wwPDB X-ray Structure Validation Summary Report (i)

Jan 19, 2022 – 07:19 pm GMT

PDB ID	:	7Q89
Title	:	OleP mutant G92W in complex with 6DEB
Authors	:	Savino, C.; Montemiglio, L.C.; Vallone, B.; Exertier, C.; Freda, I.; Gugole, E.
Deposited on	:	2021-11-10
Resolution	:	2.08 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:

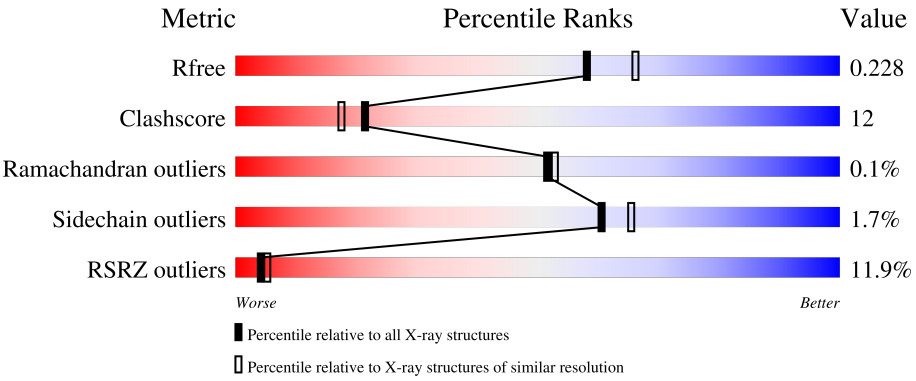
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	408	7% 78% 18%
1	B	408	5% 82% 16%
1	C	408	4% 88% 12%
1	D	408	9% 74% 22%
1	E	408	20% 78% 18%

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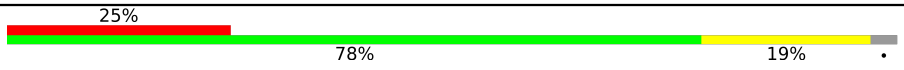
Mol	Chain	Length	Quality of chain
1	F	408	

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
4	FMT	A	509	-	-	-	X
4	FMT	A	510	-	-	X	-
4	FMT	A	525	-	-	X	-
4	FMT	A	526	-	-	X	-
4	FMT	A	531	-	-	-	X
4	FMT	A	535	-	-	-	X
4	FMT	A	537	-	-	-	X
4	FMT	B	506	-	-	X	-
4	FMT	B	511	-	-	X	-
4	FMT	B	512	-	-	X	-
4	FMT	B	513	-	-	X	-
4	FMT	B	516	-	-	-	X
4	FMT	B	520	-	-	X	-
4	FMT	B	524	-	-	-	X
4	FMT	B	525	-	-	-	X
4	FMT	B	534	-	-	-	X
4	FMT	B	537	-	-	X	-
4	FMT	B	538	-	-	X	-
4	FMT	C	513	-	-	-	X
4	FMT	C	514	-	-	-	X
4	FMT	C	520	-	-	-	X
4	FMT	C	522	-	-	X	-
4	FMT	C	524	-	-	X	-
4	FMT	D	508	-	-	X	-
4	FMT	D	515	-	-	X	-
4	FMT	E	506	-	-	X	-
4	FMT	E	507	-	-	-	X
4	FMT	E	510	-	-	-	X
4	FMT	F	507	-	-	-	X
6	GOL	A	542	-	-	-	X
6	GOL	B	543[A]	-	-	X	-
6	GOL	B	543[B]	-	-	X	-
6	GOL	C	532	-	-	-	X
6	GOL	E	515[A]	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 21704 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.

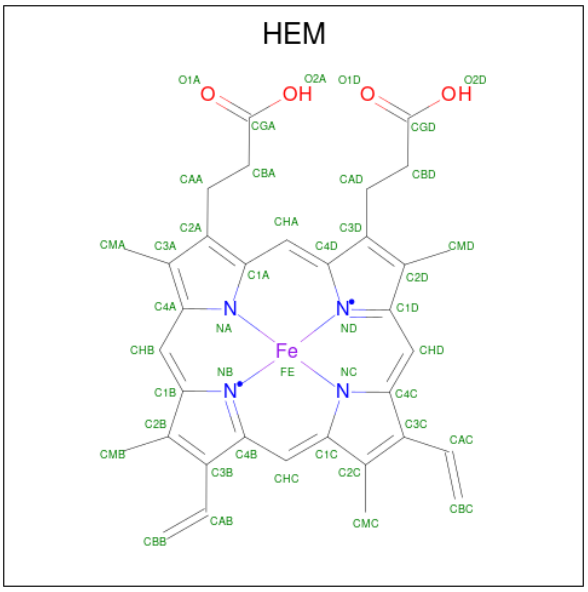
- Molecule 1 is a protein called Cytochrome P-450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	32	0
			3298	2092	595	596	15			
1	B	402	Total	C	N	O	S	0	33	0
			3331	2113	597	606	15			
1	C	408	Total	C	N	O	S	0	29	0
			3354	2128	598	611	17			
1	D	396	Total	C	N	O	S	0	16	0
			3186	2018	564	589	15			
1	E	395	Total	C	N	O	S	0	9	0
			3141	1985	558	580	18			
1	F	396	Total	C	N	O	S	0	6	0
			3132	1976	556	584	16			

There are 12 discrepancies between the modelled and reference sequences:

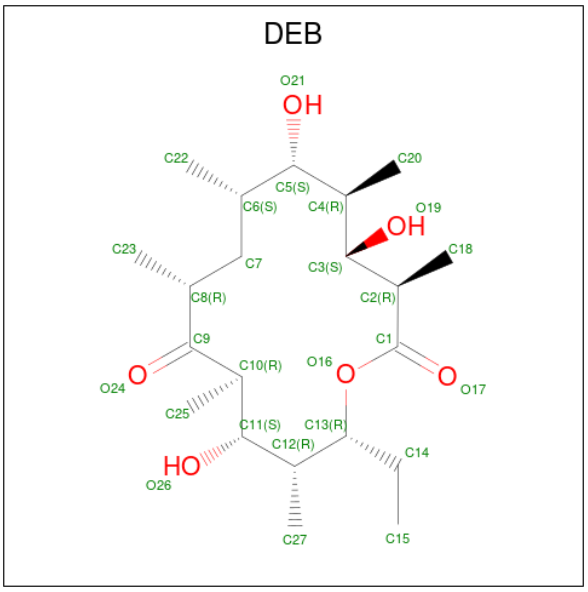
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q59819
A	92	TRP	GLY	engineered mutation	UNP Q59819
B	0	HIS	-	expression tag	UNP Q59819
B	92	TRP	GLY	engineered mutation	UNP Q59819
C	0	HIS	-	expression tag	UNP Q59819
C	92	TRP	GLY	engineered mutation	UNP Q59819
D	0	HIS	-	expression tag	UNP Q59819
D	92	TRP	GLY	engineered mutation	UNP Q59819
E	0	HIS	-	expression tag	UNP Q59819
E	92	TRP	GLY	engineered mutation	UNP Q59819
F	0	HIS	-	expression tag	UNP Q59819
F	92	TRP	GLY	engineered mutation	UNP Q59819

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



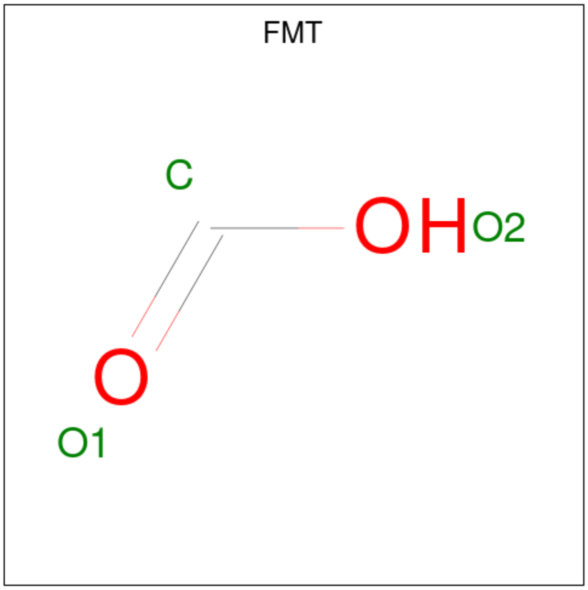
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 6-DEOXYERYTHRONOLIDE B (three-letter code: DEB) (formula: $C_{21}H_{38}O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

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

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	B	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0

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

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

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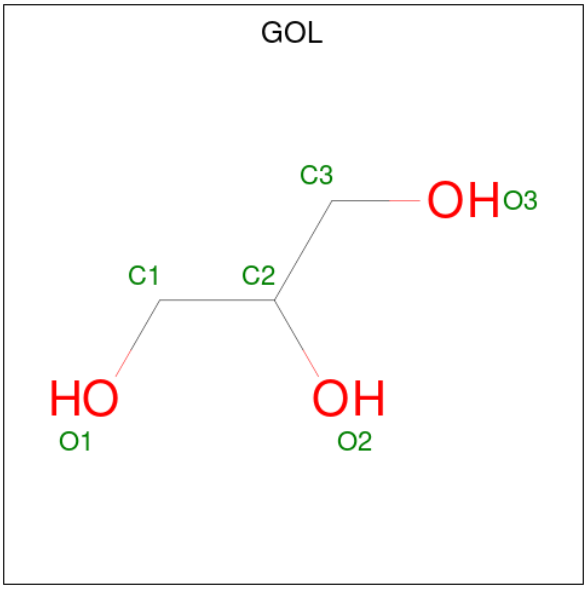
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0
4	E	1	Total C O 3 1 2	0	0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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Na 2 2	0	0
5	B	2	Total Na 2 2	0	0
5	C	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0
5	E	1	Total Na 1 1	0	0
5	F	1	Total Na 1 1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 12 6 6	0	1
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 12 6 6	0	1
6	C	1	Total C O 12 6 6	0	1
6	C	1	Total C O 6 3 3	0	0
6	E	1	Total C O 12 6 6	0	1

- Molecule 7 is water.

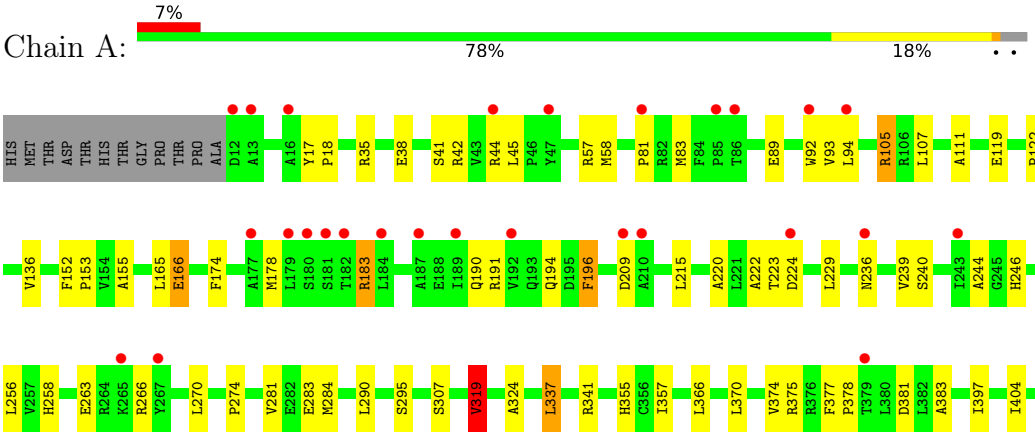
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	301	Total O 301 301	0	0
7	B	258	Total O 258 258	0	0
7	C	308	Total O 308 308	0	0
7	D	169	Total O 169 169	0	0
7	E	146	Total O 146 146	0	0
7	F	157	Total O 157 157	0	0

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.

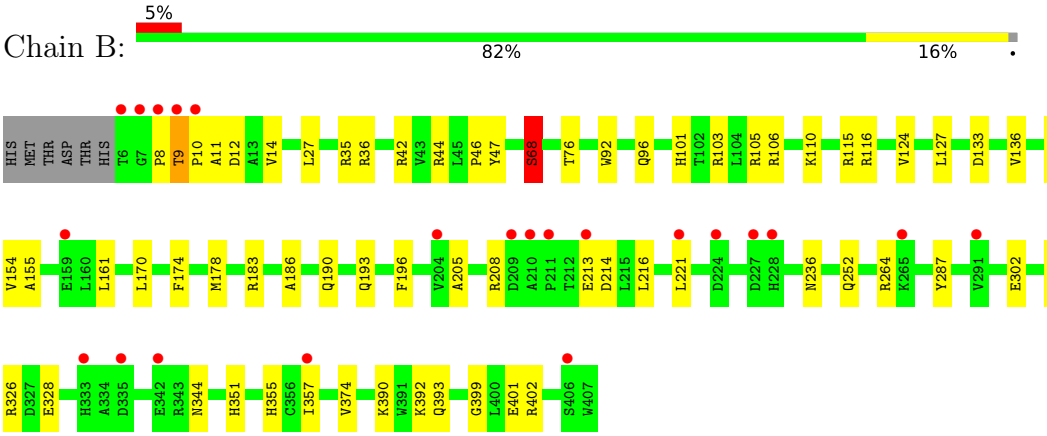
• Molecule 1: Cytochrome P-450

Chain A:



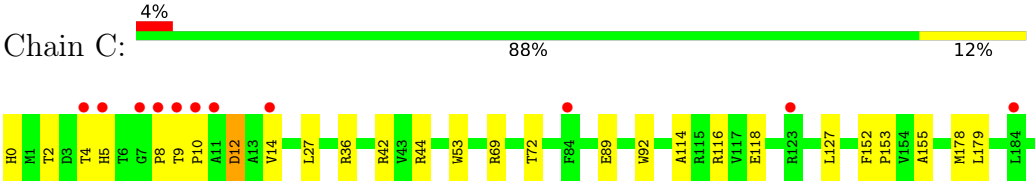
• Molecule 1: Cytochrome P-450

Chain B:

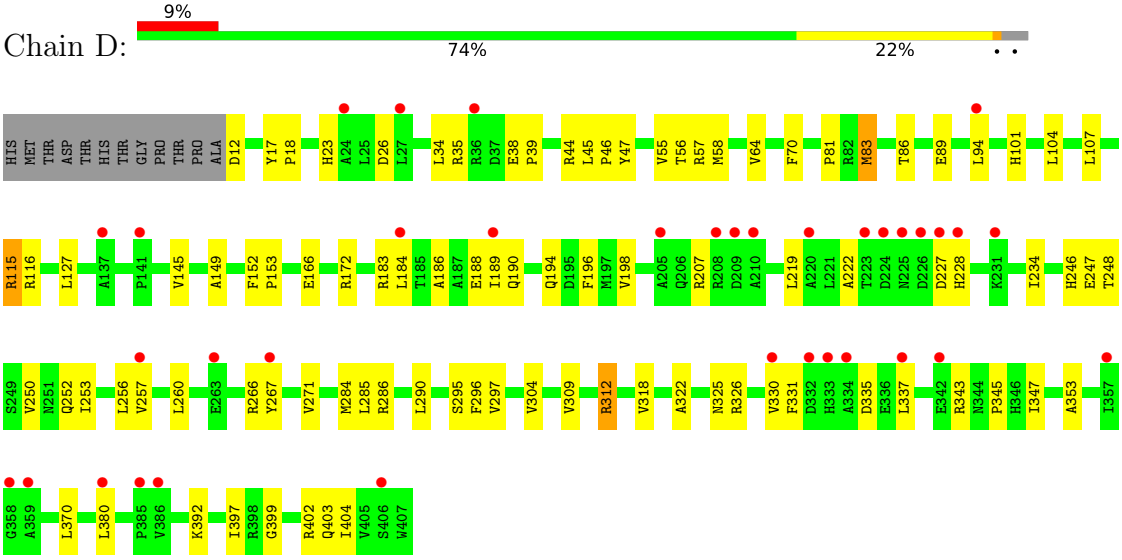


• Molecule 1: Cytochrome P-450

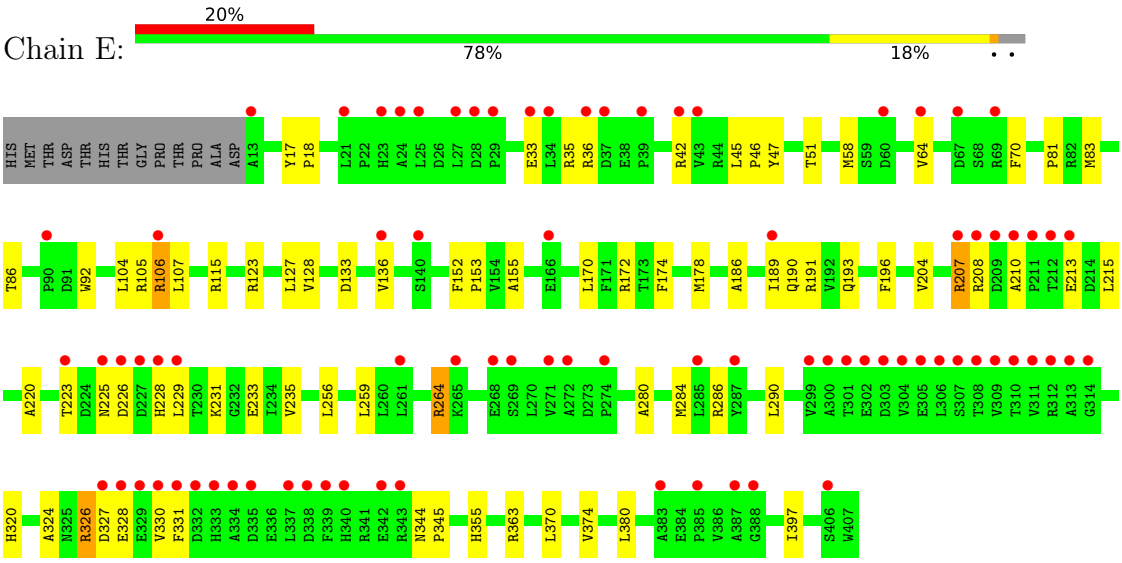
Chain C:



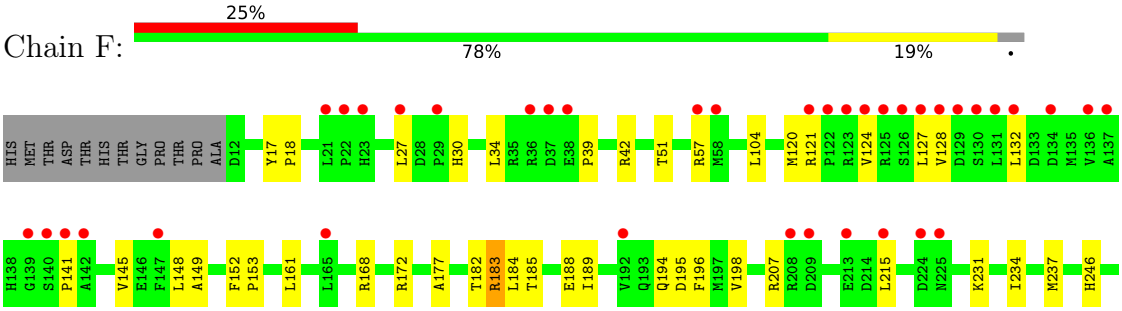
• Molecule 1: Cytochrome P-450

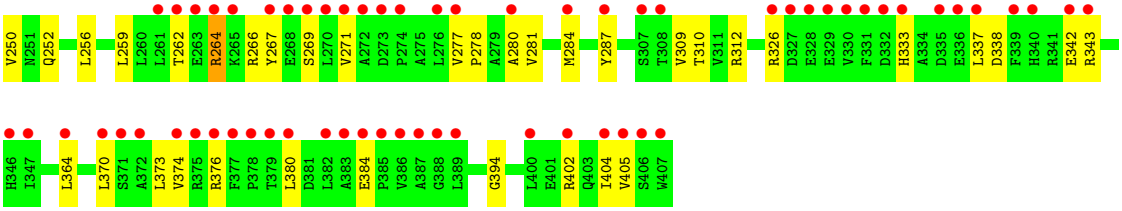


• Molecule 1: Cytochrome P-450



• Molecule 1: Cytochrome P-450




V250
N251
Q252
L256
L259
L260
L261
T262
E263
R264
K265
R266
Y267
E268
S269
L270
V271
A272
D273
P274
A275
L276
V277
P278
A279
A280
V281
M284
Y287
S307
T308
V309
T310
V311
R312
R326
D327
E328
E329
V330
F331
D332
H333
A334
D335
E336
L337
D338
F339
H340
R341
E342
R343
H346
I347
L364
L370
S371
A372
L373
V374
R375
R376
F377
P378
T379
L380
D381
L382
A383
E384
P385
V386
A387
G388
L389
G394
L400
E401
R402
Q403
I404
V405
S406
W407

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	247.76Å 110.49Å 159.82Å 90.00° 129.66° 90.00°	Depositor
Resolution (Å)	48.03 – 2.08 47.98 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.03-2.08) 99.7 (47.98-1.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.170 , 0.228 0.181 , 0.228	Depositor DCC
R_{free} test set	11825 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21704	wwPDB-VP
Average B, all atoms (Å^2)	59.0	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 37.94 % 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 3.9742e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.80	0/3456	0.98	9/4701 (0.2%)
1	B	0.80	0/3491	0.94	2/4750 (0.0%)
1	C	0.80	0/3516	0.94	1/4785 (0.0%)
1	D	0.82	0/3303	0.99	3/4499 (0.1%)
1	E	0.75	0/3231	0.90	2/4400 (0.0%)
1	F	0.74	0/3213	0.90	0/4378
All	All	0.79	0/20210	0.94	17/27513 (0.1%)

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	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	319[A]	VAL	CA-C-O	-8.17	102.95	120.10
1	A	319[B]	VAL	CA-C-O	-8.17	102.95	120.10
1	B	68	SER	N-CA-C	7.91	132.36	111.00
1	A	319[A]	VAL	CA-C-N	6.10	130.62	117.20
1	A	319[B]	VAL	CA-C-N	6.10	130.62	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	319[A]	VAL	Mainchain
1	A	319[B]	VAL	Mainchain
1	A	42	ARG	Sidechain
1	B	68	SER	Mainchain

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	3298	0	3371	100	0
1	B	3331	0	3408	95	1
1	C	3354	0	3421	60	1
1	D	3186	0	3212	88	0
1	E	3141	0	3143	70	0
1	F	3132	0	3113	68	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
2	C	43	0	30	0	0
2	D	43	0	30	4	0
2	E	43	0	30	2	0
2	F	43	0	30	3	0
3	A	27	0	38	8	0
3	B	27	0	38	2	0
3	C	27	0	38	6	0
3	D	27	0	38	0	0
3	E	27	0	38	0	0
3	F	27	0	38	0	0
4	A	111	0	37	11	0
4	B	111	0	37	23	0
4	C	84	0	28	6	0
4	D	48	0	16	6	0
4	E	33	0	11	3	0
4	F	30	0	10	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	30	0	40	9	0
6	B	18	0	24	14	0
6	C	18	0	24	3	0
6	E	12	0	16	7	0
7	A	301	0	0	6	0
7	B	258	0	0	7	0
7	C	308	0	0	7	0
7	D	169	0	0	3	0
7	E	146	0	0	4	0
7	F	157	0	0	1	0
All	All	21704	0	20319	488	1

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 12.

The worst 5 of 488 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236[A]:ASN:OD1	6:B:543[A]:GOL:H2	1.22	1.24
1:B:236[A]:ASN:OD1	6:B:543[A]:GOL:C2	2.04	1.05
1:D:115[A]:ARG:HH11	1:D:115[A]:ARG:CG	1.70	1.04
1:A:92[B]:TRP:HH2	3:A:502:DEB:H223	1.25	1.02
1:B:92:TRP:HA	1:B:236[A]:ASN:ND2	1.74	1.01

All (1) 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)
1:B:302:GLU:OE2	1:C:208:ARG:NH2[4_556]	2.14	0.06

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	426/408 (104%)	413 (97%)	13 (3%)	0	100	100
1	B	433/408 (106%)	415 (96%)	17 (4%)	1 (0%)	47	47
1	C	435/408 (107%)	426 (98%)	9 (2%)	0	100	100
1	D	410/408 (100%)	388 (95%)	22 (5%)	0	100	100
1	E	402/408 (98%)	385 (96%)	17 (4%)	0	100	100
1	F	400/408 (98%)	375 (94%)	24 (6%)	1 (0%)	41	39
All	All	2506/2448 (102%)	2402 (96%)	102 (4%)	2 (0%)	51	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	264	ARG
1	B	68	SER

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	365/343 (106%)	356 (98%)	9 (2%)	47	50
1	B	369/343 (108%)	362 (98%)	7 (2%)	57	61
1	C	372/343 (108%)	367 (99%)	5 (1%)	69	74
1	D	349/343 (102%)	342 (98%)	7 (2%)	55	59
1	E	341/343 (99%)	334 (98%)	7 (2%)	53	57
1	F	339/343 (99%)	334 (98%)	5 (2%)	65	69
All	All	2135/2058 (104%)	2095 (98%)	40 (2%)	60	61

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	42	ARG
1	F	42	ARG
1	E	106[A]	ARG

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Mol	Chain	Res	Type
1	E	225	ASN
1	F	196	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	190	GLN
1	C	236	ASN
1	F	333	HIS
1	E	225	ASN
1	C	0	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)

Of 172 ligands modelled in this entry, 8 are monoatomic - leaving 164 for Mogul analysis.

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	$\#\|Z\| > 2$
4	FMT	C	508	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	519	-	0,2,2	-	-	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FMT	F	503	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	521	-	0,2,2	-	-	0,1,1	-	-
4	FMT	E	505	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	507	-	0,2,2	-	-	0,1,1	-	-
4	FMT	F	512	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	538	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	528	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	527	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	507	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	502	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	518	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	535	-	0,2,2	-	-	0,1,1	-	-
6	GOL	A	542	-	5,5,5	0.13	0	5,5,5	0.31	0
4	FMT	B	537	-	0,2,2	-	-	0,1,1	-	-
4	FMT	F	507	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	525	-	0,2,2	-	-	0,1,1	-	-
4	FMT	E	509	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	509	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	511	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	531	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	519	-	0,2,2	-	-	0,1,1	-	-
6	GOL	A	545	-	5,5,5	0.20	0	5,5,5	0.65	0
4	FMT	C	507	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	510	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	529	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	527	-	0,2,2	-	-	0,1,1	-	-
2	HEM	E	501	1	27,50,50	1.44	5 (18%)	17,82,82	2.35	7 (41%)
4	FMT	C	524	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	509	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	527	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	535	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	514	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	514	-	0,2,2	-	-	0,1,1	-	-
4	FMT	F	505	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	539	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	516	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	530	-	0,2,2	-	-	0,1,1	-	-
3	DEB	D	502	-	27,27,27	0.22	0	35,39,39	0.47	0
4	FMT	B	504	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	524	-	0,2,2	-	-	0,1,1	-	-
4	FMT	E	507	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	521	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	523	-	0,2,2	-	-	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FMT	A	512	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	538	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	513	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	526	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	512	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	518	-	0,2,2	-	-	0,1,1	-	-
3	DEB	C	533	-	27,27,27	0.27	0	35,39,39	0.61	1 (2%)
4	FMT	D	508	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	516	-	0,2,2	-	-	0,1,1	-	-
6	GOL	C	531[A]	-	5,5,5	0.09	0	5,5,5	0.41	0
6	GOL	B	543[B]	-	5,5,5	0.23	0	5,5,5	0.43	0
4	FMT	D	514	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	511	-	0,2,2	-	-	0,1,1	-	-
3	DEB	E	502	-	27,27,27	0.50	0	35,39,39	0.77	0
4	FMT	B	539	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	511	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	519	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	513	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	520	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	518	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	510	5	0,2,2	-	-	0,1,1	-	-
4	FMT	C	506	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	503	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	534	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	517	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	511	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	528	-	0,2,2	-	-	0,1,1	-	-
3	DEB	B	502	-	27,27,27	0.51	0	35,39,39	1.08	2 (5%)
4	FMT	F	511	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	534	-	0,2,2	-	-	0,1,1	-	-
4	FMT	F	504	-	0,2,2	-	-	0,1,1	-	-
6	GOL	C	531[B]	-	5,5,5	0.22	0	5,5,5	0.65	0
4	FMT	A	525	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	525	-	0,2,2	-	-	0,1,1	-	-
4	FMT	F	510	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	506	-	0,2,2	-	-	0,1,1	-	-
6	GOL	B	543[A]	-	5,5,5	0.32	0	5,5,5	0.38	0
4	FMT	B	505	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	520	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	504	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	506	-	0,2,2	-	-	0,1,1	-	-
4	FMT	E	508	-	0,2,2	-	-	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FMT	B	515	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	531	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	526	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	522	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	506	-	0,2,2	-	-	0,1,1	-	-
6	GOL	E	515[A]	-	5,5,5	0.09	0	5,5,5	0.30	0
4	FMT	B	516	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	508	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	536	-	0,2,2	-	-	0,1,1	-	-
4	FMT	E	511	-	0,2,2	-	-	0,1,1	-	-
6	GOL	C	532	-	5,5,5	0.14	0	5,5,5	0.32	0
4	FMT	A	504	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	521	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	505	-	0,2,2	-	-	0,1,1	-	-
6	GOL	A	543[A]	-	5,5,5	0.24	0	5,5,5	0.48	0
4	FMT	D	512	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	513	-	0,2,2	-	-	0,1,1	-	-
4	FMT	E	510	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	522	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	536	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	517	-	0,2,2	-	-	0,1,1	-	-
4	FMT	E	504	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	523	-	0,2,2	-	-	0,1,1	-	-
6	GOL	E	515[B]	-	5,5,5	0.09	0	5,5,5	0.29	0
2	HEM	F	501	1	27,50,50	0.90	1 (3%)	17,82,82	1.64	4 (23%)
4	FMT	C	512	-	0,2,2	-	-	0,1,1	-	-
6	GOL	B	542	-	5,5,5	0.22	0	5,5,5	0.59	0
4	FMT	B	503	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	507	-	0,2,2	-	-	0,1,1	-	-
6	GOL	A	544	-	5,5,5	0.26	0	5,5,5	0.56	0
4	FMT	C	516	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	529	-	0,2,2	-	-	0,1,1	-	-
6	GOL	A	543[B]	-	5,5,5	0.10	0	5,5,5	0.28	0
4	FMT	F	506	-	0,2,2	-	-	0,1,1	-	-
2	HEM	B	501	1	27,50,50	0.99	2 (7%)	17,82,82	2.56	8 (47%)
4	FMT	D	510	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	503	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	520	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	510	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	533	-	0,2,2	-	-	0,1,1	-	-
4	FMT	E	506	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	524	-	0,2,2	-	-	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	FMT	C	515	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	513	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	517	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	522	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	517	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	528	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	532	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	532	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	503	-	0,2,2	-	-	0,1,1	-	-
4	FMT	E	512	-	0,2,2	-	-	0,1,1	-	-
4	FMT	D	515	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	514	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	537	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	529	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	533	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	509	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	530	-	0,2,2	-	-	0,1,1	-	-
4	FMT	F	509	-	0,2,2	-	-	0,1,1	-	-
4	FMT	B	509	-	0,2,2	-	-	0,1,1	-	-
4	FMT	A	515	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	505	-	0,2,2	-	-	0,1,1	-	-
3	DEB	F	502	-	27,27,27	0.59	1 (3%)	35,39,39	0.95	1 (2%)
4	FMT	C	523	-	0,2,2	-	-	0,1,1	-	-
2	HEM	C	501	1	27,50,50	1.15	4 (14%)	17,82,82	1.77	6 (35%)
4	FMT	A	508	-	0,2,2	-	-	0,1,1	-	-
4	FMT	E	513	-	0,2,2	-	-	0,1,1	-	-
3	DEB	A	502	-	27,27,27	0.26	0	35,39,39	0.51	0
4	FMT	A	505	-	0,2,2	-	-	0,1,1	-	-
2	HEM	A	501	1	27,50,50	1.21	3 (11%)	17,82,82	1.65	5 (29%)
4	FMT	B	518	-	0,2,2	-	-	0,1,1	-	-
4	FMT	E	503	-	0,2,2	-	-	0,1,1	-	-
4	FMT	F	508	-	0,2,2	-	-	0,1,1	-	-
2	HEM	D	501	1	27,50,50	1.47	2 (7%)	17,82,82	2.10	7 (41%)
4	FMT	D	504	-	0,2,2	-	-	0,1,1	-	-
4	FMT	C	526	-	0,2,2	-	-	0,1,1	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DEB	D	502	-	-	8/50/50/50	0/1/1/1
2	HEM	B	501	1	-	0/6/54/54	-
6	GOL	B	543[A]	-	-	4/4/4/4	-
3	DEB	C	533	-	-	10/50/50/50	0/1/1/1
6	GOL	A	542	-	-	2/4/4/4	-
6	GOL	E	515[A]	-	-	2/4/4/4	-
6	GOL	C	531[A]	-	-	3/4/4/4	-
6	GOL	B	543[B]	-	-	1/4/4/4	-
3	DEB	E	502	-	-	9/50/50/50	0/1/1/1
6	GOL	C	532	-	-	3/4/4/4	-
6	GOL	A	543[A]	-	-	4/4/4/4	-
6	GOL	A	545	-	-	2/4/4/4	-
3	DEB	F	502	-	-	8/50/50/50	0/1/1/1
2	HEM	C	501	1	-	0/6/54/54	-
2	HEM	E	501	1	-	0/6/54/54	-
3	DEB	A	502	-	-	8/50/50/50	0/1/1/1
3	DEB	B	502	-	-	7/50/50/50	0/1/1/1
2	HEM	A	501	1	-	0/6/54/54	-
6	GOL	E	515[B]	-	-	4/4/4/4	-
2	HEM	F	501	1	-	0/6/54/54	-
6	GOL	C	531[B]	-	-	1/4/4/4	-
6	GOL	B	542	-	-	4/4/4/4	-
2	HEM	D	501	1	-	0/6/54/54	-
6	GOL	A	544	-	-	2/4/4/4	-
6	GOL	A	543[B]	-	-	2/4/4/4	-

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C3B-C2B	-4.22	1.34	1.40
2	E	501	HEM	C3B-C2B	-3.78	1.35	1.40
2	E	501	HEM	C3D-C4D	3.55	1.50	1.42
2	E	501	HEM	CAA-C2A	2.78	1.56	1.52
2	D	501	HEM	C1D-ND	-2.74	1.30	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	HEM	CMA-C3A-C4A	-5.43	120.12	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	501	HEM	C4A-C3A-C2A	5.11	110.55	107.00
2	B	501	HEM	CAD-CBD-CGD	4.30	119.89	112.67
2	B	501	HEM	CMC-C2C-C3C	4.05	132.25	124.68
2	C	501	HEM	C4A-C3A-C2A	3.88	109.69	107.00

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	533	DEB	C3-C4-C5-O21
3	C	533	DEB	C20-C4-C5-O21
3	C	533	DEB	O16-C13-C14-C15
6	A	542	GOL	C1-C2-C3-O3
6	A	542	GOL	O2-C2-C3-O3

There are no ring outliers.

48 monomers are involved in 108 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	507	FMT	1	0
4	A	538	FMT	1	0
4	B	528	FMT	1	0
4	C	527	FMT	1	0
4	B	537	FMT	3	0
4	B	511	FMT	2	0
4	A	519	FMT	1	0
6	A	545	GOL	3	0
4	B	529	FMT	1	0
2	E	501	HEM	2	0
4	C	524	FMT	2	0
4	A	535	FMT	1	0
4	F	505	FMT	1	0
4	A	516	FMT	1	0
4	B	538	FMT	2	0
4	C	513	FMT	1	0
4	B	512	FMT	2	0
3	C	533	DEB	6	0
4	D	508	FMT	3	0
6	C	531[A]	GOL	1	0
6	B	543[B]	GOL	4	0
4	A	510	FMT	2	0

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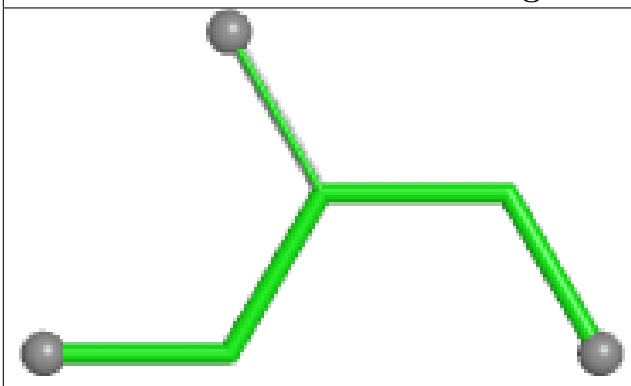
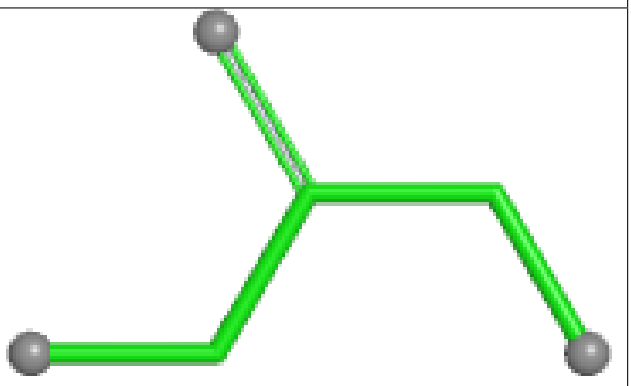
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	DEB	2	0
6	C	531[B]	GOL	2	0
4	A	525	FMT	2	0
6	B	543[A]	GOL	9	0
4	B	520	FMT	2	0
4	B	506	FMT	4	0
4	B	515	FMT	1	0
4	A	526	FMT	2	0
6	E	515[A]	GOL	7	0
6	A	543[A]	GOL	3	0
4	E	510	FMT	1	0
4	C	522	FMT	2	0
2	F	501	HEM	3	0
6	B	542	GOL	1	0
4	A	529	FMT	1	0
6	A	543[B]	GOL	3	0
2	B	501	HEM	1	0
4	D	510	FMT	1	0
4	E	506	FMT	2	0
4	B	524	FMT	1	0
4	B	513	FMT	2	0
4	B	532	FMT	1	0
4	D	515	FMT	2	0
3	A	502	DEB	8	0
2	A	501	HEM	3	0
2	D	501	HEM	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

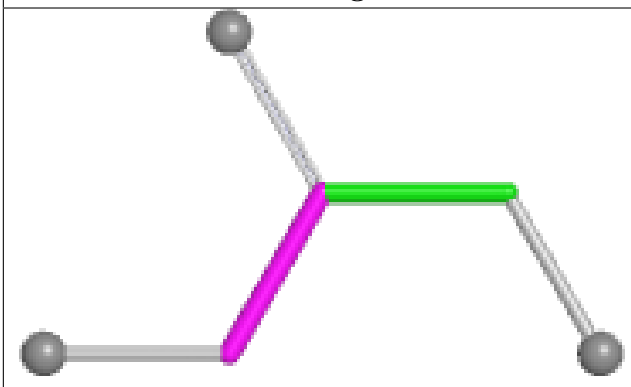
Ligand GOL A 542



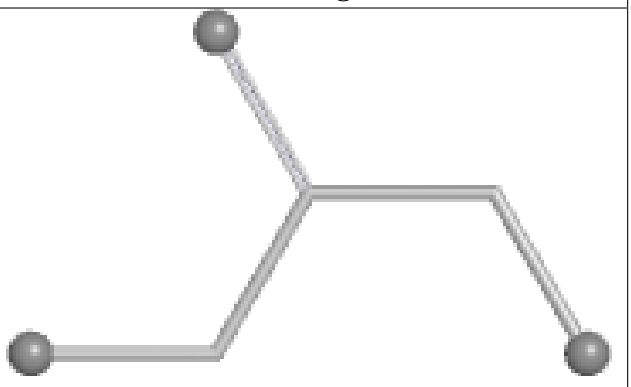
Bond lengths



Bond angles

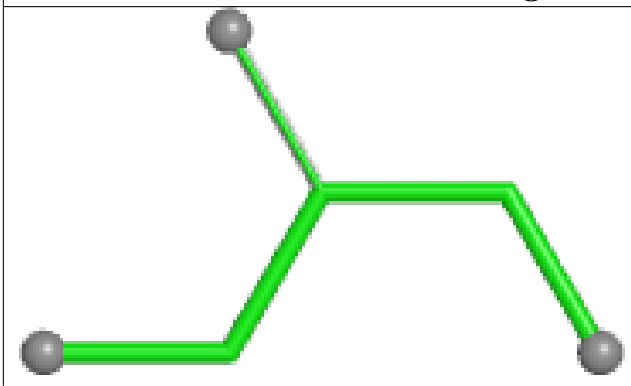


Torsions

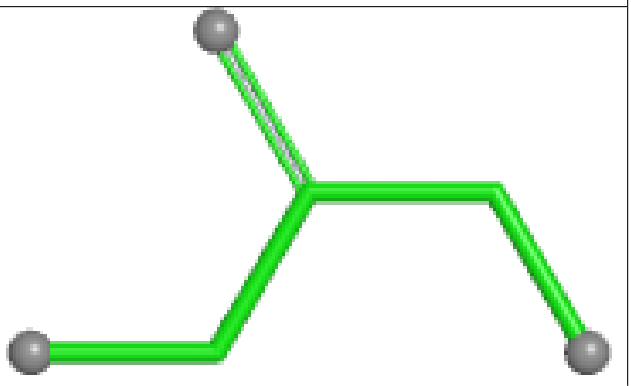


Rings

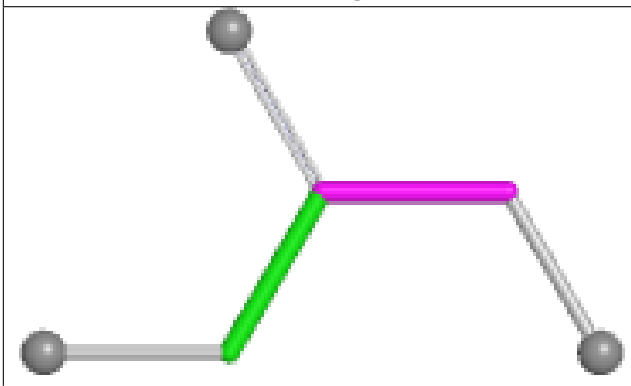
Ligand GOL A 545



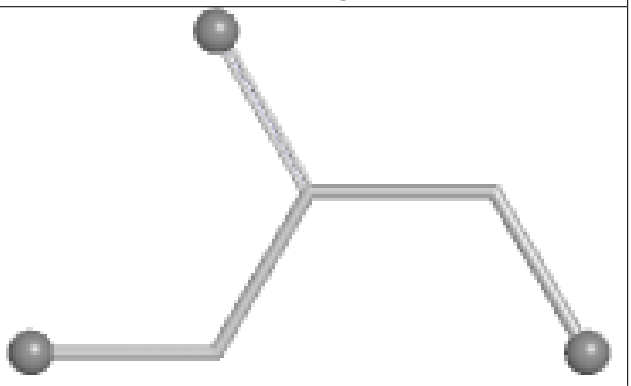
Bond lengths



Bond angles

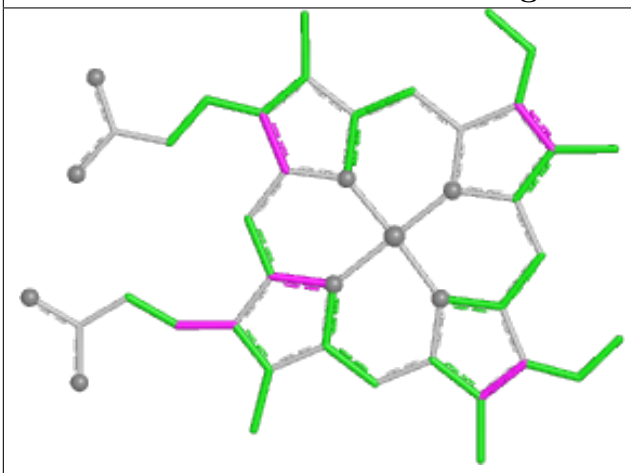


Torsions

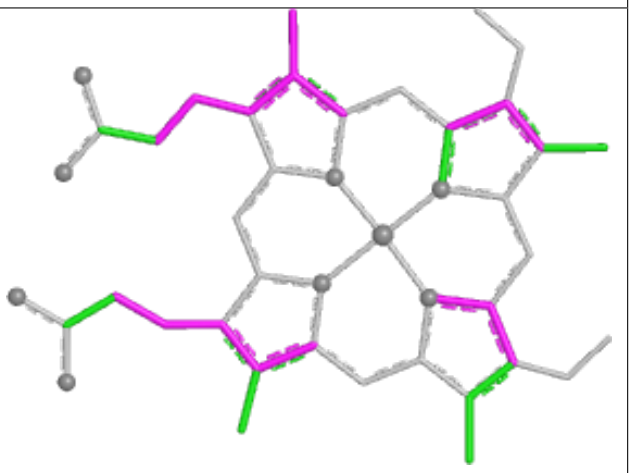


Rings

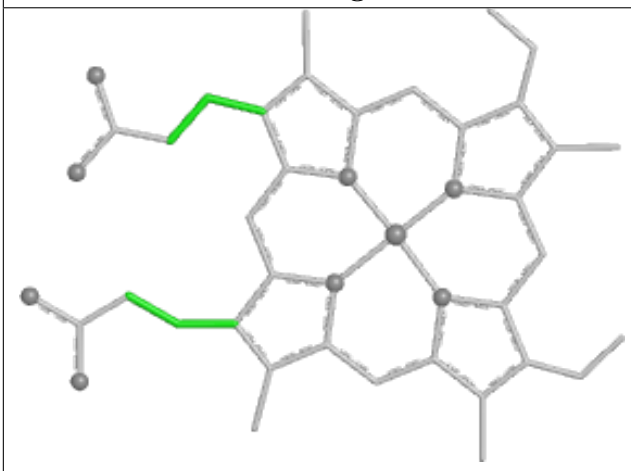
Ligand HEM E 501



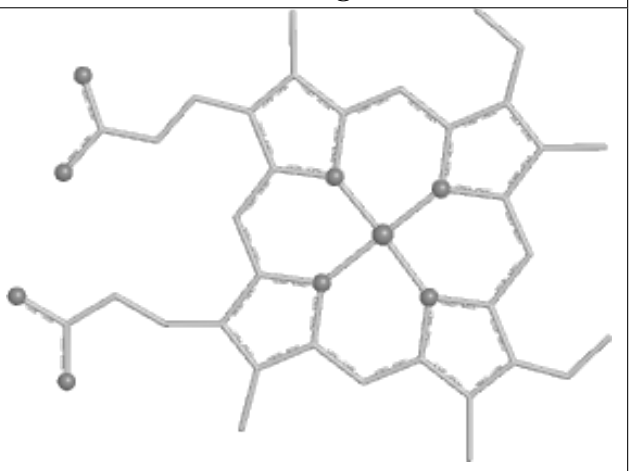
Bond lengths



Bond angles

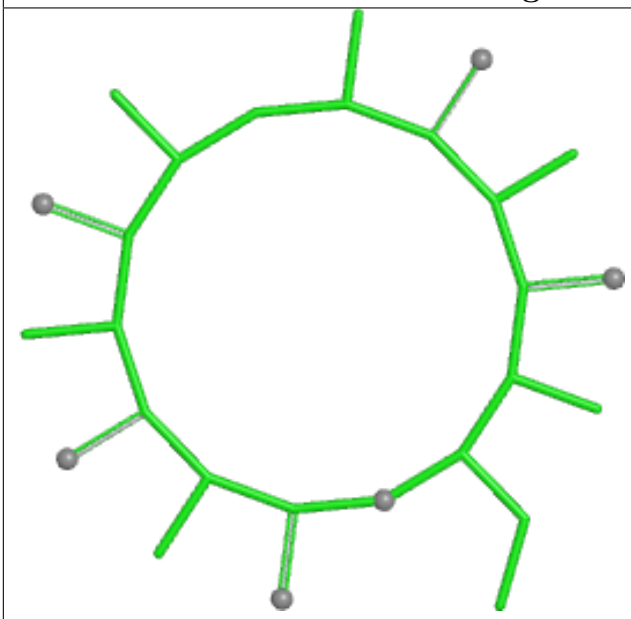


Torsions

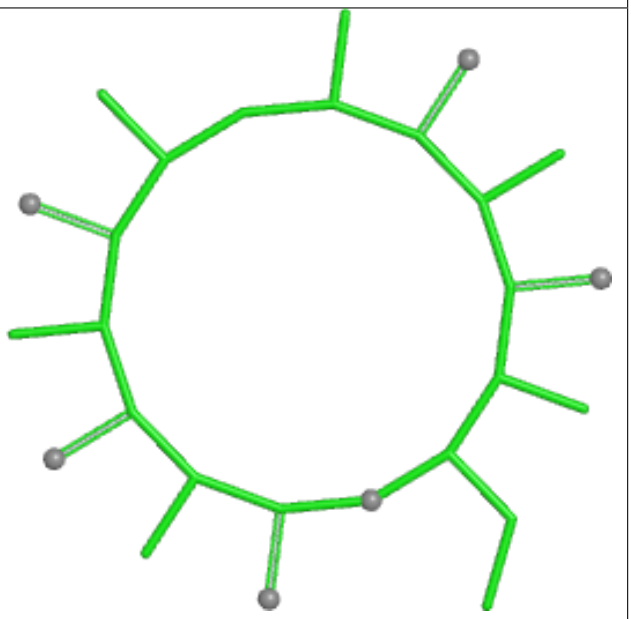


Rings

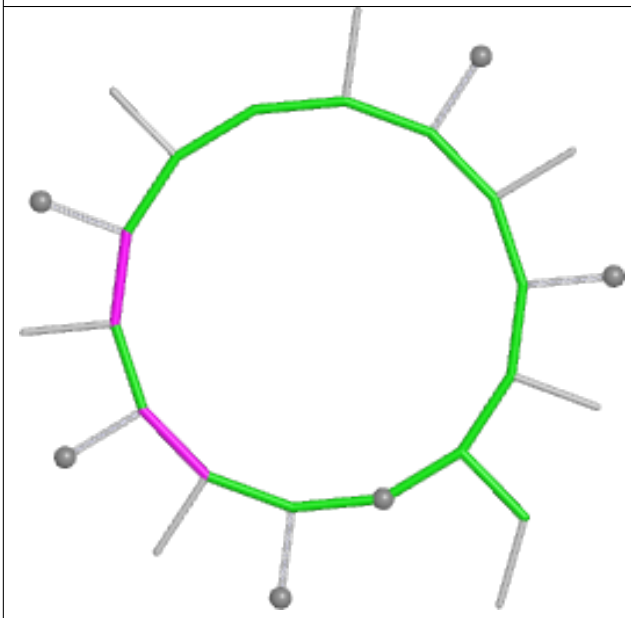
Ligand DEB D 502



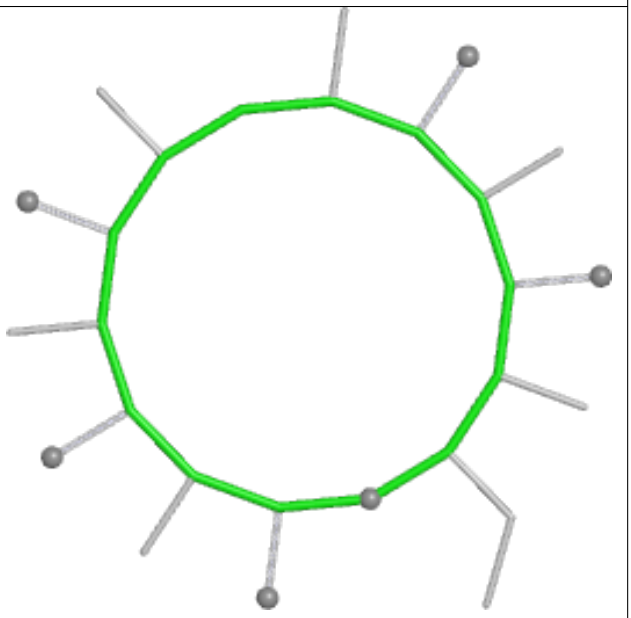
Bond lengths



Bond angles

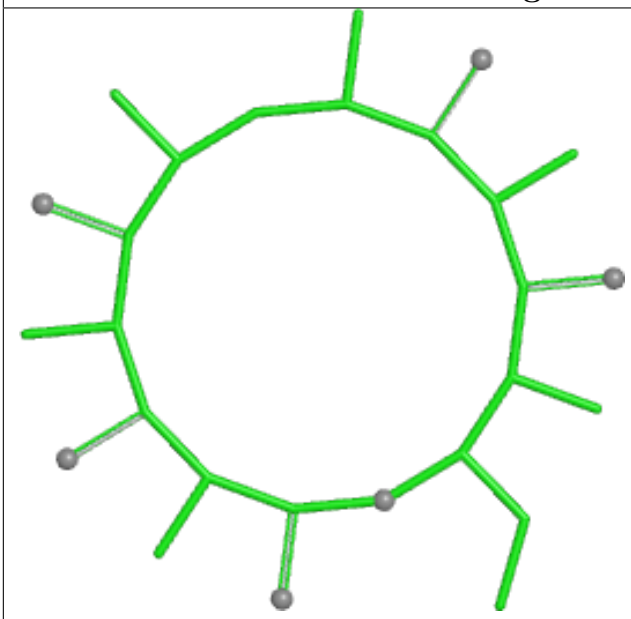


Torsions

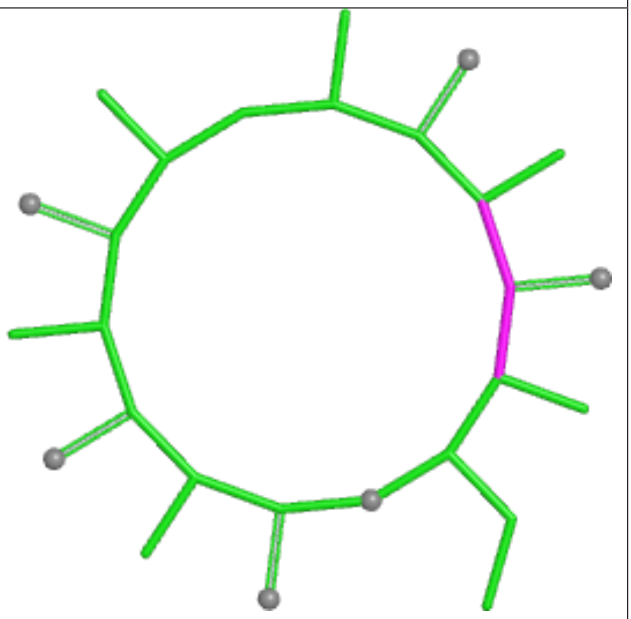


Rings

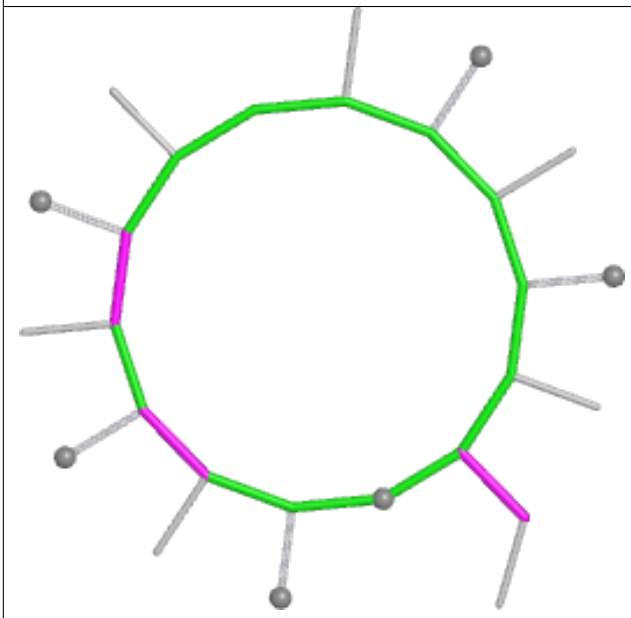
Ligand DEB C 533



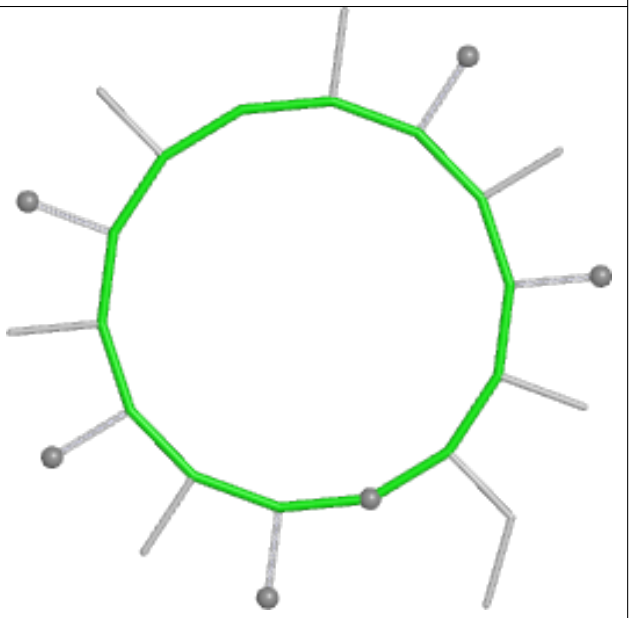
Bond lengths



Bond angles

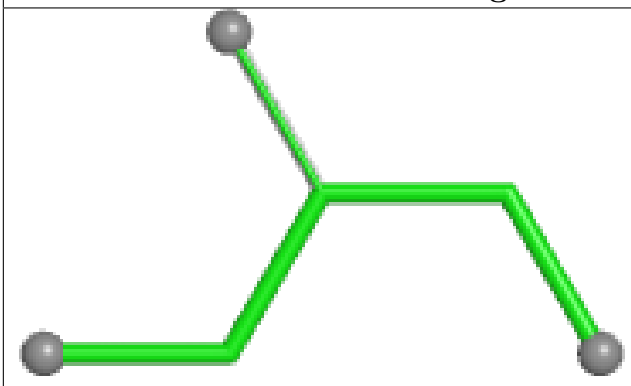


Torsions

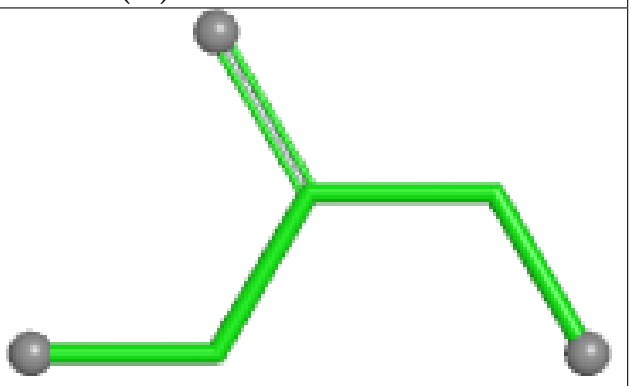


Rings

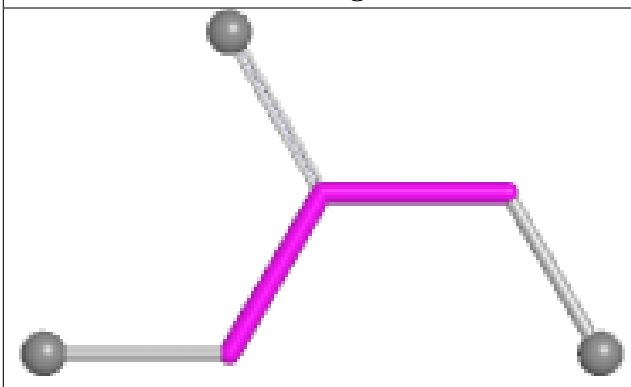
Ligand GOL C 531 (A)



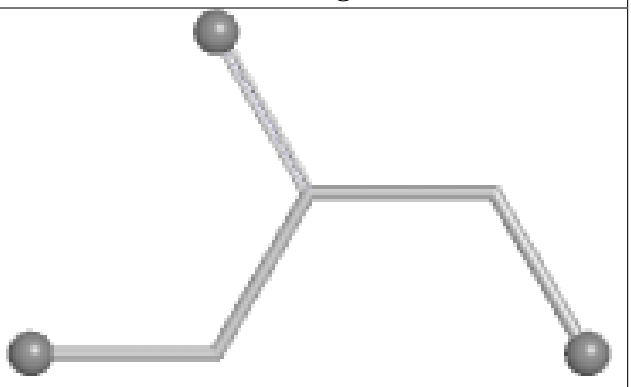
Bond lengths



Bond angles

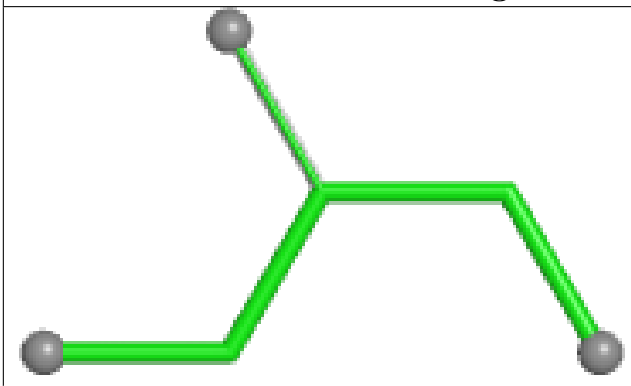


Torsions

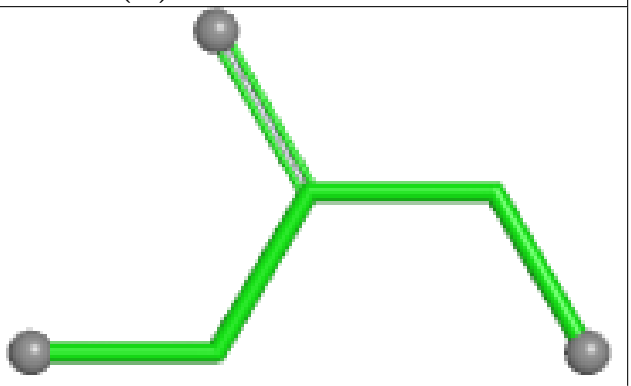


Rings

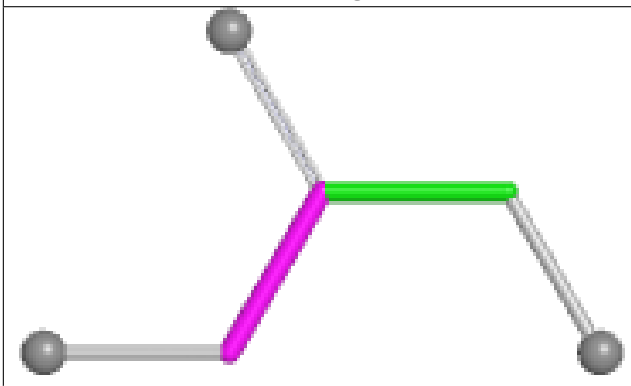
Ligand GOL B 543 (B)



Bond lengths



Bond angles



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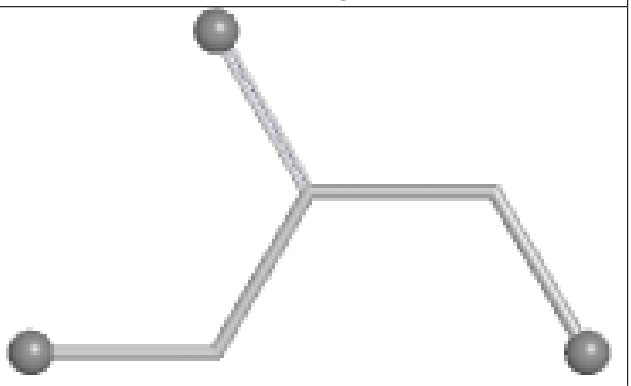
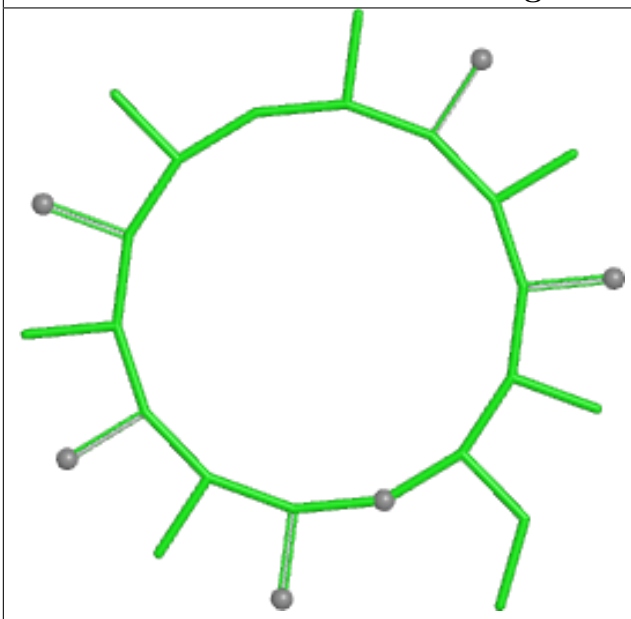
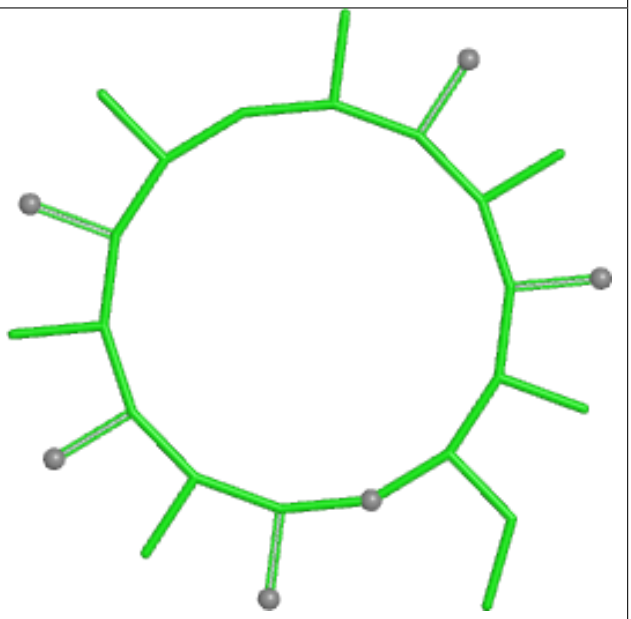


Rings

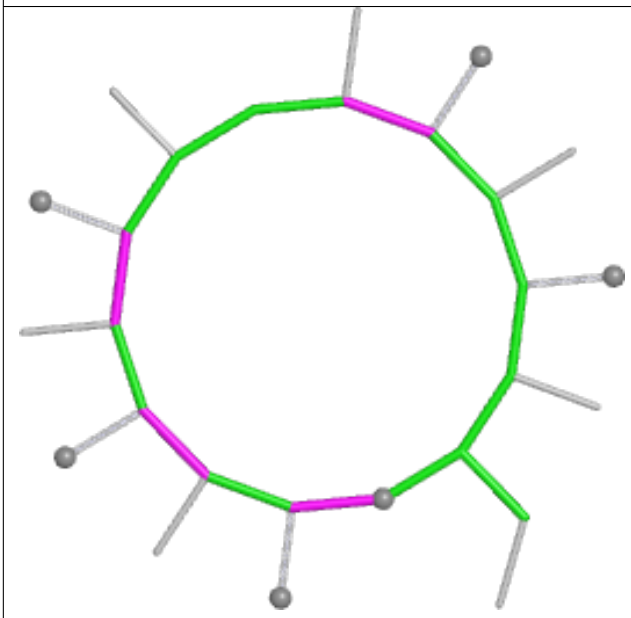
Ligand DEB E 502



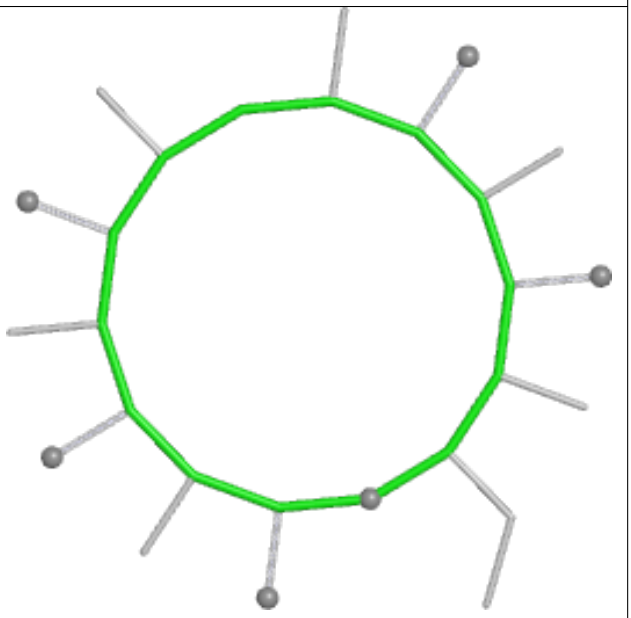
Bond lengths



Bond angles

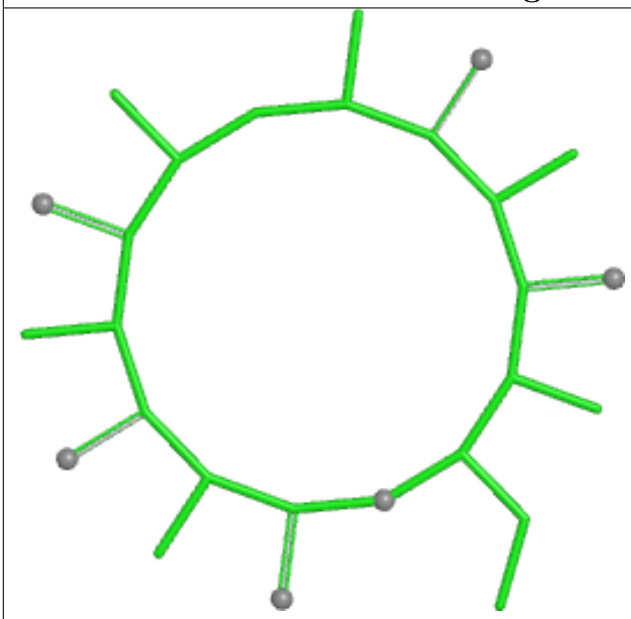


Torsions

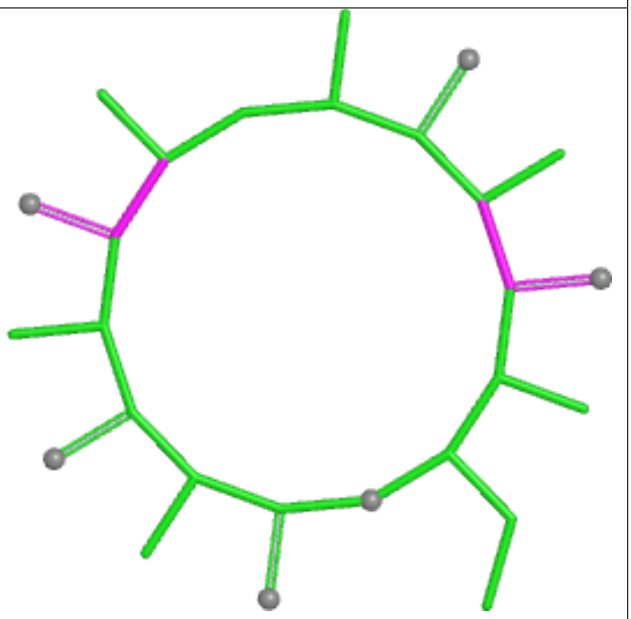


Rings

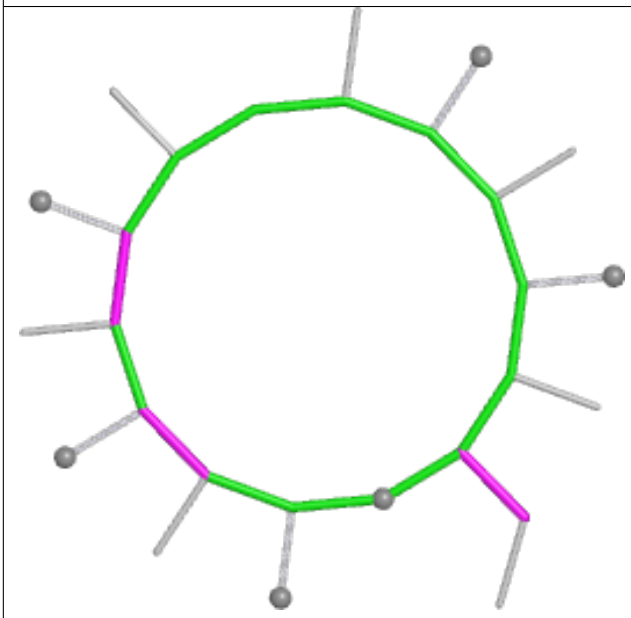
Ligand DEB B 502



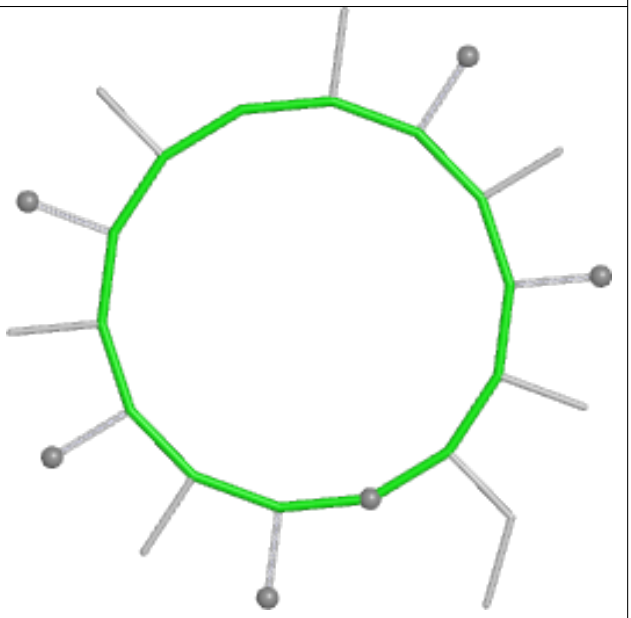
Bond lengths



Bond angles

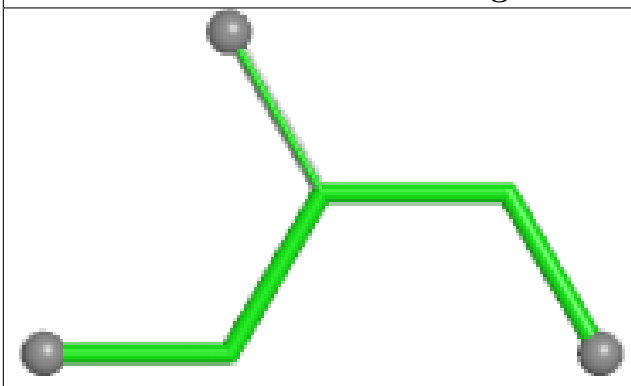


Torsions

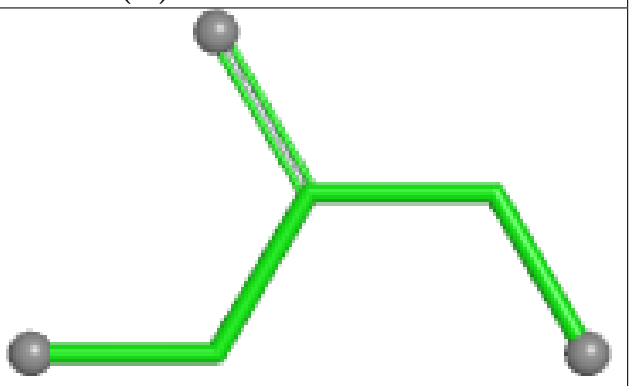


Rings

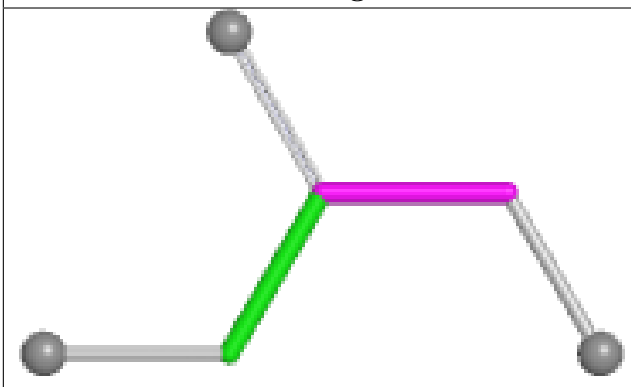
Ligand GOL C 531 (B)



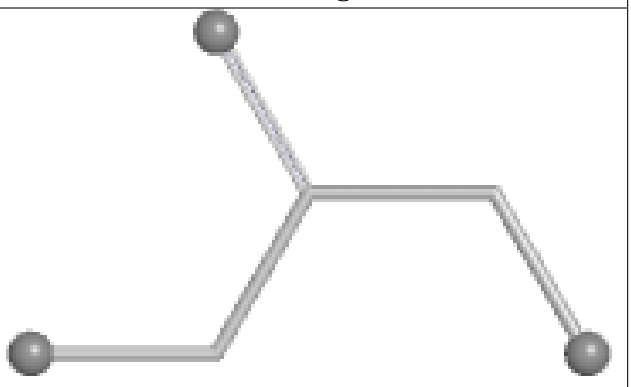
Bond lengths



Bond angles

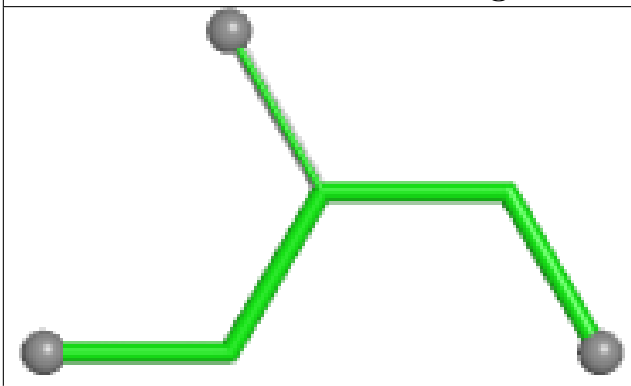


Torsions

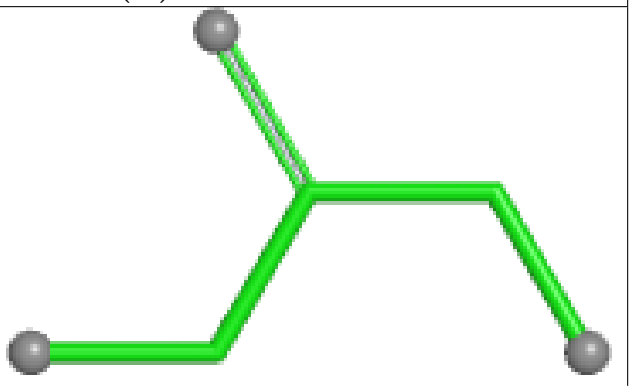


Rings

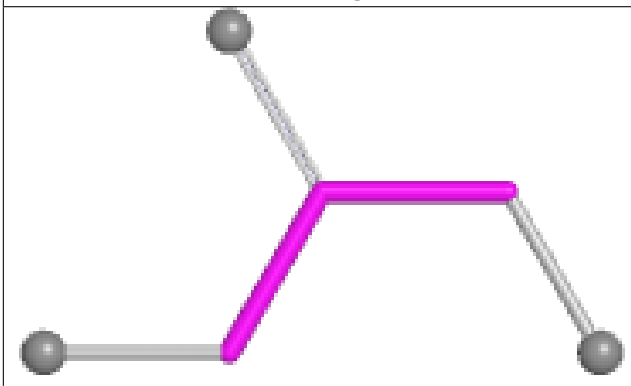
Ligand GOL B 543 (A)



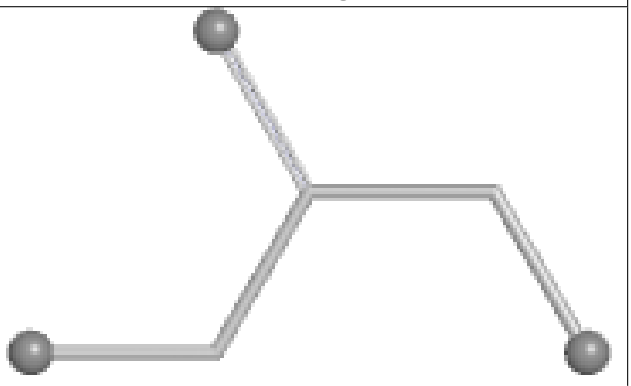
Bond lengths



Bond angles

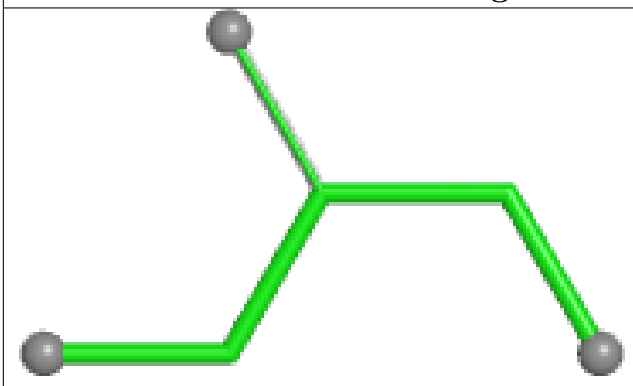


Torsions



Rings

Ligand GOL E 515 (A)



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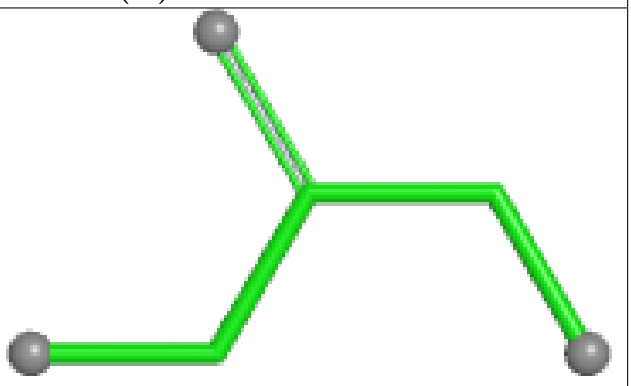
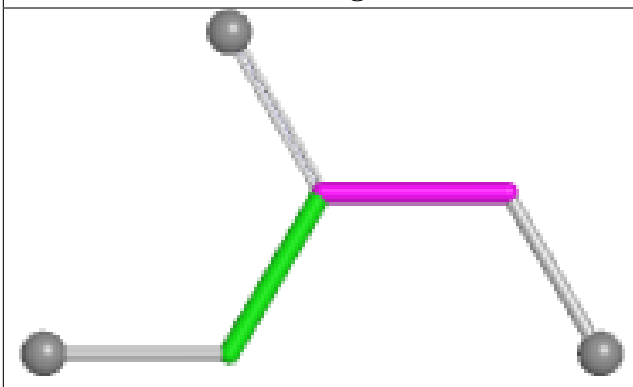
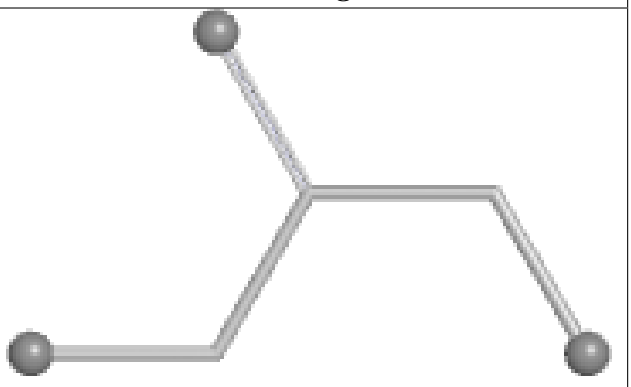


Bond angles

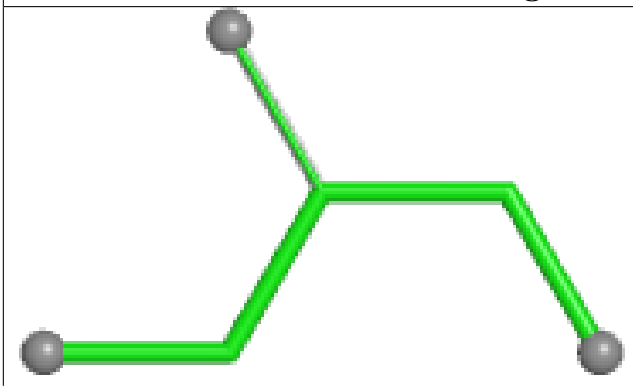


Torsions

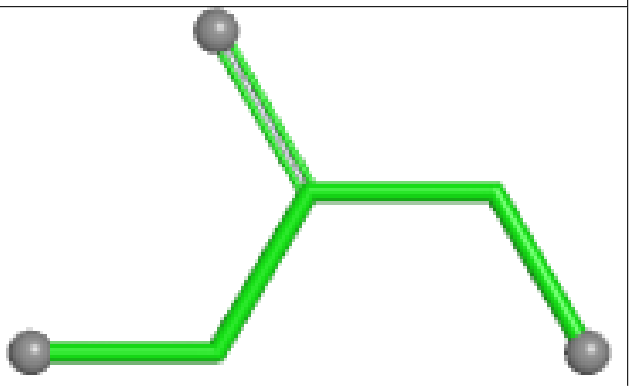


Rings

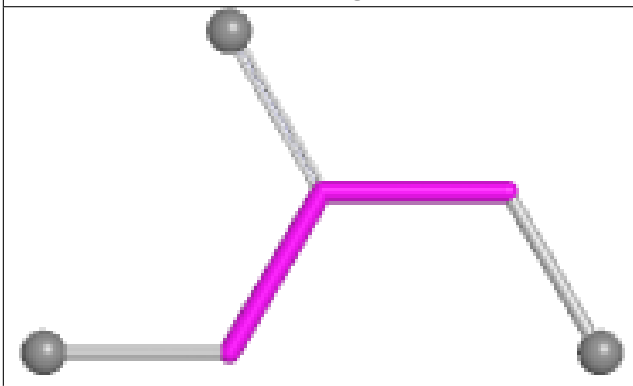
Ligand GOL C 532



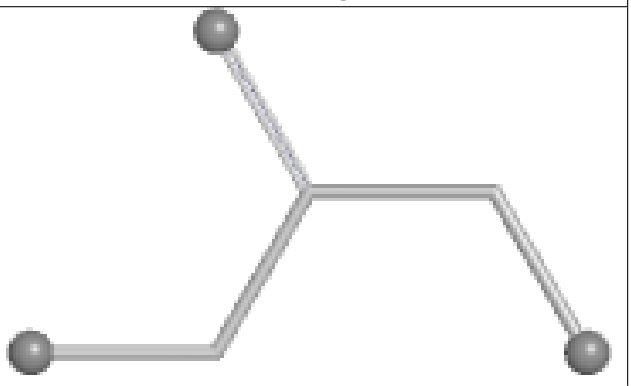
Bond lengths



Bond angles

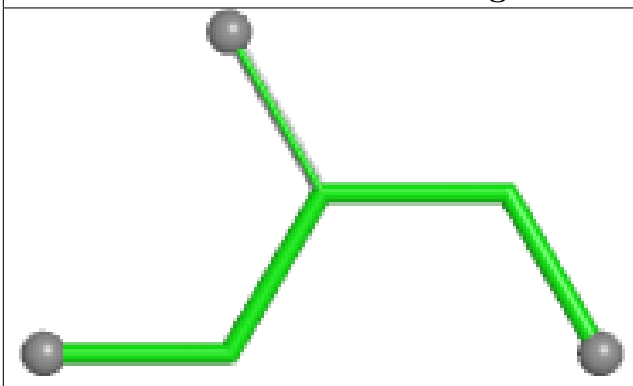


Torsions



Rings

Ligand GOL A 543 (A)



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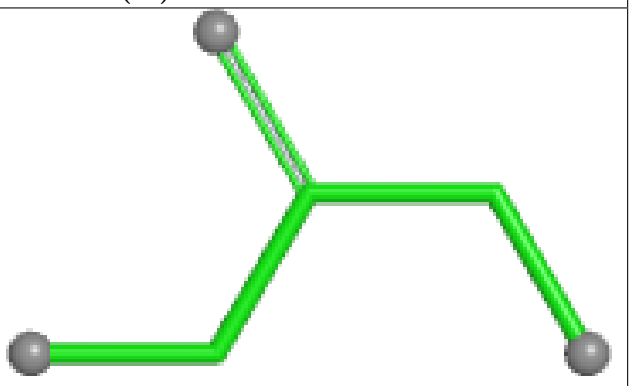
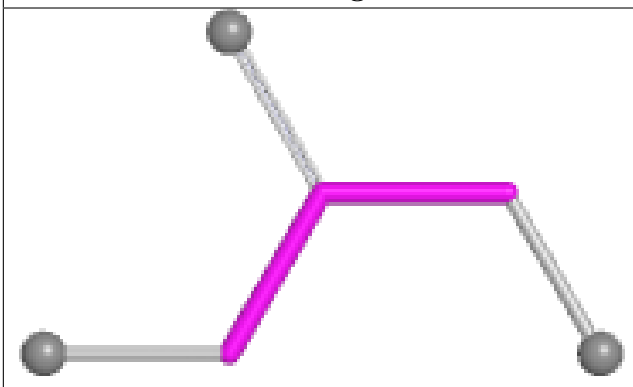
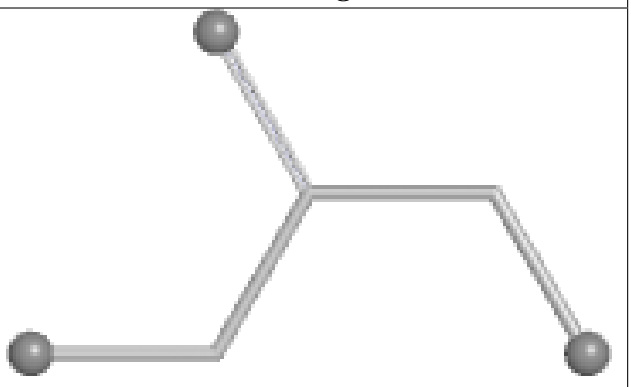


Bond angles

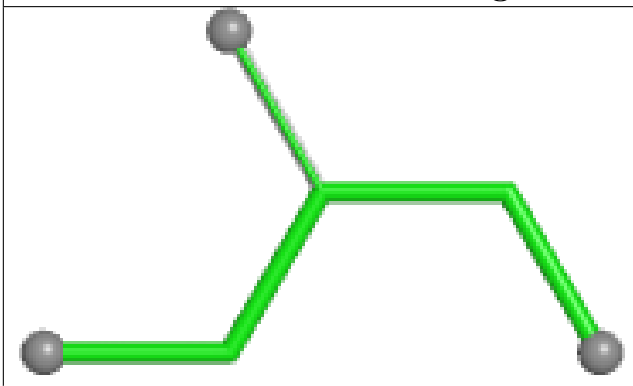


Torsions

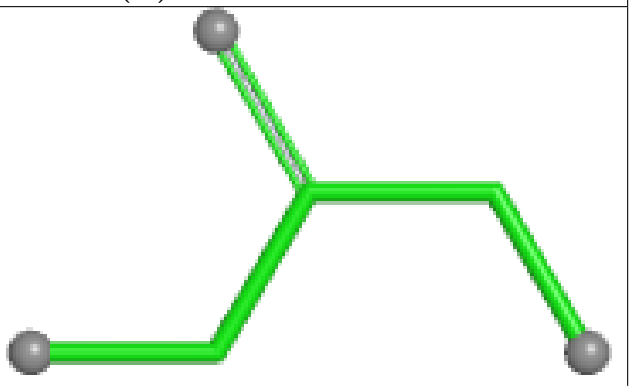


Rings

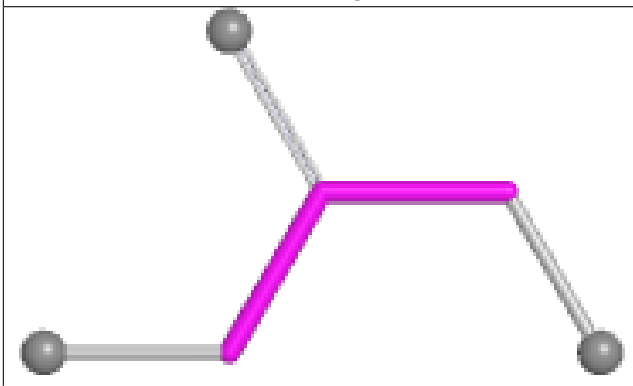
Ligand GOL E 515 (B)



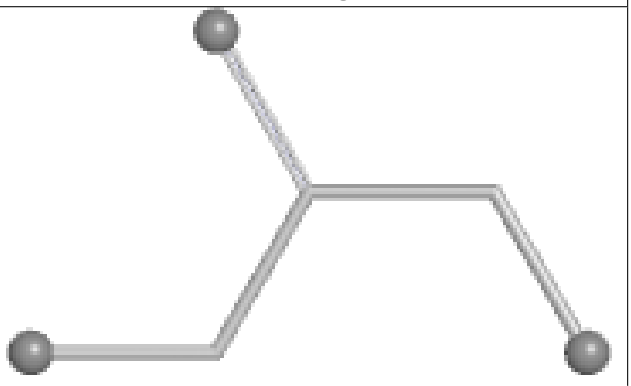
Bond lengths



Bond angles

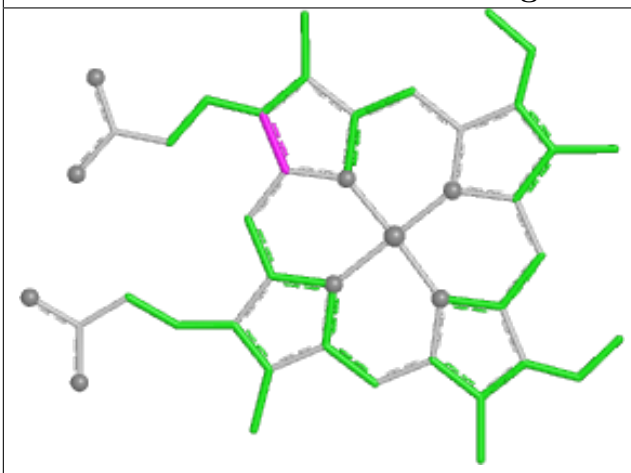


Torsions



Rings

Ligand HEM F 501



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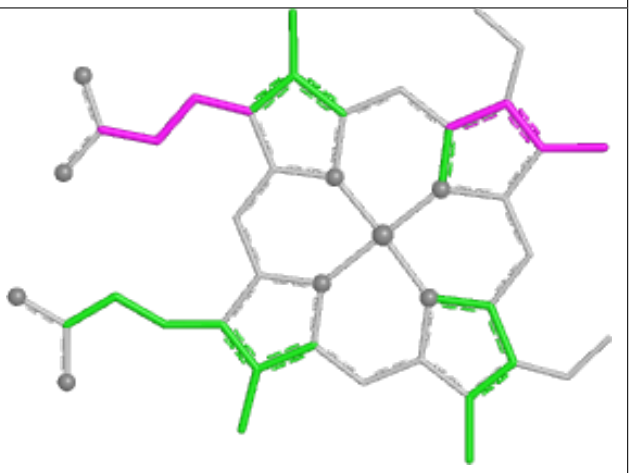
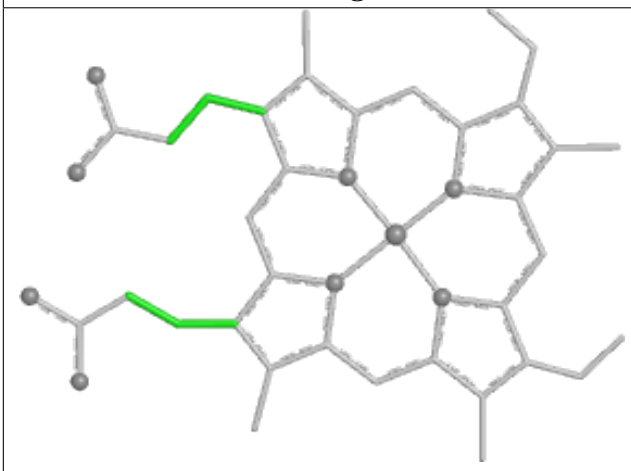
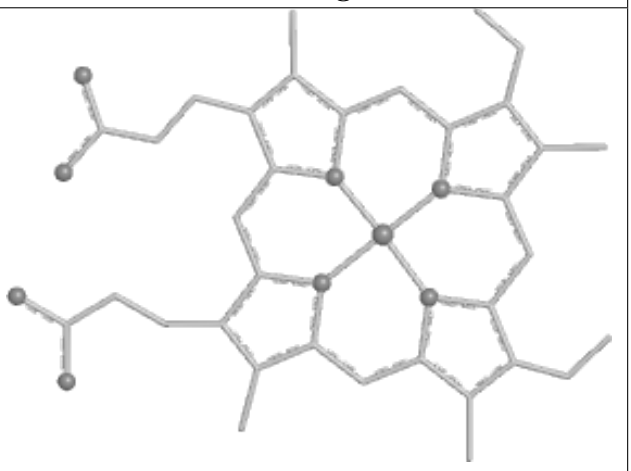


Bond angles

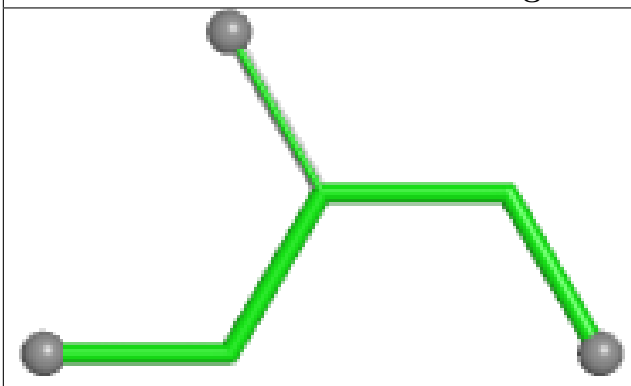


Torsions

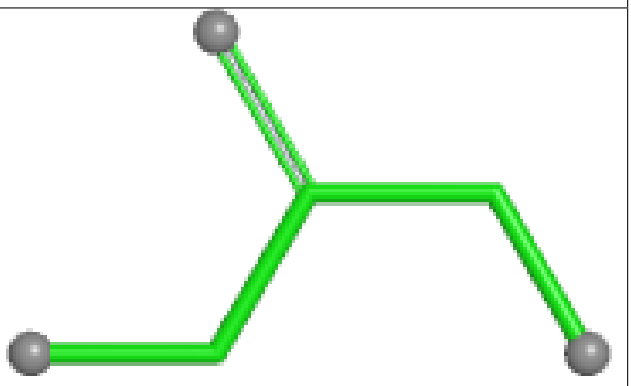


Rings

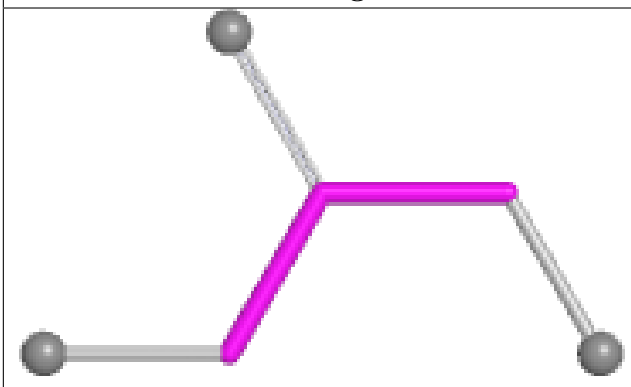
Ligand GOL B 542



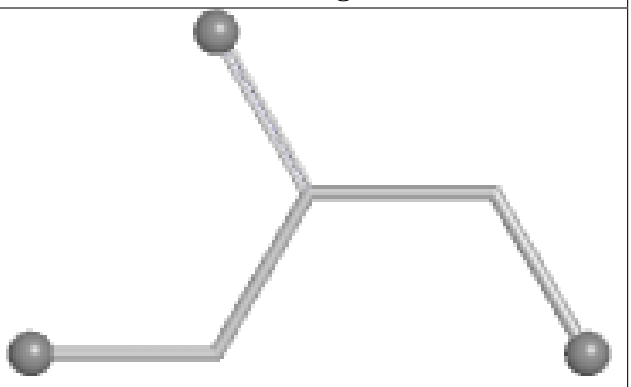
Bond lengths



Bond angles

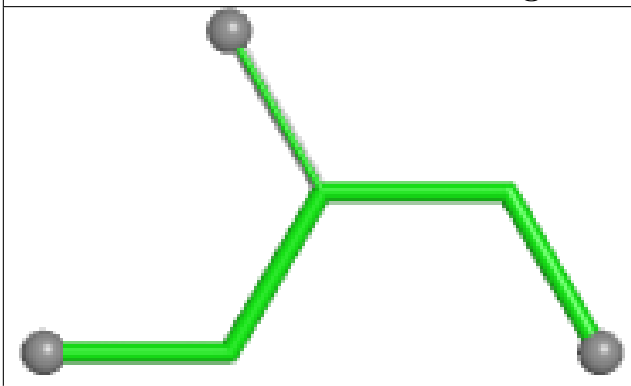


Torsions



Rings

Ligand GOL A 544



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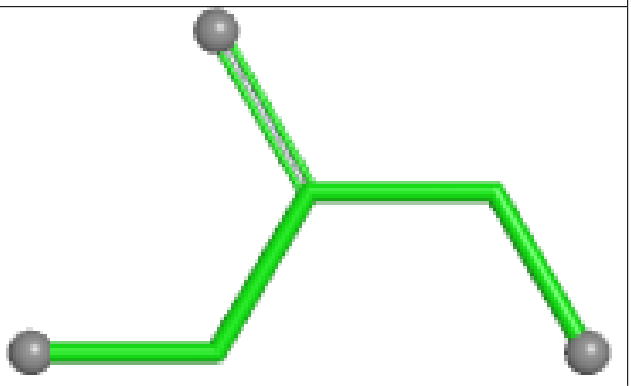
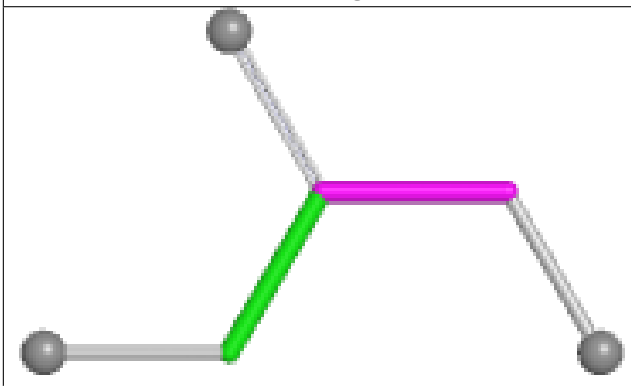
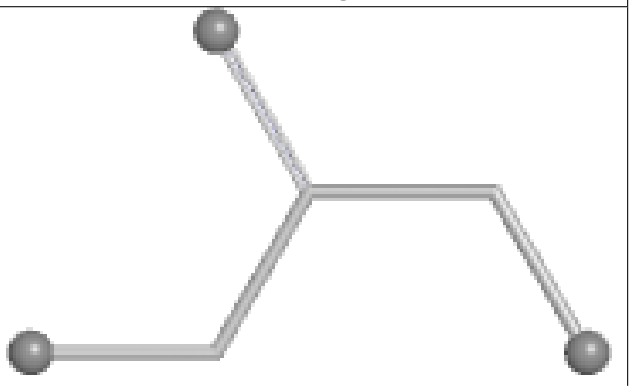


Bond angles

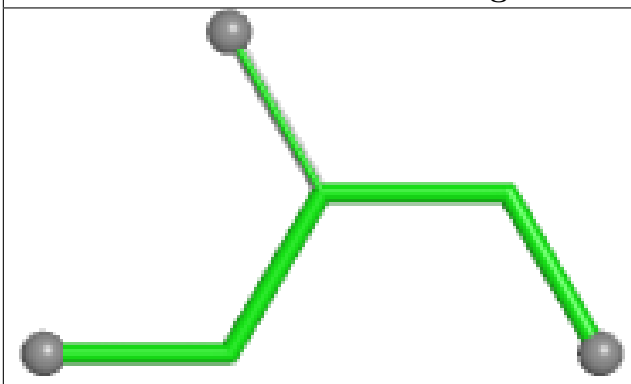


Torsions

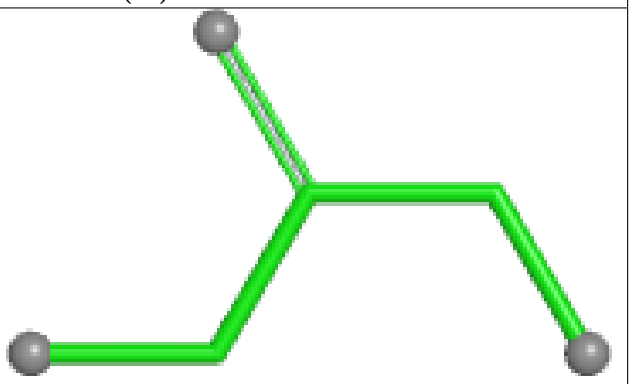


Rings

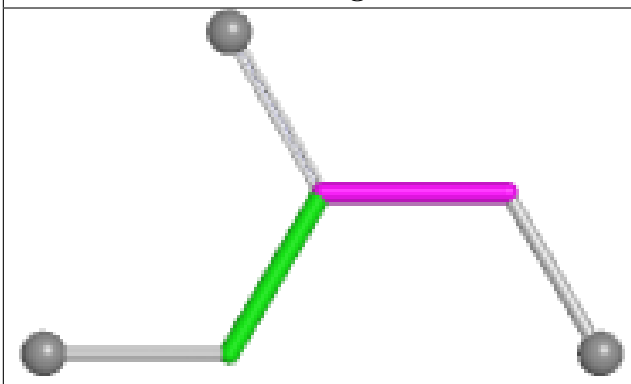
Ligand GOL A 543 (B)



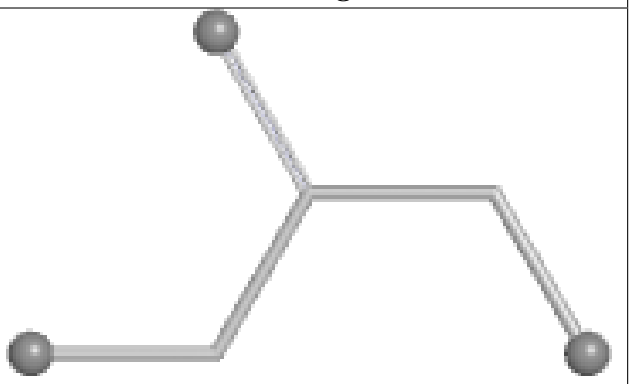
Bond lengths



Bond angles

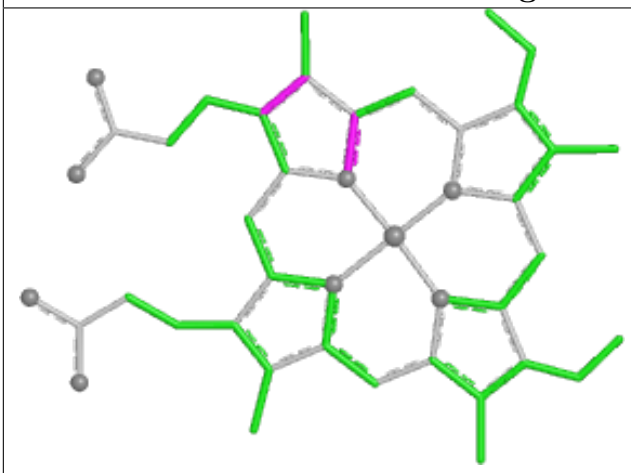


Torsions

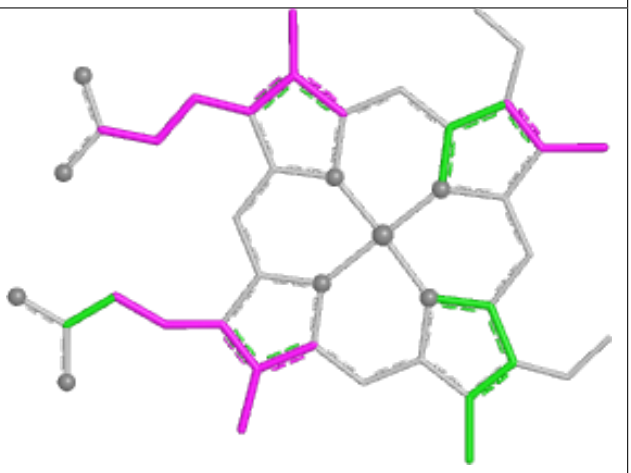


Rings

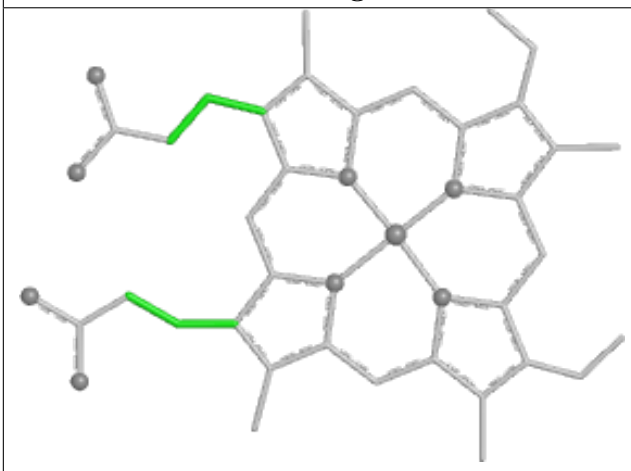
Ligand HEM B 501



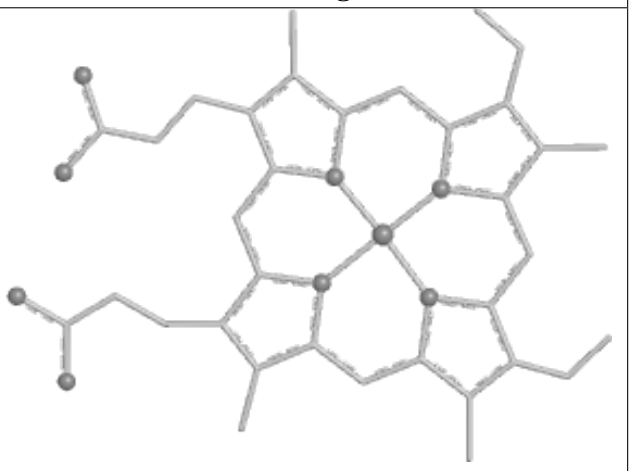
Bond lengths



Bond angles

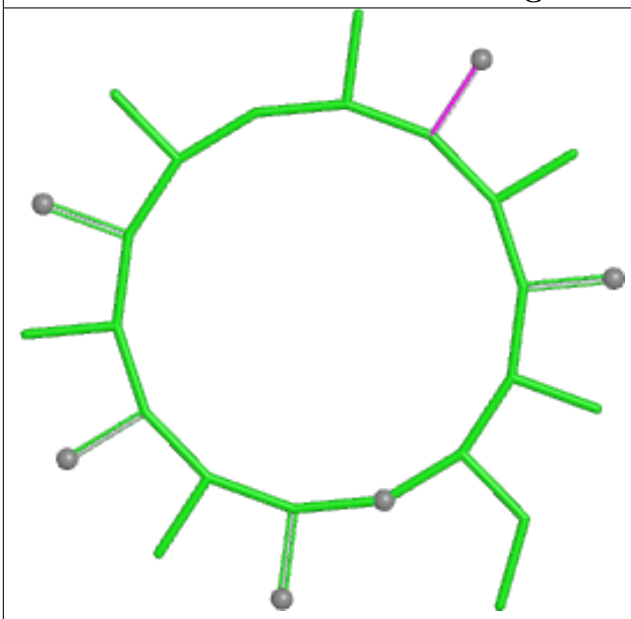


Torsions

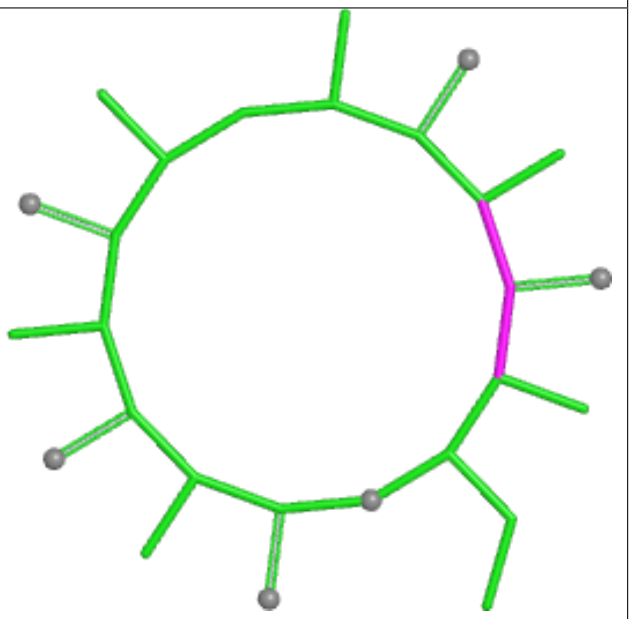


Rings

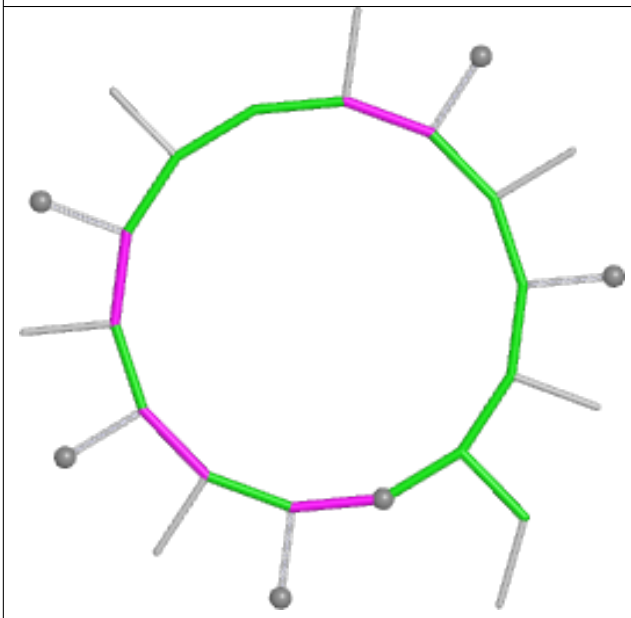
Ligand DEB F 502



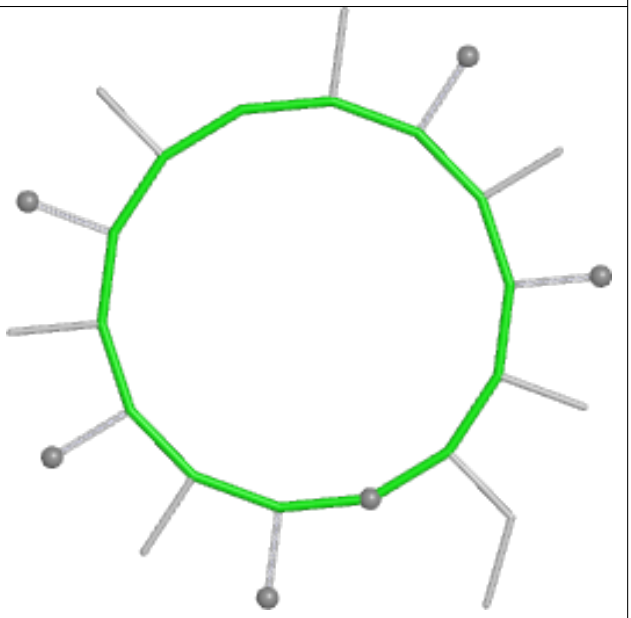
Bond lengths



Bond angles

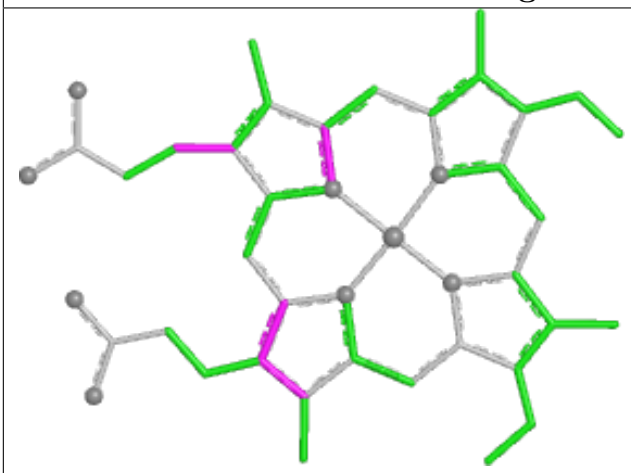


Torsions

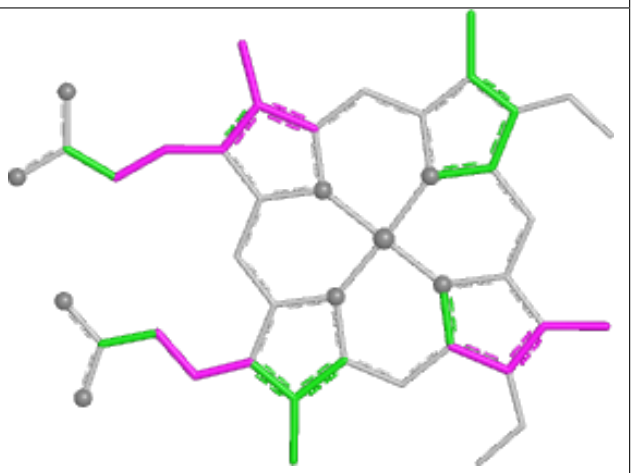


Rings

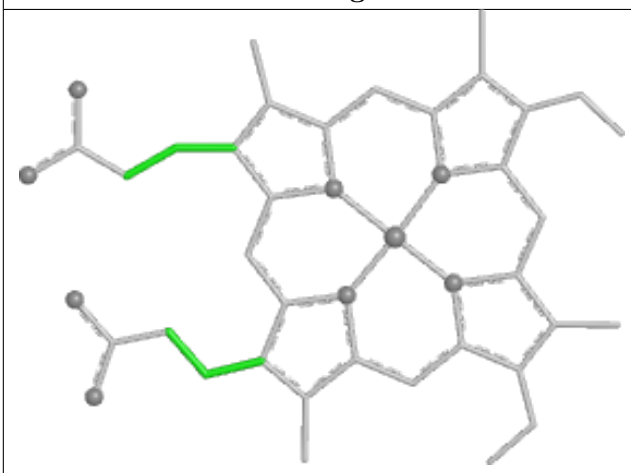
Ligand HEM C 501



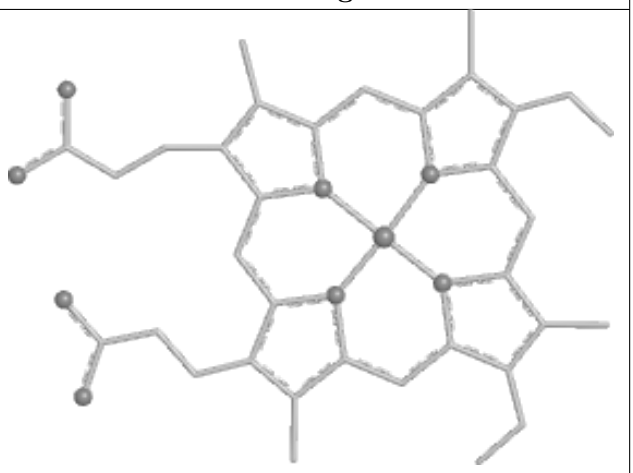
Bond lengths



Bond angles

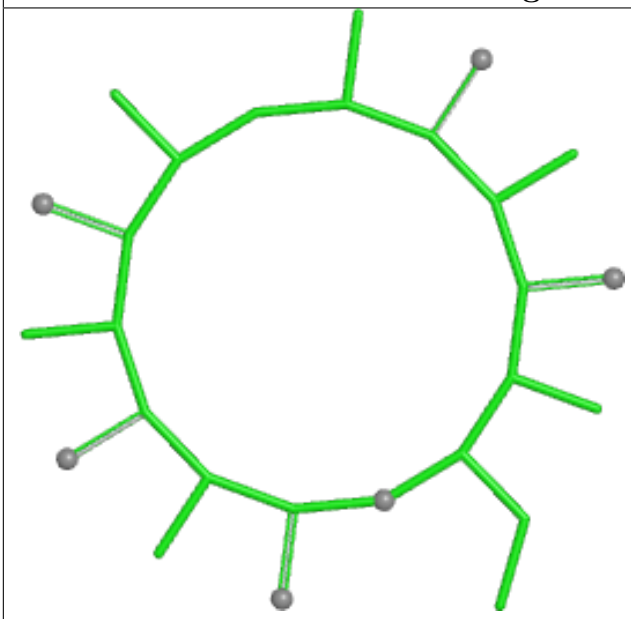


Torsions

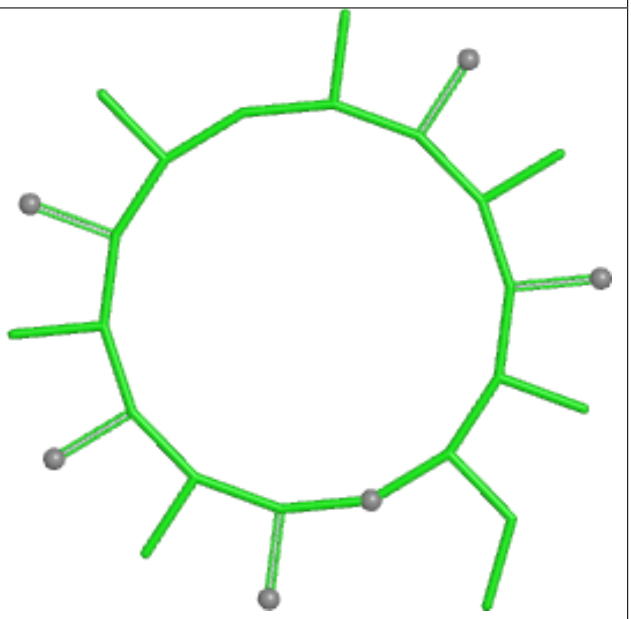


Rings

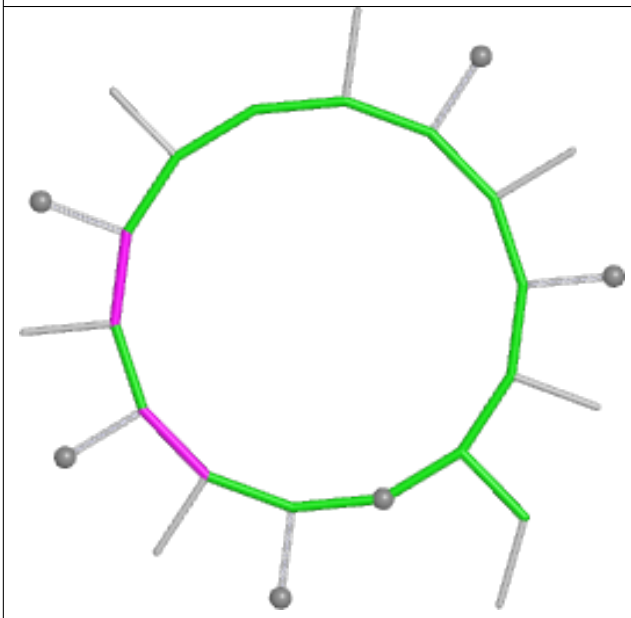
Ligand DEB A 502



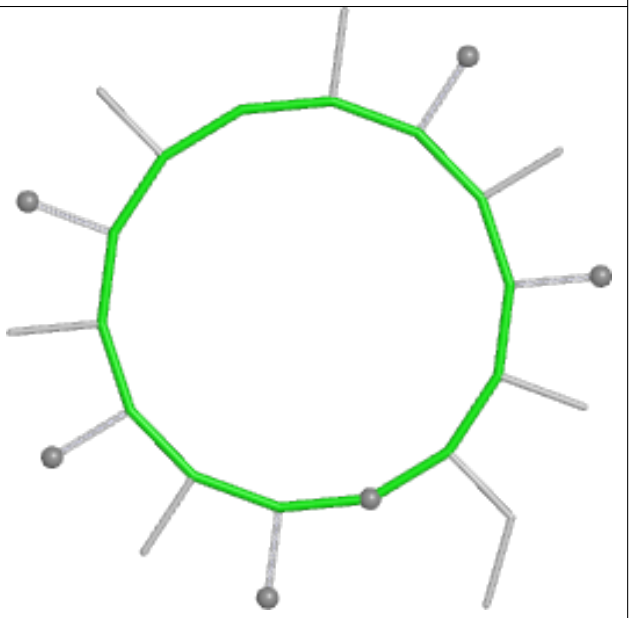
Bond lengths



Bond angles

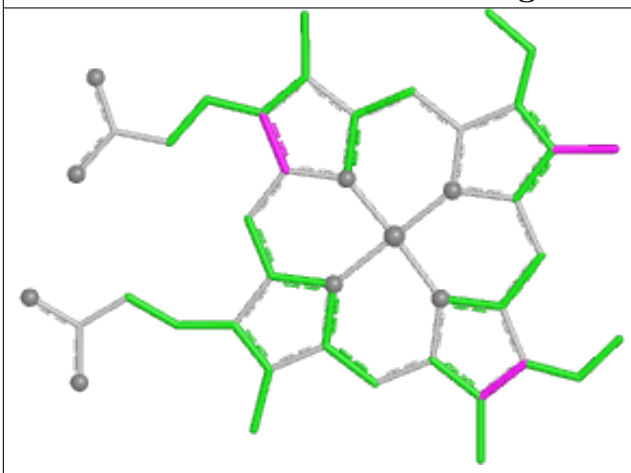


Torsions

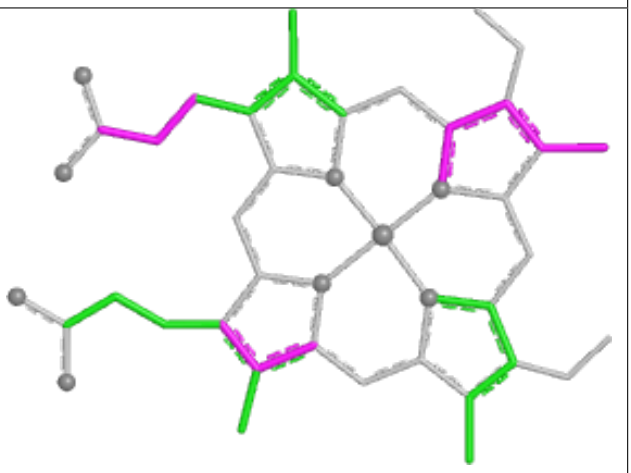


Rings

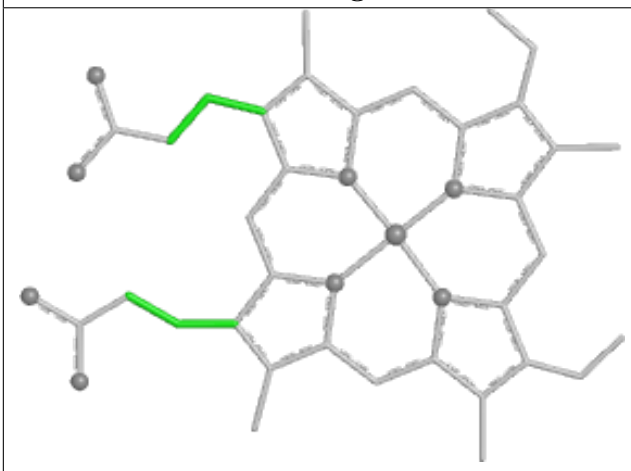
Ligand HEM A 501



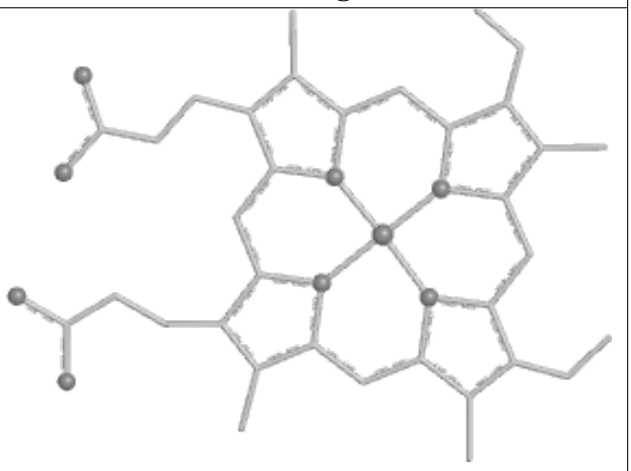
Bond lengths



Bond angles

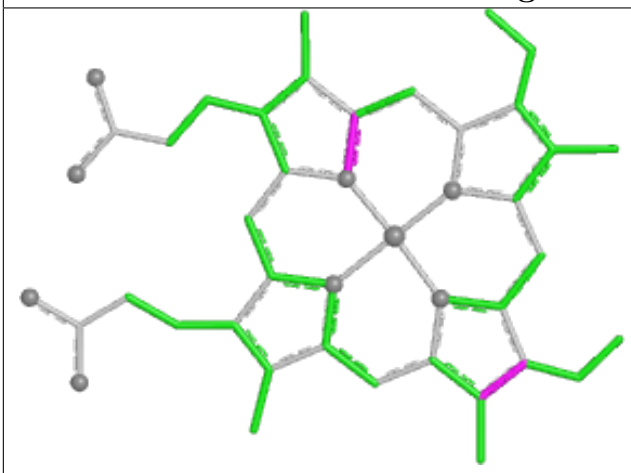


Torsions

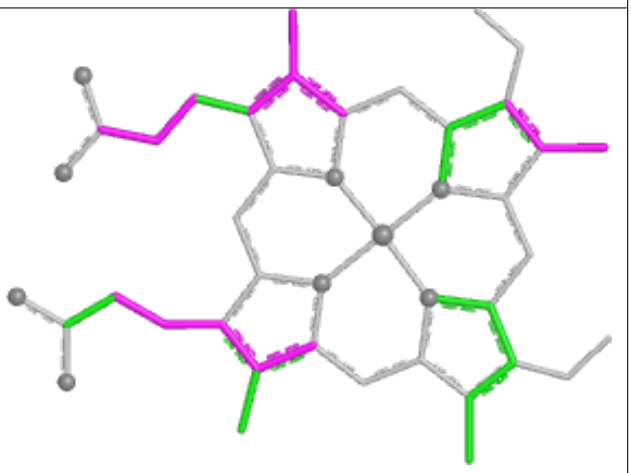


Rings

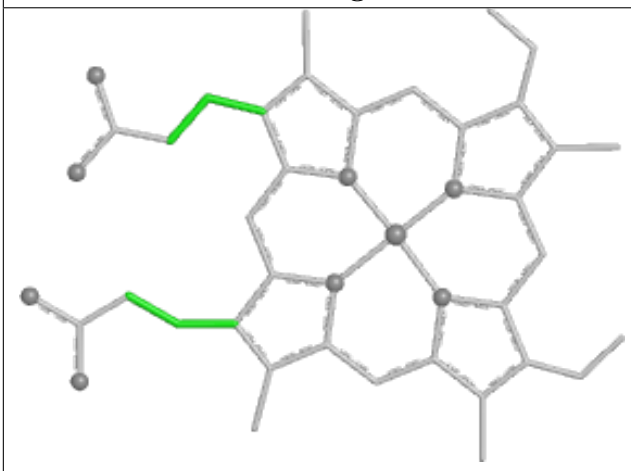
Ligand HEM D 501



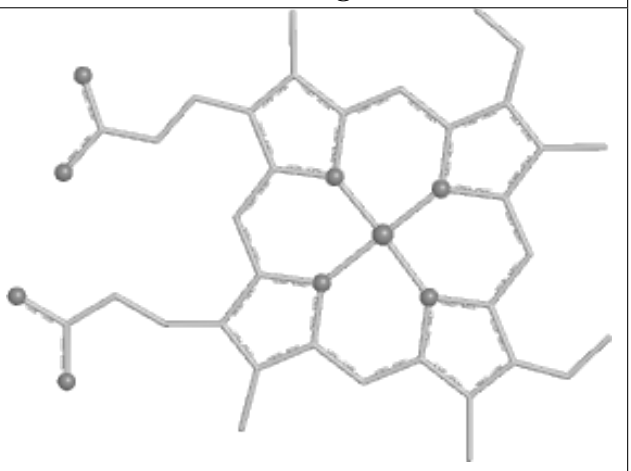
Bond lengths



Bond angles



Torsions



Rings

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	396/408 (97%)	0.42	27 (6%) 17 21	31, 47, 70, 110	0
1	B	402/408 (98%)	0.33	22 (5%) 25 30	33, 49, 76, 136	0
1	C	408/408 (100%)	0.26	17 (4%) 36 41	34, 46, 71, 145	0
1	D	396/408 (97%)	0.56	36 (9%) 9 11	39, 57, 84, 153	0
1	E	395/408 (96%)	0.87	83 (21%) 1 0	44, 63, 96, 166	0
1	F	396/408 (97%)	1.31	100 (25%) 0 0	42, 68, 107, 127	0
All	All	2393/2448 (97%)	0.62	285 (11%) 4 5	31, 54, 95, 166	0

The worst 5 of 285 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	212	THR	11.4
1	F	405	VAL	10.9
1	F	262	THR	9.7
1	B	10[A]	PRO	9.1
1	F	127	LEU	8.7

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

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

6.3 Carbohydrates

There are no 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
4	FMT	C	507	3/3	-0.11	0.38	98,98,105,106	0
4	FMT	A	504	3/3	0.27	0.27	94,94,106,108	0
4	FMT	C	514	3/3	0.33	0.44	88,88,95,108	0
4	FMT	D	507	3/3	0.34	0.40	86,86,95,100	0
4	FMT	A	512	3/3	0.35	0.34	95,95,108,112	0
4	FMT	A	514	3/3	0.36	0.24	90,90,95,99	0
4	FMT	E	510	3/3	0.36	0.41	89,89,102,105	0
4	FMT	B	515	3/3	0.39	0.32	66,66,85,86	0
4	FMT	C	518	3/3	0.40	0.36	73,73,82,94	0
4	FMT	B	512	3/3	0.42	0.22	85,85,106,110	0
4	FMT	B	539	3/3	0.43	0.28	91,91,92,97	0
4	FMT	A	537	3/3	0.44	0.63	75,75,80,94	0
4	FMT	B	503	3/3	0.45	0.35	83,83,83,88	0
4	FMT	B	525	3/3	0.46	0.48	86,86,94,101	0
4	FMT	B	534	3/3	0.46	0.51	94,94,101,105	0
4	FMT	A	508	3/3	0.47	0.14	94,94,104,106	0
4	FMT	F	503	3/3	0.48	0.17	76,76,87,92	0
4	FMT	A	524	3/3	0.49	0.33	99,99,102,106	0
4	FMT	E	509	3/3	0.49	0.25	78,78,91,94	0
4	FMT	E	511	3/3	0.50	0.16	92,92,107,121	0
4	FMT	A	534	3/3	0.50	0.30	78,78,93,93	0
4	FMT	F	505	3/3	0.51	0.22	78,78,80,96	0
4	FMT	A	529	3/3	0.52	0.21	88,88,88,101	0
4	FMT	B	524	3/3	0.52	0.52	73,73,88,91	0
4	FMT	E	504	3/3	0.53	0.32	84,84,95,97	0
4	FMT	C	521	3/3	0.54	0.15	106,106,107,108	0
6	GOL	C	532	6/6	0.55	0.51	76,93,96,109	0
4	FMT	E	512	3/3	0.56	0.33	81,81,92,92	0
4	FMT	D	508	3/3	0.57	0.24	64,64,65,76	0
4	FMT	D	516	3/3	0.58	0.20	71,71,92,93	0
4	FMT	C	516	3/3	0.59	0.27	75,75,80,81	0
4	FMT	F	507	3/3	0.59	0.52	86,86,93,103	0
4	FMT	A	522	3/3	0.59	0.22	76,76,77,92	0
4	FMT	C	513	3/3	0.60	0.47	85,85,99,101	0
6	GOL	B	542	6/6	0.60	0.26	70,88,89,89	0
4	FMT	C	523	3/3	0.60	0.25	74,74,87,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FMT	A	513	3/3	0.61	0.34	78,78,87,100	0
4	FMT	C	524	3/3	0.61	0.39	71,71,74,83	0
4	FMT	A	535	3/3	0.61	0.47	83,83,95,112	0
4	FMT	C	505	3/3	0.62	0.31	50,50,61,75	0
4	FMT	A	532	3/3	0.62	0.20	102,102,102,106	0
4	FMT	B	526	3/3	0.62	0.16	73,73,73,81	0
4	FMT	C	520	3/3	0.62	0.40	78,78,83,97	0
4	FMT	C	528	3/3	0.63	0.38	72,72,77,79	0
4	FMT	B	516	3/3	0.64	0.44	68,68,84,86	0
4	FMT	A	520	3/3	0.65	0.18	61,61,74,90	0
4	FMT	B	519	3/3	0.66	0.20	79,79,91,92	0
4	FMT	E	507	3/3	0.67	0.43	59,59,73,85	0
6	GOL	A	542	6/6	0.68	0.40	58,72,83,91	0
4	FMT	C	511	3/3	0.68	0.32	89,89,99,101	0
4	FMT	A	516	3/3	0.68	0.29	79,79,90,95	0
4	FMT	A	507	3/3	0.69	0.31	63,63,85,89	0
4	FMT	B	536	3/3	0.69	0.22	65,65,73,78	0
4	FMT	E	506	3/3	0.70	0.15	68,68,73,84	0
4	FMT	A	527	3/3	0.70	0.23	79,79,85,87	0
4	FMT	D	512	3/3	0.71	0.17	93,93,96,100	0
4	FMT	B	533	3/3	0.71	0.22	91,91,93,97	0
4	FMT	D	505	3/3	0.71	0.31	86,86,87,94	0
4	FMT	A	517	3/3	0.71	0.21	85,85,94,101	0
4	FMT	A	539	3/3	0.71	0.33	86,86,87,89	0
4	FMT	D	509	3/3	0.73	0.24	79,79,81,83	0
4	FMT	B	506	3/3	0.73	0.24	64,64,78,79	0
4	FMT	C	525	3/3	0.73	0.14	69,69,78,78	0
4	FMT	B	529	3/3	0.73	0.19	73,73,88,93	0
4	FMT	F	509	3/3	0.74	0.17	64,64,78,89	0
4	FMT	F	511	3/3	0.74	0.30	92,92,98,106	0
4	FMT	A	531	3/3	0.74	0.49	95,95,101,103	0
4	FMT	D	518	3/3	0.74	0.22	93,93,95,99	0
4	FMT	C	526	3/3	0.74	0.39	86,86,91,92	0
4	FMT	C	529	3/3	0.75	0.21	83,83,87,101	0
4	FMT	C	517	3/3	0.75	0.20	60,60,64,84	0
4	FMT	D	514	3/3	0.75	0.23	69,69,70,86	0
4	FMT	A	509	3/3	0.75	0.43	86,86,90,92	0
4	FMT	B	535	3/3	0.75	0.19	66,66,72,84	0
4	FMT	F	508	3/3	0.76	0.26	80,80,89,93	0
4	FMT	B	520	3/3	0.76	0.16	78,78,83,96	0
4	FMT	B	510	3/3	0.76	0.15	73,73,78,86	0
4	FMT	B	518	3/3	0.77	0.14	81,81,86,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FMT	D	511	3/3	0.77	0.19	75,75,83,83	0
4	FMT	E	508	3/3	0.77	0.33	91,91,93,96	0
4	FMT	D	515	3/3	0.77	0.40	68,68,71,80	0
6	GOL	E	515[A]	6/6	0.77	0.37	45,57,59,60	6
6	GOL	E	515[B]	6/6	0.77	0.37	121,125,127,128	6
4	FMT	C	503	3/3	0.79	0.23	61,61,71,83	0
4	FMT	A	530	3/3	0.79	0.16	74,74,81,89	0
4	FMT	B	528	3/3	0.79	0.23	69,69,71,89	0
6	GOL	A	544	6/6	0.79	0.27	68,80,81,83	6
4	FMT	D	510	3/3	0.80	0.17	66,66,67,79	0
6	GOL	A	545	6/6	0.80	0.28	46,63,70,80	6
4	FMT	F	510	3/3	0.80	0.13	92,92,95,97	0
4	FMT	B	513	3/3	0.81	0.25	67,67,87,87	0
4	FMT	A	525	3/3	0.81	0.71	73,73,74,77	0
4	FMT	E	505	3/3	0.81	0.17	55,55,59,74	0
4	FMT	D	513	3/3	0.81	0.41	82,82,83,89	0
4	FMT	A	511	3/3	0.82	0.22	62,62,75,80	0
4	FMT	B	514	3/3	0.82	0.43	90,90,95,98	0
4	FMT	B	523	3/3	0.82	0.24	64,64,72,79	0
4	FMT	A	536	3/3	0.82	0.37	72,72,79,82	0
4	FMT	A	533	3/3	0.82	0.29	84,84,87,100	0
4	FMT	A	519	3/3	0.82	0.33	74,74,80,84	0
4	FMT	D	503	3/3	0.82	0.34	89,89,93,96	0
6	GOL	C	531[A]	6/6	0.83	0.26	53,57,60,61	6
6	GOL	C	531[B]	6/6	0.83	0.26	26,40,43,47	6
4	FMT	C	510	3/3	0.83	0.11	86,86,105,106	0
4	FMT	B	521	3/3	0.83	0.23	75,75,79,90	0
4	FMT	C	508	3/3	0.83	0.16	82,82,90,98	0
4	FMT	B	508	3/3	0.84	0.15	77,77,93,94	0
6	GOL	B	543[A]	6/6	0.84	0.28	36,39,43,45	6
6	GOL	B	543[B]	6/6	0.84	0.28	66,72,80,83	6
3	DEB	F	502	27/27	0.84	0.18	56,64,74,83	0
4	FMT	B	531	3/3	0.84	0.16	84,84,86,88	0
4	FMT	B	532	3/3	0.84	0.22	84,84,90,92	0
4	FMT	D	504	3/3	0.84	0.20	58,58,60,64	0
4	FMT	A	503	3/3	0.84	0.16	80,80,85,87	0
4	FMT	C	522	3/3	0.85	0.15	87,87,91,93	0
4	FMT	C	515	3/3	0.85	0.25	66,66,77,79	0
4	FMT	C	527	3/3	0.85	0.33	50,50,51,73	3
4	FMT	F	512	3/3	0.85	0.28	85,85,86,90	0
4	FMT	B	505	3/3	0.85	0.34	70,70,80,90	0
4	FMT	B	509	3/3	0.86	0.22	73,73,74,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FMT	B	537	3/3	0.86	0.11	59,59,83,96	0
4	FMT	B	517	3/3	0.86	0.28	61,61,70,75	0
4	FMT	E	503	3/3	0.86	0.19	75,75,84,84	0
4	FMT	B	527	3/3	0.86	0.15	74,74,89,93	0
4	FMT	A	523	3/3	0.86	0.25	76,76,81,84	0
4	FMT	A	528	3/3	0.86	0.39	85,85,88,106	0
4	FMT	F	504	3/3	0.86	0.27	57,57,64,72	0
6	GOL	A	543[A]	6/6	0.86	0.38	32,46,51,56	6
6	GOL	A	543[B]	6/6	0.86	0.38	32,40,45,45	6
4	FMT	C	502	3/3	0.87	0.14	65,65,75,85	0
4	FMT	D	517	3/3	0.87	0.08	84,84,86,89	0
3	DEB	D	502	27/27	0.87	0.17	32,42,46,47	0
4	FMT	D	506	3/3	0.87	0.12	85,85,87,89	0
3	DEB	C	533	27/27	0.87	0.16	30,37,50,54	0
4	FMT	C	506	3/3	0.87	0.20	69,69,75,81	0
4	FMT	B	504	3/3	0.87	0.23	68,68,72,75	0
4	FMT	F	506	3/3	0.88	0.18	74,74,76,84	0
5	NA	F	513	1/1	0.88	0.29	63,63,63,63	0
4	FMT	B	522	3/3	0.88	0.27	78,78,79,80	0
3	DEB	E	502	27/27	0.89	0.14	47,53,61,74	0
4	FMT	C	512	3/3	0.89	0.19	76,76,80,87	0
5	NA	A	540	1/1	0.89	0.11	56,56,56,56	0
5	NA	D	519	1/1	0.89	0.20	56,56,56,56	0
4	FMT	A	518	3/3	0.89	0.15	83,83,88,91	0
4	FMT	A	506	3/3	0.89	0.15	63,63,66,68	0
2	HEM	F	501	43/43	0.90	0.16	47,54,64,92	0
4	FMT	B	507	3/3	0.90	0.31	63,63,64,82	0
4	FMT	C	504	3/3	0.91	0.15	59,59,63,68	0
3	DEB	A	502	27/27	0.91	0.21	30,37,50,54	0
4	FMT	B	530	3/3	0.92	0.26	52,52,83,96	0
4	FMT	A	538	3/3	0.92	0.29	71,71,72,93	0
4	FMT	A	515	3/3	0.92	0.89	82,82,94,98	0
2	HEM	E	501	43/43	0.93	0.13	39,44,53,66	0
5	NA	E	514	1/1	0.93	0.21	63,63,63,63	0
3	DEB	B	502	27/27	0.93	0.18	33,40,51,59	0
4	FMT	A	505	3/3	0.93	0.34	65,65,70,79	0
4	FMT	B	538	3/3	0.94	0.28	50,50,71,78	0
4	FMT	A	521	3/3	0.94	0.18	62,62,79,96	0
4	FMT	A	510	3/3	0.94	0.14	46,46,67,70	0
4	FMT	C	509	3/3	0.94	0.17	71,71,73,91	0
4	FMT	E	513	3/3	0.95	0.17	67,67,71,76	0
4	FMT	A	526	3/3	0.95	0.11	58,58,68,70	0

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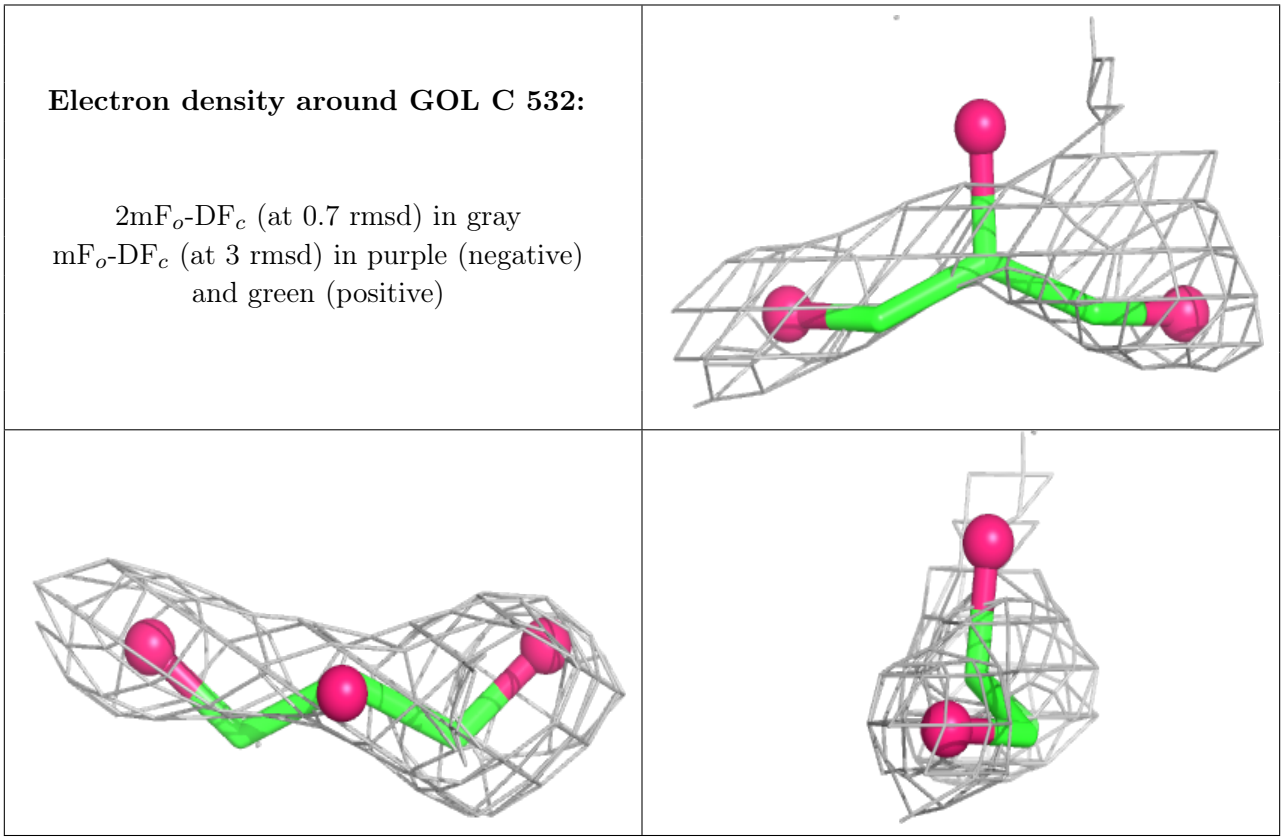
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	D	501	43/43	0.96	0.18	25,36,49,62	0
2	HEM	B	501	43/43	0.96	0.18	29,34,45,51	0
4	FMT	B	511	3/3	0.96	0.15	62,62,64,66	0
4	FMT	C	519	3/3	0.96	0.15	52,52,54,61	0
2	HEM	A	501	43/43	0.97	0.16	29,35,43,61	0
5	NA	A	541	1/1	0.97	0.26	47,47,47,47	0
5	NA	B	540	1/1	0.97	0.14	52,52,52,52	0
5	NA	C	530	1/1	0.97	0.13	47,47,47,47	0
2	HEM	C	501	43/43	0.97	0.16	31,36,41,55	0
5	NA	B	541	1/1	0.98	0.18	50,50,50,50	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.

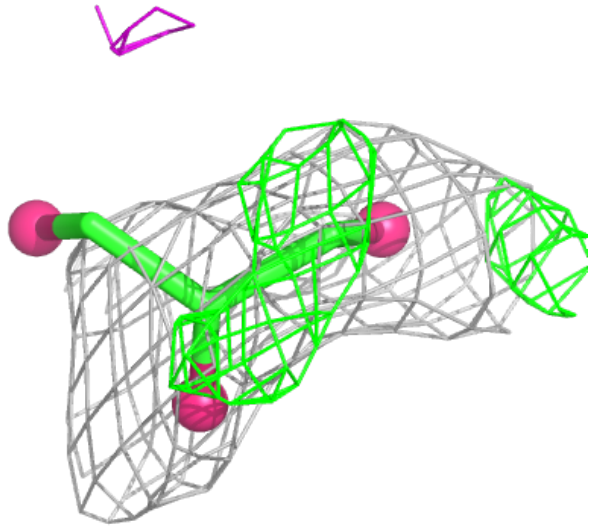
Electron density around GOL C 532:

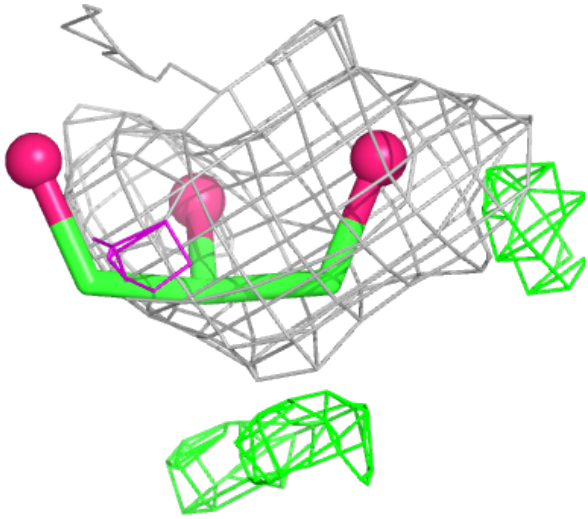
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

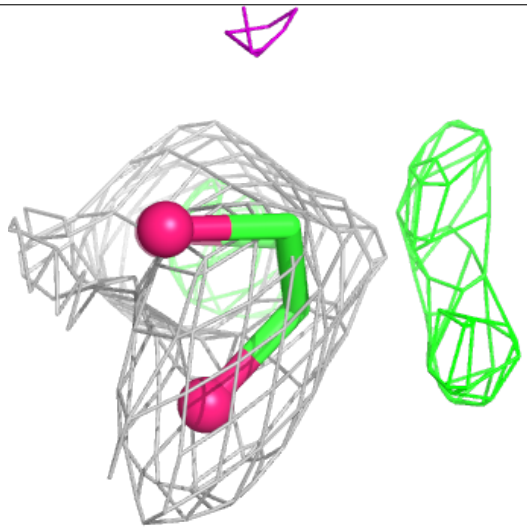


Electron density around GOL B 542:

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

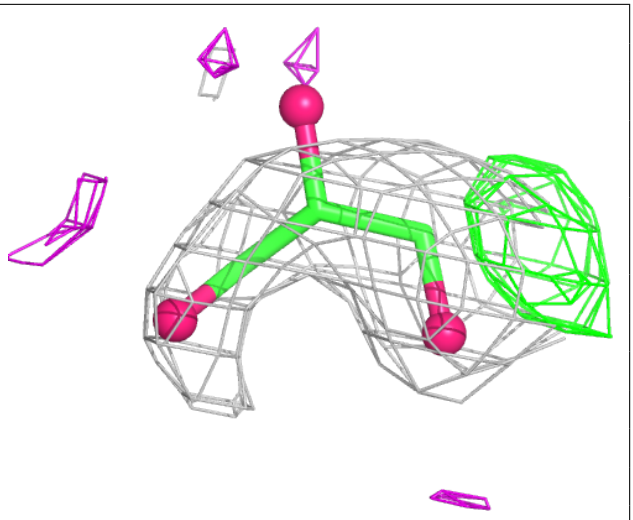


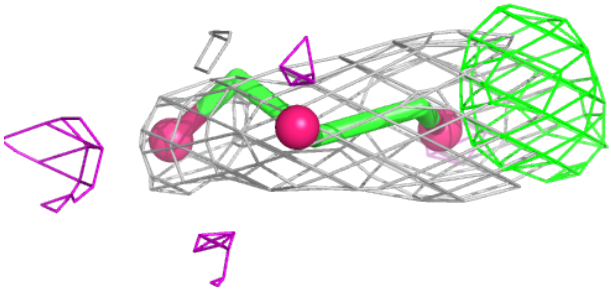


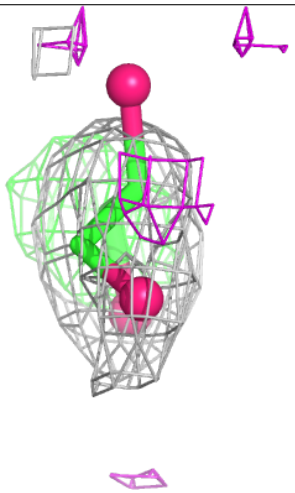


Electron density around GOL A 542:

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

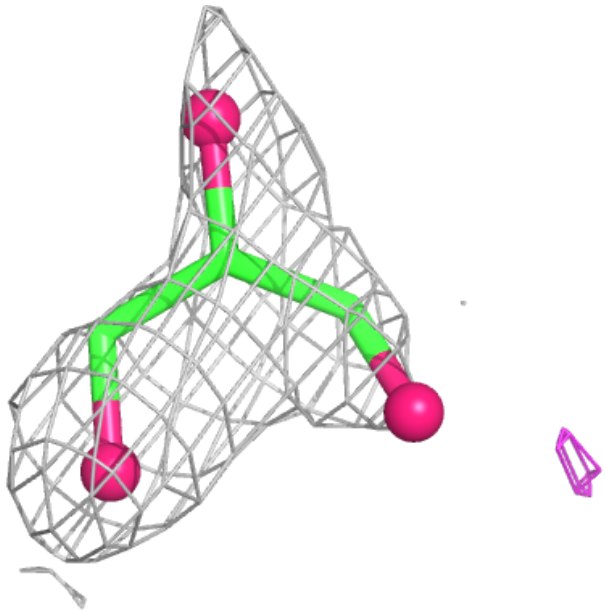


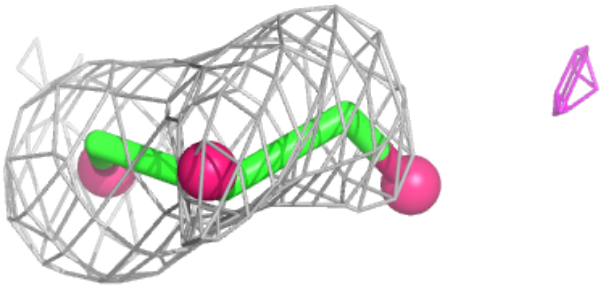


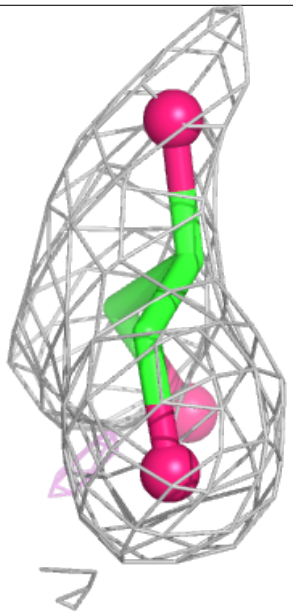


Electron density around GOL E 515 (A):

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

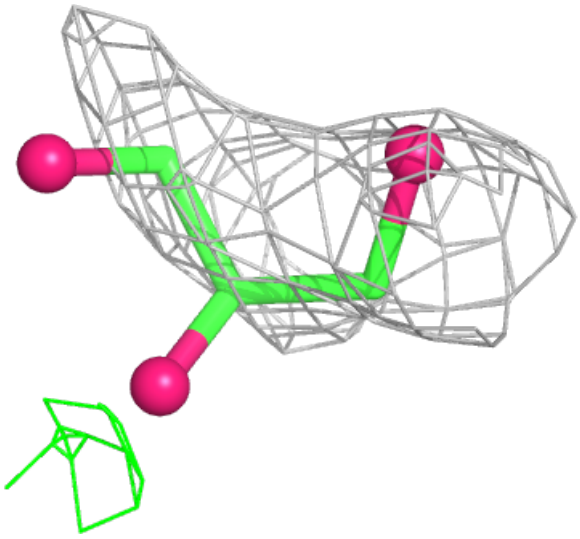


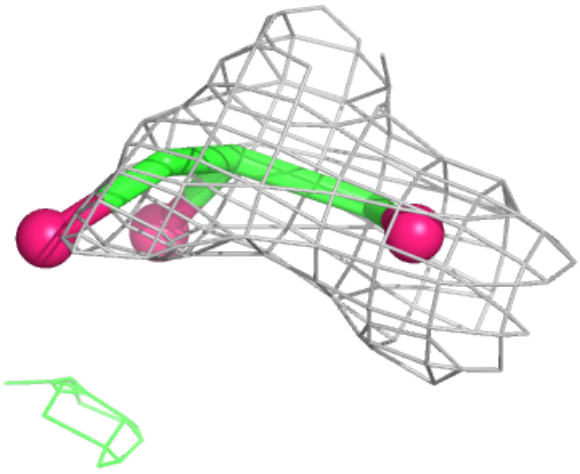


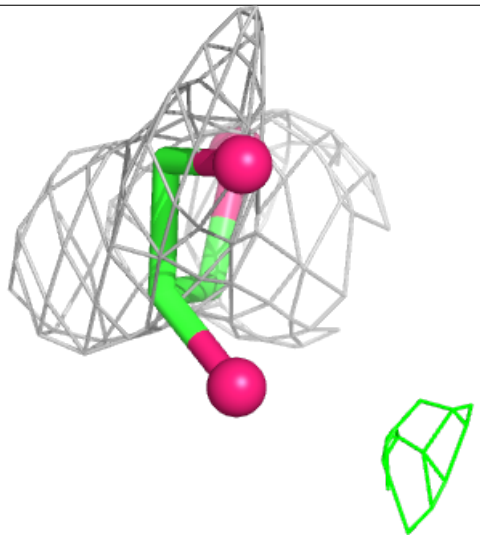


Electron density around GOL E 515 (B):

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

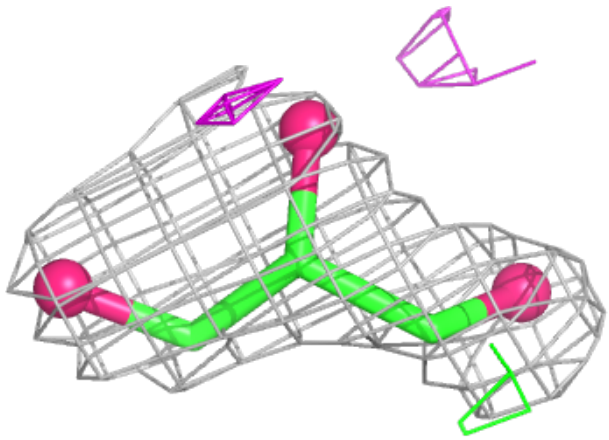


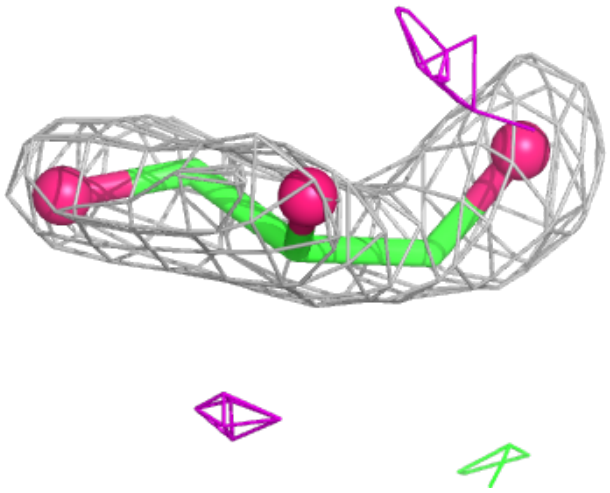


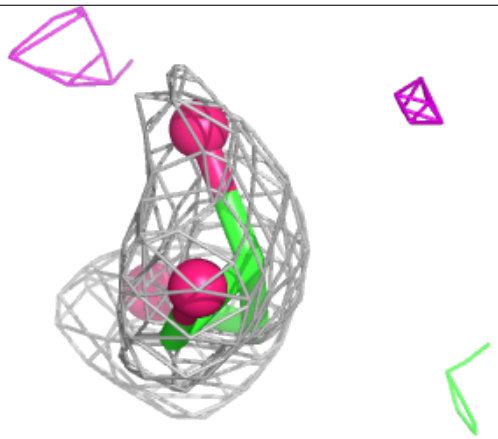


Electron density around GOL A 544:

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

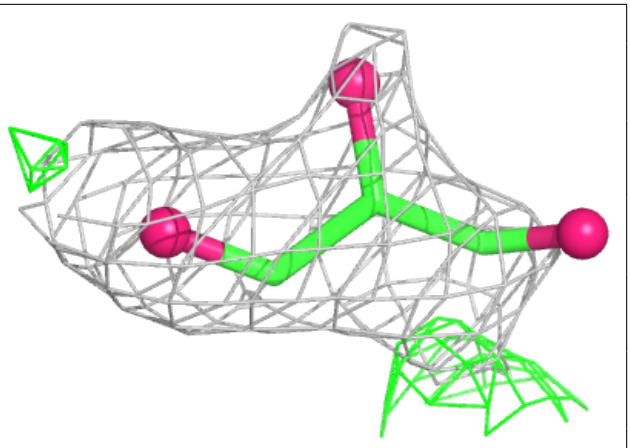


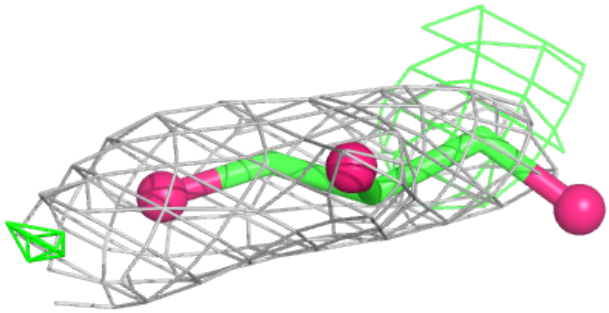


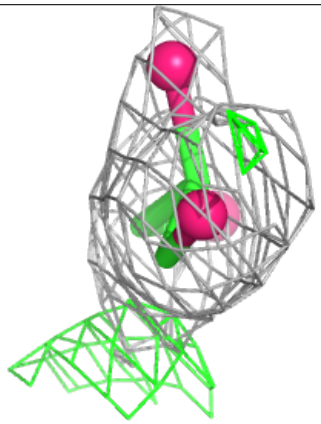


Electron density around GOL A 545:

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

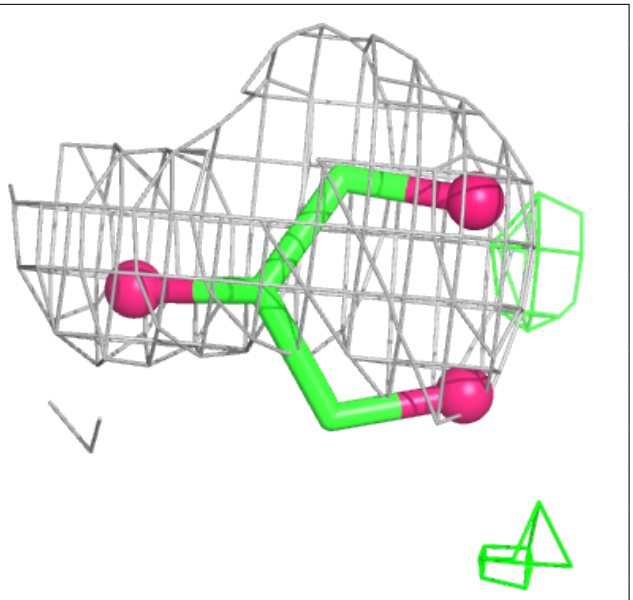


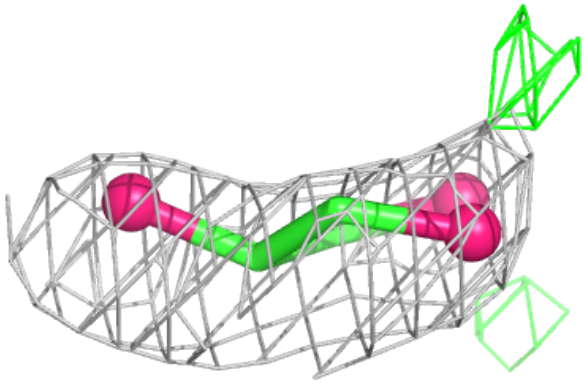


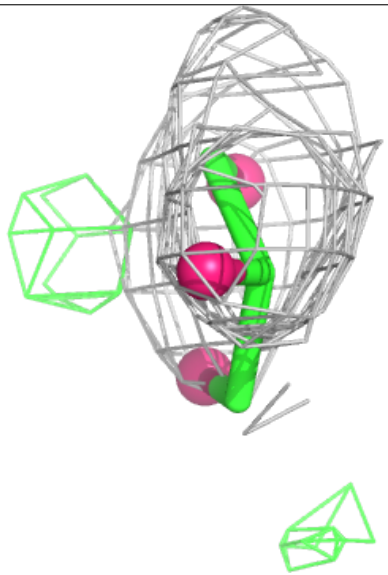


Electron density around GOL C 531 (A):

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

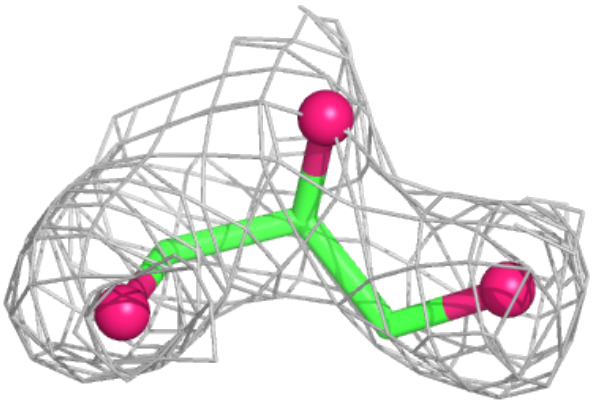


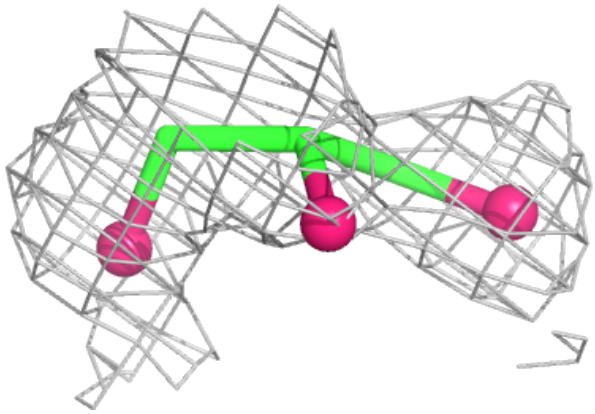


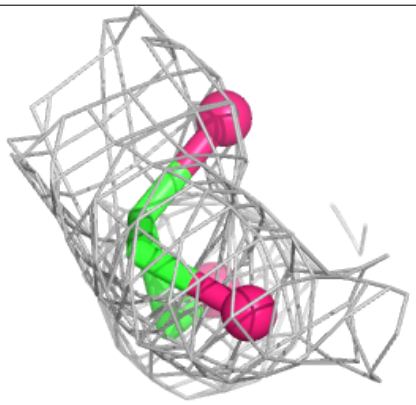


Electron density around GOL C 531 (B):

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

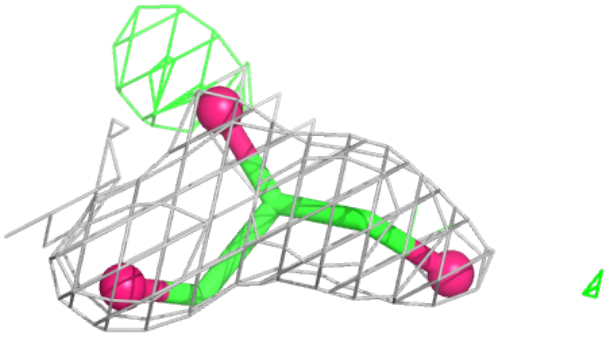


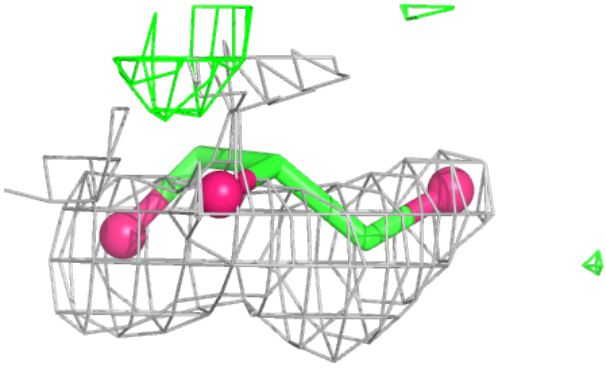


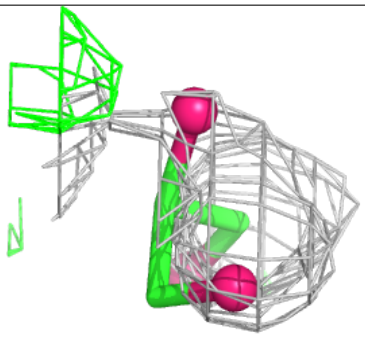


Electron density around GOL B 543 (A):

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

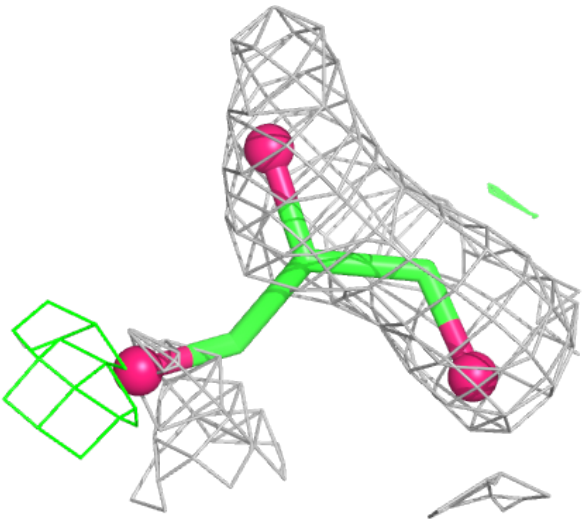


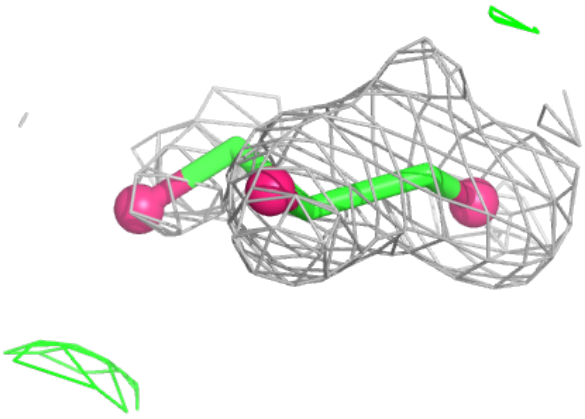


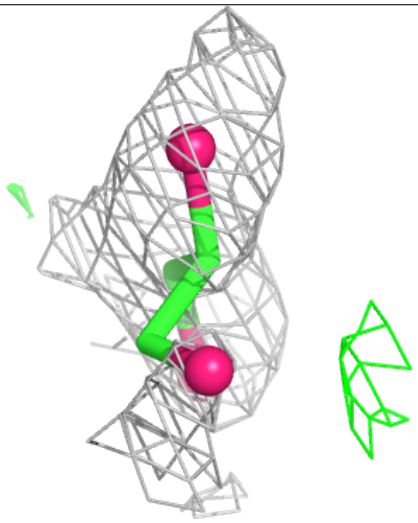


Electron density around GOL B 543 (B):

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

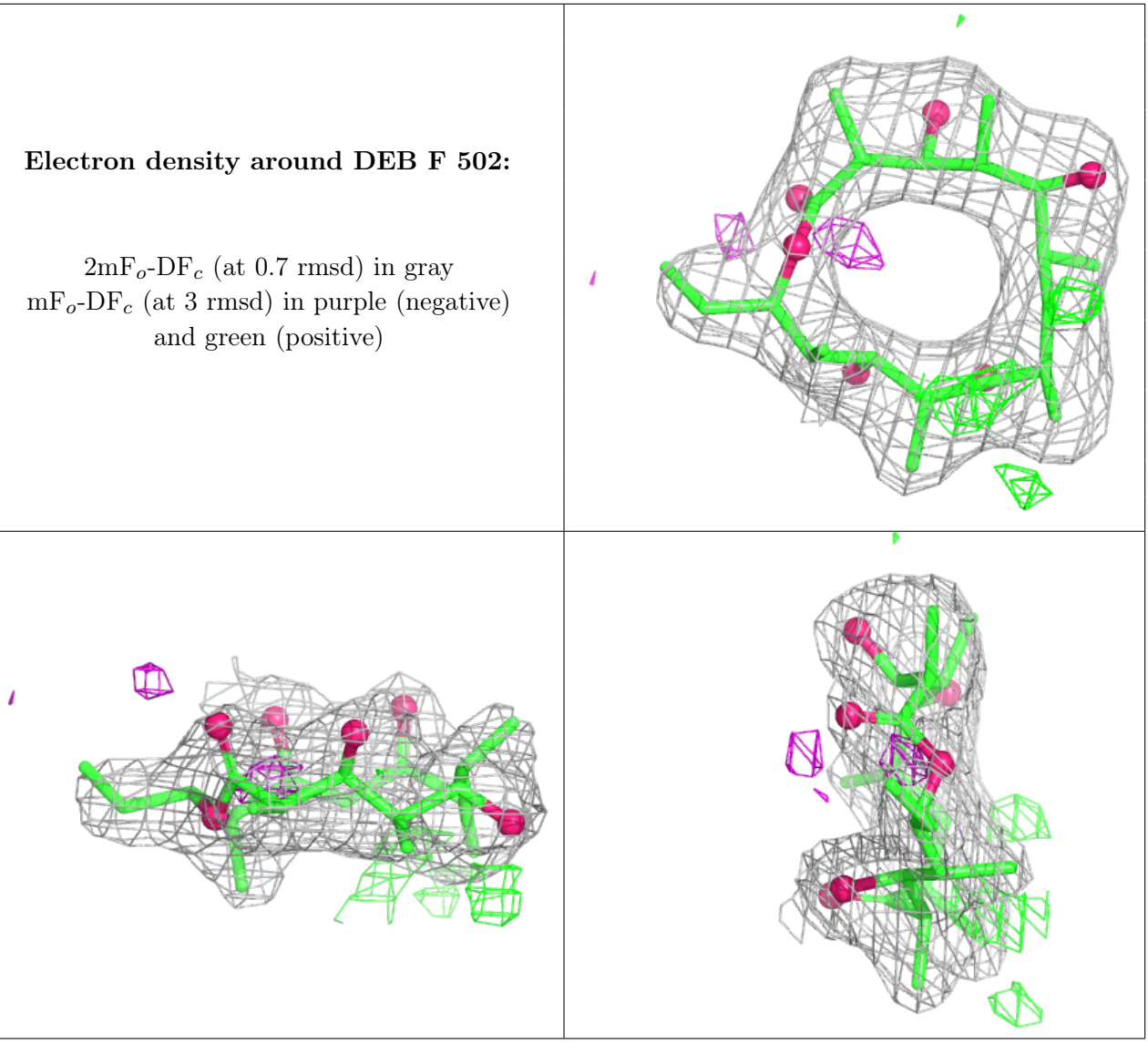






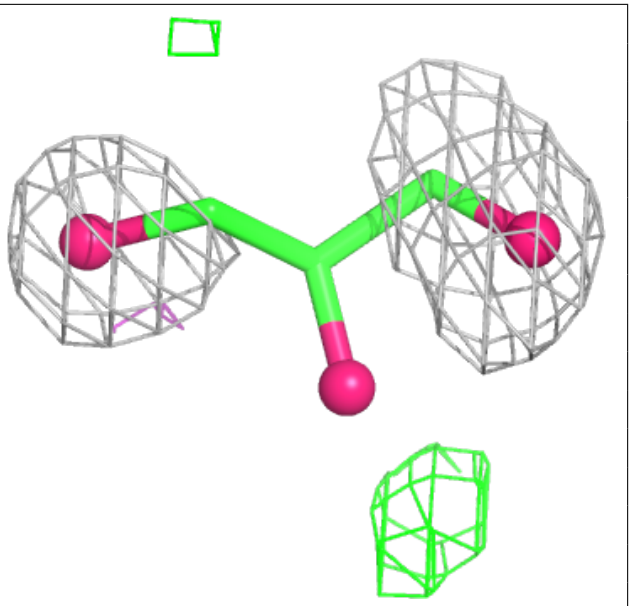
Electron density around DEB F 502:

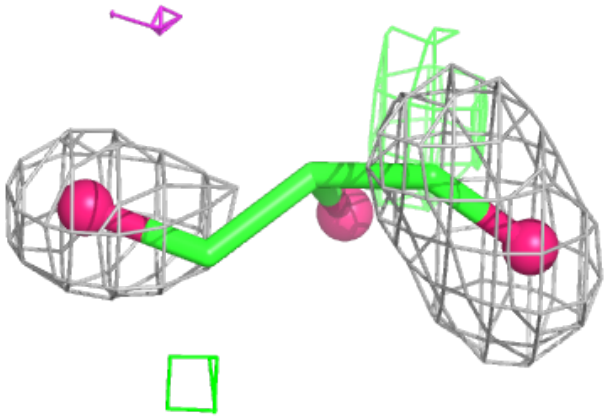
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

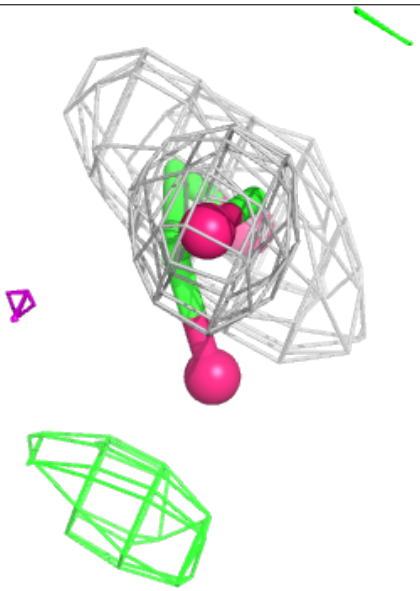


Electron density around GOL A 543 (A):

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

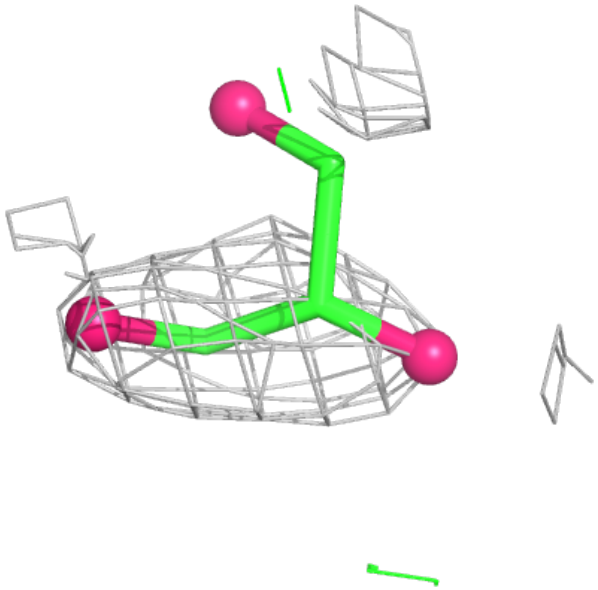


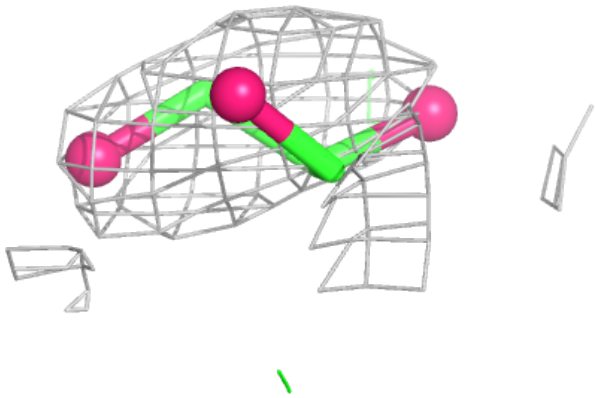


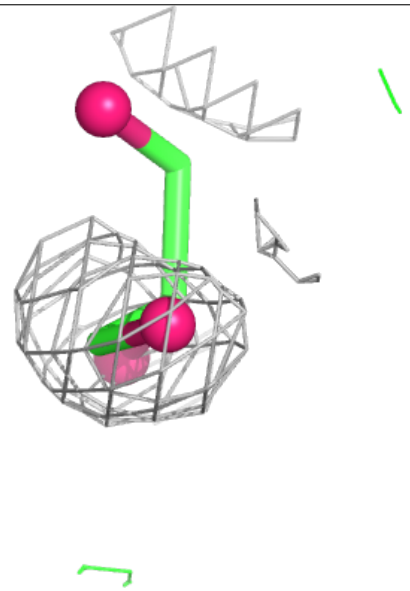


Electron density around GOL A 543 (B):

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

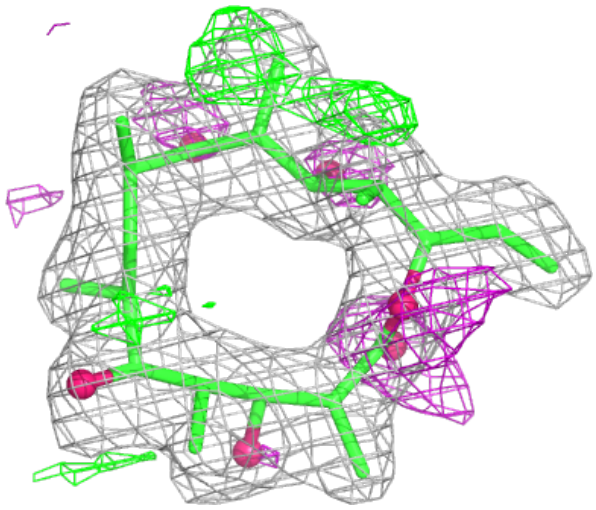


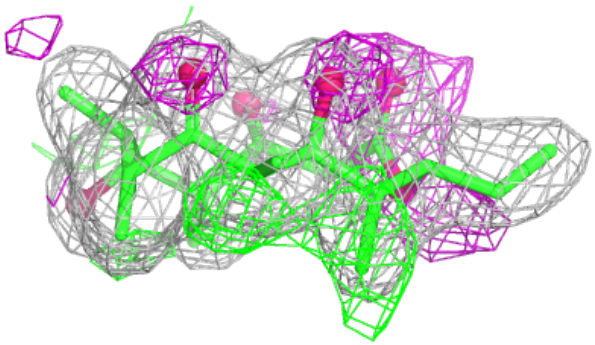




Electron density around DEB D 502:

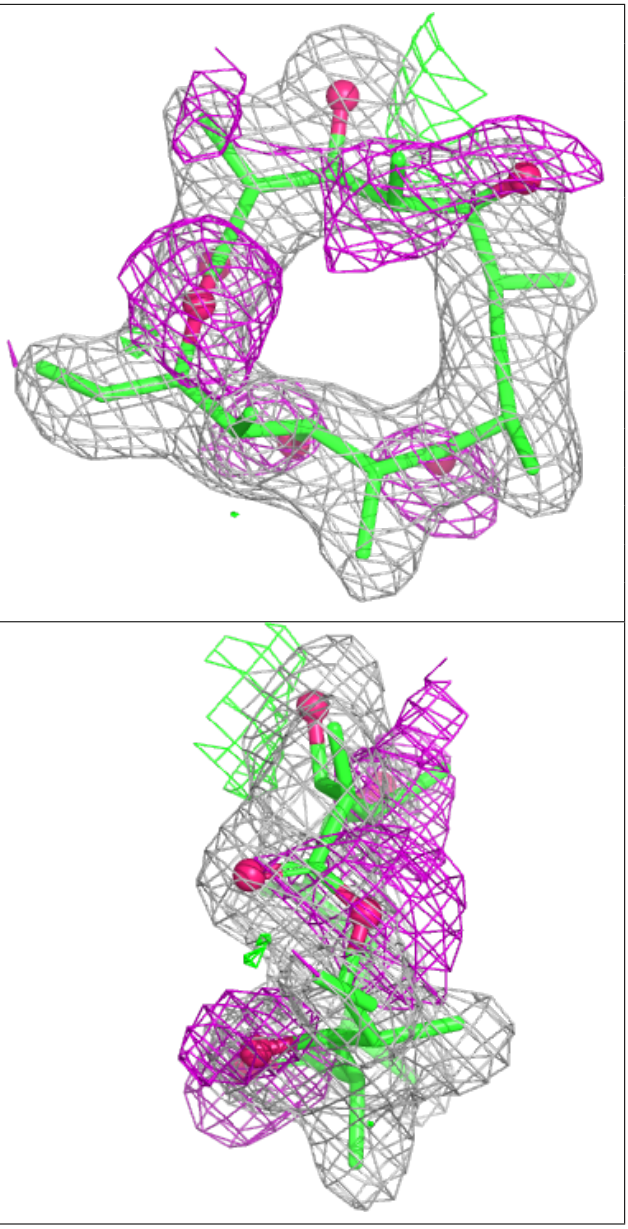
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

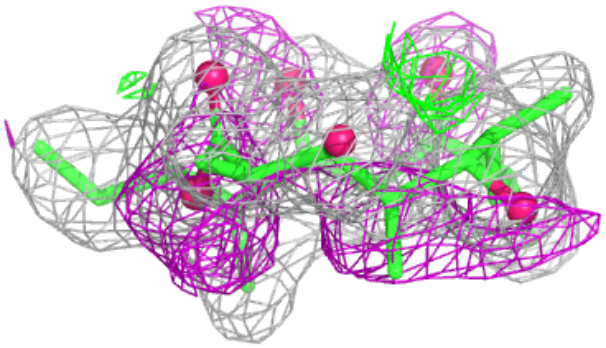




Electron density around DEB C 533:

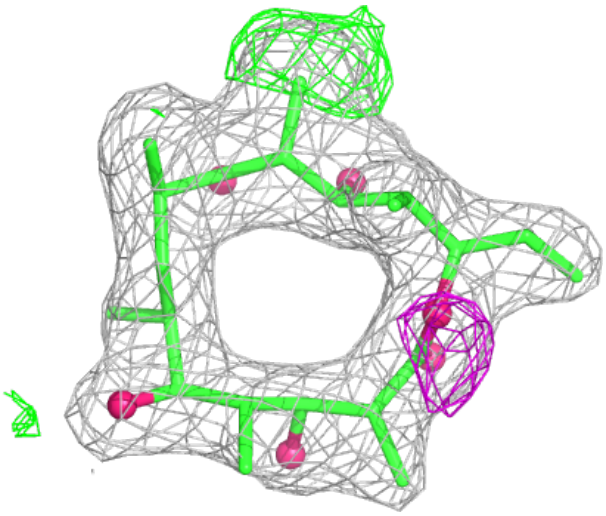
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

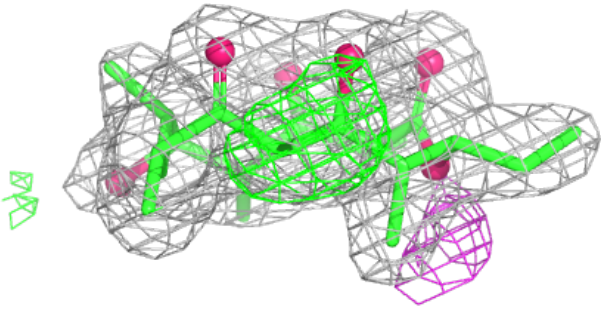


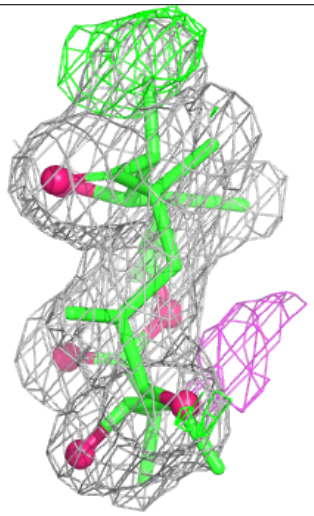


Electron density around DEB E 502:

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

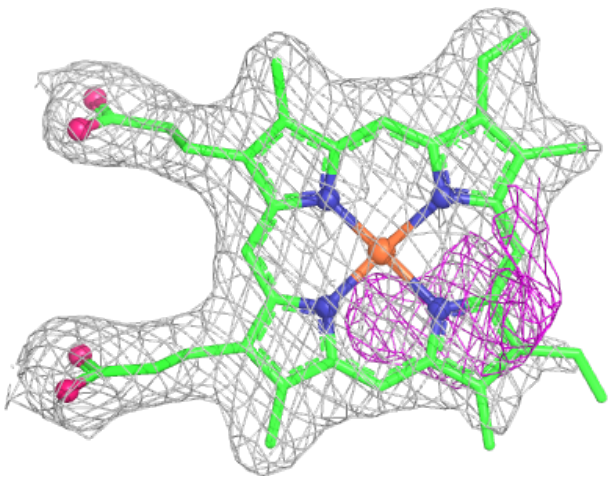


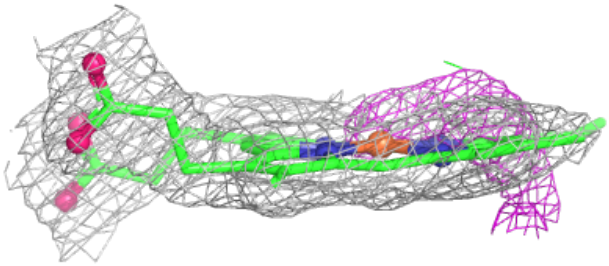




Electron density around HEM F 501:

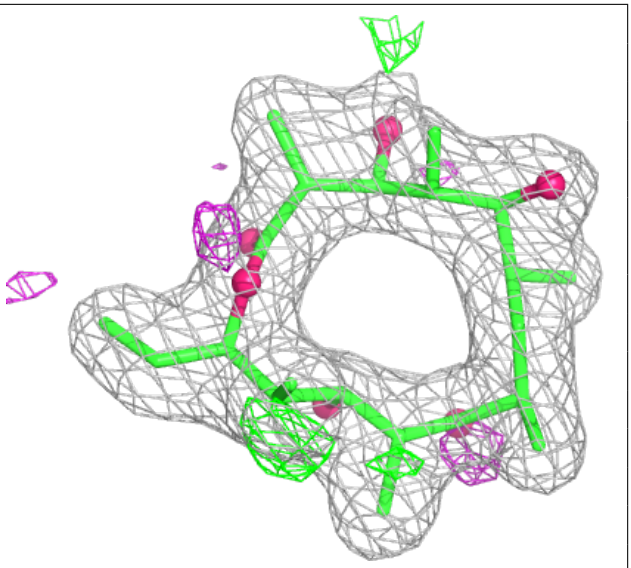
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

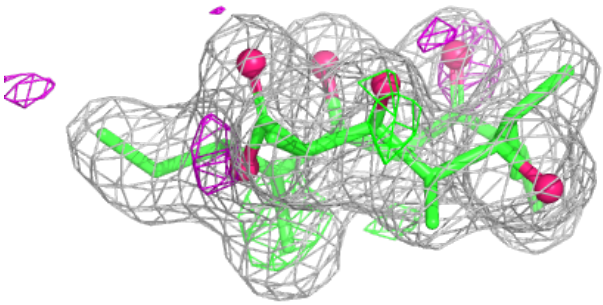


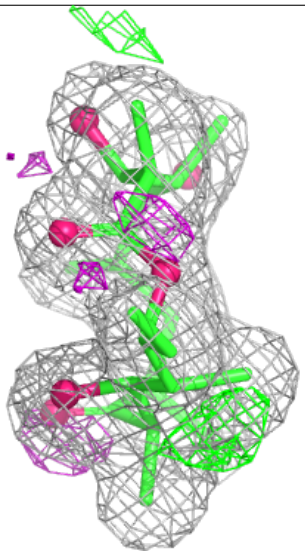


Electron density around DEB A 502:

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

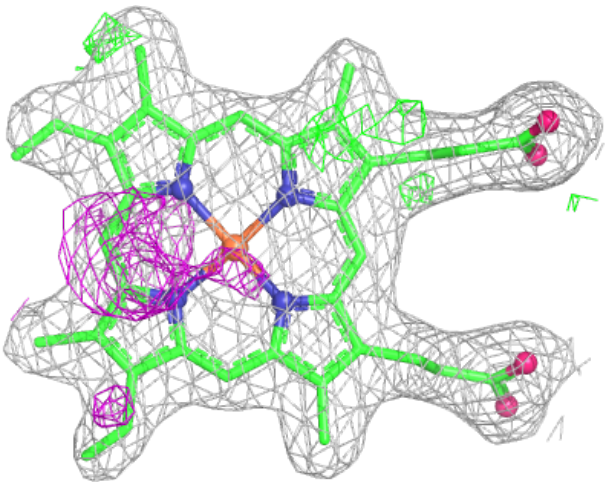


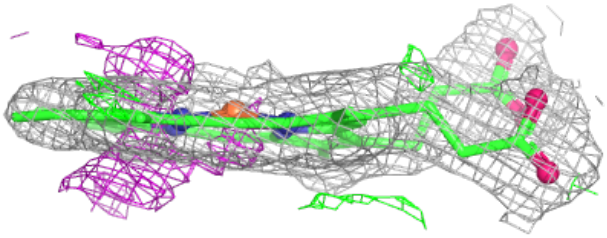


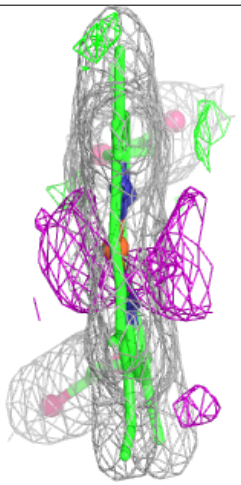


Electron density around HEM E 501:

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

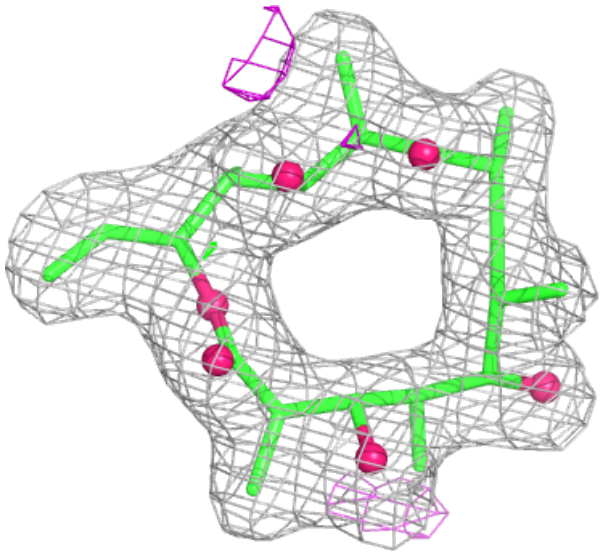


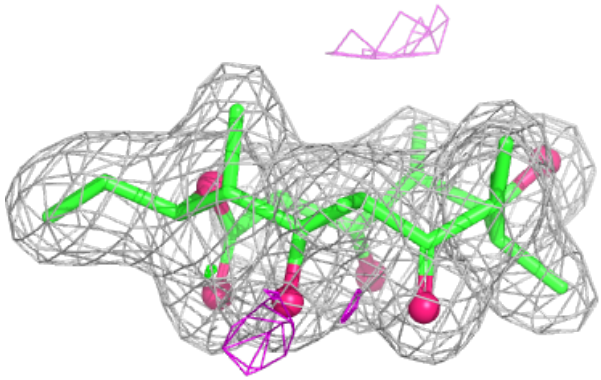


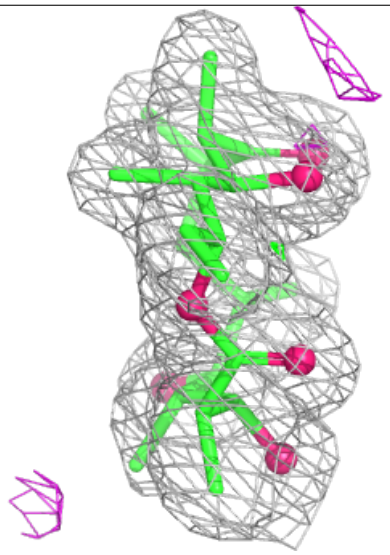


Electron density around DEB B 502:

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

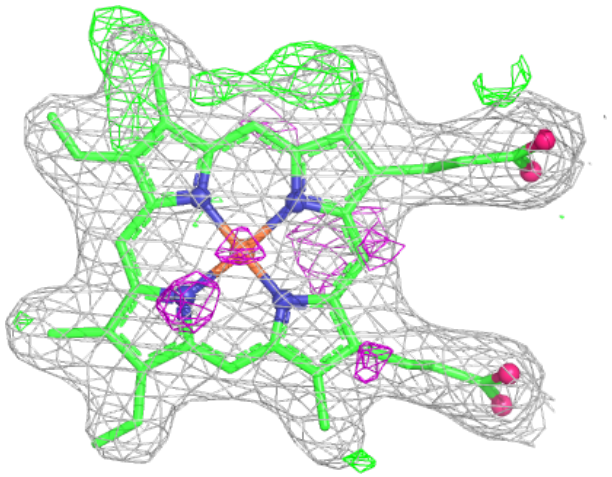


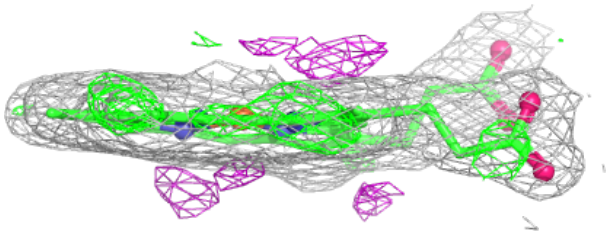


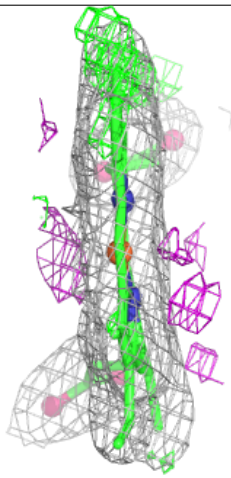


Electron density around HEM D 501:

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

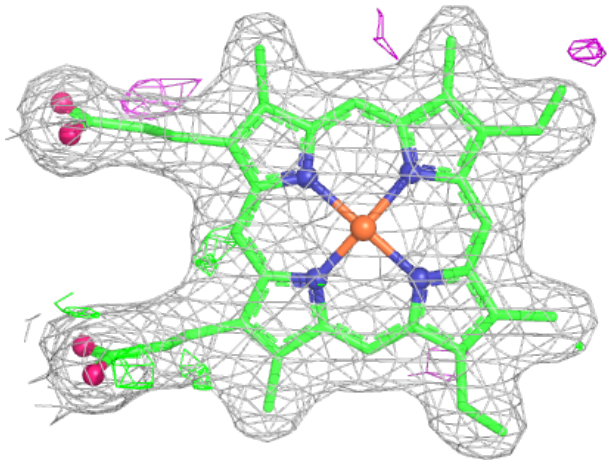


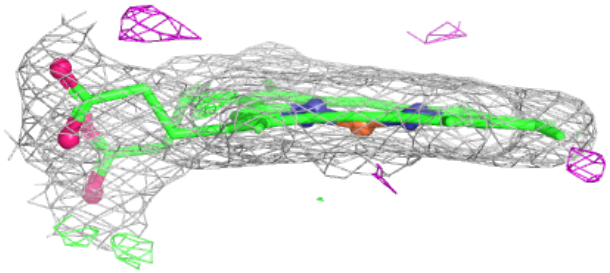




Electron density around HEM B 501:

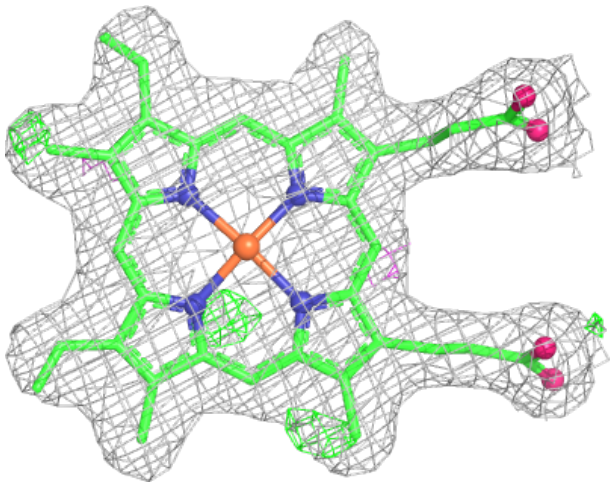
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

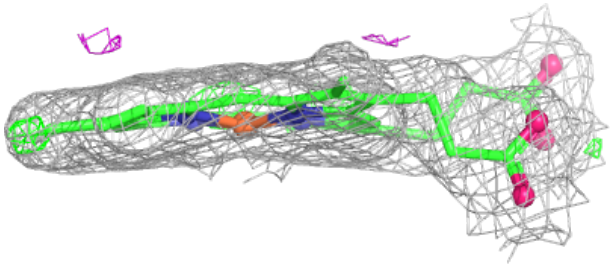


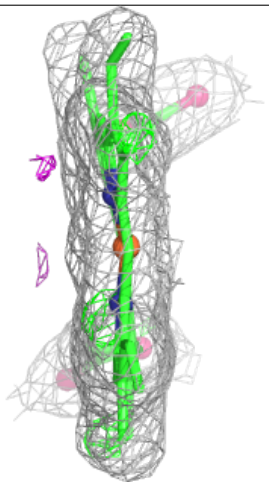


Electron density around HEM A 501:

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

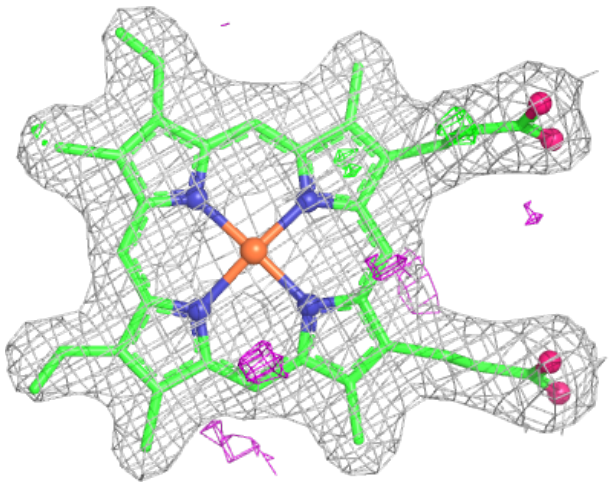


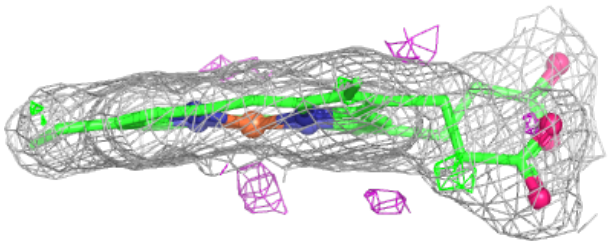


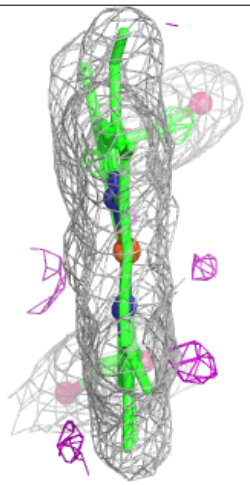


Electron density around HEM C 501:

$2mF_o$-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.