Full wwPDB X-ray Structure Validation Report ⓘ

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 Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

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

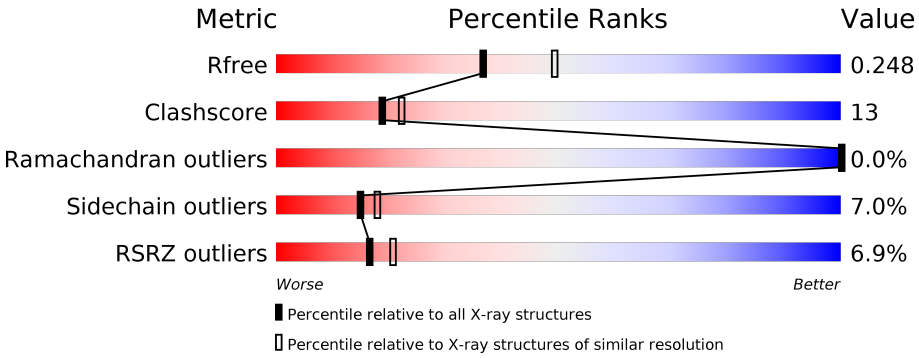
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

Continued on next page...

Continued from previous page...

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

2 Entry composition

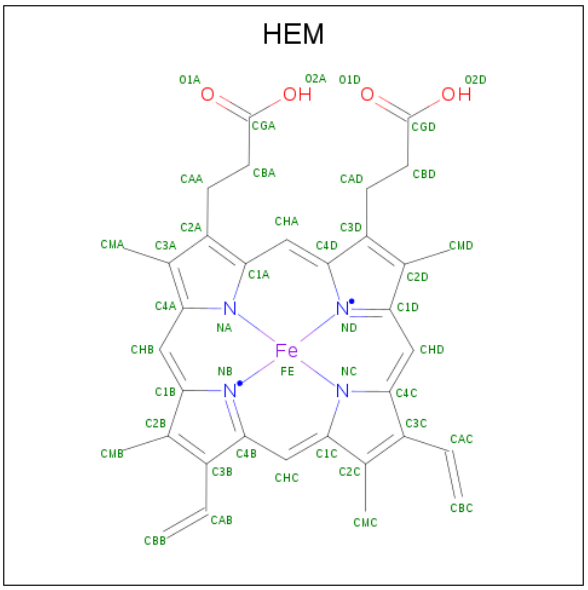
There are 7 unique types of molecules in this entry. The entry contains 22307 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

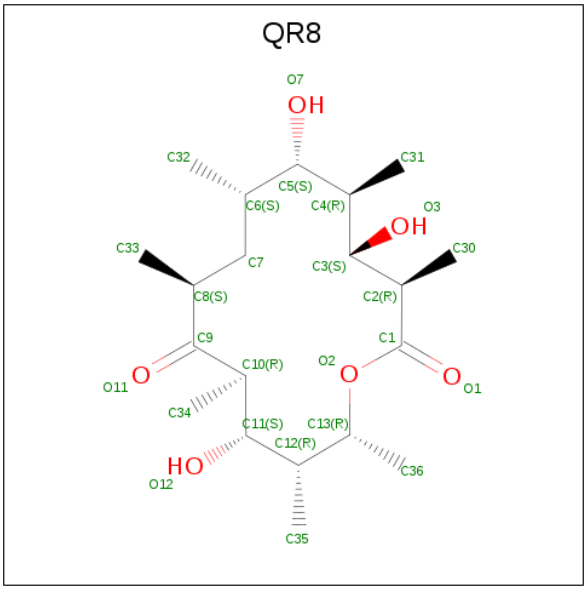
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	36	0
			3303	2099	587	599	18			
1	B	400	Total	C	N	O	S	0	22	0
			3249	2052	574	606	17			
1	C	400	Total	C	N	O	S	0	22	0
			3248	2053	577	603	15			
1	D	400	Total	C	N	O	S	0	42	0
			3372	2142	603	612	15			
1	E	397	Total	C	N	O	S	0	36	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).



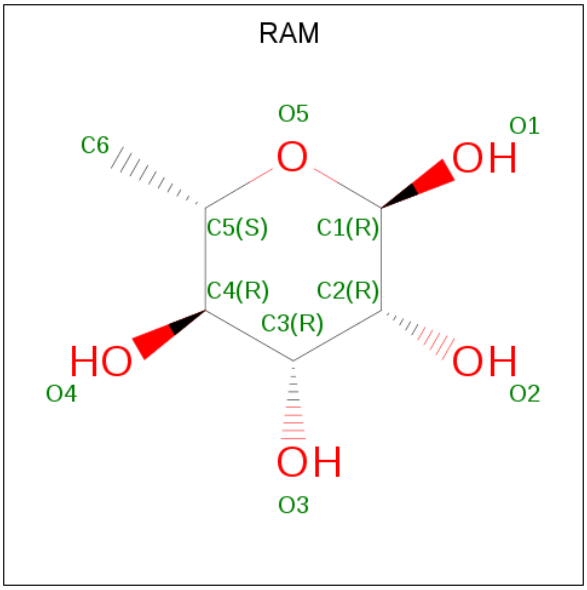
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			26	20	6		
3	B	1	Total	C	O	0	0
			26	20	6		
3	C	1	Total	C	O	0	0
			26	20	6		
3	D	1	Total	C	O	0	0
			26	20	6		
3	E	1	Total	C	O	0	0
			26	20	6		

Continued on next page...

Continued from previous page...

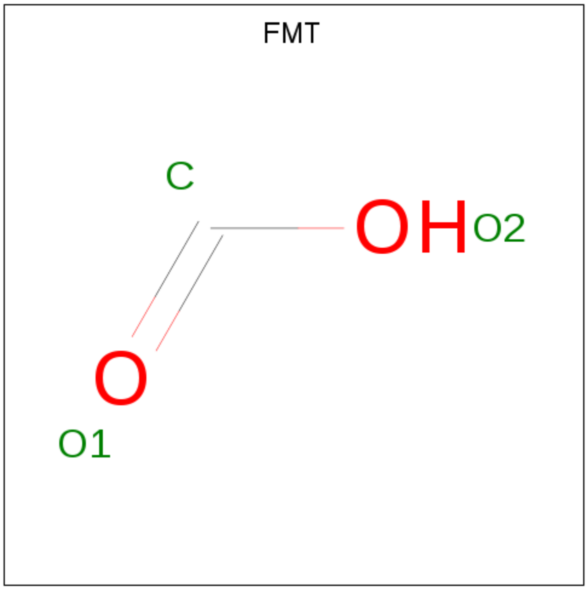
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 26 20 6	0	0

- 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
5	C	1	Total C O 3 1 2	0	0

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	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	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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.

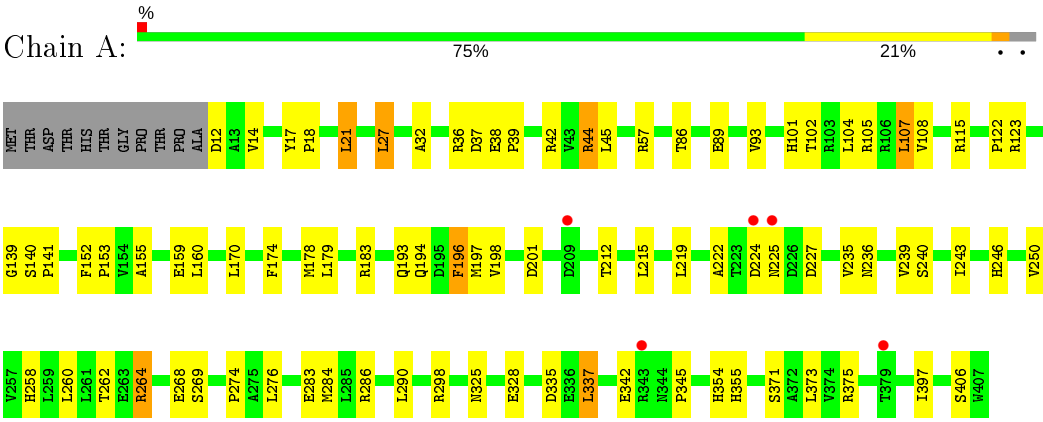
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	260	Total O 260 260	0	1
7	B	281	Total O 281 281	0	3
7	C	384	Total O 384 384	0	3
7	D	158	Total O 158 158	0	2
7	E	137	Total O 137 137	0	4
7	F	135	Total O 135 135	0	2

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.

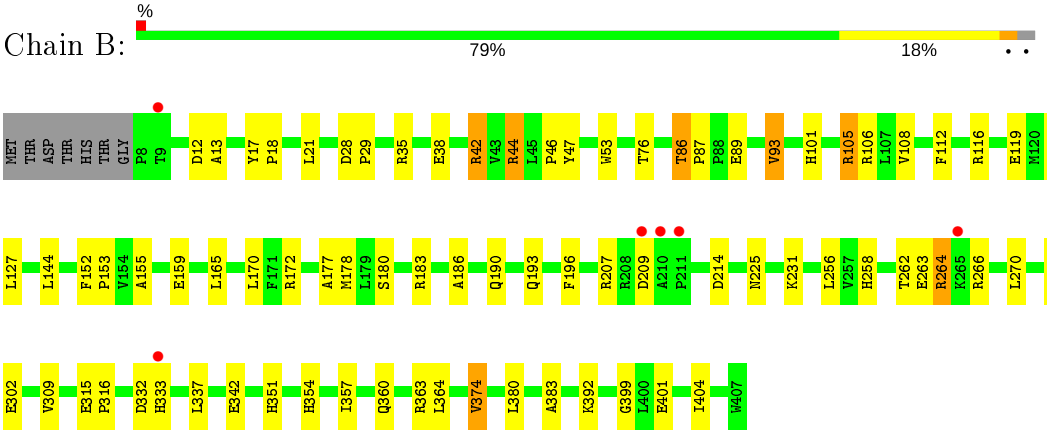
- Molecule 1: Cytochrome P-450

Chain A:



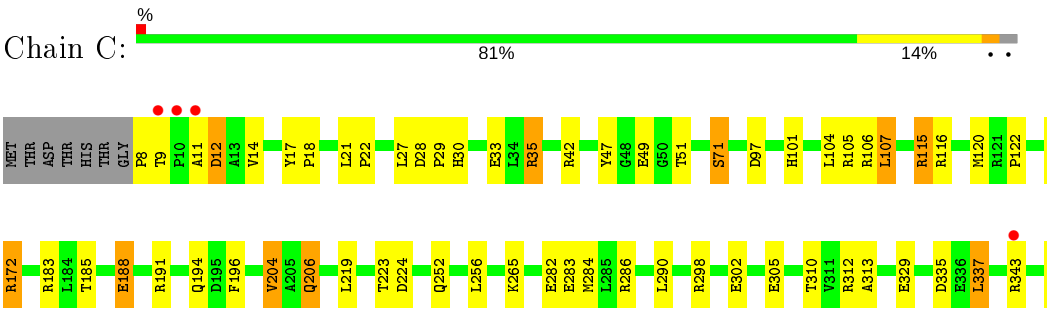
- Molecule 1: Cytochrome P-450

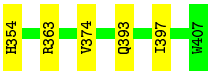
Chain B:



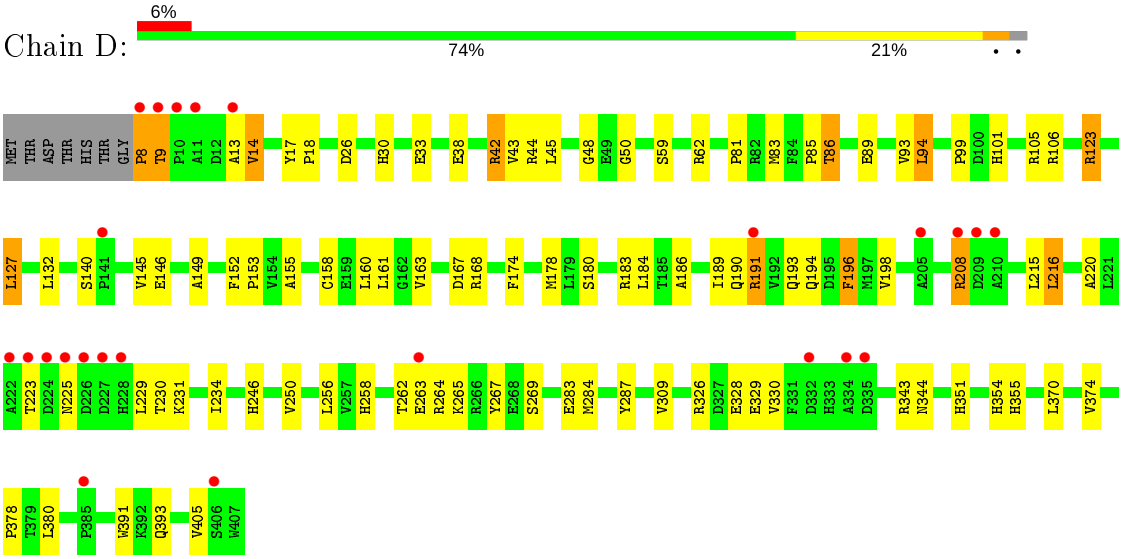
- Molecule 1: Cytochrome P-450

Chain C:

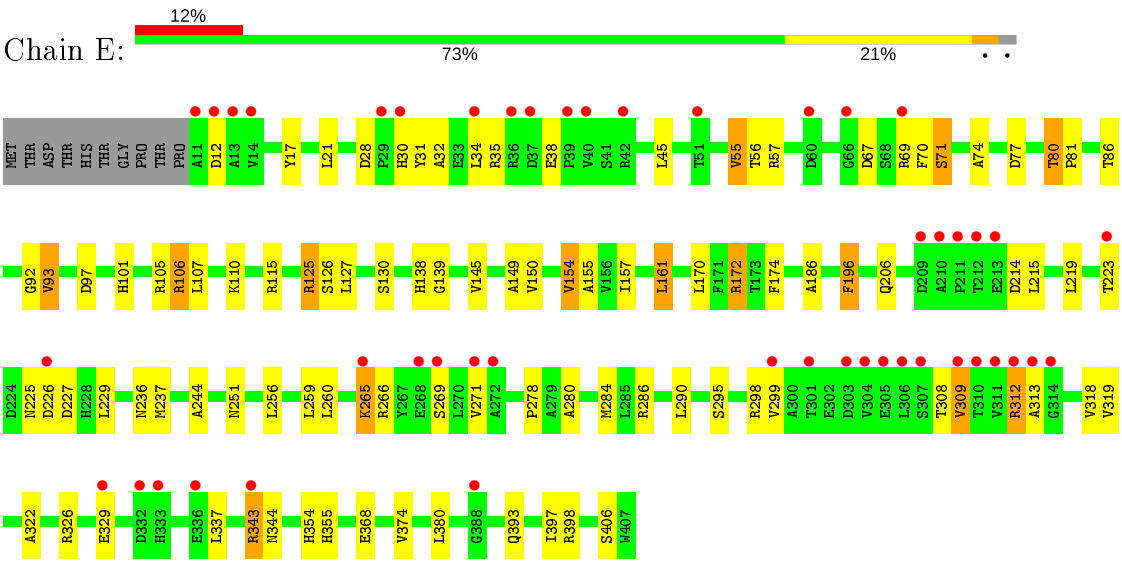




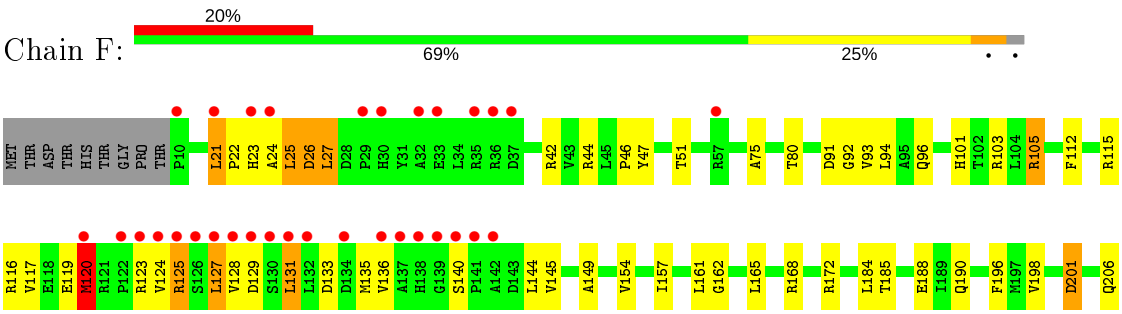
• Molecule 1: Cytochrome P-450

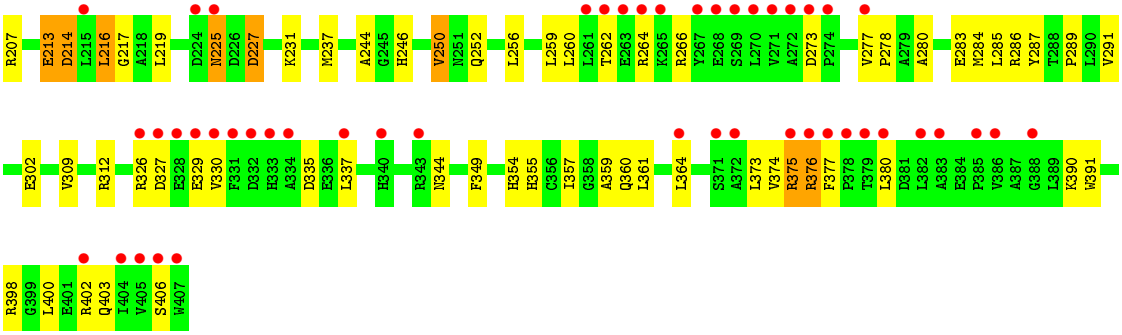


• Molecule 1: Cytochrome P-450



• Molecule 1: Cytochrome P-450




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

All (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
1	C	188	GLU	CD-OE2	5.18	1.31	1.25

All (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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	120[B]	MET	N-CA-CB	-14.58	84.36	110.60
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
1	F	26[A]	ASP	CB-CA-C	-8.36	93.68	110.40
1	F	26[B]	ASP	CB-CA-C	-8.36	93.68	110.40
1	A	105	ARG	NE-CZ-NH2	-8.25	116.18	120.30
1	C	363	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	B	363	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	F	25	LEU	C-N-CA	-7.37	103.27	121.70
1	F	120[A]	MET	N-CA-C	7.28	130.65	111.00
1	F	120[B]	MET	N-CA-C	7.28	130.65	111.00
1	C	35	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	E	214	ASP	CB-CA-C	-7.00	96.39	110.40
1	B	363	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	F	119	GLU	C-N-CA	-6.47	105.52	121.70
1	D	106	ARG	CB-CA-C	6.46	123.33	110.40
1	C	172	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	F	26[A]	ASP	N-CA-CB	-6.28	99.29	110.60
1	F	26[B]	ASP	N-CA-CB	-6.28	99.29	110.60
1	F	105	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	93	VAL	CB-CA-C	-6.00	100.00	111.40
1	A	375	ARG	CG-CD-NE	-5.84	99.54	111.80
1	C	105	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	C	298	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	D	8	PRO	N-CA-CB	5.64	110.07	103.30
1	C	286	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	363	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	C	47	TYR	CB-CG-CD1	5.50	124.30	121.00
1	B	183	ARG	CB-CA-C	-5.42	99.55	110.40
1	B	105	ARG	CB-CG-CD	-5.40	97.56	111.60
1	B	302	GLU	CB-CA-C	-5.32	99.75	110.40
1	B	44	ARG	NE-CZ-NH2	5.31	122.96	120.30
1	A	375	ARG	NE-CZ-NH1	-5.23	117.68	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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
7:A:715:HOH:O	1:D:13:ALA:HB3	1.41	1.16
1:B:89:GLU:HB3	4:B:513:RAM:H2	1.25	1.11
1:A:197[A]:MET:HE1	1:A:235[A]:VAL:CG2	1.82	1.09
1:D:89:GLU:HB2	4:D:503:RAM:H62	1.30	1.08
1:E:343[A]:ARG:HG2	1:E:343[A]:ARG:HH11	0.95	1.08
1:F:120[A]:MET:HE2	1:F:361[A]:LEU:HD21	1.17	1.08
1:F:185[A]:THR:OG1	7:F:601[A]:HOH:O	1.72	1.06
1:C:30[A]:HIS:ND1	1:C:33[A]:GLU:OE2	1.90	1.04
1:D:208[A]:ARG:HH11	1:D:208[A]:ARG:CB	1.72	1.03
1:A:197[A]:MET:HE2	1:A:235[A]:VAL:CG2	1.87	1.03
1:E:93[A]:VAL:HG11	1:E:237[A]:MET:HE1	1.05	1.02
1:A:193:GLN:HE21	4:A:503[A]:RAM:H1	1.23	1.00
1:B:42[B]:ARG:HG2	1:B:42[B]:ARG:HH21	1.23	0.99
1:E:343[A]:ARG:HG2	1:E:343[A]:ARG:NH1	1.74	0.98
1:F:120[A]:MET:HE1	1:F:361[A]:LEU:HD11	1.43	0.98
1:E:172:ARG:NH1	7:E:601:HOH:O	1.96	0.97
1:E:93[A]:VAL:CG1	1:E:237[A]:MET:CE	2.41	0.96
1:F:21:LEU:HD13	1:F:23[B]:HIS:CE1	2.01	0.95
1:E:280:ALA:O	1:E:284[A]:MET:HG3	1.68	0.94
1:A:197[A]:MET:HE2	1:A:235[A]:VAL:HG23	1.47	0.93
1:C:335:ASP:HB2	5:C:552:FMT:O2	1.69	0.93
1:D:123[A]:ARG:HH11	1:D:123[A]:ARG:HG3	1.34	0.92
1:D:30[B]:HIS:ND1	1:D:33[B]:GLU:OE2	2.03	0.92
1:B:89:GLU:HB2	4:B:513:RAM:H2	1.51	0.92
1:E:93[A]:VAL:CG1	1:E:237[A]:MET:SD	2.57	0.92
1:A:86:THR:OG1	4:A:503[A]:RAM:H63	1.68	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:GLN:CD	4:D:503:RAM:H63	1.90	0.91
1:E:93[A]:VAL:HG11	1:E:237[A]:MET:SD	2.11	0.91
1:D:123[A]:ARG:CG	1:D:123[A]:ARG:HH11	1.83	0.90
1:B:42[B]:ARG:CG	1:B:42[B]:ARG:HH21	1.85	0.90
4:A:503[B]:RAM:O2	5:A:565:FMT:C	2.20	0.89
1:A:193:GLN:NE2	4:A:503[A]:RAM:H1	1.86	0.89
1:D:105:ARG:NH1	1:D:355:HIS:O	2.06	0.88
1:C:101[B]:HIS:CE1	1:C:354[B]:HIS:CD2	2.62	0.87
1:E:172:ARG:HH11	1:E:172:ARG:HG2	1.35	0.87
1:F:21:LEU:HD23	1:F:22:PRO:HD2	1.56	0.87
1:C:256:LEU:HD22	1:C:284:MET:HB3	1.57	0.87
1:C:185[B]:THR:HG22	7:C:617:HOH:O	1.75	0.86
1:F:237[B]:MET:HA	1:F:237[B]:MET:HE3	1.58	0.86
1:A:345:PRO:HB3	1:D:8:PRO:HA	1.56	0.86
1:B:89:GLU:HB2	4:B:513:RAM:C2	2.06	0.85
1:E:93[A]:VAL:CG1	1:E:237[A]:MET:HE1	2.00	0.85
1:A:86:THR:OG1	4:A:503[A]:RAM:C6	2.24	0.85
1:D:89:GLU:HB2	4:D:503:RAM:C6	2.06	0.84
1:E:343[A]:ARG:HH11	1:E:343[A]:ARG:CG	1.85	0.84
1:A:197[A]:MET:HE2	1:A:235[A]:VAL:HG21	1.60	0.84
1:A:355:HIS:NE2	5:A:504:FMT:O1	2.11	0.84
1:A:197[A]:MET:HE1	1:A:235[A]:VAL:CB	2.07	0.83
1:C:30[A]:HIS:CE1	1:C:33[A]:GLU:OE2	2.31	0.83
1:A:335[B]:ASP:OD1	7:A:601:HOH:O	1.96	0.83
1:A:42:ARG:NH2	7:A:603:HOH:O	2.11	0.83
1:A:197[A]:MET:CE	1:A:235[A]:VAL:HG21	2.09	0.82
1:A:39:PRO:CB	1:A:57[B]:ARG:HD3	2.09	0.82
1:F:237[B]:MET:HA	1:F:237[B]:MET:CE	2.09	0.82
1:F:120[A]:MET:HE2	1:F:361[A]:LEU:CD2	2.07	0.82
1:D:178:MET:HE2	1:D:193:GLN:HA	1.62	0.82
1:C:42[B]:ARG:HH11	1:C:42[B]:ARG:HG2	1.45	0.82
1:F:21:LEU:HD13	1:F:23[B]:HIS:HE1	1.41	0.81
3:B:502:QR8:O3	4:B:513:RAM:O4	1.99	0.81
1:F:188[A]:GLU:OE1	7:F:601[A]:HOH:O	1.97	0.81
1:C:106[B]:ARG:NH2	7:C:604:HOH:O	2.12	0.81
1:F:256:LEU:O	1:F:284:MET:HE1	1.80	0.81
1:A:89:GLU:OE2	4:A:503[A]:RAM:O3	1.98	0.80
1:A:39:PRO:HB2	1:A:57[B]:ARG:HD3	1.62	0.80
1:C:188:GLU:HG3	7:C:749:HOH:O	1.82	0.80
3:A:502:QR8:O3	4:A:503[B]:RAM:H2	1.82	0.79
5:A:550:FMT:O2	7:A:602:HOH:O	2.00	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197[A]:MET:HE1	1:A:235[A]:VAL:HB	1.63	0.79
1:C:185[B]:THR:CG2	7:C:617:HOH:O	2.31	0.79
1:A:193:GLN:HE21	4:A:503[A]:RAM:C1	1.97	0.78
1:E:93[A]:VAL:HG13	1:E:237[A]:MET:SD	2.21	0.78
1:D:45:LEU:HD12	1:D:81:PRO:HB2	1.66	0.78
1:B:266:ARG:HD3	7:B:693:HOH:O	1.84	0.77
1:C:120[A]:MET:CE	7:C:773:HOH:O	2.33	0.76
1:D:208[A]:ARG:CG	1:D:208[A]:ARG:HH11	1.98	0.76
1:B:86[B]:THR:OG1	7:B:602:HOH:O	2.02	0.76
1:F:120[A]:MET:HE1	1:F:361[A]:LEU:HD21	1.68	0.76
1:A:236:ASN:HD21	4:A:503[B]:RAM:H4	1.50	0.75
1:C:33[A]:GLU:OE1	7:C:601:HOH:O	2.05	0.75
1:F:277:VAL:HG23	1:F:278:PRO:HD3	1.69	0.75
1:B:309:VAL:HB	1:C:122:PRO:HB3	1.69	0.75
1:E:125:ARG:HD3	1:E:368:GLU:OE2	1.86	0.75
1:E:256:LEU:HD22	1:E:284[B]:MET:HB3	1.70	0.74
4:A:503[A]:RAM:O4	5:A:565:FMT:C	2.35	0.74
1:A:101[B]:HIS:CE1	1:A:354[B]:HIS:CD2	2.75	0.74
1:F:27:LEU:HD23	1:F:326[B]:ARG:NE	2.03	0.74
1:F:93[B]:VAL:HG13	1:F:237[B]:MET:SD	2.27	0.74
4:B:513:RAM:H5	7:B:635:HOH:O	1.88	0.73
1:D:208[A]:ARG:HH11	1:D:208[A]:ARG:HB2	1.53	0.73
4:A:503[A]:RAM:O4	5:A:565:FMT:H	1.88	0.72
1:F:188[A]:GLU:HB2	7:F:601[A]:HOH:O	1.88	0.72
2:E:502:HEM:HHC	2:E:502:HEM:HBB2	1.72	0.72
1:F:120[A]:MET:HE1	1:F:361[A]:LEU:CD1	2.20	0.72
1:D:123[A]:ARG:HG3	1:D:123[A]:ARG:NH1	2.01	0.71
1:A:197[A]:MET:HE1	1:A:235[A]:VAL:HG23	1.48	0.71
1:B:42[B]:ARG:HG2	1:B:42[B]:ARG:NH2	1.90	0.71
1:C:126[B]:SER:OG	7:C:603:HOH:O	2.09	0.70
5:C:521:FMT:O1	7:C:602:HOH:O	2.08	0.70
1:D:193:GLN:OE1	4:D:503:RAM:H63	1.91	0.70
1:C:354[B]:HIS:HE1	7:C:636:HOH:O	1.72	0.70
1:D:183[A]:ARG:HD2	1:D:184:LEU:CD1	2.22	0.70
1:B:89:GLU:CB	4:B:513:RAM:C2	2.57	0.69
1:B:354[B]:HIS:HD2	2:B:501:HEM:O1D	1.74	0.69
1:F:120[A]:MET:CE	1:F:361[A]:LEU:CD2	2.61	0.69
1:A:178:MET:O	4:A:503[A]:RAM:O1	2.11	0.69
1:B:89:GLU:HB2	4:B:513:RAM:O2	1.91	0.69
1:A:298:ARG:HE	5:A:514:FMT:C	2.06	0.69
1:D:220:ALA:O	1:D:223:THR:OG1	2.09	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123[B]:ARG:HE	5:A:510:FMT:C	2.06	0.69
1:C:283:GLU:HG3	1:C:337:LEU:HD22	1.75	0.68
1:D:256[A]:LEU:HD22	1:D:284:MET:HB3	1.76	0.68
2:A:501:HEM:HMB2	2:A:501:HEM:HBB2	1.75	0.68
1:B:170:LEU:HB2	5:F:509:FMT:H	1.76	0.67
1:D:178:MET:CE	1:D:193:GLN:HA	2.24	0.67
1:C:35:ARG:HH11	5:C:504:FMT:C	2.08	0.67
1:B:13:ALA:HB1	1:C:115:ARG:HG2	1.76	0.67
1:A:138[A]:HIS:ND1	1:A:139:GLY:O	2.28	0.67
1:F:188[A]:GLU:CD	7:F:601[A]:HOH:O	2.33	0.67
1:D:48:GLY:O	7:D:601:HOH:O	2.13	0.66
1:C:30[A]:HIS:NE2	7:C:612:HOH:O	2.29	0.66
1:D:355:HIS:NE2	5:D:508:FMT:O1	2.26	0.65
1:F:93[B]:VAL:CG1	1:F:237[B]:MET:SD	2.84	0.65
1:B:266:ARG:HD2	1:B:337:LEU:HD23	1.79	0.65
1:A:39:PRO:HB3	1:A:57[B]:ARG:HD3	1.79	0.65
2:A:501:HEM:CMB	2:A:501:HEM:HBB2	2.27	0.65
1:D:230:THR:O	1:D:234:ILE:HD12	1.97	0.65
1:F:24:ALA:HB2	1:F:391:TRP:NE1	2.12	0.64
1:F:133:ASP:O	1:F:136[B]:VAL:HG12	1.96	0.64
5:B:503:FMT:H	7:B:735:HOH:O	1.97	0.63
1:F:24:ALA:HB2	1:F:391:TRP:CD1	2.34	0.63
1:B:392:LYS:HG2	1:B:401[A]:GLU:HG3	1.80	0.63
1:E:17:TYR:HE1	1:E:31:TYR:HH	1.45	0.63
1:A:256:LEU:HD22	1:A:284[A]:MET:HB3	1.81	0.62
1:D:89:GLU:HB3	4:D:503:RAM:H5	1.82	0.62
1:F:390[A]:LYS:NZ	1:F:402[A]:ARG:HE	1.97	0.62
1:C:101[B]:HIS:CE1	1:C:354[B]:HIS:HD2	2.18	0.62
1:B:13:ALA:HB2	5:B:507:FMT:O1	2.00	0.61
1:A:240:SER:HA	4:A:503[B]:RAM:C6	2.31	0.61
1:A:138[A]:HIS:HE1	1:A:141:PRO:O	1.84	0.61
5:D:528:FMT:C	7:D:619:HOH:O	2.47	0.61
1:F:277:VAL:CG2	1:F:278:PRO:HD3	2.30	0.60
1:F:91:ASP:O	5:F:514:FMT:O1	2.19	0.60
1:E:150:VAL:O	1:E:154:VAL:HG13	2.01	0.60
1:F:201:ASP:OD1	7:F:602:HOH:O	2.17	0.60
1:A:243:ILE:HD12	4:A:503[B]:RAM:C6	2.32	0.60
1:B:123:ARG:HD3	5:B:534:FMT:O1	2.01	0.60
3:D:502:QR8:O3	4:D:503:RAM:O1	2.18	0.60
1:D:101[B]:HIS:NE2	1:D:354[B]:HIS:CD2	2.70	0.60
1:D:145:VAL:HA	1:D:149:ALA:HB3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PHE:HB3	1:A:196:PHE:CD2	2.37	0.60
1:F:354[B]:HIS:HE1	7:F:626:HOH:O	1.83	0.59
1:F:133:ASP:OD1	1:F:376[A]:ARG:NH1	2.34	0.59
1:E:172:ARG:HH11	1:E:172:ARG:CG	2.08	0.59
1:F:103:ARG:HE	5:F:509:FMT:C	2.16	0.59
1:B:86[A]:THR:HG23	7:B:602:HOH:O	2.02	0.59
1:D:127:LEU:HD11	1:D:155:ALA:HB3	1.84	0.59
1:E:125:ARG:CD	1:E:368:GLU:OE2	2.51	0.59
1:F:112:PHE:HB3	1:F:357:ILE:O	2.02	0.59
1:D:193:GLN:NE2	4:D:503:RAM:H63	2.18	0.59
1:E:290:LEU:O	1:E:397:ILE:HA	2.03	0.58
1:A:12:ASP:HB2	7:A:722:HOH:O	2.03	0.58
1:A:240:SER:HA	4:A:503[B]:RAM:H63	1.86	0.58
1:F:21:LEU:HB3	1:F:23[B]:HIS:NE2	2.19	0.58
1:F:93[A]:VAL:HG23	5:F:514:FMT:C	2.33	0.58
1:A:115[A]:ARG:HD3	7:A:770:HOH:O	2.04	0.57
1:E:322:ALA:O	1:E:326:ARG:HG2	2.04	0.57
1:D:101[B]:HIS:CD2	1:D:354[B]:HIS:CD2	2.93	0.57
1:C:335:ASP:HB2	5:C:552:FMT:C	2.33	0.57
1:F:125:ARG:O	1:F:128[B]:VAL:HG12	2.03	0.57
1:D:17:TYR:CD1	1:D:18:PRO:HA	2.39	0.56
1:D:208[A]:ARG:HH11	1:D:208[A]:ARG:HB3	1.67	0.56
1:D:287:TYR:O	1:D:287:TYR:CD1	2.57	0.56
1:C:343[A]:ARG:NH2	7:C:619:HOH:O	2.38	0.56
1:E:312[B]:ARG:HH11	1:E:312[B]:ARG:HG2	1.70	0.56
1:F:244:ALA:HB1	2:F:502:HEM:CHD	2.35	0.56
1:A:243:ILE:HD12	4:A:503[B]:RAM:H61	1.86	0.56
1:F:101[A]:HIS:CE1	1:F:354[A]:HIS:CE1	2.94	0.56
1:C:393[B]:GLN:OE1	7:C:605:HOH:O	2.18	0.56
1:D:208[A]:ARG:CG	1:D:208[A]:ARG:NH1	2.64	0.56
1:F:266:ARG:NH2	1:F:337[B]:LEU:HD12	2.21	0.56
1:C:172:ARG:HH12	5:C:507:FMT:C	2.19	0.55
1:E:74:ALA:HB3	1:E:299:VAL:HB	1.88	0.55
1:F:349:PHE:CE1	1:F:359:ALA:HA	2.40	0.55
1:A:86:THR:OG1	4:A:503[A]:RAM:H61	2.05	0.55
1:D:152:PHE:HB3	1:D:153:PRO:HD3	1.88	0.55
1:D:183[A]:ARG:HD2	1:D:184:LEU:HD11	1.87	0.55
1:D:160:LEU:HG	1:D:215[B]:LEU:HD22	1.88	0.55
1:F:161:LEU:O	1:F:216:LEU:HB2	2.05	0.55
1:E:286:ARG:HD3	1:E:344:ASN:OD1	2.06	0.55
1:A:115[B]:ARG:HG3	1:A:115[B]:ARG:HH21	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:HEM:HBC2	2:A:501:HEM:HMC2	1.89	0.55
2:B:501:HEM:HBB2	2:B:501:HEM:HMB2	1.87	0.55
1:A:159:GLU:HG2	5:A:510:FMT:H	1.89	0.55
1:C:305[B]:GLU:OE1	1:C:310:THR:OG1	2.21	0.55
1:E:115:ARG:HB3	5:E:501:FMT:C	2.37	0.54
1:D:178:MET:HE3	1:D:196:PHE:HD2	1.72	0.54
1:A:283:GLU:HG3	1:A:337:LEU:HD22	1.89	0.54
1:B:105:ARG:HD3	1:B:357:ILE:HD12	1.88	0.54
1:B:264:ARG:NH1	1:B:380:LEU:O	2.40	0.54
1:E:77:ASP:HB3	1:E:80:THR:CG2	2.37	0.54
1:F:286[A]:ARG:HD3	1:F:344:ASN:OD1	2.08	0.54
1:D:178:MET:HE2	1:D:193:GLN:CA	2.37	0.54
1:A:36[B]:ARG:HG2	1:A:37:ASP:OD1	2.08	0.54
1:D:158:CYS:HB3	1:D:163:VAL:O	2.08	0.54
1:B:207:ARG:NH2	1:B:214:ASP:OD1	2.40	0.53
1:A:260:LEU:HG	1:A:284[A]:MET:HE1	1.90	0.53
1:D:326:ARG:HG3	5:D:507:FMT:H	1.89	0.53
1:E:92:GLY:HA2	1:E:236:ASN:ND2	2.23	0.53
1:F:244:ALA:HB1	2:F:502:HEM:C4C	2.43	0.53
1:E:256:LEU:O	1:E:284[A]:MET:HE1	2.09	0.53
1:F:145[B]:VAL:HA	1:F:149:ALA:HB3	1.90	0.53
1:A:274:PRO:O	5:A:550:FMT:O1	2.26	0.53
4:A:503[A]:RAM:HO4	5:A:565:FMT:C	2.18	0.53
1:B:38:GLU:OE1	5:B:510:FMT:O2	2.26	0.53
1:E:266:ARG:HD3	1:E:337:LEU:HD23	1.89	0.53
1:F:145[A]:VAL:HA	1:F:149:ALA:HB3	1.90	0.53
1:F:326[B]:ARG:NH2	1:F:335[B]:ASP:OD2	2.40	0.53
1:A:38:GLU:HG3	5:A:531:FMT:O2	2.09	0.53
1:A:38:GLU:HG3	5:A:531:FMT:C	2.38	0.53
1:D:89:GLU:CB	4:D:503:RAM:C6	2.84	0.53
1:A:239:VAL:HG12	4:A:503[B]:RAM:H62	1.90	0.53
4:A:503[B]:RAM:O2	5:A:565:FMT:O1	2.25	0.53
1:A:371:SER:HB3	5:A:506:FMT:C	2.39	0.52
1:F:375[B]:ARG:HG2	1:F:376[B]:ARG:HG3	1.89	0.52
1:D:208[A]:ARG:NH1	1:D:208[A]:ARG:HB2	2.23	0.52
1:E:256:LEU:HD22	1:E:284[B]:MET:CB	2.39	0.52
1:B:383:ALA:HB3	1:B:404:ILE:HG22	1.91	0.52
1:C:21:LEU:HD12	1:C:22:PRO:HD2	1.91	0.52
1:E:101[B]:HIS:CD2	1:E:354[B]:HIS:CD2	2.97	0.52
1:F:327:ASP:OD1	1:F:329:GLU:OE1	2.26	0.52
1:F:127[B]:LEU:HD13	7:F:629[B]:HOH:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ARG:NH2	7:B:611:HOH:O	2.43	0.52
1:B:17:TYR:HA	1:B:18:PRO:C	2.29	0.52
1:F:24:ALA:CB	1:F:391:TRP:NE1	2.73	0.52
1:F:289:PRO:HA	5:F:505:FMT:H	1.92	0.52
1:A:127:LEU:HD21	1:A:155:ALA:HB3	1.92	0.51
1:B:101[B]:HIS:HE1	2:B:501:HEM:O2D	1.92	0.51
1:E:256:LEU:HD22	1:E:284[A]:MET:HB3	1.91	0.51
1:F:287:TYR:CD1	1:F:337[B]:LEU:HG	2.44	0.51
1:C:28:ASP:OD1	1:C:29:PRO:HD2	2.11	0.51
1:D:89:GLU:CB	4:D:503:RAM:H62	2.21	0.51
1:E:32:ALA:HA	1:E:35[B]:ARG:NH1	2.26	0.51
1:F:168[B]:ARG:CG	1:F:168[B]:ARG:HH11	2.22	0.51
1:F:21:LEU:HD23	1:F:22:PRO:CD	2.37	0.51
1:C:30[A]:HIS:HD1	1:C:33[A]:GLU:CD	2.08	0.51
1:F:162:GLY:HA3	1:F:214:ASP:OD2	2.11	0.51
1:C:9:THR:CG2	1:C:11:ALA:HB3	2.41	0.51
1:E:145:VAL:HA	1:E:149:ALA:HB3	1.92	0.51
3:A:502:QR8:O3	4:A:503[A]:RAM:H3	2.11	0.50
1:E:101[B]:HIS:CD2	1:E:354[B]:HIS:NE2	2.79	0.50
1:E:170:LEU:HD22	1:E:174:PHE:CZ	2.46	0.50
1:C:120[A]:MET:HE2	7:C:773:HOH:O	2.02	0.50
1:E:256:LEU:HD22	1:E:284[A]:MET:CB	2.39	0.50
1:A:44[B]:ARG:HD2	5:A:511:FMT:C	2.41	0.50
1:E:35[A]:ARG:HG2	1:E:57:ARG:HG2	1.92	0.50
1:A:160:LEU:HG	1:A:215[A]:LEU:HD22	1.92	0.50
1:B:172:ARG:HD2	7:B:670:HOH:O	2.10	0.50
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.41	0.50
2:D:501:HEM:HMC2	2:D:501:HEM:HBC2	1.93	0.50
1:D:9:THR:HG22	1:D:9:THR:O	2.12	0.50
1:A:240:SER:CA	4:A:503[B]:RAM:H63	2.42	0.50
2:C:501:HEM:HBB2	2:C:501:HEM:HMB2	1.94	0.50
1:D:193:GLN:HG2	4:D:503:RAM:H4	1.93	0.50
1:D:258[B]:HIS:NE2	1:D:391:TRP:HZ2	2.10	0.50
1:E:251:ASN:HD22	1:E:397:ILE:HD12	1.76	0.50
1:A:32:ALA:HB2	5:A:530:FMT:H	1.94	0.50
1:A:258:HIS:O	1:A:262:THR:HG23	2.12	0.50
1:F:168[A]:ARG:HG2	1:F:172:ARG:HD3	1.93	0.49
1:F:46:PRO:HB2	1:F:47:TYR:CD1	2.47	0.49
1:F:291:VAL:H	5:F:505:FMT:C	2.25	0.49
1:F:42:ARG:HD2	1:F:51:THR:HG23	1.93	0.49
1:D:123[A]:ARG:CG	1:D:123[A]:ARG:NH1	2.54	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42[A]:ARG:NH1	5:C:523:FMT:O2	2.45	0.49
1:B:401[A]:GLU:OE2	7:B:603[A]:HOH:O	2.19	0.49
1:F:21:LEU:HD22	1:F:23[B]:HIS:CE1	2.47	0.49
1:D:189:ILE:HG21	5:D:504:FMT:C	2.43	0.49
1:E:28:ASP:OD1	1:E:30:HIS:HB2	2.12	0.49
1:B:256:LEU:HD22	1:B:284[B]:MET:HB3	1.94	0.49
1:C:14:VAL:HG21	1:C:51[B]:THR:HG23	1.94	0.49
1:F:237[B]:MET:HA	5:F:514:FMT:H	1.95	0.49
1:A:122:PRO:HB3	1:D:309:VAL:HB	1.94	0.48
1:A:240:SER:OG	4:A:503[B]:RAM:C1	2.61	0.48
1:F:252:GLN:OE1	1:F:252:GLN:HA	2.12	0.48
1:D:178:MET:CE	1:D:196:PHE:HB2	2.42	0.48
1:E:251:ASN:HB3	1:E:398:ARG:O	2.12	0.48
1:F:172:ARG:HG2	1:F:172:ARG:HH11	1.78	0.48
1:C:71:SER:OG	1:C:97:ASP:OD2	2.22	0.48
1:B:280:ALA:O	1:B:284[A]:MET:HG3	2.14	0.48
1:A:328:GLU:HB2	5:A:505:FMT:C	2.44	0.48
1:E:86:THR:HG22	1:E:186:ALA:HA	1.95	0.48
1:E:70:PHE:HB3	1:E:298:ARG:HB3	1.94	0.48
1:E:35[A]:ARG:HG2	1:E:57:ARG:CG	2.43	0.48
1:F:259:LEU:HB2	1:F:284:MET:CE	2.43	0.48
1:F:24:ALA:CB	1:F:391:TRP:CE2	2.97	0.48
1:A:115[B]:ARG:HH21	1:A:115[B]:ARG:CG	2.26	0.47
1:A:44[B]:ARG:HD2	5:A:511:FMT:O2	2.14	0.47
1:D:89:GLU:CB	4:D:503:RAM:H5	2.43	0.47
1:D:101[B]:HIS:NE2	1:D:354[B]:HIS:HD2	2.11	0.47
1:A:89:GLU:HB2	4:A:503[B]:RAM:O3	2.13	0.47
2:B:501:HEM:HMC2	2:B:501:HEM:HBC2	1.96	0.47
1:D:208[A]:ARG:NH1	1:D:208[A]:ARG:CB	2.57	0.47
4:A:503[A]:RAM:O4	5:A:565:FMT:O2	2.27	0.47
1:B:177:ALA:O	1:B:180:SER:HB3	2.14	0.47
5:B:503:FMT:C	7:B:735:HOH:O	2.59	0.47
1:E:271:VAL:HA	1:E:374:VAL:HG13	1.95	0.47
1:A:107[A]:LEU:HD13	1:A:219:LEU:CD2	2.44	0.47
1:D:256[A]:LEU:HD22	1:D:284:MET:CB	2.44	0.47
1:E:380:LEU:HA	1:E:406:SER:O	2.15	0.47
1:E:312[B]:ARG:HH11	1:E:312[B]:ARG:CG	2.28	0.47
1:F:117:VAL:O	1:F:120[A]:MET:HG2	2.15	0.47
1:F:206[B]:GLN:HG2	7:F:657:HOH:O	2.15	0.47
1:B:392:LYS:HG3	1:B:399:GLY:O	2.15	0.47
1:C:42[B]:ARG:HH11	1:C:42[B]:ARG:CG	2.23	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLN:CD	4:B:513:RAM:O2	2.53	0.47
1:B:159:GLU:HG2	5:B:534:FMT:O1	2.15	0.47
1:C:185[B]:THR:HG23	1:C:188:GLU:HB3	1.97	0.47
1:D:83:MET:O	7:D:602:HOH:O	2.21	0.47
1:F:27:LEU:HD23	1:F:326[B]:ARG:HE	1.79	0.47
1:D:101[B]:HIS:CD2	1:D:354[B]:HIS:NE2	2.83	0.46
1:F:27:LEU:HD23	1:F:326[B]:ARG:CZ	2.44	0.46
1:A:39:PRO:HB3	1:A:57[B]:ARG:CD	2.43	0.46
1:F:168[B]:ARG:NH1	1:F:168[B]:ARG:CG	2.79	0.46
1:A:240:SER:OG	4:A:503[B]:RAM:H1	2.15	0.46
1:B:152:PHE:HB3	1:B:153:PRO:HD3	1.96	0.46
1:D:178:MET:HE3	1:D:196:PHE:HB2	1.96	0.46
1:B:101[B]:HIS:CE1	1:B:354[B]:HIS:CD2	3.03	0.46
1:D:86[A]:THR:HG22	1:D:186:ALA:HA	1.98	0.46
1:C:219:LEU:O	1:C:223:THR:HG23	2.15	0.46
7:A:759:HOH:O	1:D:38:GLU:HG3	2.15	0.46
1:E:115:ARG:HB3	5:E:501:FMT:H	1.97	0.46
1:A:264:ARG:HH11	1:A:264:ARG:CG	2.29	0.46
1:C:206:GLN:HE22	5:C:514:FMT:H	1.81	0.46
1:A:193:GLN:HG2	4:A:503[A]:RAM:O2	2.16	0.46
1:B:12[B]:ASP:CG	1:B:44:ARG:HH21	2.19	0.46
1:F:144[B]:LEU:HD23	1:F:144[B]:LEU:HA	1.72	0.46
1:F:93[B]:VAL:HG11	1:F:237[B]:MET:SD	2.57	0.46
1:F:287:TYR:CE1	1:F:337[B]:LEU:HG	2.51	0.46
1:D:167:ASP:O	1:D:168:ARG:C	2.54	0.45
1:E:30:HIS:O	1:E:34[A]:LEU:HG	2.16	0.45
1:D:190[B]:GLN:HA	1:D:190[B]:GLN:HE21	1.80	0.45
1:E:172:ARG:NH1	1:E:172:ARG:CG	2.73	0.45
1:E:295:SER:H	1:E:318[A]:VAL:CG2	2.29	0.45
1:F:260[B]:LEU:HD12	1:F:260[B]:LEU:HA	1.79	0.45
1:F:361[A]:LEU:HD23	1:F:361[A]:LEU:HA	1.83	0.45
1:F:373:LEU:HD22	1:F:380[B]:LEU:HD11	1.98	0.45
1:F:92:GLY:O	1:F:96:GLN:HG2	2.17	0.45
1:A:152:PHE:HB3	1:A:153:PRO:HD3	1.99	0.45
1:D:123[B]:ARG:HG3	7:D:720:HOH:O	2.17	0.45
1:E:101[B]:HIS:NE2	1:E:354[B]:HIS:CD2	2.84	0.45
1:F:237[B]:MET:CA	1:F:237[B]:MET:CE	2.84	0.45
1:F:237[A]:MET:HA	5:F:514:FMT:H	1.98	0.45
5:B:511:FMT:C	7:B:618:HOH:O	2.63	0.45
1:E:106:ARG:CG	1:E:106:ARG:HH11	2.29	0.45
1:E:138[B]:HIS:HD2	1:E:139:GLY:O	2.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:MET:HE3	4:B:513:RAM:H4	1.97	0.45
1:B:270:LEU:HB2	1:B:374:VAL:HG21	1.98	0.45
2:C:501:HEM:HMC1	2:C:501:HEM:HBC2	1.98	0.45
1:D:94:LEU:HD21	3:D:502:QR8:O12	2.17	0.45
1:A:101[B]:HIS:CE1	1:A:354[B]:HIS:HD2	2.33	0.45
1:A:264:ARG:HG2	1:A:268:GLU:OE2	2.16	0.45
1:C:120[A]:MET:HE3	7:C:773:HOH:O	2.09	0.45
1:C:393[B]:GLN:CD	7:C:605:HOH:O	2.54	0.45
1:A:12:ASP:N	7:A:615:HOH:O	2.49	0.45
1:A:240:SER:HA	4:A:503[B]:RAM:H61	1.98	0.45
1:A:290:LEU:O	1:A:397:ILE:HA	2.17	0.45
3:A:502:QR8:C5	4:A:503[B]:RAM:O5	2.65	0.45
1:C:283:GLU:HG3	1:C:337:LEU:CD2	2.46	0.45
1:C:290:LEU:O	1:C:397:ILE:HA	2.16	0.45
1:D:93:VAL:N	5:D:528:FMT:O2	2.50	0.45
1:A:178:MET:CE	4:A:503[A]:RAM:O2	2.65	0.44
1:D:123[A]:ARG:HD2	5:D:512:FMT:O2	2.17	0.44
1:F:280:ALA:O	1:F:284:MET:HG3	2.17	0.44
1:A:107[B]:LEU:HD21	1:A:222:ALA:CB	2.47	0.44
1:A:243:ILE:HD12	4:A:503[B]:RAM:H62	2.00	0.44
1:C:312:ARG:O	1:C:313:ALA:C	2.54	0.44
1:C:12[A]:ASP:HB2	1:C:51[A]:THR:CG2	2.47	0.44
1:E:35[A]:ARG:HG3	1:E:56:THR:HB	2.00	0.44
1:F:120[A]:MET:HE1	1:F:361[A]:LEU:CD2	2.37	0.44
1:F:46:PRO:HB2	1:F:47:TYR:CE1	2.53	0.44
1:A:140:SER:OG	1:A:406:SER:HA	2.17	0.44
1:D:146:GLU:O	7:D:603:HOH:O	2.21	0.44
1:D:178:MET:SD	4:D:503:RAM:O3	2.76	0.44
1:D:62:ARG:HH11	1:D:351[A]:HIS:CD2	2.35	0.44
1:E:259:LEU:HB2	1:E:284[A]:MET:CE	2.47	0.44
1:E:312[B]:ARG:HG3	1:E:313:ALA:N	2.32	0.44
1:F:184:LEU:HD22	1:F:188[A]:GLU:OE1	2.18	0.44
1:B:315:GLU:HA	1:B:316:PRO:HD3	1.83	0.44
1:F:131[A]:LEU:HA	1:F:131[A]:LEU:HD13	1.74	0.44
1:F:400:LEU:HD13	1:F:403:GLN:CG	2.48	0.44
1:A:138[A]:HIS:CE1	1:A:139:GLY:O	2.71	0.44
1:D:101[B]:HIS:HE2	1:D:354[B]:HIS:HD2	1.66	0.44
1:D:246:HIS:O	1:D:250:VAL:HG23	2.18	0.44
5:F:504:FMT:C	7:F:628:HOH:O	2.65	0.44
1:B:144:LEU:HA	1:B:144:LEU:HD12	1.89	0.44
1:D:94:LEU:HA	1:D:354[A]:HIS:CE1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:503[B]:RAM:H4	4:A:503[B]:RAM:H1	1.63	0.44
5:B:511:FMT:H	7:B:618:HOH:O	2.18	0.44
1:C:256:LEU:HD22	1:C:284:MET:CB	2.37	0.44
1:D:174:PHE:HB3	1:D:196:PHE:CD2	2.53	0.44
1:F:376[A]:ARG:NH2	1:F:377[A]:PHE:CZ	2.86	0.44
2:B:501:HEM:HBB2	2:B:501:HEM:CMB	2.48	0.44
1:E:127[B]:LEU:HD21	1:E:155:ALA:HB3	1.99	0.43
1:B:354[B]:HIS:HE1	7:B:713:HOH:O	2.00	0.43
1:D:178:MET:HE3	1:D:196:PHE:CD2	2.52	0.43
1:F:129[A]:ASP:OD1	1:F:376[A]:ARG:HD2	2.18	0.43
1:F:244:ALA:CB	2:F:502:HEM:CHD	2.96	0.43
1:F:25:LEU:N	1:F:25:LEU:HD23	2.33	0.43
1:A:246:HIS:O	1:A:250:VAL:HG23	2.18	0.43
1:C:101[B]:HIS:HE1	2:C:501:HEM:O2D	2.01	0.43
1:C:346[A]:HIS:HD2	1:C:348:ALA:H	1.66	0.43
1:A:258:HIS:CE1	1:A:262:THR:HG21	2.53	0.43
1:D:283:GLU:HA	1:D:344:ASN:HD21	1.82	0.43
1:F:214:ASP:HB3	1:F:217:GLY:H	1.82	0.43
1:F:285:LEU:HA	1:F:285:LEU:HD23	1.90	0.43
1:B:263:GLU:O	1:B:266:ARG:HG3	2.18	0.43
1:D:193:GLN:CG	4:D:503:RAM:H4	2.48	0.43
1:D:256[B]:LEU:HD23	1:D:370:LEU:HD11	1.99	0.43
1:F:168[B]:ARG:HG2	1:F:168[B]:ARG:HH11	1.83	0.43
1:A:256:LEU:HD22	1:A:284[B]:MET:HB3	2.00	0.43
1:B:101[B]:HIS:CE1	2:B:501:HEM:O2D	2.71	0.43
1:B:193:GLN:HG2	4:B:513:RAM:H1	2.00	0.43
1:D:85:PRO:HD2	5:D:504:FMT:O1	2.19	0.43
1:E:55:VAL:HG22	1:E:319:VAL:HG22	2.00	0.43
1:F:283:GLU:HG3	1:F:337[A]:LEU:HD12	2.01	0.43
2:F:502:HEM:HMB2	2:F:502:HEM:HBB2	2.01	0.43
1:B:17:TYR:O	1:B:46:PRO:HD3	2.19	0.43
1:C:8:PRO:N	7:C:639:HOH:O	2.51	0.43
1:D:264[A]:ARG:NH2	1:D:378:PRO:O	2.51	0.43
1:D:393[B]:GLN:NE2	5:D:518:FMT:O2	2.46	0.43
1:F:101[A]:HIS:CE1	1:F:354[A]:HIS:ND1	2.87	0.43
1:F:123:ARG:CZ	1:F:127[B]:LEU:HD11	2.48	0.43
1:D:180:SER:HB2	1:D:189:ILE:HD11	2.01	0.43
1:D:258[B]:HIS:CD2	1:D:391:TRP:CZ2	3.07	0.43
1:E:215:LEU:HD23	1:E:215:LEU:HA	1.75	0.43
1:B:121:ARG:HG3	1:B:364:LEU:HD11	2.01	0.42
1:A:104:LEU:O	1:A:107[A]:LEU:HB2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:VAL:HG11	1:F:360:GLN:C	2.40	0.42
1:B:127:LEU:HD21	1:B:155:ALA:HB3	2.01	0.42
1:B:86[A]:THR:HG22	1:B:186:ALA:HA	2.01	0.42
1:D:44[B]:ARG:HD2	1:D:50:GLY:O	2.19	0.42
1:E:308:THR:O	1:E:309:VAL:HG23	2.19	0.42
1:F:277:VAL:HG23	1:F:278:PRO:CD	2.44	0.42
1:E:157:ILE:HG13	1:E:161:LEU:HD22	2.00	0.42
1:F:283:GLU:OE1	1:F:344:ASN:ND2	2.52	0.42
1:B:46:PRO:HB2	1:B:47:TYR:CD1	2.54	0.42
1:D:380:LEU:HD11	1:D:405:VAL:HG21	2.02	0.42
2:D:501:HEM:HHC	2:D:501:HEM:HAB	1.66	0.42
1:E:226:ASP:HB2	1:E:229:LEU:O	2.19	0.42
1:E:265[A]:LYS:NZ	1:E:265[A]:LYS:HB2	2.35	0.42
1:A:179:LEU:HA	1:A:179:LEU:HD23	1.86	0.42
1:D:89:GLU:HB2	4:D:503:RAM:C5	2.49	0.42
2:E:502:HEM:HMC2	2:E:502:HEM:HBC2	2.02	0.42
1:F:105:ARG:NH2	1:F:355:HIS:O	2.38	0.42
1:B:351[A]:HIS:HE1	7:B:809:HOH:O	2.03	0.42
1:C:150:VAL:CG2	5:C:507:FMT:H	2.49	0.42
1:D:14:VAL:O	1:D:44[A]:ARG:NH1	2.44	0.42
1:F:225:ASN:ND2	1:F:227:ASP:OD1	2.53	0.42
1:A:101[B]:HIS:HE1	2:A:501:HEM:O2D	2.01	0.42
1:A:193:GLN:HE22	4:A:503[A]:RAM:H63	1.85	0.42
1:B:42[B]:ARG:HD2	1:B:53:TRP:CH2	2.54	0.42
1:E:174:PHE:HB3	1:E:196:PHE:CD2	2.54	0.42
1:A:212:THR:O	5:A:546:FMT:O1	2.38	0.42
1:A:354[B]:HIS:HE1	7:A:680:HOH:O	2.03	0.42
1:A:21:LEU:HD12	5:A:524:FMT:C	2.50	0.42
1:D:161:LEU:O	1:D:216:LEU:HB2	2.19	0.42
1:D:99:PRO:HD2	7:D:651:HOH:O	2.20	0.42
1:D:190[B]:GLN:HE21	1:D:190[B]:GLN:CA	2.32	0.42
1:F:94:LEU:HA	1:F:94:LEU:HD12	1.94	0.42
1:A:21:LEU:HA	1:A:21:LEU:HD12	1.92	0.41
1:F:120[A]:MET:HE1	1:F:361[A]:LEU:CG	2.50	0.41
1:A:27:LEU:HD12	1:A:27:LEU:HA	1.86	0.41
1:B:28:ASP:HA	1:B:29:PRO:HD3	1.92	0.41
1:C:194:GLN:O	5:C:512:FMT:O1	2.38	0.41
1:D:123[A]:ARG:HH11	1:D:123[A]:ARG:HG2	1.79	0.41
1:D:42:ARG:O	1:D:43:VAL:CG1	2.68	0.41
1:F:154:VAL:HG11	1:F:168[A]:ARG:HE	1.84	0.41
1:A:373[B]:LEU:HD12	1:A:373[B]:LEU:HA	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:TYR:HA	1:C:18:PRO:C	2.41	0.41
2:D:501:HEM:HMB2	2:D:501:HEM:HBB2	2.02	0.41
1:E:219:LEU:O	1:E:223[B]:THR:HG23	2.20	0.41
1:F:75:ALA:HA	1:F:80:THR:HG21	2.01	0.41
1:A:107[B]:LEU:HD21	1:A:222:ALA:HB1	2.02	0.41
1:B:258:HIS:CE1	1:B:262:THR:HG21	2.55	0.41
1:F:24:ALA:HB1	1:F:391:TRP:CE2	2.55	0.41
1:F:140:SER:HB2	1:F:406:SER:HA	2.02	0.41
1:A:283:GLU:HG3	1:A:337:LEU:CD2	2.49	0.41
1:C:107:LEU:HD12	1:C:107:LEU:HA	1.80	0.41
1:C:252:GLN:HA	1:C:252:GLN:OE1	2.19	0.41
1:E:45:LEU:HD22	1:E:81:PRO:CB	2.51	0.41
1:F:144[A]:LEU:HD12	1:F:144[A]:LEU:HA	1.92	0.41
1:F:246:HIS:O	1:F:250:VAL:HG12	2.21	0.41
1:A:36[B]:ARG:NE	1:A:37:ASP:OD1	2.54	0.41
1:B:76:THR:OG1	5:B:538:FMT:O2	2.36	0.41
1:D:191[A]:ARG:HA	1:D:191[A]:ARG:HD3	1.58	0.41
1:F:22:PRO:HB3	1:F:398:ARG:NH2	2.36	0.41
1:F:93[B]:VAL:H	5:F:514:FMT:C	2.34	0.41
1:D:101[A]:HIS:HE1	2:D:501:HEM:O2D	2.03	0.41
1:E:260:LEU:HG	1:E:284[A]:MET:CE	2.51	0.41
1:A:170:LEU:HD23	1:A:170:LEU:C	2.40	0.41
1:A:286:ARG:HG2	1:A:325:ASN:HB3	2.03	0.41
1:B:332:ASP:C	1:B:333[A]:HIS:CG	2.94	0.41
1:E:71:SER:HB2	1:E:97:ASP:OD2	2.20	0.41
1:A:17:TYR:HA	1:A:18:PRO:C	2.41	0.41
1:C:12[A]:ASP:N	1:C:12[A]:ASP:OD1	2.53	0.41
1:C:185[B]:THR:HG23	1:C:188:GLU:CB	2.51	0.41
1:C:282:GLU:OE1	1:C:346[A]:HIS:HE1	2.04	0.41
1:B:108:VAL:HG13	1:B:112:PHE:CE2	2.56	0.40
1:E:244:ALA:CB	2:E:502:HEM:CHD	2.98	0.40
1:E:67:ASP:OD1	1:E:69:ARG:HG3	2.21	0.40
1:F:157:ILE:HD12	1:F:157:ILE:HA	1.90	0.40
1:F:42:ARG:HD2	1:F:51:THR:CG2	2.51	0.40
1:C:104:LEU:O	1:C:107:LEU:HB2	2.20	0.40
1:A:252:GLN:O	1:A:256:LEU:HG	2.21	0.40
1:C:204:VAL:HG22	7:C:777:HOH:O	2.20	0.40
1:F:124:VAL:HG21	1:F:364:LEU:HD21	2.03	0.40
1:A:256:LEU:HB3	1:A:284[A]:MET:SD	2.62	0.40
1:B:165:LEU:HA	1:B:165:LEU:HD23	1.91	0.40
1:E:77:ASP:HB3	1:E:80:THR:HG23	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.90	0.40
1:A:178:MET:HE3	4:A:503[A]:RAM:O2	2.21	0.40
1:C:12[A]:ASP:CB	1:C:51[A]:THR:HG21	2.52	0.40
1:F:237[B]:MET:CA	1:F:237[B]:MET:HE2	2.52	0.40

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
All	All	2204/2046 (108%)	2026 (92%)	178 (8%)	15	13

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	21	LEU
1	A	27	LEU
1	A	44[A]	ARG
1	A	44[B]	ARG
1	A	45	LEU
1	A	93	VAL
1	A	102	THR
1	A	107[A]	LEU
1	A	107[B]	LEU
1	A	108[A]	VAL
1	A	108[B]	VAL
1	A	126	SER
1	A	183	ARG
1	A	194[A]	GLN
1	A	194[B]	GLN
1	A	196	PHE
1	A	198	VAL
1	A	201	ASP
1	A	225[A]	ASN
1	A	225[B]	ASN
1	A	227	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	264	ARG
1	A	269	SER
1	A	276	LEU
1	A	337	LEU
1	A	342[A]	GLU
1	A	342[B]	GLU
1	B	21	LEU
1	B	42[A]	ARG
1	B	42[B]	ARG
1	B	86[A]	THR
1	B	86[B]	THR
1	B	93	VAL
1	B	106	ARG
1	B	116	ARG
1	B	123	ARG
1	B	190[A]	GLN
1	B	190[B]	GLN
1	B	196	PHE
1	B	209[A]	ASP
1	B	209[B]	ASP
1	B	209[C]	ASP
1	B	225	ASN
1	B	231	LYS
1	B	264	ARG
1	B	342[A]	GLU
1	B	342[B]	GLU
1	B	374	VAL
1	C	12[A]	ASP
1	C	12[B]	ASP
1	C	27	LEU
1	C	49[A]	GLU
1	C	49[B]	GLU
1	C	107	LEU
1	C	115	ARG
1	C	116	ARG
1	C	183	ARG
1	C	191	ARG
1	C	196	PHE
1	C	204	VAL
1	C	206	GLN
1	C	265[A]	LYS
1	C	265[B]	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	302	GLU
1	C	329	GLU
1	C	337	LEU
1	C	374	VAL
1	D	9	THR
1	D	14	VAL
1	D	26	ASP
1	D	42	ARG
1	D	59	SER
1	D	86[A]	THR
1	D	86[B]	THR
1	D	94	LEU
1	D	123[A]	ARG
1	D	123[B]	ARG
1	D	127	LEU
1	D	132	LEU
1	D	140	SER
1	D	191[A]	ARG
1	D	191[B]	ARG
1	D	196	PHE
1	D	208[A]	ARG
1	D	208[B]	ARG
1	D	216	LEU
1	D	225	ASN
1	D	229[A]	LEU
1	D	229[B]	LEU
1	D	231[A]	LYS
1	D	231[B]	LYS
1	D	262	THR
1	D	263[A]	GLU
1	D	263[B]	GLU
1	D	265[A]	LYS
1	D	265[B]	LYS
1	D	269	SER
1	D	329	GLU
1	D	330	VAL
1	D	343[A]	ARG
1	D	343[B]	ARG
1	D	374	VAL
1	E	12	ASP
1	E	21	LEU
1	E	55	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	71	SER
1	E	80	THR
1	E	93[A]	VAL
1	E	93[B]	VAL
1	E	106	ARG
1	E	107	LEU
1	E	110	LYS
1	E	125	ARG
1	E	126	SER
1	E	130	SER
1	E	154	VAL
1	E	161	LEU
1	E	172	ARG
1	E	196	PHE
1	E	206	GLN
1	E	225	ASN
1	E	227[A]	ASP
1	E	227[B]	ASP
1	E	265[A]	LYS
1	E	265[B]	LYS
1	E	269	SER
1	E	278	PRO
1	E	309	VAL
1	E	312[A]	ARG
1	E	312[B]	ARG
1	E	329[A]	GLU
1	E	329[B]	GLU
1	E	343[A]	ARG
1	E	343[B]	ARG
1	E	355[A]	HIS
1	E	355[B]	HIS
1	E	393[A]	GLN
1	E	393[B]	GLN
1	F	21	LEU
1	F	27	LEU
1	F	44	ARG
1	F	115	ARG
1	F	116	ARG
1	F	120[A]	MET
1	F	120[B]	MET
1	F	125	ARG
1	F	127[A]	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	127[B]	LEU
1	F	131[A]	LEU
1	F	131[B]	LEU
1	F	135	MET
1	F	165	LEU
1	F	190[A]	GLN
1	F	190[B]	GLN
1	F	196	PHE
1	F	198	VAL
1	F	201	ASP
1	F	207	ARG
1	F	213	GLU
1	F	214	ASP
1	F	216	LEU
1	F	219	LEU
1	F	225	ASN
1	F	227	ASP
1	F	231	LYS
1	F	250	VAL
1	F	262	THR
1	F	264	ARG
1	F	302	GLU
1	F	309	VAL
1	F	312	ARG
1	F	330	VAL
1	F	374	VAL
1	F	375[A]	ARG
1	F	375[B]	ARG
1	F	376[A]	ARG
1	F	376[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
1	A	236	ASN
1	A	258	HIS
1	A	393	GLN
1	B	193	GLN
1	B	258	HIS
1	C	206	GLN
1	C	225	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	360	GLN
1	D	96	GLN
1	D	193	GLN
1	D	225	ASN
1	D	320	HIS
1	E	193	GLN
1	E	206	GLN
1	E	236	ASN
1	F	193	GLN
1	F	225	ASN
1	F	236	ASN

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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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	-
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	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
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
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

All (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
3	D	502	QR8	O2-C13	-4.63	1.39	1.46
3	F	503	QR8	O2-C13	-4.34	1.39	1.46
2	D	501	HEM	C1D-ND	-4.29	1.27	1.36
2	D	501	HEM	C3B-C2B	-4.24	1.34	1.40
3	E	503	QR8	O2-C13	-4.13	1.39	1.46
3	F	503	QR8	O2-C1	4.02	1.43	1.34
3	D	502	QR8	C10-C9	-3.89	1.46	1.52
3	E	503	QR8	O2-C1	3.78	1.43	1.34
2	C	501	HEM	C3B-CAB	-3.68	1.40	1.47
3	F	503	QR8	C10-C9	-3.53	1.47	1.52
2	B	501	HEM	C3C-C2C	-3.50	1.35	1.40
3	A	502	QR8	O2-C1	3.39	1.42	1.34
3	D	502	QR8	O2-C1	3.28	1.41	1.34
3	B	502	QR8	O2-C1	3.25	1.41	1.34
3	B	502	QR8	C10-C9	-3.22	1.47	1.52
4	B	513	RAM	O3-C3	3.10	1.50	1.43
2	B	501	HEM	C3B-C2B	-3.07	1.36	1.40
4	B	513	RAM	C4-C5	3.05	1.59	1.52
2	A	501	HEM	C1D-CHD	-3.03	1.32	1.41
2	A	501	HEM	C4D-C3D	2.96	1.49	1.42
3	C	502	QR8	O2-C1	2.87	1.41	1.34
2	D	501	HEM	C4D-C3D	2.85	1.49	1.42
4	A	503[B]	RAM	C6-C5	-2.85	1.44	1.51
4	B	513	RAM	C3-C2	2.67	1.59	1.52
2	E	502	HEM	C3B-C2B	-2.66	1.36	1.40
2	D	501	HEM	C3C-C2C	-2.65	1.36	1.40
2	B	501	HEM	CMD-C2D	-2.65	1.46	1.51
3	A	502	QR8	C10-C9	-2.59	1.48	1.52
3	E	503	QR8	C10-C9	-2.55	1.48	1.52
4	A	503[B]	RAM	O5-C1	2.47	1.49	1.42
4	D	503	RAM	O3-C3	2.40	1.48	1.43
2	C	501	HEM	C1D-CHD	-2.40	1.34	1.41
2	E	502	HEM	C4D-C3D	2.38	1.48	1.42
3	A	502	QR8	C7-C6	-2.37	1.50	1.54
4	A	503[A]	RAM	C6-C5	-2.36	1.45	1.51
4	B	513	RAM	C6-C5	2.35	1.57	1.51
2	A	501	HEM	C4A-NA	2.33	1.41	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C1A-CHA	-2.32	1.34	1.41
2	E	502	HEM	C4A-NA	2.29	1.40	1.36
3	D	502	QR8	C7-C6	-2.28	1.50	1.54
2	E	502	HEM	C1A-NA	2.26	1.40	1.36
3	B	502	QR8	C7-C6	-2.25	1.50	1.54
4	A	503[A]	RAM	O3-C3	-2.24	1.37	1.43
2	B	501	HEM	C3C-CAC	-2.16	1.43	1.47
2	B	501	HEM	C1D-ND	-2.12	1.31	1.36
2	F	502	HEM	C4D-C3D	2.05	1.47	1.42
3	E	503	QR8	C10-C11	-2.04	1.49	1.53
4	A	503[A]	RAM	C1-C2	-2.04	1.47	1.52
2	B	501	HEM	C1A-NA	2.01	1.40	1.36
2	A	501	HEM	CAA-C2A	2.01	1.55	1.52

All (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
4	B	513	RAM	C4-C3-C2	-5.02	102.06	110.82
3	A	502	QR8	C8-C9-C10	-4.94	110.53	119.10
4	A	503[A]	RAM	O4-C4-C3	4.78	121.40	110.35
4	B	513	RAM	O2-C2-C3	4.72	121.27	110.35
2	D	501	HEM	CBD-CAD-C3D	-4.72	103.78	112.48
2	A	501	HEM	CAD-CBD-CGD	4.70	120.56	112.67
4	B	513	RAM	C3-C4-C5	-4.66	102.51	109.77
4	B	513	RAM	O3-C3-C4	4.57	120.92	110.35
3	C	502	QR8	C8-C9-C10	-4.50	111.29	119.10
4	A	503[B]	RAM	C6-C5-C4	-4.49	104.78	113.07
2	B	501	HEM	CMA-C3A-C4A	-4.40	121.69	128.46
2	B	501	HEM	C4A-C3A-C2A	4.23	109.94	107.00
3	B	502	QR8	C36-C13-C12	-4.23	108.26	114.39
4	D	503	RAM	O1-C1-C2	4.19	120.82	109.03
4	A	503[B]	RAM	O3-C3-C4	-4.11	100.84	110.35
3	D	502	QR8	C8-C9-C10	-4.11	111.96	119.10
4	B	513	RAM	O4-C4-C5	4.09	118.74	109.67
2	A	501	HEM	C4A-C3A-C2A	4.02	109.79	107.00
3	D	502	QR8	O11-C9-C8	3.96	128.61	121.26
2	E	502	HEM	CBD-CAD-C3D	-3.95	105.20	112.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	502	QR8	C34-C10-C11	3.94	118.95	112.37
2	E	502	HEM	CBA-CAA-C2A	3.93	119.73	112.49
2	C	501	HEM	CMA-C3A-C4A	3.92	134.49	128.46
4	D	503	RAM	O2-C2-C1	3.83	118.04	109.16
4	D	503	RAM	O5-C1-C2	-3.83	103.46	110.28
4	D	503	RAM	O3-C3-C2	3.82	119.19	110.35
3	A	502	QR8	O11-C9-C8	3.78	128.28	121.26
3	D	502	QR8	C36-C13-C12	-3.76	108.94	114.39
2	C	501	HEM	CMA-C3A-C2A	-3.70	117.97	124.94
4	A	503[B]	RAM	C1-C2-C3	-3.63	102.79	110.31
2	B	501	HEM	CMC-C2C-C3C	3.59	131.40	124.68
3	B	502	QR8	C8-C9-C10	-3.56	112.92	119.10
3	E	503	QR8	C8-C9-C10	-3.55	112.93	119.10
2	E	502	HEM	C1D-C2D-C3D	-3.55	104.53	107.00
4	D	503	RAM	C4-C3-C2	-3.50	104.71	110.82
3	C	502	QR8	C34-C10-C9	3.48	114.13	108.08
3	E	503	QR8	O2-C1-C2	3.42	119.07	111.56
2	B	501	HEM	C4C-C3C-C2C	3.41	109.28	106.90
3	F	503	QR8	C32-C6-C5	-3.40	105.24	111.54
2	E	502	HEM	CMC-C2C-C3C	3.39	131.02	124.68
3	E	503	QR8	C36-C13-C12	-3.36	109.53	114.39
4	B	513	RAM	C1-C2-C3	3.32	117.21	110.31
3	A	502	QR8	C7-C8-C9	3.32	118.64	110.85
3	F	503	QR8	O2-C1-C2	3.31	118.83	111.56
4	A	503[A]	RAM	O2-C2-C1	-3.30	101.51	109.16
3	C	502	QR8	C34-C10-C11	3.30	117.87	112.37
4	D	503	RAM	C1-C2-C3	-3.22	103.63	110.31
3	E	503	QR8	C32-C6-C7	-3.20	105.89	110.69
2	A	501	HEM	CBA-CAA-C2A	3.18	118.35	112.49
4	A	503[B]	RAM	O5-C1-C2	-3.16	104.65	110.28
3	A	502	QR8	C32-C6-C7	-3.15	105.97	110.69
4	A	503[B]	RAM	O3-C3-C2	3.13	117.59	110.35
2	C	501	HEM	CMC-C2C-C3C	3.13	130.53	124.68
2	F	502	HEM	CMC-C2C-C3C	3.11	130.49	124.68
3	C	502	QR8	O11-C9-C10	3.10	125.01	120.60
3	B	502	QR8	O2-C1-C2	3.04	118.22	111.56
3	A	502	QR8	C34-C10-C11	3.03	117.43	112.37
3	B	502	QR8	C34-C10-C11	3.01	117.40	112.37
4	A	503[B]	RAM	O1-C1-O5	2.98	119.31	110.38
3	B	502	QR8	C32-C6-C7	-2.95	106.28	110.69
3	C	502	QR8	O2-C1-O1	-2.94	118.45	123.94
3	F	503	QR8	C36-C13-C12	-2.90	110.19	114.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	503	QR8	C7-C8-C9	2.90	117.66	110.85
3	D	502	QR8	O2-C1-C2	2.89	117.89	111.56
3	A	502	QR8	C36-C13-C12	-2.88	110.22	114.39
4	D	503	RAM	O5-C5-C4	-2.85	104.40	109.52
3	F	503	QR8	C10-C11-C12	-2.83	108.57	114.41
3	A	502	QR8	C32-C6-C5	-2.80	106.34	111.54
3	E	503	QR8	C32-C6-C5	-2.78	106.38	111.54
2	A	501	HEM	CMA-C3A-C4A	-2.77	124.21	128.46
2	D	501	HEM	CMA-C3A-C4A	-2.76	124.22	128.46
3	A	502	QR8	C2-C3-C4	-2.76	108.72	114.41
2	B	501	HEM	CAD-CBD-CGD	2.74	117.27	112.67
3	F	503	QR8	O7-C5-C6	-2.72	104.72	109.83
3	C	502	QR8	O2-C1-C2	2.72	117.52	111.56
3	B	502	QR8	C7-C8-C9	2.71	117.22	110.85
3	D	502	QR8	C7-C8-C9	2.67	117.13	110.85
3	D	502	QR8	C2-C3-C4	-2.65	108.94	114.41
4	D	503	RAM	O4-C4-C5	2.65	115.53	109.67
2	D	501	HEM	C4A-C3A-C2A	2.65	108.84	107.00
3	C	502	QR8	C7-C8-C9	2.65	117.06	110.85
2	F	502	HEM	C4A-C3A-C2A	2.64	108.83	107.00
2	F	502	HEM	CBD-CAD-C3D	-2.62	107.65	112.48
3	E	503	QR8	O2-C1-O1	-2.61	119.06	123.94
4	A	503[A]	RAM	O5-C1-C2	2.61	114.94	110.28
3	A	502	QR8	O2-C1-C2	2.58	117.23	111.56
2	C	501	HEM	CAD-CBD-CGD	2.57	116.98	112.67
3	F	503	QR8	C35-C12-C13	-2.57	108.86	112.18
4	A	503[B]	RAM	O5-C5-C6	2.55	112.22	106.70
3	D	502	QR8	C11-C10-C9	-2.54	105.76	110.36
3	F	503	QR8	C2-C3-C4	-2.53	109.19	114.41
3	B	502	QR8	O11-C9-C8	2.44	125.80	121.26
3	B	502	QR8	C2-C3-C4	-2.38	109.51	114.41
4	A	503[A]	RAM	C6-C5-C4	-2.37	108.69	113.07
3	E	503	QR8	C6-C5-C4	-2.33	112.66	116.27
3	F	503	QR8	O2-C1-O1	-2.33	119.59	123.94
3	B	502	QR8	C32-C6-C5	-2.31	107.25	111.54
2	D	501	HEM	CBA-CAA-C2A	2.29	116.70	112.49
3	E	503	QR8	C11-C10-C9	-2.29	106.22	110.36
3	E	503	QR8	C34-C10-C9	2.27	112.03	108.08
3	B	502	QR8	C11-C10-C9	-2.27	106.24	110.36
2	A	501	HEM	CBD-CAD-C3D	-2.27	108.30	112.48
3	F	503	QR8	C13-O2-C1	-2.25	114.25	117.51
4	A	503[B]	RAM	O2-C2-C3	2.24	115.52	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	503[A]	RAM	O2-C2-C3	2.24	115.52	110.35
2	F	502	HEM	C1D-C2D-C3D	-2.21	105.45	107.00
2	A	501	HEM	CMC-C2C-C3C	2.20	128.79	124.68
4	A	503[A]	RAM	O3-C3-C4	2.20	115.43	110.35
4	A	503[B]	RAM	O5-C5-C4	-2.19	105.59	109.52
2	C	501	HEM	CMD-C2D-C1D	-2.19	125.10	128.46
2	F	502	HEM	CBA-CAA-C2A	2.17	116.49	112.49
3	D	502	QR8	O2-C1-O1	-2.16	119.91	123.94
4	A	503[A]	RAM	C3-C4-C5	-2.14	106.43	109.77
2	E	502	HEM	C3B-C4B-NB	-2.11	106.48	109.21
2	B	501	HEM	CMB-C2B-C3B	2.10	128.61	124.68
2	D	501	HEM	CAD-CBD-CGD	2.10	116.20	112.67
2	C	501	HEM	C1D-C2D-C3D	2.08	108.44	107.00
4	D	503	RAM	O2-C2-C3	2.08	115.15	110.35
2	F	502	HEM	CMA-C3A-C4A	-2.03	125.35	128.46
4	D	503	RAM	O5-C5-C6	2.02	111.05	106.70

There are no chirality outliers.

All (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
3	C	502	QR8	C6-C7-C8-C33
3	C	502	QR8	C1-C2-C3-O3
3	D	502	QR8	C6-C7-C8-C9
3	D	502	QR8	C6-C7-C8-C33
3	D	502	QR8	C31-C4-C5-O7
3	D	502	QR8	C3-C4-C5-O7
3	D	502	QR8	C30-C2-C3-C4
3	D	502	QR8	C1-C2-C3-O3
3	F	503	QR8	C30-C2-C3-C4
3	E	503	QR8	C6-C7-C8-C9
3	A	502	QR8	C3-C4-C5-O7
3	B	502	QR8	C3-C4-C5-O7
3	F	503	QR8	C3-C4-C5-O7
3	E	503	QR8	C3-C4-C5-O7
3	C	502	QR8	C3-C4-C5-O7
3	A	502	QR8	C30-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	502	QR8	C30-C2-C3-O3
3	C	502	QR8	C30-C2-C3-O3
3	D	502	QR8	C30-C2-C3-O3
3	F	503	QR8	C30-C2-C3-O3
3	A	502	QR8	C30-C2-C3-C4
3	B	502	QR8	C30-C2-C3-C4
3	C	502	QR8	C30-C2-C3-C4
3	A	502	QR8	C31-C4-C5-O7
3	B	502	QR8	C31-C4-C5-O7
3	C	502	QR8	C31-C4-C5-O7
3	F	503	QR8	C31-C4-C5-O7
3	E	503	QR8	C31-C4-C5-O7
3	A	502	QR8	C6-C7-C8-C33
3	E	503	QR8	C6-C7-C8-C33
3	D	502	QR8	C3-C4-C5-C6
3	F	503	QR8	C3-C4-C5-C6
3	E	503	QR8	C30-C2-C3-C4
3	D	502	QR8	C31-C4-C5-C6
3	B	502	QR8	C5-C6-C7-C8
3	E	503	QR8	C30-C2-C3-O3
3	F	503	QR8	C7-C8-C9-C10
3	A	502	QR8	C31-C4-C5-C6
3	C	502	QR8	C31-C4-C5-C6
3	F	503	QR8	C31-C4-C5-C6
3	B	502	QR8	C31-C4-C5-C6
3	E	503	QR8	C31-C4-C5-C6
3	B	502	QR8	C3-C4-C5-C6
3	C	502	QR8	C3-C4-C5-C6
3	E	503	QR8	C3-C4-C5-C6
3	A	502	QR8	C3-C4-C5-C6
3	A	502	QR8	C32-C6-C7-C8
3	D	502	QR8	C32-C6-C7-C8
3	A	502	QR8	C1-C2-C3-C4
3	B	502	QR8	C1-C2-C3-C4
3	C	502	QR8	C1-C2-C3-C4
3	D	502	QR8	C1-C2-C3-C4
3	F	503	QR8	C1-C2-C3-C4
3	F	503	QR8	C1-C2-C3-O3
3	E	503	QR8	C1-C2-C3-C4
3	E	503	QR8	C1-C2-C3-O3
3	B	502	QR8	O7-C5-C6-C7
3	B	502	QR8	C6-C7-C8-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	502	QR8	C5-C6-C7-C8
3	D	502	QR8	C5-C6-C7-C8
3	E	503	QR8	C5-C6-C7-C8
3	A	502	QR8	C33-C8-C9-C10
3	F	503	QR8	C33-C8-C9-C10
3	B	502	QR8	C32-C6-C7-C8
3	E	503	QR8	C32-C6-C7-C8
3	F	503	QR8	C33-C8-C9-O11
3	B	502	QR8	C4-C5-C6-C7
3	C	502	QR8	O1-C1-O2-C13
3	E	503	QR8	C2-C1-O2-C13
3	C	502	QR8	C32-C6-C7-C8
3	C	502	QR8	C12-C13-O2-C1
3	F	503	QR8	O12-C11-C12-C35
3	C	502	QR8	C2-C1-O2-C13
3	D	502	QR8	C33-C8-C9-C10
3	E	503	QR8	C33-C8-C9-C10
3	F	503	QR8	C7-C8-C9-O11
3	E	503	QR8	C4-C5-C6-C7

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
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

Continued on next page...

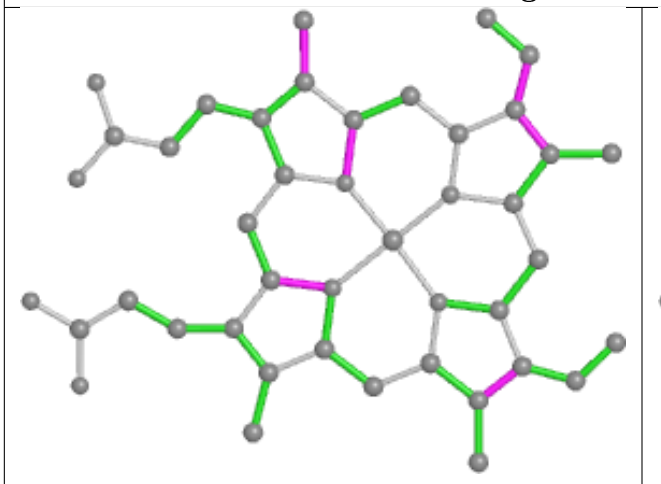
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

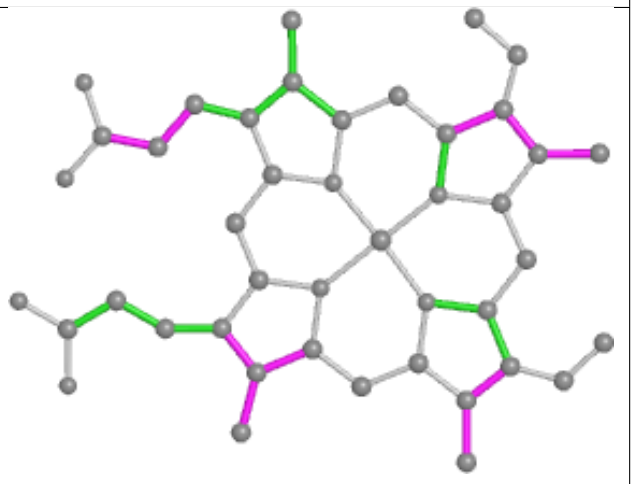
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

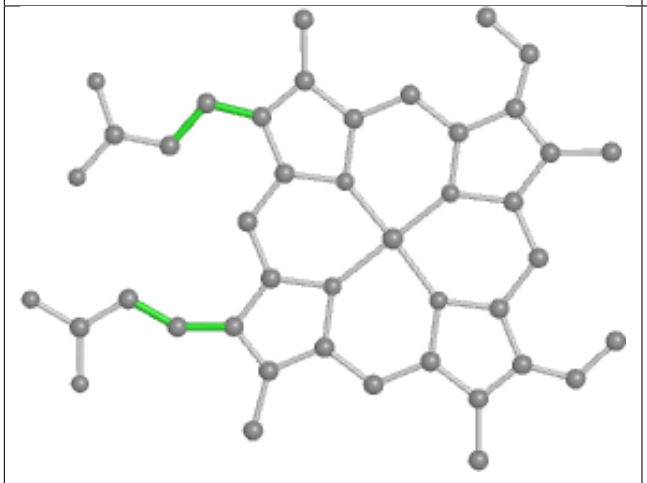
Ligand HEM B 501



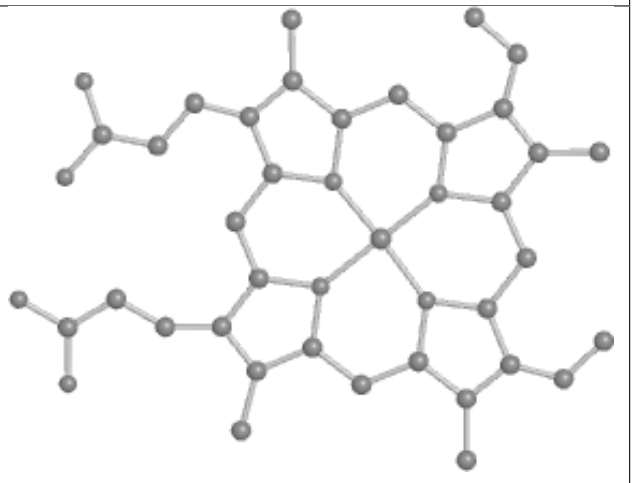
Bond lengths



Bond angles

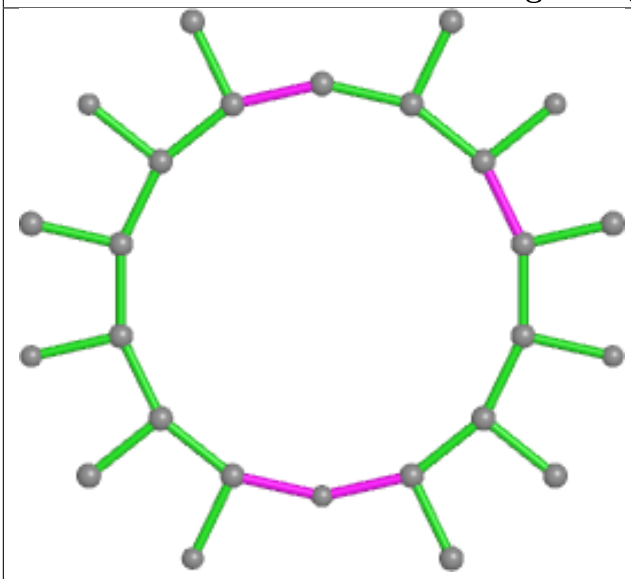


Torsions

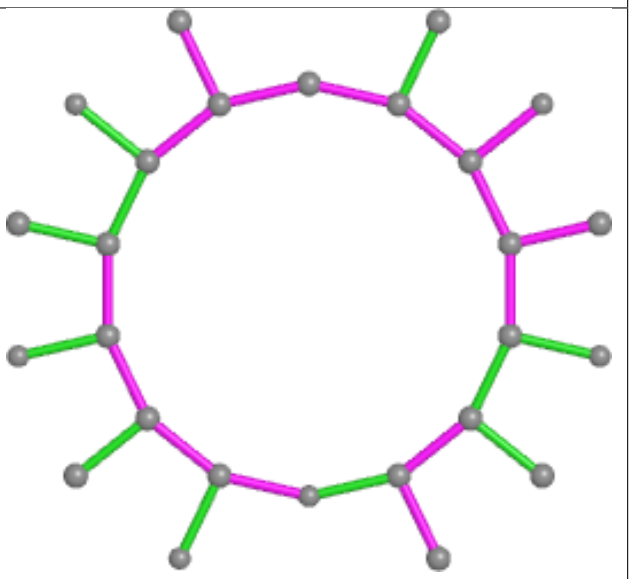


Rings

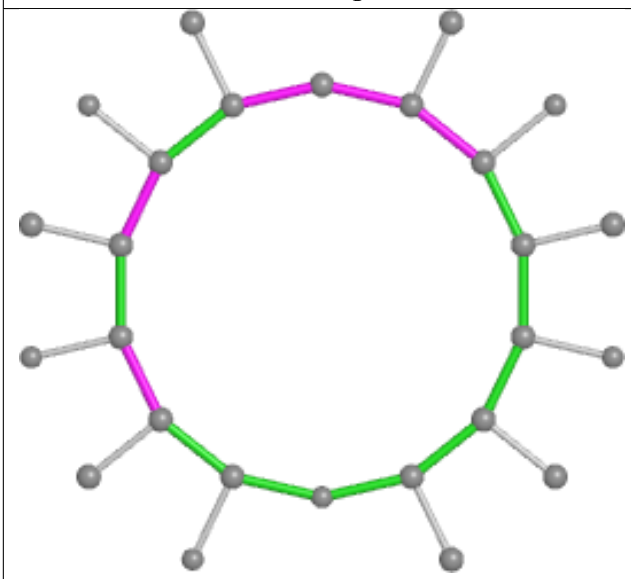
Ligand QR8 A 502



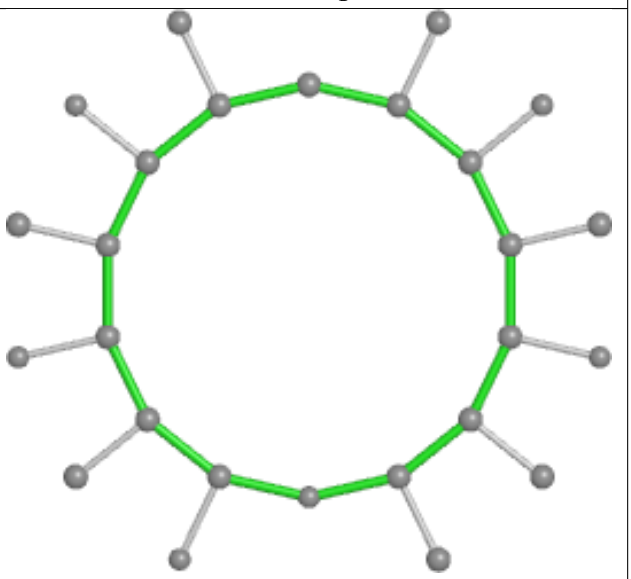
Bond lengths



Bond angles

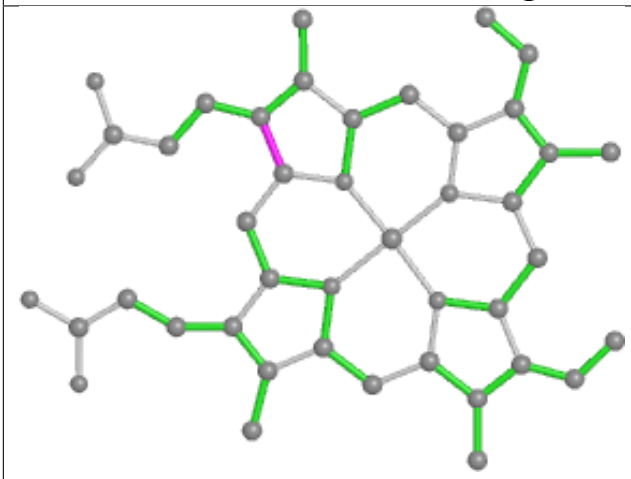


Torsions

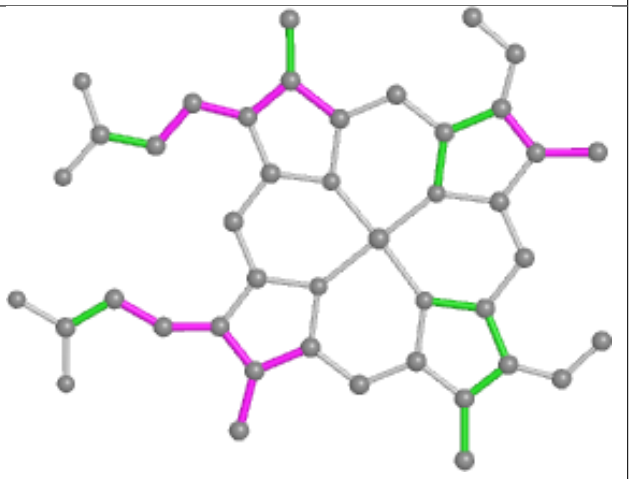


Rings

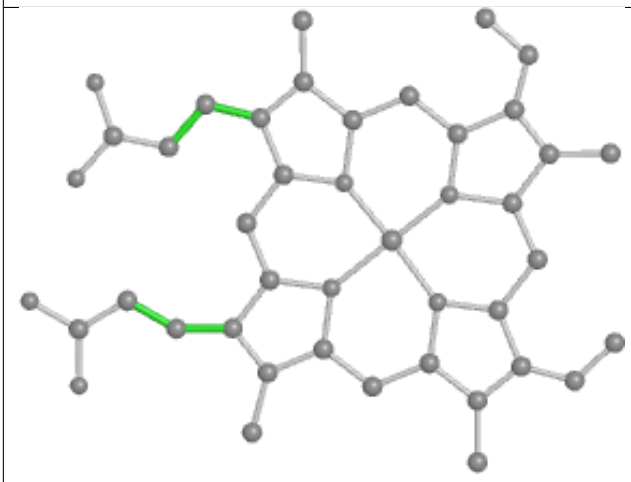
Ligand HEM F 502



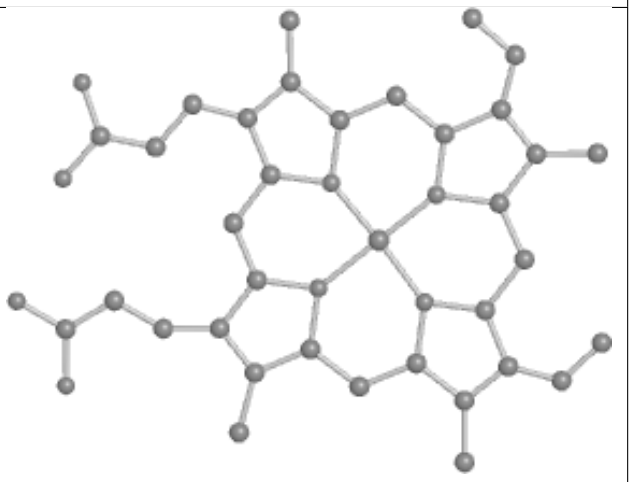
Bond lengths



Bond angles

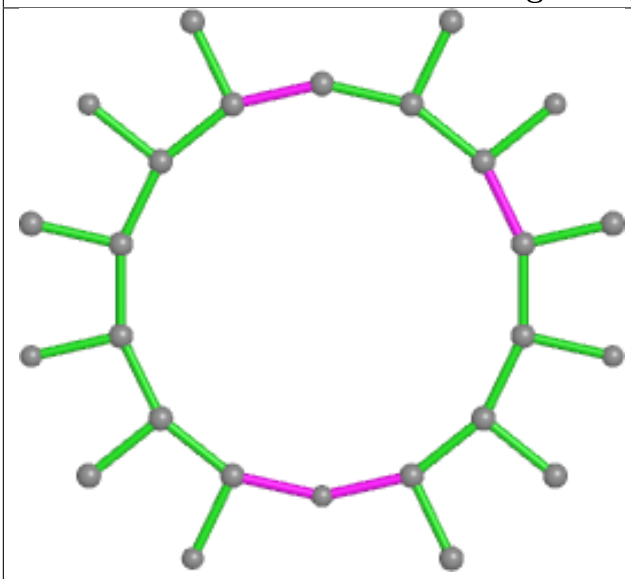


Torsions

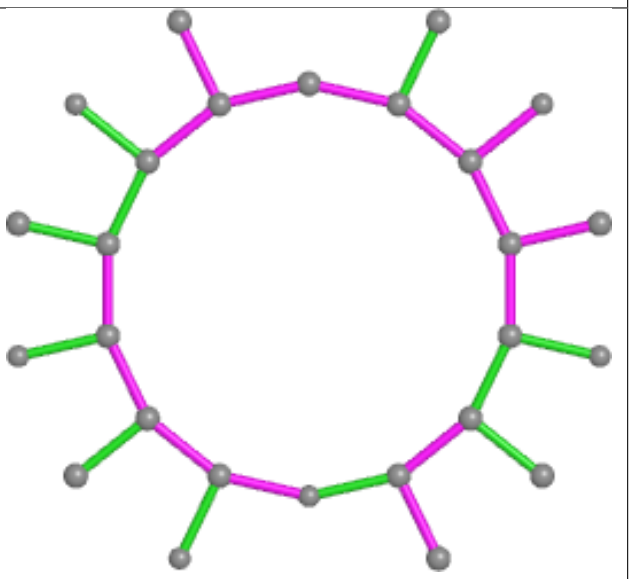


Rings

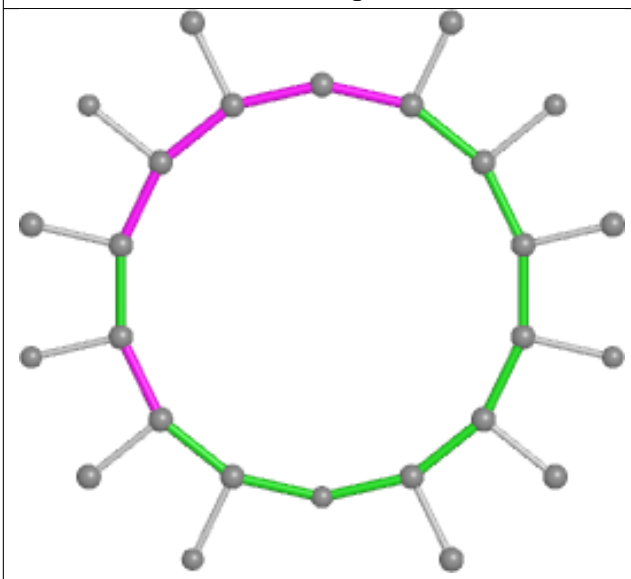
Ligand QR8 B 502



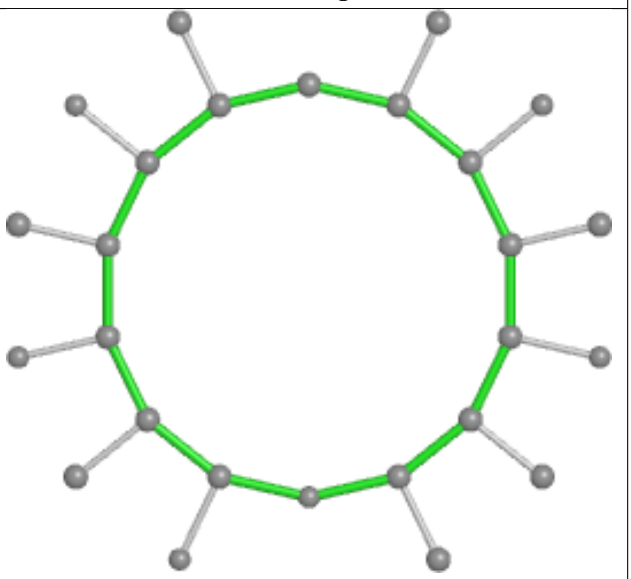
Bond lengths



Bond angles

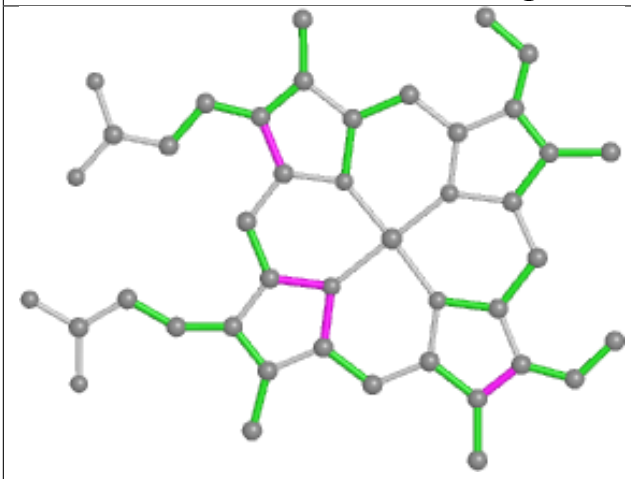


Torsions

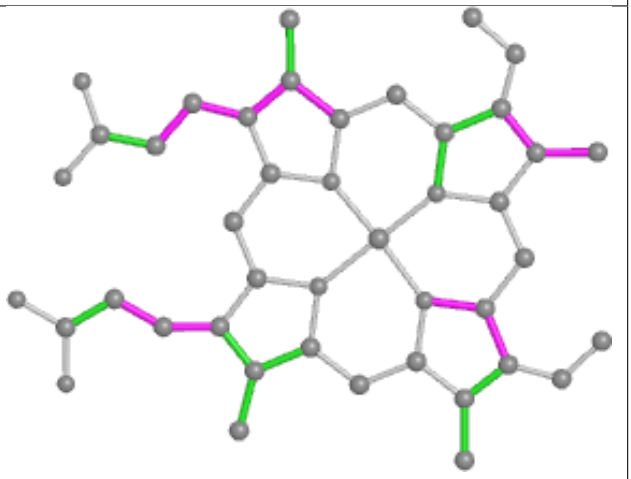


Rings

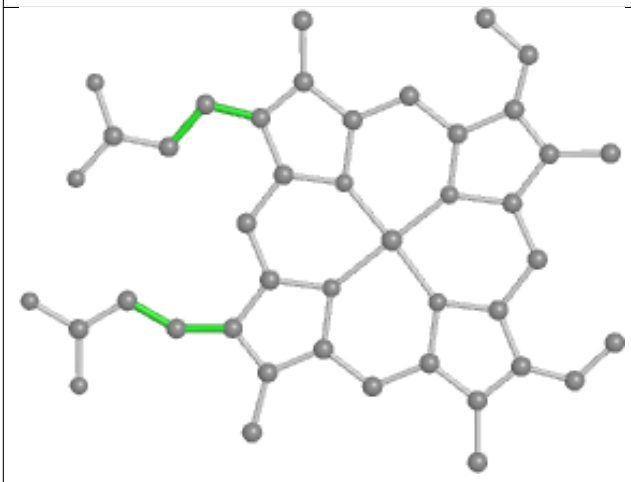
Ligand HEM E 502



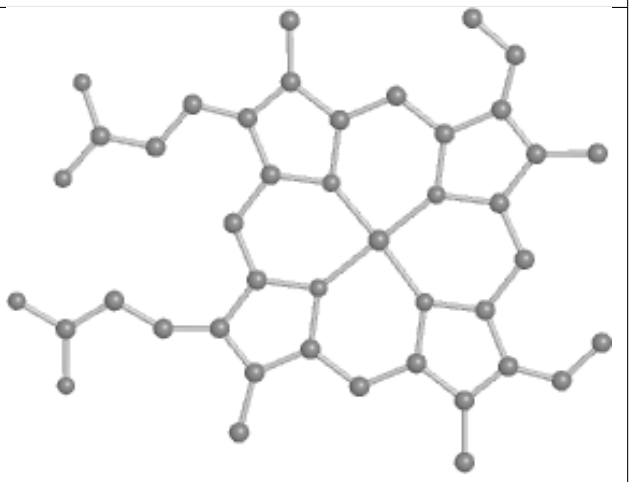
Bond lengths



Bond angles

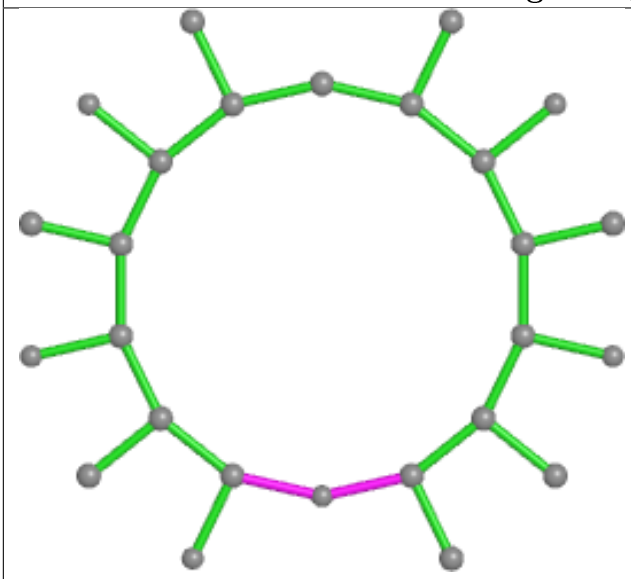


Torsions

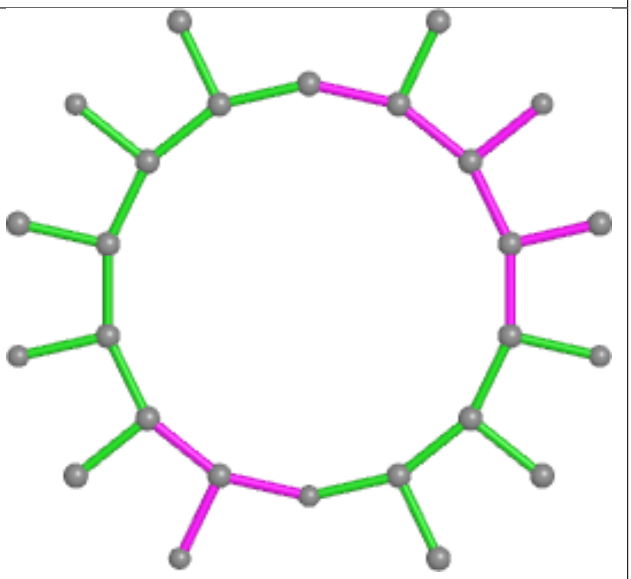


Rings

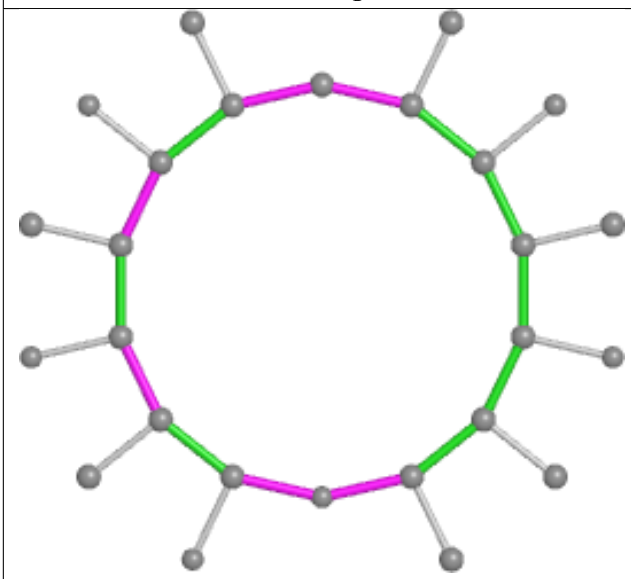
Ligand QR8 C 502



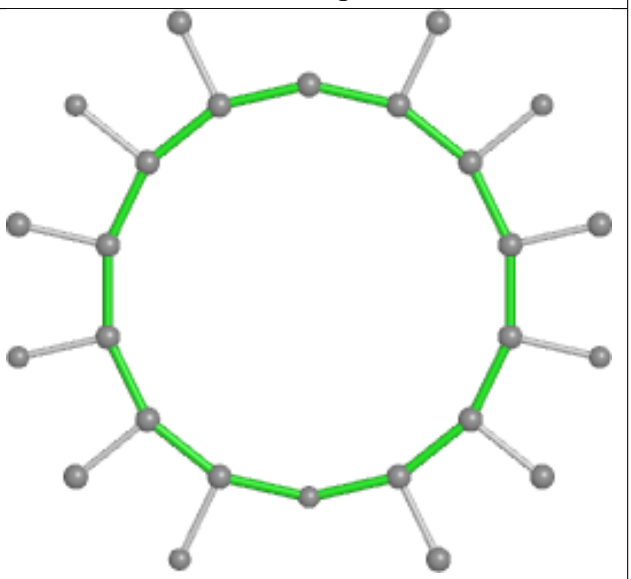
Bond lengths



Bond angles

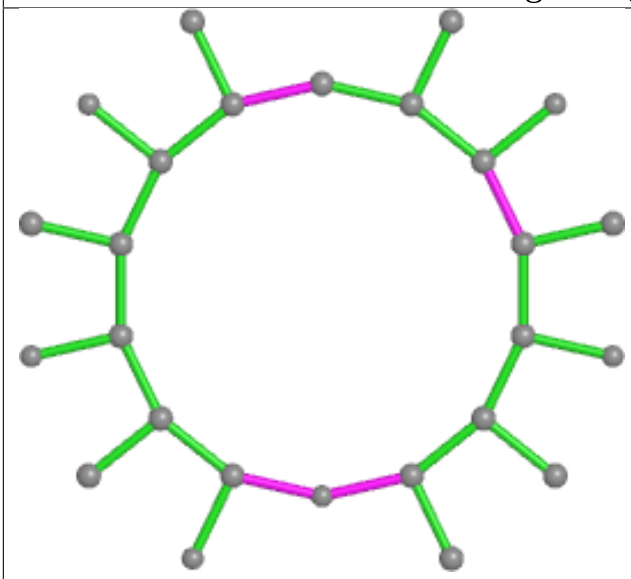


Torsions

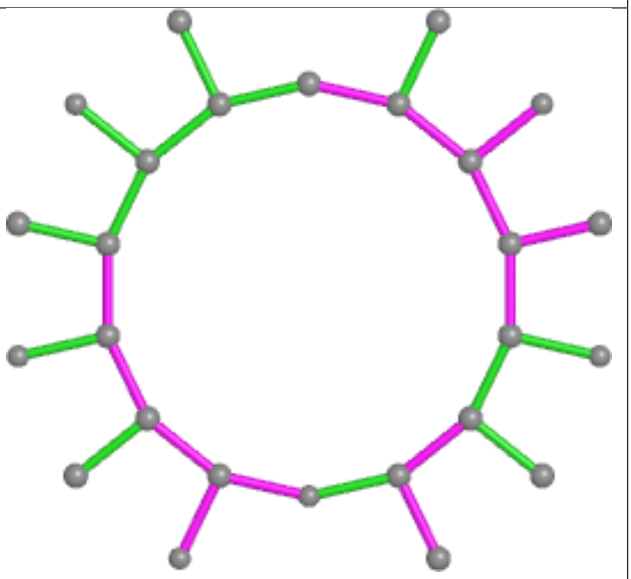


Rings

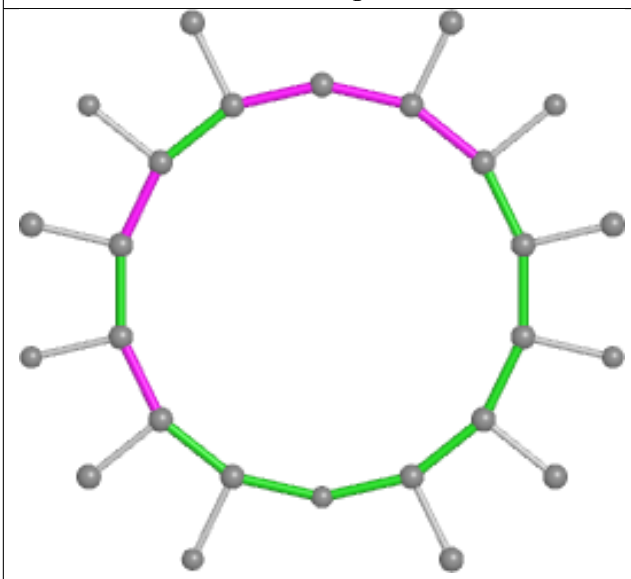
Ligand QR8 D 502



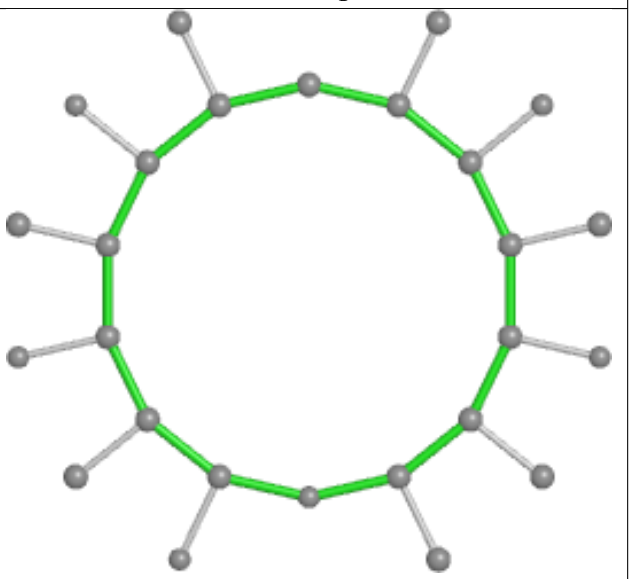
Bond lengths



Bond angles

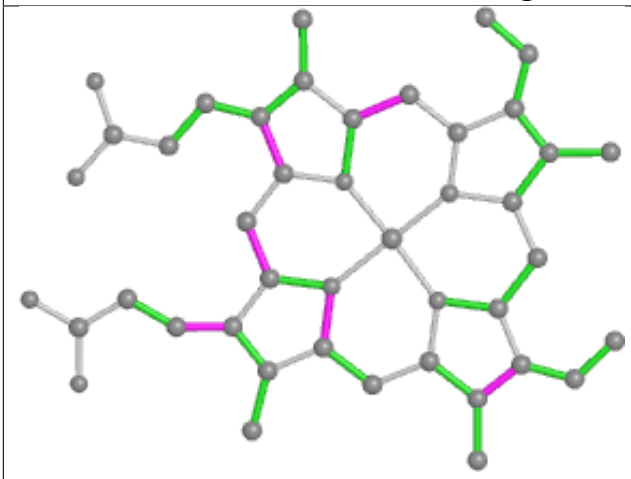


Torsions

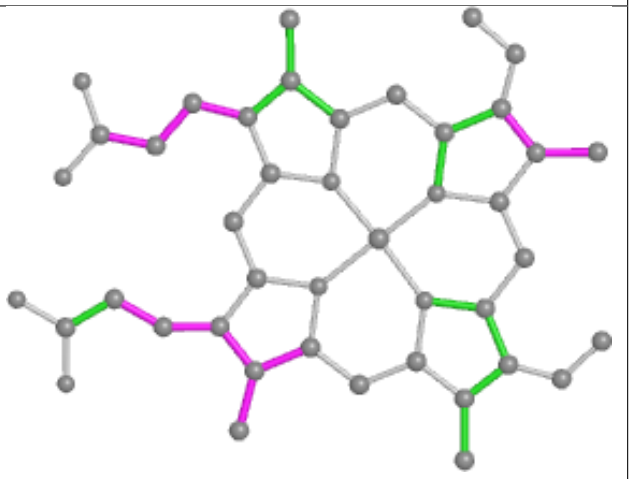


Rings

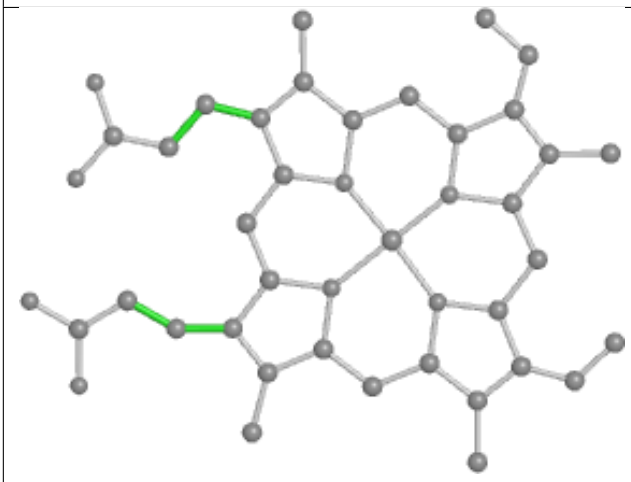
Ligand HEM A 501



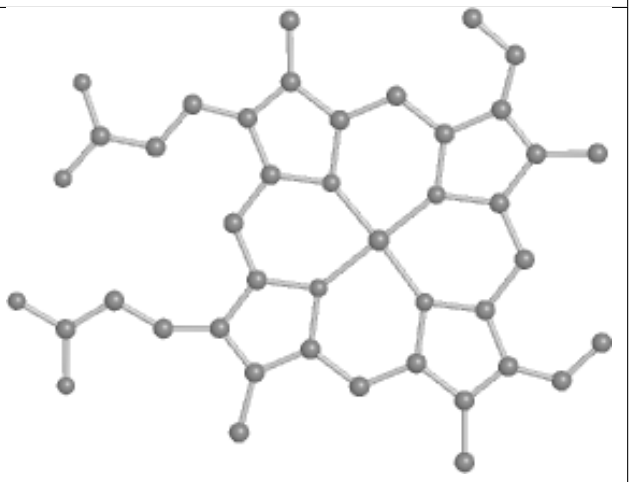
Bond lengths



Bond angles

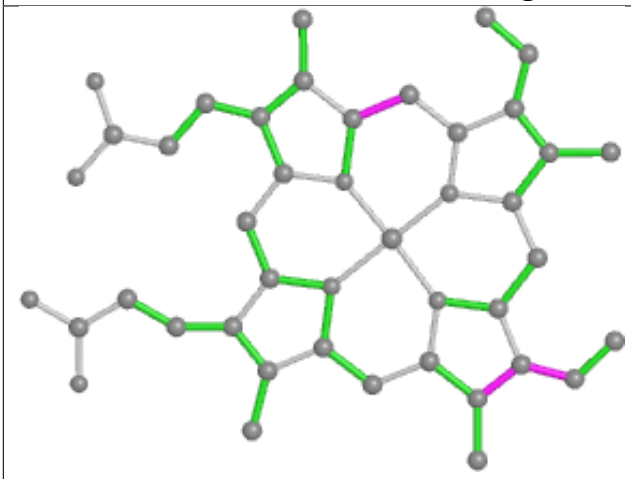


Torsions

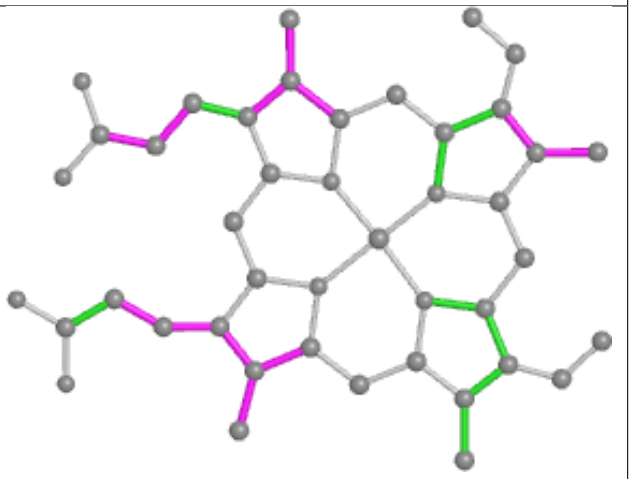


Rings

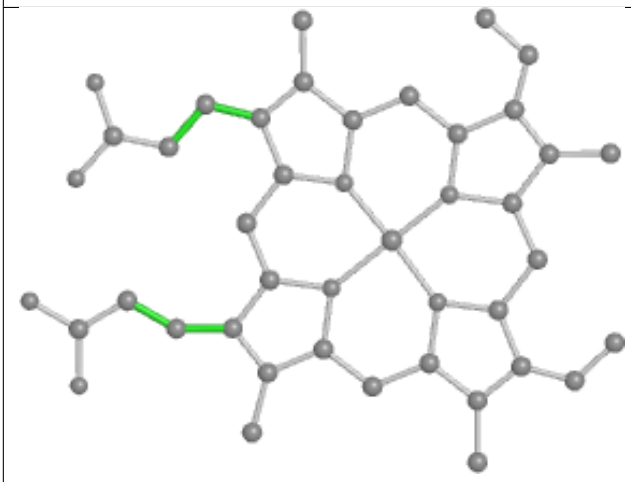
Ligand HEM C 501



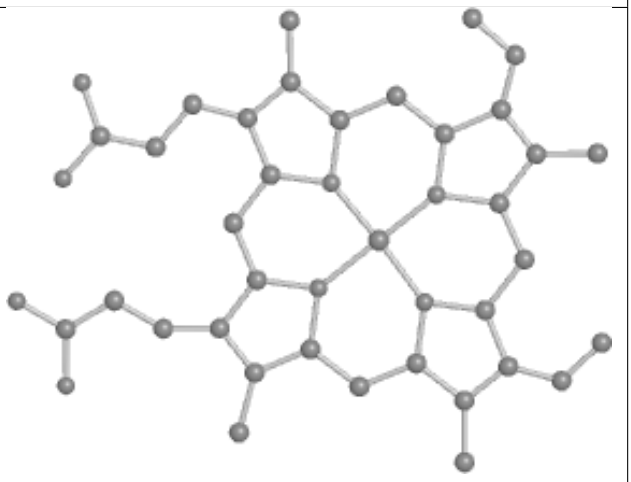
Bond lengths



Bond angles

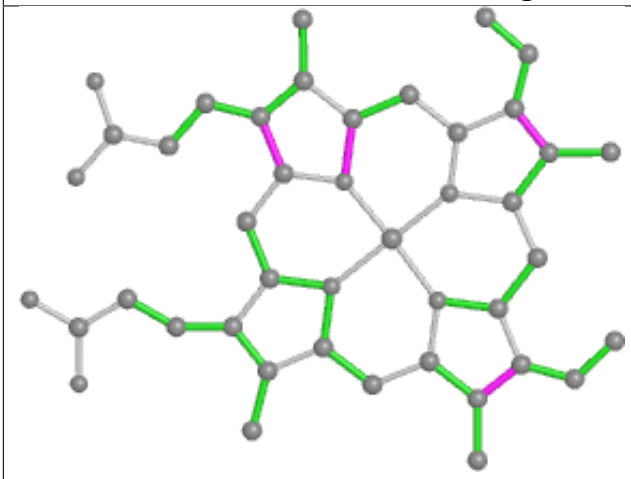


Torsions

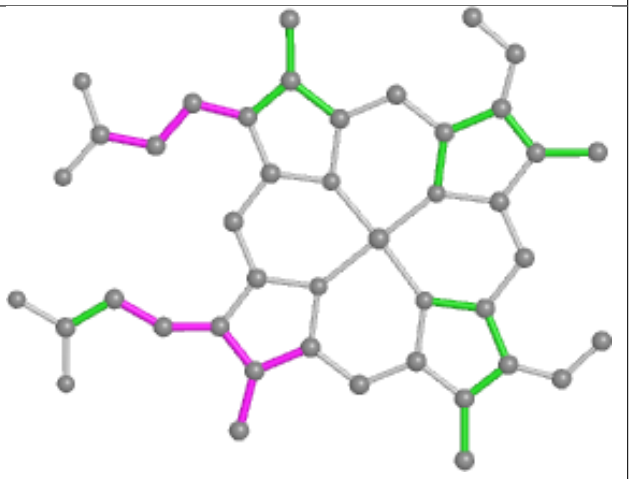


Rings

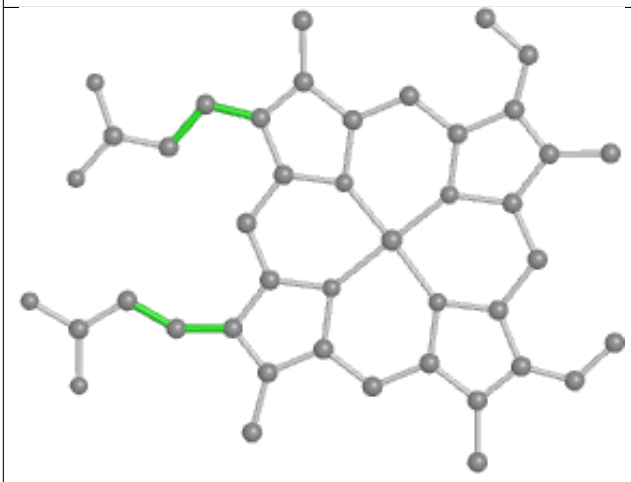
Ligand HEM D 501



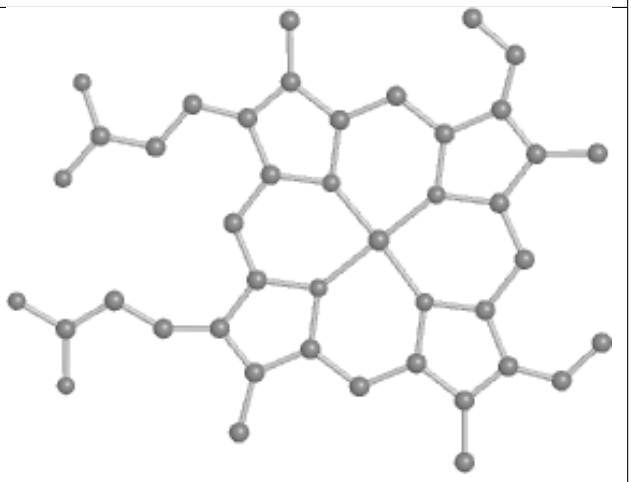
Bond lengths



Bond angles

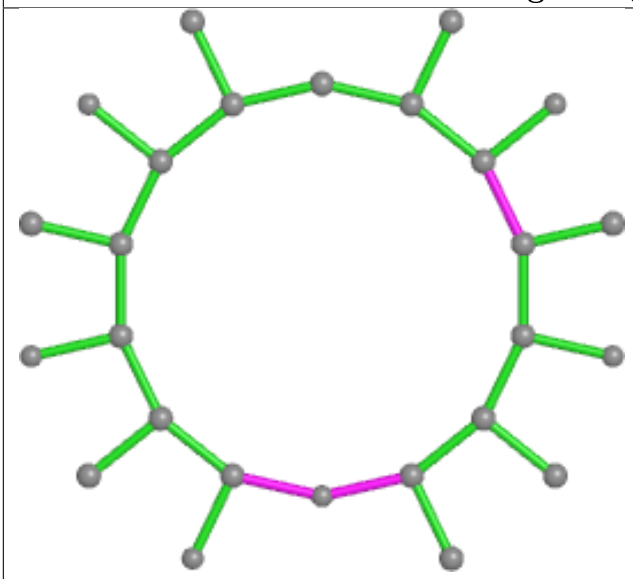


Torsions

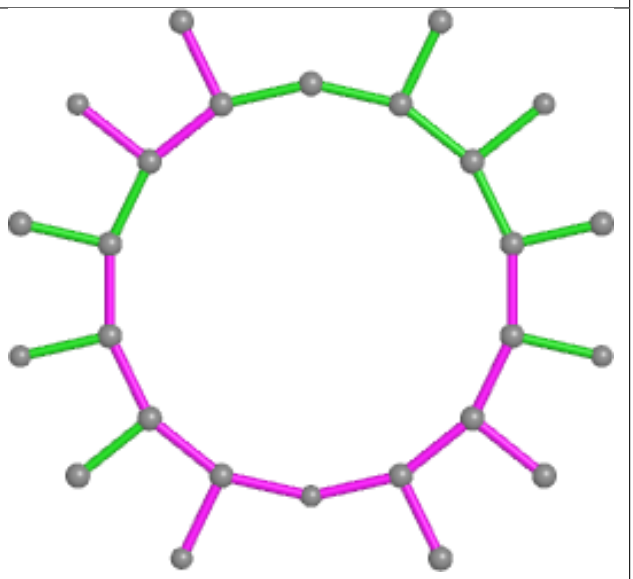


Rings

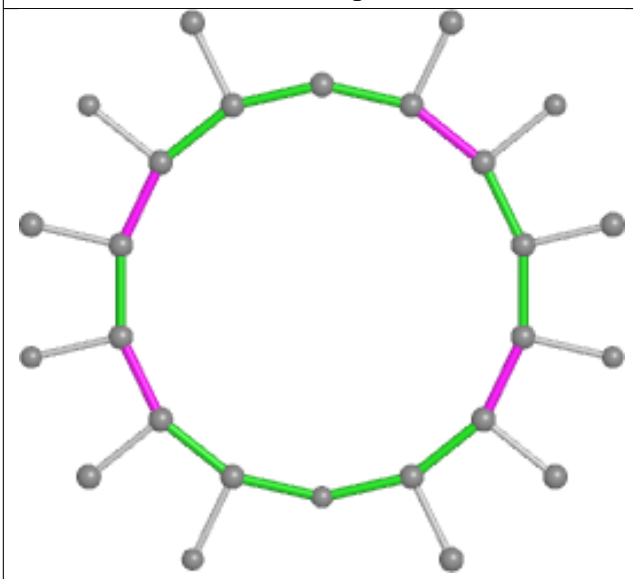
Ligand QR8 F 503



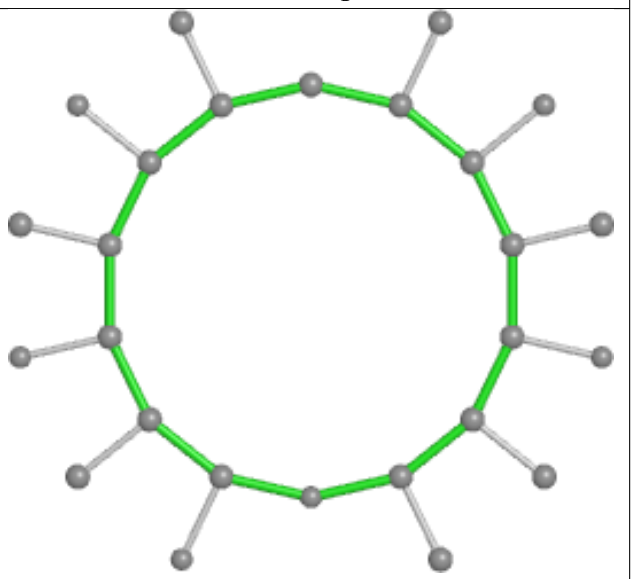
Bond lengths



Bond angles

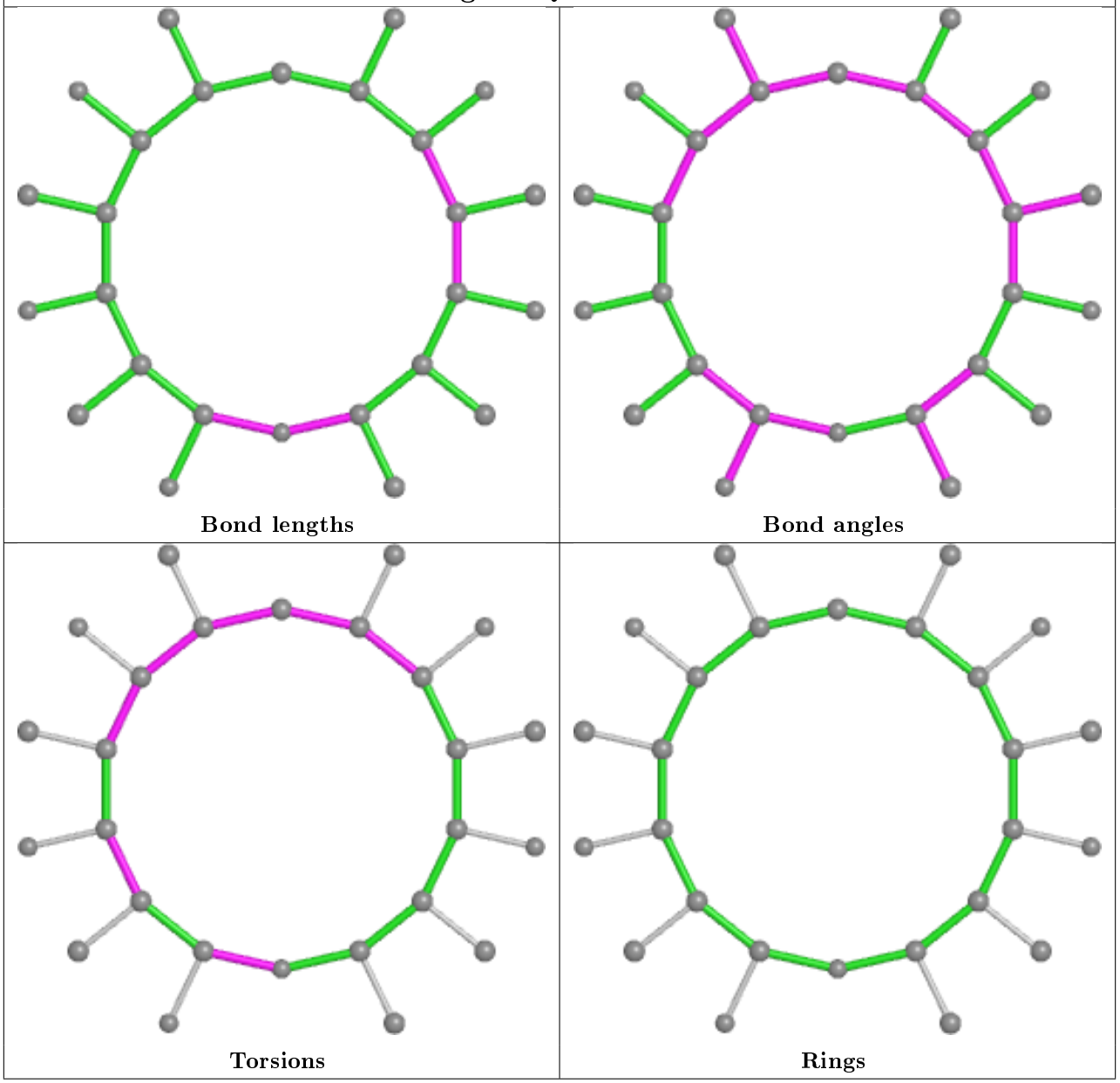


Torsions



Rings

Ligand QR8 E 503



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

All (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
1	D	10	PRO	7.6
1	E	313	ALA	7.6
1	F	377[A]	PHE	7.5
1	F	380[A]	LEU	7.4
1	F	129[A]	ASP	7.4
1	B	9	THR	7.1
1	F	124	VAL	6.7
1	B	209[A]	ASP	6.4
1	F	132[A]	LEU	6.2
1	F	125	ARG	5.9
1	F	262	THR	5.9
1	F	141	PRO	5.8
1	F	123	ARG	5.7
1	F	23[A]	HIS	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	379[A]	THR	5.4
1	F	271	VAL	5.2
1	E	312[A]	ARG	5.1
1	D	208[A]	ARG	5.0
1	F	273	ASP	5.0
1	D	226	ASP	4.8
1	F	404	ILE	4.8
1	F	36	ARG	4.8
1	F	277	VAL	4.8
1	D	225	ASN	4.8
1	F	382[A]	LEU	4.7
1	C	9	THR	4.7
1	D	224	ASP	4.7
1	F	270	LEU	4.7
1	D	210	ALA	4.6
1	F	265	LYS	4.6
1	F	385	PRO	4.6
1	F	142	ALA	4.5
1	E	304	VAL	4.5
1	F	332	ASP	4.5
1	E	209[A]	ASP	4.4
1	E	311[A]	VAL	4.4
1	E	11	ALA	4.4
1	D	209[A]	ASP	4.3
1	F	126	SER	4.3
1	D	205	ALA	4.3
1	E	305[A]	GLU	4.2
1	F	267	TYR	4.1
1	F	388	GLY	4.1
1	D	223	THR	4.1
1	F	407	TRP	4.0
1	F	406	SER	4.0
1	F	364	LEU	4.0
1	E	307	SER	4.0
1	E	212	THR	4.0
1	E	306	LEU	3.9
1	E	213	GLU	3.9
1	E	13	ALA	3.9
1	D	228[A]	HIS	3.9
1	F	140	SER	3.8
1	F	264	ARG	3.8
1	E	265[A]	LYS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	13	ALA	3.8
1	F	24	ALA	3.7
1	F	131[A]	LEU	3.7
1	E	12	ASP	3.7
1	B	210	ALA	3.7
1	A	209[A]	ASP	3.7
1	F	272	ALA	3.6
1	E	333	HIS	3.6
1	E	310[A]	THR	3.6
1	E	301	THR	3.5
1	F	376[A]	ARG	3.4
1	D	191[A]	ARG	3.4
1	F	386	VAL	3.4
1	F	375[A]	ARG	3.3
1	D	222	ALA	3.3
1	E	14[A]	VAL	3.3
1	F	328	GLU	3.3
1	E	332	ASP	3.3
1	E	36[A]	ARG	3.2
1	E	39	PRO	3.2
1	F	215	LEU	3.2
1	F	225	ASN	3.2
1	E	37	ASP	3.2
1	F	120[A]	MET	3.2
1	F	130[A]	SER	3.1
1	E	309	VAL	3.1
1	D	263[A]	GLU	3.1
1	F	261	LEU	3.1
1	F	139	GLY	3.1
1	F	343	ARG	3.1
1	F	334	ALA	3.0
1	F	371	SER	3.0
1	F	383	ALA	3.0
1	E	314	GLY	3.0
1	F	329	GLU	2.9
1	E	34[A]	LEU	2.9
1	E	42	ARG	2.9
1	F	224[A]	ASP	2.9
1	F	330	VAL	2.8
1	D	141	PRO	2.8
1	F	378	PRO	2.8
1	A	225[A]	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	66	GLY	2.8
1	E	210	ALA	2.8
1	E	272	ALA	2.8
1	E	29	PRO	2.8
1	F	21	LEU	2.8
1	F	333	HIS	2.8
1	F	340	HIS	2.8
1	B	265[A]	LYS	2.8
1	E	69	ARG	2.8
1	F	134	ASP	2.7
1	F	402[A]	ARG	2.8
1	A	224[A]	ASP	2.7
1	F	331	PHE	2.7
1	E	303	ASP	2.7
1	F	29	PRO	2.7
1	D	8	PRO	2.6
1	E	388	GLY	2.6
1	F	37	ASP	2.6
1	E	223[A]	THR	2.6
1	F	269	SER	2.6
1	E	30	HIS	2.6
1	A	379	THR	2.6
1	D	227[A]	ASP	2.5
1	F	57[A]	ARG	2.5
1	F	274	PRO	2.5
1	F	372	ALA	2.5
1	E	60	ASP	2.5
1	F	138	HIS	2.4
1	F	32	ALA	2.4
1	B	333[A]	HIS	2.4
1	F	268	GLU	2.4
1	F	326[A]	ARG	2.4
1	F	136[A]	VAL	2.4
1	F	263	GLU	2.3
1	F	137	ALA	2.3
1	F	128[A]	VAL	2.3
1	F	122	PRO	2.3
1	C	10	PRO	2.3
1	F	327	ASP	2.3
1	E	329[A]	GLU	2.2
1	E	336[A]	GLU	2.2
1	E	51	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	343[A]	ARG	2.2
1	E	269	SER	2.2
1	F	10	PRO	2.2
1	D	335[A]	ASP	2.2
1	F	35	ARG	2.1
1	E	211	PRO	2.1
1	C	11	ALA	2.1
1	D	385	PRO	2.1
1	D	406	SER	2.1
1	E	268	GLU	2.1
1	F	30	HIS	2.1
1	E	271	VAL	2.1
1	C	343[A]	ARG	2.1
1	B	211	PRO	2.1
1	F	33[A]	GLU	2.0
1	E	40	VAL	2.0
1	E	299	VAL	2.0
1	D	334	ALA	2.0
1	D	332[A]	ASP	2.0
1	F	337[A]	LEU	2.0
1	A	343	ARG	2.0

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

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

6.3 Carbohydrates (i)

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
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

Continued on next page...

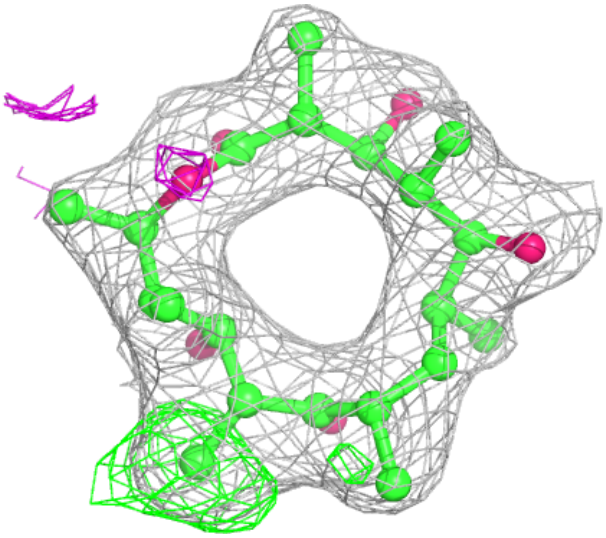
Continued from previous page...

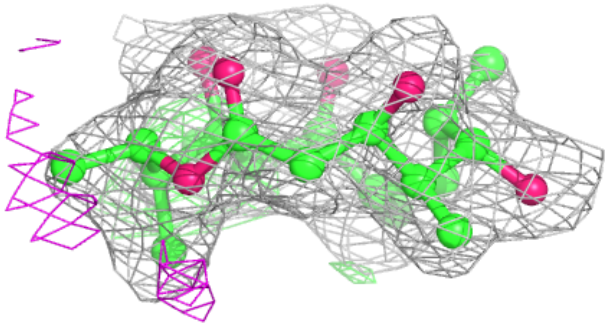
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	QR8	A	502	26/26	0.93	0.17	33,38,42,43	0
5	FMT	B	505	3/3	0.93	0.08	62,62,65,69	0
3	QR8	D	502	26/26	0.94	0.16	43,48,51,58	0
5	FMT	B	503	3/3	0.94	0.07	53,53,58,63	0
6	NA	D	513	1/1	0.94	0.14	54,54,54,54	0
3	QR8	C	502	26/26	0.94	0.15	30,35,37,42	0
5	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

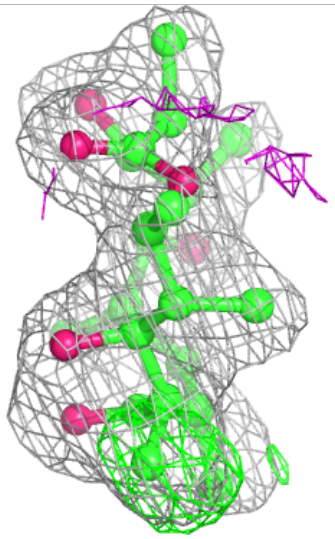
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

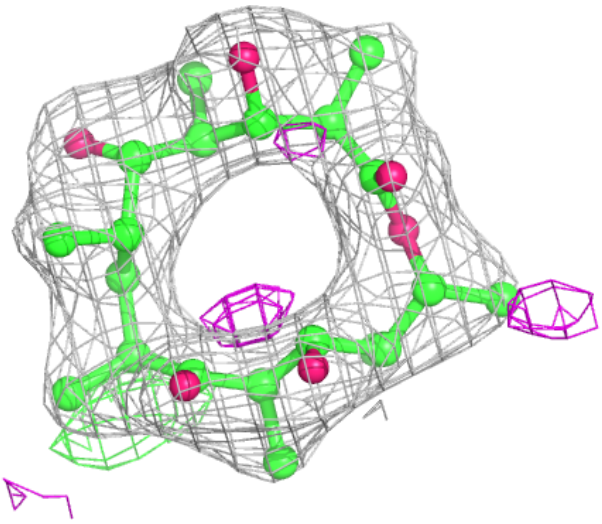


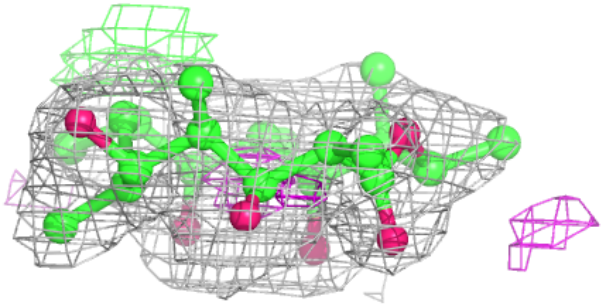


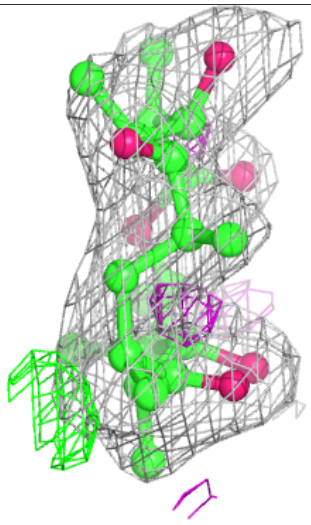


Electron density around QR8 F 503:

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

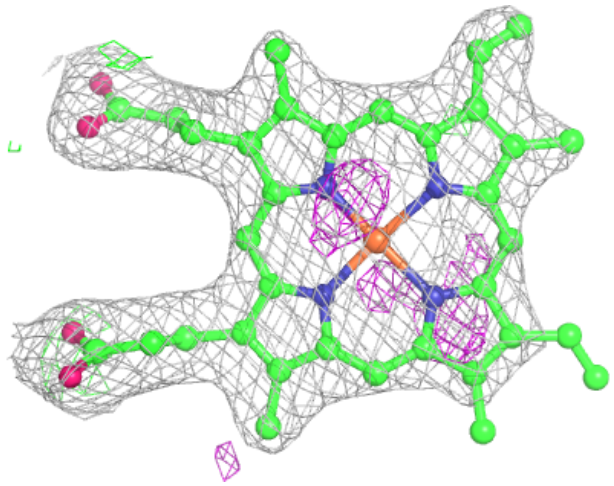


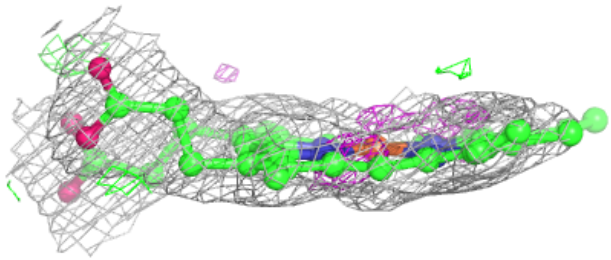


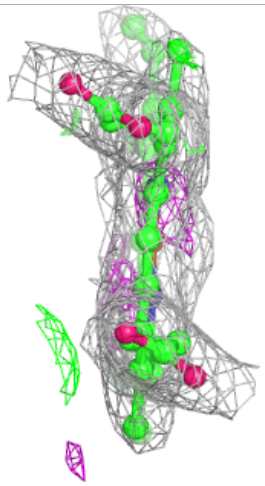


Electron density around HEM F 502:

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

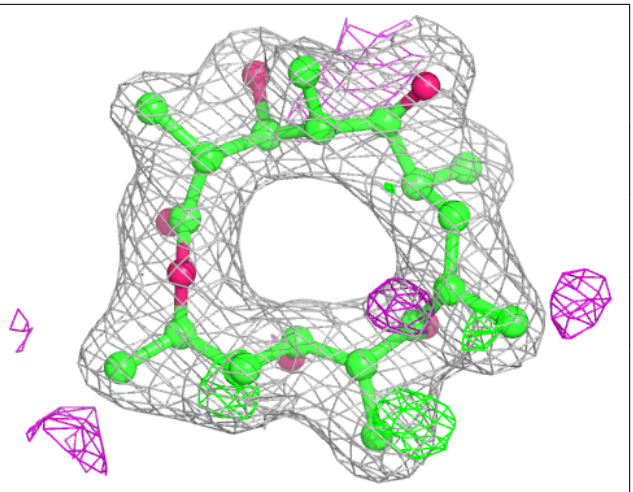


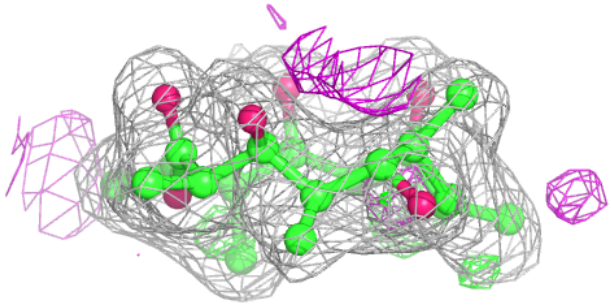


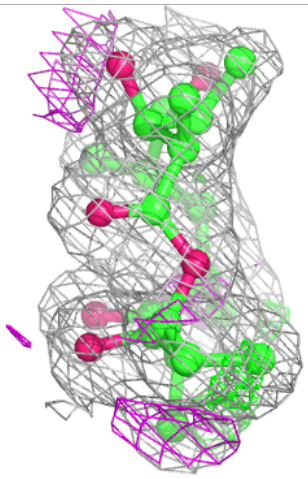


Electron density around QR8 A 502:

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

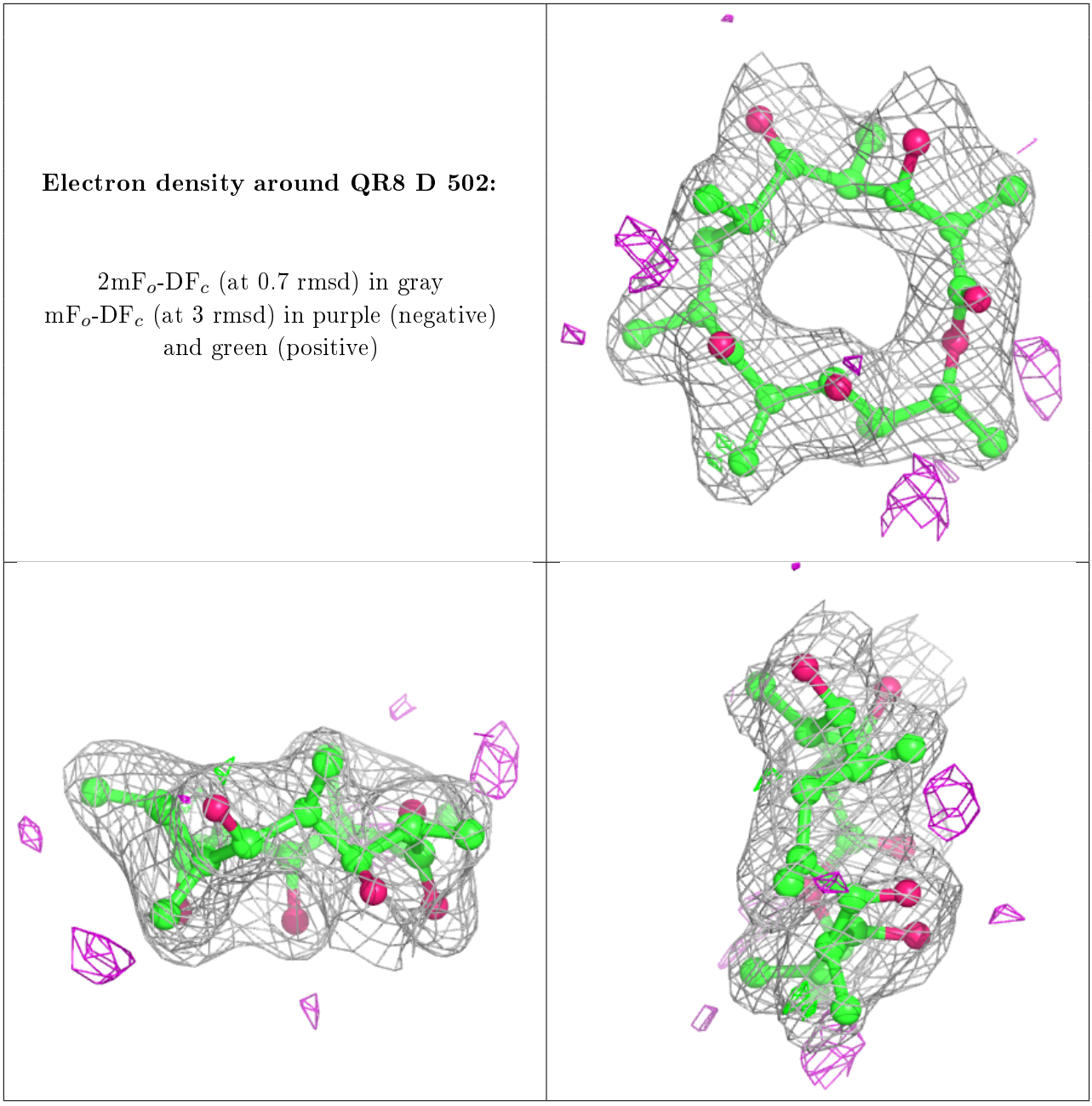






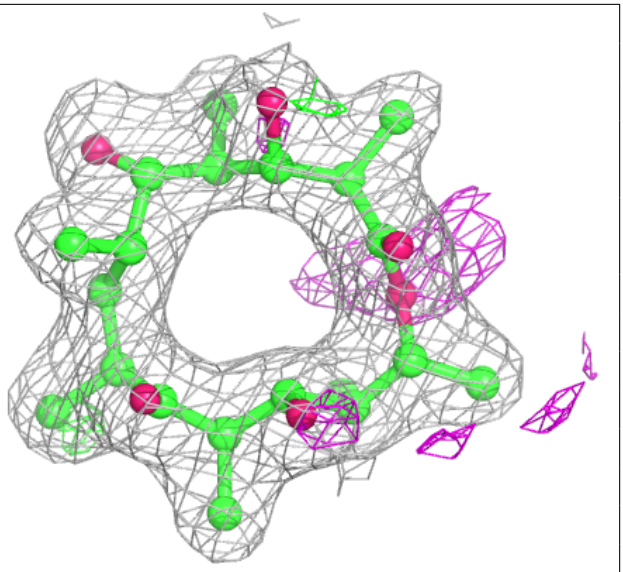
Electron density around QR8 D 502:

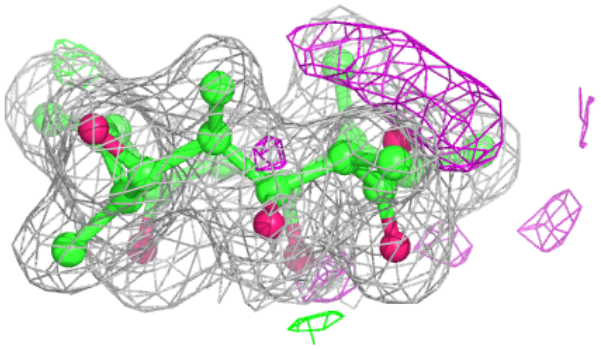
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around QR8 C 502:

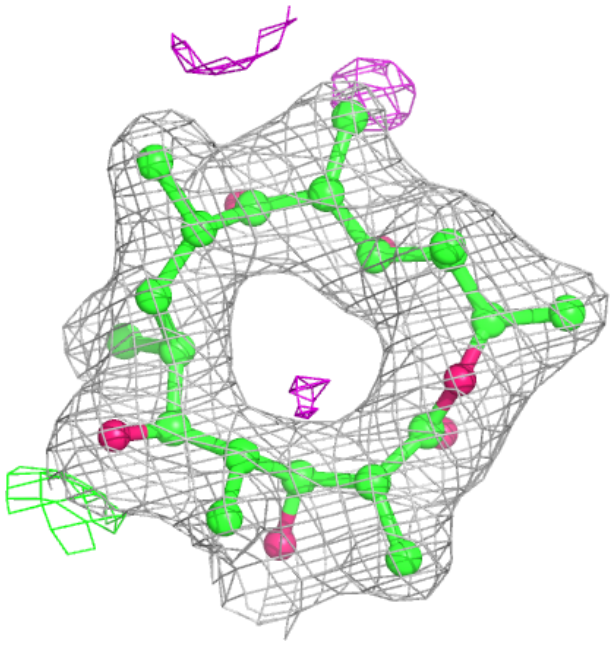
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

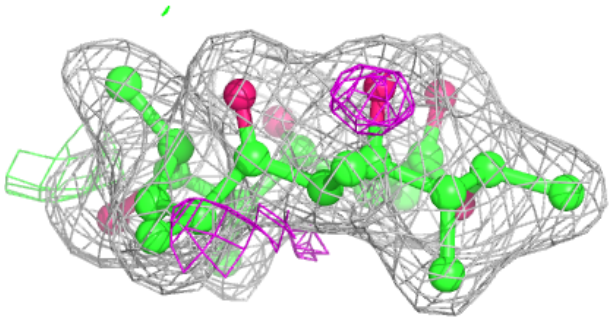


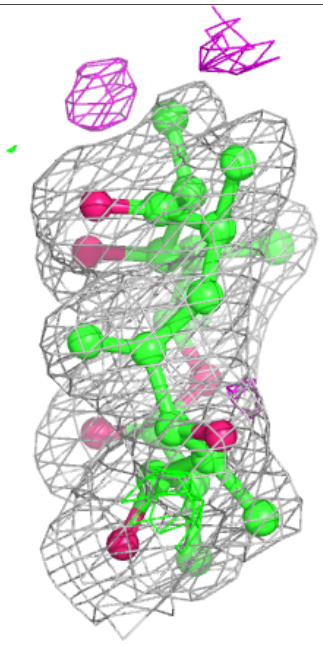


Electron density around QR8 B 502:

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

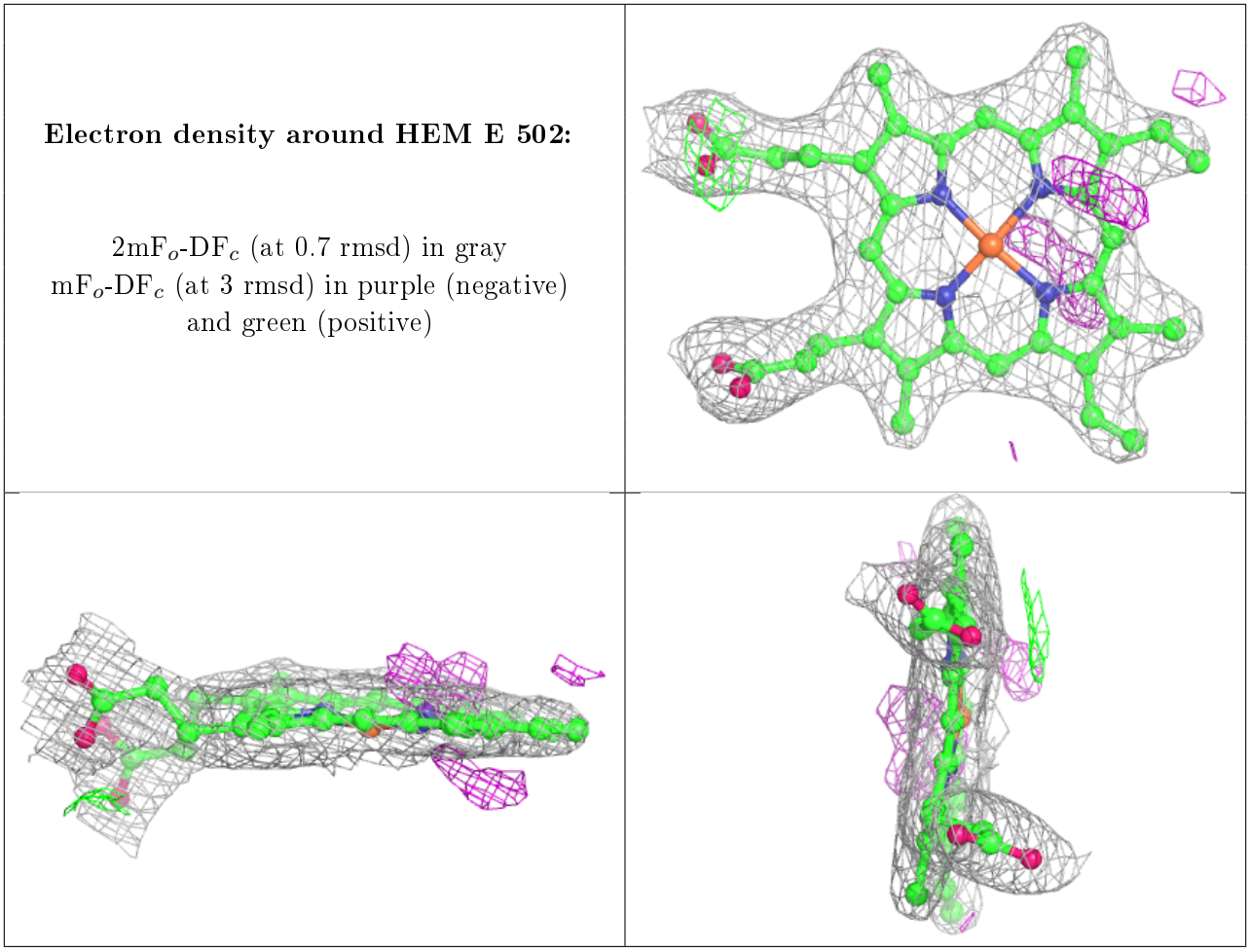






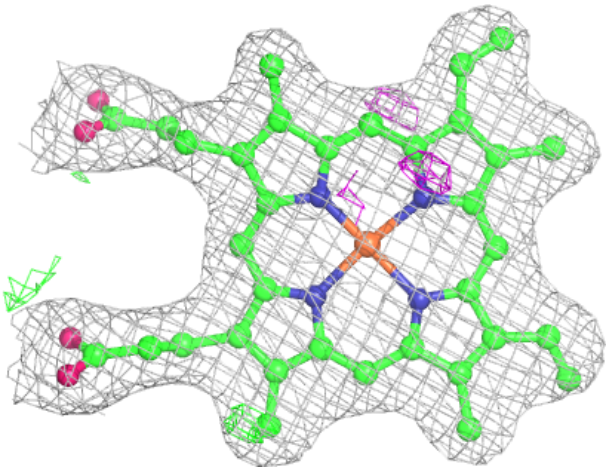
Electron density around HEM E 502:

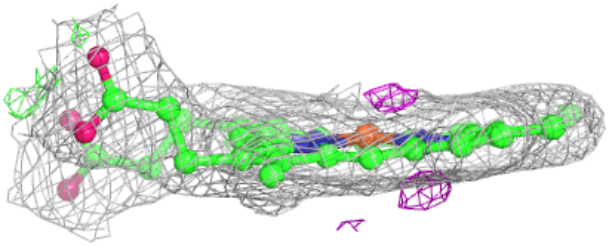
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

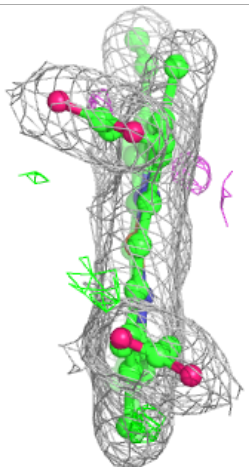


Electron density around HEM A 501:

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

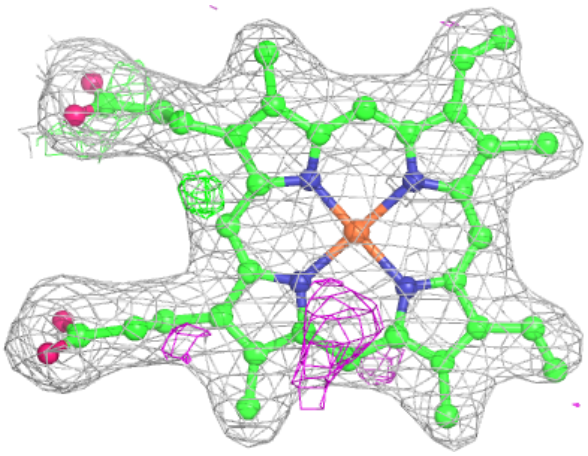


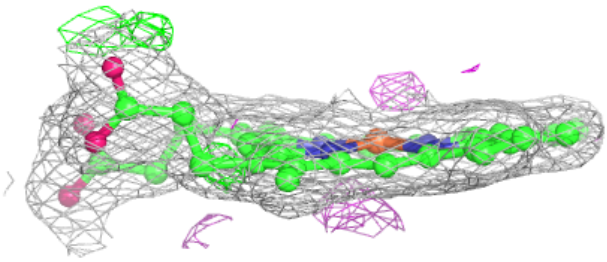


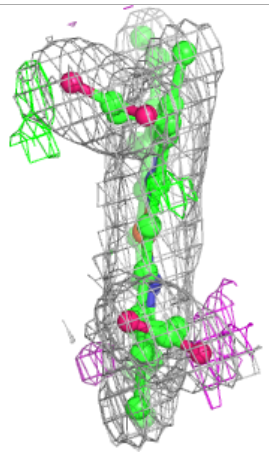


Electron density around HEM B 501:

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

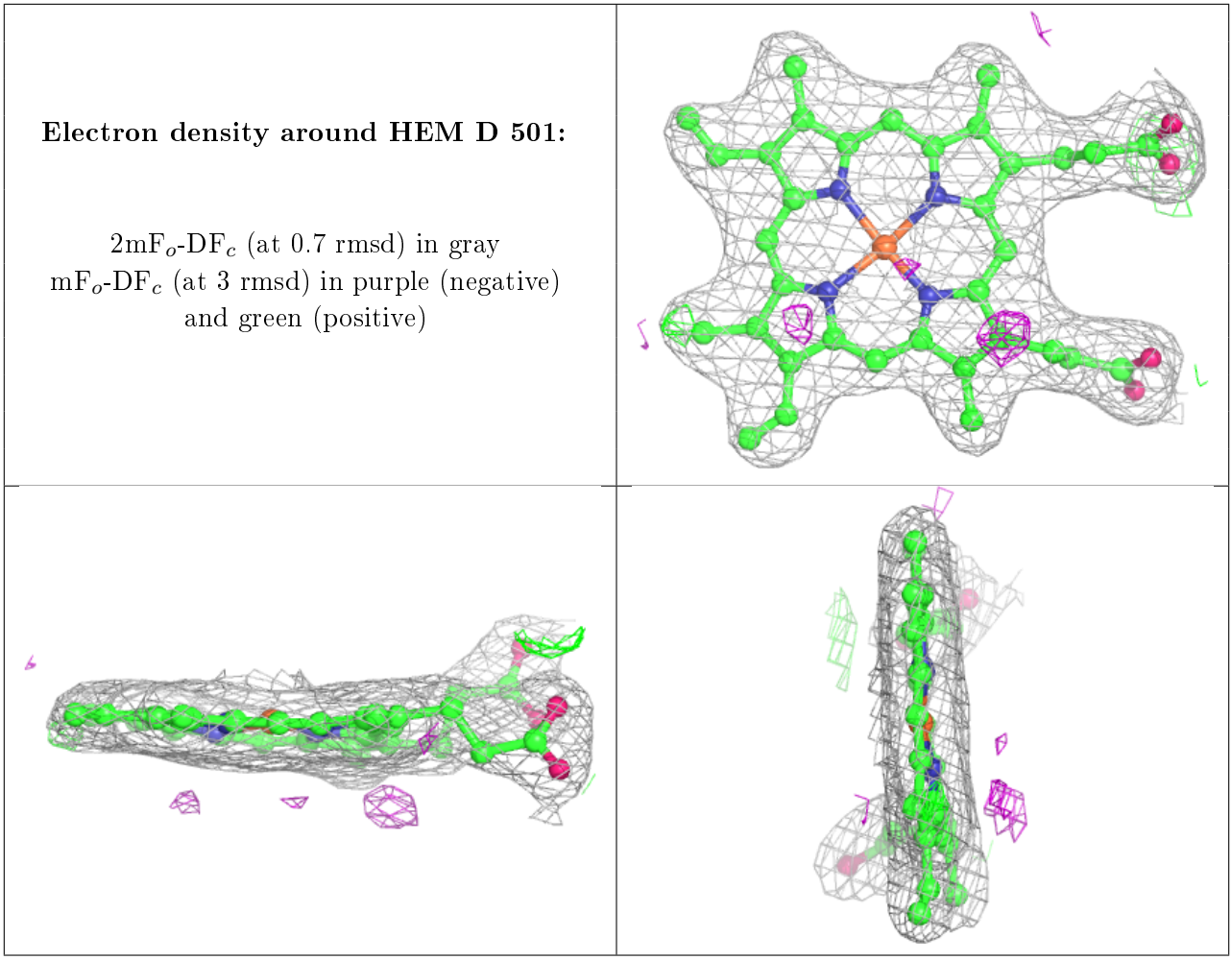






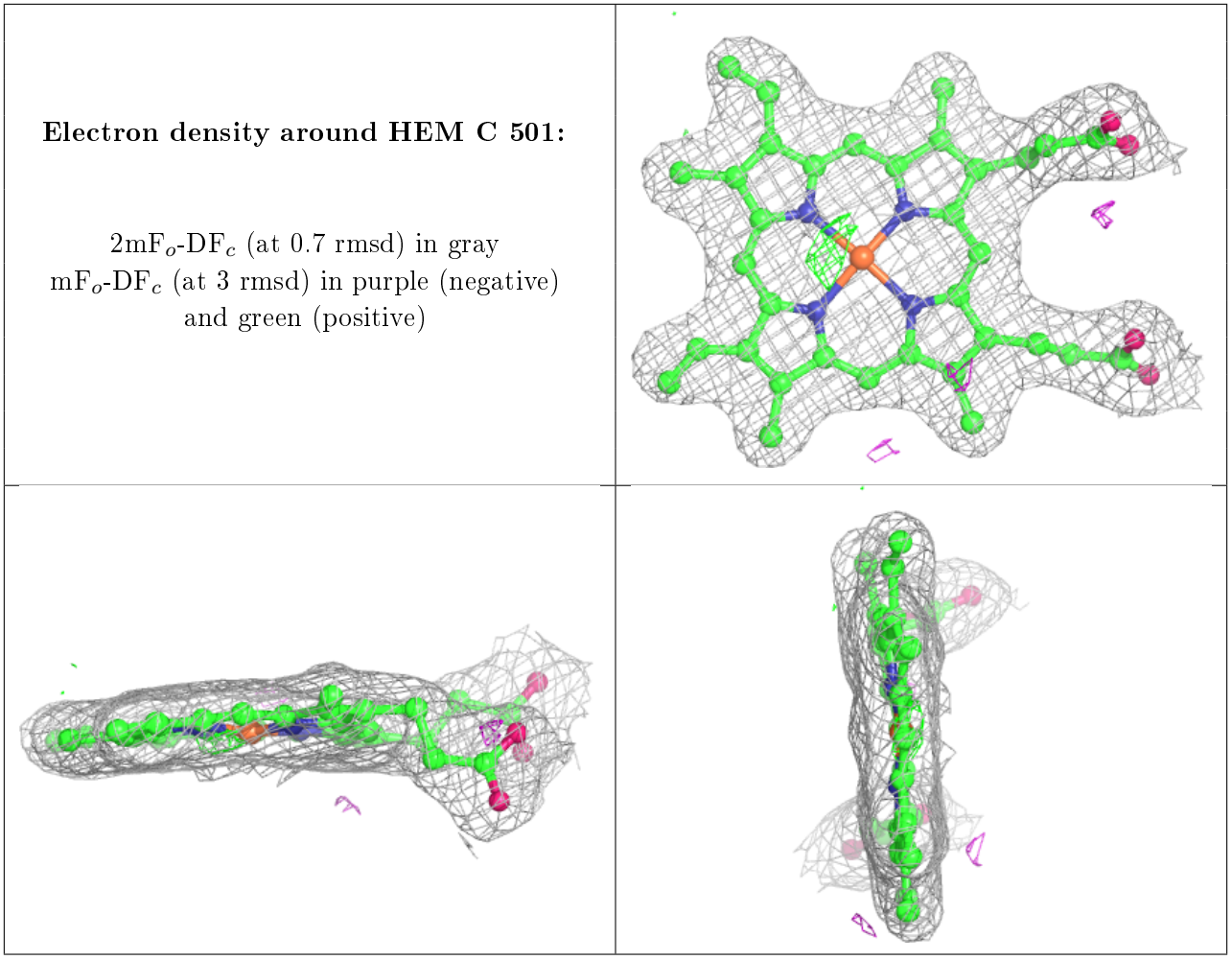
Electron density around HEM D 501:

$2mF_o$-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.