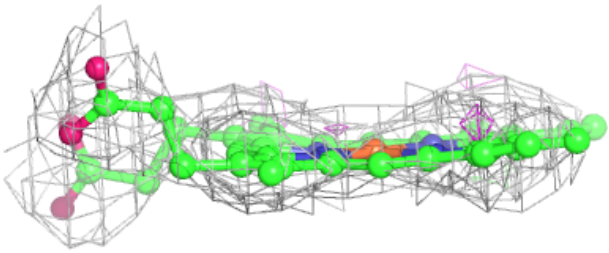
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

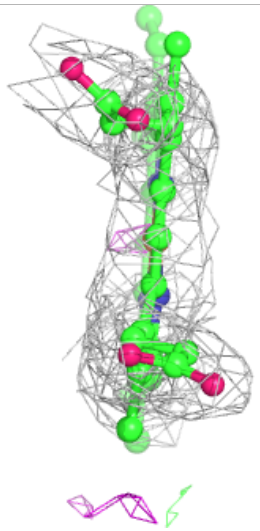


Electron density around HEM F 501:

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

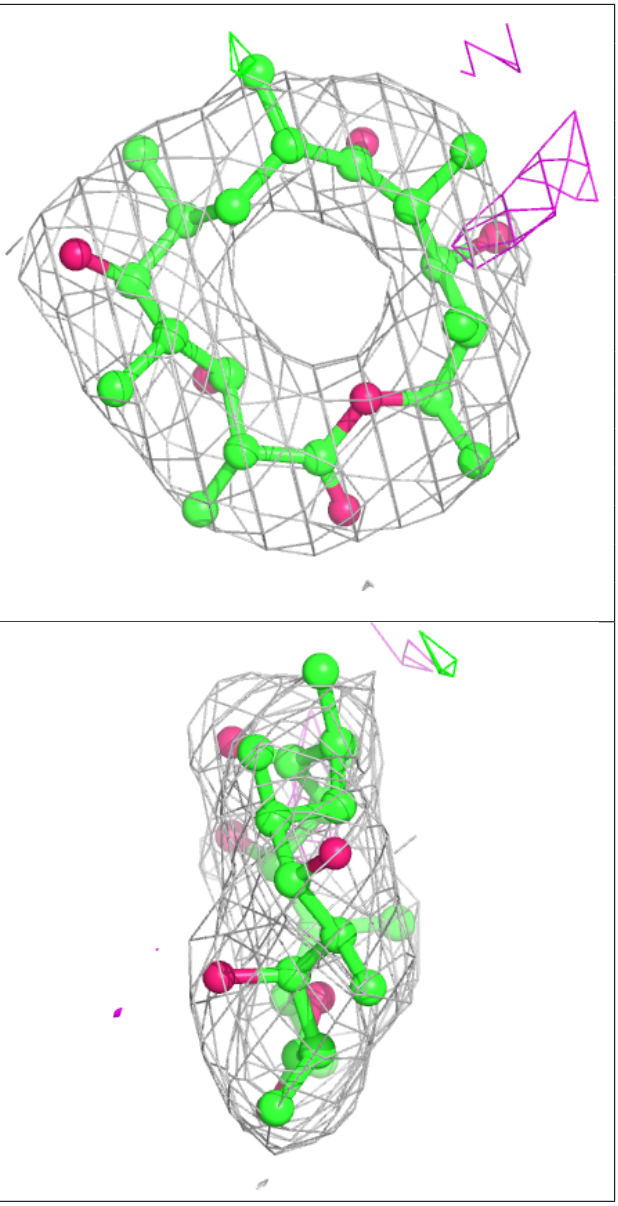


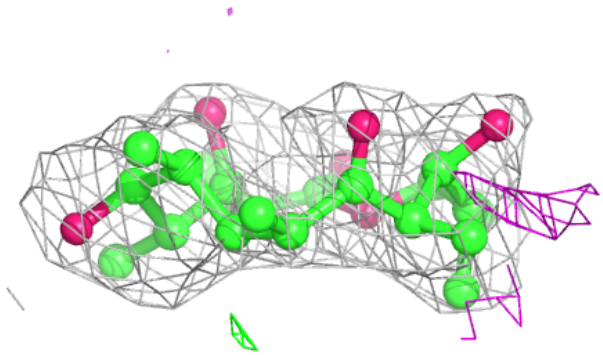




Electron density around QR8 B 502:

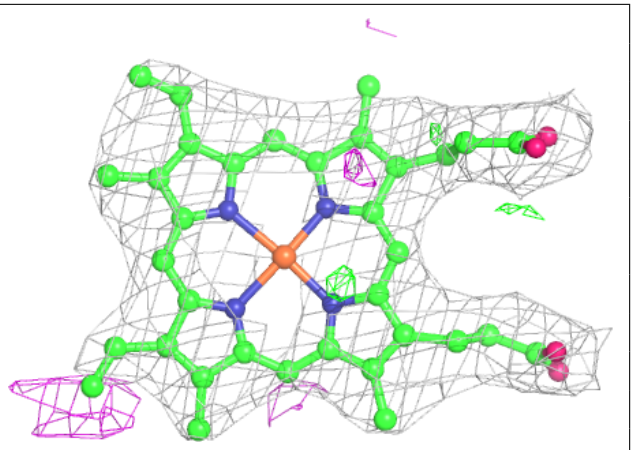
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

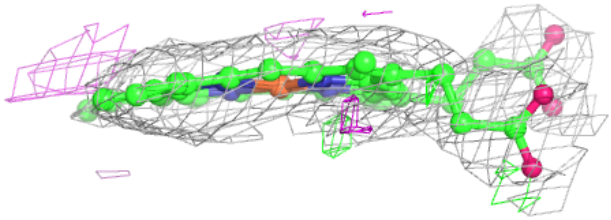


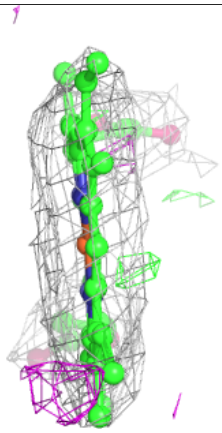


Electron density around HEM B 501:

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

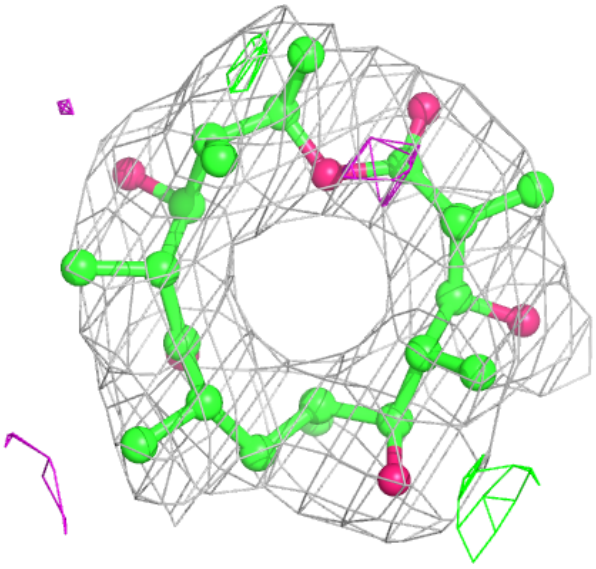


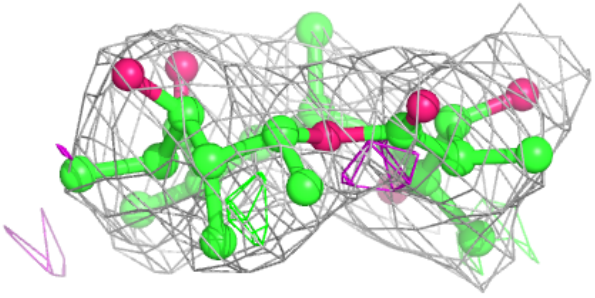


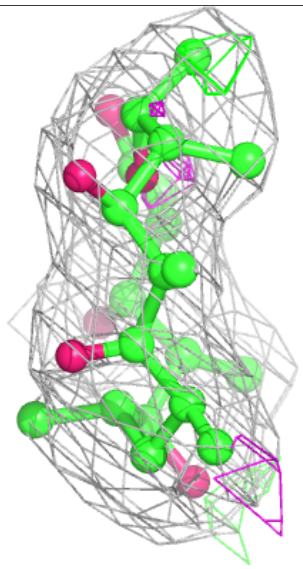


Electron density around QR8 C 502:

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

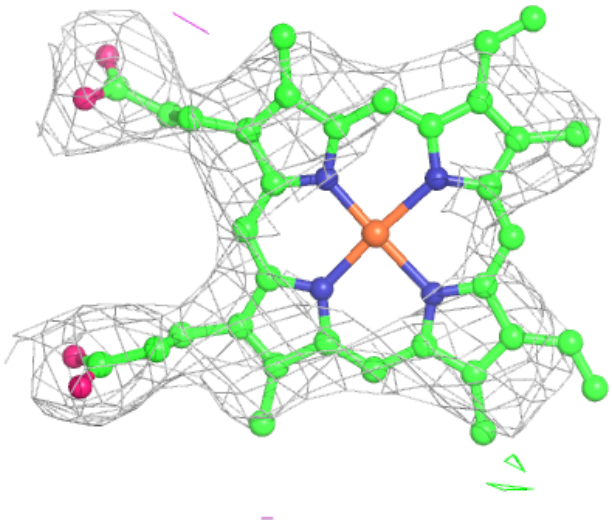


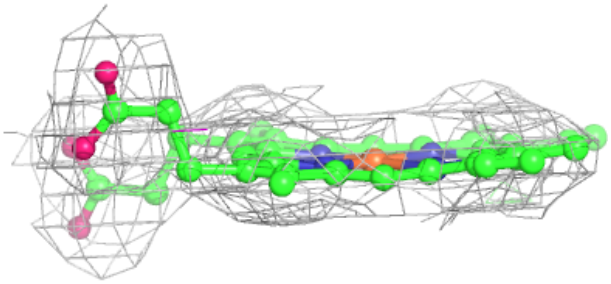


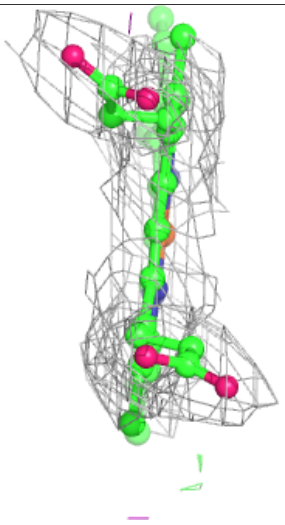


Electron density around HEM H 501:

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

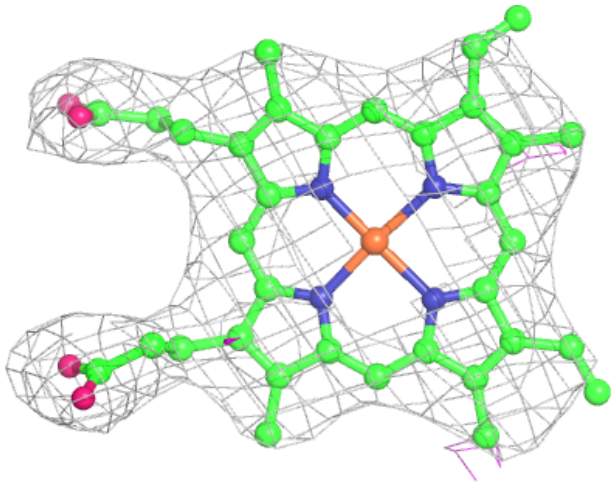


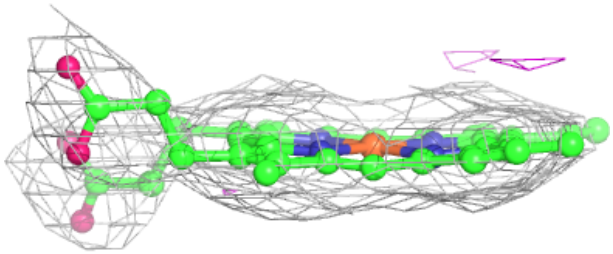


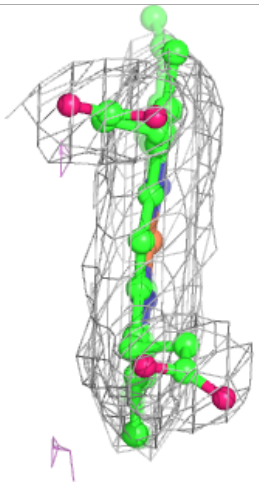


Electron density around HEM E 501:

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

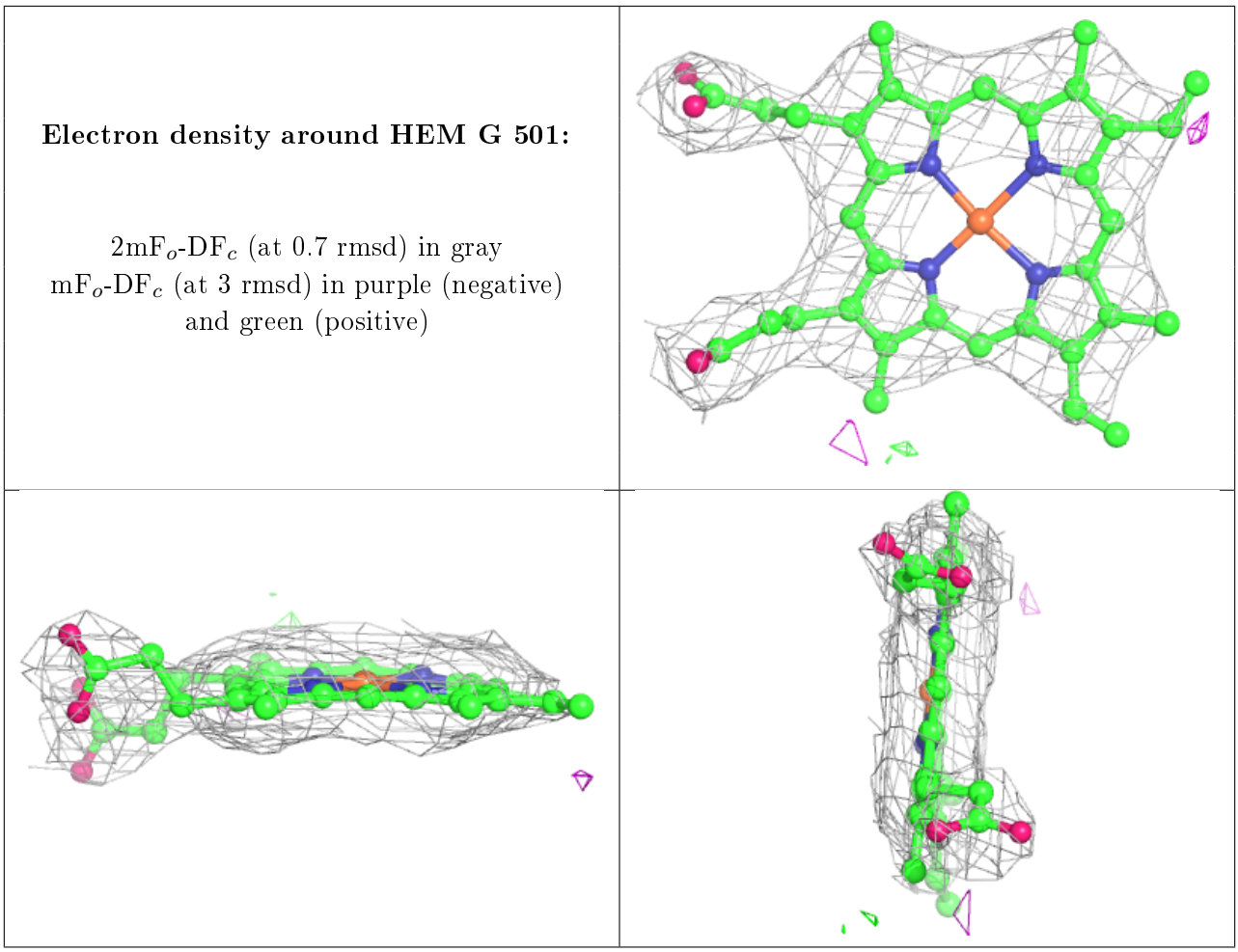






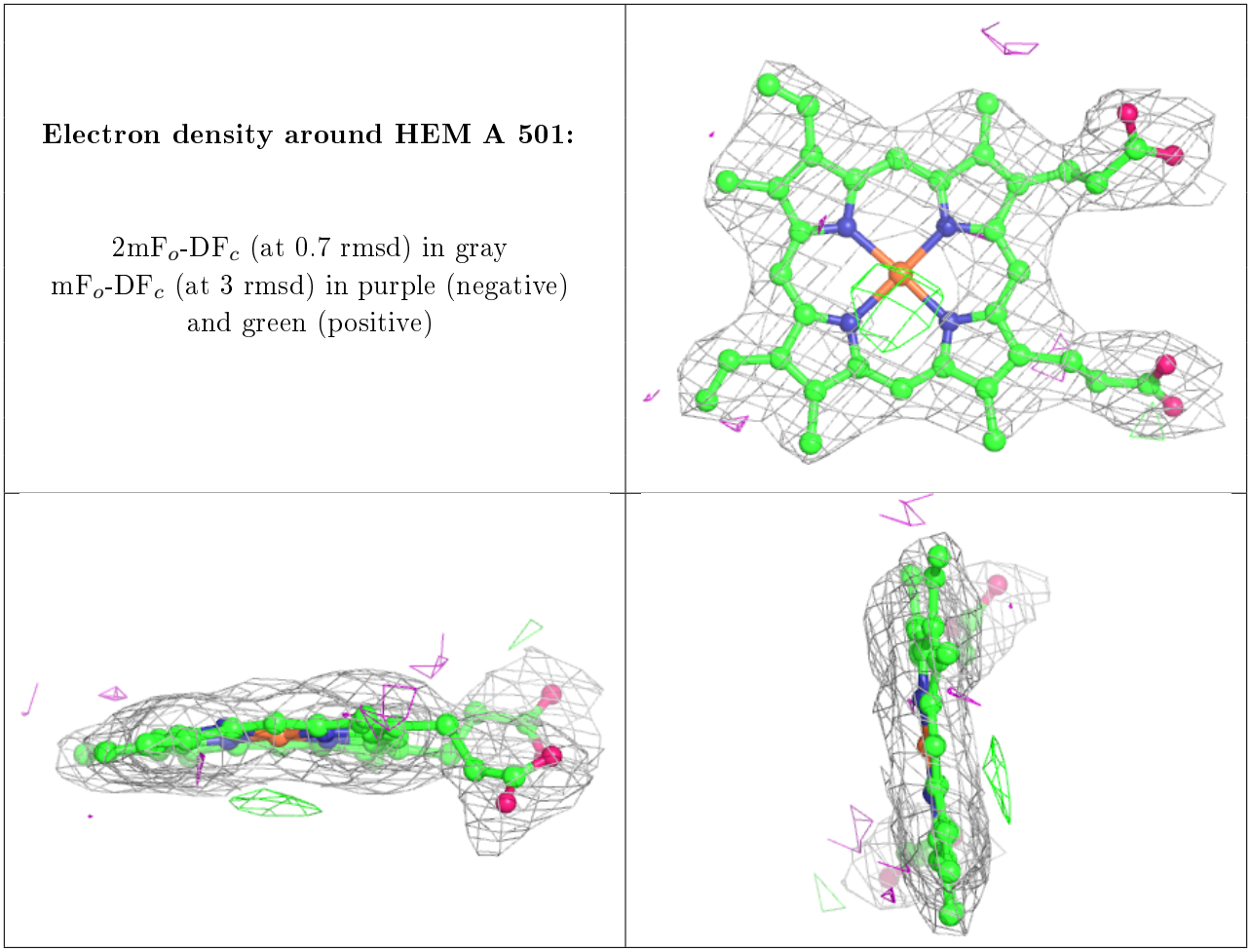
Electron density around HEM G 501:

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



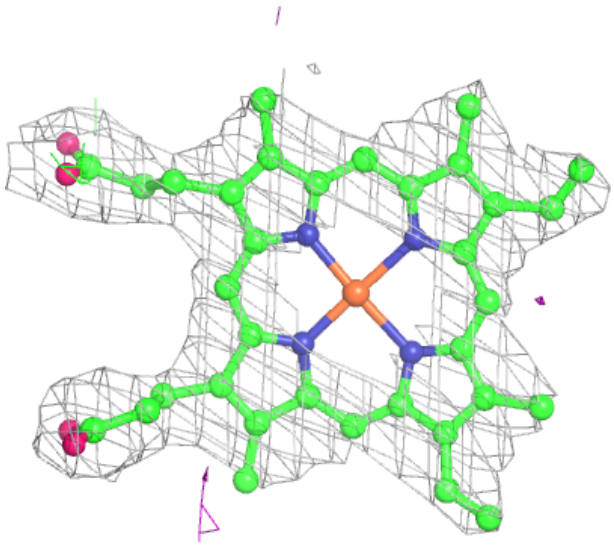
Electron density around HEM A 501:

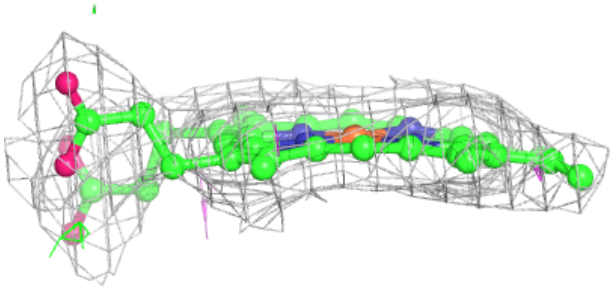
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

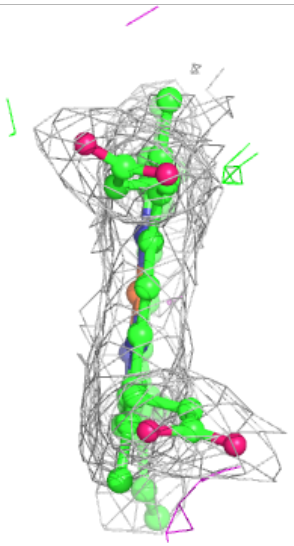


Electron density around HEM D 501:

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

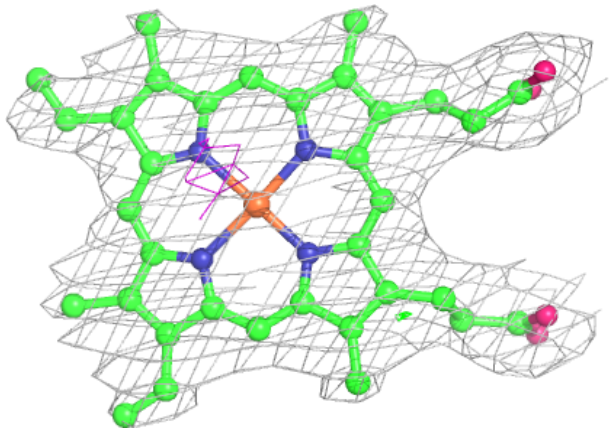


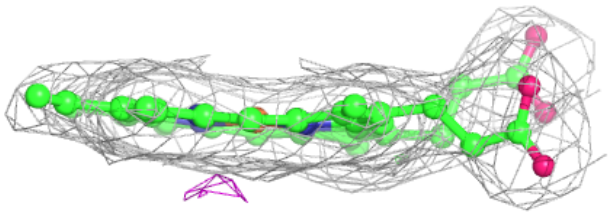


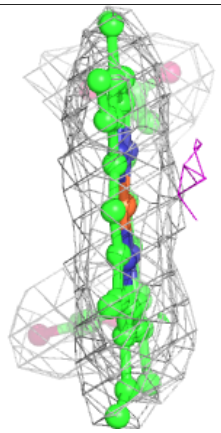


Electron density around HEM C 501:

$2mF_o$-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.