wwPDB X-ray Structure Validation Summary Report (i)

Sep 15, 2026 – 01:49 pm BST

PDB ID	:	5MNS / pdb_00005mns
Title	:	Structural and functional characterization of OleP in complex with 6DEB in sodium formate
Authors	:	Parisi, G.; Savino, C.; Montemiglio, L.C.; Vallone, B.
Deposited on	:	2016-12-13
Resolution	:	2.62 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

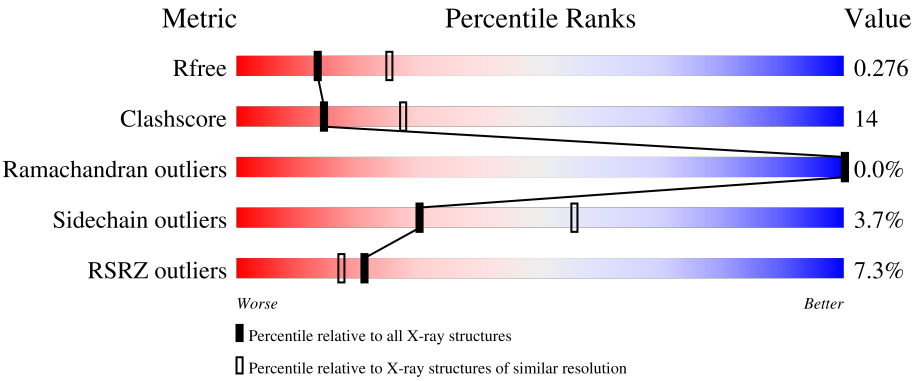
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.62 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	407	3% 77% 19%
1	B	407	3% 78% 17%
1	C	407	% 82% 13%
1	D	407	7% 70% 24%
1	E	407	9% 76% 18%

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Mol	Chain	Length	Quality of chain
1	F	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
2	HEC	A	501	X	-	-	-

2 Entry composition (i)

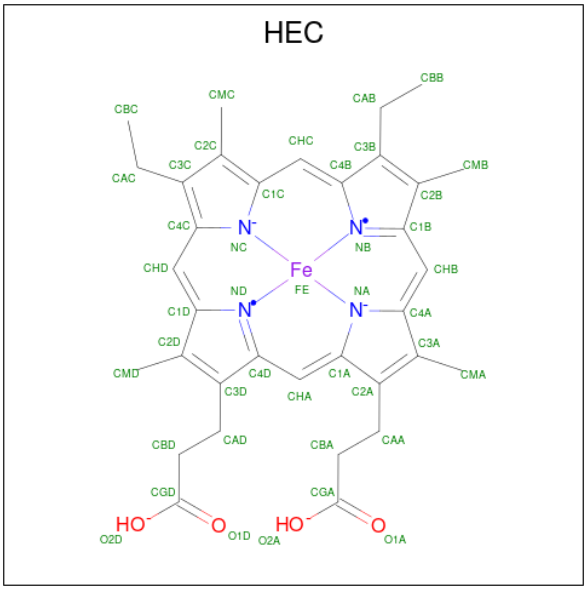
There are 5 unique types of molecules in this entry. The entry contains 19457 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

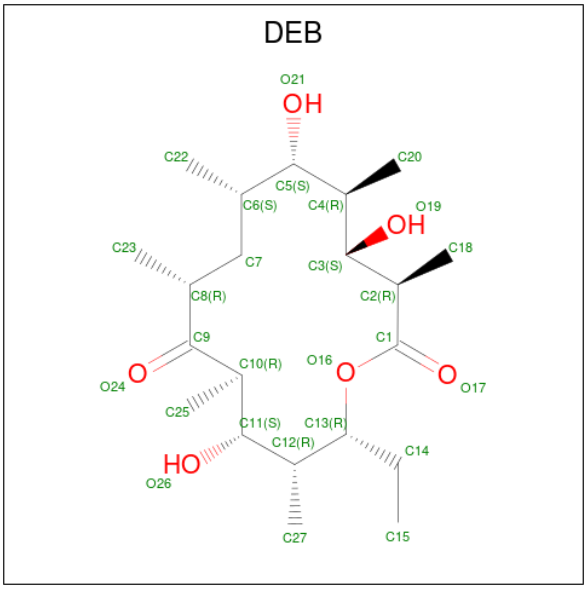
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			3077	1937	552	575	13			
1	B	395	Total	C	N	O	S	0	2	0
			3094	1947	556	578	13			
1	C	395	Total	C	N	O	S	0	0	0
			3077	1937	552	575	13			
1	D	395	Total	C	N	O	S	0	0	0
			3077	1937	552	575	13			
1	E	395	Total	C	N	O	S	0	1	0
			3085	1942	555	575	13			
1	F	393	Total	C	N	O	S	0	0	0
			3062	1928	550	571	13			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



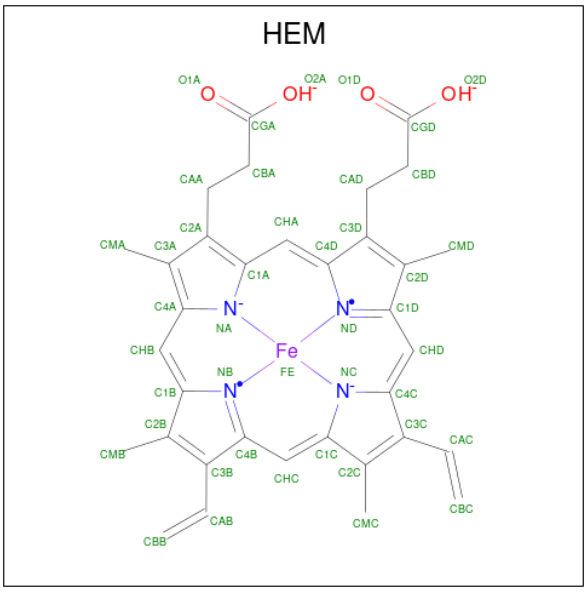
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is water.

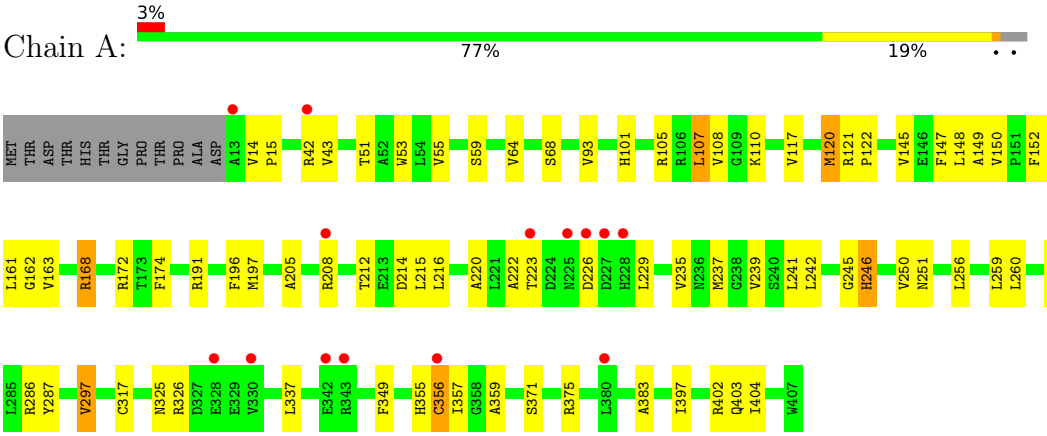
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	89	Total O 89 89	0	0
5	B	126	Total O 126 126	0	0
5	C	184	Total O 184 184	0	0
5	D	56	Total O 56 56	0	0
5	E	53	Total O 53 53	0	0
5	F	57	Total O 57 57	0	0

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.

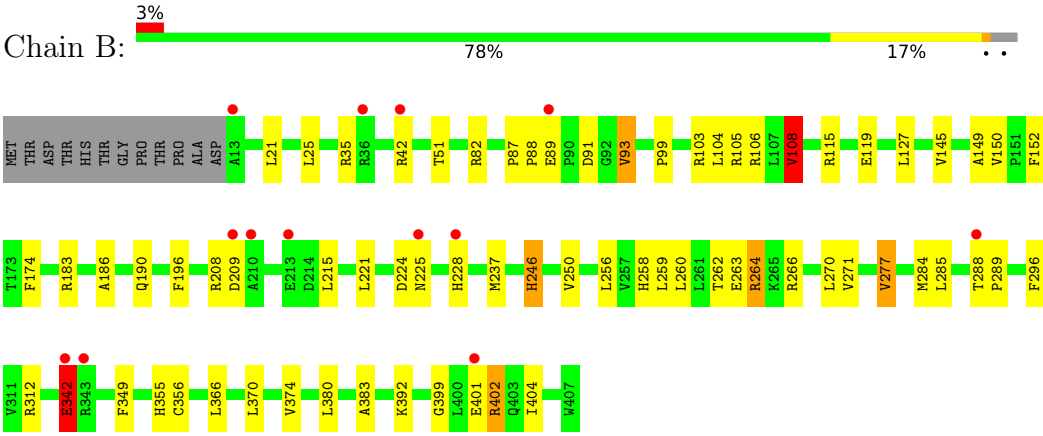
• Molecule 1: Cytochrome P-450

Chain A:



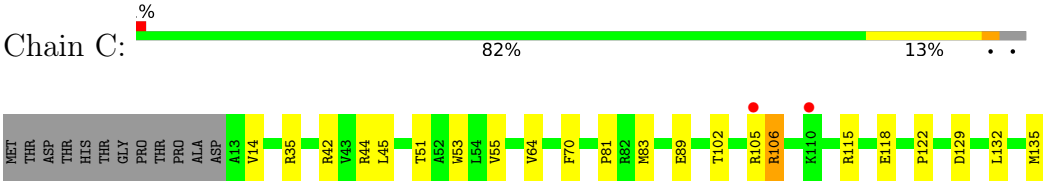
• Molecule 1: Cytochrome P-450

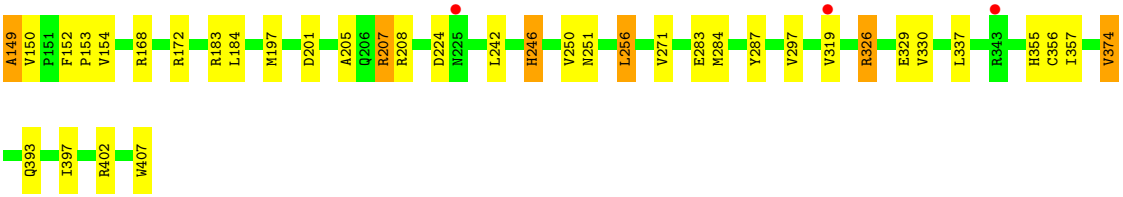
Chain B:



• Molecule 1: Cytochrome P-450

Chain C:

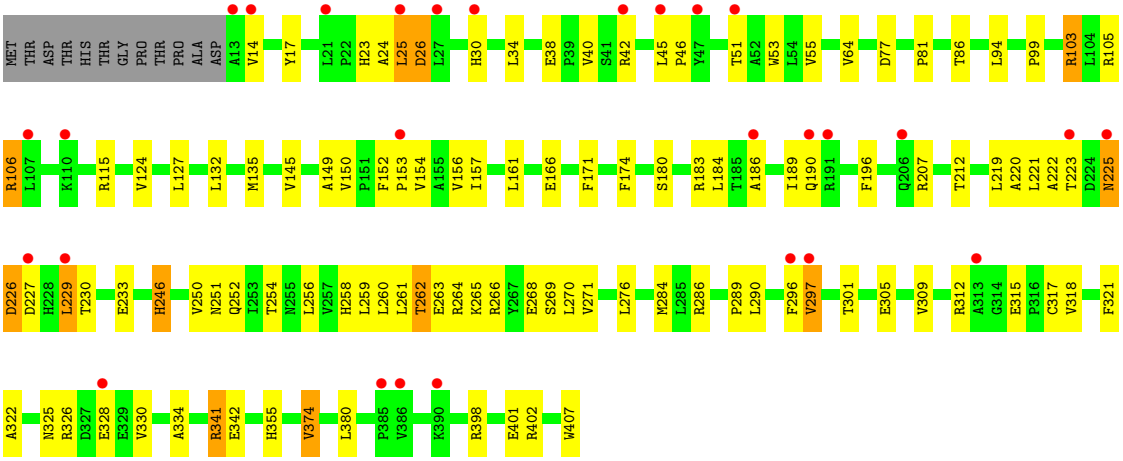




• Molecule 1: Cytochrome P-450

Chain D:

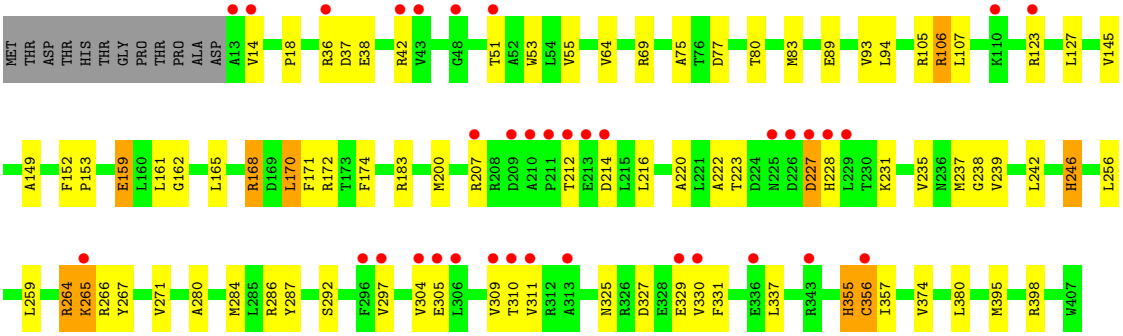




• Molecule 1: Cytochrome P-450

Chain E:

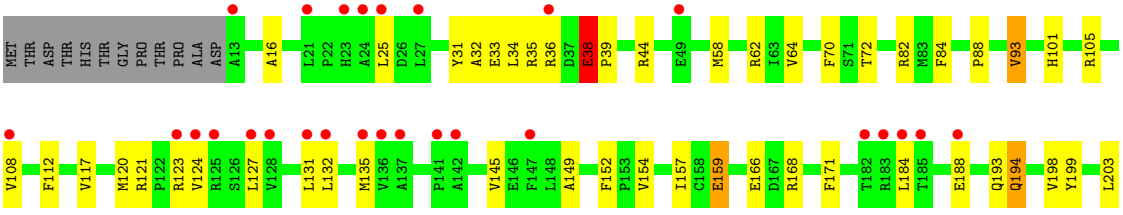


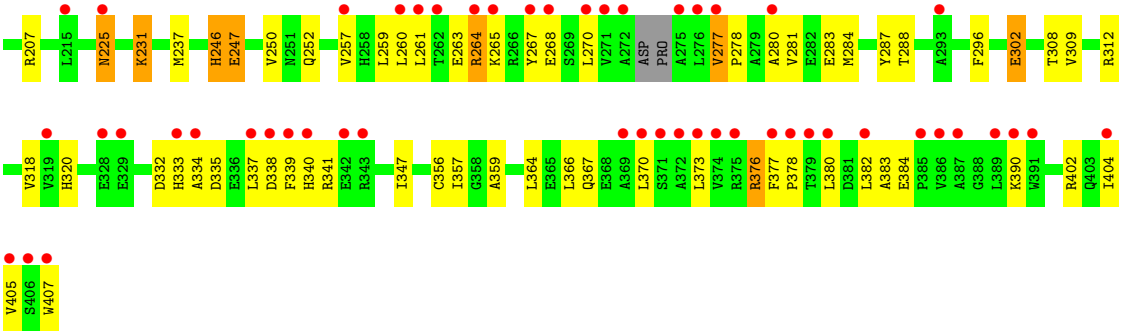


• Molecule 1: Cytochrome P-450

Chain F:






R207
L215
N225
K231
M237
H246
E247
V250
N251
Q252
V257
H258
L259
L260
L261
T262
E263
R264
K265
R266
Y267
E268
S269
L270
V271
A272
ASP
PRO
A275
L276
V277
P278
A279
A280
V281
E282
E283
M284
Y287
T288
A293
F296
E302
T308
V309
R312
V318
V319
H320
E328
E329
D332
H333
A334
D335
E336
L337
D338
F339
H340
R341
E342
R343
I347
C356
I357
G358
A359
L364
E365
L366
Q367
E368
A369
L370
S371
A372
L373
V374
R375
R376
F377
P378
T379
L380
D381
L382
A383
E384
P385
V386
A387
G388
L389
K390
W391
R402
Q403
I404
V405
S406
W407

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	247.60Å 110.80Å 159.10Å 90.00° 129.60° 90.00°	Depositor
Resolution (Å)	120.00 – 2.62 120.00 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.6 (120.00-2.62) 99.6 (120.00-2.62)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.50 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.208 , 0.258 0.234 , 0.276	Depositor DCC
R_{free} test set	4932 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.019 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19457	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4422e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEC, 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	0.73	2/3144 (0.1%)	0.95	3/4284 (0.1%)
1	B	0.71	3/3164 (0.1%)	0.98	8/4310 (0.2%)
1	C	0.73	2/3144 (0.1%)	0.90	2/4284 (0.0%)
1	D	0.75	2/3144 (0.1%)	1.05	11/4284 (0.3%)
1	E	0.72	1/3155 (0.0%)	0.99	7/4298 (0.2%)
1	F	0.72	1/3127 (0.0%)	1.03	9/4258 (0.2%)
All	All	0.73	11/18878 (0.1%)	0.99	40/25718 (0.2%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	HIS	CG-ND1	-6.79	1.30	1.38
1	A	246	HIS	CG-ND1	-6.59	1.31	1.38
1	B	246	HIS	CD2-NE2	-6.21	1.31	1.37
1	B	277	VAL	CA-CB	6.05	1.57	1.54
1	C	246	HIS	CG-ND1	-6.04	1.31	1.38

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	227	ASP	N-CA-C	10.80	122.62	111.07
1	D	26	ASP	N-CA-C	-10.54	96.32	110.55
1	D	227	ASP	N-CA-C	10.14	122.33	111.28
1	D	24	ALA	N-CA-C	8.50	123.12	111.39
1	A	147	PHE	N-CA-C	8.10	120.19	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3077	0	3056	81	2
1	B	3094	0	3074	69	0
1	C	3077	0	3056	51	0
1	D	3077	0	3056	97	1
1	E	3085	0	3070	110	0
1	F	3062	0	3044	123	1
2	A	43	0	32	5	0
3	A	27	0	38	0	0
3	B	27	0	38	1	0
3	C	27	0	38	0	0
3	D	27	0	38	1	0
3	E	27	0	38	0	0
3	F	27	0	38	0	0
4	B	43	0	30	4	0
4	C	43	0	30	2	0
4	D	43	0	30	4	0
4	E	43	0	30	12	0
4	F	43	0	30	4	0
5	A	89	0	0	0	0
5	B	126	0	0	3	1
5	C	184	0	0	6	0
5	D	56	0	0	5	0
5	E	53	0	0	1	0
5	F	57	0	0	4	0
All	All	19457	0	18766	529	3

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 14.

The worst 5 of 529 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:E:356:CYS:SG	4:E:501:HEM:FE	0.96	1.56
1:A:42:ARG:HH11	1:A:51:THR:CG2	1.30	1.44
1:E:123:ARG:NH1	1:E:127:LEU:HD12	1.42	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:CYS:SG	4:E:501:HEM:ND	2.00	1.34
1:E:200:MET:HE3	1:E:238:GLY:C	1.56	1.28

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:723:HOH:O	5:B:723:HOH:O[2_656]	2.11	0.09
1:A:208:ARG:NH1	1:D:301:THR:OG1[4_445]	2.16	0.04
1:A:68:SER:OG	1:F:231:LYS:NZ[4_546]	2.19	0.01

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	393/407 (97%)	383 (98%)	10 (2%)	0	100	100
1	B	395/407 (97%)	384 (97%)	11 (3%)	0	100	100
1	C	393/407 (97%)	380 (97%)	13 (3%)	0	100	100
1	D	393/407 (97%)	371 (94%)	22 (6%)	0	100	100
1	E	394/407 (97%)	378 (96%)	15 (4%)	1 (0%)	36	56
1	F	389/407 (96%)	372 (96%)	17 (4%)	0	100	100
All	All	2357/2442 (96%)	2268 (96%)	88 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	265	LYS

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	331/341 (97%)	323 (98%)	8 (2%)	43	69
1	B	333/341 (98%)	325 (98%)	8 (2%)	43	69
1	C	331/341 (97%)	321 (97%)	10 (3%)	36	62
1	D	331/341 (97%)	314 (95%)	17 (5%)	21	43
1	E	332/341 (97%)	320 (96%)	12 (4%)	31	56
1	F	329/341 (96%)	309 (94%)	20 (6%)	17	35
All	All	1987/2046 (97%)	1912 (96%)	75 (4%)	30	54

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	154	VAL
1	F	370	LEU
1	F	166	GLU
1	F	264	ARG
1	C	374	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	246	HIS
1	E	193	GLN
1	F	246	HIS
1	E	246	HIS
1	E	101	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	HEC	A	501	-	50,50,50	1.80	9 (18%)	68,82,82	1.90	19 (27%)
3	DEB	F	502	-	27,27,27	1.12	1 (3%)	35,39,39	1.16	4 (11%)
4	HEM	E	501	-	50,50,50	2.02	19 (38%)	66,82,82	1.64	12 (18%)
3	DEB	B	502	-	27,27,27	1.55	3 (11%)	35,39,39	1.38	3 (8%)
4	HEM	F	501	1	50,50,50	1.62	5 (10%)	66,82,82	1.56	11 (16%)
4	HEM	D	501	1	50,50,50	1.69	9 (18%)	66,82,82	1.70	13 (19%)
3	DEB	E	502	-	27,27,27	1.52	4 (14%)	35,39,39	1.56	7 (20%)
4	HEM	B	501	1	50,50,50	1.59	9 (18%)	66,82,82	1.70	13 (19%)
3	DEB	C	502	-	27,27,27	1.10	1 (3%)	35,39,39	1.06	2 (5%)
4	HEM	C	501	1	50,50,50	1.63	7 (14%)	66,82,82	1.72	15 (22%)
3	DEB	D	502	-	27,27,27	1.16	1 (3%)	35,39,39	1.27	2 (5%)
3	DEB	A	502	-	27,27,27	1.13	1 (3%)	35,39,39	1.18	2 (5%)

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	HEC	A	501	-	1/1/3/7	6/14/54/54	-
3	DEB	F	502	-	-	10/50/50/50	0/1/1/1
4	HEM	E	501	-	-	1/14/54/54	-
3	DEB	B	502	-	-	8/50/50/50	0/1/1/1
4	HEM	F	501	1	-	0/14/54/54	-
4	HEM	D	501	1	-	5/14/54/54	-
3	DEB	E	502	-	-	6/50/50/50	0/1/1/1
4	HEM	B	501	1	-	2/14/54/54	-
3	DEB	C	502	-	-	10/50/50/50	0/1/1/1
4	HEM	C	501	1	-	2/14/54/54	-
3	DEB	D	502	-	-	8/50/50/50	0/1/1/1
3	DEB	A	502	-	-	7/50/50/50	0/1/1/1

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	501	HEM	FE-NB	5.91	2.13	1.94
3	A	502	DEB	O16-C1	5.54	1.47	1.34
3	D	502	DEB	O16-C1	5.46	1.47	1.34
3	F	502	DEB	O16-C1	5.20	1.46	1.34
4	D	501	HEM	FE-NB	4.94	2.10	1.94

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	501	HEM	C1B-NB-C4B	5.89	111.16	105.07
4	C	501	HEM	CHC-C4B-NB	5.66	130.57	124.42
4	B	501	HEM	C1B-NB-C4B	5.46	110.72	105.07
2	A	501	HEC	C4B-NB-C1B	5.41	110.66	105.07
4	B	501	HEM	CHC-C4B-NB	5.05	129.91	124.42

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	501	HEC	NA

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	DEB	C3-C4-C5-O21

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Mol	Chain	Res	Type	Atoms
3	A	502	DEB	C20-C4-C5-O21
3	C	502	DEB	C18-C2-C3-C4
3	D	502	DEB	C3-C4-C5-O21
3	E	502	DEB	C3-C4-C5-O21

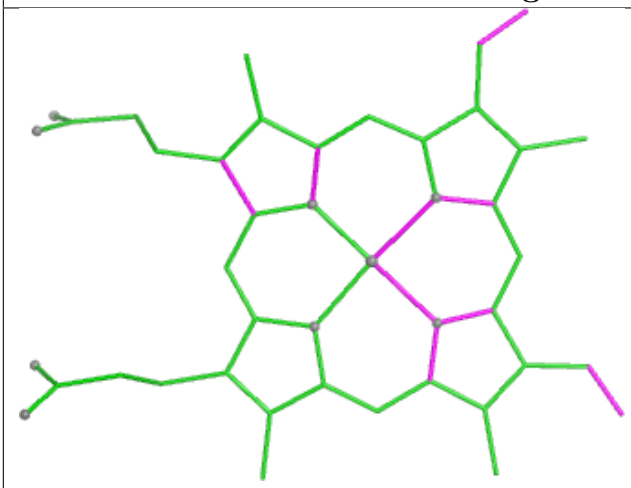
There are no ring outliers.

8 monomers are involved in 33 short contacts:

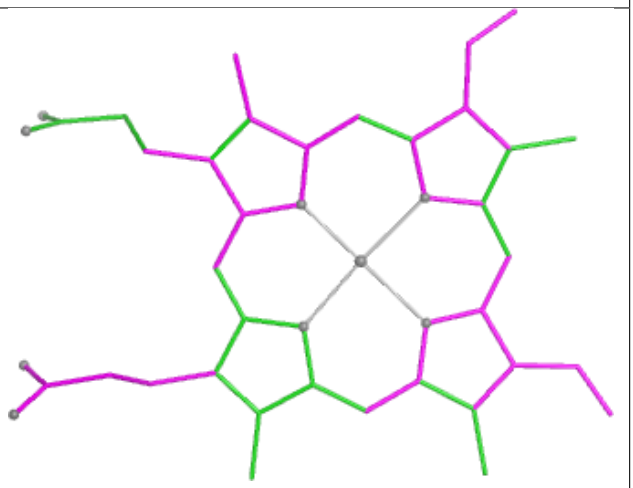
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEC	5	0
4	E	501	HEM	12	0
3	B	502	DEB	1	0
4	F	501	HEM	4	0
4	D	501	HEM	4	0
4	B	501	HEM	4	0
4	C	501	HEM	2	0
3	D	502	DEB	1	0

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

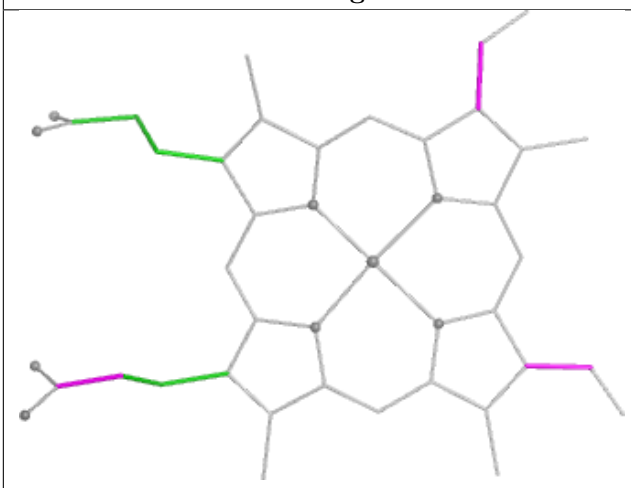
Ligand HEC A 501



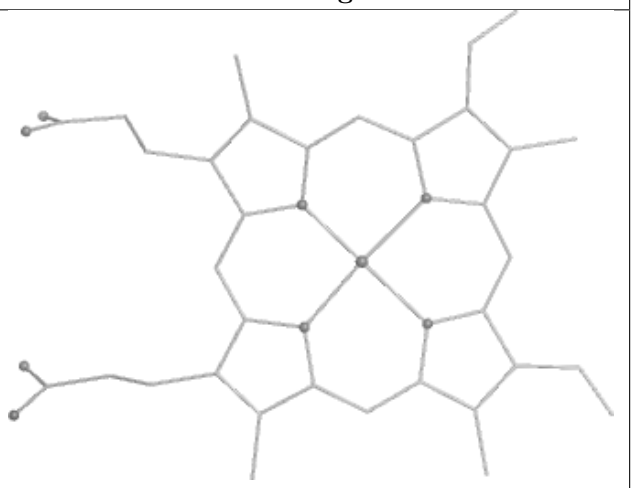
Bond lengths



Bond angles

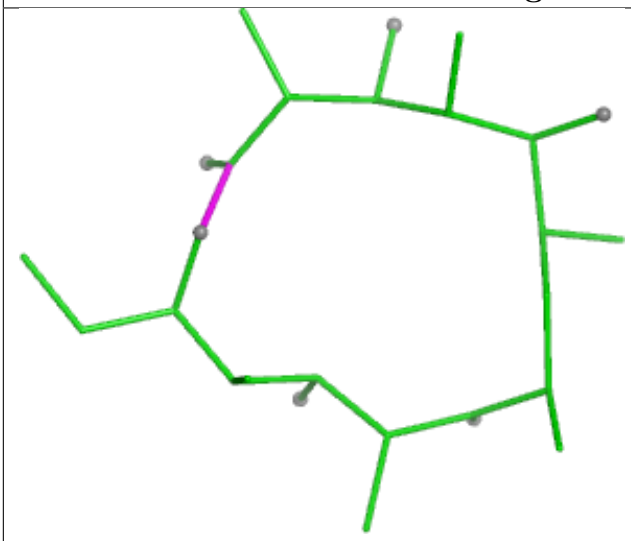


Torsions

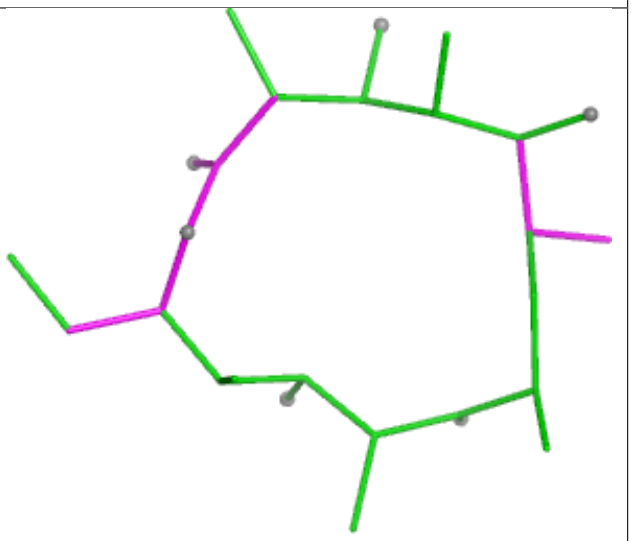


Rings

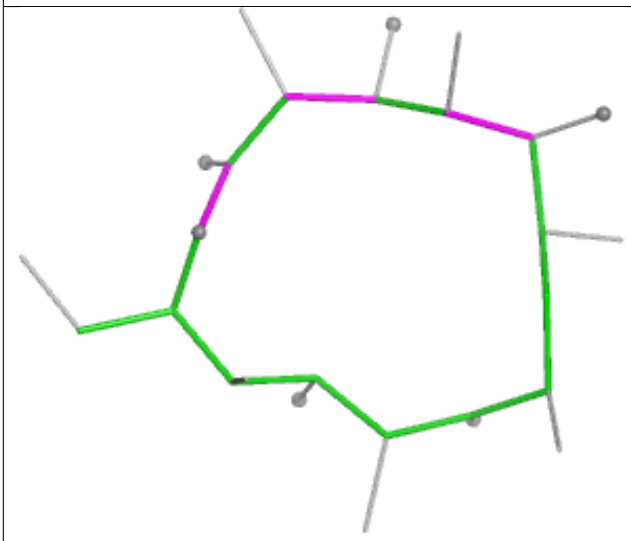
Ligand DEB F 502



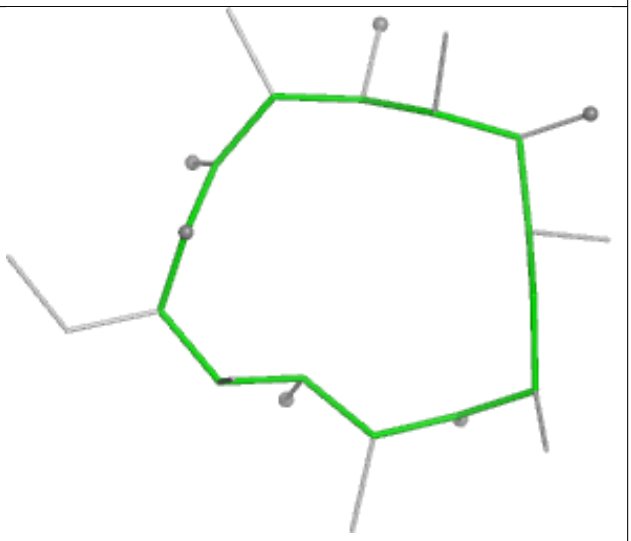
Bond lengths



Bond angles

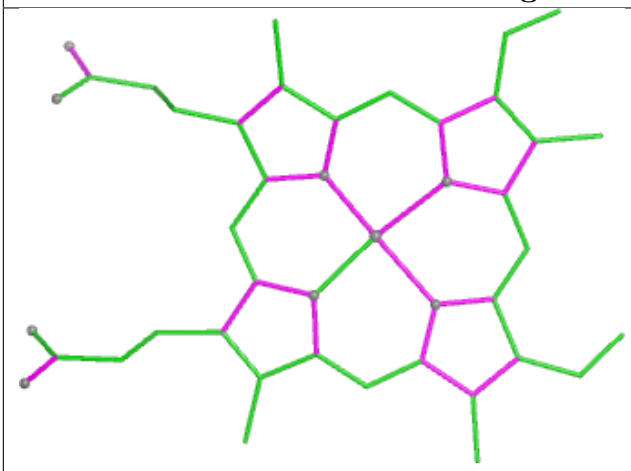


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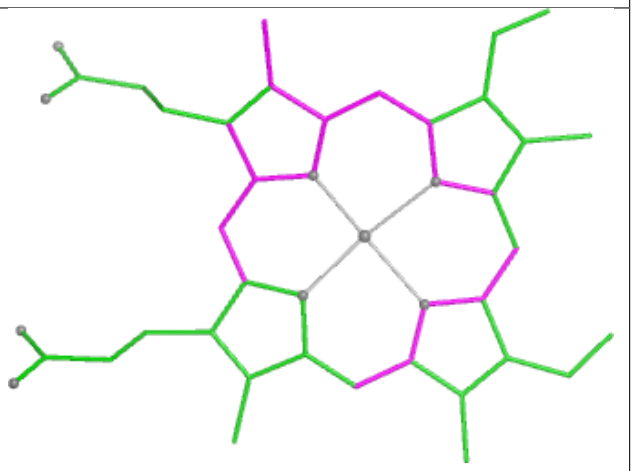


Rings

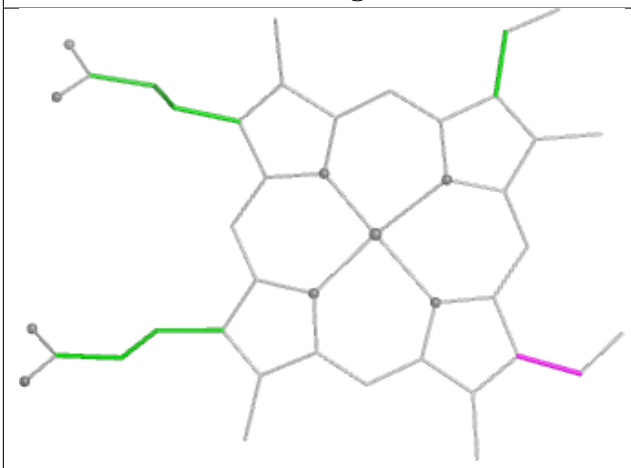
Ligand HEM E 501



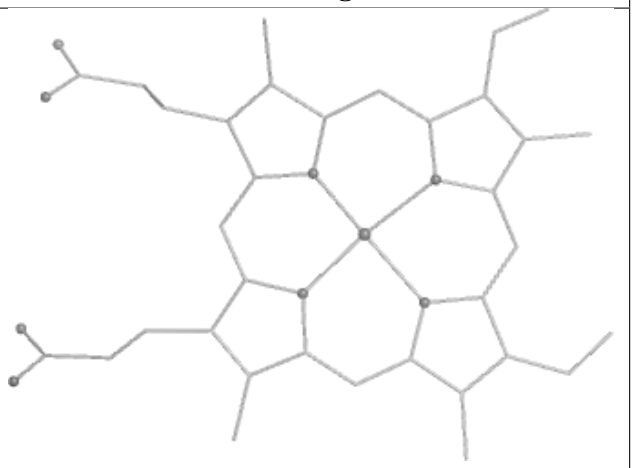
Bond lengths



Bond angles

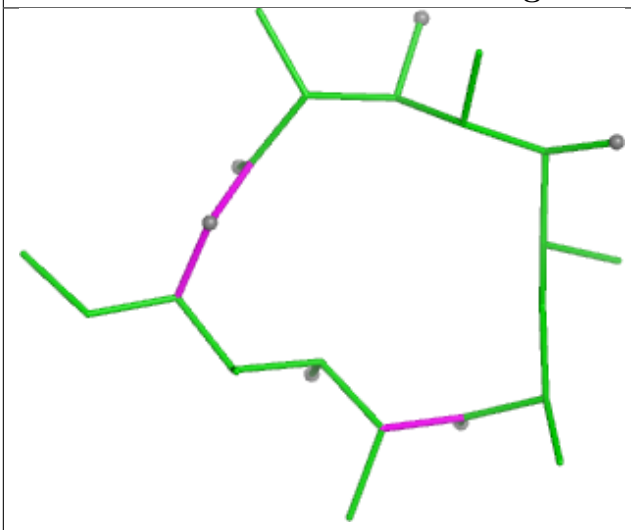


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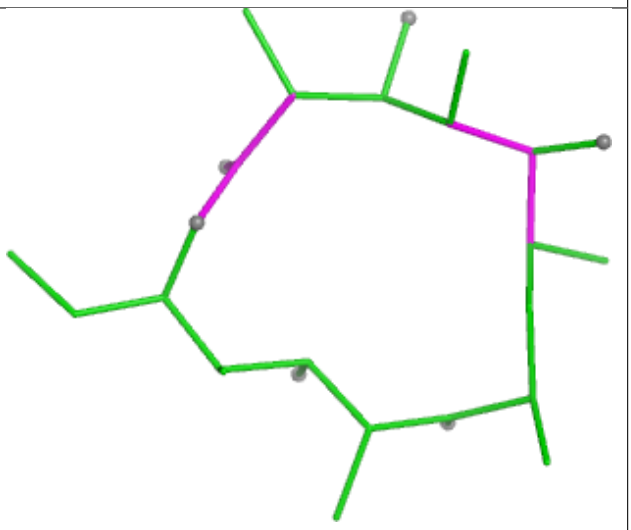


Rings

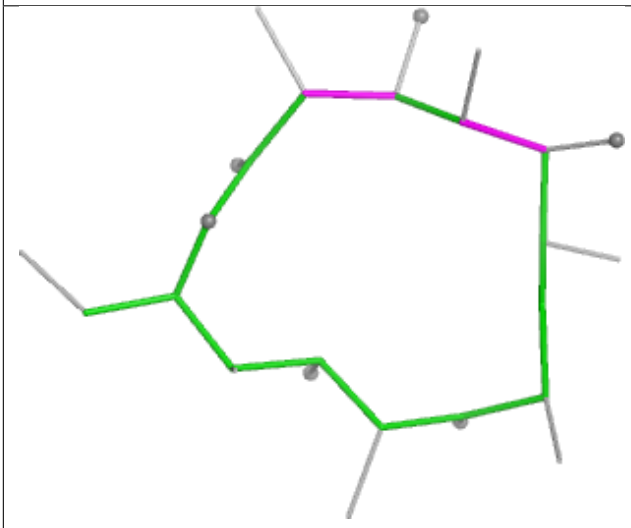
Ligand DEB B 502



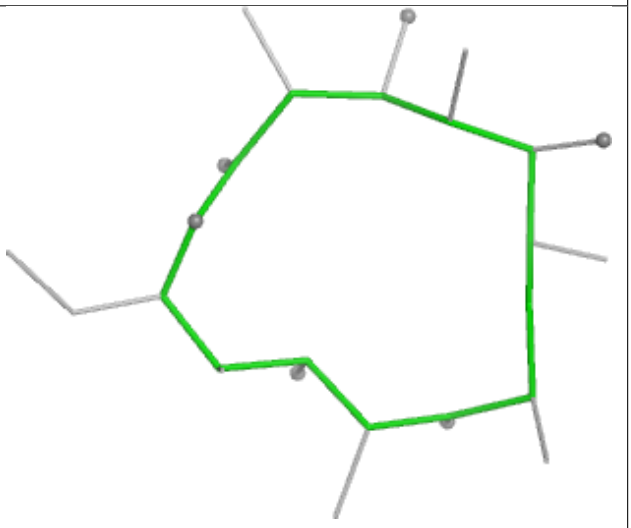
Bond lengths



Bond angles

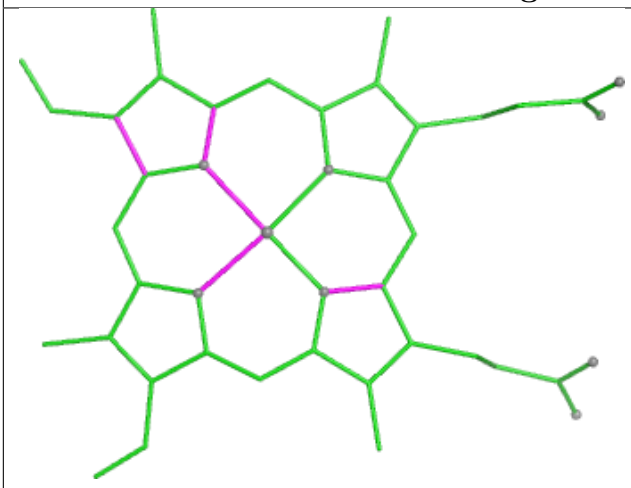


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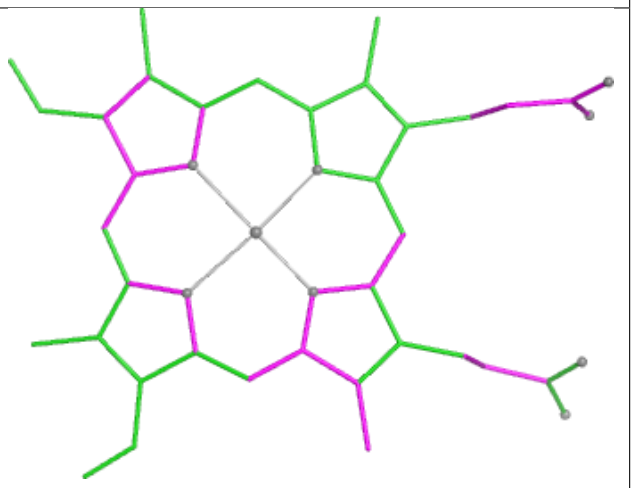


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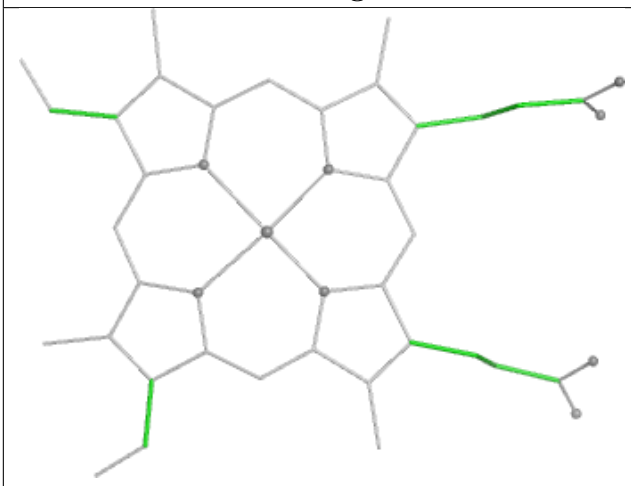
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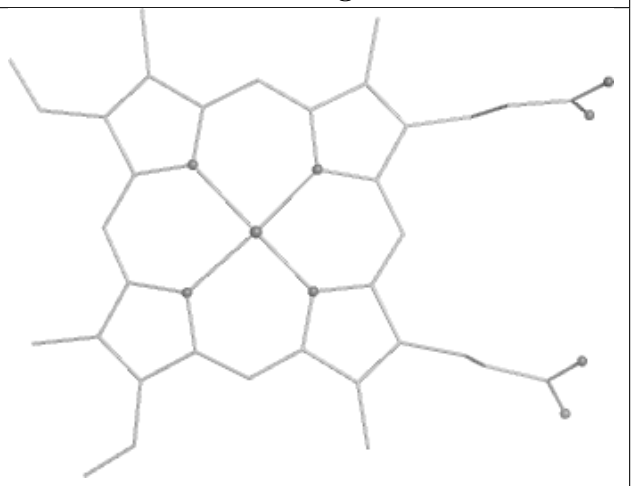
Bond lengths



Bond angles

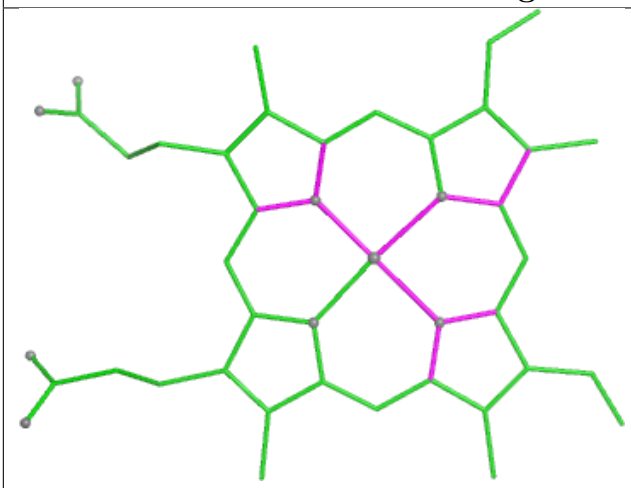


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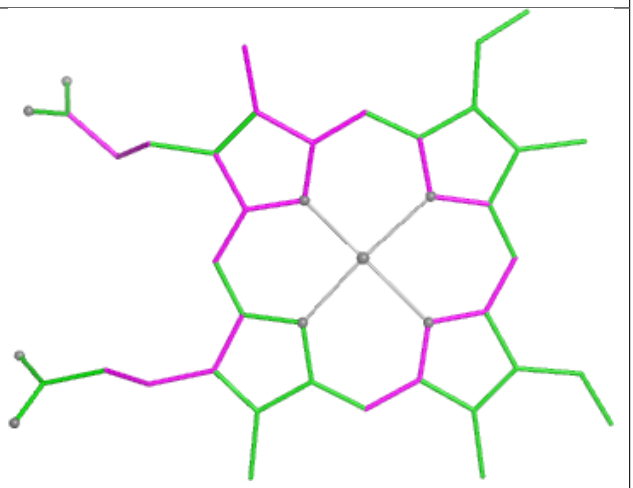


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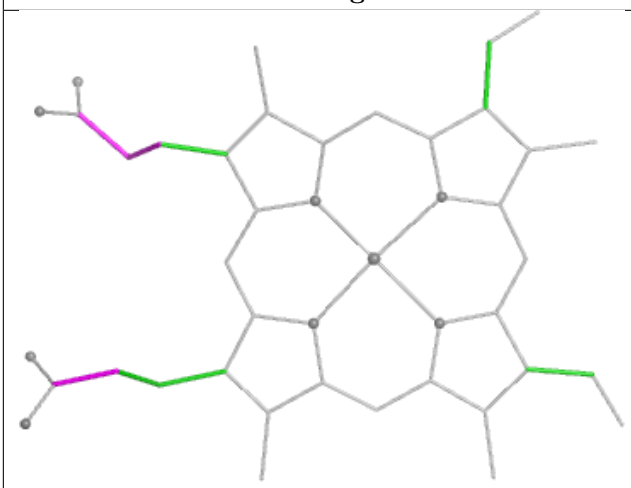
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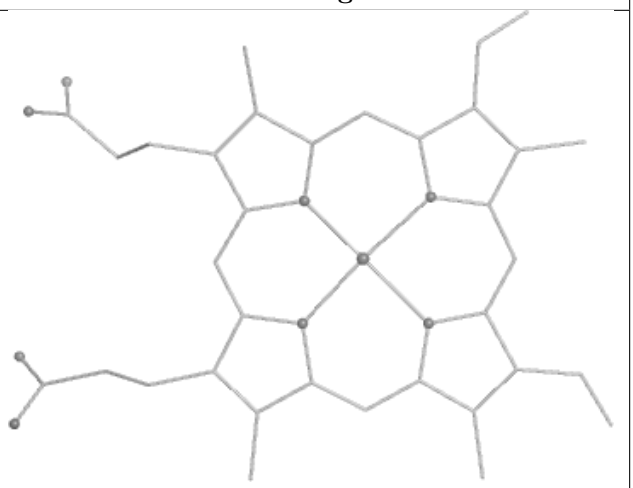
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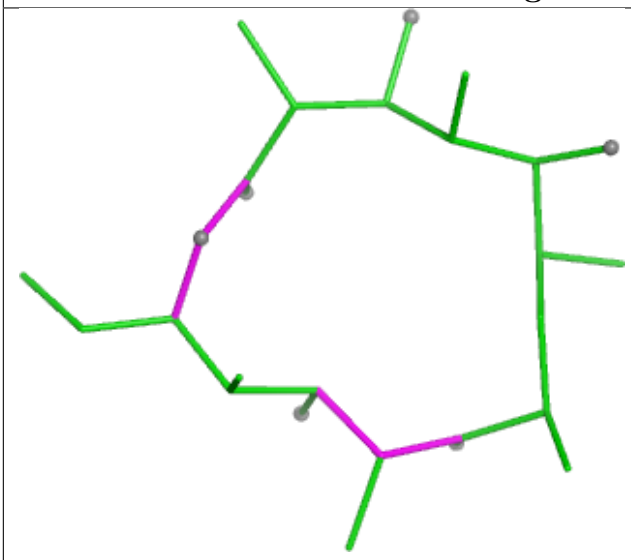


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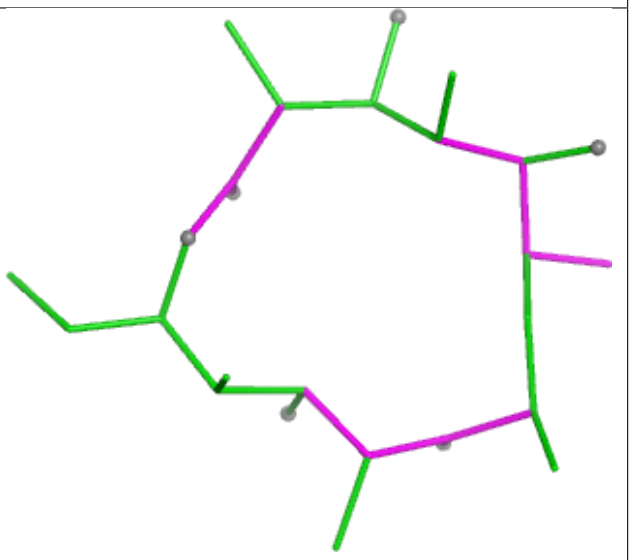


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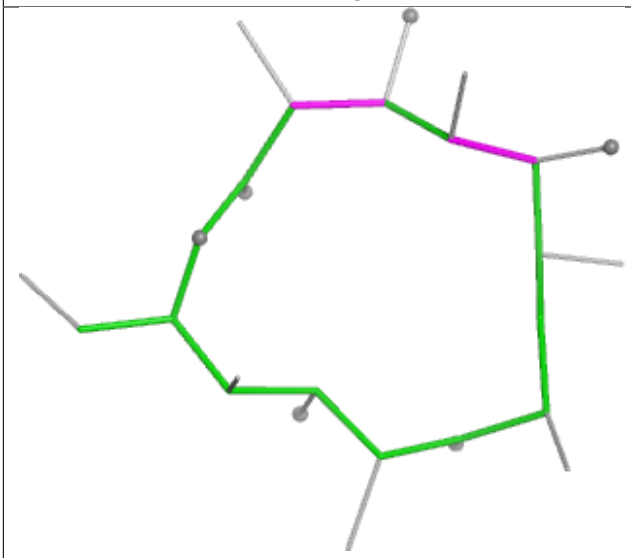
Ligand DEB E 502



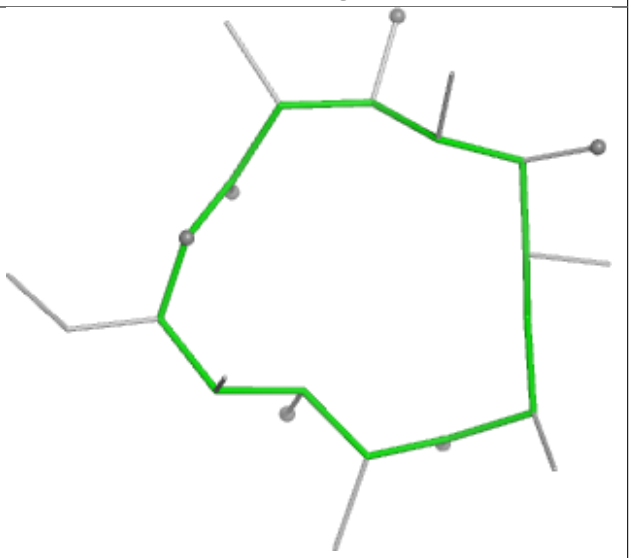
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Bond angles

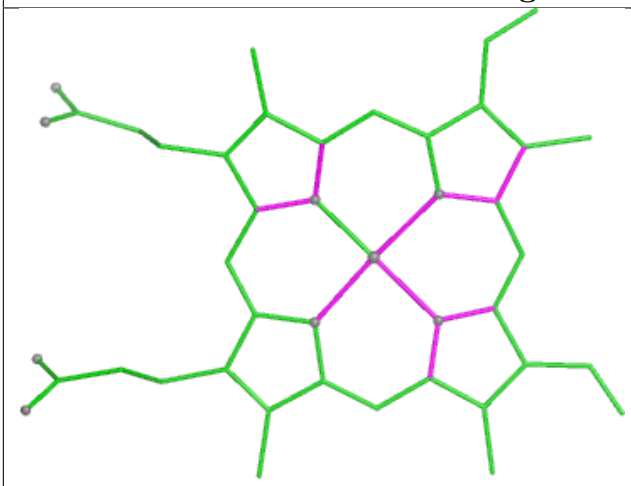


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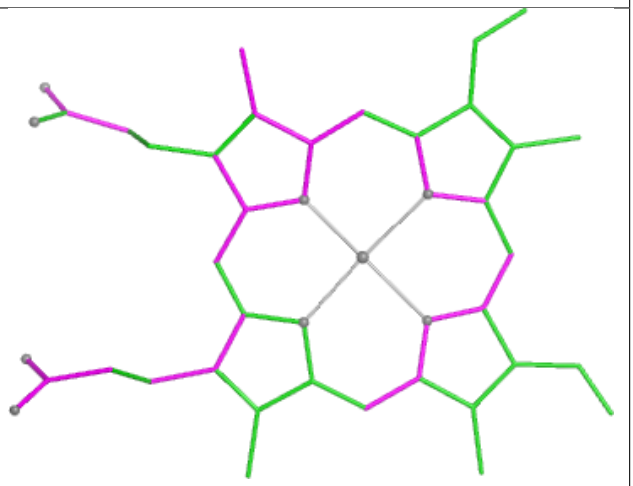


Rings

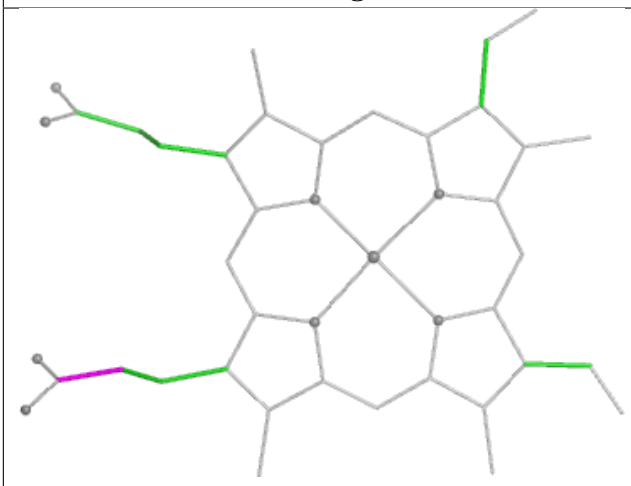
Ligand HEM B 501



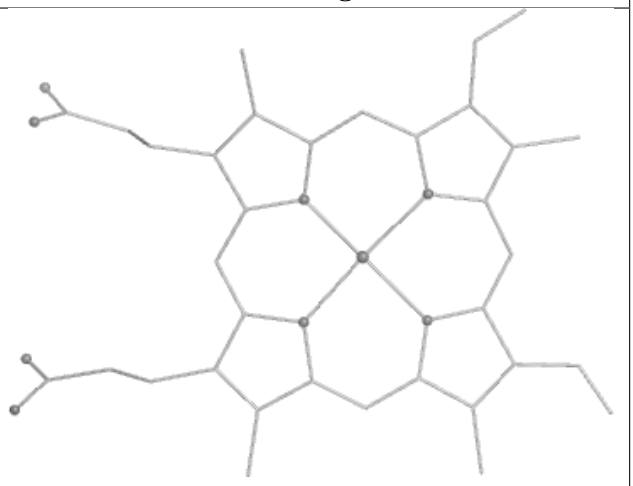
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Bond angles

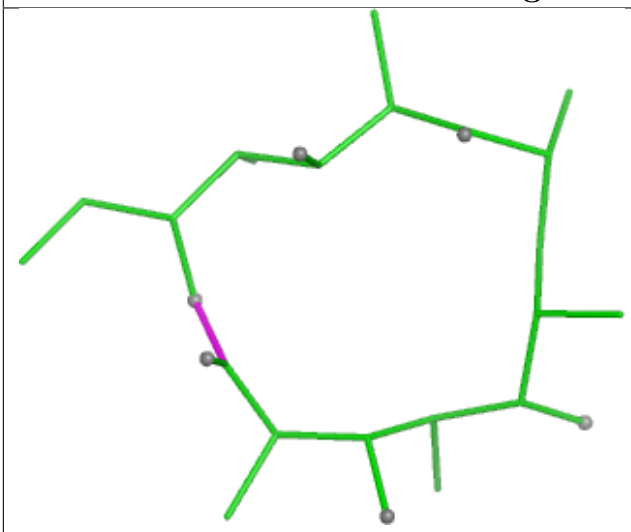


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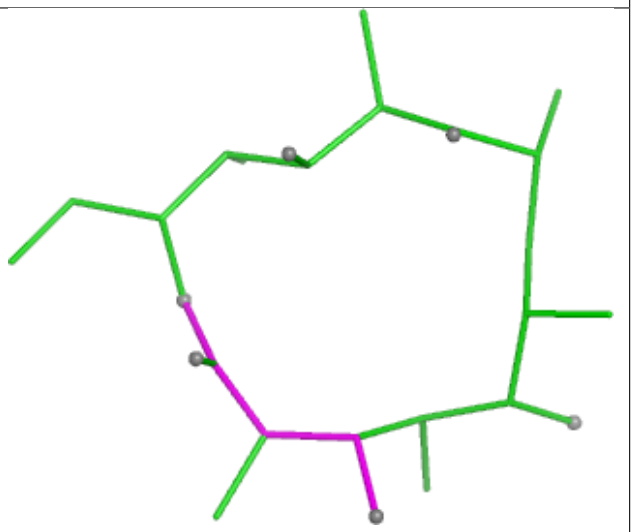


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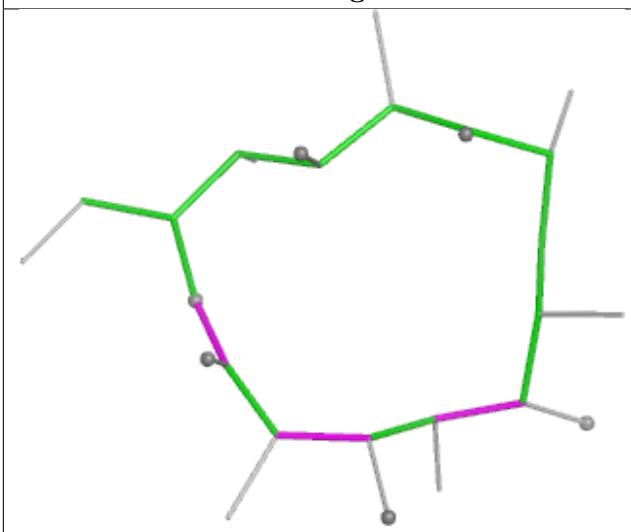
Ligand DEB C 502



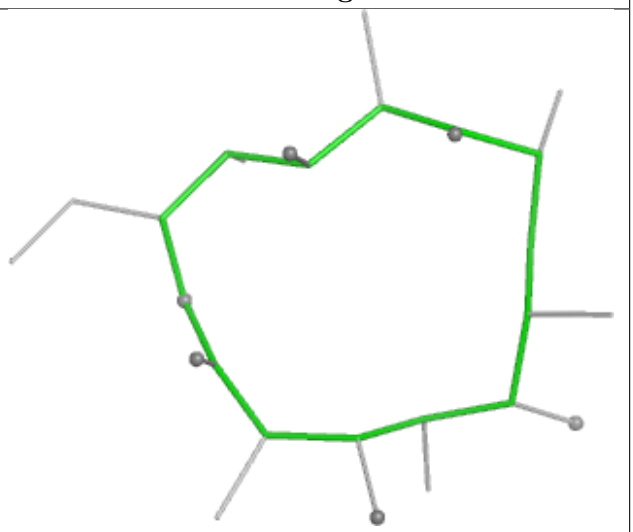
Bond lengths



Bond angles

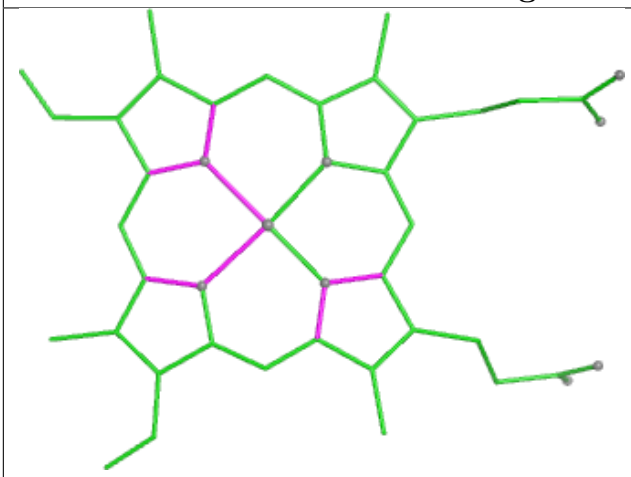


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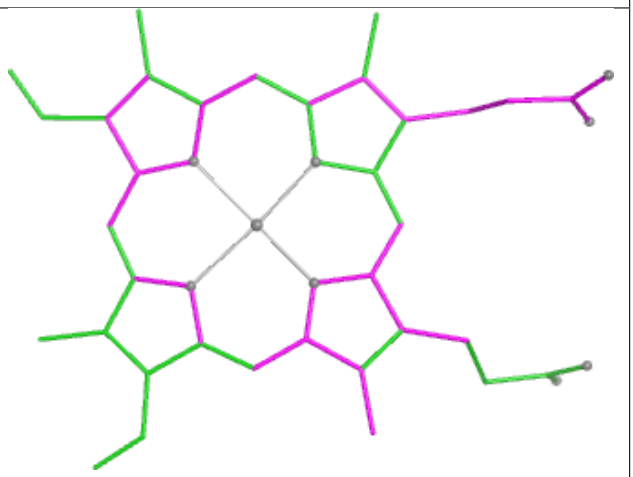


Rings

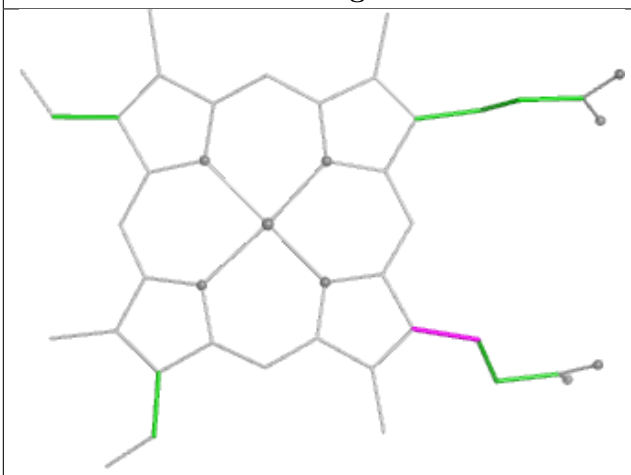
Ligand HEM C 501



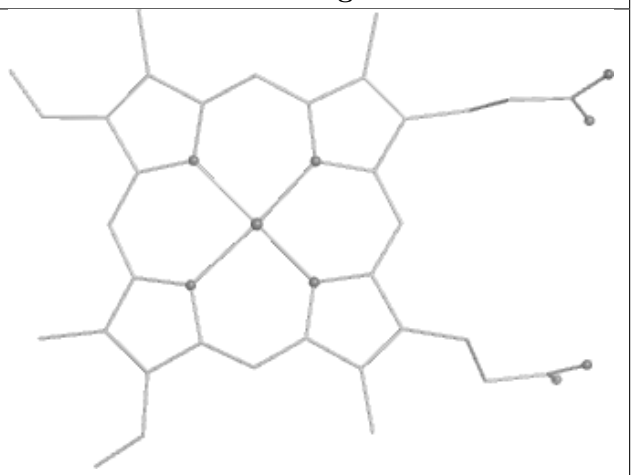
Bond lengths



Bond angles

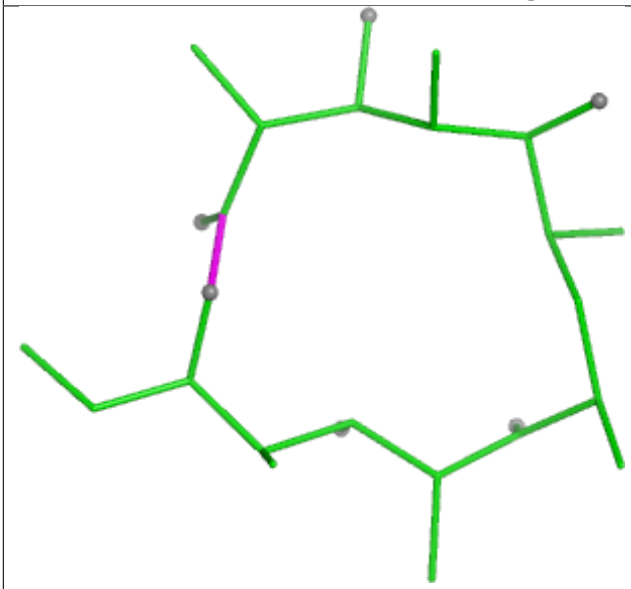


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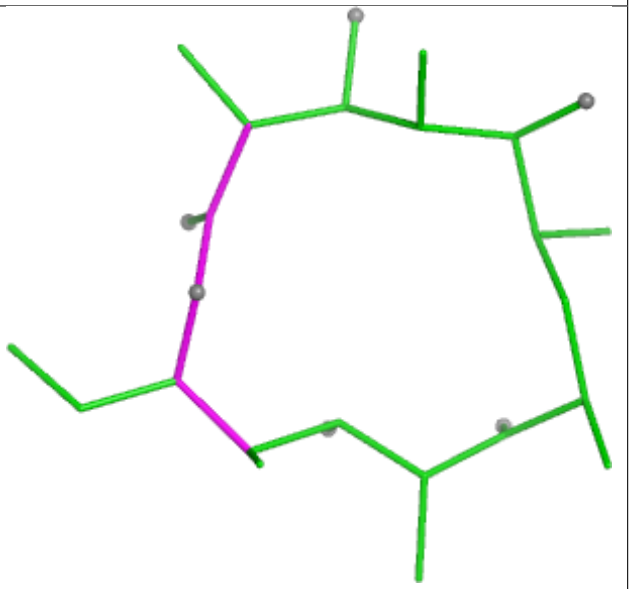


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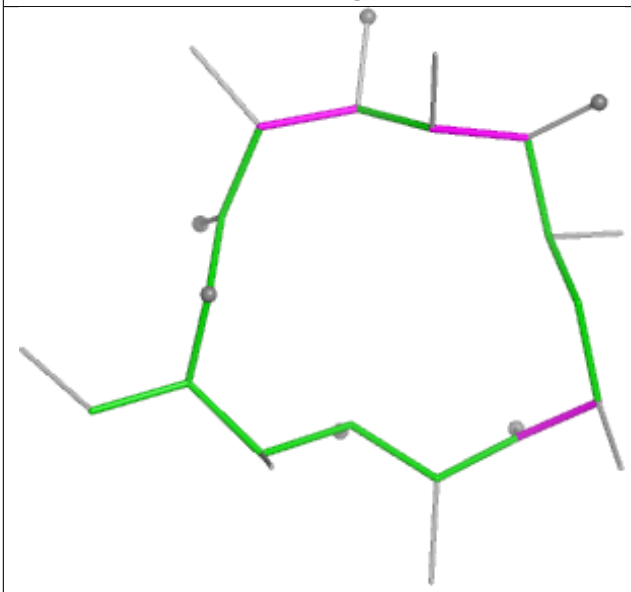
Ligand DEB D 502



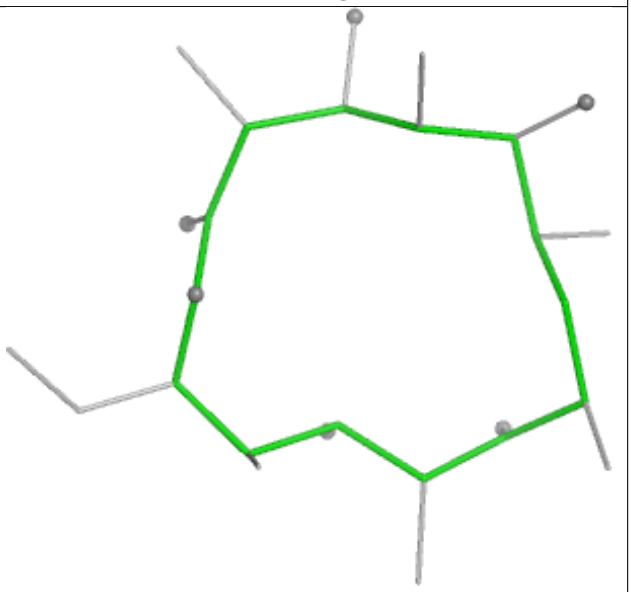
Bond lengths



Bond angles

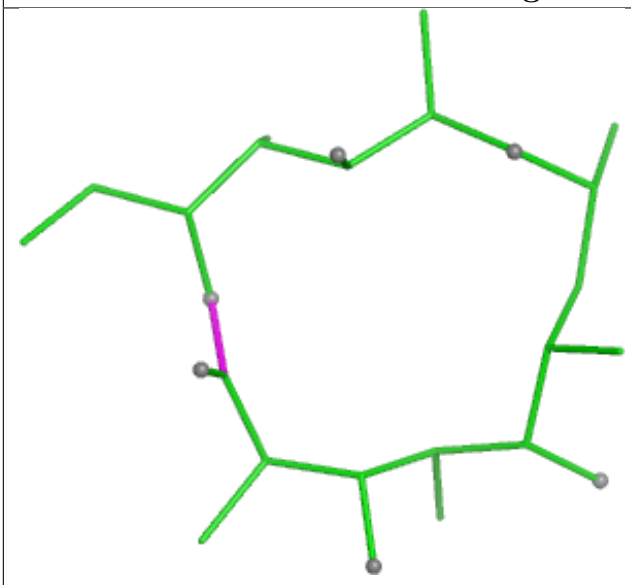


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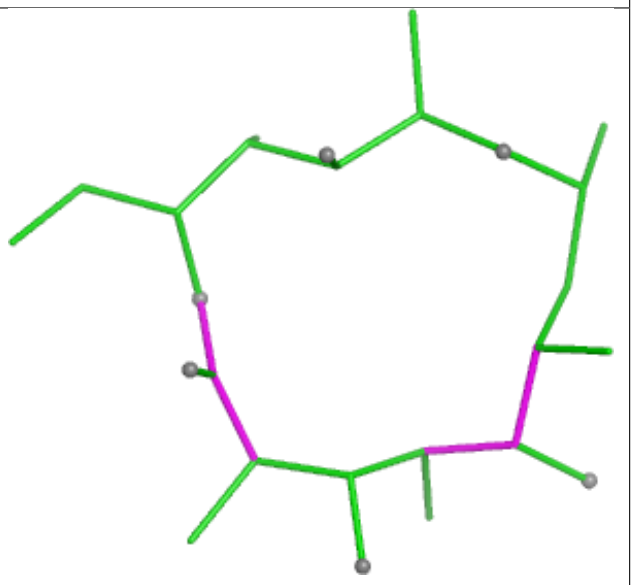


Rings

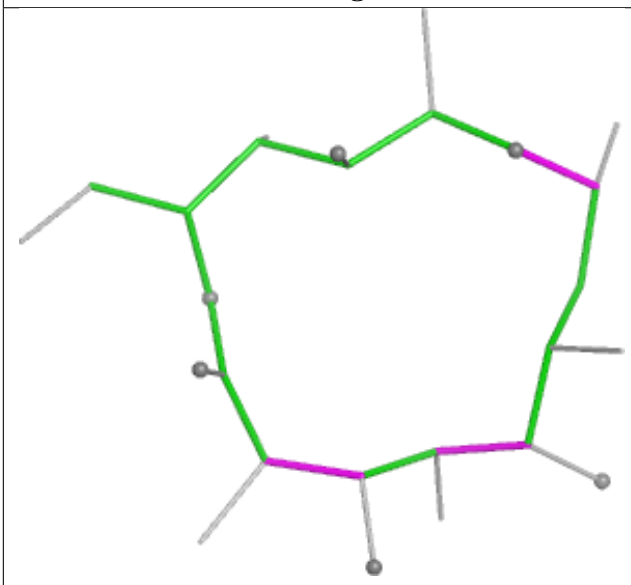
Ligand DEB A 502



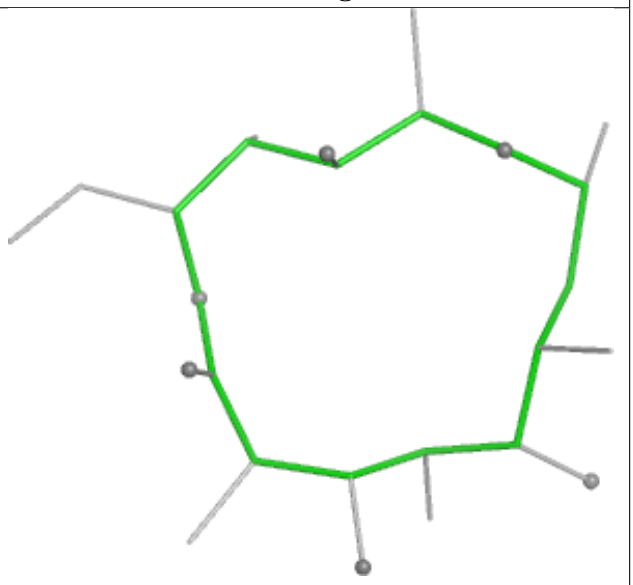
Bond lengths



Bond angles



Torsions



Rings

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	395/407 (97%)	0.19	14 (3%) 47 41	26, 48, 75, 102	0
1	B	395/407 (97%)	0.02	13 (3%) 49 44	18, 43, 66, 111	2 (0%)
1	C	395/407 (97%)	-0.25	5 (1%) 75 71	24, 37, 54, 88	0
1	D	395/407 (97%)	0.64	28 (7%) 22 18	33, 58, 86, 121	0
1	E	395/407 (97%)	0.63	36 (9%) 15 11	29, 64, 93, 120	1 (0%)
1	F	393/407 (96%)	1.21	78 (19%) 3 2	42, 72, 106, 121	0
All	All	2368/2442 (96%)	0.41	174 (7%) 21 17	18, 53, 91, 121	3 (0%)

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	227	ASP	5.7
1	F	276	LEU	5.4
1	F	267	TYR	5.2
1	B	225	ASN	5.0
1	E	212	THR	4.9

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

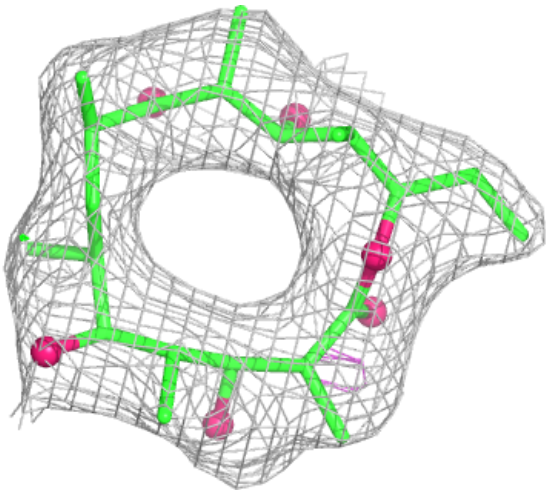
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

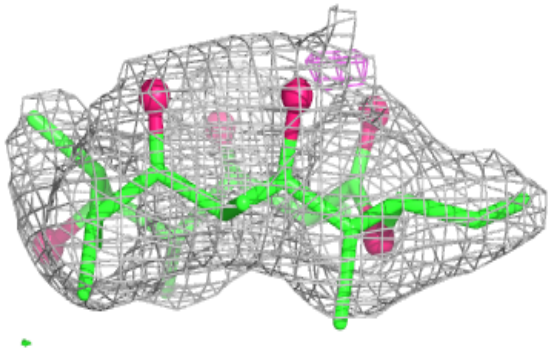
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DEB	F	502	27/27	0.92	0.12	54,58,61,61	0
3	DEB	D	502	27/27	0.93	0.11	39,43,47,50	0
4	HEM	E	501	43/43	0.93	0.11	39,44,50,60	0
3	DEB	E	502	27/27	0.94	0.09	40,43,45,45	0
4	HEM	F	501	43/43	0.94	0.12	50,70,76,84	0
3	DEB	C	502	27/27	0.95	0.08	25,28,31,32	0
2	HEC	A	501	43/43	0.96	0.08	24,26,29,34	0
3	DEB	A	502	27/27	0.96	0.09	27,28,29,30	0
3	DEB	B	502	27/27	0.96	0.08	29,32,33,33	0
4	HEM	D	501	43/43	0.97	0.07	22,24,36,44	0
4	HEM	C	501	43/43	0.98	0.06	23,25,29,36	0
4	HEM	B	501	43/43	0.98	0.06	20,22,26,29	0

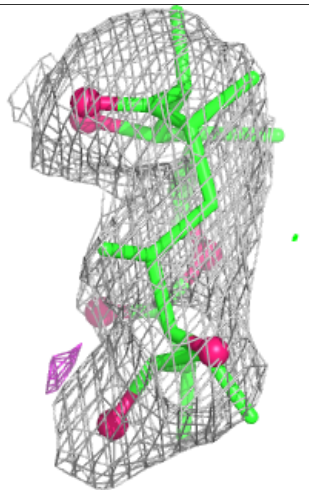
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DEB 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)

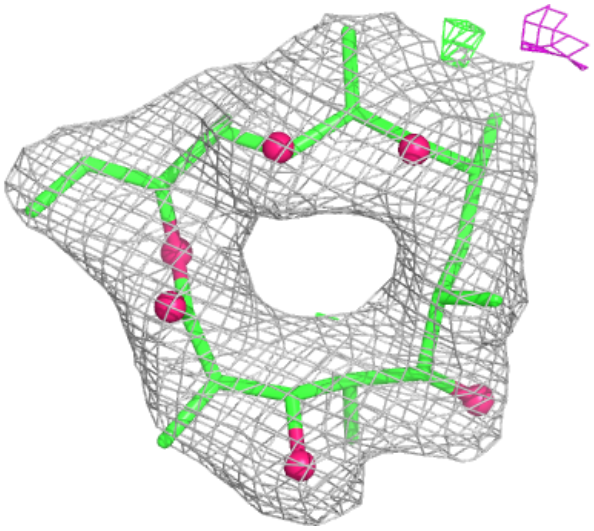


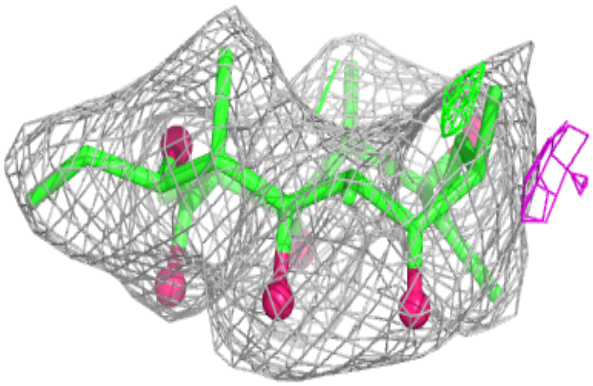


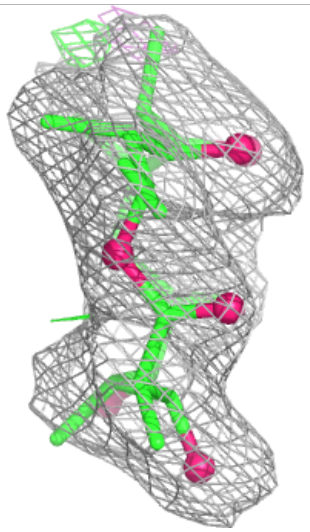


Electron density around DEB D 502:

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

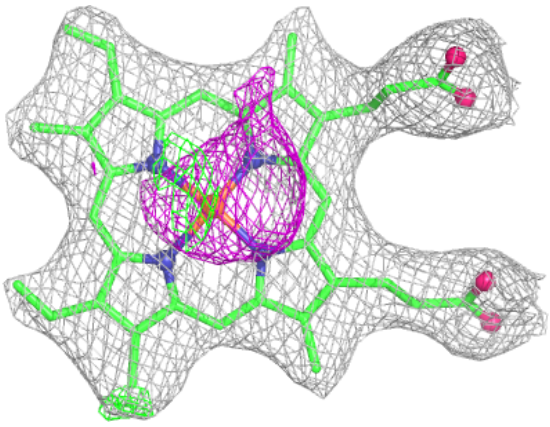


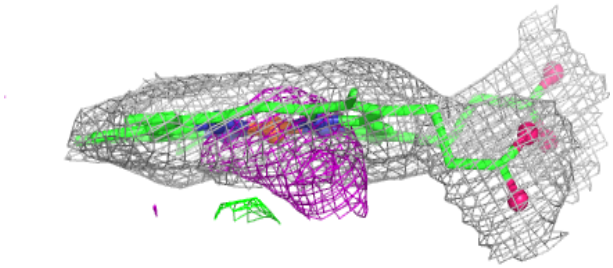


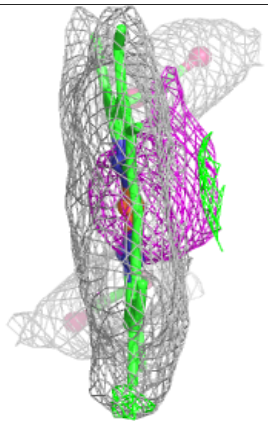


Electron density around HEM E 501:

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

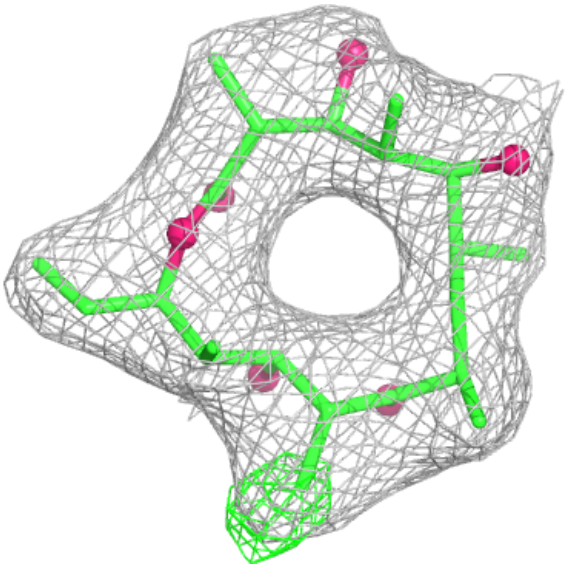


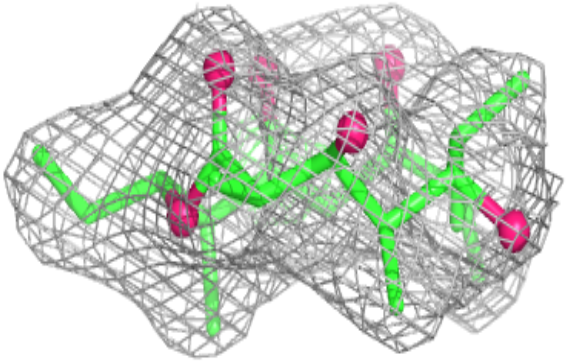


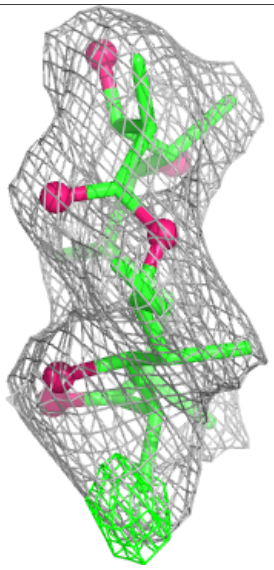


Electron density around DEB E 502:

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

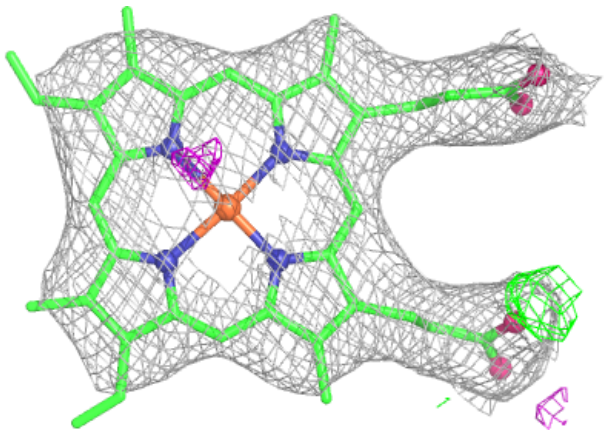


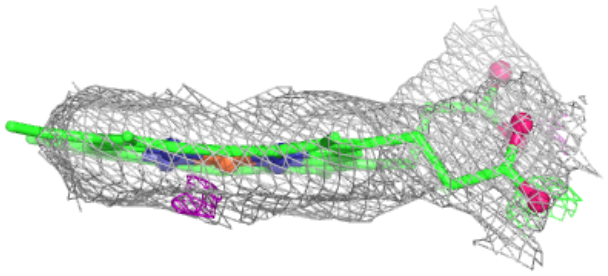


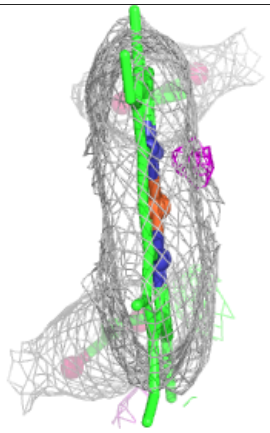


Electron density around HEM F 501:

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

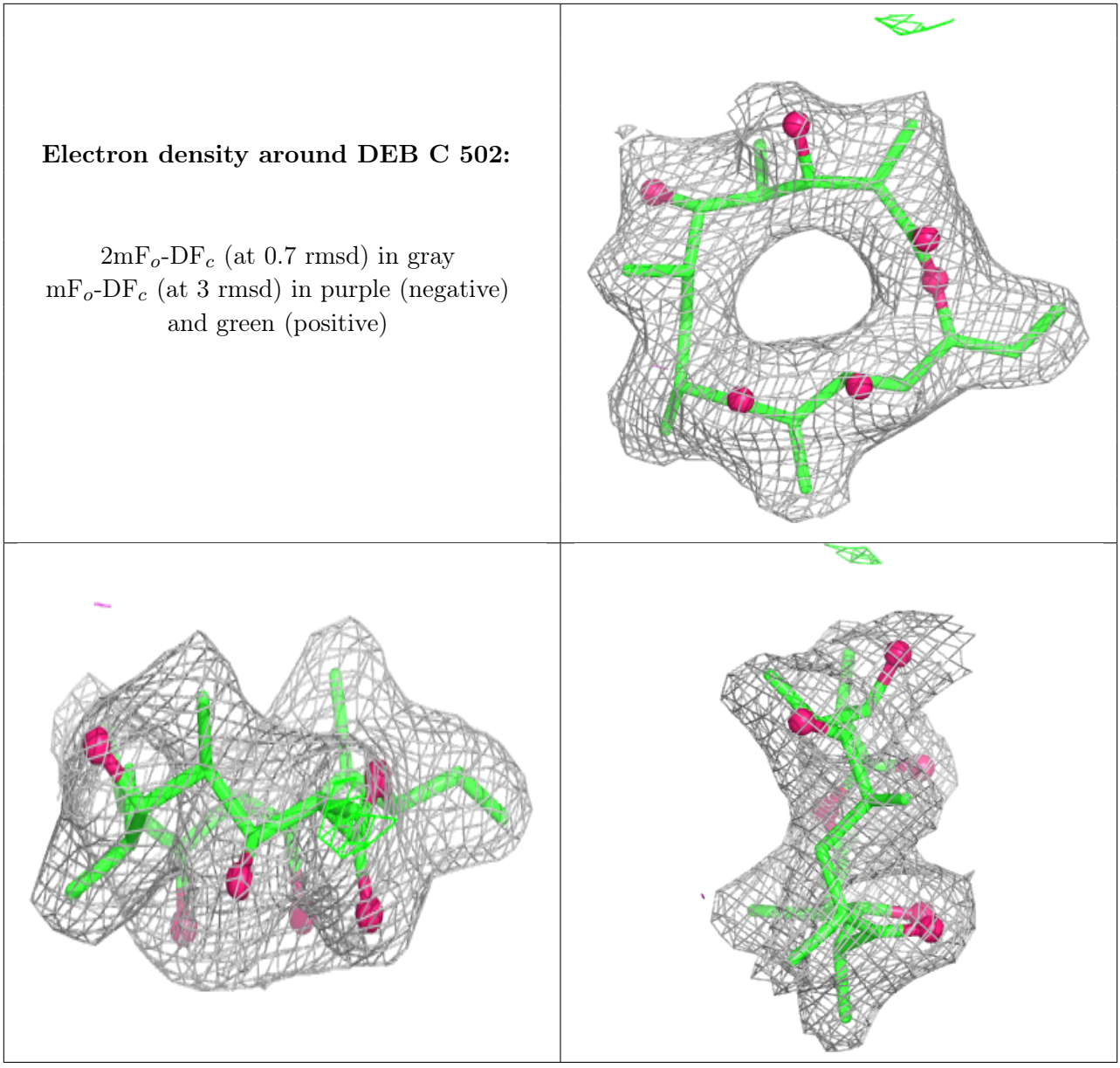






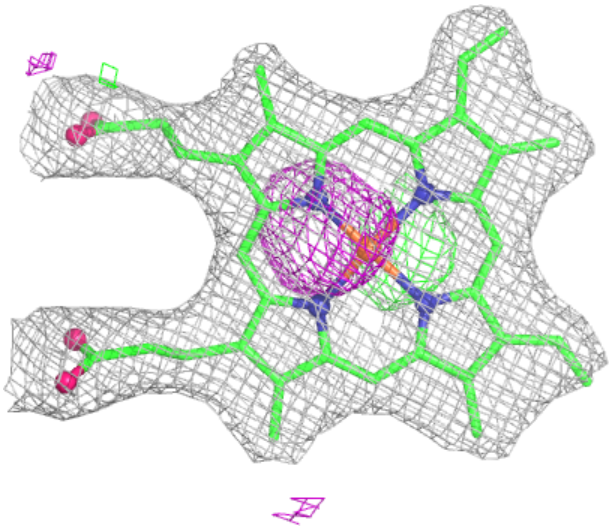
Electron density around DEB C 502:

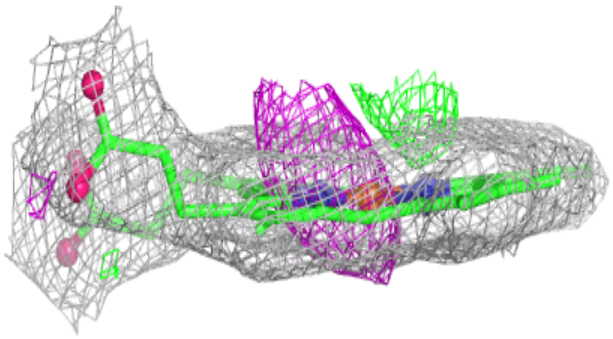
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

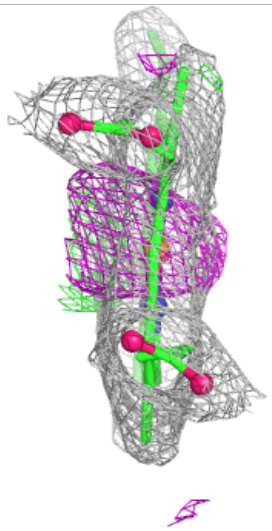


Electron density around HEC A 501:

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

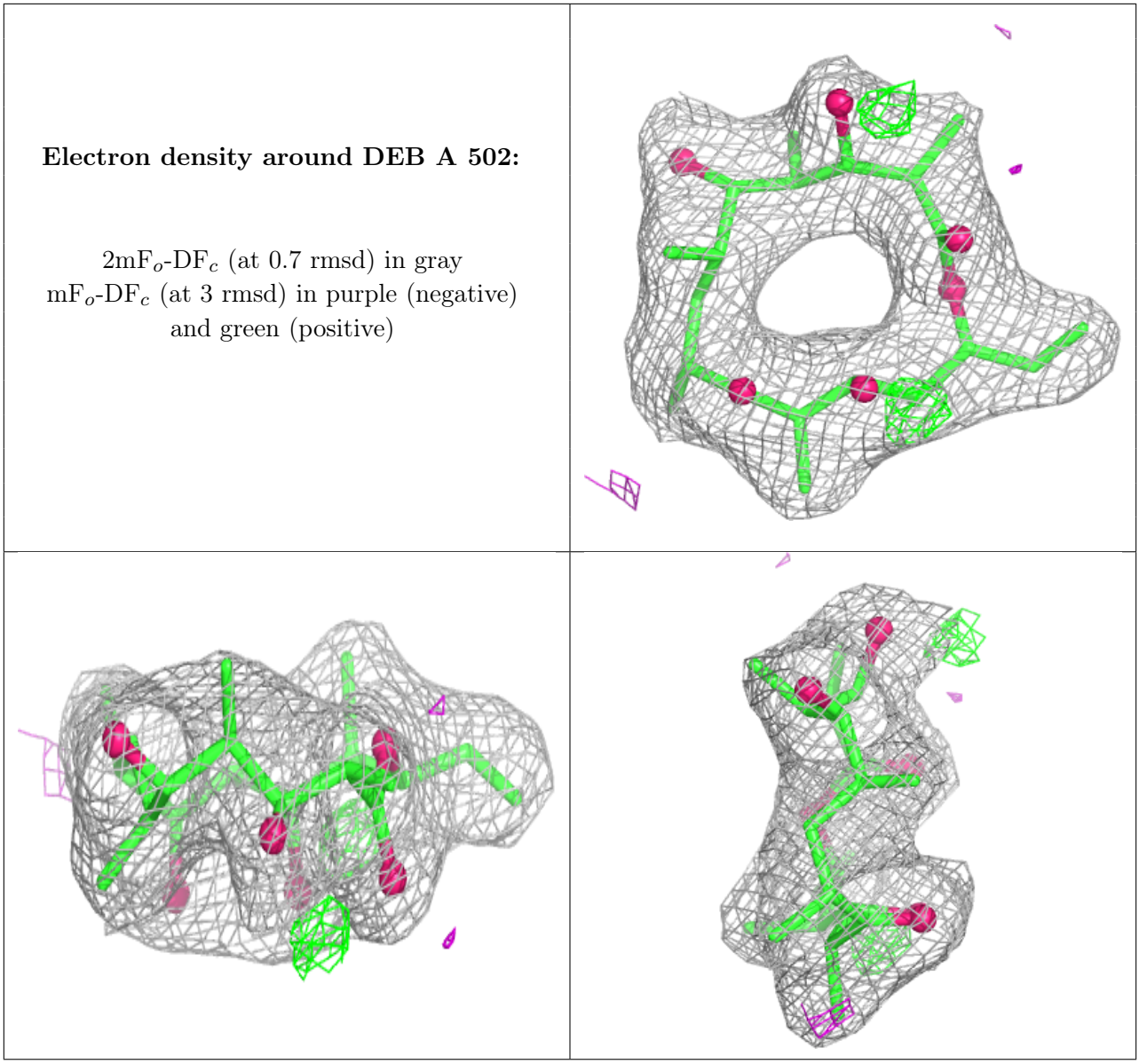






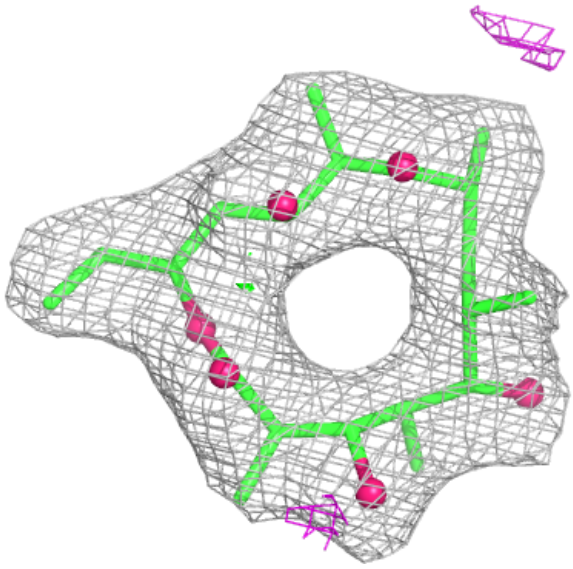
Electron density around DEB A 502:

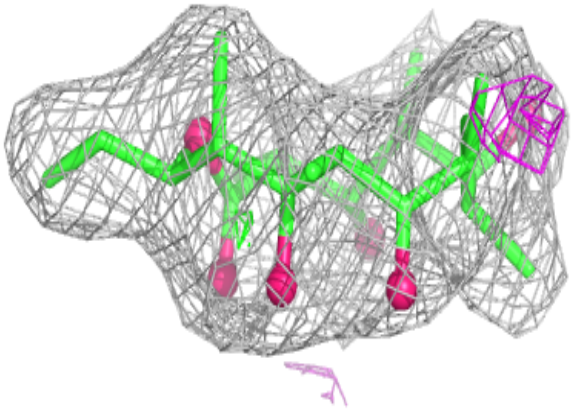
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

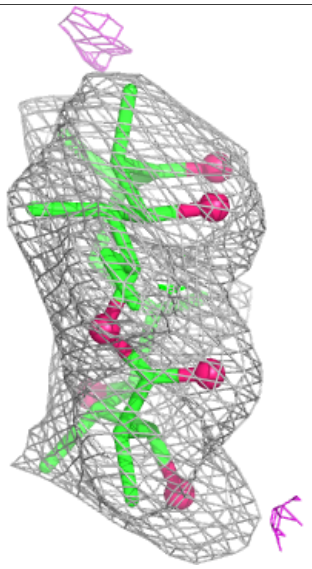


Electron density around DEB B 502:

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

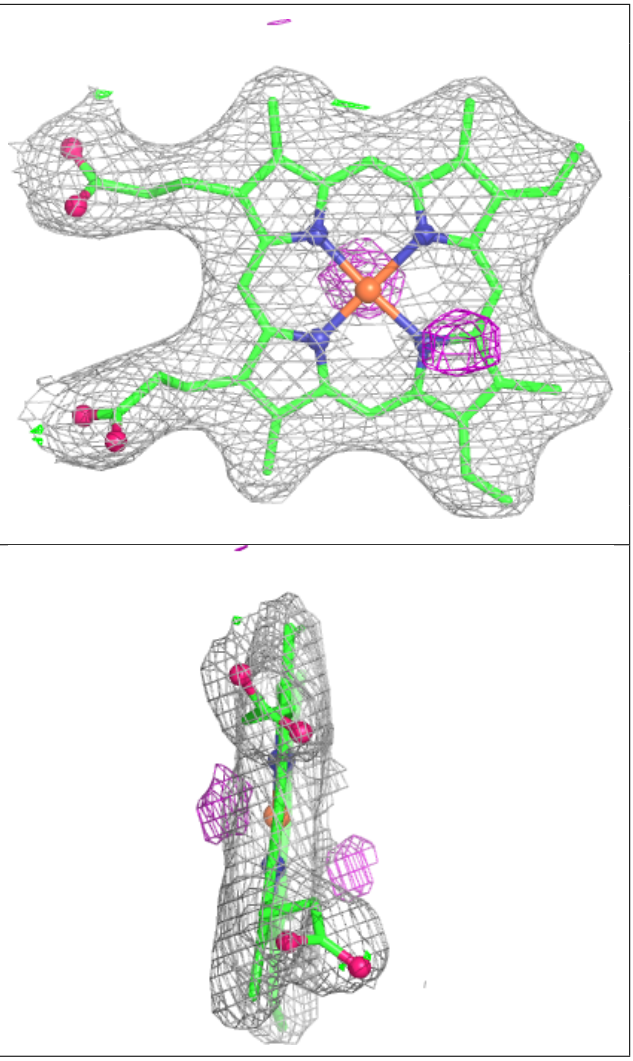






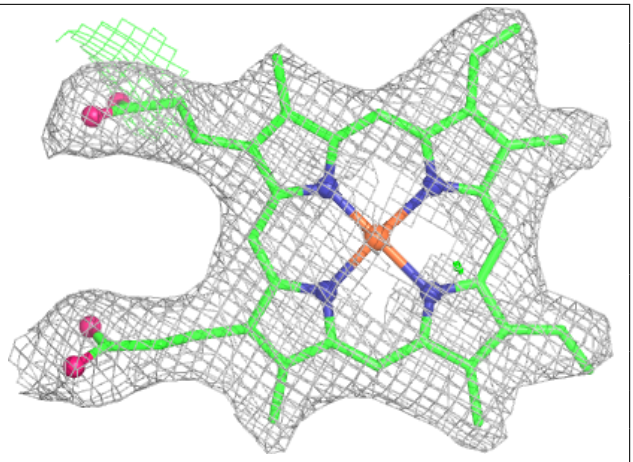
Electron density around HEM D 501:

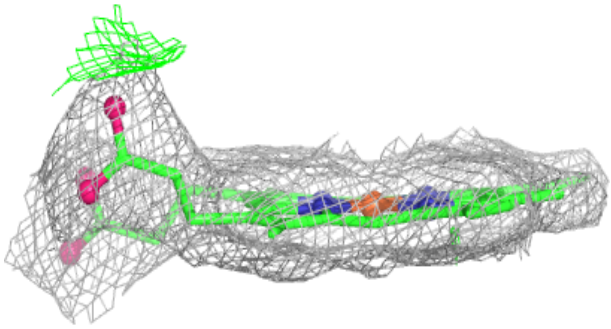
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

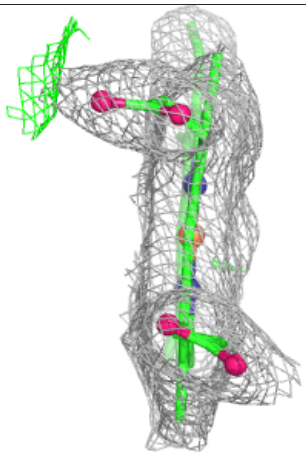


Electron density around HEM C 501:

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

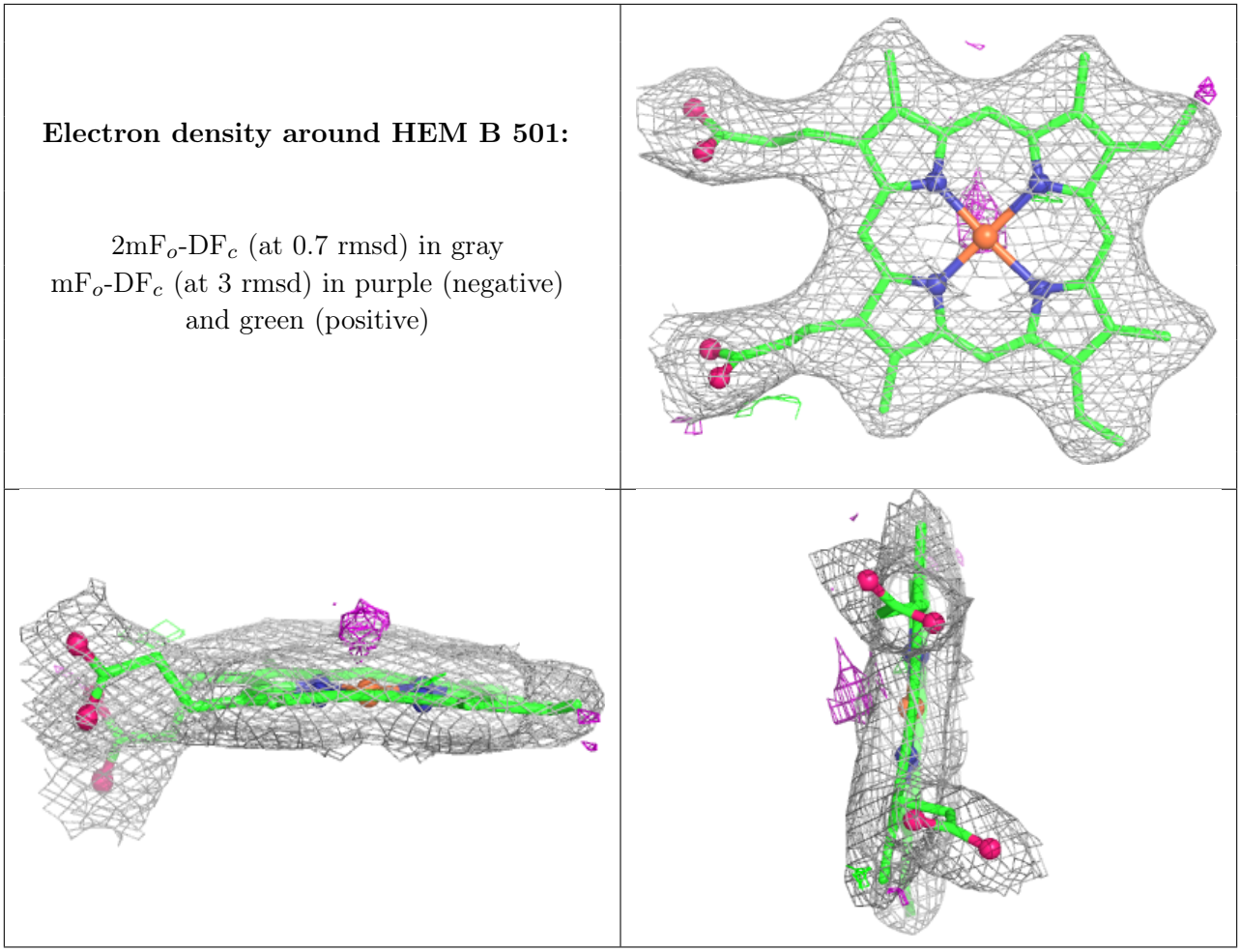






Electron density around HEM B 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.