wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 09:21 AM EDT

PDB ID	:	6ZHZ
Title	:	OleP-oleandolide(DEO) in high salt crystallization conditions
Authors	:	Montemiglio, L.C.; Savino, C.; Vallone, B.; Parisi, G.; Cecchetti, C.
Deposited on	:	2020-06-24
Resolution	:	2.20 Å(reported)

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

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

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

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

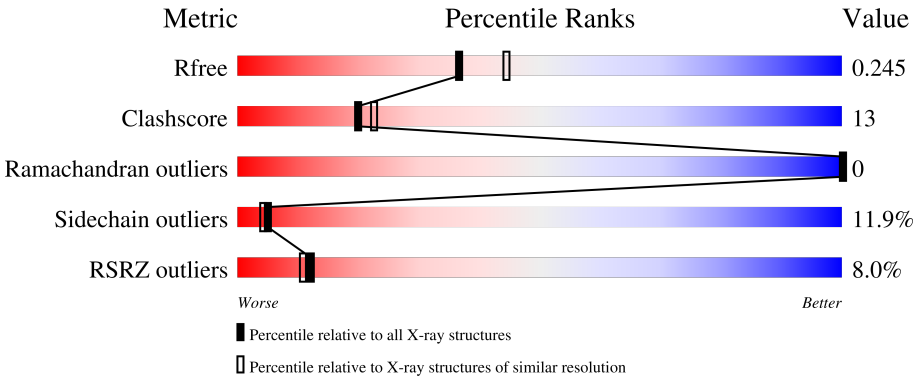
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	407	5% 70% 22% 6% ·
1	B	407	4% 72% 21% · ·
1	C	407	3% 75% 18% · ·
1	D	407	7% 63% 28% 6% ·
1	E	407	10% 70% 21% 6% ·

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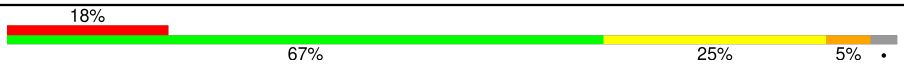
Mol	Chain	Length	Quality of chain
1	F	407	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TRS	D	503	-	-	X	-
5	FMT	A	505	-	-	-	X
5	FMT	A	511	-	-	-	X
5	FMT	A	515	-	-	-	X
5	FMT	B	508	-	-	X	-
5	FMT	B	522	-	-	-	X
5	FMT	B	525	-	-	-	X
5	FMT	C	505	-	-	-	X
5	FMT	C	507	-	-	X	-
5	FMT	C	516	-	-	X	-
5	FMT	D	507	-	-	-	X
5	FMT	D	508	-	-	-	X
5	FMT	E	504	-	-	-	X
5	FMT	E	510	-	-	-	X
5	FMT	F	507	-	-	-	X

2 Entry composition (i)

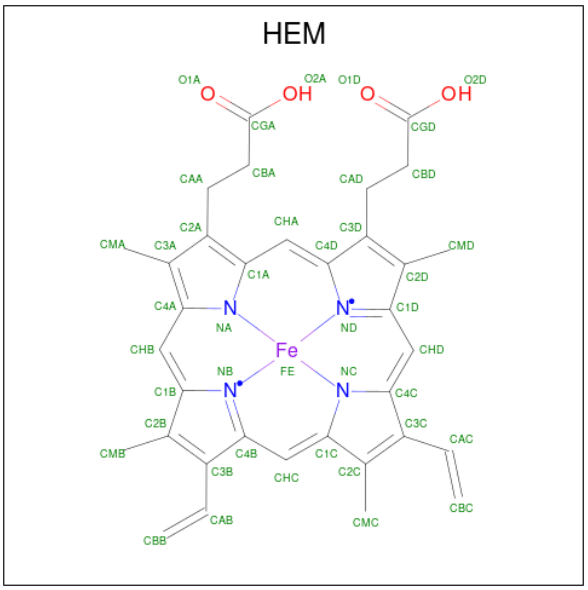
There are 8 unique types of molecules in this entry. The entry contains 20348 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

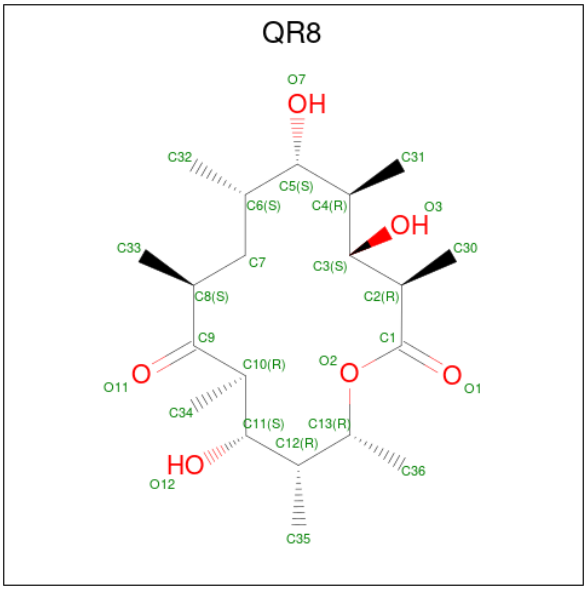
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	7	0
			3135	1978	561	583	13			
1	B	397	Total	C	N	O	S	0	8	0
			3148	1980	563	591	14			
1	C	396	Total	C	N	O	S	0	7	0
			3136	1976	563	584	13			
1	D	395	Total	C	N	O	S	0	1	0
			3082	1942	552	575	13			
1	E	395	Total	C	N	O	S	0	13	0
			3200	2006	580	601	13			
1	F	395	Total	C	N	O	S	0	3	0
			3102	1952	555	582	13			

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



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

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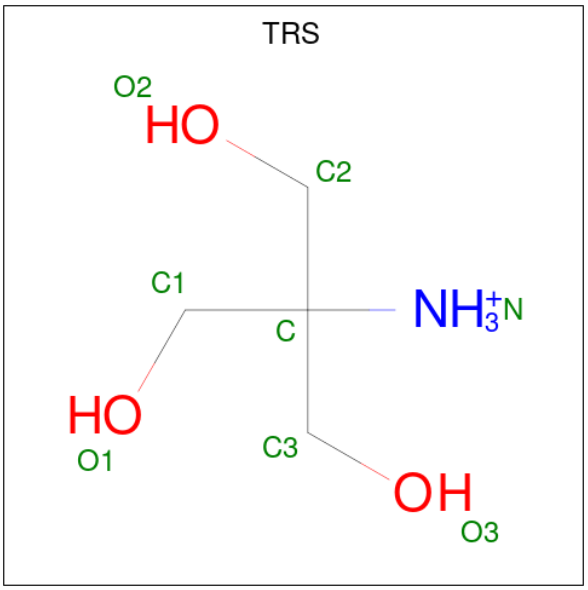
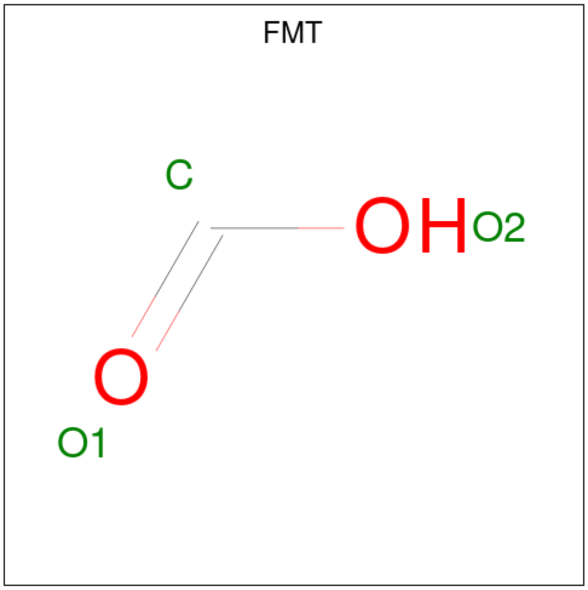
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 26 20 6	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 1 3	0	0
4	D	1	Total C N O 8 4 1 3	0	0
4	F	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

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

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

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

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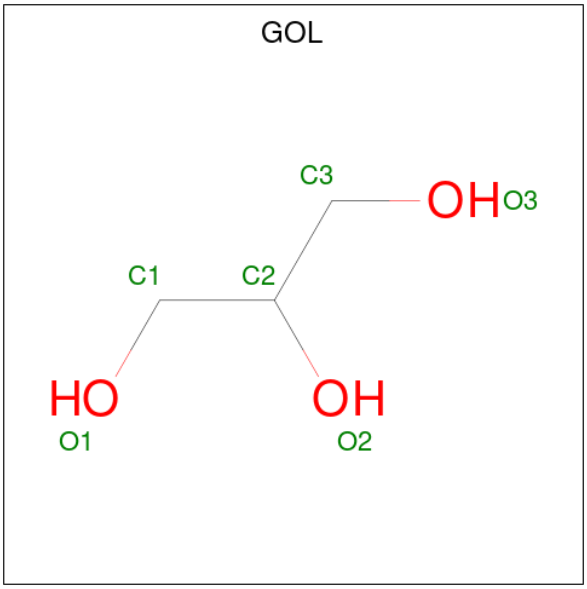
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C O 3 1 2	0	0
5	F	1	Total C O 3 1 2	0	0
5	F	1	Total C O 3 1 2	0	0
5	F	1	Total C O 3 1 2	0	0
5	F	1	Total C O 3 1 2	0	0
5	F	1	Total C O 3 1 2	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	B	1	Total Na 1 1	0	0
7	C	1	Total Na 1 1	0	0
7	D	1	Total Na 1 1	0	0
7	F	1	Total Na 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	138	Total O 138 138	0	0
8	B	157	Total O 157 157	0	0

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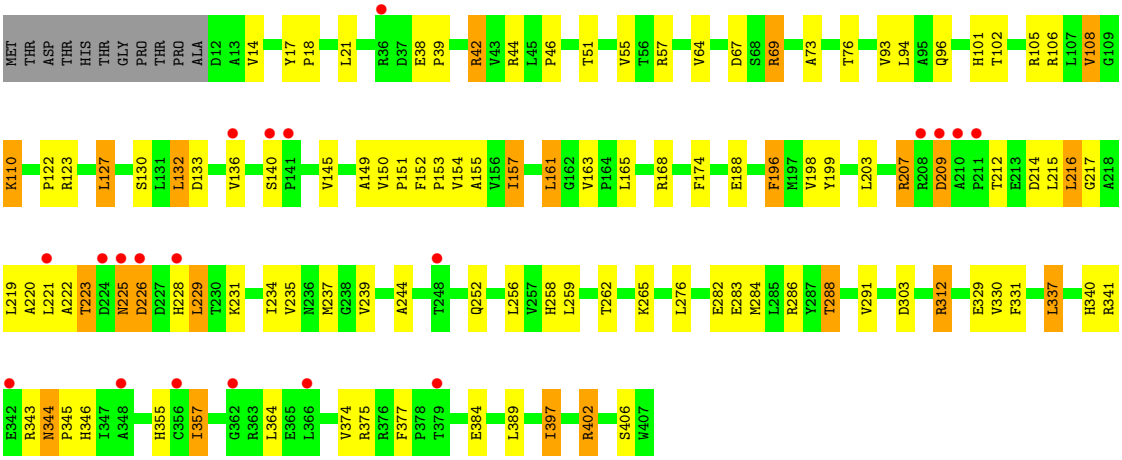
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	229	Total O 229 229	0	0
8	D	84	Total O 84 84	0	0
8	E	76	Total O 76 76	0	0
8	F	79	Total O 79 79	0	0

3 Residue-property plots (i)

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

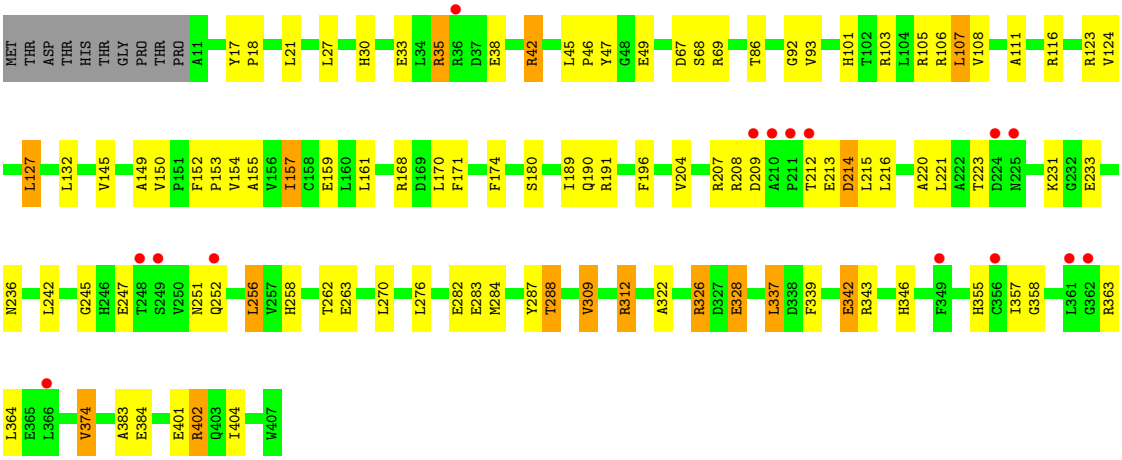
• Molecule 1: Cytochrome P-450

Chain A:



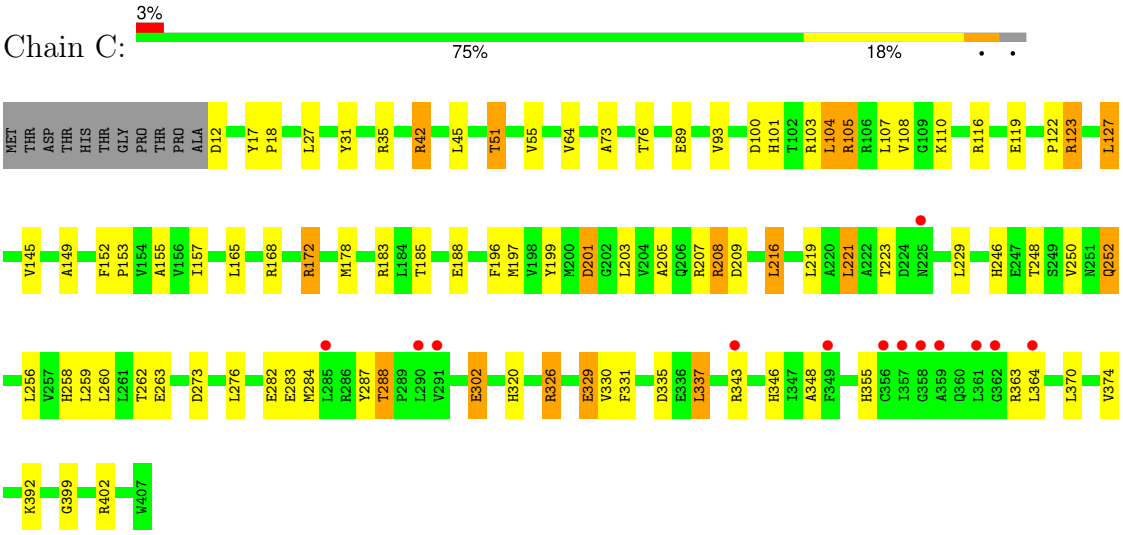
• Molecule 1: Cytochrome P-450

Chain B:



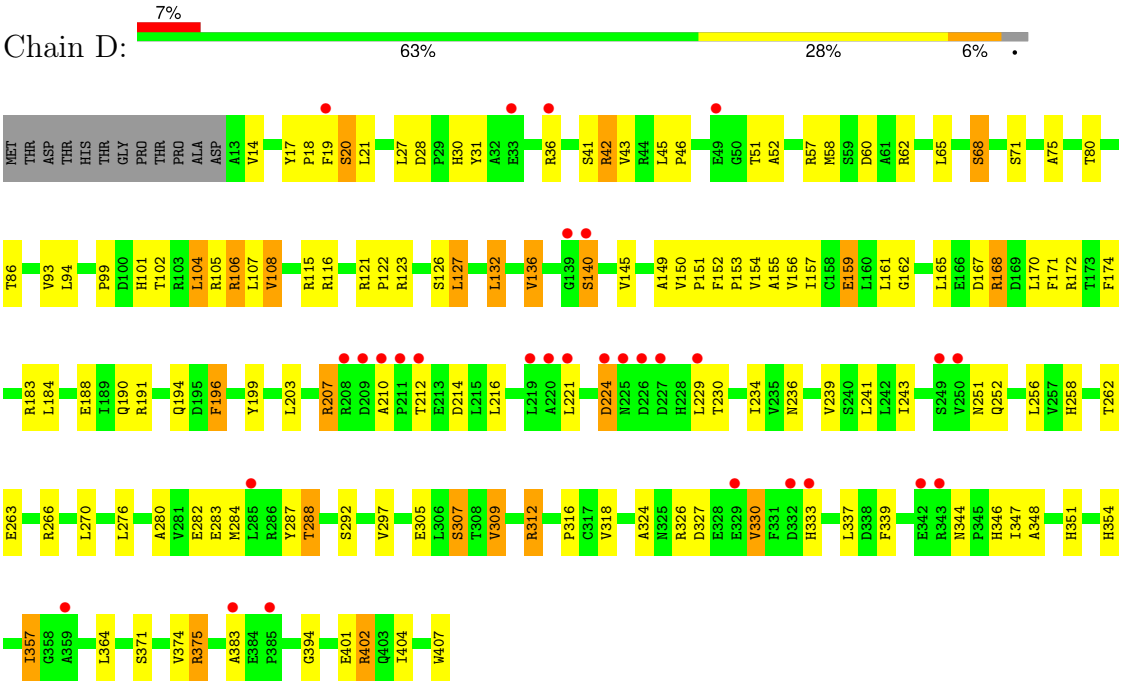
• Molecule 1: Cytochrome P-450

Chain C:



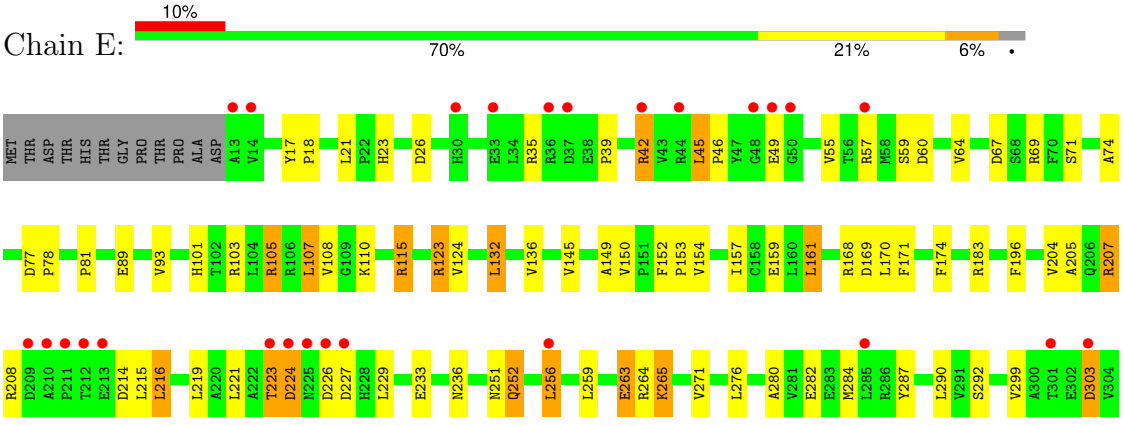
• Molecule 1: Cytochrome P-450

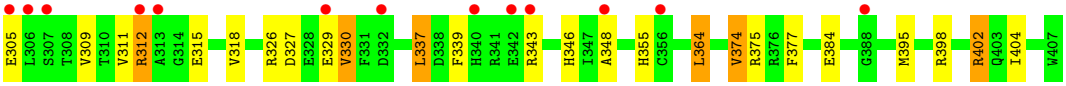
Chain D:



• Molecule 1: Cytochrome P-450

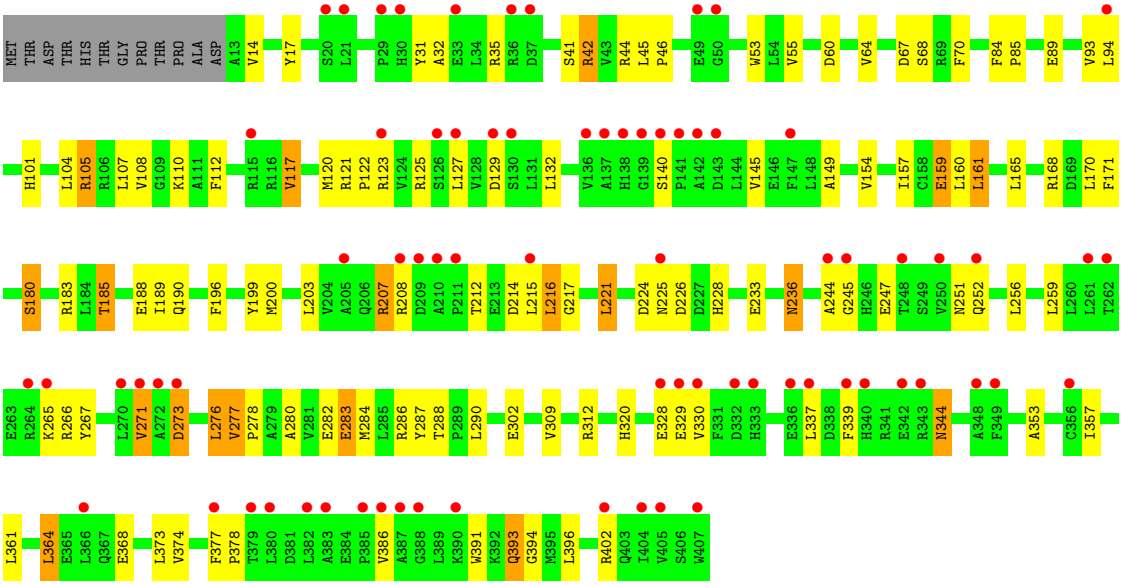
Chain E:





• Molecule 1: Cytochrome P-450

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	247.47Å 111.22Å 159.20Å 90.00° 129.39° 90.00°	Depositor
Resolution (Å)	37.73 – 2.20 37.70 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.73-2.20) 99.5 (37.70-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.187 , 0.243 0.192 , 0.245	Depositor DCC
R_{free} test set	8476 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	20348	wwPDB-VP
Average B, all atoms (Å^2)	65.0	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 42.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0173e-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: NA, TRS, GOL, QR8, FMT, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.82	1/3214 (0.0%)	1.01	3/4376 (0.1%)
1	B	0.86	2/3227 (0.1%)	1.09	11/4395 (0.3%)
1	C	0.86	1/3218 (0.0%)	1.09	12/4380 (0.3%)
1	D	0.80	1/3152 (0.0%)	1.01	3/4295 (0.1%)
1	E	0.77	0/3270	0.95	1/4448 (0.0%)
1	F	0.84	2/3169 (0.1%)	0.97	1/4318 (0.0%)
All	All	0.83	7/19250 (0.0%)	1.02	31/26212 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	283	GLU	CD-OE2	15.47	1.42	1.25
1	B	49	GLU	CD-OE2	6.67	1.32	1.25
1	F	283	GLU	CD-OE1	6.48	1.32	1.25
1	A	188	GLU	CD-OE2	6.06	1.32	1.25
1	B	38	GLU	CD-OE1	5.62	1.31	1.25

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	103	ARG	NE-CZ-NH1	-13.20	113.70	120.30
1	B	103	ARG	NE-CZ-NH2	12.35	126.48	120.30
1	C	105	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	C	35	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	B	363	ARG	NE-CZ-NH2	-7.13	116.74	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3135	0	3135	75	0
1	B	3148	0	3127	77	0
1	C	3136	0	3133	65	2
1	D	3082	0	3066	100	0
1	E	3200	0	3162	79	2
1	F	3102	0	3074	83	0
2	A	43	0	30	5	0
2	B	43	0	30	4	0
2	C	43	0	30	1	0
2	D	43	0	30	10	0
2	E	43	0	30	4	0
2	F	43	0	30	7	0
3	A	26	0	0	0	0
3	B	26	0	0	0	0
3	C	26	0	0	0	0
3	D	26	0	0	1	0
3	E	26	0	0	0	0
3	F	26	0	0	1	0
4	A	8	0	12	0	0
4	D	8	0	12	8	0
4	F	8	0	12	1	0
5	A	42	0	14	1	0
5	B	72	0	24	3	0
5	C	63	0	21	6	0
5	D	24	0	8	0	0
5	E	24	0	8	0	0
5	F	24	0	8	2	0
6	A	6	0	8	0	0
6	B	36	0	48	6	0
6	C	36	0	48	2	0
6	D	6	0	8	0	0
6	F	6	0	8	3	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	138	0	0	4	0
8	B	157	0	0	4	0
8	C	229	0	0	11	0
8	D	84	0	0	5	0
8	E	76	0	0	4	0
8	F	79	0	0	2	0
All	All	20348	0	19116	487	2

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 13.

The worst 5 of 487 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:C:207[A]:ARG:NH2	5:C:516:FMT:O2	1.84	1.10
1:E:375[B]:ARG:HH21	1:E:375[B]:ARG:HG2	0.86	1.02
1:E:226:ASP:OD1	1:E:229:LEU:N	1.93	1.01
1:E:375[B]:ARG:HH21	1:E:375[B]:ARG:CG	1.74	1.00
1:D:140:SER:O	1:D:407:TRP:CZ3	2.16	0.99

All (2) 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:C:302:GLU:OE1	1:E:205:ALA:O[4_646]	2.07	0.13
1:C:103:ARG:NH1	1:E:169:ASP:OD2[4_646]	2.09	0.11

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	401/407 (98%)	388 (97%)	13 (3%)	0	100	100
1	B	403/407 (99%)	389 (96%)	14 (4%)	0	100	100
1	C	401/407 (98%)	389 (97%)	12 (3%)	0	100	100
1	D	394/407 (97%)	364 (92%)	30 (8%)	0	100	100
1	E	406/407 (100%)	386 (95%)	20 (5%)	0	100	100
1	F	396/407 (97%)	372 (94%)	24 (6%)	0	100	100
All	All	2401/2442 (98%)	2288 (95%)	113 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	339/341 (99%)	294 (87%)	45 (13%)	4	3
1	B	340/341 (100%)	307 (90%)	33 (10%)	8	7
1	C	339/341 (99%)	311 (92%)	28 (8%)	11	11
1	D	332/341 (97%)	284 (86%)	48 (14%)	3	2
1	E	344/341 (101%)	295 (86%)	49 (14%)	3	2
1	F	334/341 (98%)	289 (86%)	45 (14%)	4	3
All	All	2028/2046 (99%)	1780 (88%)	248 (12%)	5	4

5 of 248 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	71	SER
1	F	180	SER
1	D	307	SER
1	F	159	GLU
1	F	277	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	346	HIS
1	F	96	GLN
1	F	344	ASN
1	B	393	GLN
1	B	360	GLN

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 118 ligands modelled in this entry, 5 are monoatomic - leaving 113 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	$\#\|Z\| > 2$
6	GOL	C	525	-	5,5,5	0.10	0	5,5,5	0.22	0
6	GOL	B	528	-	5,5,5	0.13	0	5,5,5	0.40	0
5	FMT	D	508	-	2,2,2	0.23	0	1,1,1	0.18	0
5	FMT	B	510	-	2,2,2	0.43	0	1,1,1	0.10	0
5	FMT	A	506	-	2,2,2	0.30	0	1,1,1	0.13	0
5	FMT	A	504	-	2,2,2	0.26	0	1,1,1	0.14	0
3	QR8	E	502	-	26,26,26	1.63	4 (15%)	37,38,38	1.55	8 (21%)
5	FMT	E	504	-	2,2,2	0.22	0	1,1,1	0.20	0
5	FMT	C	514	-	2,2,2	0.24	0	1,1,1	0.15	0
5	FMT	A	517	-	2,2,2	0.41	0	1,1,1	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FMT	D	510	-	2,2,2	0.36	0	1,1,1	0.12	0
5	FMT	C	517	-	2,2,2	0.48	0	1,1,1	0.00	0
5	FMT	C	503	-	2,2,2	0.27	0	1,1,1	0.18	0
5	FMT	E	503	-	2,2,2	0.33	0	1,1,1	0.15	0
5	FMT	B	503	-	2,2,2	0.29	0	1,1,1	0.11	0
5	FMT	B	526	-	2,2,2	0.39	0	1,1,1	0.09	0
6	GOL	C	527	-	5,5,5	0.10	0	5,5,5	0.13	0
5	FMT	A	513	-	2,2,2	0.23	0	1,1,1	0.17	0
5	FMT	A	507	-	2,2,2	0.23	0	1,1,1	0.17	0
5	FMT	E	507	-	2,2,2	0.43	0	1,1,1	0.03	0
5	FMT	B	504	-	2,2,2	0.35	0	1,1,1	0.11	0
5	FMT	B	511	-	2,2,2	0.33	0	1,1,1	0.13	0
5	FMT	F	505	-	2,2,2	0.39	0	1,1,1	0.11	0
5	FMT	A	510	-	2,2,2	0.27	0	1,1,1	0.14	0
5	FMT	C	510	-	2,2,2	0.35	0	1,1,1	0.11	0
5	FMT	C	520	-	2,2,2	0.38	0	1,1,1	0.03	0
5	FMT	A	505	-	2,2,2	0.32	0	1,1,1	0.13	0
3	QR8	C	502	-	26,26,26	1.56	4 (15%)	37,38,38	1.77	8 (21%)
5	FMT	E	505	-	2,2,2	0.30	0	1,1,1	0.14	0
4	TRS	F	503	-	7,7,7	0.52	0	9,9,9	0.88	1 (11%)
5	FMT	B	508	-	2,2,2	0.20	0	1,1,1	0.19	0
5	FMT	C	513	-	2,2,2	0.45	0	1,1,1	0.05	0
5	FMT	D	507	-	2,2,2	0.24	0	1,1,1	0.18	0
5	FMT	D	509	-	2,2,2	0.35	0	1,1,1	0.08	0
5	FMT	C	511	-	2,2,2	0.35	0	1,1,1	0.07	0
5	FMT	C	506	-	2,2,2	0.39	0	1,1,1	0.06	0
3	QR8	B	502	-	26,26,26	1.78	5 (19%)	37,38,38	1.81	10 (27%)
5	FMT	C	516	-	2,2,2	0.37	0	1,1,1	0.10	0
5	FMT	A	514	-	2,2,2	0.28	0	1,1,1	0.17	0
5	FMT	B	515	-	2,2,2	0.34	0	1,1,1	0.11	0
5	FMT	B	513	-	2,2,2	0.32	0	1,1,1	0.10	0
5	FMT	D	511	-	2,2,2	0.36	0	1,1,1	0.11	0
2	HEM	F	501	1	42,50,50	1.43	7 (16%)	46,82,82	2.15	13 (28%)
5	FMT	B	509	-	2,2,2	0.36	0	1,1,1	0.11	0
5	FMT	B	520	-	2,2,2	0.37	0	1,1,1	0.14	0
6	GOL	D	512	-	5,5,5	0.08	0	5,5,5	0.21	0
5	FMT	C	523	-	2,2,2	0.30	0	1,1,1	0.12	0
6	GOL	C	528	-	5,5,5	0.13	0	5,5,5	0.34	0
5	FMT	A	516	-	2,2,2	0.30	0	1,1,1	0.13	0
5	FMT	E	508	-	2,2,2	0.39	0	1,1,1	0.10	0
5	FMT	E	510	-	2,2,2	0.25	0	1,1,1	0.19	0
6	GOL	C	529	-	5,5,5	0.15	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FMT	F	508	-	2,2,2	0.22	0	1,1,1	0.16	0
6	GOL	F	512	-	5,5,5	0.12	0	5,5,5	0.33	0
5	FMT	A	515	-	2,2,2	0.28	0	1,1,1	0.16	0
6	GOL	B	529	-	5,5,5	0.10	0	5,5,5	0.28	0
2	HEM	E	501	1	42,50,50	1.50	6 (14%)	46,82,82	2.26	13 (28%)
2	HEM	B	501	1	42,50,50	2.09	9 (21%)	46,82,82	2.18	20 (43%)
5	FMT	C	518	-	2,2,2	0.19	0	1,1,1	0.23	0
5	FMT	F	507	-	2,2,2	0.24	0	1,1,1	0.18	0
6	GOL	C	526	-	5,5,5	0.32	0	5,5,5	0.88	0
3	QR8	A	502	-	26,26,26	1.53	3 (11%)	37,38,38	1.57	7 (18%)
5	FMT	E	509	-	2,2,2	0.24	0	1,1,1	0.20	0
5	FMT	F	510	-	2,2,2	0.35	0	1,1,1	0.15	0
5	FMT	C	504	-	2,2,2	0.49	0	1,1,1	0.10	0
5	FMT	C	515	-	2,2,2	0.23	0	1,1,1	0.17	0
6	GOL	B	532	-	5,5,5	0.16	0	5,5,5	0.36	0
5	FMT	E	506	-	2,2,2	0.28	0	1,1,1	0.15	0
2	HEM	A	501	1	42,50,50	1.51	3 (7%)	46,82,82	2.13	17 (36%)
5	FMT	C	521	-	2,2,2	0.64	0	1,1,1	0.08	0
5	FMT	C	507	-	2,2,2	0.43	0	1,1,1	0.02	0
5	FMT	B	521	-	2,2,2	0.20	0	1,1,1	0.19	0
5	FMT	D	506	-	2,2,2	0.25	0	1,1,1	0.12	0
5	FMT	C	522	-	2,2,2	0.22	0	1,1,1	0.21	0
3	QR8	D	502	-	26,26,26	1.68	3 (11%)	37,38,38	1.82	9 (24%)
2	HEM	D	501	1	42,50,50	2.03	8 (19%)	46,82,82	2.29	18 (39%)
5	FMT	B	512	-	2,2,2	0.25	0	1,1,1	0.18	0
5	FMT	C	508	-	2,2,2	0.33	0	1,1,1	0.15	0
4	TRS	A	503	-	7,7,7	0.32	0	9,9,9	0.90	0
5	FMT	D	504	-	2,2,2	0.32	0	1,1,1	0.05	0
2	HEM	C	501	1	42,50,50	1.70	6 (14%)	46,82,82	2.40	17 (36%)
5	FMT	B	523	-	2,2,2	0.41	0	1,1,1	0.26	0
5	FMT	B	514	-	2,2,2	0.34	0	1,1,1	0.14	0
5	FMT	C	505	-	2,2,2	0.21	0	1,1,1	0.21	0
5	FMT	B	525	-	2,2,2	0.33	0	1,1,1	0.11	0
5	FMT	B	517	-	2,2,2	0.43	0	1,1,1	0.08	0
5	FMT	F	509	-	2,2,2	0.32	0	1,1,1	0.10	0
5	FMT	B	505	-	2,2,2	0.22	0	1,1,1	0.17	0
6	GOL	B	527	-	5,5,5	0.10	0	5,5,5	0.32	0
5	FMT	D	505	-	2,2,2	0.28	0	1,1,1	0.16	0
5	FMT	A	512	-	2,2,2	0.30	0	1,1,1	0.12	0
5	FMT	B	522	-	2,2,2	0.25	0	1,1,1	0.17	0
6	GOL	C	524	-	5,5,5	0.20	0	5,5,5	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	B	531	-	5,5,5	0.16	0	5,5,5	0.33	0
5	FMT	A	511	-	2,2,2	0.20	0	1,1,1	0.21	0
5	FMT	F	511	-	2,2,2	0.23	0	1,1,1	0.13	0
5	FMT	B	518	-	2,2,2	0.28	0	1,1,1	0.18	0
5	FMT	B	519	-	2,2,2	0.35	0	1,1,1	0.10	0
5	FMT	C	512	-	2,2,2	0.34	0	1,1,1	0.17	0
4	TRS	D	503	-	7,7,7	0.34	0	9,9,9	0.89	0
5	FMT	B	506	-	2,2,2	0.26	0	1,1,1	0.16	0
6	GOL	B	530	-	5,5,5	0.12	0	5,5,5	0.38	0
5	FMT	A	508	-	2,2,2	0.25	0	1,1,1	0.17	0
5	FMT	B	524	-	2,2,2	0.24	0	1,1,1	0.20	0
3	QR8	F	502	-	26,26,26	1.54	3 (11%)	37,38,38	1.79	13 (35%)
5	FMT	A	509	-	2,2,2	0.33	0	1,1,1	0.03	0
5	FMT	F	504	-	2,2,2	0.53	0	1,1,1	0.04	0
5	FMT	B	507	-	2,2,2	0.27	0	1,1,1	0.16	0
5	FMT	F	506	-	2,2,2	0.24	0	1,1,1	0.17	0
5	FMT	B	516	-	2,2,2	0.43	0	1,1,1	0.03	0
6	GOL	A	518	-	5,5,5	0.14	0	5,5,5	0.43	0
5	FMT	C	509	-	2,2,2	0.30	0	1,1,1	0.11	0
5	FMT	C	519	-	2,2,2	0.27	0	1,1,1	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	525	-	-	2/4/4/4	-
6	GOL	B	529	-	-	4/4/4/4	-
2	HEM	E	501	1	-	0/12/54/54	-
6	GOL	B	528	-	-	2/4/4/4	-
2	HEM	B	501	1	-	0/12/54/54	-
3	QR8	C	502	-	-	12/48/48/48	0/1/1/1
6	GOL	B	527	-	-	0/4/4/4	-
6	GOL	C	526	-	-	2/4/4/4	-
3	QR8	A	502	-	-	12/48/48/48	0/1/1/1
4	TRS	F	503	-	-	7/9/9/9	-
6	GOL	C	524	-	-	2/4/4/4	-
6	GOL	B	531	-	-	2/4/4/4	-
3	QR8	B	502	-	-	12/48/48/48	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	532	-	-	4/4/4/4	-
6	GOL	F	512	-	-	1/4/4/4	-
4	TRS	D	503	-	-	9/9/9/9	-
3	QR8	E	502	-	-	14/48/48/48	0/1/1/1
6	GOL	B	530	-	-	2/4/4/4	-
2	HEM	A	501	1	-	0/12/54/54	-
2	HEM	F	501	1	-	0/12/54/54	-
6	GOL	C	527	-	-	2/4/4/4	-
3	QR8	F	502	-	-	17/48/48/48	0/1/1/1
6	GOL	D	512	-	-	0/4/4/4	-
3	QR8	D	502	-	-	12/48/48/48	0/1/1/1
2	HEM	D	501	1	-	2/12/54/54	-
6	GOL	C	528	-	-	2/4/4/4	-
6	GOL	A	518	-	-	4/4/4/4	-
6	GOL	C	529	-	-	2/4/4/4	-
4	TRS	A	503	-	-	9/9/9/9	-
2	HEM	C	501	1	-	0/12/54/54	-

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C1B-NB	-6.66	1.28	1.40
2	D	501	HEM	C4B-NB	-5.85	1.27	1.38
2	C	501	HEM	C1B-NB	-5.58	1.30	1.40
3	B	502	QR8	O2-C13	-5.30	1.38	1.46
2	D	501	HEM	C1D-ND	-5.24	1.28	1.38

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	CHC-C4B-NB	8.23	133.29	124.44
2	F	501	HEM	CHC-C4B-NB	7.35	132.34	124.44
2	E	501	HEM	CHC-C4B-NB	6.75	131.70	124.44
2	A	501	HEM	CHC-C4B-NB	6.44	131.36	124.44
2	D	501	HEM	CHC-C4B-NB	6.30	131.21	124.44

There are no chirality outliers.

5 of 137 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	QR8	C6-C7-C8-C9
3	A	502	QR8	C6-C7-C8-C33
3	A	502	QR8	C3-C4-C5-O7
3	B	502	QR8	C6-C7-C8-C9
3	B	502	QR8	C31-C4-C5-O7

There are no ring outliers.

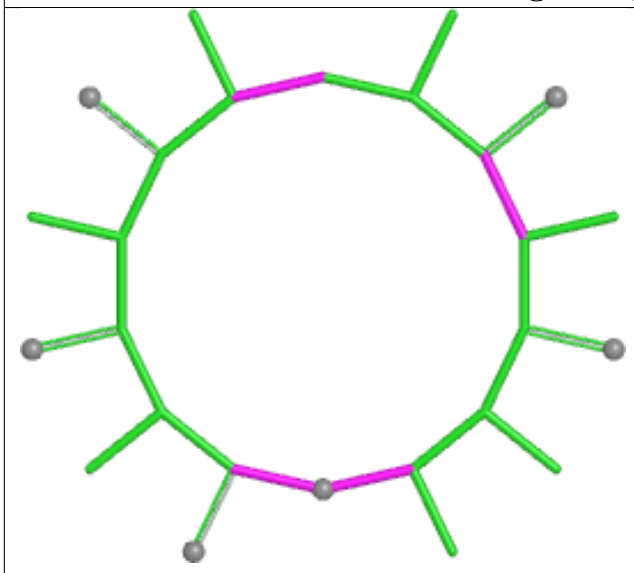
26 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	528	GOL	2	0
6	C	527	GOL	1	0
4	F	503	TRS	1	0
5	B	508	FMT	2	0
5	C	511	FMT	1	0
5	C	516	FMT	2	0
5	B	513	FMT	1	0
2	F	501	HEM	7	0
6	C	529	GOL	1	0
6	F	512	GOL	3	0
6	B	529	GOL	1	0
2	E	501	HEM	4	0
2	B	501	HEM	4	0
2	A	501	HEM	5	0
5	C	507	FMT	2	0
5	C	522	FMT	1	0
3	D	502	QR8	1	0
2	D	501	HEM	10	0
2	C	501	HEM	1	0
6	B	527	GOL	2	0
5	A	512	FMT	1	0
5	F	511	FMT	1	0
4	D	503	TRS	8	0
6	B	530	GOL	1	0
3	F	502	QR8	1	0
5	F	506	FMT	1	0

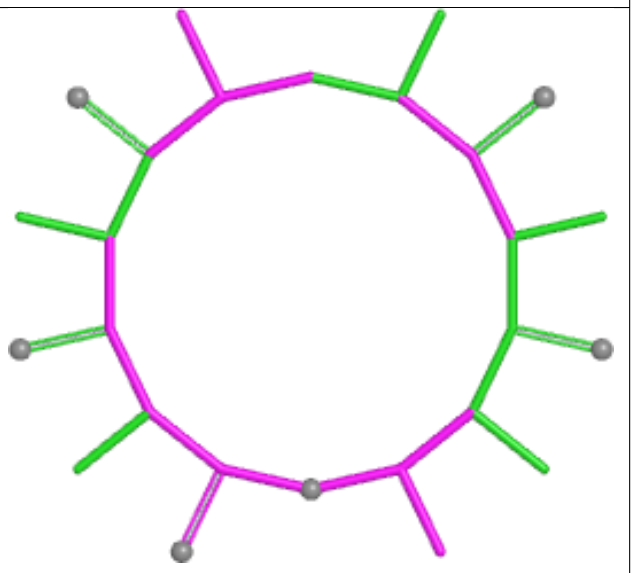
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

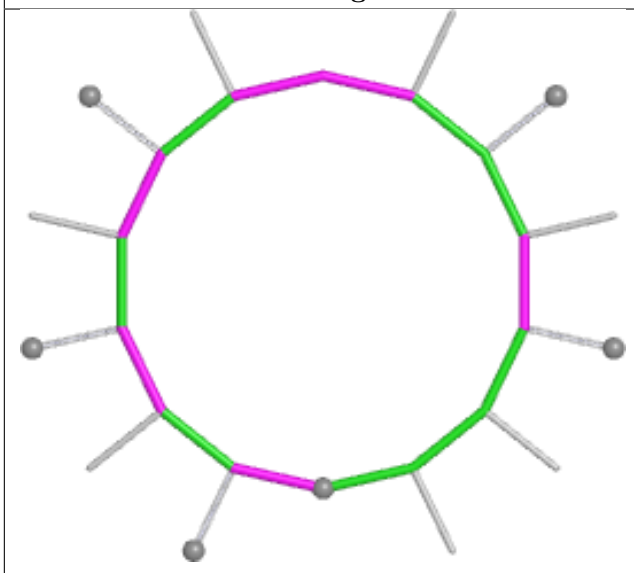
Ligand QR8 E 502



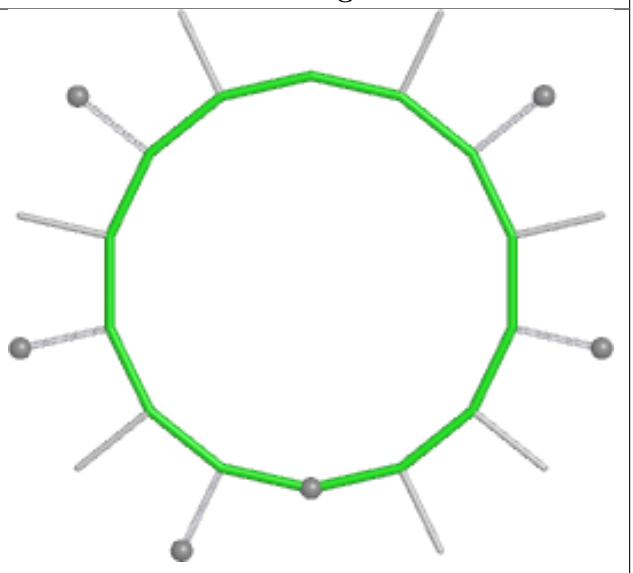
Bond lengths



Bond angles

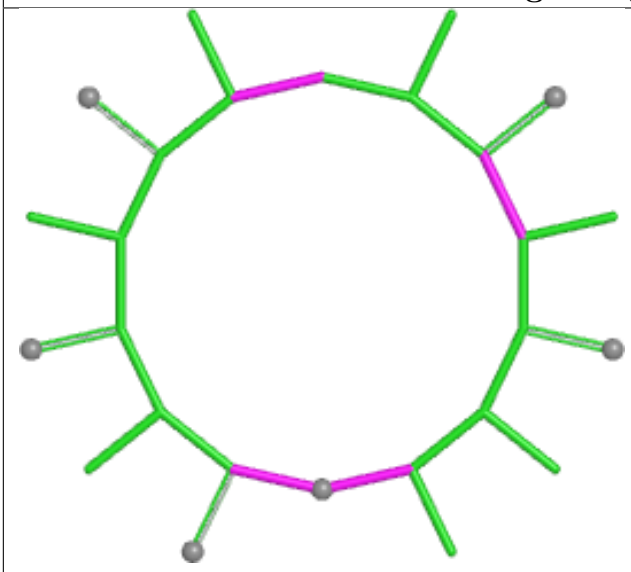


Torsions

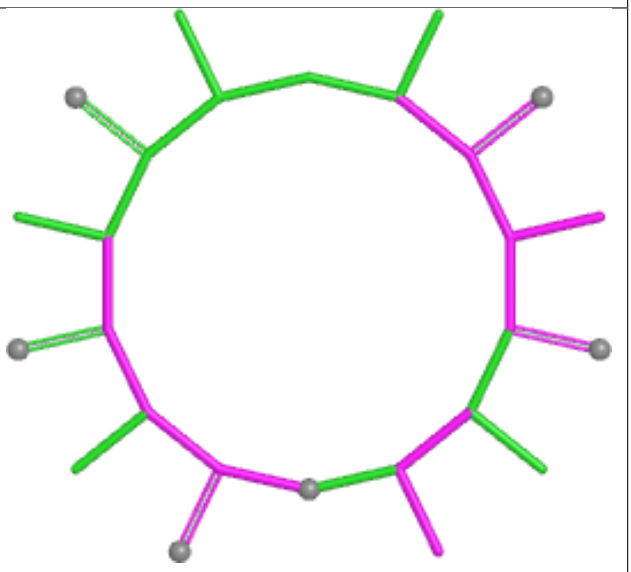


Rings

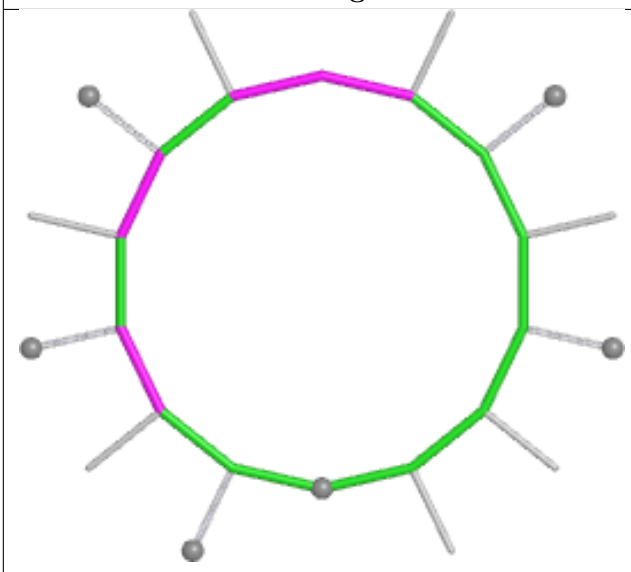
Ligand QR8 C 502



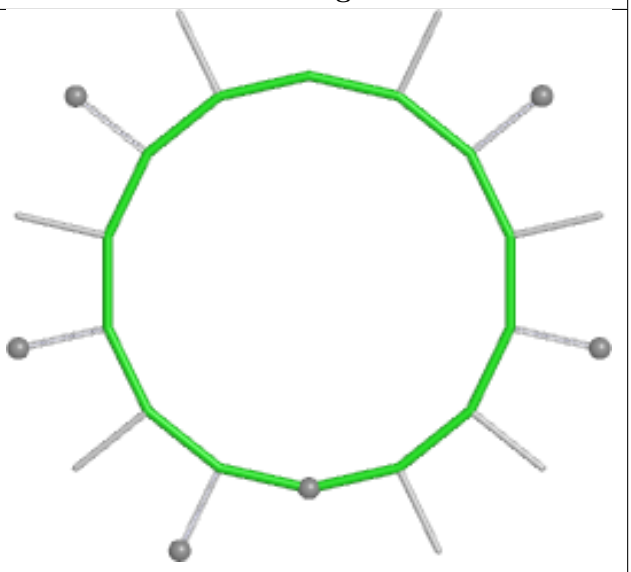
Bond lengths



Bond angles

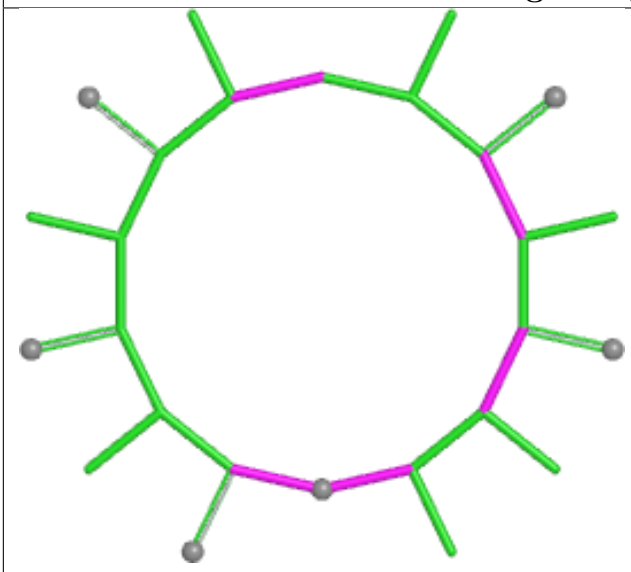


Torsions

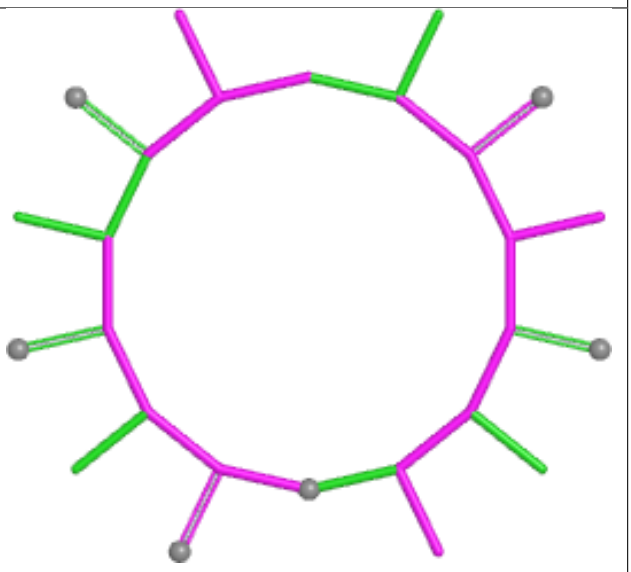


Rings

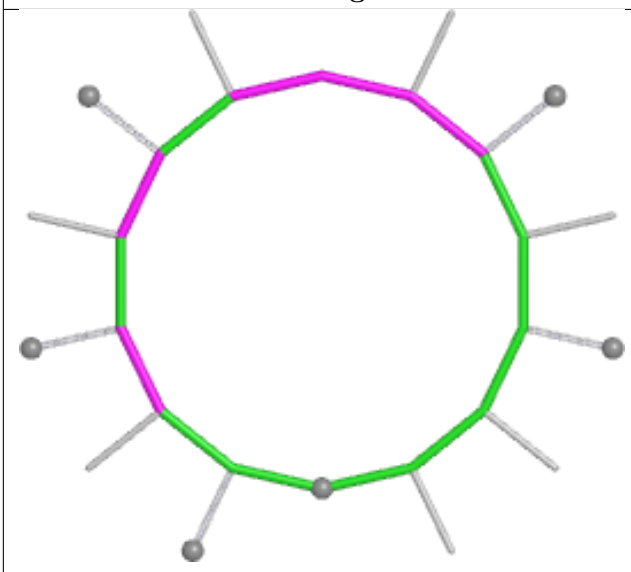
Ligand QR8 B 502



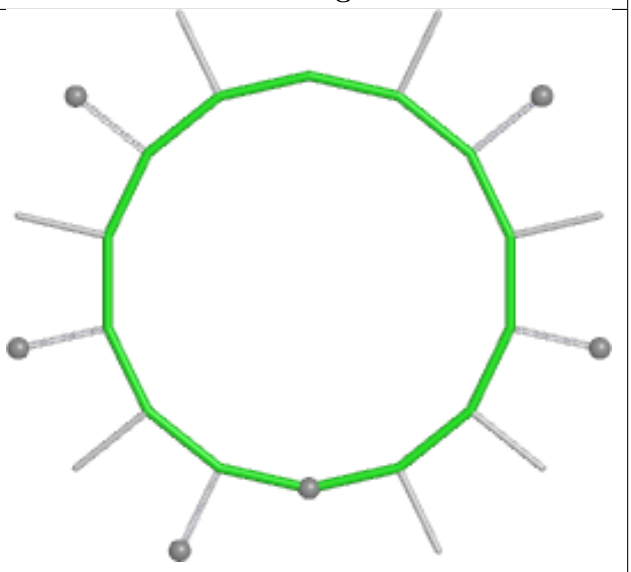
Bond lengths



Bond angles

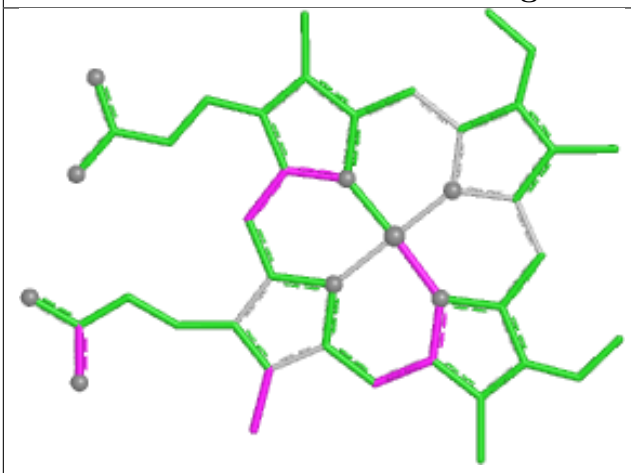


Torsions

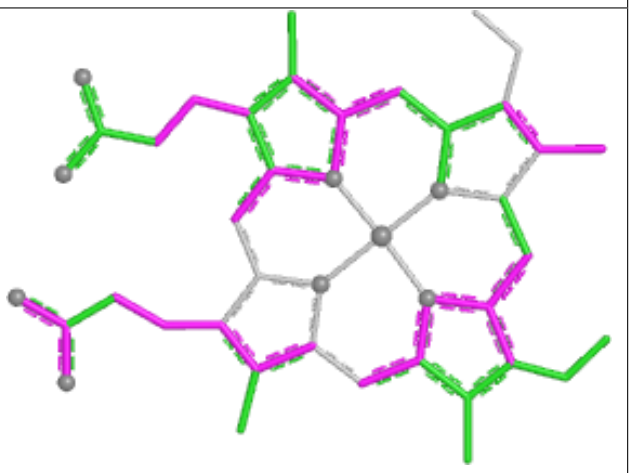


Rings

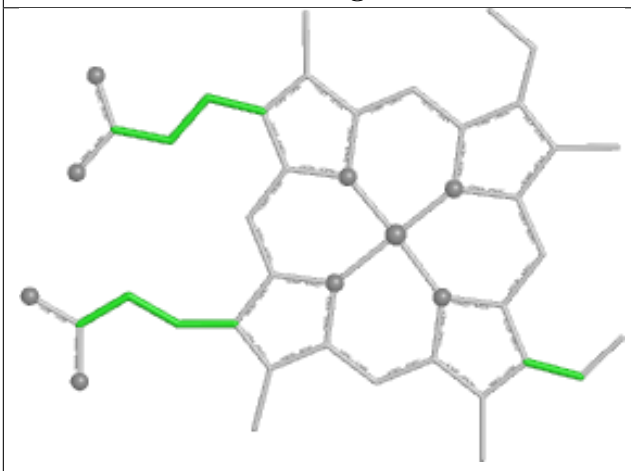
Ligand HEM F 501



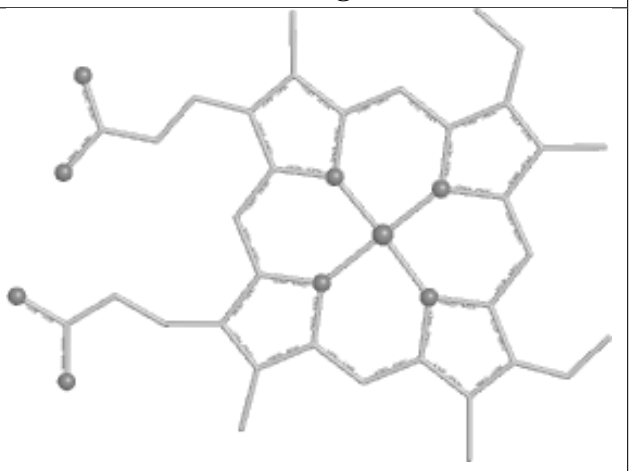
Bond lengths



Bond angles

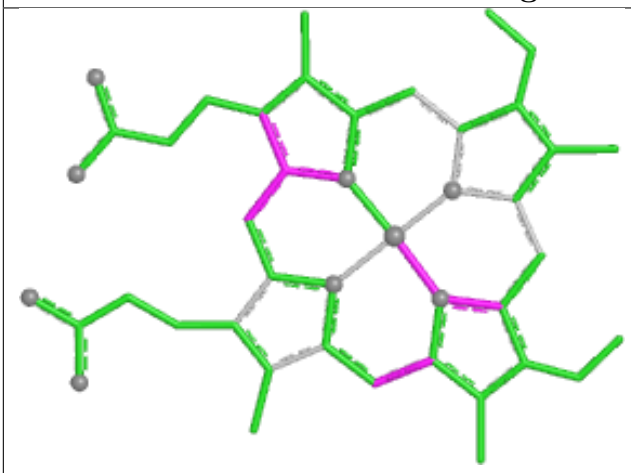


Torsions

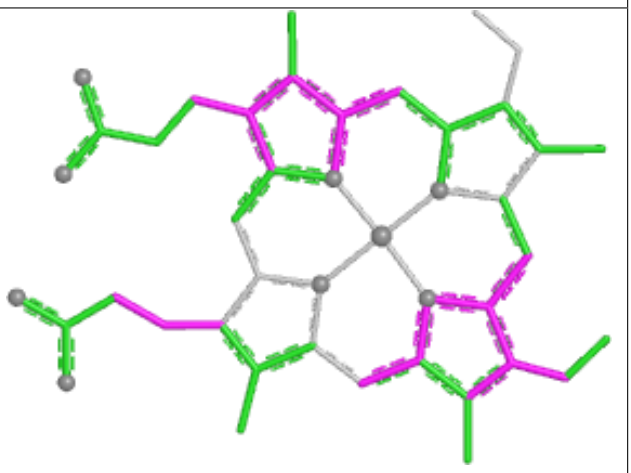


Rings

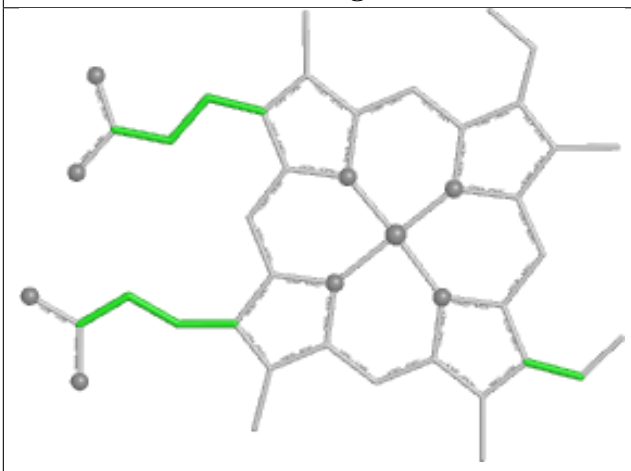
Ligand HEM E 501



Bond lengths



Bond angles



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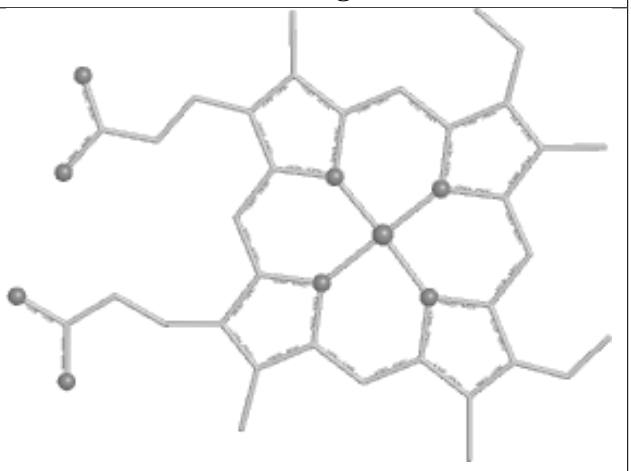
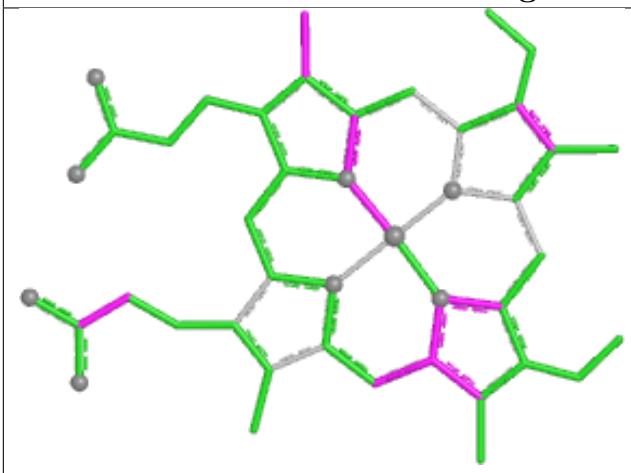


Rings

Ligand HEM B 501



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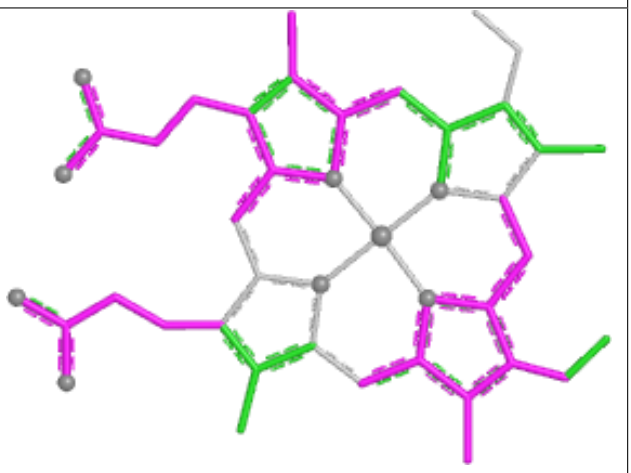
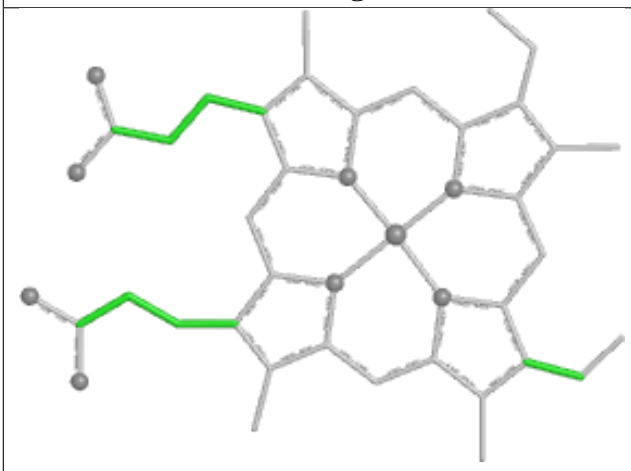
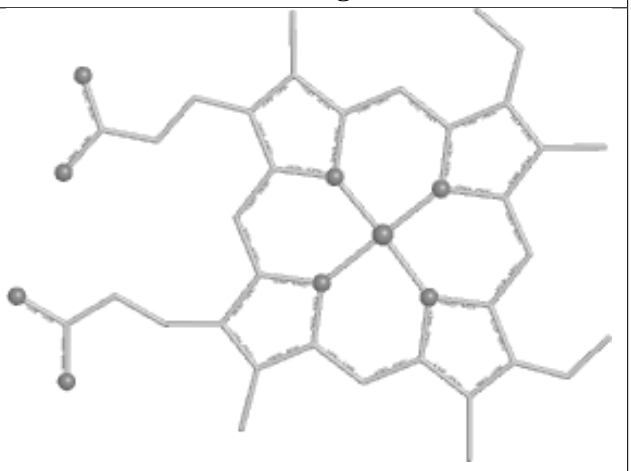


Bond angles

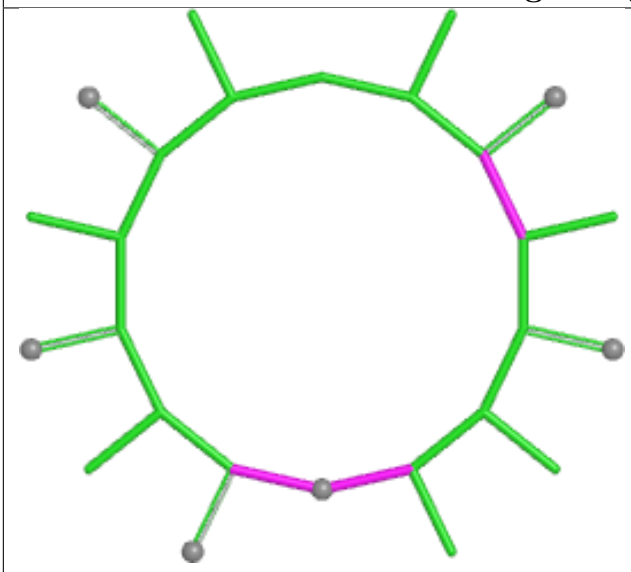


Torsions



Rings

Ligand QR8 A 502



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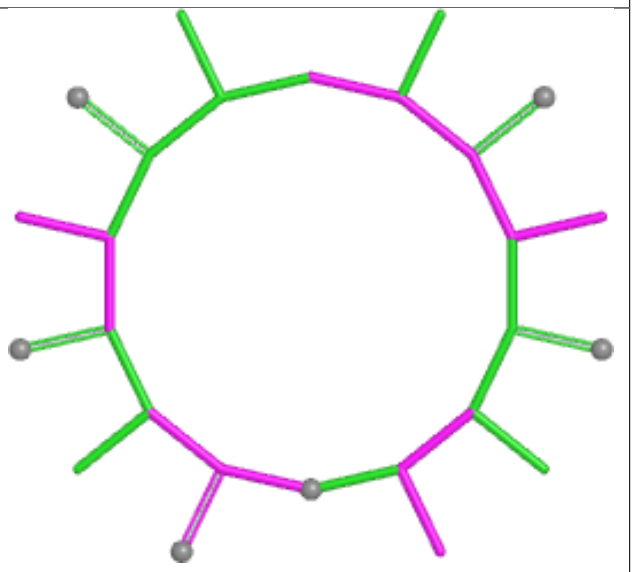

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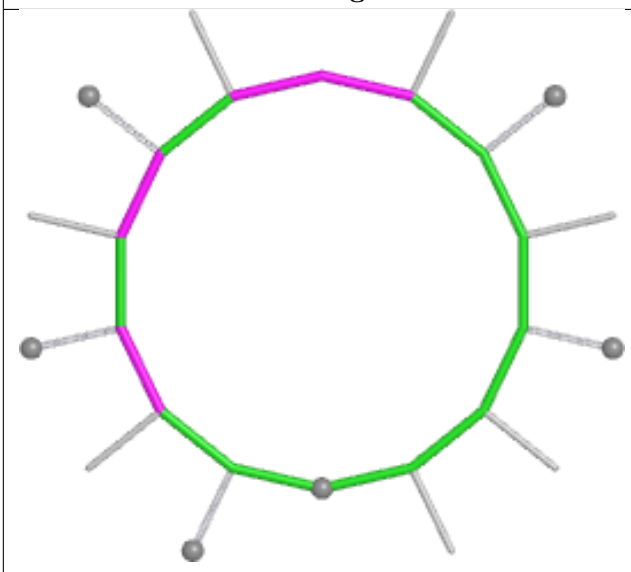

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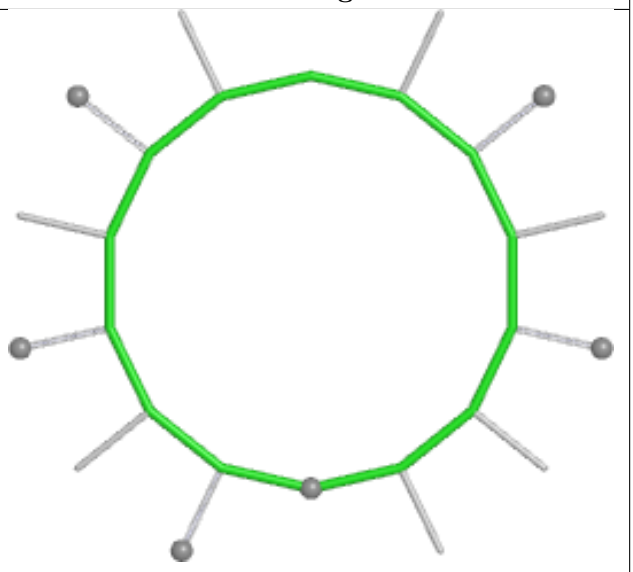
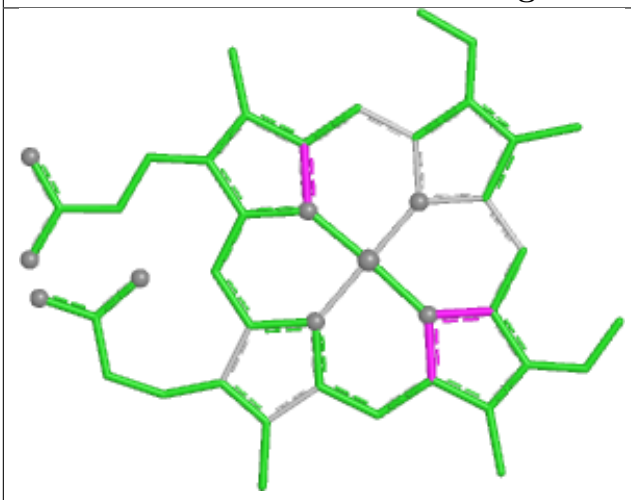


Rings

Ligand HEM A 501



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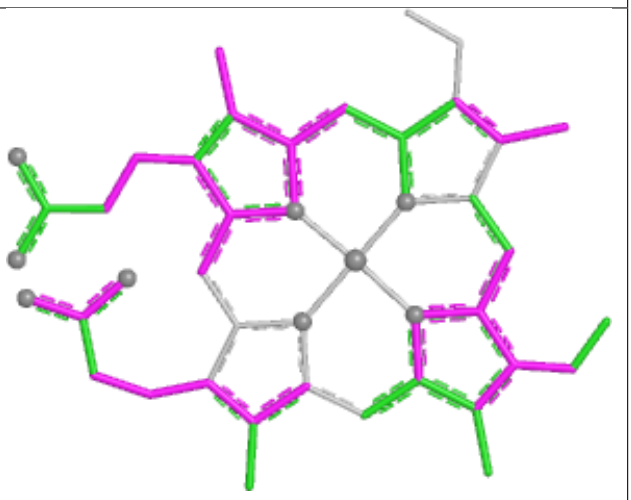
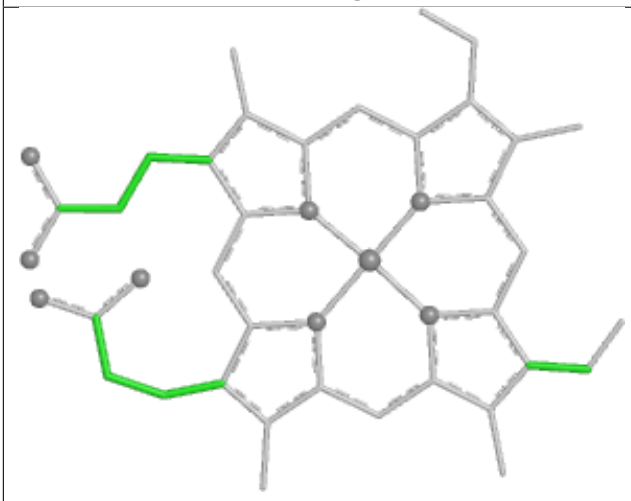
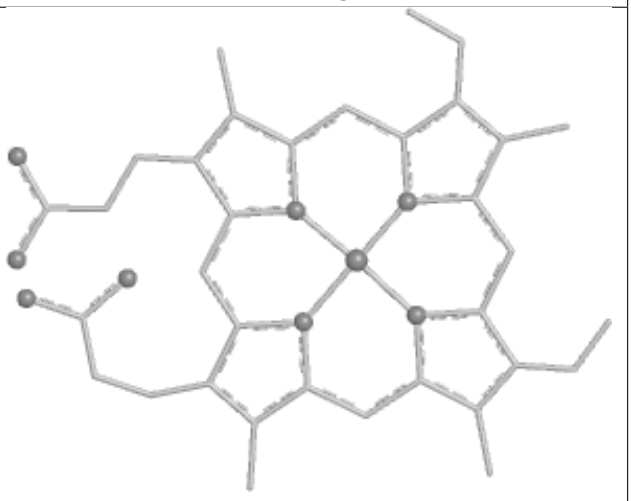


Bond angles

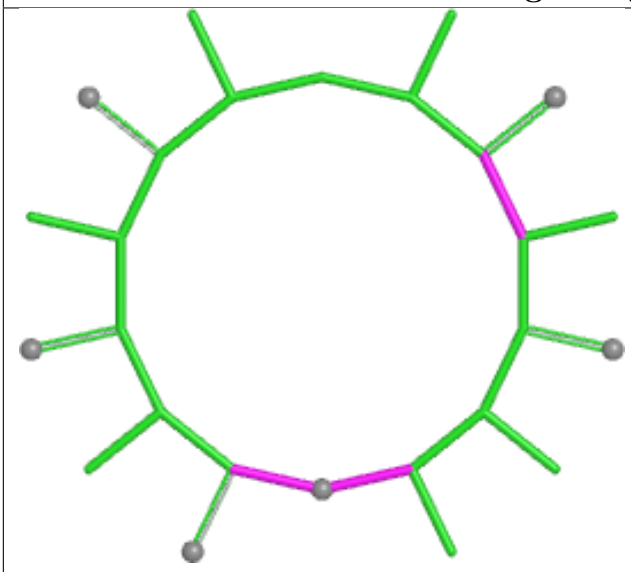


Torsions

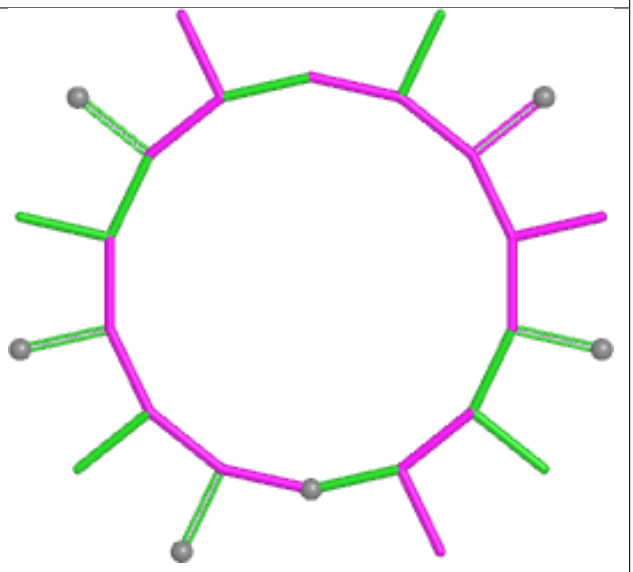


Rings

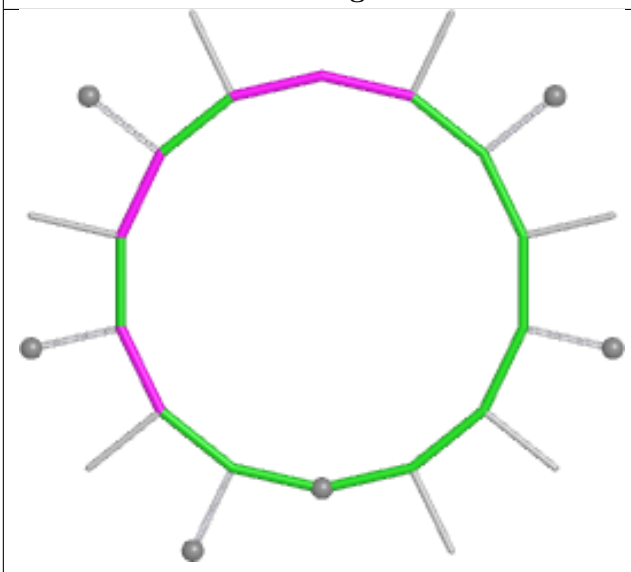
Ligand QR8 D 502



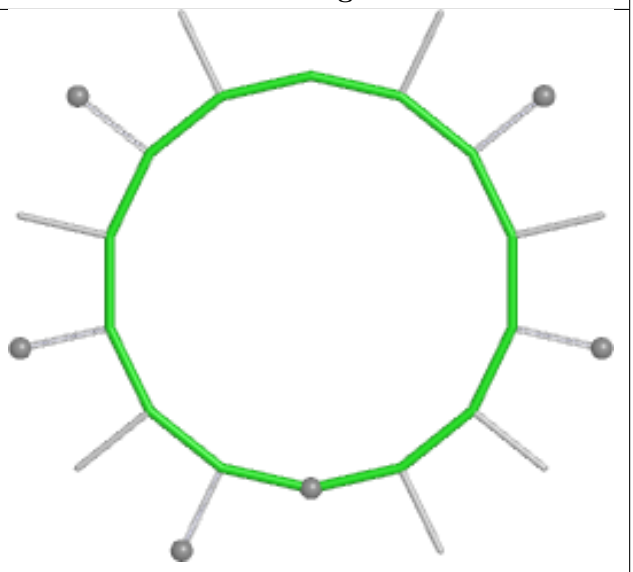
Bond lengths



Bond angles

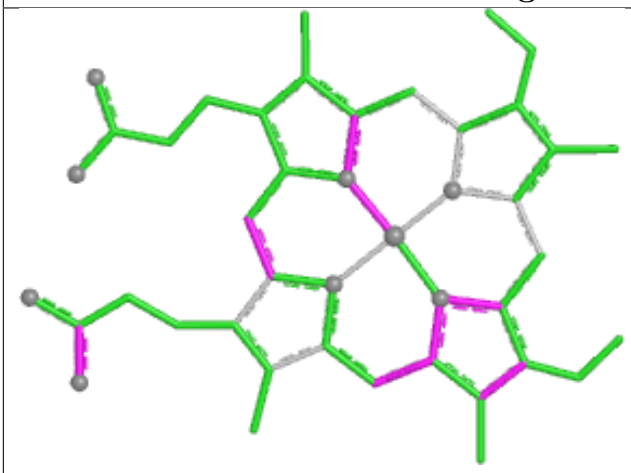


Torsions

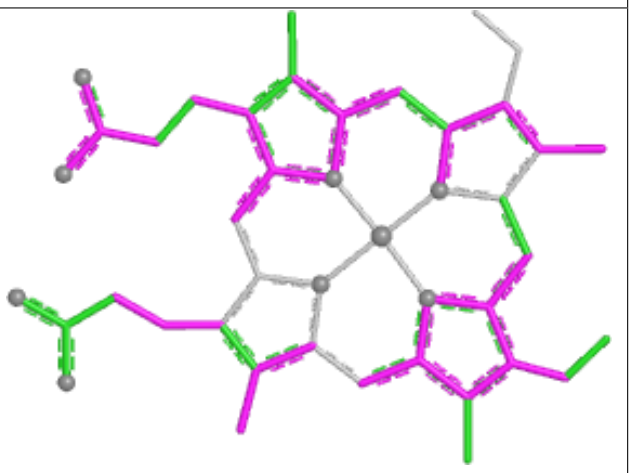


Rings

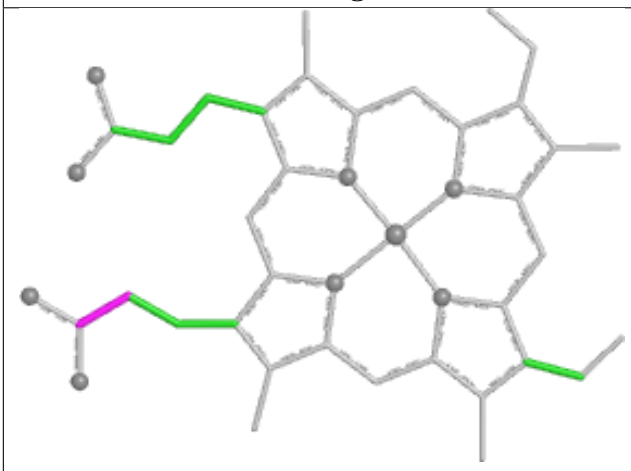
Ligand HEM D 501



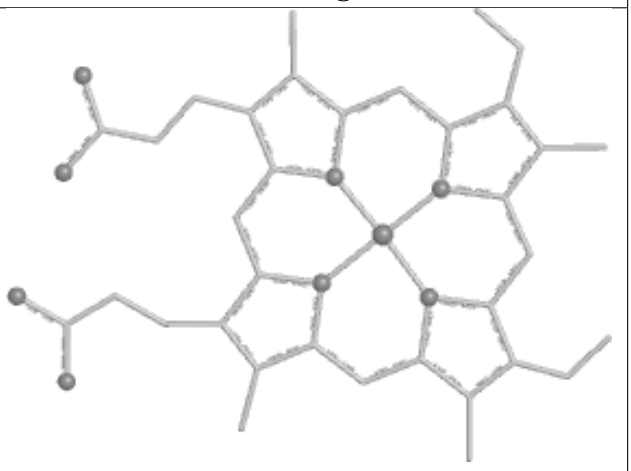
Bond lengths



Bond angles

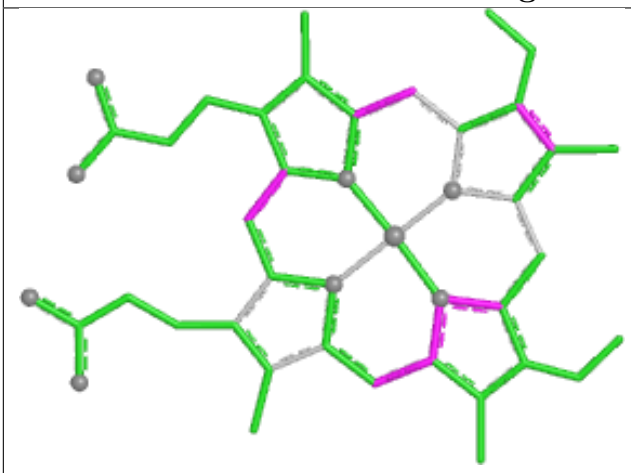


Torsions

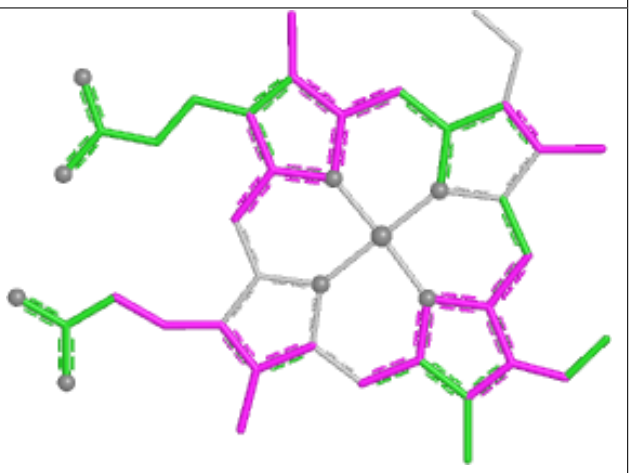


Rings

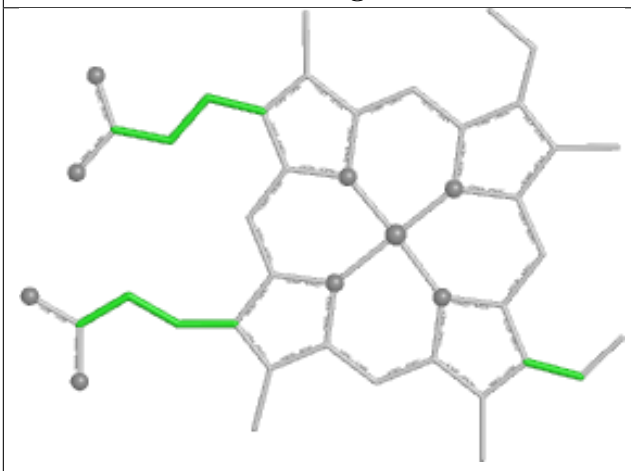
Ligand HEM C 501



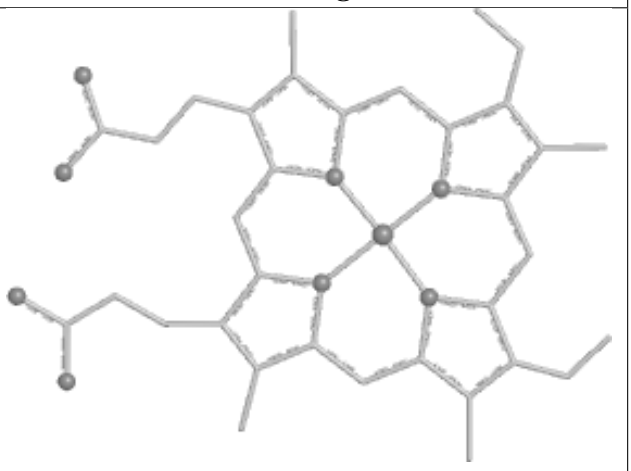
Bond lengths



Bond angles

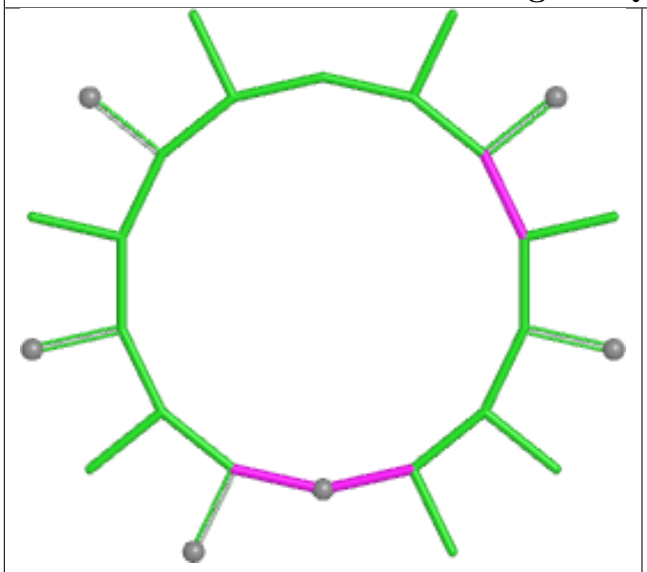


Torsions

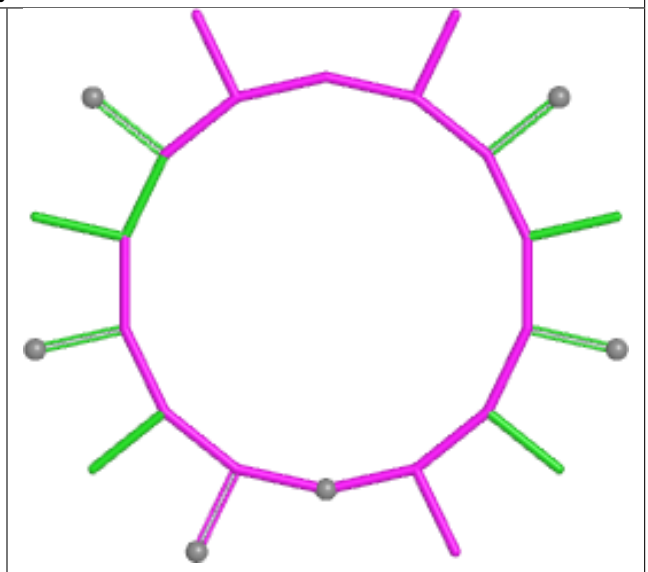


Rings

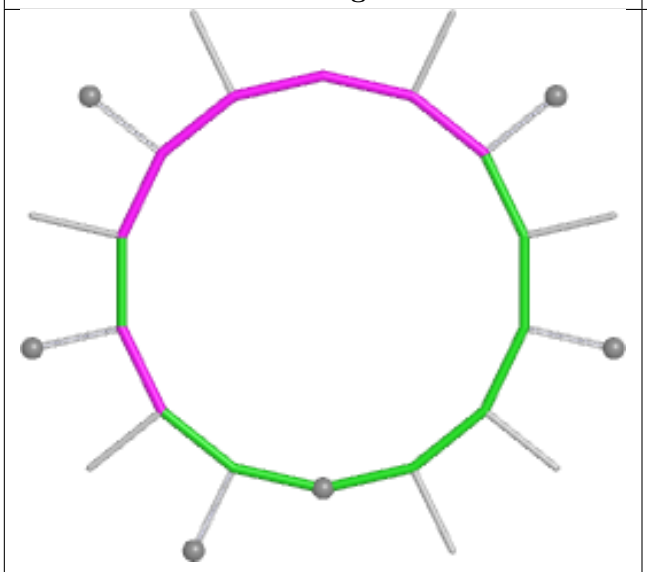
Ligand QR8 F 502



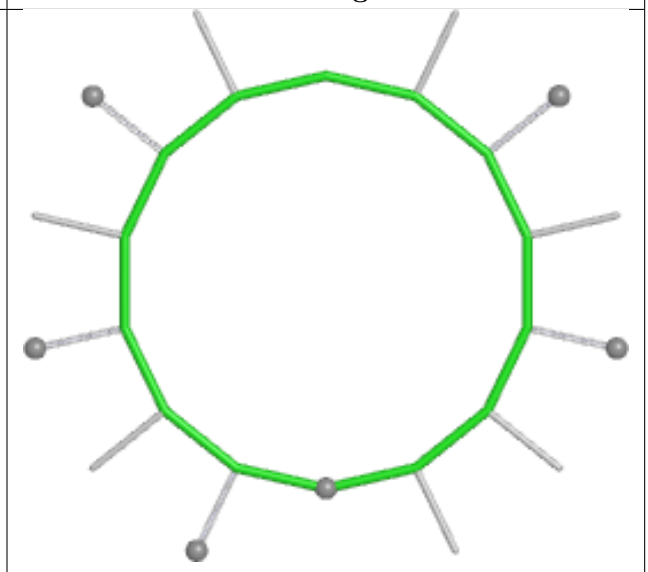
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	396/407 (97%)	-0.02	20 (5%)	28	26	35, 58, 87, 137	0
1	B	397/407 (97%)	-0.07	15 (3%)	40	38	32, 50, 74, 150	0
1	C	396/407 (97%)	-0.22	13 (3%)	46	44	31, 44, 64, 103	0
1	D	395/407 (97%)	0.19	30 (7%)	13	12	44, 69, 100, 147	1 (0%)
1	E	395/407 (97%)	0.43	39 (9%)	7	6	45, 70, 102, 154	0
1	F	395/407 (97%)	0.69	74 (18%)	1	1	49, 79, 124, 142	0
All	All	2374/2442 (97%)	0.17	191 (8%)	12	11	31, 62, 105, 154	1 (0%)

The worst 5 of 191 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	212	THR	7.6
1	E	209	ASP	7.2
1	E	343	ARG	6.4
1	E	210	ALA	6.1
1	E	42[A]	ARG	6.0

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
5	FMT	A	515	3/3	0.07	0.45	98,98,101,106	0
5	FMT	E	509	3/3	0.41	0.35	96,96,100,105	0
5	FMT	F	507	3/3	0.46	0.67	91,91,95,101	0
5	FMT	C	505	3/3	0.52	0.43	113,113,113,113	0
5	FMT	C	518	3/3	0.52	0.26	93,93,94,94	0
5	FMT	B	514	3/3	0.55	0.36	97,97,107,107	0
5	FMT	C	509	3/3	0.56	0.35	85,85,89,96	0
5	FMT	E	506	3/3	0.58	0.18	85,85,89,96	0
5	FMT	B	525	3/3	0.59	0.69	92,92,98,102	0
5	FMT	E	504	3/3	0.62	0.51	91,91,97,99	0
5	FMT	A	504	3/3	0.62	0.37	78,78,89,90	0
5	FMT	A	514	3/3	0.63	0.34	87,87,88,91	0
5	FMT	B	505	3/3	0.65	0.22	94,94,101,102	0
5	FMT	E	505	3/3	0.66	0.30	89,89,97,97	0
5	FMT	D	507	3/3	0.67	0.42	87,87,90,91	0
5	FMT	A	516	3/3	0.67	0.25	83,83,88,99	0
5	FMT	D	505	3/3	0.67	0.40	99,99,109,111	0
6	GOL	B	531	6/6	0.67	0.27	82,99,102,104	0
5	FMT	C	513	3/3	0.68	0.23	78,78,78,93	0
5	FMT	E	510	3/3	0.69	0.49	98,98,105,113	0
5	FMT	C	506	3/3	0.69	0.39	75,75,76,84	0
5	FMT	D	511	3/3	0.69	0.38	82,82,94,94	0
6	GOL	B	532	6/6	0.69	0.24	87,98,100,102	0
5	FMT	C	516	3/3	0.71	0.29	41,41,42,44	3
5	FMT	D	506	3/3	0.72	0.26	85,85,91,95	0
6	GOL	B	528	6/6	0.72	0.25	88,95,102,104	0
5	FMT	D	508	3/3	0.73	0.50	108,108,113,114	0
5	FMT	D	509	3/3	0.73	0.27	78,78,81,86	0
5	FMT	A	505	3/3	0.73	0.47	85,85,92,95	0
5	FMT	B	522	3/3	0.74	0.45	92,92,97,98	0
5	FMT	C	514	3/3	0.74	0.18	100,100,103,104	0
5	FMT	F	509	3/3	0.74	0.19	90,90,107,107	0
5	FMT	D	510	3/3	0.75	0.32	93,93,95,99	0
5	FMT	B	515	3/3	0.75	0.24	76,76,82,84	0
5	FMT	C	515	3/3	0.75	0.32	92,92,93,97	0
5	FMT	B	518	3/3	0.75	0.31	85,85,86,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FMT	A	513	3/3	0.76	0.31	103,103,106,108	0
5	FMT	C	510	3/3	0.77	0.26	83,83,90,94	0
5	FMT	A	511	3/3	0.77	0.57	95,95,95,96	0
5	FMT	F	510	3/3	0.77	0.34	79,79,83,86	0
5	FMT	B	523	3/3	0.79	0.27	61,61,73,78	0
5	FMT	C	519	3/3	0.79	0.22	88,88,92,93	0
5	FMT	C	504	3/3	0.80	0.34	64,64,70,74	0
5	FMT	B	519	3/3	0.80	0.29	89,89,92,100	0
6	GOL	B	527	6/6	0.80	0.26	82,88,98,105	0
5	FMT	A	509	3/3	0.81	0.28	72,72,73,74	0
5	FMT	B	504	3/3	0.81	0.26	74,74,74,78	0
5	FMT	A	510	3/3	0.81	0.12	95,95,99,100	0
5	FMT	C	503	3/3	0.81	0.51	94,94,98,101	0
5	FMT	B	507	3/3	0.81	0.35	90,90,97,100	0
5	FMT	C	523	3/3	0.81	0.37	80,80,83,87	0
5	FMT	F	505	3/3	0.81	0.16	86,86,93,99	0
5	FMT	F	504	3/3	0.82	0.26	79,79,82,92	0
5	FMT	B	511	3/3	0.83	0.33	78,78,86,92	0
5	FMT	C	520	3/3	0.83	0.15	70,70,80,85	0
5	FMT	B	524	3/3	0.83	0.57	99,99,102,102	0
5	FMT	B	521	3/3	0.83	0.42	92,92,94,97	0
5	FMT	B	526	3/3	0.83	0.29	79,79,87,90	0
5	FMT	A	507	3/3	0.83	0.11	88,88,97,101	0
5	FMT	E	508	3/3	0.84	0.20	78,78,89,94	0
5	FMT	B	517	3/3	0.84	0.19	73,73,75,80	0
5	FMT	C	517	3/3	0.84	0.34	62,62,77,85	0
6	GOL	C	528	6/6	0.84	0.20	80,89,92,94	0
5	FMT	B	513	3/3	0.85	0.37	85,85,94,94	0
5	FMT	F	508	3/3	0.85	0.44	104,104,109,113	0
5	FMT	B	520	3/3	0.85	0.22	80,80,82,92	0
6	GOL	C	529	6/6	0.85	0.17	65,76,82,84	0
5	FMT	B	503	3/3	0.86	0.30	74,74,76,80	0
5	FMT	A	512	3/3	0.86	0.18	94,94,99,99	0
6	GOL	F	512	6/6	0.86	0.15	71,75,82,88	0
5	FMT	F	506	3/3	0.87	0.15	65,65,77,79	0
4	TRS	A	503	8/8	0.87	0.24	88,90,95,103	0
5	FMT	C	521	3/3	0.87	0.21	66,66,72,84	0
7	NA	F	513	1/1	0.88	0.13	64,64,64,64	0
5	FMT	B	510	3/3	0.89	0.17	71,71,73,82	0
5	FMT	C	522	3/3	0.89	0.17	70,70,82,91	0
4	TRS	F	503	8/8	0.89	0.18	63,71,75,79	0
5	FMT	A	517	3/3	0.89	0.14	69,69,80,82	0

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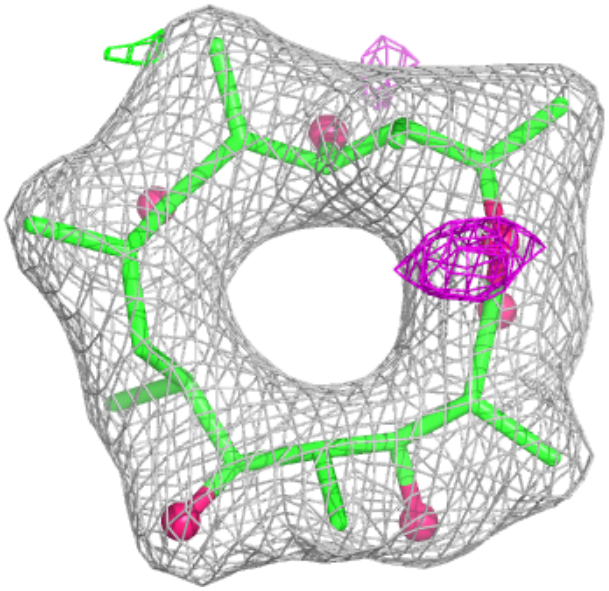
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FMT	C	512	3/3	0.89	0.31	72,72,85,86	0
6	GOL	B	530	6/6	0.89	0.14	76,87,92,107	0
6	GOL	C	527	6/6	0.90	0.14	67,73,75,77	0
5	FMT	B	516	3/3	0.90	0.15	66,66,78,85	0
5	FMT	A	506	3/3	0.90	0.13	79,79,82,82	0
5	FMT	E	503	3/3	0.90	0.21	85,85,90,95	0
6	GOL	C	526	6/6	0.90	0.18	42,50,62,64	0
5	FMT	B	506	3/3	0.91	0.21	81,81,96,100	0
6	GOL	D	512	6/6	0.91	0.19	90,93,95,100	0
4	TRS	D	503	8/8	0.92	0.19	76,82,84,86	0
5	FMT	E	507	3/3	0.92	0.17	73,73,79,87	0
5	FMT	F	511	3/3	0.92	0.17	90,90,95,95	0
3	QR8	E	502	26/26	0.93	0.22	55,61,68,69	0
6	GOL	B	529	6/6	0.93	0.16	52,75,82,84	0
5	FMT	B	512	3/3	0.93	0.08	74,74,80,81	0
7	NA	C	530	1/1	0.93	0.15	51,51,51,51	0
5	FMT	C	511	3/3	0.93	0.28	72,72,77,78	0
3	QR8	F	502	26/26	0.94	0.23	65,76,79,82	0
3	QR8	C	502	26/26	0.94	0.20	38,45,53,59	0
5	FMT	B	509	3/3	0.94	0.33	70,70,71,73	0
6	GOL	A	518	6/6	0.94	0.16	56,75,81,95	0
5	FMT	C	507	3/3	0.94	0.20	55,55,73,81	0
5	FMT	C	508	3/3	0.94	0.12	68,68,72,73	0
5	FMT	D	504	3/3	0.95	0.21	63,63,70,78	0
3	QR8	B	502	26/26	0.95	0.22	42,48,54,59	0
3	QR8	D	502	26/26	0.95	0.15	55,63,70,73	0
7	NA	A	519	1/1	0.96	0.28	55,55,55,55	0
7	NA	B	533	1/1	0.96	0.09	52,52,52,52	0
3	QR8	A	502	26/26	0.96	0.21	47,52,60,66	0
7	NA	D	513	1/1	0.96	0.39	67,67,67,67	0
6	GOL	C	525	6/6	0.96	0.18	68,76,80,83	0
2	HEM	F	501	43/43	0.97	0.20	59,65,76,86	0
5	FMT	B	508	3/3	0.97	0.13	56,56,56,60	0
6	GOL	C	524	6/6	0.97	0.11	50,58,61,62	0
2	HEM	D	501	43/43	0.98	0.19	41,45,54,59	0
2	HEM	E	501	43/43	0.98	0.21	44,49,56,63	0
2	HEM	A	501	43/43	0.99	0.19	32,37,42,47	0
5	FMT	A	508	3/3	0.99	0.10	52,52,54,54	0
2	HEM	B	501	43/43	0.99	0.22	30,33,39,44	0
2	HEM	C	501	43/43	0.99	0.21	28,32,38,40	0

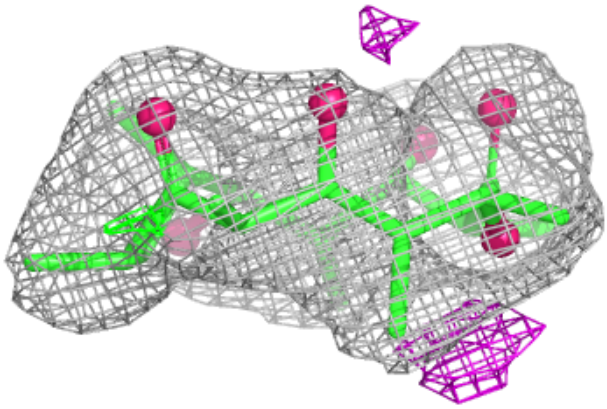
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around QR8 E 502:

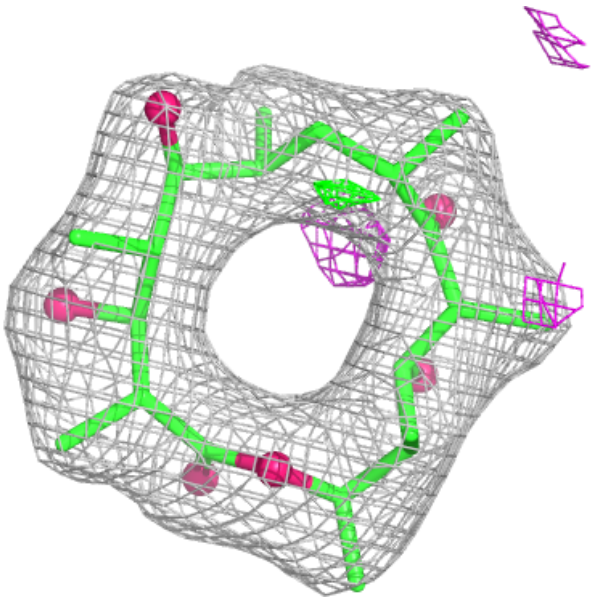
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

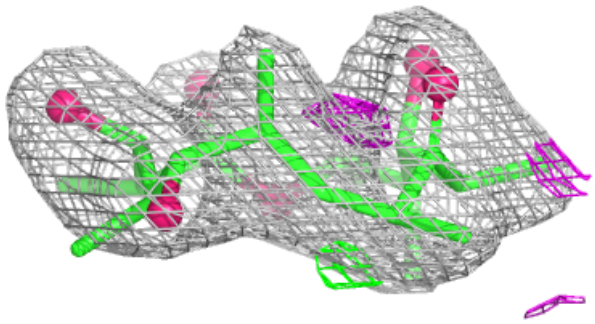


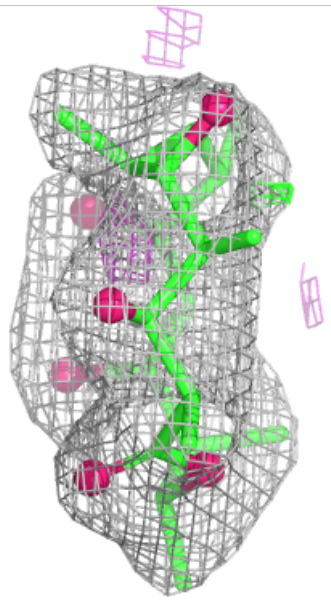


Electron density around QR8 F 502:

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

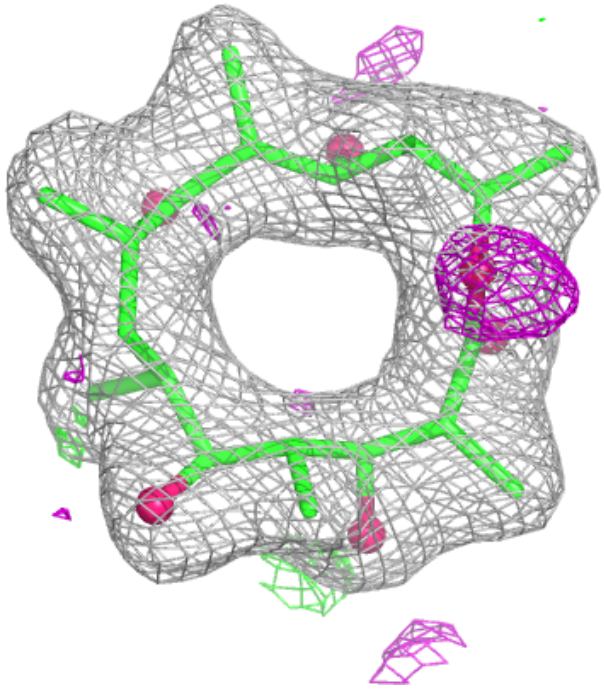


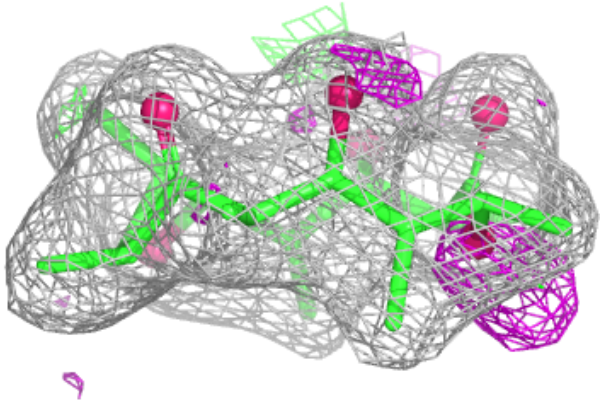


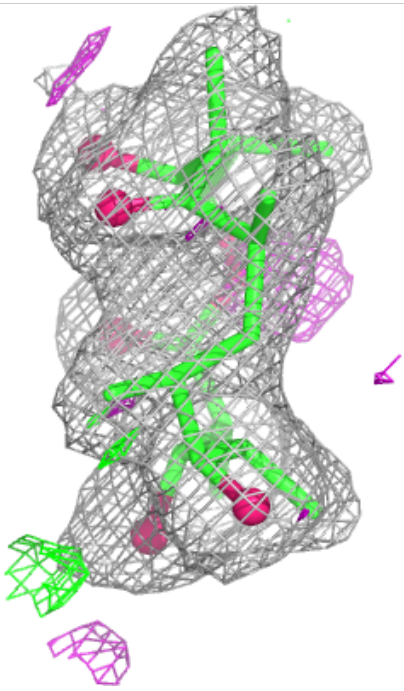


Electron density around QR8 C 502:

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

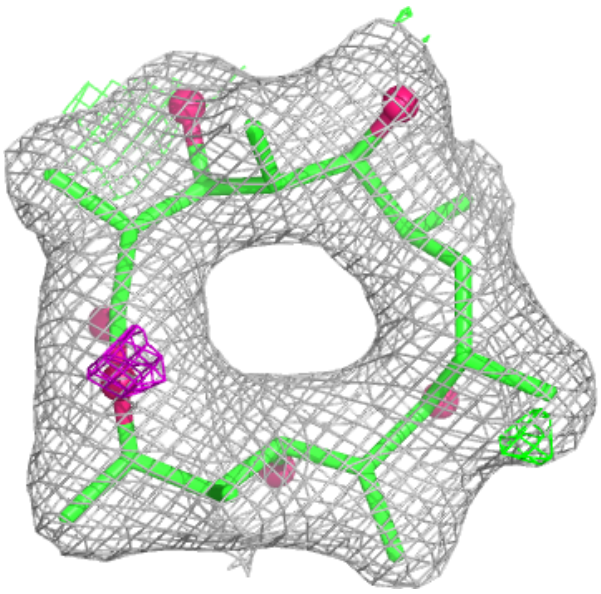


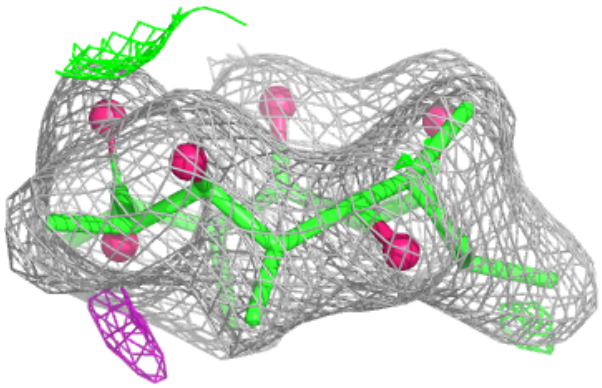


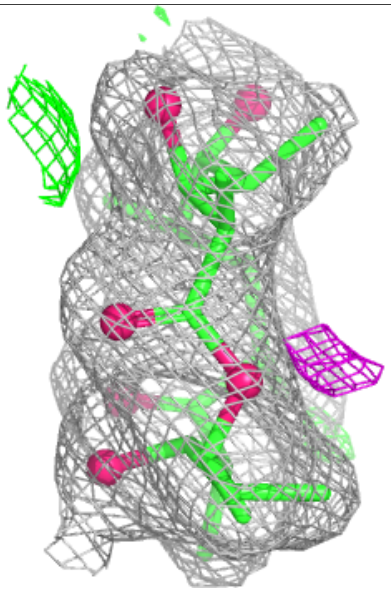


Electron density around QR8 B 502:

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

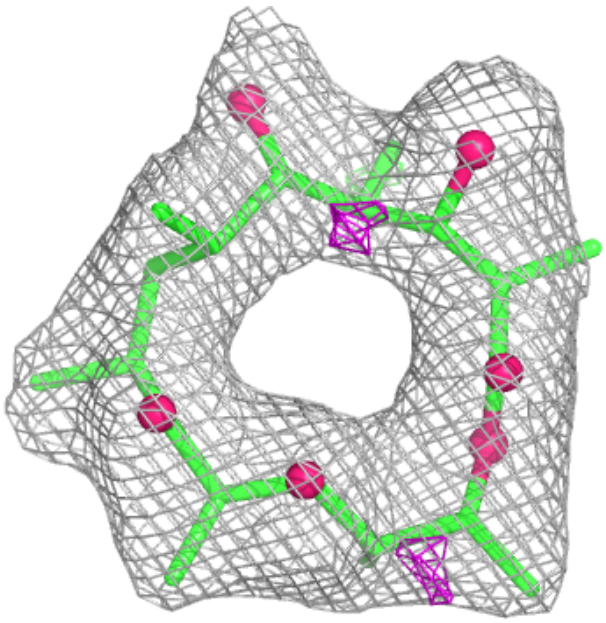


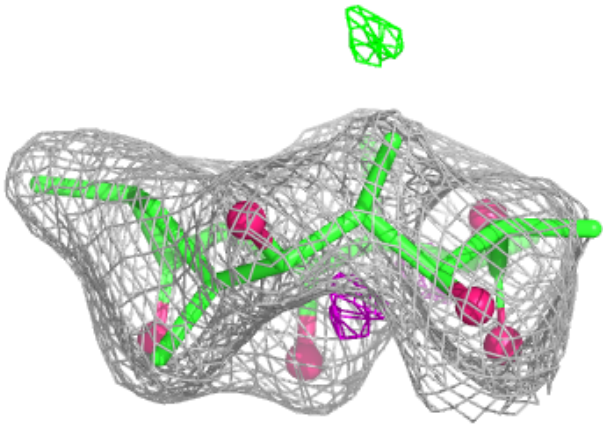


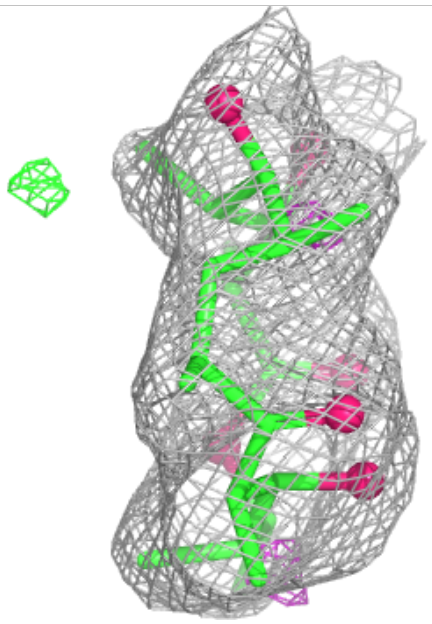


Electron density around QR8 D 502:

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

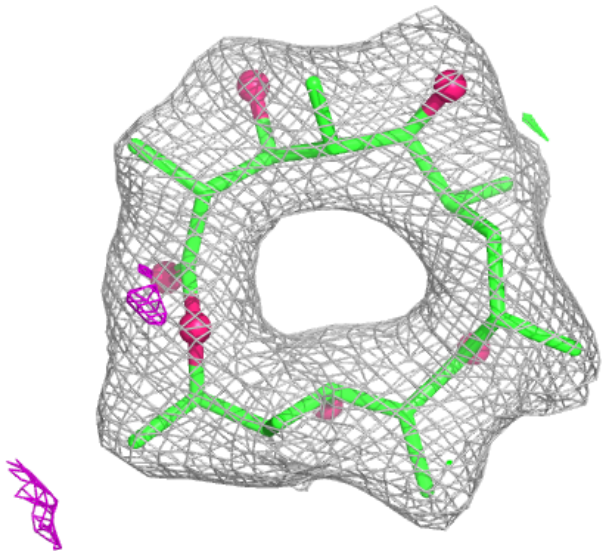


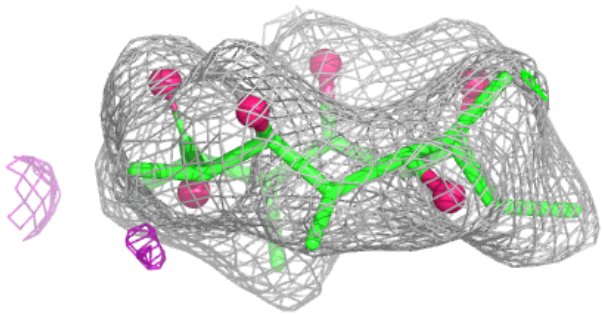


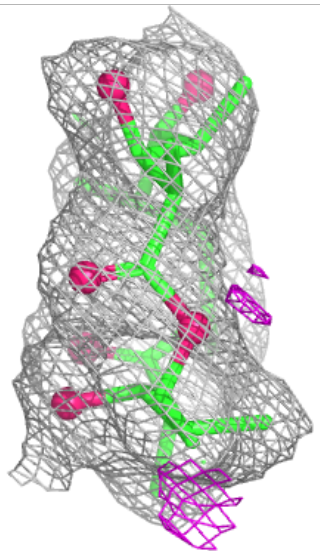


Electron density around QR8 A 502:

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

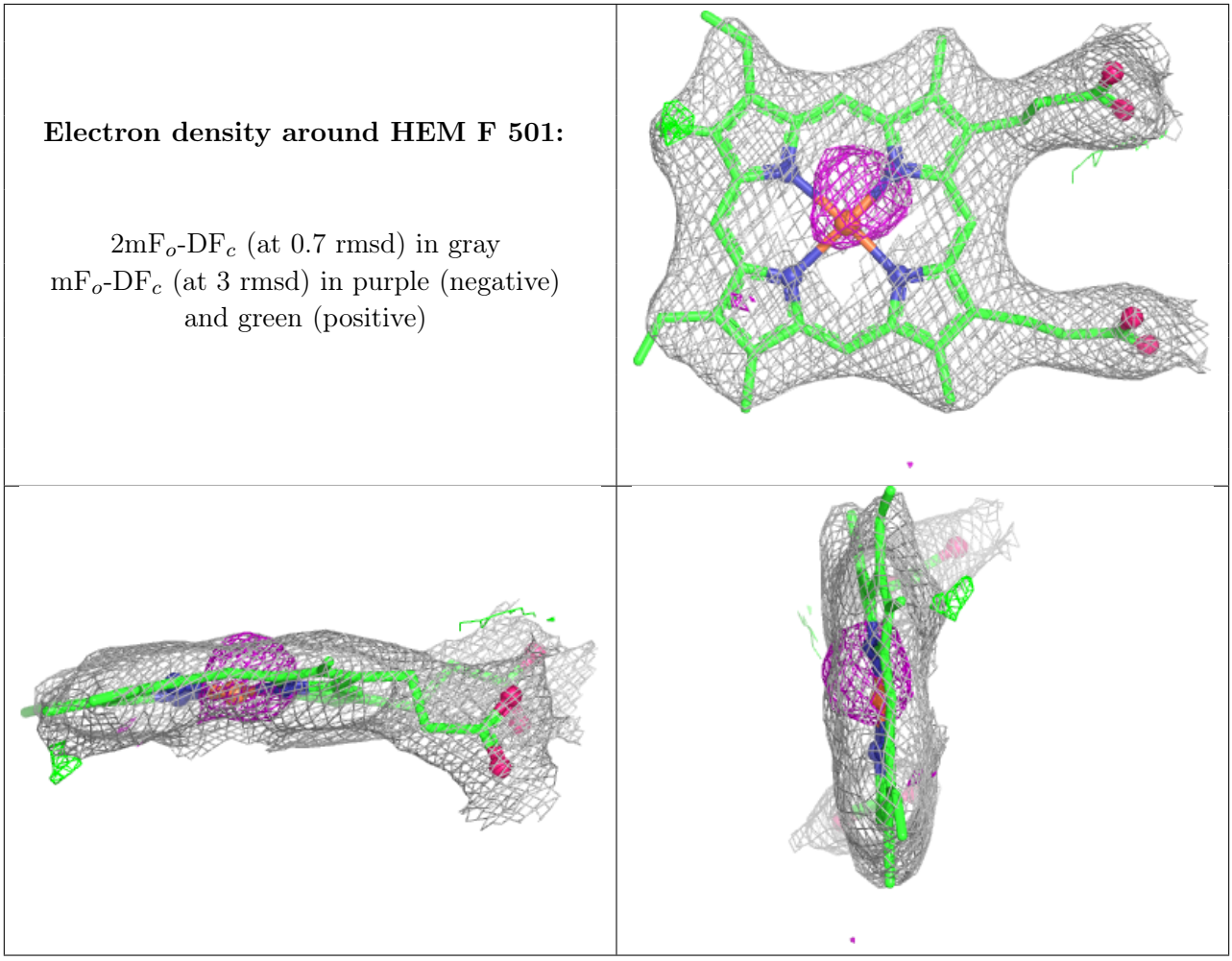






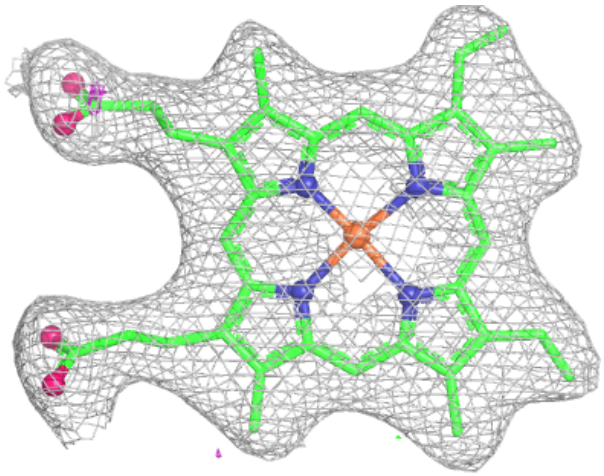
Electron density around HEM F 501:

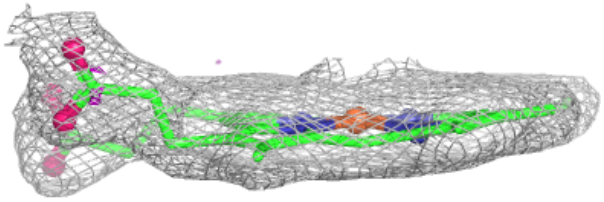
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

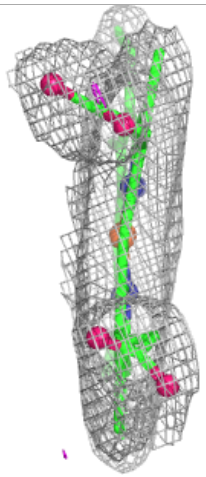


Electron density around HEM D 501:

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

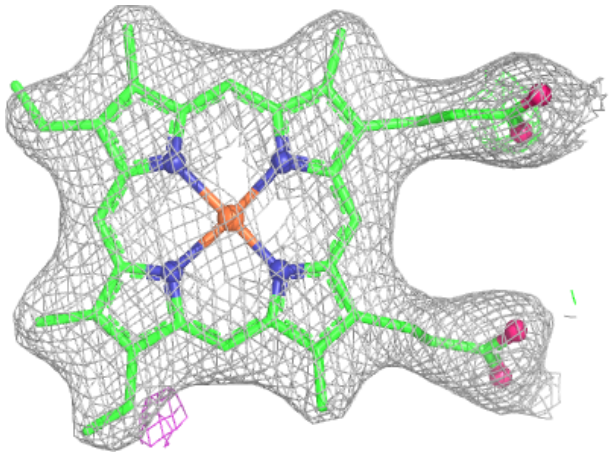


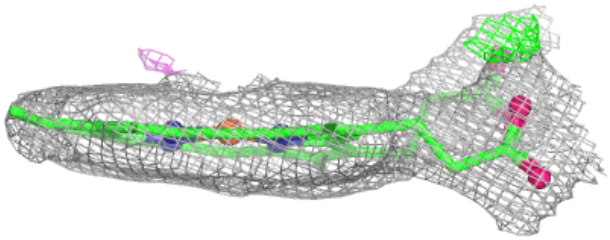


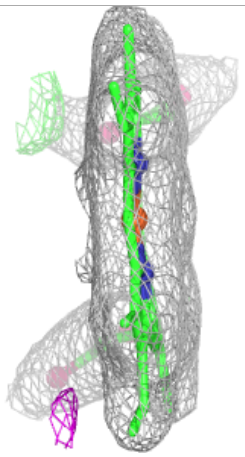


Electron density around HEM E 501:

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

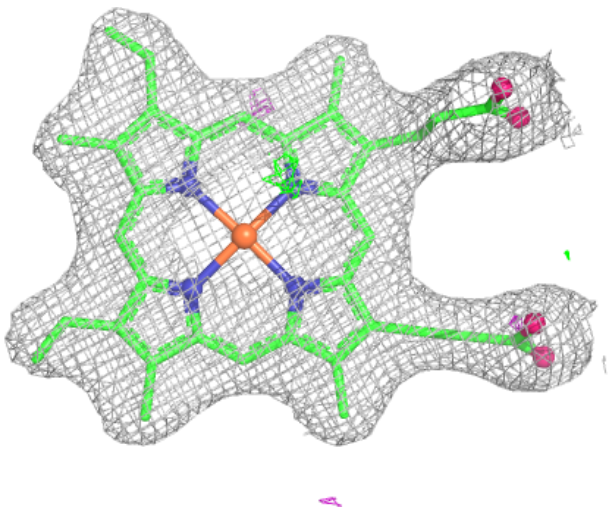


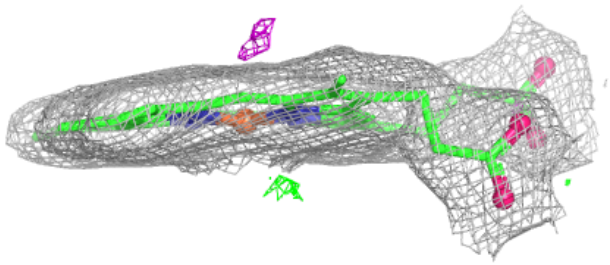


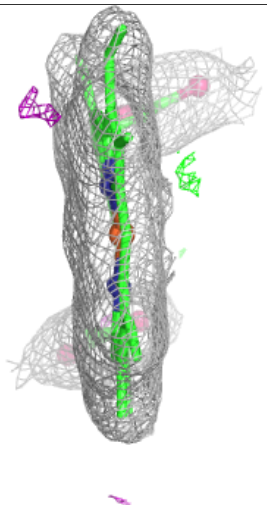


Electron density around HEM A 501:

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

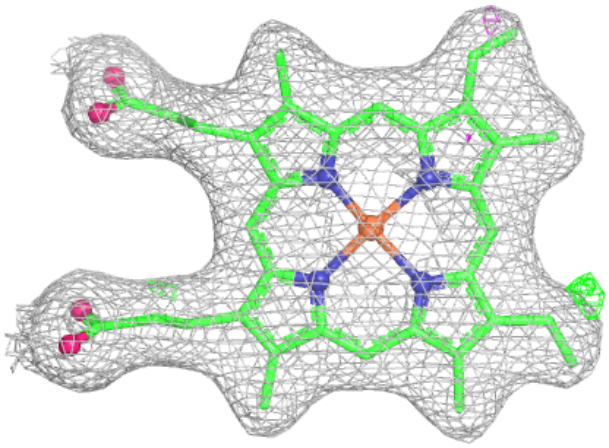


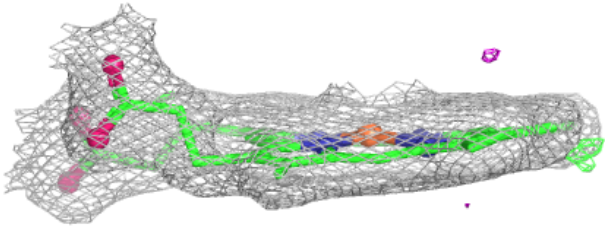


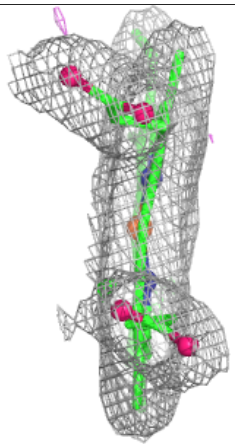


Electron density around HEM B 501:

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

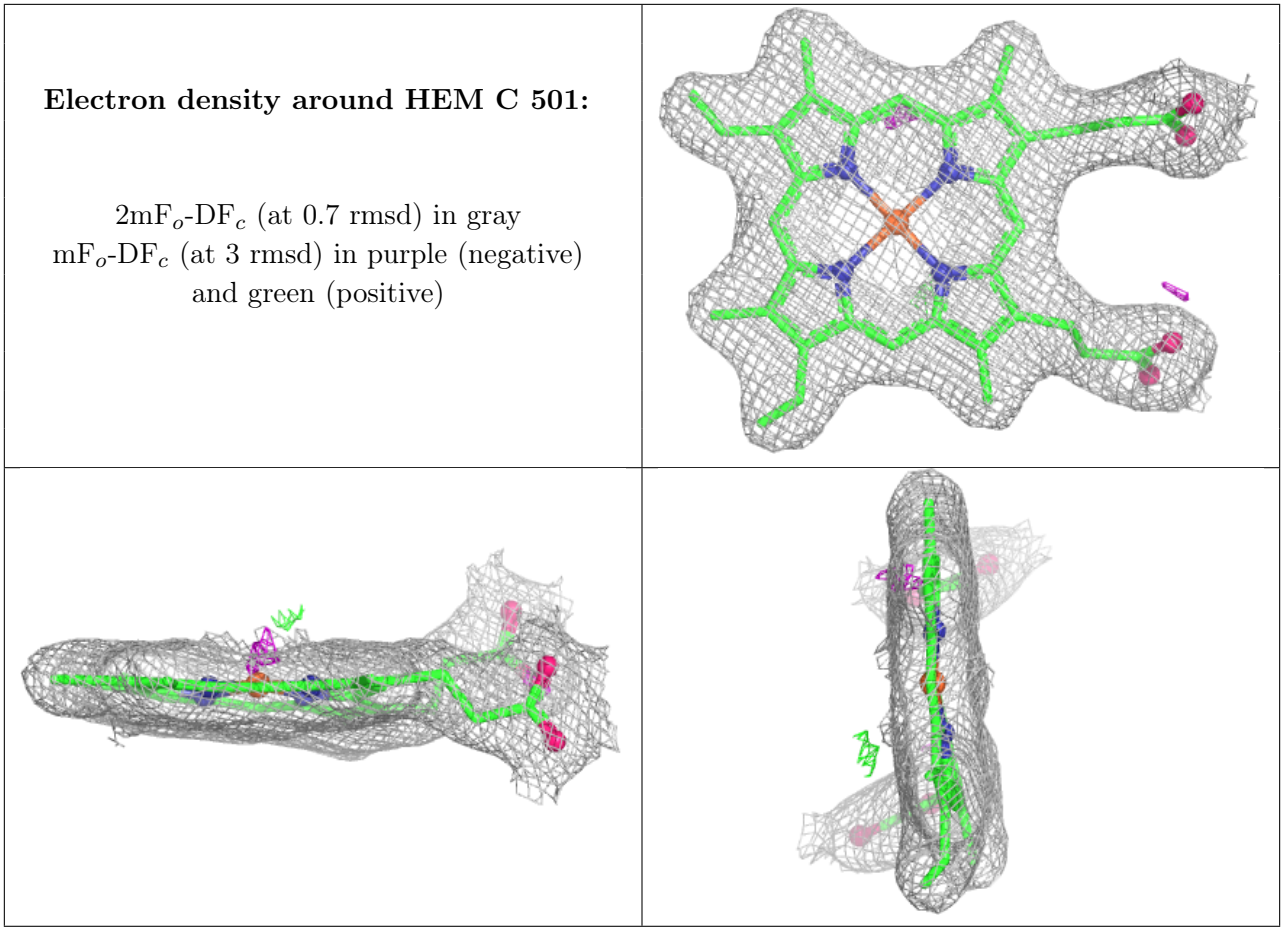






Electron density around HEM C 501:

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



6.5 Other polymers

There are no such residues in this entry.