wwPDB X-ray Structure Validation Summary Report (i)

Oct 13, 2020 – 01:10 AM BST

PDB ID	:	6ZI7
Title	:	Crystal structure of OleP-oleandolide(DEO) bound to L-rhamnose
Authors	:	Montemiglio, L.C.; Savino, C.; Vallone, B.; Parisi, G.; Freda, I.
Deposited on	:	2020-06-25
Resolution	:	2.28 Å(reported)

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

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

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

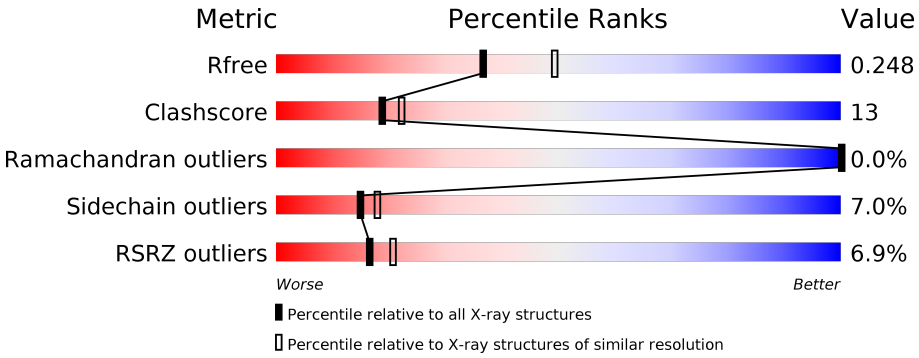
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	407	% 75% 21%
1	B	407	% 79% 18%
1	C	407	% 81% 14%
1	D	407	6% 74% 21%
1	E	407	12% 73% 21%
1	F	407	20% 69% 25%

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	RAM	A	503[A]	-	-	X	X
4	RAM	A	503[B]	-	-	X	X
4	RAM	B	513	-	-	X	-
4	RAM	D	503	-	-	X	-
5	FMT	A	510	-	-	X	-
5	FMT	A	511	-	-	X	-
5	FMT	A	517	-	-	-	X
5	FMT	A	529	-	-	-	X
5	FMT	A	531	-	-	X	-
5	FMT	A	546	-	-	-	X
5	FMT	A	549	-	-	-	X
5	FMT	A	550	-	-	X	-
5	FMT	A	563	-	-	-	X
5	FMT	A	565	-	-	X	-
5	FMT	A	574	-	-	-	X
5	FMT	B	503	-	-	X	-
5	FMT	B	511	-	-	X	-
5	FMT	B	522	-	-	-	X
5	FMT	B	534	-	-	X	-
5	FMT	B	538	-	-	-	X
5	FMT	B	539	-	-	-	X
5	FMT	C	507	-	-	X	-
5	FMT	C	528	-	-	-	X
5	FMT	C	539	-	-	-	X
5	FMT	C	543	-	-	-	X
5	FMT	C	544	-	-	-	X
5	FMT	C	545	-	-	-	X
5	FMT	C	551	-	-	-	X
5	FMT	C	552	-	-	X	-
5	FMT	D	504	-	-	X	-
5	FMT	D	517	-	-	-	X
5	FMT	D	527	-	-	-	X
5	FMT	D	528	-	-	X	-
5	FMT	D	530	-	-	-	X
5	FMT	D	536	-	-	-	X
5	FMT	E	501	-	-	X	-
5	FMT	E	509	-	-	-	X
5	FMT	E	511	-	-	-	X
5	FMT	E	517	-	-	-	X
5	FMT	F	505	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FMT	F	509	-	-	X	-
5	FMT	F	514	-	-	X	-

2 Entry composition

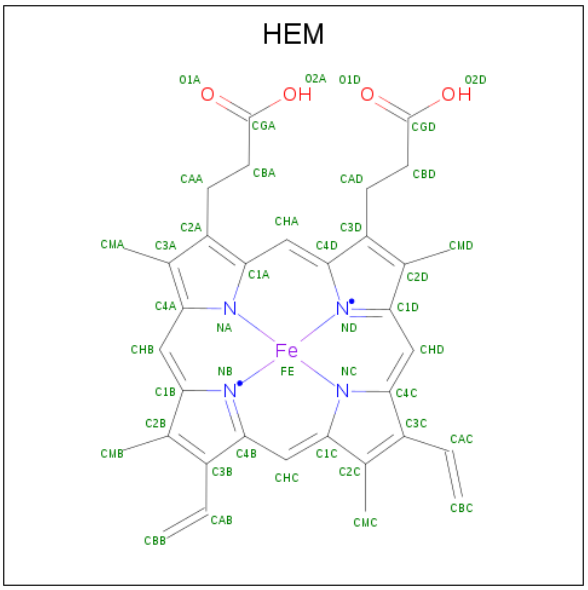
There are 7 unique types of molecules in this entry. The entry contains 22307 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

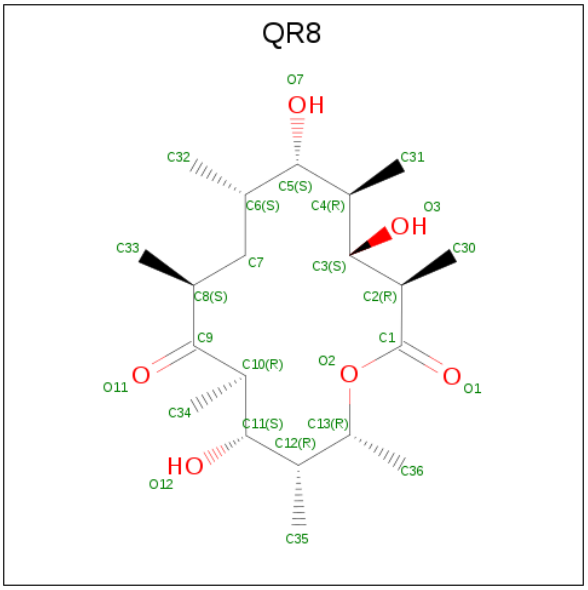
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	36	0
			3303	2099	587	599	18			
1	B	400	Total	C	N	O	S	0	22	0
			3249	2052	574	606	17			
1	C	400	Total	C	N	O	S	0	22	0
			3248	2053	577	603	15			
1	D	400	Total	C	N	O	S	0	42	0
			3372	2142	603	612	15			
1	E	397	Total	C	N	O	S	0	36	0
			3316	2107	591	601	17			
1	F	398	Total	C	N	O	S	0	46	0
			3358	2149	588	606	15			

- 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 author).



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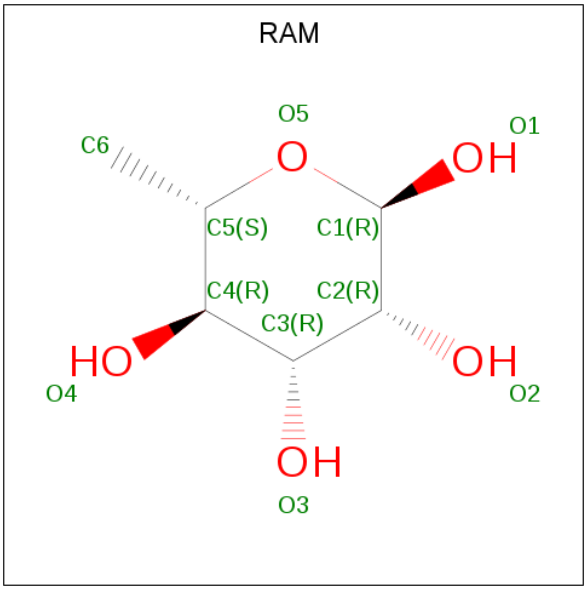
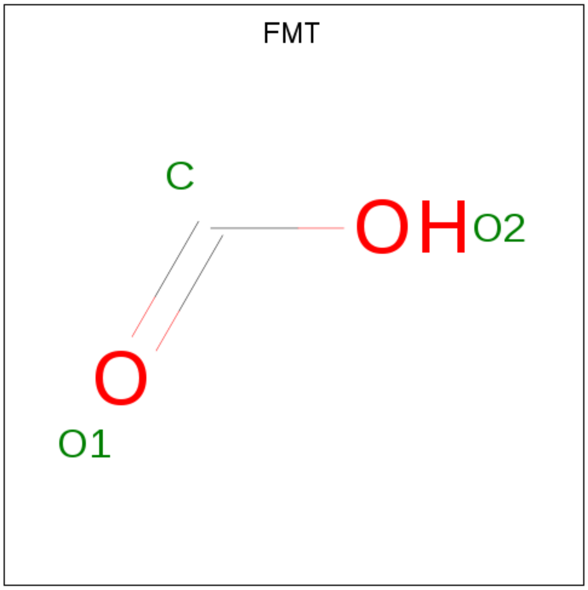
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 26 20 6	0	0

- Molecule 4 is alpha-L-rhamnopyranose (three-letter code: RAM) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 22 12 10	0	1
4	B	1	Total C O 11 6 5	0	0
4	D	1	Total C O 11 6 5	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	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
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	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
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	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
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	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	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	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	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	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	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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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
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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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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	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

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

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

- Molecule 7 is water.

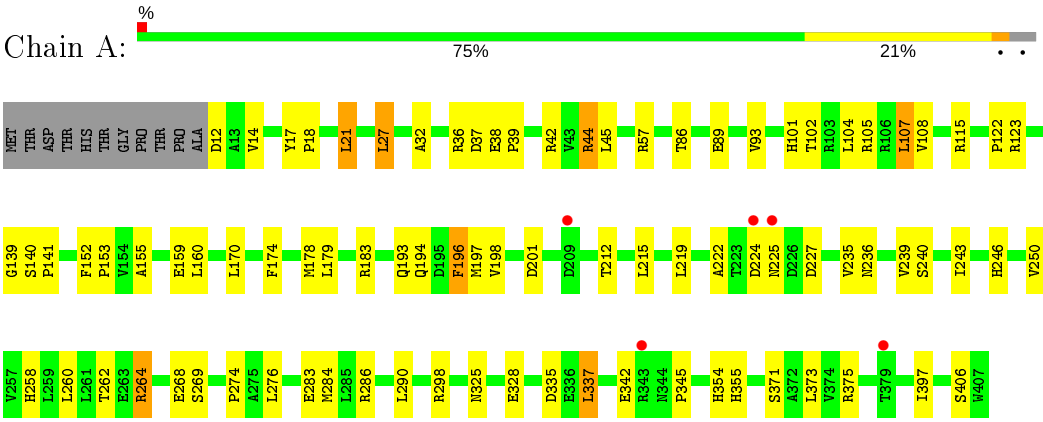
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	260	Total O 260 260	0	1
7	B	281	Total O 281 281	0	3
7	C	384	Total O 384 384	0	3
7	D	158	Total O 158 158	0	2
7	E	137	Total O 137 137	0	4
7	F	135	Total O 135 135	0	2

3 Residue-property plots (i)

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

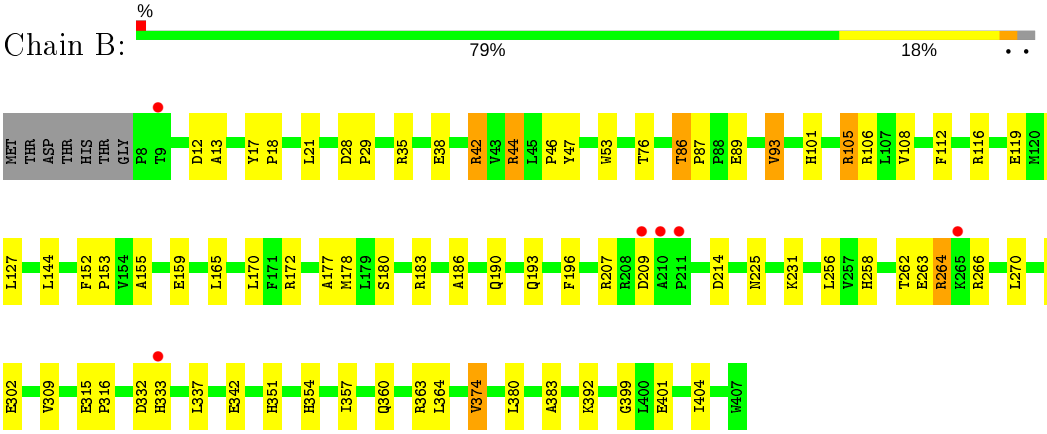
- Molecule 1: Cytochrome P-450

Chain A:



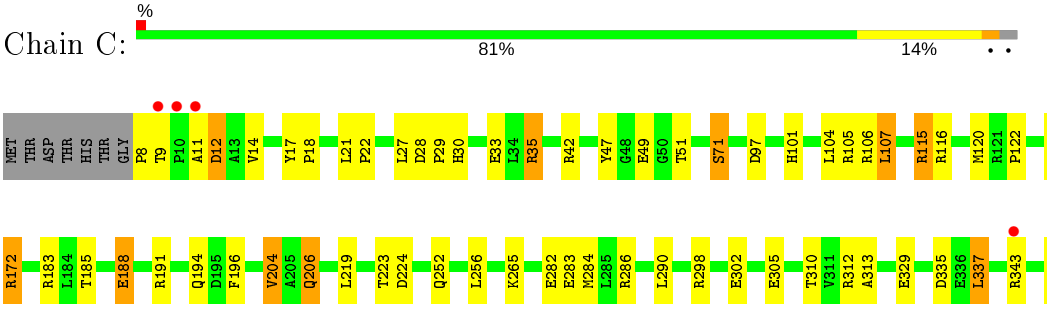
- Molecule 1: Cytochrome P-450

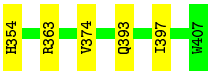
Chain B:



- Molecule 1: Cytochrome P-450

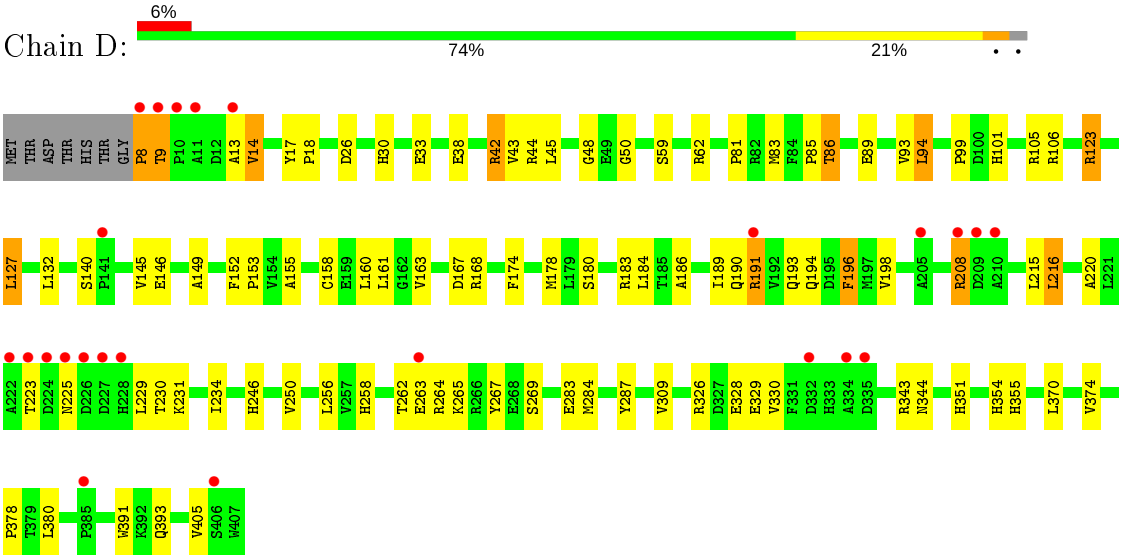
Chain C:





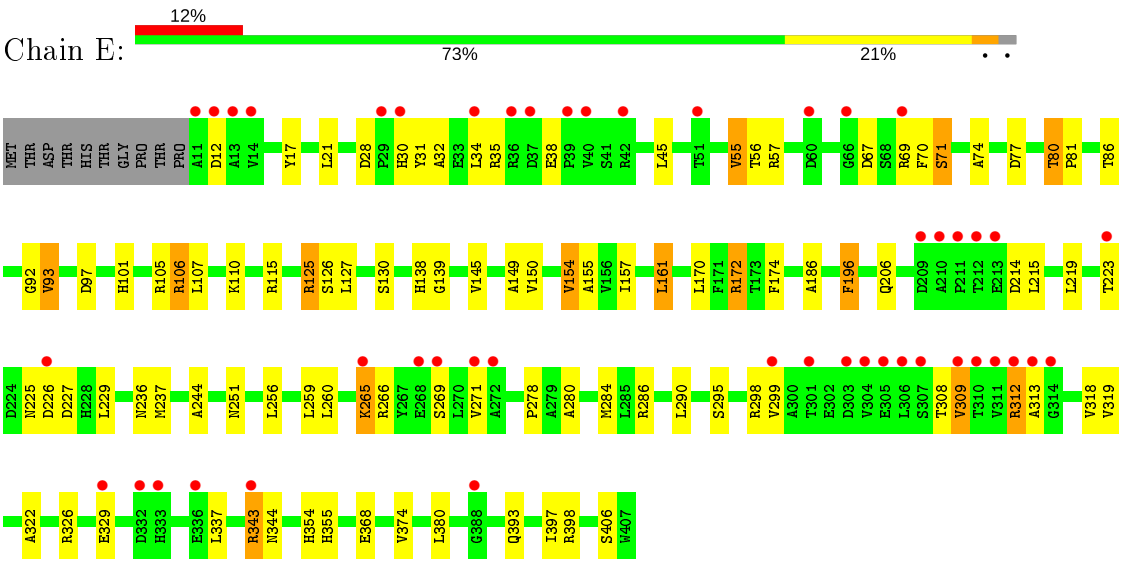
• Molecule 1: Cytochrome P-450

Chain D:



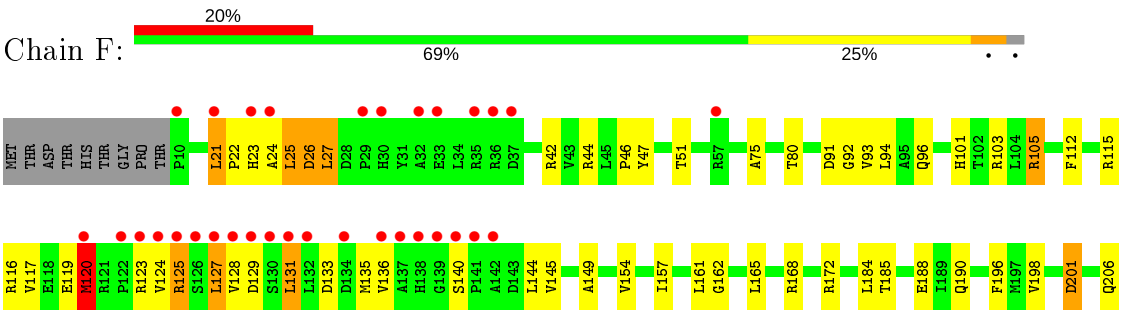
• Molecule 1: Cytochrome P-450

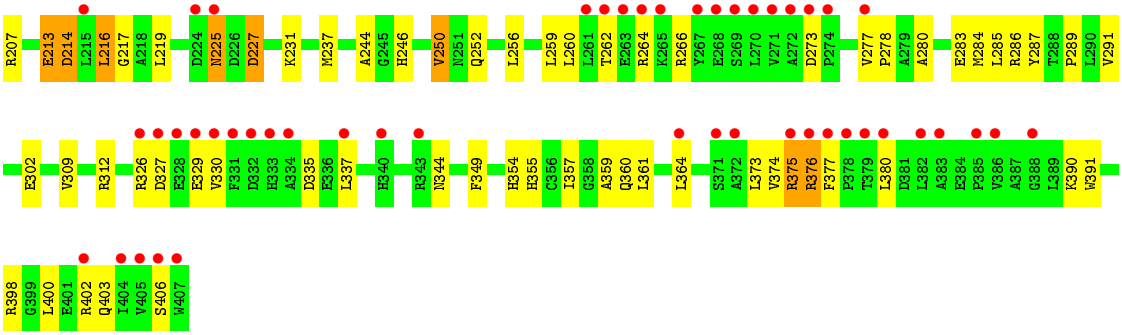
Chain E:



• Molecule 1: Cytochrome P-450

Chain F:




R207
E213
D214
L215
L216
G217
A218
L219
D224
N225
D226
D227
K231
M237
A244
G245
H246
V250
N251
Q252
L256
L259
L260
L261
T262
E263
R264
K265
R266
Y267
E268
S269
L270
V271
A272
D273
P274
V277
P278
A279
A280
E283
M284
L285
R286
Y287
T288
P289
L290
V291
E302
V309
R312
R326
D327
E328
E329
V330
F331
D332
H333
A334
D335
E336
L337
H340
R343
N344
F349
H354
H355
C356
I357
G358
A359
Q360
L361
L364
S371
A372
L373
V374
R375
R376
F377
P378
T379
L380
D381
L382
A383
E384
P385
V386
A387
G388
L389
K390
W391
R398
G399
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	247.53Å 110.68Å 159.28Å 90.00° 129.46° 90.00°	Depositor
Resolution (Å)	47.92 – 2.28 47.87 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.92-2.28) 94.7 (47.87-1.86)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.184 , 0.247 0.190 , 0.248	Depositor DCC
R_{free} test set	13326 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	56.7	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.2	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	22307	wwPDB-VP
Average B, all atoms (Å^2)	60.0	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 40.86 % 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 2.5720e-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: QR8, NA, FMT, RAM, 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	0.86	0/3483	1.02	3/4732 (0.1%)
1	B	0.89	1/3385 (0.0%)	1.05	7/4606 (0.2%)
1	C	0.90	3/3385 (0.1%)	1.08	9/4606 (0.2%)
1	D	0.84	0/3572	1.01	2/4852 (0.0%)
1	E	0.81	0/3489	0.96	1/4744 (0.0%)
1	F	0.85	2/3561 (0.1%)	1.06	13/4843 (0.3%)
All	All	0.86	6/20875 (0.0%)	1.03	35/28383 (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	F	0	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	26[A]	ASP	CA-C	8.04	1.73	1.52
1	F	26[B]	ASP	CA-C	8.04	1.73	1.52
1	C	188	GLU	CD-OE1	5.81	1.32	1.25
1	B	119	GLU	CD-OE1	5.61	1.31	1.25
1	C	71	SER	CA-CB	-5.35	1.45	1.52

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	120[A]	MET	N-CA-CB	-14.58	84.36	110.60
1	F	120[B]	MET	N-CA-CB	-14.58	84.36	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	26[A]	ASP	CA-C-O	-11.16	96.66	120.10
1	F	26[B]	ASP	CA-C-O	-11.16	96.66	120.10
1	C	35	ARG	NE-CZ-NH2	-10.81	114.89	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	213	GLU	Peptide
1	F	26[A]	ASP	Mainchain
1	F	26[B]	ASP	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	3303	0	3379	104	0
1	B	3249	0	3256	61	1
1	C	3248	0	3258	59	0
1	D	3372	0	3458	98	0
1	E	3316	0	3380	74	0
1	F	3358	0	3479	115	0
2	A	43	0	30	4	0
2	B	43	0	30	7	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
2	E	43	0	30	3	0
2	F	43	0	30	4	0
3	A	26	0	0	3	0
3	B	26	0	0	1	0
3	C	26	0	0	0	0
3	D	26	0	0	2	0
3	E	26	0	0	0	0
3	F	26	0	0	0	0
4	A	22	0	23	34	0
4	B	11	0	12	11	0
4	D	11	0	12	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	210	0	71	21	1
5	B	108	0	36	9	0
5	C	147	0	49	9	0
5	D	99	0	33	8	0
5	E	42	0	14	2	0
5	F	36	0	12	10	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	260	0	0	9	0
7	B	281	0	0	14	0
7	C	384	0	0	17	0
7	D	158	0	0	6	0
7	E	137	0	0	1	0
7	F	135	0	0	9	0
All	All	22307	0	20652	544	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 13.

The worst 5 of 544 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93[A]:VAL:HG11	1:E:237[A]:MET:CE	1.54	1.37
1:F:120[A]:MET:CE	1:F:361[A]:LEU:HD21	1.69	1.22
1:A:197[A]:MET:CE	1:A:235[A]:VAL:HG23	1.73	1.19
1:B:89:GLU:CB	4:B:513:RAM:H2	1.71	1.17
1:A:197[A]:MET:CE	1:A:235[A]:VAL:CG2	2.23	1.17

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:360[B]:GLN:NE2	5:A:567:FMT:O2[3_555]	2.18	0.02

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	430/407 (106%)	418 (97%)	12 (3%)	0	100	100
1	B	421/407 (103%)	407 (97%)	14 (3%)	0	100	100
1	C	420/407 (103%)	406 (97%)	14 (3%)	0	100	100
1	D	440/407 (108%)	409 (93%)	31 (7%)	0	100	100
1	E	431/407 (106%)	410 (95%)	21 (5%)	0	100	100
1	F	442/407 (109%)	413 (93%)	28 (6%)	1 (0%)	47	57
All	All	2584/2442 (106%)	2463 (95%)	120 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	273	ASP

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	368/341 (108%)	340 (92%)	28 (8%)	13	15
1	B	358/341 (105%)	337 (94%)	21 (6%)	19	24
1	C	357/341 (105%)	338 (95%)	19 (5%)	22	29
1	D	376/341 (110%)	341 (91%)	35 (9%)	9	9
1	E	368/341 (108%)	332 (90%)	36 (10%)	8	8
1	F	377/341 (111%)	338 (90%)	39 (10%)	7	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2204/2046 (108%)	2026 (92%)	178 (8%)	15 13

5 of 178 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	140	SER
1	D	330	VAL
1	F	227	ASP
1	D	191[B]	ARG
1	D	231[A]	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	360	GLN
1	D	193	GLN
1	E	236	ASN
1	C	225	ASN
1	F	193	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 236 ligands modelled in this entry, 6 are monoatomic - leaving 230 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	RAM	A	503[B]	-	11,11,11	1.37	2 (18%)	15,16,16	2.60	9 (60%)
5	FMT	A	565	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	527	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	543	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	530	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	532	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	517	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	510	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	F	514	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	509	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	569	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	523	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	518	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	545	-	0,2,2	0.00	-	0,1,1	0.00	-
4	RAM	B	513	-	11,11,11	1.77	4 (36%)	15,16,16	3.53	8 (53%)
5	FMT	A	520	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	542	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	526	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	523	-	0,2,2	0.00	-	0,1,1	0.00	-
2	HEM	B	501	1	27,50,50	1.52	6 (22%)	17,82,82	2.30	6 (35%)
5	FMT	A	563	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	532	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	559	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	560	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	534	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	552	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	537	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	552	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	520	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	516	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	538	-	0,2,2	0.00	-	0,1,1	0.00	-
3	QR8	A	502	-	26,26,26	1.69	4 (15%)	35,38,38	1.83	9 (25%)
5	FMT	B	523	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	547	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	526	-	0,2,2	0.00	-	0,1,1	0.00	-
2	HEM	F	502	1	27,50,50	0.85	1 (3%)	17,82,82	1.59	6 (35%)
5	FMT	D	532	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FMT	D	512	-	0,2,2	0.00	-	0,1,1	0.00	-
3	QR8	B	502	-	26,26,26	1.79	4 (15%)	35,38,38	1.73	10 (28%)
5	FMT	A	549	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	528	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	537	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	544	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	514	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	570	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	521	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	514	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	508	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	503	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	508	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	519	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	573	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	541	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	501	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	504	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	542	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	516	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	512	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	525	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	F	504	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	508	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	505	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	531	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	511	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	F	511	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	536	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	523	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	512	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	504	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	F	512	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	524	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	517	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	515	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	547	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	544	-	0,2,2	0.00	-	0,1,1	0.00	-
2	HEM	E	502	1	27,50,50	1.12	4 (14%)	17,82,82	2.15	5 (29%)
5	FMT	A	574	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	546	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	513	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	QR8	C	502	-	26,26,26	1.53	2 (7%)	35,38,38	1.70	7 (20%)
5	FMT	B	524	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	538	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	520	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	550	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	534	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	503	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	506	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	521	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	531	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	539	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	507	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	535	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	540	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	518	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	506	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	558	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	549	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	516	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	519	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	522	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	504	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	532	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	530	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	510	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	526	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	529	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	555	-	0,2,2	0.00	-	0,1,1	0.00	-
3	QR8	D	502	-	26,26,26	1.64	4 (15%)	35,38,38	1.90	9 (25%)
5	FMT	C	533	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	539	-	0,2,2	0.00	-	0,1,1	0.00	-
2	HEM	A	501	1	27,50,50	1.68	6 (22%)	17,82,82	2.06	6 (35%)
4	RAM	A	503[A]	-	11,11,11	1.32	3 (27%)	15,16,16	3.59	9 (60%)
5	FMT	A	524	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	519	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	534	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	533	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	521	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	543	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	511	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	504	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	571	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FMT	C	535	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	522	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	540	-	0,2,2	0.00	-	0,1,1	0.00	-
2	HEM	C	501	1	27,50,50	1.73	3 (11%)	17,82,82	2.36	7 (41%)
5	FMT	C	509	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	572	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	538	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	519	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	531	-	0,2,2	0.00	-	0,1,1	0.00	-
2	HEM	D	501	1	27,50,50	1.64	4 (14%)	17,82,82	1.87	5 (29%)
5	FMT	D	529	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	507	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	513	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	540	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	514	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	504	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	520	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	527	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	530	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	516	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	548	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	561	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	529	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	511	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	F	513	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	551	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	508	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	509	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	534	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	518	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	530	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	505	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	533	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	F	509	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	508	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	525	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	517	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	535	-	0,2,2	0.00	-	0,1,1	0.00	-
3	QR8	F	503	-	26,26,26	1.68	3 (11%)	35,38,38	1.59	9 (25%)
5	FMT	A	567	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	F	515	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	528	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FMT	A	551	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	548	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	537	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	F	506	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	533	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	514	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	525	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	527	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	557	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	510	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	535	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	510	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	521	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	505	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	556	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	517	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	512	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	553	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	512	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	546	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	550	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	537	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	506	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	F	507	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	506	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	536	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	509	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	531	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	510	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	514	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	518	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	F	510	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	515	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	564	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	511	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	515	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	513	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	515	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	554	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	536	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	509	-	0,2,2	0.00	-	0,1,1	0.00	-
4	RAM	D	503	-	11,11,11	1.14	1 (9%)	15,16,16	2.77	10 (66%)
5	FMT	A	562	-	0,2,2	0.00	-	0,1,1	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	FMT	A	568	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	507	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	516	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	522	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	536	-	0,2,2	0.00	-	0,1,1	0.00	-
3	QR8	E	503	-	26,26,26	1.55	4 (15%)	35,38,38	1.77	10 (28%)
5	FMT	B	525	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	505	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	566	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	505	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	F	505	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	541	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	524	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	511	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	528	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	539	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	D	506	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	522	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	529	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	507	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	517	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	528	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	545	-	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	F	501	-	0,2,2	0.00	-	0,1,1	0.00	-

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
4	RAM	A	503[B]	-	-	-	0/1/1/1
4	RAM	B	513	-	-	-	0/1/1/1
2	HEM	D	501	1	-	0/6/54/54	-
3	QR8	A	502	-	-	13/48/48/48	0/1/1/1
2	HEM	B	501	1	-	0/6/54/54	-
3	QR8	E	503	-	-	15/48/48/48	0/1/1/1
2	HEM	F	502	1	-	0/6/54/54	-
2	HEM	E	502	1	-	0/6/54/54	-
3	QR8	F	503	-	-	13/48/48/48	0/1/1/1
4	RAM	A	503[A]	-	-	-	0/1/1/1
3	QR8	D	502	-	-	13/48/48/48	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	501	1	-	0/6/54/54	-
2	HEM	A	501	1	-	0/6/54/54	-
3	QR8	B	502	-	-	14/48/48/48	0/1/1/1
3	QR8	C	502	-	-	14/48/48/48	0/1/1/1
4	RAM	D	503	-	-	-	0/1/1/1

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	QR8	O2-C13	-5.69	1.37	1.46
2	C	501	HEM	C3B-C2B	-5.33	1.33	1.40
3	C	502	QR8	O2-C13	-5.12	1.38	1.46
2	A	501	HEM	C3B-C2B	-4.86	1.33	1.40
3	A	502	QR8	O2-C13	-4.73	1.39	1.46

The worst 5 of 125 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503[A]	RAM	O1-C1-C2	-8.65	84.68	109.03
4	A	503[A]	RAM	O3-C3-C2	-6.69	94.89	110.35
4	B	513	RAM	C6-C5-C4	5.66	123.54	113.07
4	B	513	RAM	O3-C3-C2	5.50	123.06	110.35
2	C	501	HEM	CBA-CAA-C2A	5.40	122.44	112.49

There are no chirality outliers.

5 of 82 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	QR8	C6-C7-C8-C9
3	A	502	QR8	C1-C2-C3-O3
3	B	502	QR8	C6-C7-C8-C9
3	B	502	QR8	C1-C2-C3-O3
3	C	502	QR8	C6-C7-C8-C9

There are no ring outliers.

50 monomers are involved in 139 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503[B]	RAM	17	0
5	A	565	FMT	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	510	FMT	2	0
5	F	514	FMT	5	0
4	B	513	RAM	11	0
2	B	501	HEM	7	0
5	C	552	FMT	2	0
3	A	502	QR8	3	0
2	F	502	HEM	4	0
5	D	512	FMT	1	0
3	B	502	QR8	1	0
5	E	501	FMT	2	0
5	A	504	FMT	1	0
5	F	504	FMT	1	0
5	D	508	FMT	1	0
5	B	511	FMT	2	0
5	C	523	FMT	1	0
2	E	502	HEM	3	0
5	B	538	FMT	1	0
5	A	550	FMT	2	0
5	B	534	FMT	2	0
5	B	503	FMT	2	0
3	D	502	QR8	2	0
2	A	501	HEM	4	0
4	A	503[A]	RAM	17	0
5	A	524	FMT	1	0
5	C	521	FMT	1	0
5	D	504	FMT	2	0
2	C	501	HEM	3	0
5	A	531	FMT	2	0
2	D	501	HEM	4	0
5	C	507	FMT	2	0
5	C	514	FMT	1	0
5	C	504	FMT	1	0
5	D	518	FMT	1	0
5	A	530	FMT	1	0
5	A	505	FMT	1	0
5	F	509	FMT	2	0
5	A	567	FMT	0	1
5	D	528	FMT	2	0
5	C	512	FMT	1	0
5	A	546	FMT	1	0
5	A	506	FMT	1	0
5	B	510	FMT	1	0

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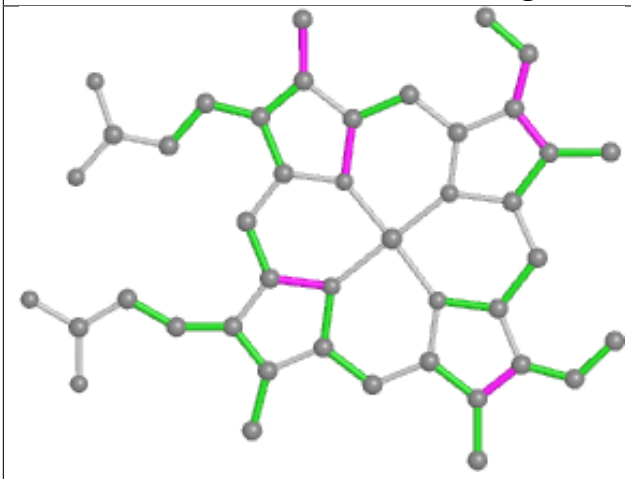
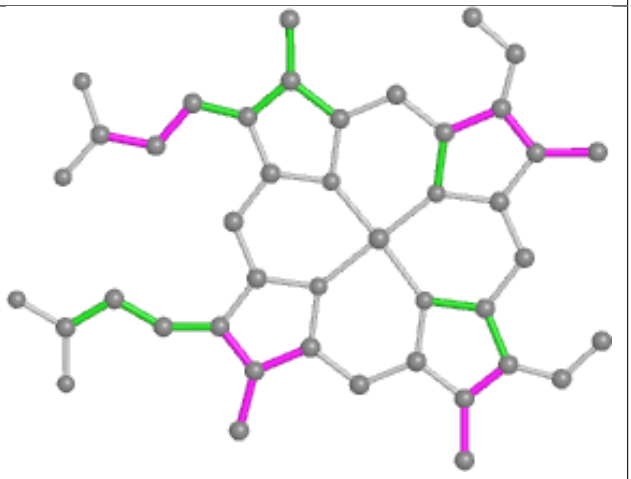
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	514	FMT	1	0
4	D	503	RAM	14	0
5	D	507	FMT	1	0
5	F	505	FMT	2	0
5	A	511	FMT	2	0
5	B	507	FMT	1	0

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.

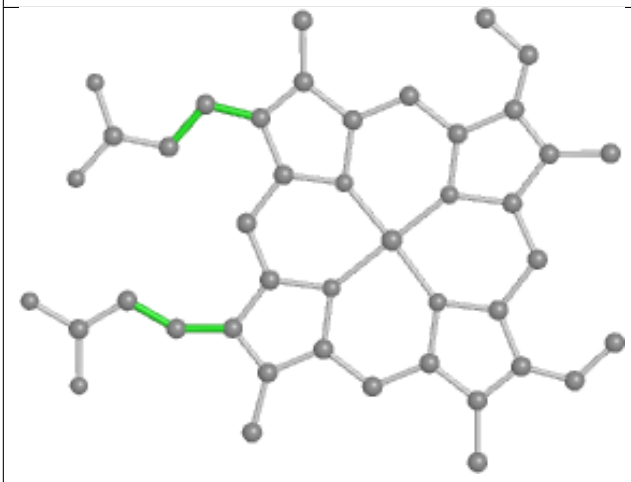
Ligand HEM B 501



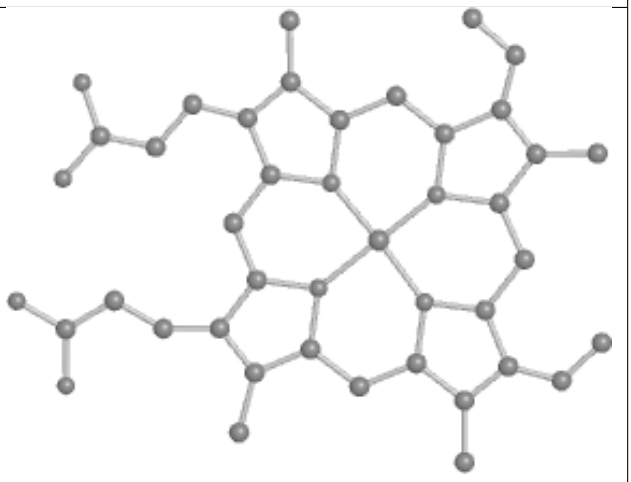
Bond lengths



Bond angles

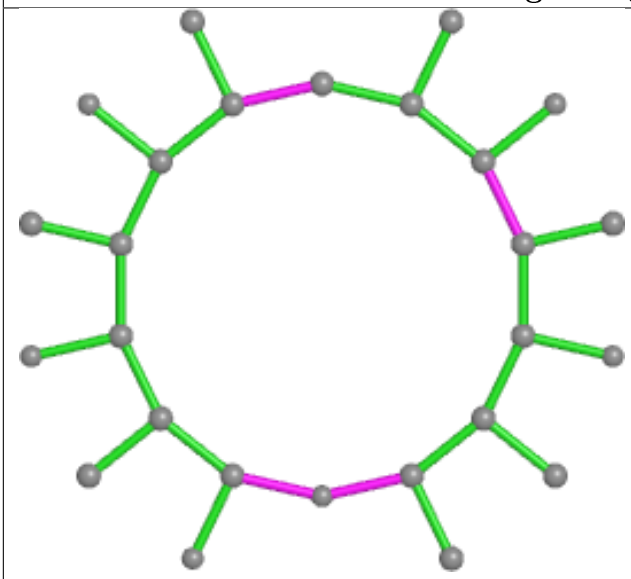


Torsions



Rings

Ligand QR8 A 502



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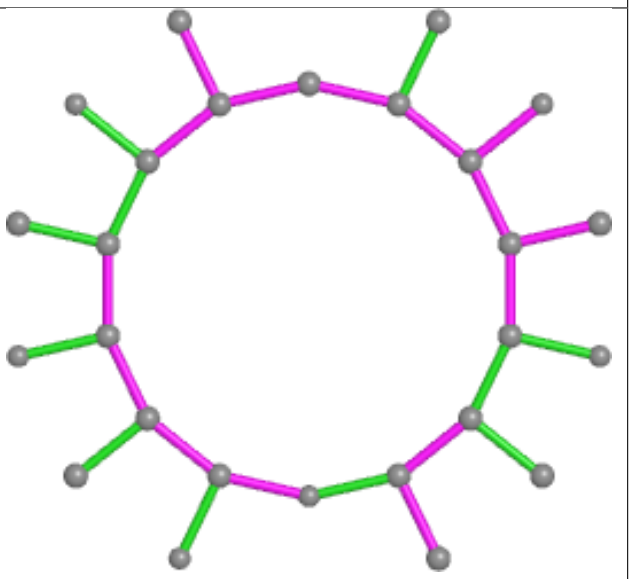
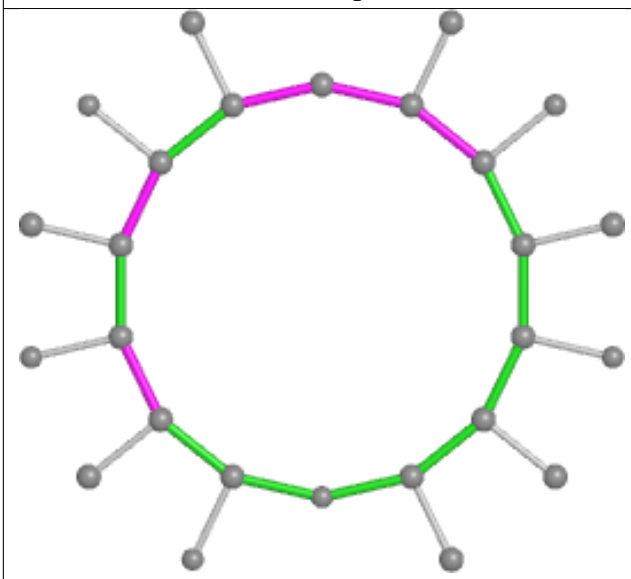
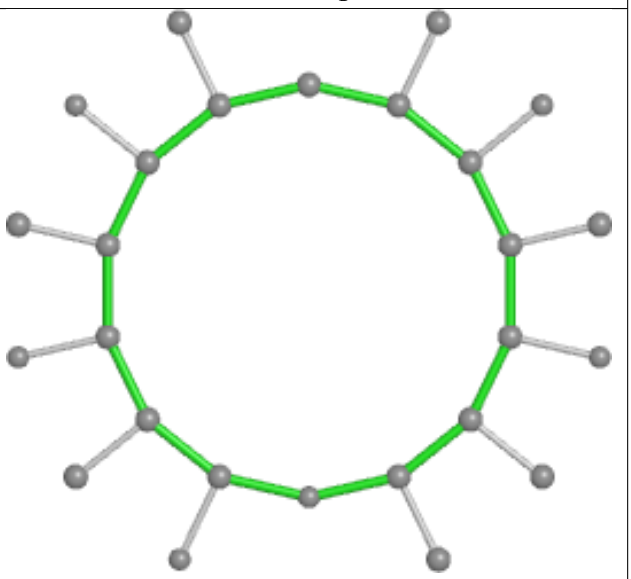


Bond angles

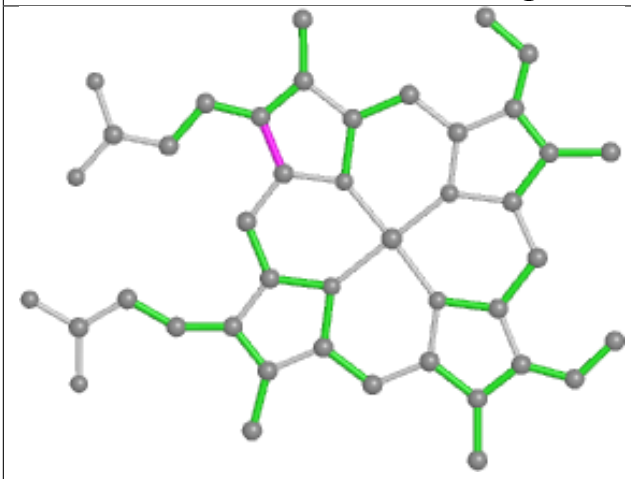


Torsions

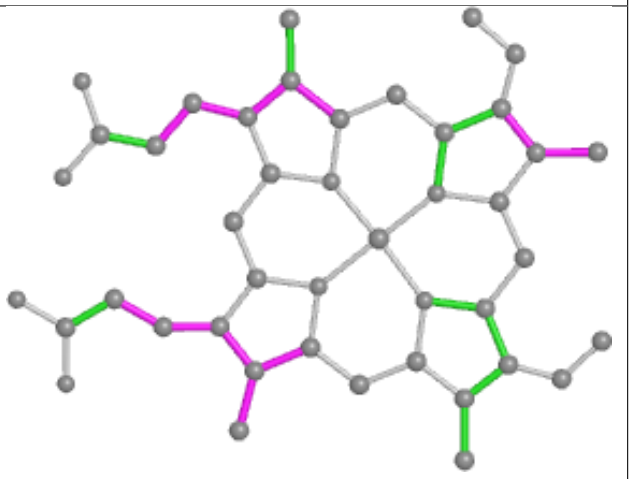


Rings

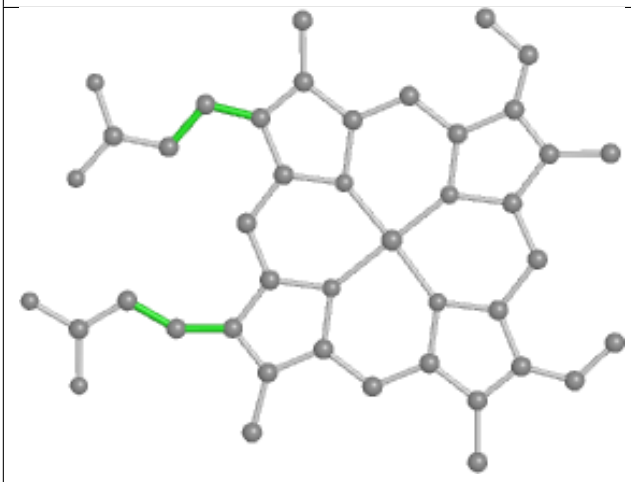
Ligand HEM F 502



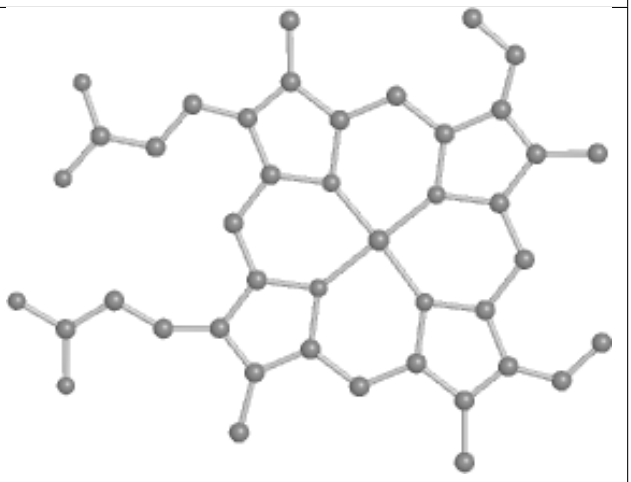
Bond lengths



Bond angles

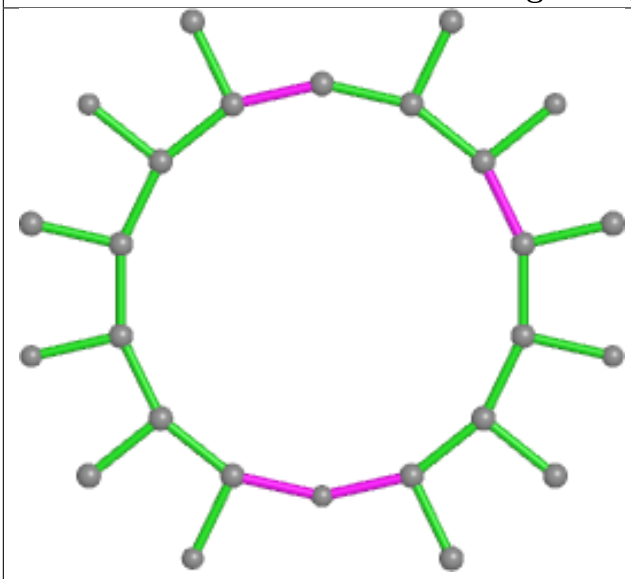


Torsions



Rings

Ligand QR8 B 502



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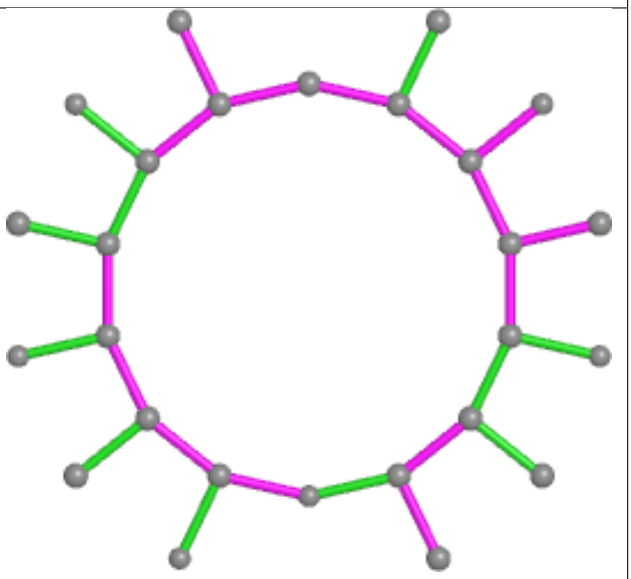
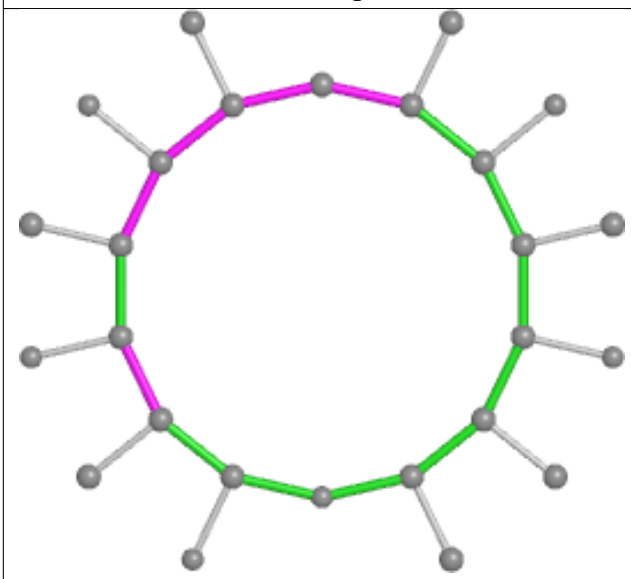


Bond angles



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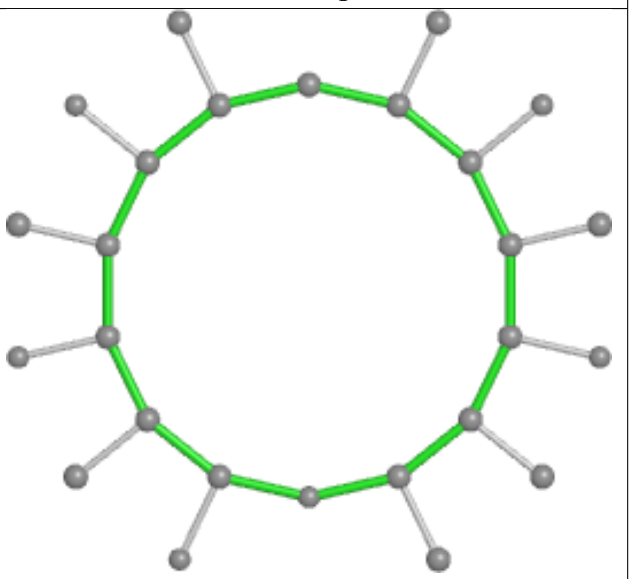
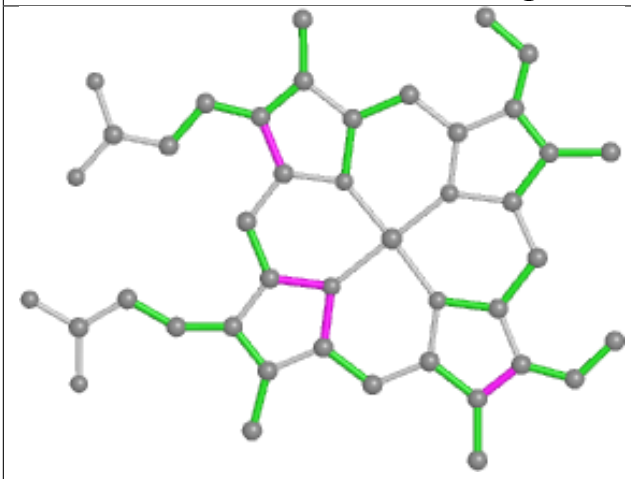
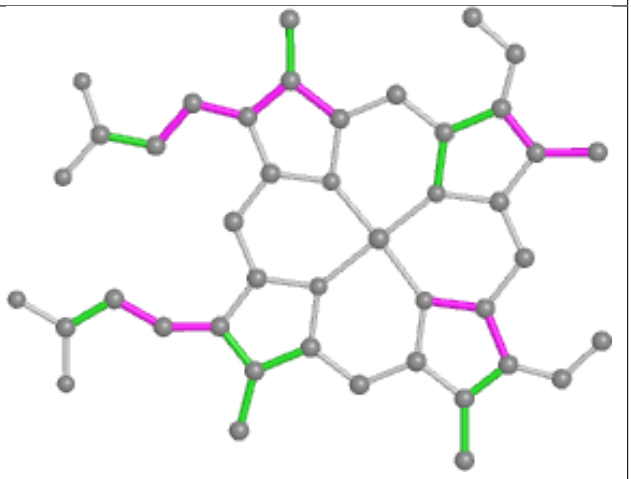


Rings

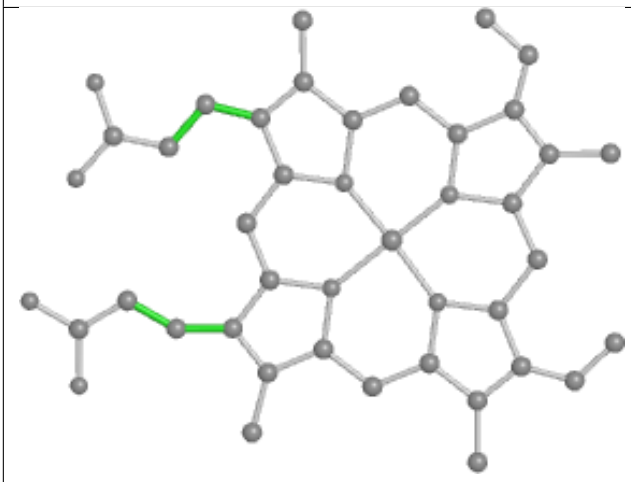
Ligand HEM E 502



Bond lengths



Bond angles



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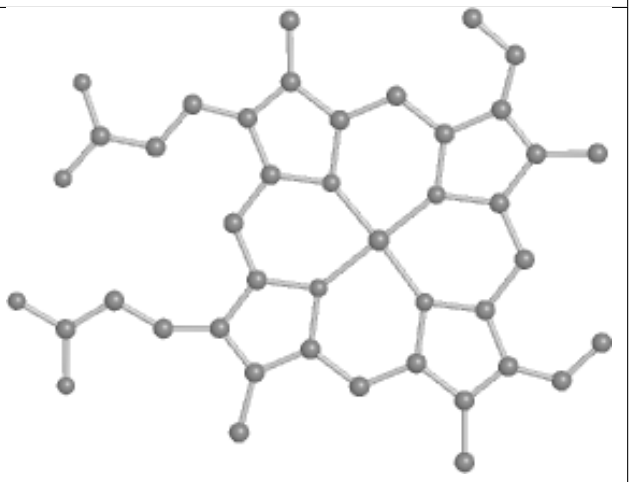
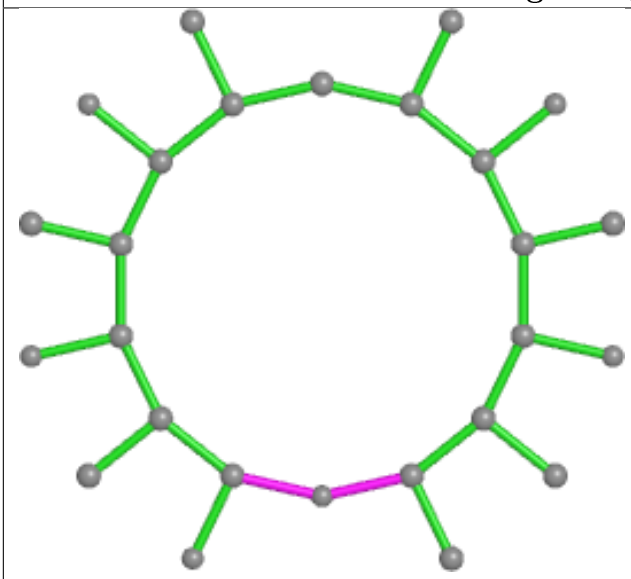


Rings

Ligand QR8 C 502



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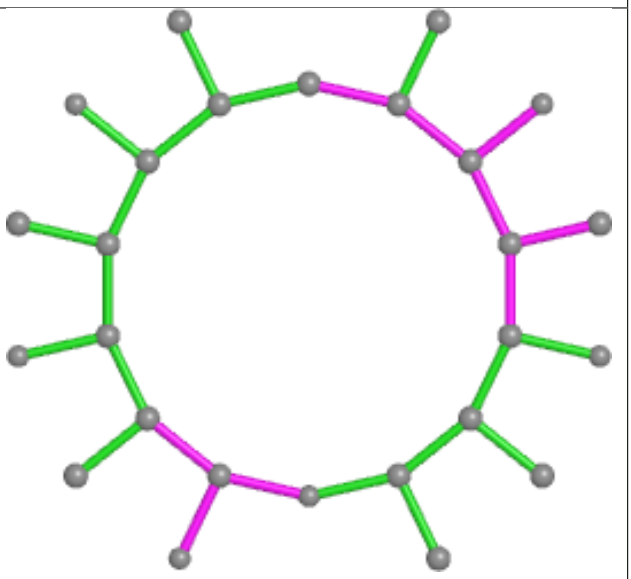

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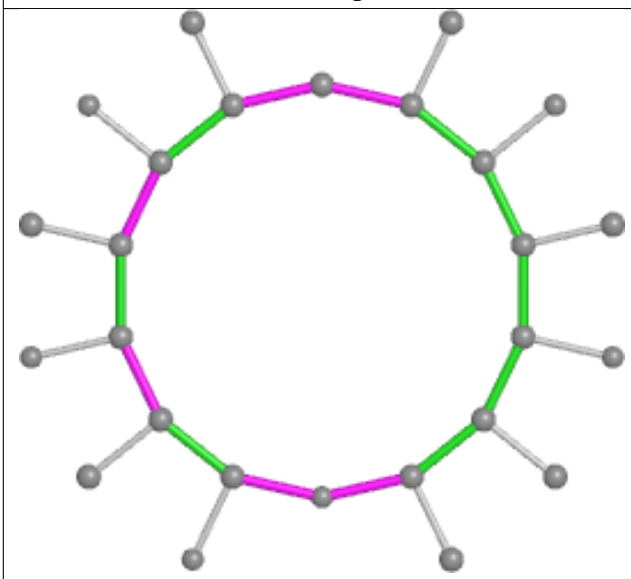

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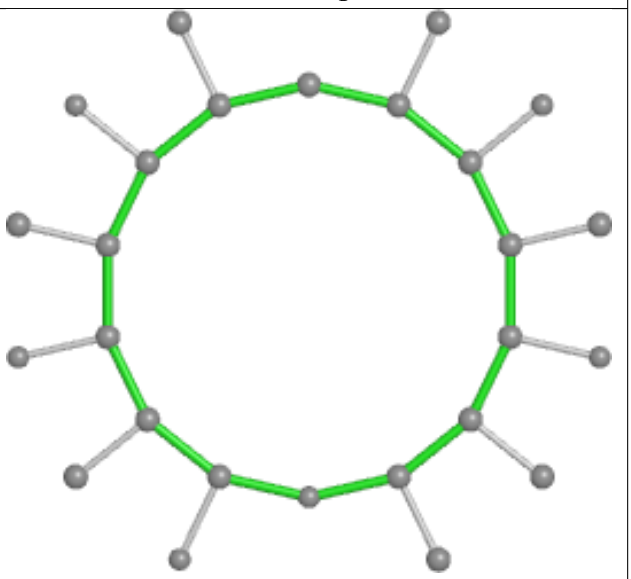
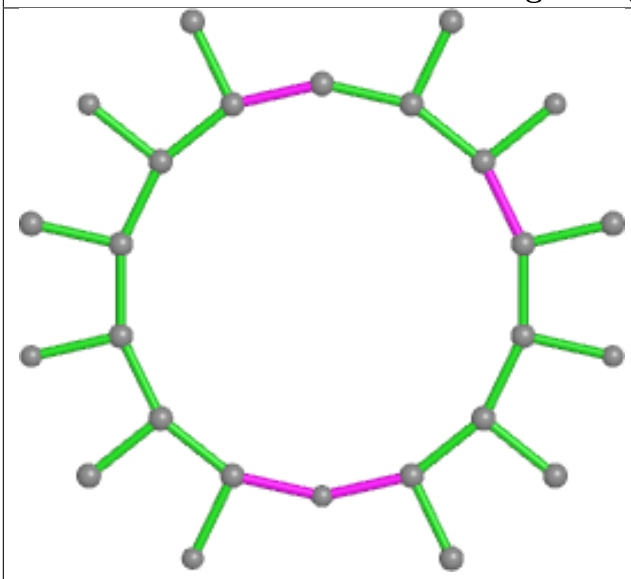


Rings

Ligand QR8 D 502



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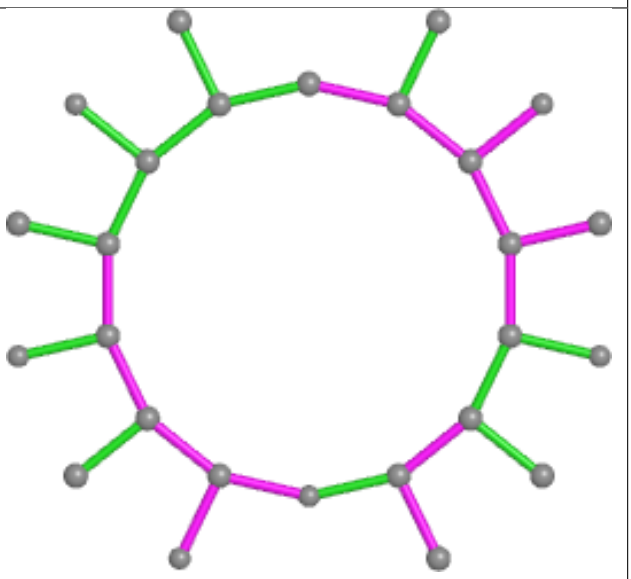

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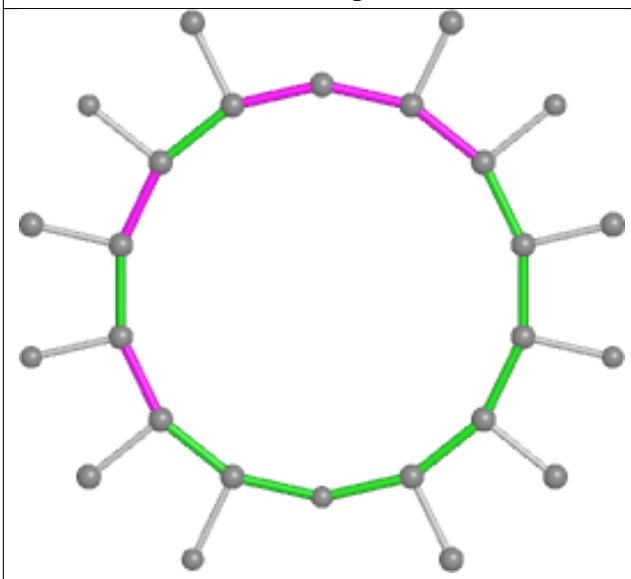

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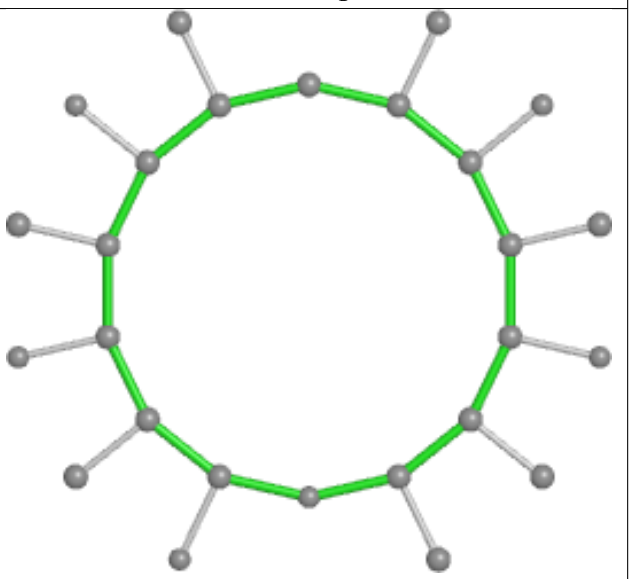
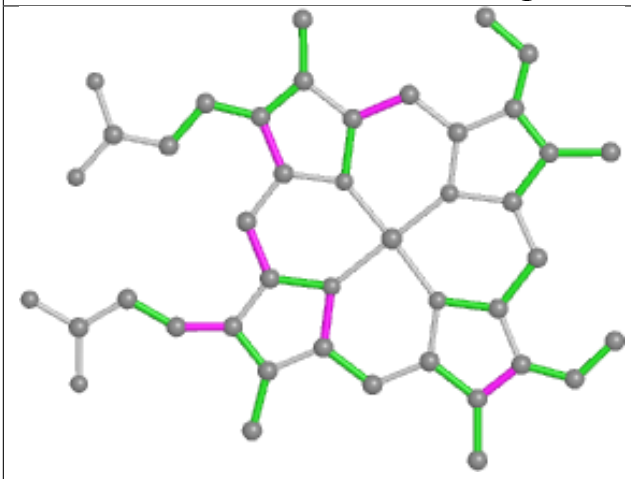


Rings

Ligand HEM A 501



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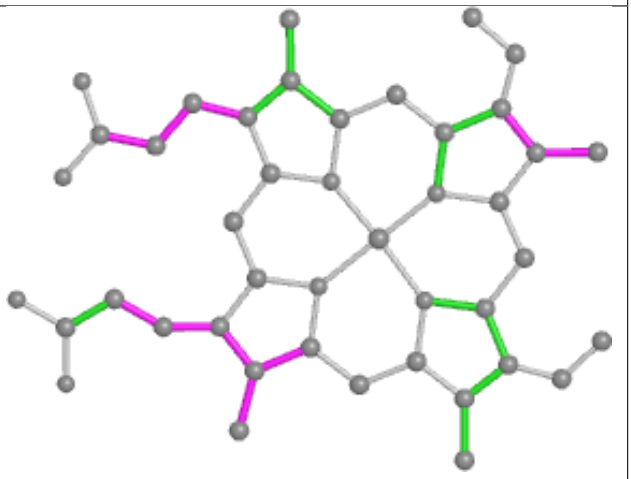

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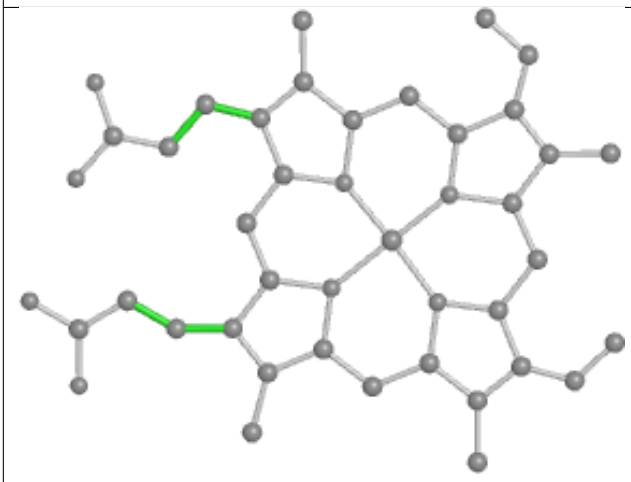

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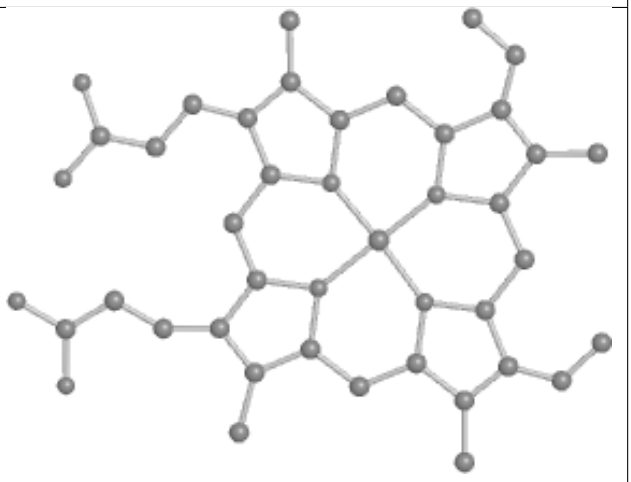
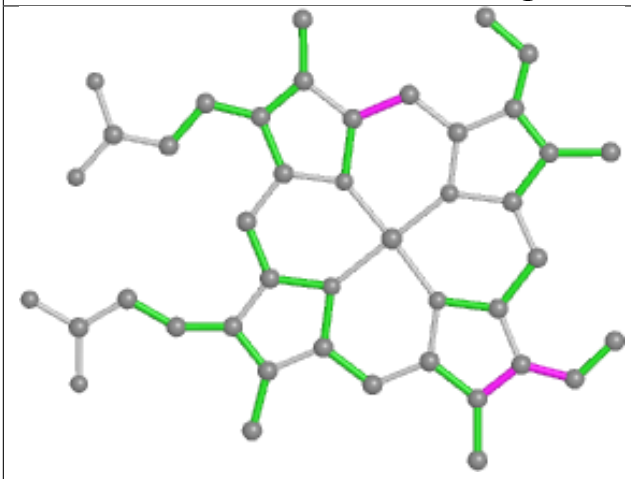


Rings

Ligand HEM C 501



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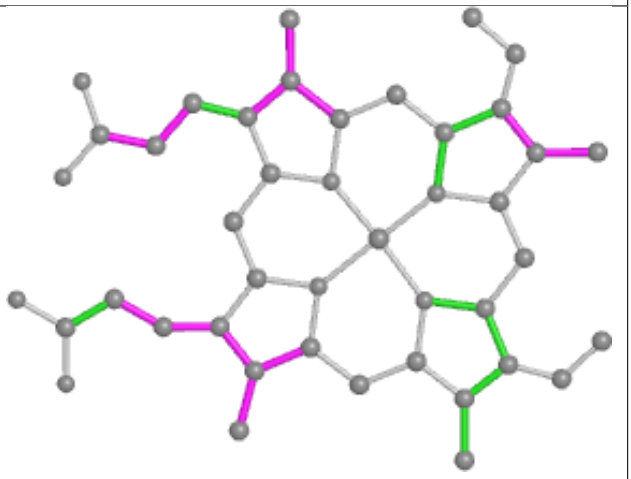
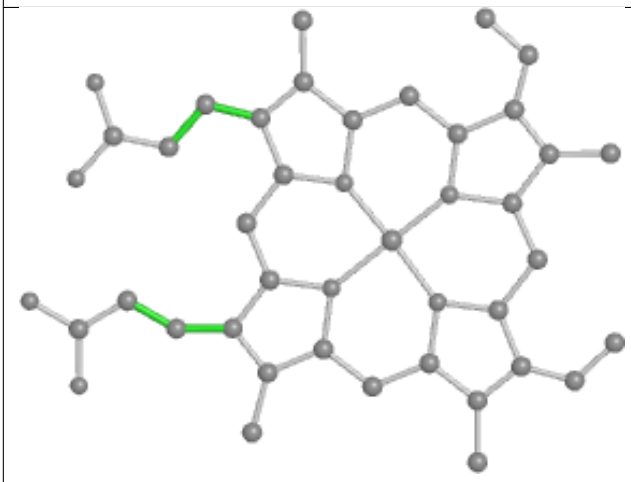
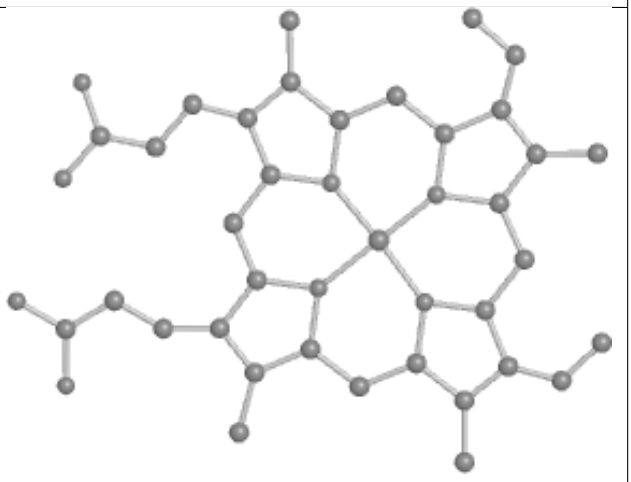


Bond angles

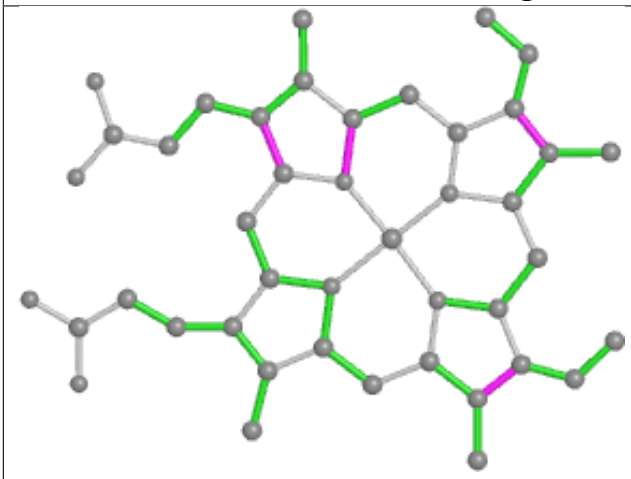


Torsions



Rings

Ligand HEM D 501



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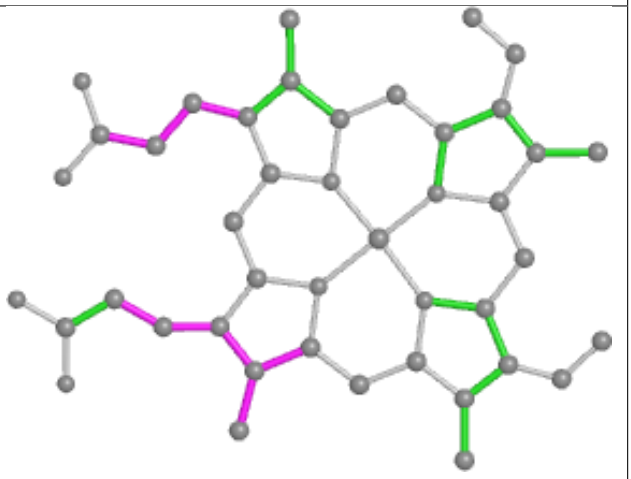
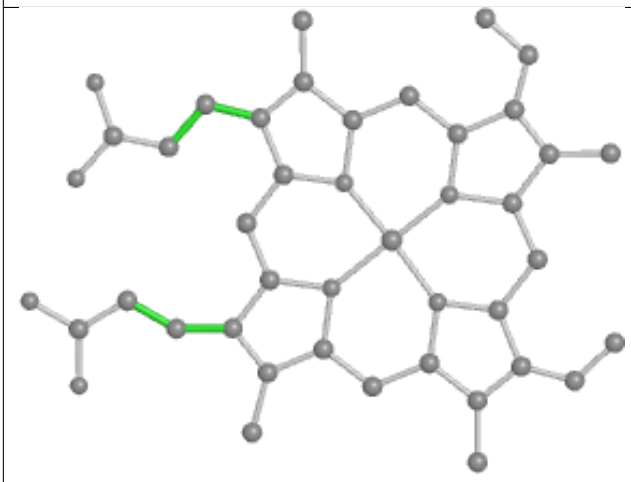


Bond angles



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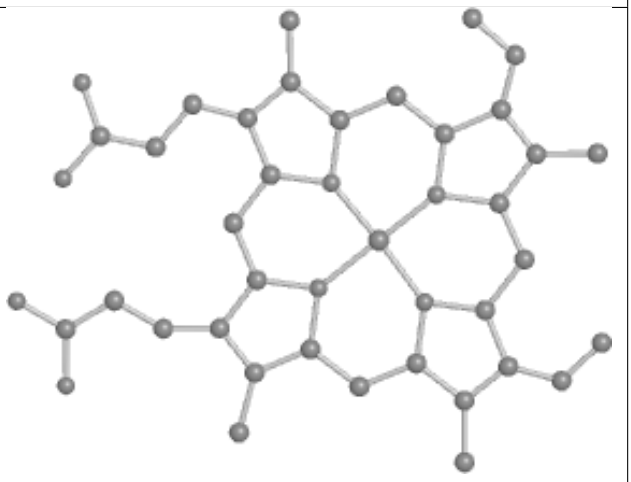
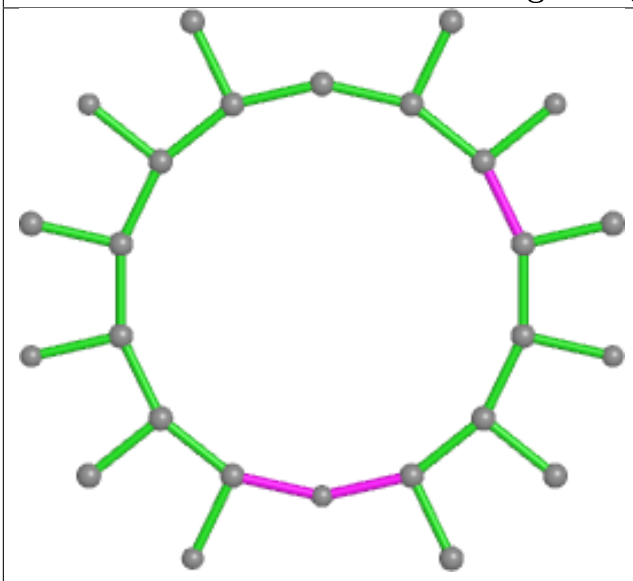


Rings

Ligand QR8 F 503



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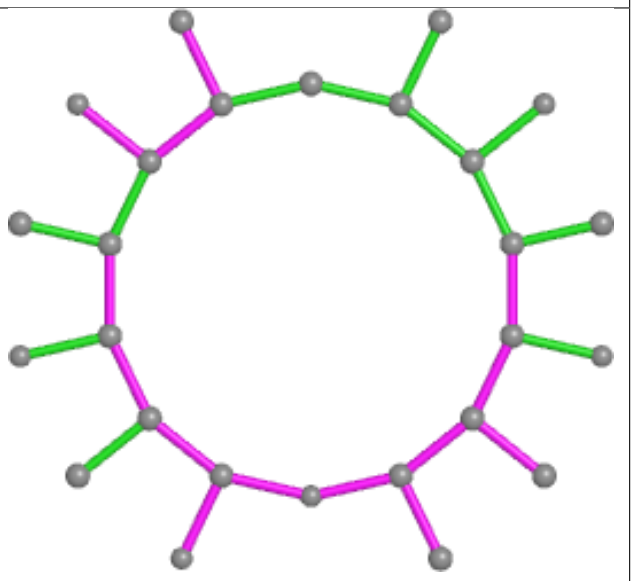
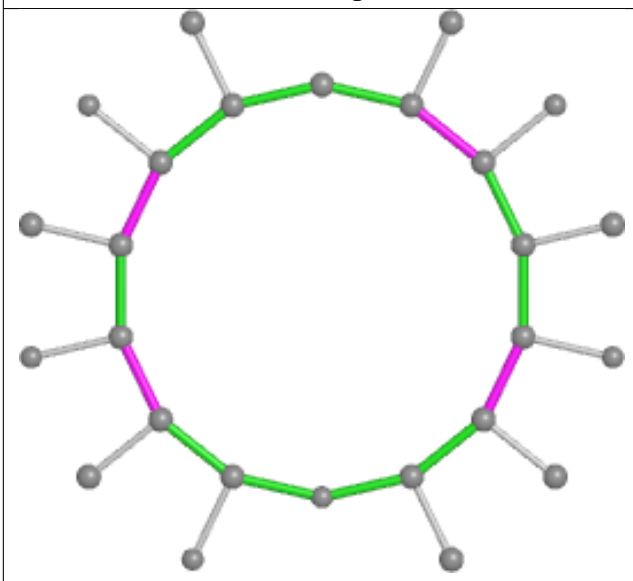


Bond angles



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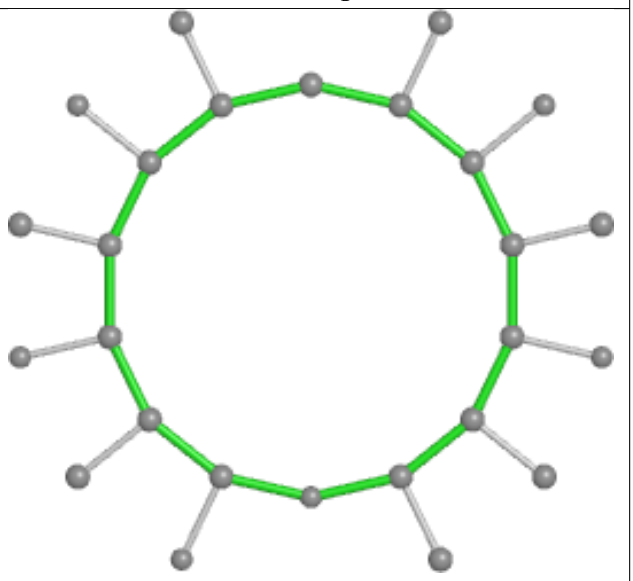
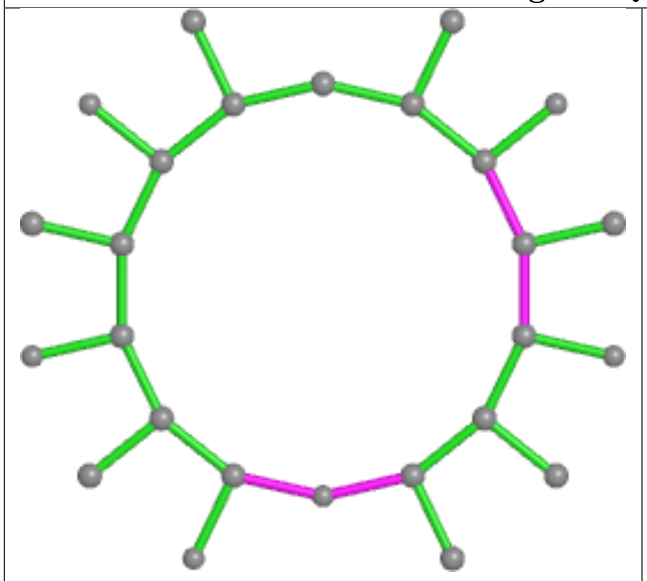
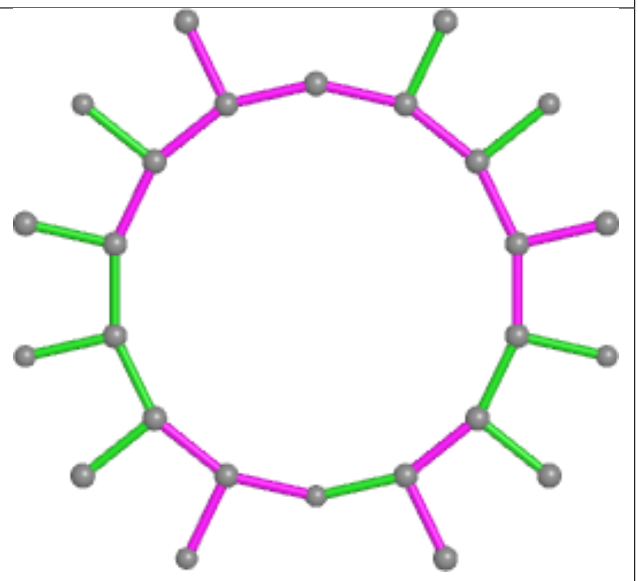


Rings

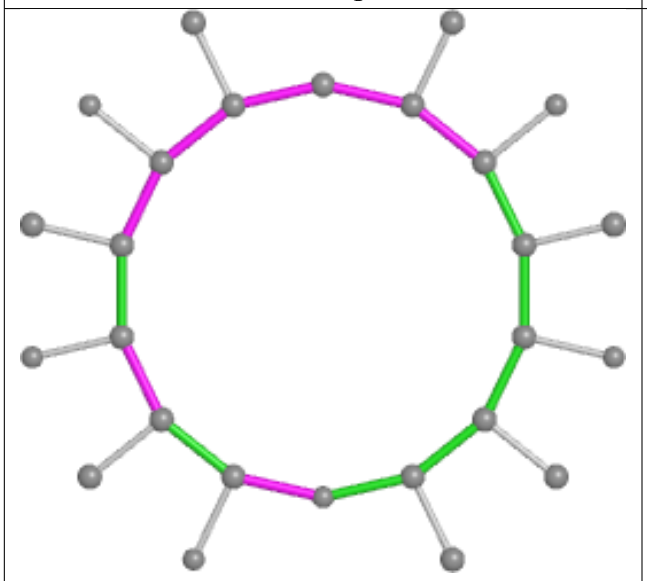
Ligand QR8 E 503



Bond lengths



Bond angles



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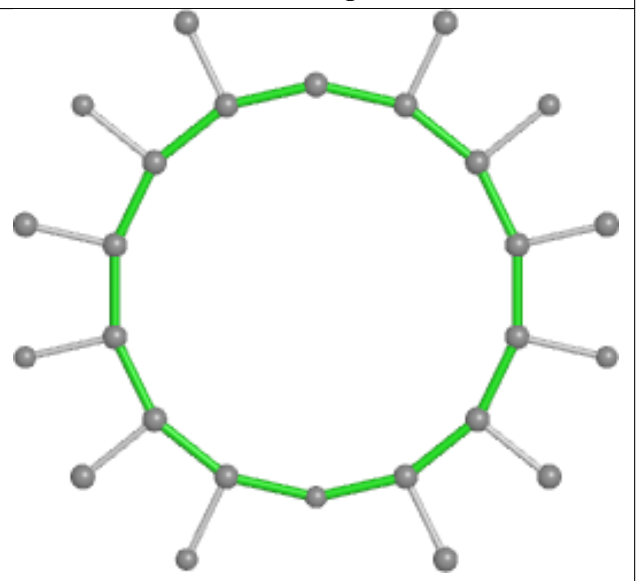

Rings

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	396/407 (97%)	-0.26	5 (1%) 77 81	31, 48, 71, 103	0
1	B	400/407 (98%)	-0.29	6 (1%) 73 78	34, 49, 74, 154	0
1	C	400/407 (98%)	-0.27	4 (1%) 82 86	29, 41, 58, 154	0
1	D	400/407 (98%)	0.07	24 (6%) 21 26	39, 60, 92, 170	0
1	E	397/407 (97%)	0.35	47 (11%) 4 6	43, 63, 94, 147	0
1	F	398/407 (97%)	0.83	80 (20%) 1 1	47, 72, 115, 146	0
All	All	2391/2442 (97%)	0.07	166 (6%) 16 21	29, 55, 97, 170	0

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	9	THR	10.0
1	E	226	ASP	8.8
1	F	405	VAL	8.7
1	F	127[A]	LEU	8.7
1	D	11	ALA	8.6

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FMT	D	530	3/3	-0.18	0.47	101,101,109,109	0
5	FMT	E	511	3/3	0.03	0.71	119,119,120,122	0
5	FMT	A	529	3/3	0.09	0.43	100,100,107,109	0
5	FMT	E	515	3/3	0.11	0.39	103,103,114,115	0
5	FMT	F	512	3/3	0.16	0.30	106,106,112,113	0
5	FMT	A	551	3/3	0.17	0.38	104,104,113,115	0
5	FMT	B	540	3/3	0.18	0.32	95,95,99,100	0
5	FMT	B	517	3/3	0.23	0.35	86,86,94,100	0
5	FMT	B	533	3/3	0.25	0.35	78,78,79,89	0
5	FMT	E	509	3/3	0.25	0.45	86,86,101,104	0
5	FMT	A	554	3/3	0.27	0.32	100,100,107,111	0
5	FMT	D	526	3/3	0.28	0.23	104,104,106,112	0
5	FMT	C	530	3/3	0.30	0.31	105,105,110,113	0
5	FMT	C	539	3/3	0.31	0.45	87,87,90,98	0
5	FMT	A	533	3/3	0.35	0.21	87,87,91,92	0
5	FMT	D	517	3/3	0.35	0.56	114,114,121,129	0
5	FMT	D	524	3/3	0.36	0.25	111,111,112,116	0
5	FMT	B	527	3/3	0.37	0.16	96,96,99,103	0
5	FMT	C	549	3/3	0.38	0.20	100,100,100,101	0
5	FMT	F	511	3/3	0.39	0.39	101,101,109,109	0
5	FMT	C	531	3/3	0.39	0.37	102,102,102,106	0
5	FMT	C	551	3/3	0.42	0.44	90,90,94,103	0
5	FMT	C	541	3/3	0.45	0.33	83,83,85,91	0
5	FMT	A	564	3/3	0.50	0.28	90,90,102,105	0
5	FMT	A	563	3/3	0.50	0.44	97,97,102,107	0
5	FMT	B	520	3/3	0.51	0.21	95,95,102,102	0
5	FMT	E	510	3/3	0.51	0.26	95,95,107,108	0
5	FMT	D	521	3/3	0.51	0.21	102,102,102,104	0
5	FMT	A	545	3/3	0.52	0.32	83,83,87,101	0
5	FMT	C	528	3/3	0.53	0.44	95,95,95,101	0
5	FMT	B	526	3/3	0.54	0.20	96,96,96,99	0
5	FMT	C	515	3/3	0.55	0.19	63,63,76,76	0
5	FMT	A	560	3/3	0.55	0.23	74,74,81,93	0
5	FMT	D	527	3/3	0.56	0.43	91,91,97,97	0
5	FMT	C	511	3/3	0.56	0.22	68,68,76,80	0
5	FMT	A	517	3/3	0.56	0.49	98,98,106,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FMT	C	526	3/3	0.57	0.20	75,75,80,83	0
5	FMT	A	574	3/3	0.58	0.43	102,102,108,111	0
5	FMT	D	519	3/3	0.59	0.38	90,90,91,96	0
5	FMT	A	537	3/3	0.59	0.35	100,100,109,109	0
5	FMT	B	511	3/3	0.60	0.20	73,73,77,78	0
5	FMT	D	525	3/3	0.60	0.32	87,87,91,92	0
5	FMT	A	552	3/3	0.60	0.25	83,83,89,92	0
5	FMT	F	510	3/3	0.61	0.31	88,88,98,100	0
5	FMT	C	540	3/3	0.61	0.31	74,74,80,83	0
5	FMT	A	542	3/3	0.62	0.21	102,102,103,104	0
4	RAM	A	503[A]	11/11	0.63	0.49	34,37,39,44	11
4	RAM	A	503[B]	11/11	0.63	0.49	37,41,44,46	11
5	FMT	A	515	3/3	0.63	0.23	80,80,82,89	0
5	FMT	A	507	3/3	0.63	0.18	69,69,73,76	0
5	FMT	E	508	3/3	0.63	0.29	86,86,89,93	0
5	FMT	C	544	3/3	0.64	0.49	68,68,73,82	0
5	FMT	E	517	3/3	0.65	0.50	95,95,99,100	0
5	FMT	C	525	3/3	0.65	0.26	90,90,91,94	0
5	FMT	B	528	3/3	0.65	0.15	85,85,86,89	0
5	FMT	A	539	3/3	0.66	0.22	101,101,110,111	0
5	FMT	C	543	3/3	0.66	0.47	82,82,87,92	0
5	FMT	B	523	3/3	0.67	0.30	86,86,87,92	0
5	FMT	B	531	3/3	0.68	0.17	98,98,102,104	0
5	FMT	A	571	3/3	0.68	0.25	94,94,108,108	0
4	RAM	B	513	11/11	0.68	0.32	50,57,63,64	11
5	FMT	B	504	3/3	0.69	0.34	69,69,74,80	0
5	FMT	A	527	3/3	0.69	0.23	88,88,93,100	0
5	FMT	C	548	3/3	0.69	0.21	85,85,91,91	0
5	FMT	C	535	3/3	0.69	0.31	89,89,112,116	0
5	FMT	C	537	3/3	0.69	0.38	97,97,109,111	0
5	FMT	A	559	3/3	0.69	0.22	90,90,91,95	0
5	FMT	B	519	3/3	0.69	0.36	100,100,101,104	0
5	FMT	A	508	3/3	0.69	0.31	74,74,76,83	0
5	FMT	C	504	3/3	0.70	0.15	48,48,52,54	0
5	FMT	B	516	3/3	0.70	0.13	100,100,103,107	0
5	FMT	C	517	3/3	0.70	0.25	70,70,71,74	0
5	FMT	B	525	3/3	0.70	0.25	98,98,105,105	0
5	FMT	A	568	3/3	0.71	0.19	85,85,90,91	0
5	FMT	D	512	3/3	0.71	0.20	85,85,88,92	0
5	FMT	C	523	3/3	0.72	0.26	69,69,75,81	0
5	FMT	D	507	3/3	0.72	0.35	85,85,90,91	0
5	FMT	B	538	3/3	0.72	0.45	82,82,83,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FMT	C	547	3/3	0.72	0.36	65,65,73,82	0
5	FMT	B	521	3/3	0.72	0.29	66,66,78,84	0
5	FMT	A	540	3/3	0.72	0.40	105,105,112,114	0
5	FMT	A	556	3/3	0.72	0.30	87,87,89,93	0
5	FMT	C	532	3/3	0.73	0.14	49,49,57,72	0
5	FMT	B	522	3/3	0.73	0.57	76,76,82,90	0
5	FMT	F	504	3/3	0.73	0.17	78,78,87,91	0
5	FMT	A	566	3/3	0.73	0.14	87,87,89,96	0
5	FMT	D	514	3/3	0.74	0.24	60,60,60,71	0
5	FMT	A	550	3/3	0.74	0.31	64,64,78,80	0
5	FMT	A	531	3/3	0.74	0.21	63,63,65,75	0
5	FMT	A	561	3/3	0.74	0.16	77,77,83,87	0
5	FMT	E	516	3/3	0.74	0.14	90,90,90,96	0
5	FMT	D	515	3/3	0.74	0.29	79,79,80,88	0
5	FMT	C	508	3/3	0.75	0.23	81,81,87,90	0
5	FMT	A	547	3/3	0.75	0.19	70,70,73,77	0
5	FMT	C	545	3/3	0.75	0.50	78,78,80,86	0
5	FMT	A	565	3/3	0.75	0.19	66,66,82,85	0
5	FMT	B	518	3/3	0.75	0.19	89,89,104,105	0
5	FMT	F	509	3/3	0.75	0.17	66,66,67,74	0
5	FMT	A	546	3/3	0.76	0.43	64,64,73,83	0
5	FMT	A	558	3/3	0.76	0.22	83,83,84,92	0
5	FMT	B	514	3/3	0.76	0.22	75,75,80,87	0
5	FMT	D	535	3/3	0.76	0.33	96,96,104,104	0
5	FMT	A	544	3/3	0.76	0.23	67,67,77,81	0
5	FMT	A	509	3/3	0.77	0.15	61,61,64,71	0
5	FMT	A	528	3/3	0.77	0.21	84,84,84,93	0
5	FMT	D	518	3/3	0.78	0.15	84,84,96,100	0
5	FMT	B	524	3/3	0.78	0.32	68,68,74,78	0
5	FMT	A	523	3/3	0.78	0.19	67,67,70,77	0
5	FMT	D	531	3/3	0.78	0.39	59,59,65,71	0
5	FMT	B	539	3/3	0.78	0.42	85,85,89,91	0
5	FMT	D	506	3/3	0.78	0.26	68,68,81,84	0
5	FMT	D	536	3/3	0.78	0.51	111,111,113,115	0
5	FMT	C	536	3/3	0.78	0.31	98,98,99,104	0
5	FMT	A	520	3/3	0.79	0.21	84,84,87,90	0
5	FMT	B	532	3/3	0.79	0.18	96,96,99,102	0
5	FMT	D	522	3/3	0.80	0.14	97,97,106,113	0
4	RAM	D	503	11/11	0.80	0.38	58,66,68,68	11
5	FMT	A	549	3/3	0.80	0.49	71,71,87,90	0
5	FMT	B	537	3/3	0.80	0.12	82,82,94,96	0
5	FMT	C	509	3/3	0.80	0.18	60,60,67,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FMT	F	513	3/3	0.81	0.28	75,75,79,82	0
5	FMT	D	505	3/3	0.81	0.20	69,69,69,73	0
5	FMT	C	510	3/3	0.81	0.15	83,83,84,91	0
5	FMT	B	535	3/3	0.81	0.25	88,88,89,94	0
5	FMT	A	553	3/3	0.81	0.22	86,86,94,95	0
5	FMT	F	515	3/3	0.81	0.13	101,101,103,108	0
5	FMT	A	572	3/3	0.81	0.51	91,91,97,98	0
5	FMT	A	548	3/3	0.81	0.18	64,64,65,76	0
5	FMT	A	510	3/3	0.81	0.15	75,75,84,85	0
5	FMT	E	514	3/3	0.81	0.38	86,86,94,97	0
5	FMT	D	523	3/3	0.81	0.26	85,85,94,95	0
5	FMT	B	529	3/3	0.81	0.16	71,71,71,79	0
5	FMT	A	513	3/3	0.81	0.17	75,75,81,88	0
5	FMT	D	534	3/3	0.82	0.40	91,91,91,93	0
5	FMT	E	501	3/3	0.82	0.15	76,76,78,79	0
5	FMT	D	520	3/3	0.82	0.14	96,96,100,108	0
5	FMT	A	538	3/3	0.82	0.16	63,63,75,85	0
5	FMT	A	562	3/3	0.82	0.29	55,55,70,72	0
5	FMT	A	524	3/3	0.82	0.30	60,60,68,74	0
5	FMT	C	546	3/3	0.82	0.17	87,87,88,91	0
5	FMT	A	567	3/3	0.82	0.21	85,85,85,85	0
5	FMT	D	529	3/3	0.82	0.17	76,76,79,82	0
5	FMT	E	512	3/3	0.83	0.16	80,80,81,86	0
5	FMT	C	534	3/3	0.83	0.19	88,88,90,92	0
5	FMT	A	516	3/3	0.83	0.27	77,77,81,85	0
5	FMT	C	506	3/3	0.83	0.33	62,62,69,73	0
5	FMT	C	512	3/3	0.83	0.17	59,59,73,74	0
5	FMT	D	533	3/3	0.84	0.35	70,70,70,73	0
5	FMT	A	543	3/3	0.84	0.14	54,54,69,69	0
5	FMT	C	529	3/3	0.84	0.18	84,84,88,92	0
5	FMT	F	514	3/3	0.84	0.25	56,56,70,72	0
5	FMT	A	530	3/3	0.84	0.20	55,55,75,77	0
5	FMT	C	507	3/3	0.85	0.15	60,60,65,68	0
5	FMT	C	518	3/3	0.85	0.26	65,65,72,77	0
5	FMT	C	516	3/3	0.85	0.09	81,81,86,87	0
5	FMT	C	505	3/3	0.85	0.24	57,57,64,68	0
5	FMT	A	522	3/3	0.85	0.26	74,74,80,83	0
5	FMT	A	512	3/3	0.85	0.13	98,98,103,109	0
5	FMT	D	516	3/3	0.86	0.23	90,90,91,91	0
5	FMT	E	513	3/3	0.86	0.20	74,74,74,75	0
5	FMT	B	512	3/3	0.86	0.13	68,68,72,74	0
5	FMT	A	534	3/3	0.86	0.19	60,60,72,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FMT	C	552	3/3	0.86	0.16	72,72,74,79	0
5	FMT	F	501	3/3	0.86	0.15	85,85,86,88	0
5	FMT	D	509	3/3	0.87	0.29	66,66,76,76	0
5	FMT	A	541	3/3	0.87	0.11	92,92,93,96	0
5	FMT	A	532	3/3	0.87	0.68	76,76,77,85	0
5	FMT	C	550	3/3	0.87	0.10	57,57,67,70	0
5	FMT	B	509	3/3	0.87	0.20	60,60,62,64	0
5	FMT	E	506	3/3	0.87	0.24	70,70,72,74	0
5	FMT	C	542	3/3	0.88	0.54	91,91,115,119	0
5	FMT	A	557	3/3	0.88	0.19	87,87,90,91	0
5	FMT	E	504	3/3	0.88	0.14	63,63,63,74	0
5	FMT	C	521	3/3	0.88	0.18	59,59,70,87	0
3	QR8	E	503	26/26	0.88	0.17	46,53,56,57	0
5	FMT	C	522	3/3	0.88	0.22	54,54,62,62	0
5	FMT	A	518	3/3	0.88	0.22	58,58,66,71	0
5	FMT	A	555	3/3	0.88	0.24	61,61,65,71	0
5	FMT	A	521	3/3	0.88	0.20	49,49,63,67	0
5	FMT	F	505	3/3	0.88	0.15	79,79,84,85	0
5	FMT	C	520	3/3	0.89	0.18	55,55,66,70	0
5	FMT	A	569	3/3	0.89	0.24	94,94,95,95	0
5	FMT	B	506	3/3	0.89	0.14	63,63,69,71	0
6	NA	E	507	1/1	0.89	0.34	81,81,81,81	0
5	FMT	D	504	3/3	0.89	0.21	67,67,71,76	0
5	FMT	B	507	3/3	0.89	0.12	75,75,84,84	0
5	FMT	A	536	3/3	0.89	0.11	71,71,71,77	0
5	FMT	A	570	3/3	0.89	0.18	92,92,98,98	0
5	FMT	A	511	3/3	0.89	0.11	61,61,66,66	0
5	FMT	D	511	3/3	0.90	0.25	68,68,73,74	0
5	FMT	C	519	3/3	0.90	0.10	69,69,76,84	0
5	FMT	A	506	3/3	0.90	0.31	66,66,73,77	0
5	FMT	A	535	3/3	0.90	0.19	89,89,103,109	0
5	FMT	B	508	3/3	0.90	0.09	73,73,79,83	0
3	QR8	F	503	26/26	0.91	0.12	55,62,66,75	0
5	FMT	F	506	3/3	0.91	0.10	74,74,75,76	0
5	FMT	E	505	3/3	0.91	0.12	72,72,79,81	0
5	FMT	A	505	3/3	0.91	0.10	59,59,68,71	0
5	FMT	D	528	3/3	0.91	0.59	79,79,80,81	0
2	HEM	F	502	43/43	0.91	0.15	53,64,75,93	0
5	FMT	B	510	3/3	0.91	0.16	86,86,91,92	0
5	FMT	C	533	3/3	0.91	0.13	68,68,69,76	0
5	FMT	C	503	3/3	0.92	0.11	48,48,55,60	0
5	FMT	B	536	3/3	0.92	0.09	69,69,76,81	0

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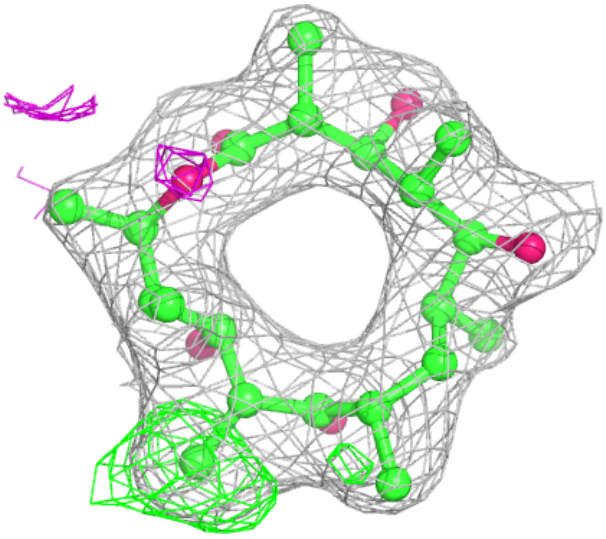
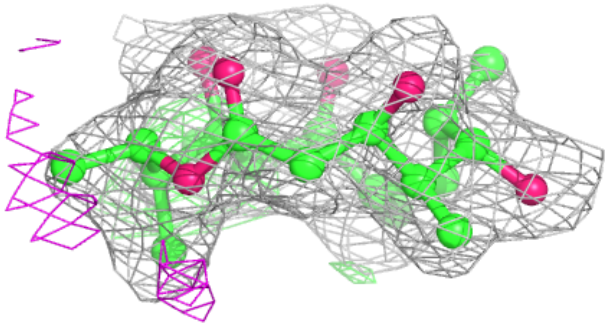
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FMT	A	525	3/3	0.92	0.34	76,76,82,83	0
5	FMT	D	537	3/3	0.92	0.21	48,48,60,65	0
6	NA	F	508	1/1	0.92	0.16	59,59,59,59	0
5	FMT	A	519	3/3	0.92	0.21	74,74,75,76	0
5	FMT	A	573	3/3	0.92	0.13	67,67,85,97	0
5	FMT	D	508	3/3	0.93	0.11	57,57,59,59	0
5	FMT	A	514	3/3	0.93	0.17	46,46,48,51	0
5	FMT	A	504	3/3	0.93	0.10	52,52,56,57	0
3	QR8	A	502	26/26	0.93	0.17	33,38,42,43	0
5	FMT	B	505	3/3	0.93	0.08	62,62,65,69	0
3	QR8	D	502	26/26	0.94	0.16	43,48,51,58	0
5	FMT	B	503	3/3	0.94	0.07	53,53,58,63	0
6	NA	D	513	1/1	0.94	0.14	54,54,54,54	0
3	QR8	C	502	26/26	0.94	0.15	30,35,37,42	0
5	FMT	B	530	3/3	0.94	0.16	71,71,80,93	0
6	NA	B	515	1/1	0.95	0.17	57,57,57,57	0
5	FMT	C	513	3/3	0.95	0.19	54,54,62,63	0
5	FMT	D	532	3/3	0.95	0.18	79,79,80,84	0
3	QR8	B	502	26/26	0.95	0.17	35,41,45,48	0
5	FMT	B	534	3/3	0.95	0.14	70,70,72,74	0
6	NA	A	526	1/1	0.95	0.15	41,41,41,41	0
2	HEM	E	502	43/43	0.95	0.12	42,48,54,58	0
5	FMT	F	507	3/3	0.96	0.10	66,66,69,72	0
5	FMT	C	538	3/3	0.96	0.25	58,58,61,64	0
5	FMT	C	514	3/3	0.96	0.12	53,53,56,64	0
2	HEM	A	501	43/43	0.97	0.14	29,32,39,41	0
2	HEM	B	501	43/43	0.97	0.14	32,36,39,47	0
2	HEM	D	501	43/43	0.97	0.13	36,40,46,49	0
5	FMT	C	524	3/3	0.97	0.12	48,48,49,52	0
5	FMT	D	510	3/3	0.97	0.14	70,70,70,72	0
6	NA	C	527	1/1	0.98	0.15	42,42,42,42	0
2	HEM	C	501	43/43	0.98	0.15	27,30,37,38	0

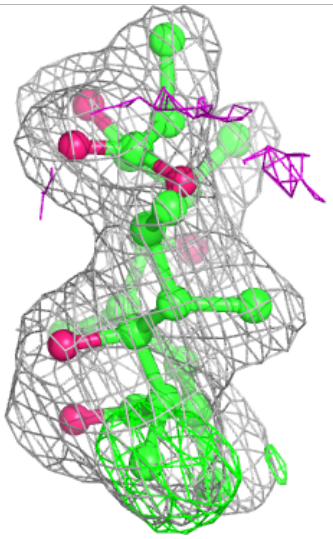
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QR8 E 503:

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

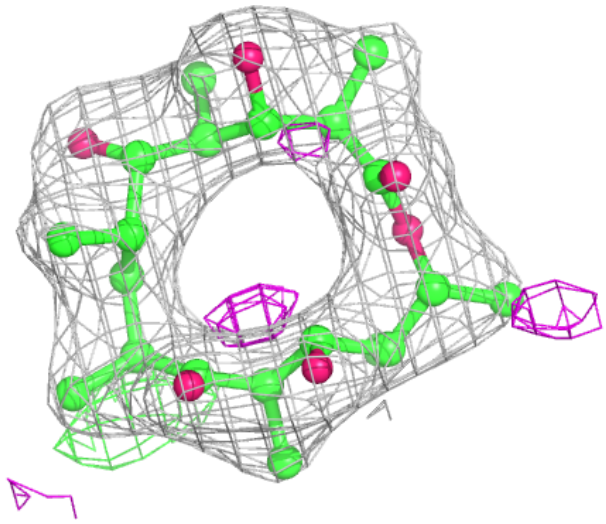


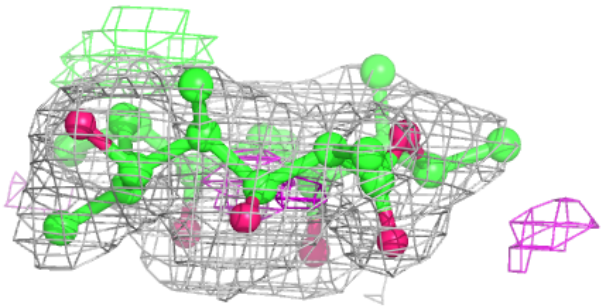


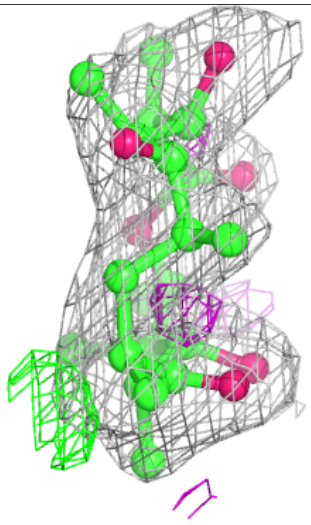


Electron density around QR8 F 503:

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

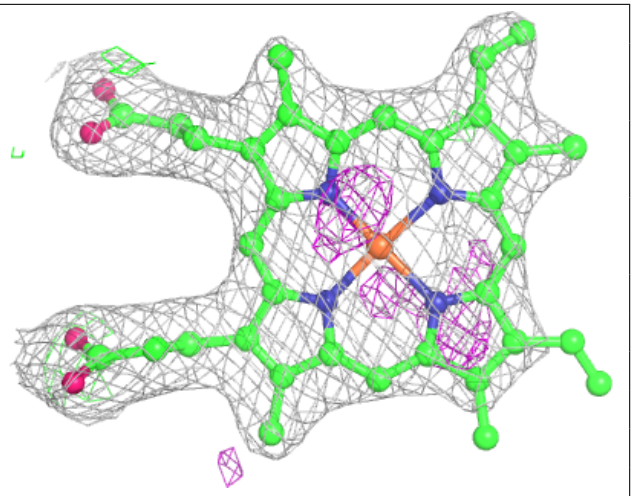


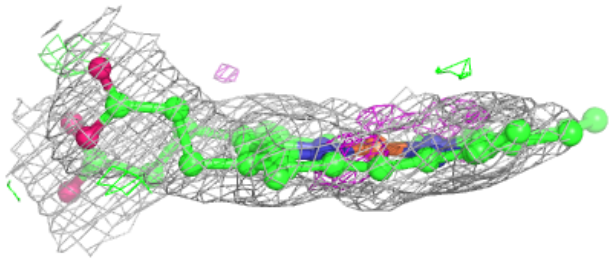


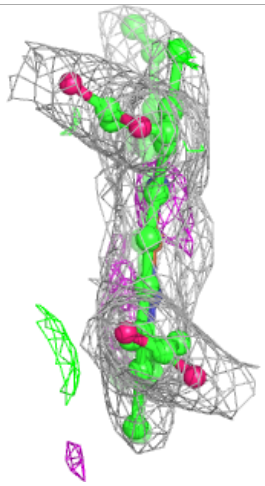


Electron density around HEM F 502:

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

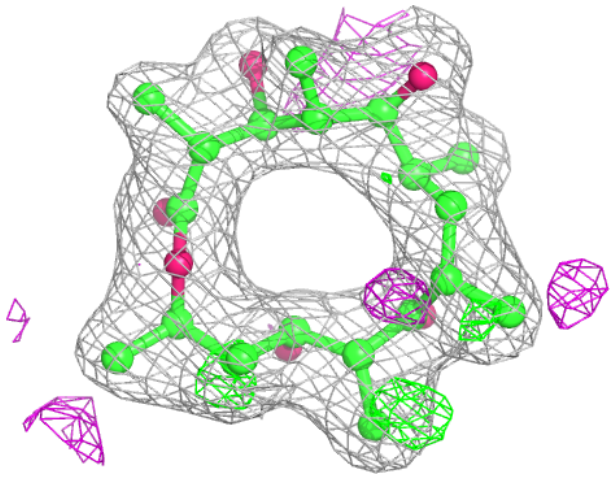


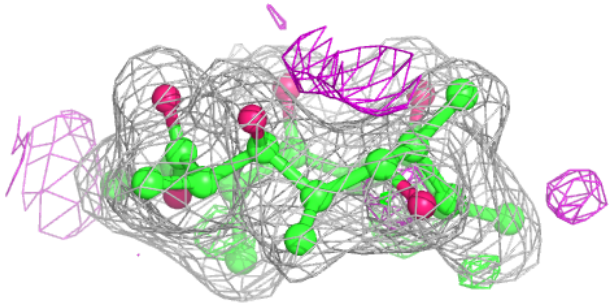


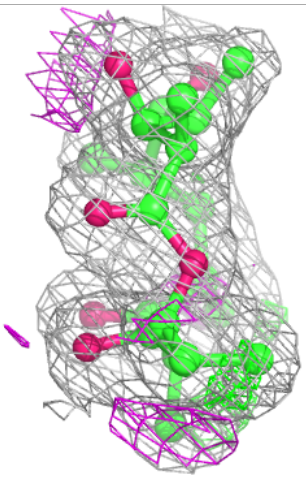


Electron density around QR8 A 502:

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

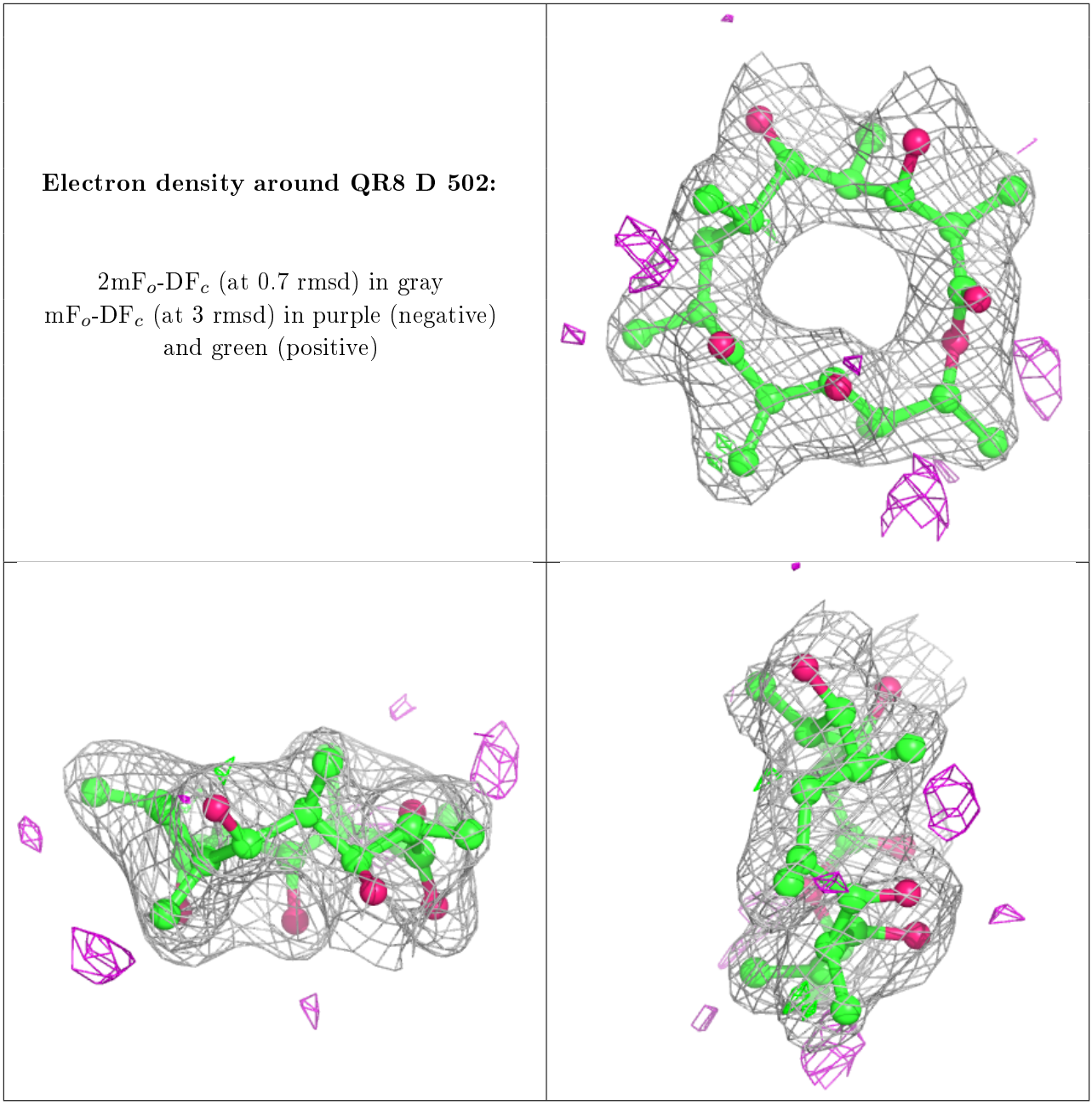






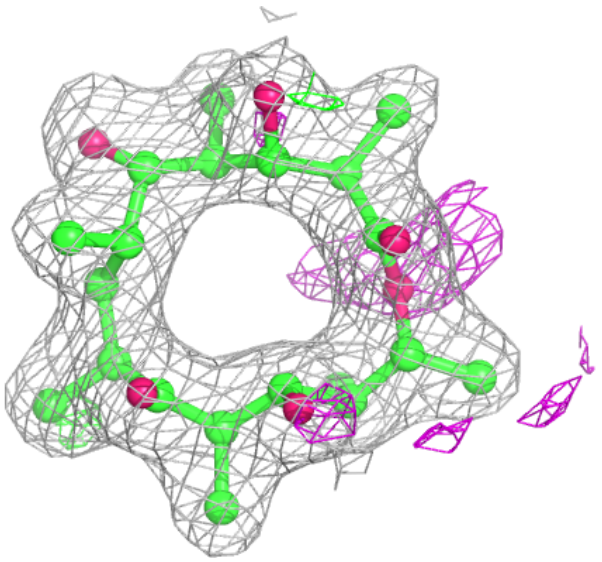
Electron density around QR8 D 502:

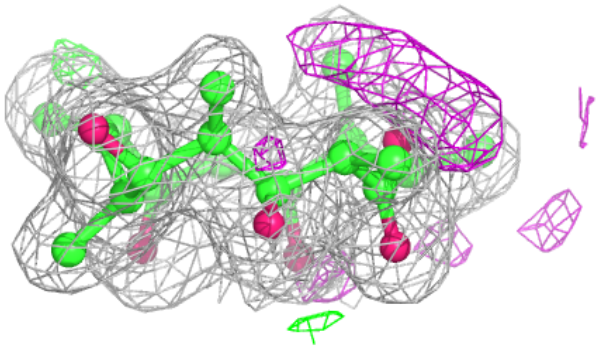
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around QR8 C 502:

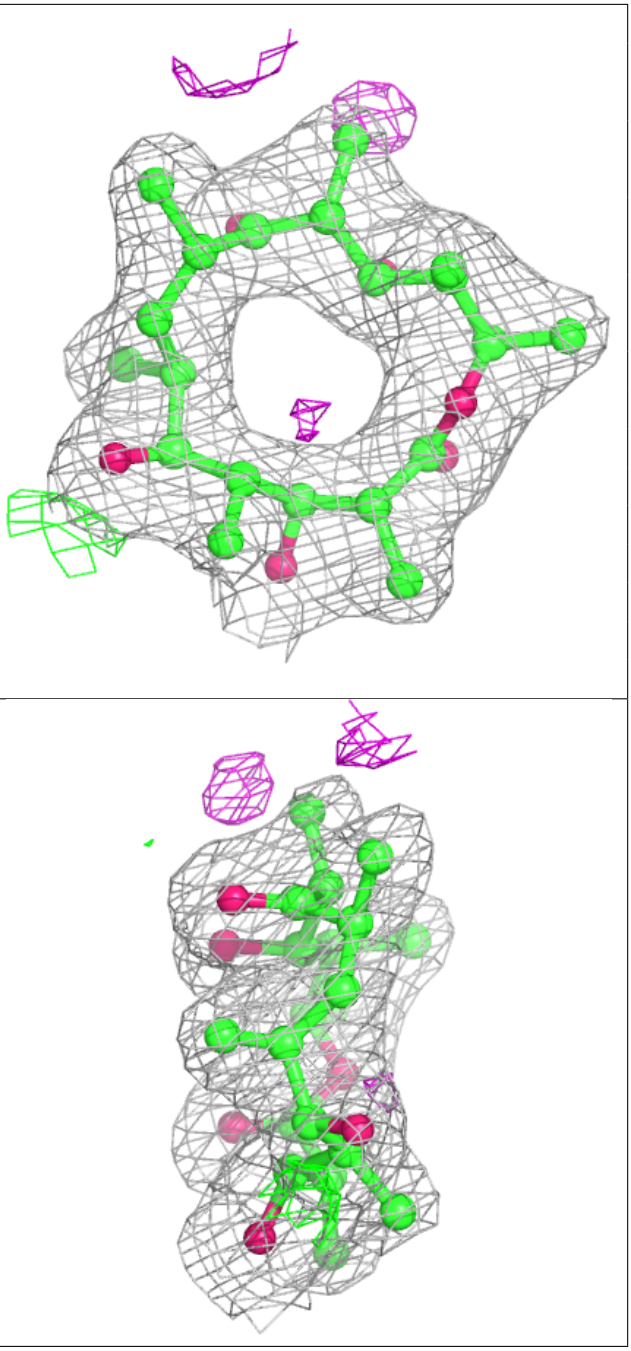
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





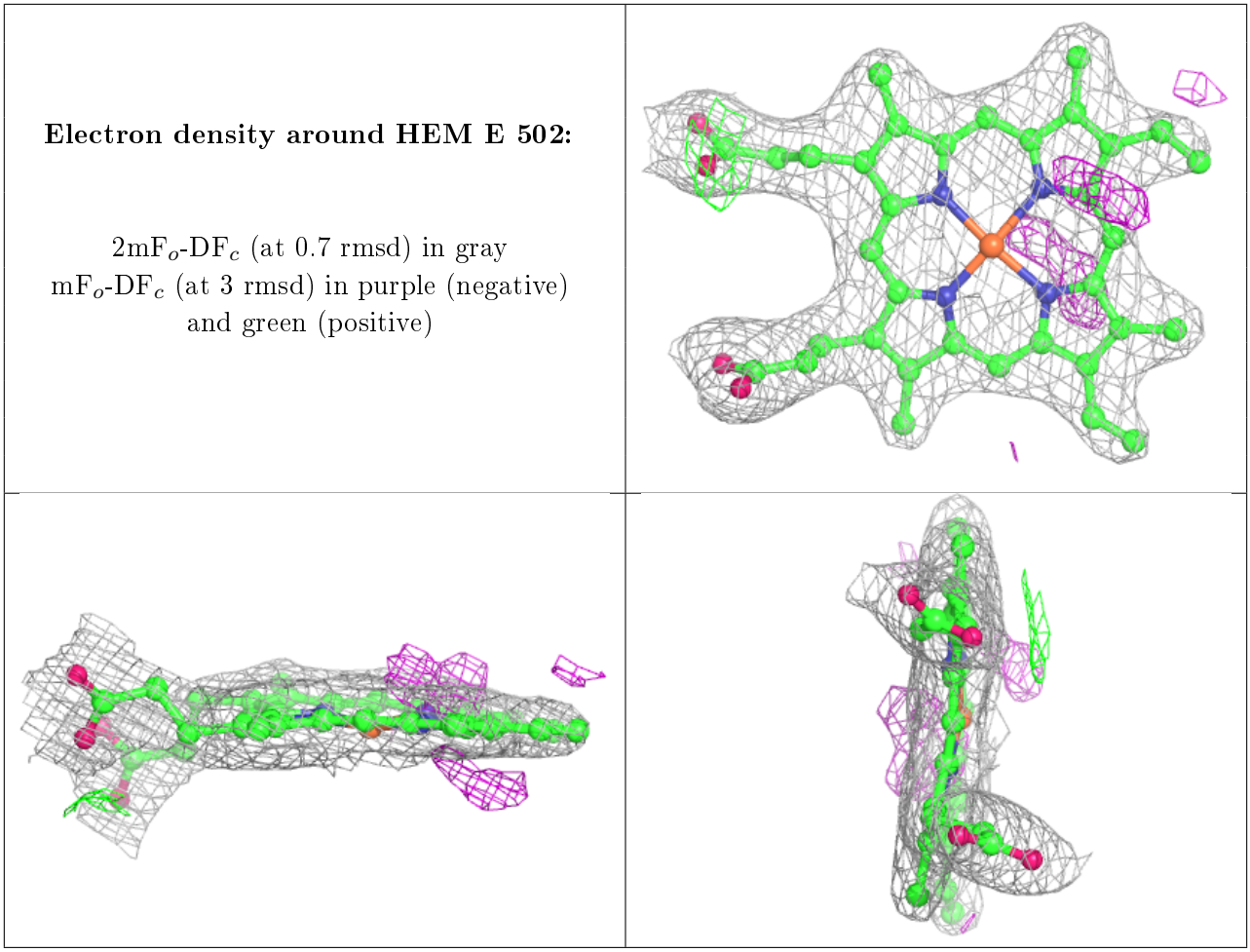
Electron density around QR8 B 502:

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



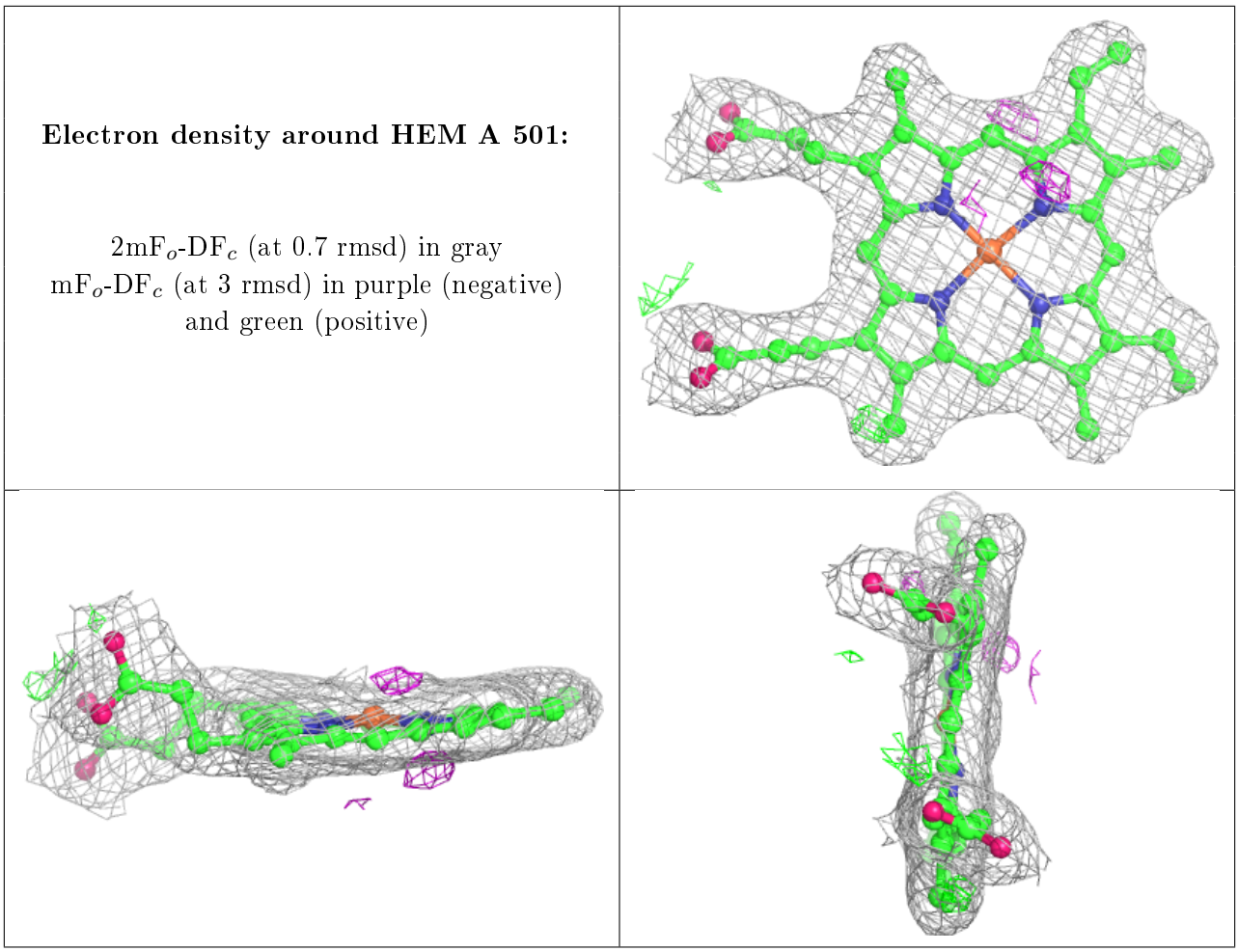
Electron density around HEM E 502:

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



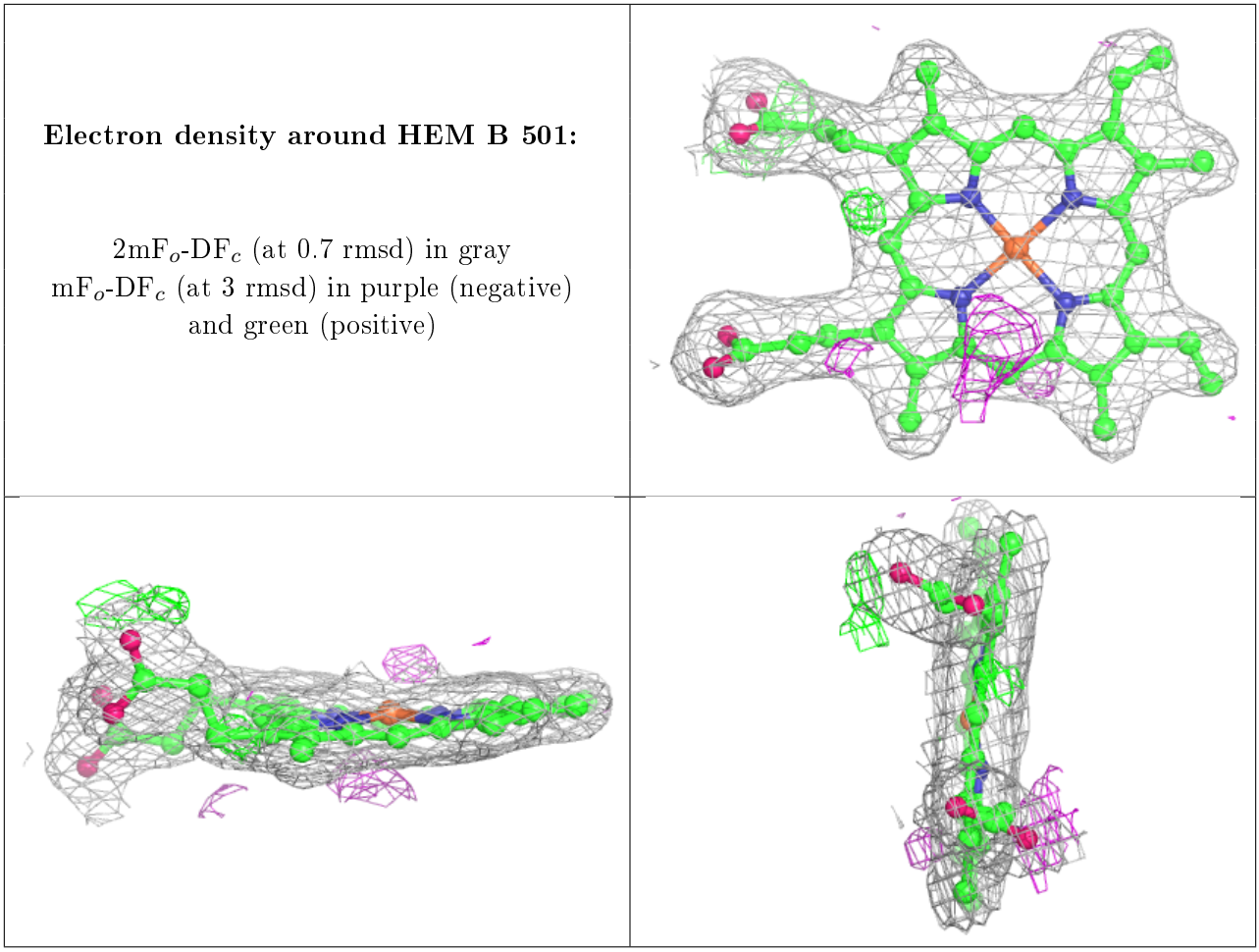
Electron density around HEM A 501:

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



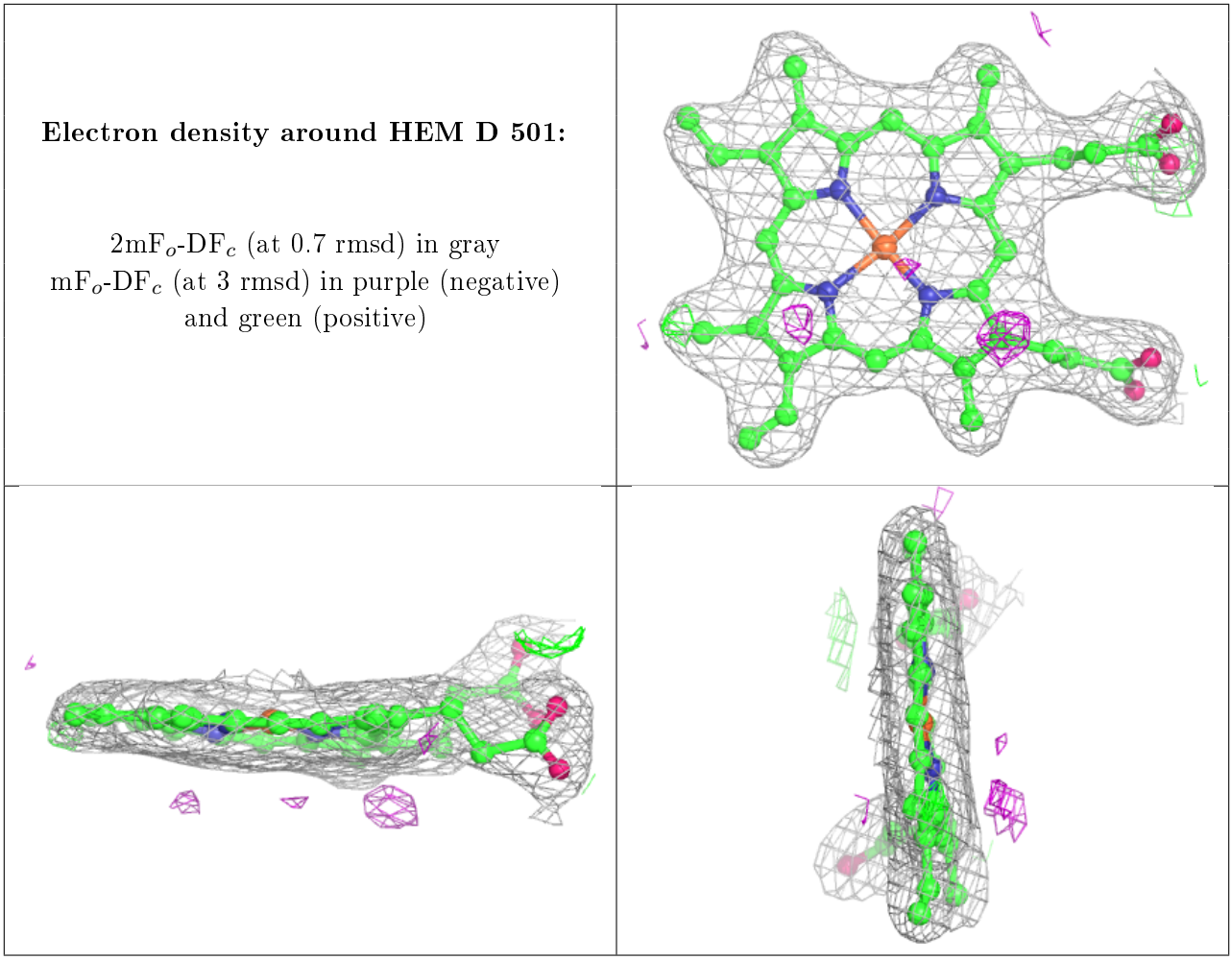
Electron density around HEM B 501:

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



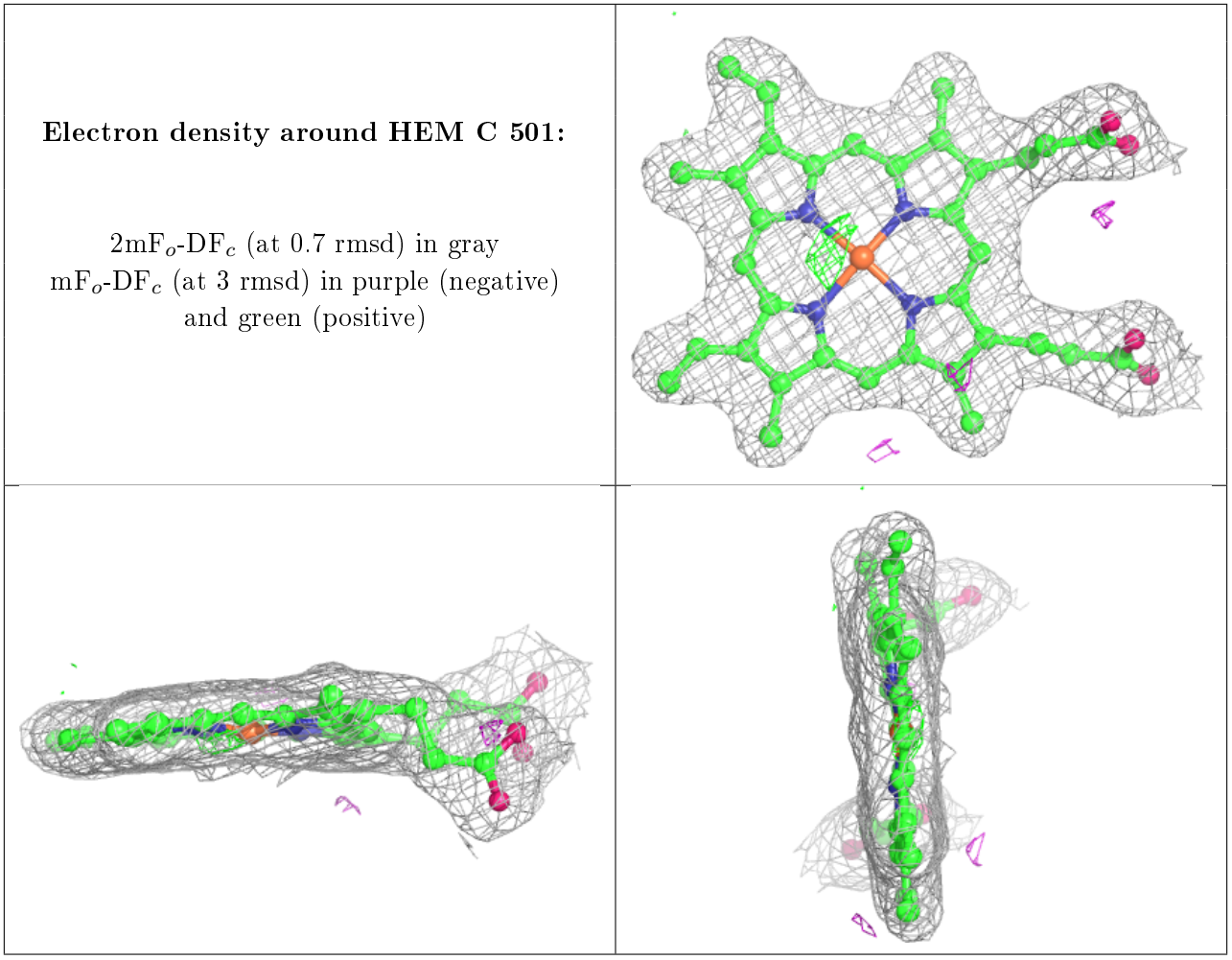
Electron density around HEM D 501:

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



Electron density around HEM C 501:

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



6.5 Other polymers

There are no such residues in this entry.