wwPDB X-ray Structure Validation Summary Report (i)

Sep 3, 2023 – 08:18 PM EDT

PDB ID	:	3T6D
Title	:	Crystal Structure of the Reaction Centre from Blastochloris viridis strain DSM 133 (ATCC 19567) substrain-08
Authors	:	Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on	:	2011-07-28
Resolution	:	1.95 Å(reported)

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

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

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

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

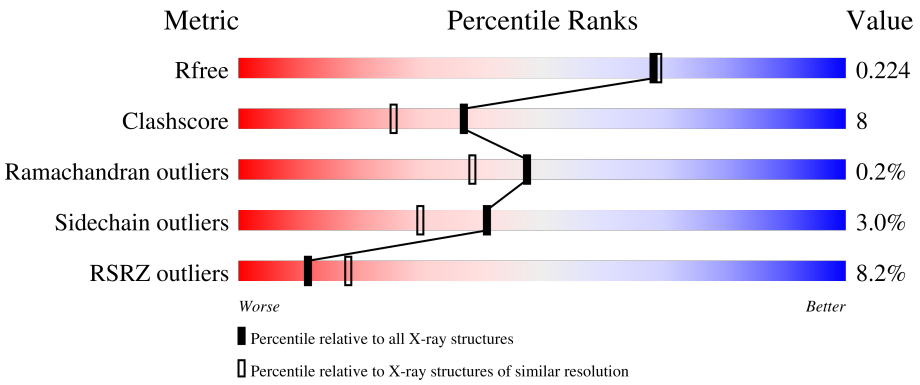
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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

Mol	Chain	Length	Quality of chain
1	C	356	11% 86% 8% 6%
2	H	258	5% 88% 12%
3	L	273	7% 90% 9% •
4	M	323	8% 93% 6% •

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
10	GOL	C	370	-	-	-	X
10	GOL	C	371	-	-	-	X
10	GOL	C	374[B]	-	-	-	X
10	GOL	C	377	-	-	X	-
10	GOL	C	378	-	-	-	X
10	GOL	H	283	-	-	X	-
10	GOL	L	288	-	-	-	X
10	GOL	M	341	-	-	-	X
6	LDA	H	718[B]	-	-	-	X
6	LDA	L	702	-	-	-	X
6	LDA	L	712	-	-	-	X
6	LDA	L	724	-	-	-	X
6	LDA	M	706	-	-	-	X
7	DGA	C	730	-	-	-	X
8	SO4	C	351	-	-	-	X
8	SO4	H	261[B]	-	-	X	-
8	SO4	L	275	-	-	-	X
8	SO4	M	326	-	-	X	-
8	SO4	M	329	-	-	-	X
8	SO4	M	330	-	-	-	X
9	HTO	C	355	-	-	X	-
9	HTO	C	356	-	X	-	-
9	HTO	C	357	-	-	-	X
9	HTO	C	358[A]	-	X	-	-
9	HTO	H	274[A]	-	-	-	X
9	HTO	M	333	-	-	-	X

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 12156 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 Photosynthetic reaction center cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	334	2647	1667	474	486	20	0	3	0

- Molecule 2 is a protein called Photosynthetic reaction center H-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	258	2035	1300	353	379	3	44	4	0

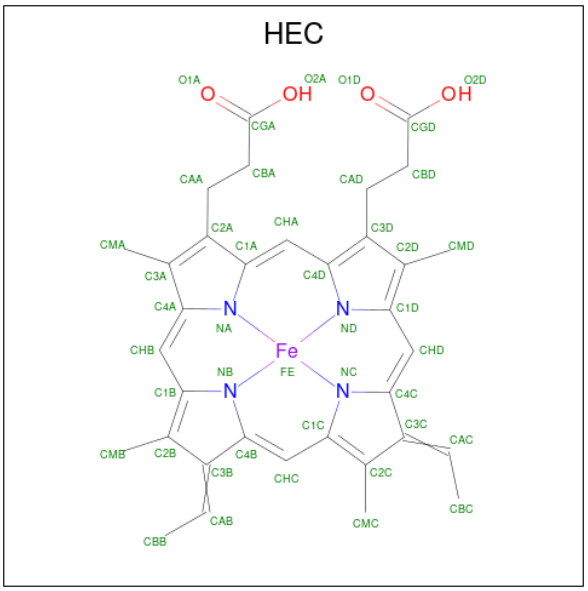
- Molecule 3 is a protein called Photosynthetic reaction center L-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	273	2191	1474	352	358	7	0	2	0

- Molecule 4 is a protein called Photosynthetic reaction center M-subunit.

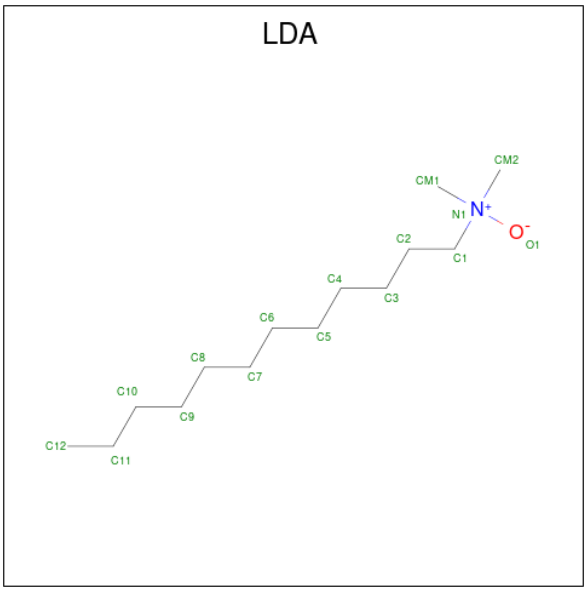
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	323	2574	1716	424	423	11	0	2	0

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	C	1	16	14	1	1	0	0
			Total	C	N	O		
6	C	1	16	14	1	1	0	0
			Total	C	N	O		
6	H	1	16	14	1	1	0	0
			Total	C	N	O		
6	H	1	16	14	1	1	0	1
			Total	C	N	O		
6	H	1	16	14	1	1	0	0
			Total	C	N	O		
6	H	1	16	14	1	1	0	0
			Total	C	N	O		
6	H	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	L	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0

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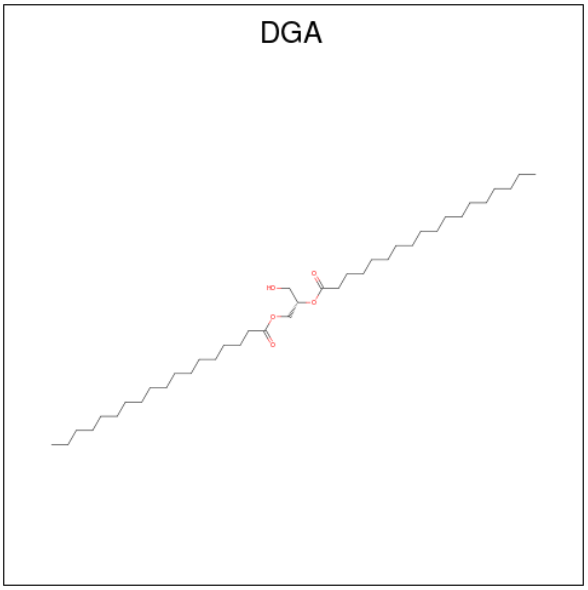
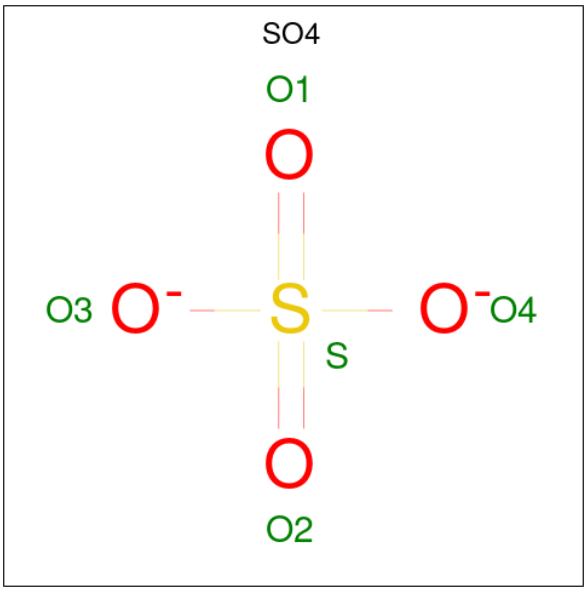
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	M	1	16	14	1	1	0	0
			Total	C	N	O		
6	M	1	16	14	1	1	0	0

- Molecule 7 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	C	1	37	33	4	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	O	S		0	1
			10	8	2			
8	C	1	Total	O	S		0	0
			5	4	1			
8	C	1	Total	O	S		0	0
			5	4	1			
8	C	1	Total	O	S		0	0
			5	4	1			
8	C	1	Total	O	S		0	0
			5	4	1			
8	C	1	Total	O	S		0	0
			5	4	1			
8	C	1	Total	O	S		0	0
			5	4	1			
8	C	1	Total	O	S		0	0
			5	4	1			
8	C	1	Total	O	S		0	0
			5	4	1			
8	C	1	Total	O	S		0	0
			5	4	1			
8	C	1	Total	O	S		0	0
			5	4	1			
8	C	1	Total	O	S		0	0
			5	4	1			
8	C	1	Total	O	S		0	0
			5	4	1			
8	C	1	Total	O	S		0	0
			5	4	1			

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
8	C	1	5	4	1	0	0
			Total	O	S		
8	C	1	5	4	1	0	0
			Total	O	S		
8	C	1	5	4	1	0	0
			Total	O	S		
8	C	1	5	4	1	0	0
			Total	O	S		
8	H	1	5	4	1	0	0
			Total	O	S		
8	H	1	5	4	1	0	0
			Total	O	S		
8	H	1	10	8	2	0	1
			Total	O	S		
8	H	1	5	4	1	0	0
			Total	O	S		
8	H	1	5	4	1	0	0
			Total	O	S		
8	H	1	5	4	1	0	0
			Total	O	S		
8	H	1	5	4	1	0	0
			Total	O	S		
8	H	1	5	4	1	0	0
			Total	O	S		
8	H	1	5	4	1	0	0
			Total	O	S		
8	H	1	5	4	1	0	0
			Total	O	S		
8	H	1	5	4	1	0	0
			Total	O	S		
8	H	1	5	4	1	0	0
			Total	O	S		
8	H	1	5	4	1	0	0
			Total	O	S		
8	L	1	5	4	1	0	0
			Total	O	S		
8	L	1	5	4	1	0	0
			Total	O	S		
8	M	1	5	4	1	0	0
			Total	O	S		
8	M	1	5	4	1	0	0

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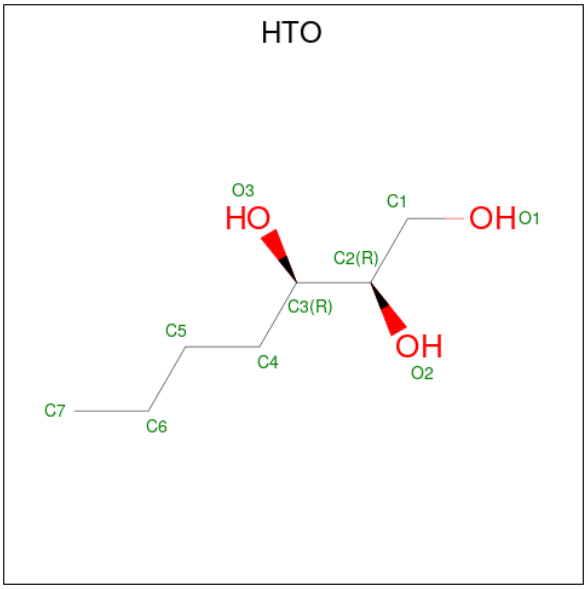
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0
8	M	1	Total O S 5 4 1	0	0

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 10 7 3	0	0
9	C	1	Total C O 10 7 3	0	0
9	C	1	Total C O 10 7 3	0	0
9	C	1	Total C O 10 7 3	0	1
9	H	1	Total C O 10 7 3	0	0

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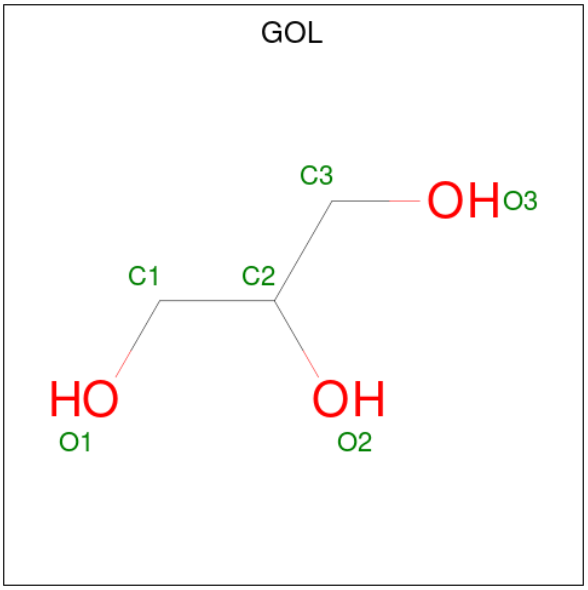
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	1	Total C O 10 7 3	0	0
9	H	1	Total C O 10 7 3	0	1
9	L	1	Total C O 10 7 3	0	0
9	L	1	Total C O 10 7 3	0	0
9	L	1	Total C O 10 7 3	0	0
9	L	1	Total C O 10 7 3	0	0
9	L	1	Total C O 10 7 3	0	0
9	M	1	Total C O 10 7 3	0	0

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C O 6 3 3	0	0
10	C	1	Total C O 6 3 3	0	0
10	C	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	1
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	C	1	6	3	3	0	0
			Total	C	O		
10	H	1	6	3	3	0	0
			Total	C	O		
10	H	1	8	4	4	0	1
			Total	C	O		
10	H	1	6	3	3	0	0
			Total	C	O		
10	H	1	6	3	3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	H	1	6	3	3	0	0
10	L	1	6	3	3	0	0
10	L	1	6	3	3	0	0
10	L	1	6	3	3	0	0
10	L	1	6	3	3	0	0
10	L	1	6	3	3	0	0
10	L	1	6	3	3	0	0
10	L	1	6	3	3	0	0
10	L	1	6	3	3	0	0

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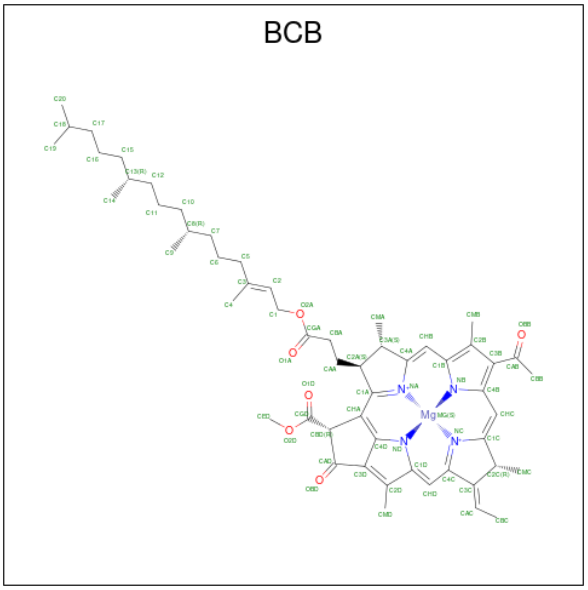
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	M	1	6	3	3	0	0
			Total	C	O		
10	M	1	6	3	3	0	0
			Total	C	O		
10	M	1	6	3	3	0	0
			Total	C	O		
10	M	1	6	3	3	0	0
			Total	C	O		
10	M	1	6	3	3	0	0
			Total	C	O		
10	M	1	6	3	3	0	0
			Total	C	O		
10	M	1	6	3	3	0	0
			Total	C	O		
10	M	1	6	3	3	0	0
			Total	C	O		
10	M	1	6	3	3	0	0

- Molecule 11 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
11	L	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
11	L	1	66	55	1	4	6	0	0

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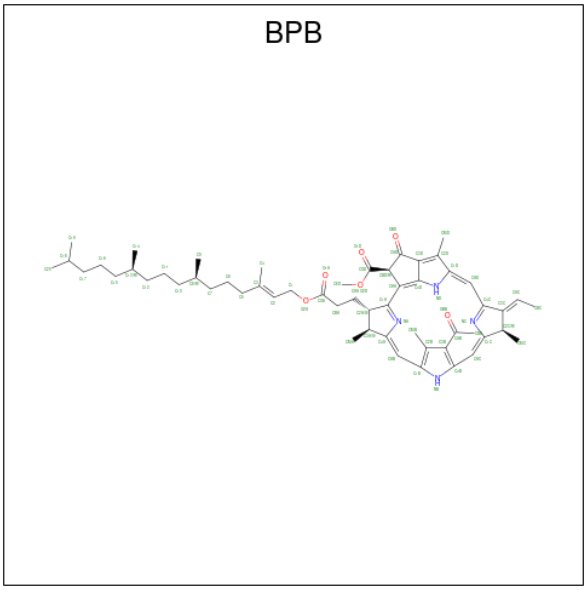
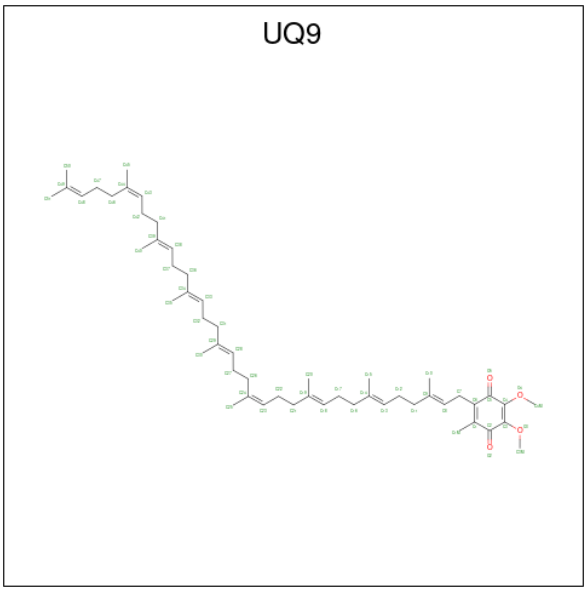
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Mg	N	O		
11	M	1	66	55	1	4	6	0	0
			Total	C	Mg	N	O		
11	M	1	66	55	1	4	6	0	0

- Molecule 12 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
12	L	1	65	55	4	6	0	0
			Total	C	N	O		
12	M	1	65	55	4	6	0	0

- Molecule 13 is Ubiquinone-9 (three-letter code: UQ9) (formula: $C_{54}H_{82}O_4$).

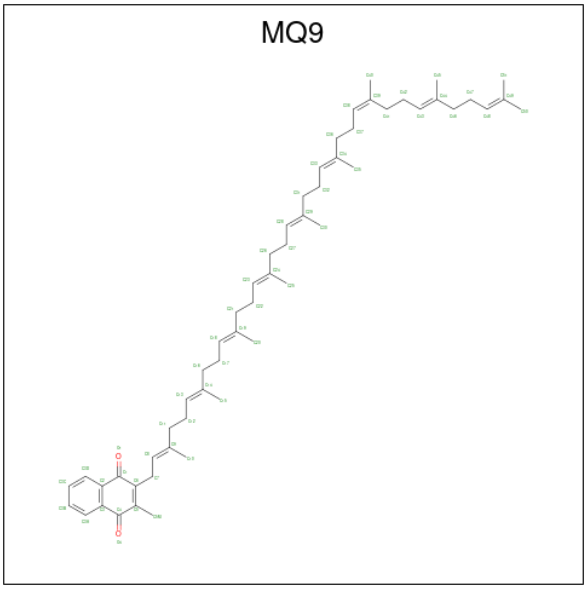


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
13	L	1	58	54	4	0	0
			Total	C	O		
13	L	1	23	19	4	0	0

- Molecule 14 is FE (II) ION (three-letter code: FE2) (formula: Fe).

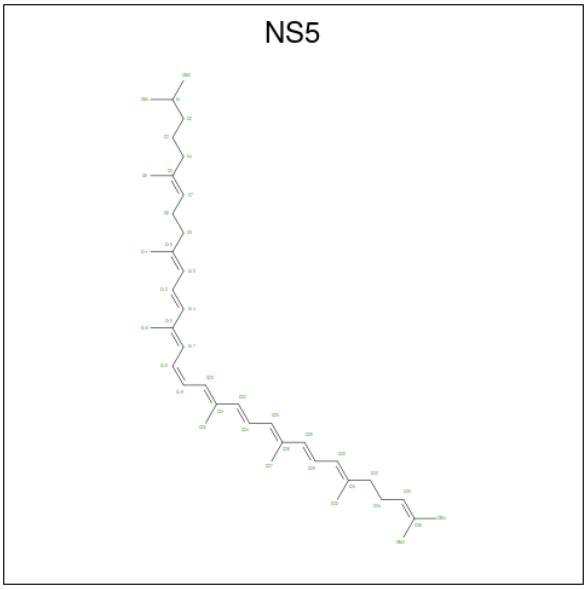
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
14	M	1	1	1	0	0

- Molecule 15 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$).



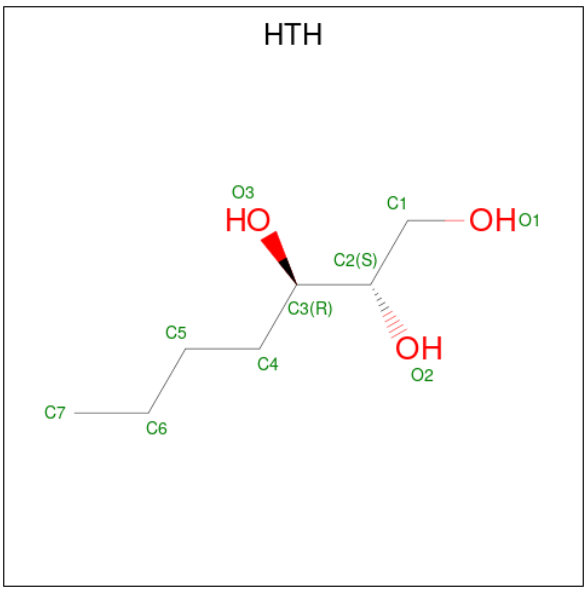
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
15	M	1	58	56	2	0	0

- Molecule 16 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
16	M	1	40	40	0	0

- Molecule 17 is (2S,3R)-heptane-1,2,3-triol (three-letter code: HTH) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
17	M	1	10	7	3	0	0

- Molecule 18 is water.

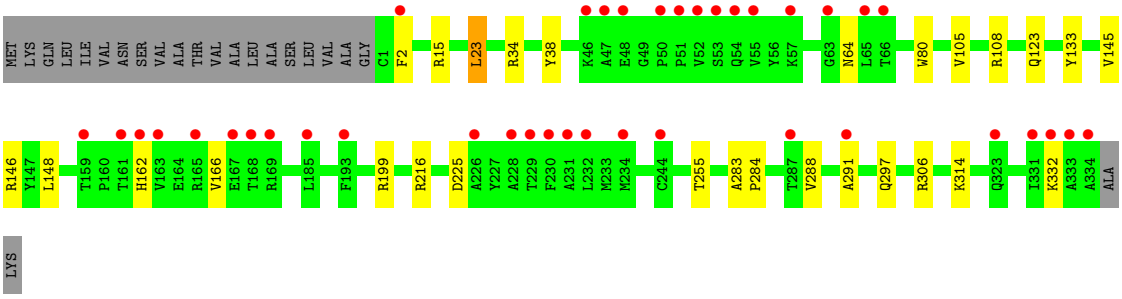
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	C	388	388	388	0	0
			Total	O		
18	H	211	211	211	0	0
			Total	O		
18	L	109	109	109	0	0
			Total	O		
18	M	153	153	153	0	0

3 Residue-property plots (i)

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

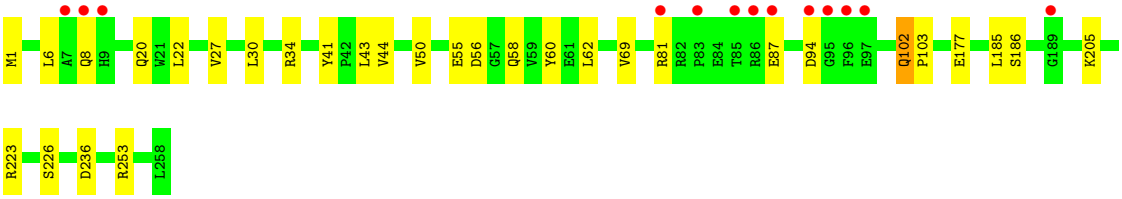
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C:



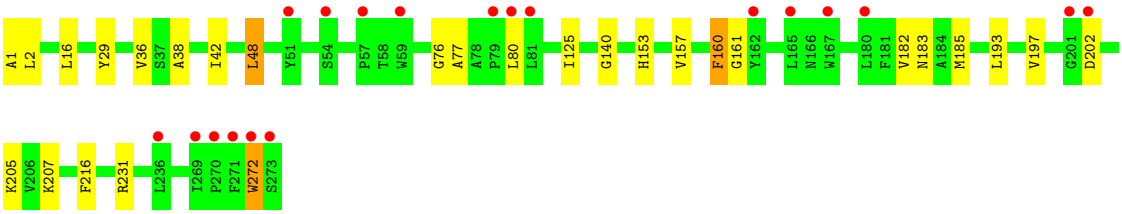
• Molecule 2: Photosynthetic reaction center H-subunit

Chain H:



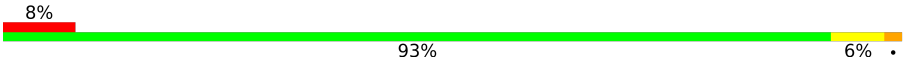
• Molecule 3: Photosynthetic reaction center L-subunit

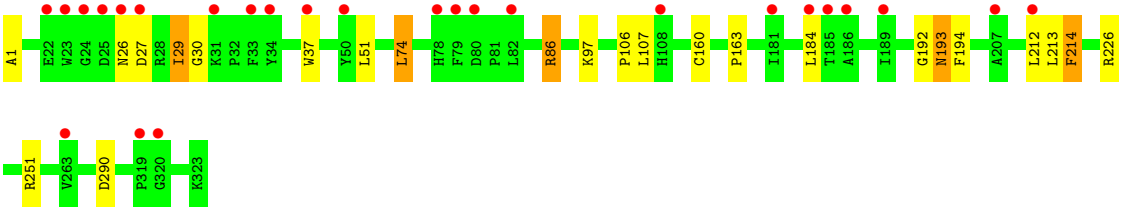
Chain L:



• Molecule 4: Photosynthetic reaction center M-subunit

Chain M:




A1
E22
W23
G24
D25
N26
D27
R28
I29
G30
K31
P32
F33
Y34
W37
Y50
L51
L74
H78
F79
D80
P81
L82
R86
K97
P106
L107
H108
C160
P163
I181
L184
T185
A186
I189
G192
N193
F194
A207
L212
L213
F214
R226
R251
V263
D290
P319
G320
K323

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	220.44Å 220.44Å 113.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 1.95 48.34 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.34-1.95) 96.2 (48.34-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.6.0101	Depositor
R, R_{free}	0.182 , 0.216 0.192 , 0.224	Depositor DCC
R_{free} test set	9677 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 75.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12156	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BCB, SO4, FE2, LDA, DGA, HTH, NS5, BPB, MQ9, FME, HTO, HEC, UQ9, GOL

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	C	0.91	0/2716	0.82	3/3701 (0.1%)
2	H	0.91	2/2069 (0.1%)	0.84	0/2827
3	L	0.94	0/2280	0.81	2/3113 (0.1%)
4	M	0.94	1/2679 (0.0%)	0.79	2/3662 (0.1%)
All	All	0.93	3/9744 (0.0%)	0.81	7/13303 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	177	GLU	CD-OE1	5.52	1.31	1.25
2	H	27	VAL	CB-CG2	5.43	1.64	1.52
4	M	160	CYS	CB-SG	-5.19	1.73	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	251	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	C	23	LEU	CA-CB-CG	5.82	128.69	115.30
3	L	160	PHE	CB-CG-CD1	5.55	124.69	120.80
4	M	86	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	15	ARG	NE-CZ-NH1	5.24	122.92	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2647	0	2610	33	0
2	H	2035	0	2017	19	0
3	L	2191	0	2116	22	0
4	M	2574	0	2470	28	0
5	C	172	0	120	4	0
6	C	32	0	62	7	0
6	H	80	0	155	9	0
6	L	144	0	279	19	0
6	M	128	0	248	12	0
7	C	37	0	58	3	0
8	C	95	0	0	3	0
8	H	70	0	0	5	0
8	L	10	0	0	0	0
8	M	40	0	0	2	0
9	C	40	0	64	8	0
9	H	30	0	48	5	0
9	L	50	0	80	3	0
9	M	10	0	16	2	0
10	C	120	0	160	15	0
10	H	104	0	135	10	0
10	L	48	0	64	1	0
10	M	54	0	72	6	0
11	L	132	0	144	9	0
11	M	132	0	144	17	0
12	L	65	0	74	2	0
12	M	65	0	74	1	0
13	L	81	0	105	16	0
14	M	1	0	0	0	0
15	M	58	0	80	2	0
16	M	40	0	60	3	0
17	M	10	0	16	0	0
18	C	388	0	0	4	0
18	H	211	0	0	4	0
18	L	109	0	0	0	0
18	M	153	0	0	1	0
All	All	12156	0	11471	178	0

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 8.

The worst 5 of 178 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)
6:H:720:LDA:H72	6:H:720:LDA:C3	1.43	1.34
6:H:720:LDA:H32	6:H:720:LDA:C7	1.62	1.27
13:L:502:UQ9:H15A	11:M:400:BCB:C9	1.75	1.15
9:M:333:HTO:O3	9:M:333:HTO:H72	1.50	1.10
13:L:502:UQ9:H15A	11:M:400:BCB:H93	1.46	0.98

There are no symmetry-related clashes.

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	C	335/356 (94%)	326 (97%)	9 (3%)	0	100	100
2	H	259/258 (100%)	247 (95%)	11 (4%)	1 (0%)	34	22
3	L	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
4	M	323/323 (100%)	315 (98%)	7 (2%)	1 (0%)	41	30
All	All	1190/1210 (98%)	1156 (97%)	32 (3%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	50	VAL
4	M	193	ASN

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	C	286/299 (96%)	283 (99%)	3 (1%)	76	74
2	H	209/211 (99%)	199 (95%)	10 (5%)	25	12
3	L	220/218 (101%)	212 (96%)	8 (4%)	35	23
4	M	249/247 (101%)	241 (97%)	8 (3%)	39	27
All	All	964/975 (99%)	935 (97%)	29 (3%)	41	30

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	16	LEU
4	M	214	PHE
3	L	160	PHE
4	M	163	PRO
3	L	80	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	239	ASN
3	L	213	ASN
2	H	220	ASN
2	H	102	GLN
3	L	183	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	H	1[A]	-	8,9,10	1.24	2 (25%)	7,9,11	3.02	3 (42%)
2	FME	H	1[B]	-	8,9,10	0.97	0	7,9,11	3.00	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	H	1[A]	-	-	3/7/9/11	-
2	FME	H	1[B]	-	-	4/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1[A]	FME	CN-N	2.23	1.40	1.33
2	H	1[A]	FME	CA-N	2.15	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1[B]	FME	CA-N-CN	-7.48	111.32	122.82
2	H	1[A]	FME	CA-N-CN	-7.16	111.81	122.82
2	H	1[A]	FME	CE-SD-CG	2.25	108.14	100.40
2	H	1[A]	FME	CG-CB-CA	2.04	118.61	112.95

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1[A]	FME	O1-CN-N-CA
2	H	1[A]	FME	CB-CA-N-CN
2	H	1[B]	FME	O1-CN-N-CA
2	H	1[A]	FME	CB-CG-SD-CE
2	H	1[B]	FME	CB-CA-N-CN

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 152 ligands modelled in this entry, 1 is monoatomic - leaving 151 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	$\#\|Z\| > 2$
10	GOL	C	361	-	5,5,5	0.58	0	5,5,5	1.05	0
8	SO4	M	327	-	4,4,4	0.42	0	6,6,6	0.25	0
8	SO4	H	261[A]	-	4,4,4	0.41	0	6,6,6	0.33	0
10	GOL	C	374[B]	-	5,5,5	0.35	0	5,5,5	0.39	0
10	GOL	C	366	-	5,5,5	0.47	0	5,5,5	0.41	0
8	SO4	M	324	-	4,4,4	0.35	0	6,6,6	0.87	0
10	GOL	H	281	-	5,5,5	0.55	0	5,5,5	0.36	0
10	GOL	C	368	-	5,5,5	0.15	0	5,5,5	0.68	0
13	UQ9	L	502	-	58,58,58	2.24	24 (41%)	70,73,73	1.58	14 (20%)
8	SO4	C	342	-	4,4,4	0.39	0	6,6,6	0.27	0
8	SO4	H	269	-	4,4,4	0.38	0	6,6,6	0.16	0
8	SO4	C	339	-	4,4,4	0.32	0	6,6,6	0.43	0
10	GOL	H	283	-	5,5,5	0.18	0	5,5,5	0.96	0
6	LDA	M	714	-	12,15,15	2.21	1 (8%)	14,17,17	0.37	0
8	SO4	C	348	-	4,4,4	0.40	0	6,6,6	0.41	0
10	GOL	H	289	-	5,5,5	0.34	0	5,5,5	0.24	0
10	GOL	M	341	-	5,5,5	0.39	0	5,5,5	0.24	0
10	GOL	L	288	-	5,5,5	0.15	0	5,5,5	0.61	0
11	BCB	L	400	3	54,74,74	1.18	4 (7%)	52,115,115	2.30	15 (28%)
16	NS5	M	600	-	39,39,39	1.82	12 (30%)	44,46,46	2.72	14 (31%)
8	SO4	L	275	-	4,4,4	0.32	0	6,6,6	0.13	0
12	BPB	L	402	-	49,70,70	0.81	0	47,101,101	1.69	10 (21%)
6	LDA	H	718[B]	-	12,15,15	1.99	1 (8%)	14,17,17	0.61	0
8	SO4	C	349	-	4,4,4	0.47	0	6,6,6	0.26	0
9	HTO	H	272	-	9,9,9	0.74	0	10,10,10	1.68	3 (30%)
8	SO4	H	260	-	4,4,4	0.35	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	GOL	C	365	-	5,5,5	0.35	0	5,5,5	0.36	0
10	GOL	C	378	-	5,5,5	0.33	0	5,5,5	0.17	0
6	LDA	C	716	-	12,15,15	2.00	1 (8%)	14,17,17	0.68	0
10	GOL	H	282	-	5,5,5	0.38	0	5,5,5	0.22	0
8	SO4	M	330	-	4,4,4	0.42	0	6,6,6	0.15	0
8	SO4	C	337[B]	-	4,4,4	0.36	0	6,6,6	0.21	0
8	SO4	C	354	-	4,4,4	0.27	0	6,6,6	0.38	0
10	GOL	C	371	-	5,5,5	0.34	0	5,5,5	0.78	0
8	SO4	H	271	-	4,4,4	0.35	0	6,6,6	0.08	0
10	GOL	H	276[B]	-	5,5,5	0.82	0	5,5,5	0.94	0
8	SO4	H	267	-	4,4,4	0.27	0	6,6,6	0.16	0
8	SO4	H	270	-	4,4,4	0.34	0	6,6,6	0.14	0
9	HTO	L	277	-	9,9,9	0.45	0	10,10,10	1.35	1 (10%)
9	HTO	H	273	-	9,9,9	0.44	0	10,10,10	1.21	1 (10%)
10	GOL	M	342	-	5,5,5	0.40	0	5,5,5	0.66	0
10	GOL	M	337	-	5,5,5	0.34	0	5,5,5	0.36	0
8	SO4	C	344	-	4,4,4	0.41	0	6,6,6	0.17	0
8	SO4	C	338	-	4,4,4	0.46	0	6,6,6	0.42	0
10	GOL	C	359	-	5,5,5	0.83	0	5,5,5	0.85	0
8	SO4	M	326	-	4,4,4	0.19	0	6,6,6	0.45	0
10	GOL	C	363	-	5,5,5	0.79	0	5,5,5	1.07	0
10	GOL	H	277	-	5,5,5	0.41	0	5,5,5	0.54	0
8	SO4	H	262	-	4,4,4	0.34	0	6,6,6	0.39	0
12	BPB	M	402	-	49,70,70	0.87	1 (2%)	47,101,101	1.49	8 (17%)
6	LDA	L	709	-	12,15,15	1.97	1 (8%)	14,17,17	0.48	0
8	SO4	C	341	-	4,4,4	0.35	0	6,6,6	0.31	0
6	LDA	M	704	-	12,15,15	2.36	1 (8%)	14,17,17	1.53	3 (21%)
6	LDA	L	710	-	12,15,15	2.09	1 (8%)	14,17,17	0.49	0
8	SO4	H	268	-	4,4,4	0.29	0	6,6,6	0.19	0
6	LDA	L	703	-	12,15,15	2.12	1 (8%)	14,17,17	0.57	0
10	GOL	L	283	-	5,5,5	0.41	0	5,5,5	0.54	0
6	LDA	M	717	-	12,15,15	1.94	1 (8%)	14,17,17	0.58	0
9	HTO	L	280	-	9,9,9	0.43	0	10,10,10	1.04	1 (10%)
9	HTO	L	278	-	9,9,9	0.67	0	10,10,10	1.63	3 (30%)
8	SO4	C	345	-	4,4,4	0.33	0	6,6,6	0.32	0
10	GOL	C	375	-	5,5,5	0.28	0	5,5,5	0.19	0
6	LDA	H	719	-	12,15,15	1.99	1 (8%)	14,17,17	0.54	0
10	GOL	H	280	-	5,5,5	0.73	0	5,5,5	1.09	0
6	LDA	L	723	-	12,15,15	2.02	1 (8%)	14,17,17	0.78	0
9	HTO	C	355	-	9,9,9	0.55	0	10,10,10	1.61	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	SO4	H	263	-	4,4,4	0.38	0	6,6,6	0.31	0
9	HTO	C	358[A]	-	9,9,9	0.73	0	10,10,10	2.66	4 (40%)
10	GOL	L	285	-	5,5,5	0.55	0	5,5,5	0.74	0
6	LDA	M	705	-	12,15,15	1.86	1 (8%)	14,17,17	0.53	0
10	GOL	H	284	-	5,5,5	0.36	0	5,5,5	0.80	0
10	GOL	L	282	-	5,5,5	0.88	0	5,5,5	1.20	1 (20%)
10	GOL	M	338	-	5,5,5	0.41	0	5,5,5	0.47	0
6	LDA	L	711	-	12,15,15	2.07	1 (8%)	14,17,17	0.61	0
10	GOL	C	372	-	5,5,5	0.29	0	5,5,5	0.61	0
8	SO4	C	337[A]	-	4,4,4	0.36	0	6,6,6	0.23	0
8	SO4	C	352	-	4,4,4	0.31	0	6,6,6	0.15	0
6	LDA	L	708	-	12,15,15	1.98	1 (8%)	14,17,17	1.25	2 (14%)
10	GOL	H	275	-	5,5,5	0.67	0	5,5,5	0.38	0
10	GOL	H	287	-	5,5,5	0.32	0	5,5,5	0.11	0
8	SO4	C	343	-	4,4,4	0.16	0	6,6,6	0.83	0
10	GOL	H	286	-	5,5,5	0.26	0	5,5,5	0.57	0
5	HEC	C	402	1	32,50,50	0.95	1 (3%)	24,82,82	1.49	4 (16%)
8	SO4	M	328	-	4,4,4	0.30	0	6,6,6	0.24	0
10	GOL	H	276[A]	-	5,5,5	0.83	0	5,5,5	0.58	0
10	GOL	C	370	-	5,5,5	0.27	0	5,5,5	0.21	0
9	HTO	C	356	-	9,9,9	0.75	0	10,10,10	1.85	3 (30%)
6	LDA	M	715	-	12,15,15	2.08	1 (8%)	14,17,17	0.46	0
8	SO4	C	340	-	4,4,4	0.36	0	6,6,6	0.65	0
10	GOL	C	367	-	5,5,5	0.25	0	5,5,5	1.07	0
8	SO4	M	325	-	4,4,4	0.17	0	6,6,6	0.60	0
10	GOL	H	278	-	5,5,5	0.47	0	5,5,5	0.79	0
10	GOL	C	376	-	5,5,5	0.33	0	5,5,5	0.31	0
5	HEC	C	401	1	32,50,50	1.15	2 (6%)	24,82,82	2.04	7 (29%)
10	GOL	C	364	-	5,5,5	0.57	0	5,5,5	0.96	0
6	LDA	H	721	-	12,15,15	1.86	1 (8%)	14,17,17	0.59	0
11	BCB	M	400	4	54,74,74	1.27	4 (7%)	52,115,115	2.22	14 (26%)
8	SO4	C	350	-	4,4,4	0.37	0	6,6,6	0.14	0
10	GOL	L	281	-	5,5,5	0.19	0	5,5,5	0.44	0
11	BCB	L	401	3	54,74,74	1.62	6 (11%)	52,115,115	2.08	13 (25%)
8	SO4	M	329	-	4,4,4	0.30	0	6,6,6	0.34	0
10	GOL	M	339	-	5,5,5	0.25	0	5,5,5	0.31	0
8	SO4	H	266	-	4,4,4	0.36	0	6,6,6	0.40	0
10	GOL	H	291	-	5,5,5	0.38	0	5,5,5	0.42	0
8	SO4	H	261[B]	-	4,4,4	0.30	0	6,6,6	0.42	0
7	DGA	C	730	1	36,36,43	0.85	2 (5%)	38,38,45	1.48	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	GOL	C	362	-	5,5,5	0.70	0	5,5,5	0.85	0
9	HTO	L	279	-	9,9,9	0.39	0	10,10,10	1.46	1 (10%)
10	GOL	C	369	-	5,5,5	0.39	0	5,5,5	0.63	0
10	GOL	L	286	-	5,5,5	0.20	0	5,5,5	0.77	0
9	HTO	M	333	-	9,9,9	0.48	0	10,10,10	2.65	4 (40%)
9	HTO	L	276	-	9,9,9	0.47	0	10,10,10	1.55	2 (20%)
13	UQ9	L	503	-	23,23,58	2.27	8 (34%)	28,31,73	1.52	4 (14%)
10	GOL	C	373	-	5,5,5	0.35	0	5,5,5	0.27	0
10	GOL	L	284	-	5,5,5	0.37	0	5,5,5	0.48	0
6	LDA	M	706	-	12,15,15	1.93	1 (8%)	14,17,17	0.57	0
17	HTH	M	332	-	9,9,9	0.43	0	10,10,10	1.20	1 (10%)
6	LDA	H	720	-	12,15,15	2.23	1 (8%)	14,17,17	0.76	0
10	GOL	H	279	-	5,5,5	0.37	0	5,5,5	0.53	0
10	GOL	H	288	-	5,5,5	0.38	0	5,5,5	0.34	0
6	LDA	M	707	-	12,15,15	2.15	1 (8%)	14,17,17	0.89	0
6	LDA	H	701	-	12,15,15	1.54	1 (8%)	14,17,17	0.93	0
5	HEC	C	404	1	32,50,50	0.99	2 (6%)	24,82,82	1.83	8 (33%)
10	GOL	C	360	-	5,5,5	0.26	0	5,5,5	0.62	0
6	LDA	C	722	-	12,15,15	1.98	1 (8%)	14,17,17	0.58	0
6	LDA	L	724	-	12,15,15	2.20	1 (8%)	14,17,17	0.59	0
8	SO4	C	353	-	4,4,4	0.48	0	6,6,6	0.27	0
9	HTO	C	357	-	9,9,9	0.58	0	10,10,10	0.76	0
8	SO4	H	264	-	4,4,4	0.33	0	6,6,6	0.16	0
11	BCB	M	401	4	54,74,74	1.55	7 (12%)	52,115,115	2.78	15 (28%)
10	GOL	M	336	-	5,5,5	0.16	0	5,5,5	1.01	0
5	HEC	C	403	1	32,50,50	1.13	3 (9%)	24,82,82	1.07	2 (8%)
15	MQ9	M	501	-	59,59,59	2.28	25 (42%)	72,75,75	1.24	9 (12%)
6	LDA	L	702	-	12,15,15	2.07	1 (8%)	14,17,17	0.64	0
10	GOL	L	287	-	5,5,5	0.35	0	5,5,5	0.60	0
8	SO4	C	346	-	4,4,4	0.40	0	6,6,6	0.41	0
10	GOL	H	290	-	5,5,5	0.34	0	5,5,5	0.52	0
10	GOL	H	285	-	5,5,5	0.18	0	5,5,5	0.56	0
8	SO4	M	331	-	4,4,4	0.35	0	6,6,6	0.13	0
8	SO4	H	259	-	4,4,4	0.26	0	6,6,6	0.43	0
10	GOL	M	340	-	5,5,5	0.47	0	5,5,5	0.57	0
8	SO4	L	274	-	4,4,4	0.29	0	6,6,6	0.34	0
10	GOL	M	335	-	5,5,5	0.45	0	5,5,5	0.37	0
10	GOL	C	377	-	5,5,5	0.18	0	5,5,5	0.34	0
8	SO4	C	351	-	4,4,4	0.32	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	SO4	H	265	-	4,4,4	0.43	0	6,6,6	0.29	0
9	HTO	H	274[A]	-	9,9,9	0.32	0	10,10,10	0.75	0
6	LDA	L	712	-	12,15,15	2.10	1 (8%)	14,17,17	0.36	0
10	GOL	M	334	-	5,5,5	0.15	0	5,5,5	0.30	0
8	SO4	C	347	-	4,4,4	0.56	0	6,6,6	0.18	0
6	LDA	M	713	-	12,15,15	1.98	1 (8%)	14,17,17	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	C	361	-	-	0/4/4/4	-
10	GOL	C	374[B]	-	-	4/4/4/4	-
10	GOL	C	366	-	-	3/4/4/4	-
10	GOL	H	281	-	-	3/4/4/4	-
10	GOL	C	368	-	-	4/4/4/4	-
13	UQ9	L	502	-	-	15/57/81/81	0/1/1/1
10	GOL	H	283	-	-	4/4/4/4	-
6	LDA	M	714	-	-	8/13/13/13	-
10	GOL	H	289	-	-	4/4/4/4	-
10	GOL	M	341	-	-	0/4/4/4	-
10	GOL	L	288	-	-	2/4/4/4	-
11	BCB	L	400	3	-	6/37/177/177	-
16	NS5	M	600	-	-	8/43/43/43	-
12	BPB	L	402	-	-	5/37/105/105	0/5/6/6
6	LDA	H	718[B]	-	-	8/13/13/13	-
9	HTO	H	272	-	-	1/10/10/10	-
10	GOL	C	365	-	-	2/4/4/4	-
10	GOL	C	378	-	-	2/4/4/4	-
6	LDA	C	716	-	-	10/13/13/13	-
10	GOL	H	282	-	-	2/4/4/4	-
10	GOL	C	371	-	-	1/4/4/4	-
10	GOL	H	276[B]	-	-	2/4/4/4	-
9	HTO	L	277	-	-	0/10/10/10	-
9	HTO	H	273	-	-	4/10/10/10	-
10	GOL	M	342	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	M	337	-	-	2/4/4/4	-
10	GOL	C	359	-	-	2/4/4/4	-
10	GOL	C	363	-	-	0/4/4/4	-
10	GOL	H	277	-	-	2/4/4/4	-
12	BPB	M	402	-	-	9/37/105/105	0/5/6/6
6	LDA	L	709	-	-	6/13/13/13	-
6	LDA	M	704	-	-	5/13/13/13	-
6	LDA	L	710	-	-	8/13/13/13	-
6	LDA	L	703	-	-	6/13/13/13	-
10	GOL	L	283	-	-	2/4/4/4	-
6	LDA	M	717	-	-	2/13/13/13	-
9	HTO	L	280	-	-	5/10/10/10	-
9	HTO	L	278	-	-	4/10/10/10	-
10	GOL	C	375	-	-	0/4/4/4	-
6	LDA	H	719	-	-	8/13/13/13	-
10	GOL	H	280	-	-	2/4/4/4	-
6	LDA	L	723	-	-	8/13/13/13	-
9	HTO	C	355	-	-	4/10/10/10	-
10	GOL	L	285	-	-	2/4/4/4	-
9	HTO	C	358[A]	-	-	10/10/10/10	-
6	LDA	M	705	-	-	6/13/13/13	-
10	GOL	H	284	-	-	2/4/4/4	-
10	GOL	L	282	-	-	2/4/4/4	-
10	GOL	M	338	-	-	4/4/4/4	-
6	LDA	L	711	-	-	4/13/13/13	-
10	GOL	C	372	-	-	2/4/4/4	-
6	LDA	L	708	-	-	8/13/13/13	-
10	GOL	H	275	-	-	2/4/4/4	-
10	GOL	H	287	-	-	4/4/4/4	-
10	GOL	H	286	-	-	3/4/4/4	-
5	HEC	C	402	1	-	5/10/54/54	-
10	GOL	H	276[A]	-	-	4/4/4/4	-
10	GOL	C	370	-	-	2/4/4/4	-
9	HTO	C	356	-	-	9/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	M	715	-	-	5/13/13/13	-
10	GOL	C	367	-	-	4/4/4/4	-
10	GOL	H	278	-	-	2/4/4/4	-
10	GOL	C	376	-	-	2/4/4/4	-
5	HEC	C	401	1	-	3/10/54/54	-
10	GOL	C	364	-	-	4/4/4/4	-
6	LDA	H	721	-	-	10/13/13/13	-
11	BCB	M	400	4	-	12/37/177/177	-
10	GOL	L	281	-	-	0/4/4/4	-
11	BCB	L	401	3	-	7/37/177/177	-
10	GOL	M	339	-	-	2/4/4/4	-
10	GOL	H	291	-	-	2/4/4/4	-
7	DGA	C	730	1	-	26/37/37/45	-
10	GOL	C	362	-	-	2/4/4/4	-
9	HTO	L	279	-	-	3/10/10/10	-
10	GOL	C	369	-	-	2/4/4/4	-
10	GOL	L	286	-	-	4/4/4/4	-
9	HTO	M	333	-	-	7/10/10/10	-
9	HTO	L	276	-	-	6/10/10/10	-
13	UQ9	L	503	-	-	3/15/39/81	0/1/1/1
10	GOL	C	373	-	-	2/4/4/4	-
10	GOL	L	284	-	-	4/4/4/4	-
6	LDA	M	706	-	-	8/13/13/13	-
17	HTH	M	332	-	-	7/10/10/10	-
6	LDA	H	720	-	-	6/13/13/13	-
10	GOL	H	279	-	-	1/4/4/4	-
10	GOL	H	288	-	-	2/4/4/4	-
6	LDA	M	707	-	-	7/13/13/13	-
6	LDA	H	701	-	-	4/13/13/13	-
5	HEC	C	404	1	-	2/10/54/54	-
10	GOL	C	360	-	-	0/4/4/4	-
6	LDA	C	722	-	-	9/13/13/13	-
6	LDA	L	724	-	-	6/13/13/13	-
9	HTO	C	357	-	-	6/10/10/10	-
11	BCB	M	401	4	-	9/37/177/177	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	M	336	-	-	4/4/4/4	-
5	HEC	C	403	1	-	0/10/54/54	-
15	MQ9	M	501	-	-	2/53/73/73	0/2/2/2
6	LDA	L	702	-	-	7/13/13/13	-
10	GOL	L	287	-	-	0/4/4/4	-
10	GOL	H	290	-	-	2/4/4/4	-
10	GOL	H	285	-	-	4/4/4/4	-
10	GOL	M	340	-	-	3/4/4/4	-
10	GOL	M	335	-	-	0/4/4/4	-
10	GOL	C	377	-	-	2/4/4/4	-
9	HTO	H	274[A]	-	-	4/10/10/10	-
6	LDA	L	712	-	-	7/13/13/13	-
10	GOL	M	334	-	-	4/4/4/4	-
6	LDA	M	713	-	-	4/13/13/13	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	704	LDA	O1-N1	-7.97	1.23	1.42
6	H	720	LDA	O1-N1	-7.66	1.24	1.42
6	M	714	LDA	O1-N1	-7.61	1.24	1.42
6	L	724	LDA	O1-N1	-7.52	1.24	1.42
6	M	707	LDA	O1-N1	-7.37	1.24	1.42

The worst 5 of 175 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	M	401	BCB	O2D-CGD-CBD	10.71	124.57	111.00
11	M	401	BCB	C4D-C3D-CAD	-9.51	102.33	116.53
11	L	400	BCB	C4D-C3D-CAD	-9.27	102.70	116.53
11	M	400	BCB	C4D-C3D-CAD	-9.11	102.93	116.53
11	L	401	BCB	C4D-C3D-CAD	-8.33	104.09	116.53

There are no chirality outliers.

5 of 468 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	716	LDA	C2-C1-N1-CM1
6	C	716	LDA	N1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	C	722	LDA	C2-C1-N1-O1
6	C	722	LDA	N1-C1-C2-C3
6	H	718[B]	LDA	C2-C1-N1-O1

There are no ring outliers.

62 monomers are involved in 144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	H	261[A]	SO4	1	0
10	C	368	GOL	1	0
13	L	502	UQ9	11	0
10	H	283	GOL	6	0
6	M	714	LDA	2	0
11	L	400	BCB	5	0
16	M	600	NS5	3	0
12	L	402	BPB	2	0
9	H	272	HTO	1	0
10	C	365	GOL	2	0
6	C	716	LDA	3	0
8	C	354	SO4	1	0
9	L	277	HTO	2	0
9	H	273	HTO	3	0
10	M	342	GOL	1	0
8	C	338	SO4	1	0
8	M	326	SO4	2	0
10	C	363	GOL	1	0
12	M	402	BPB	1	0
6	M	704	LDA	6	0
6	L	710	LDA	1	0
6	L	703	LDA	4	0
6	H	719	LDA	3	0
10	H	280	GOL	1	0
6	L	723	LDA	4	0
9	C	355	HTO	6	0
10	M	338	GOL	3	0
6	L	711	LDA	1	0
6	M	715	LDA	2	0
8	C	340	SO4	1	0
10	H	278	GOL	2	0
5	C	401	HEC	1	0
10	C	364	GOL	3	0
6	H	721	LDA	1	0

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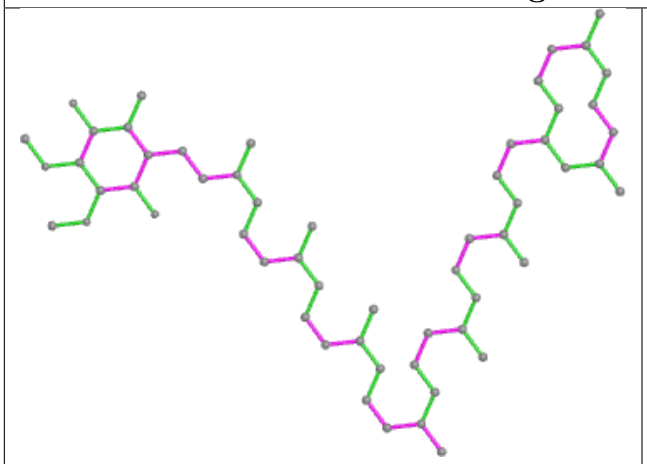
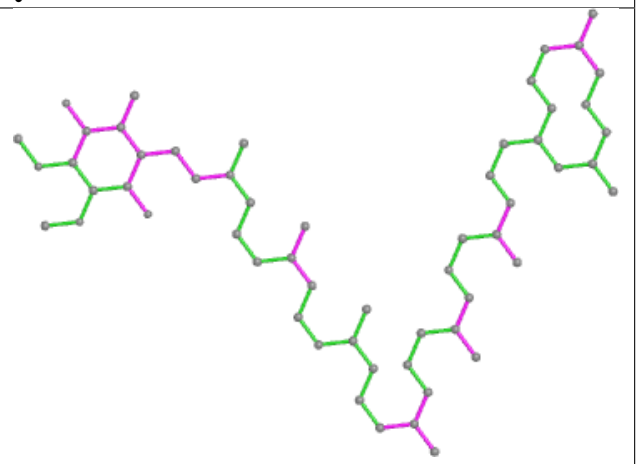
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	M	400	BCB	12	0
11	L	401	BCB	4	0
8	H	261[B]	SO4	4	0
7	C	730	DGA	3	0
9	L	279	HTO	1	0
10	C	369	GOL	3	0
10	L	286	GOL	1	0
9	M	333	HTO	2	0
13	L	503	UQ9	5	0
10	C	373	GOL	1	0
6	M	706	LDA	1	0
6	H	720	LDA	8	0
10	H	279	GOL	1	0
6	M	707	LDA	1	0
5	C	404	HEC	1	0
6	C	722	LDA	4	0
6	L	724	LDA	2	0
9	C	357	HTO	2	0
11	M	401	BCB	5	0
10	M	336	GOL	1	0
5	C	403	HEC	3	0
15	M	501	MQ9	2	0
6	L	702	LDA	6	0
10	C	377	GOL	4	0
8	C	351	SO4	1	0
9	H	274[A]	HTO	1	0
6	L	712	LDA	1	0
10	M	334	GOL	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.

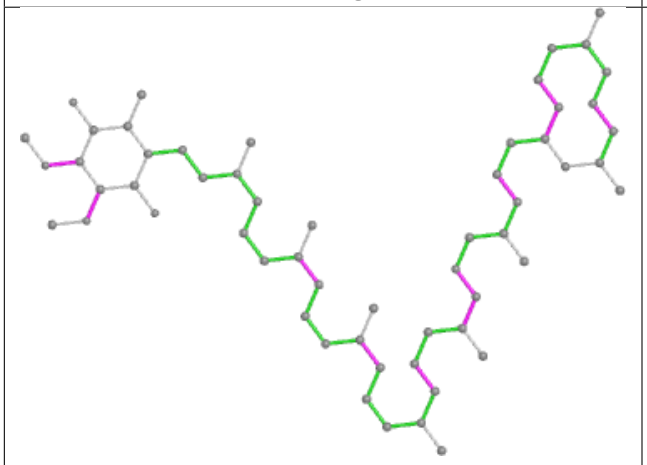
Ligand UQ9 L 502



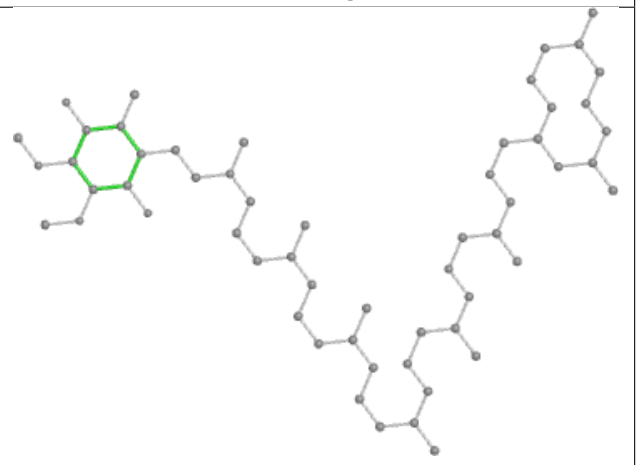
Bond lengths



Bond angles

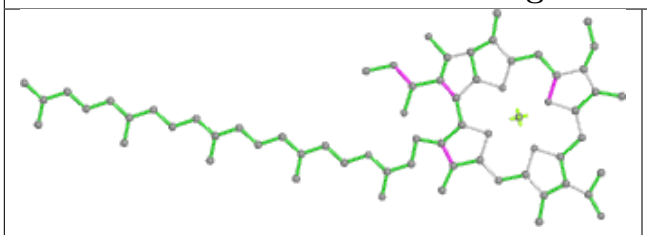


Torsions

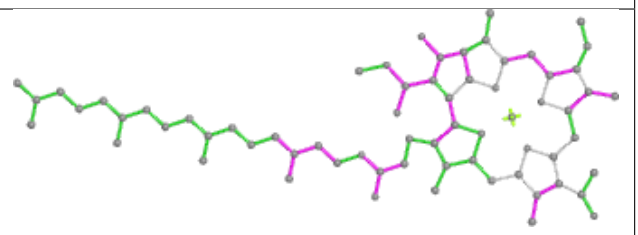


Rings

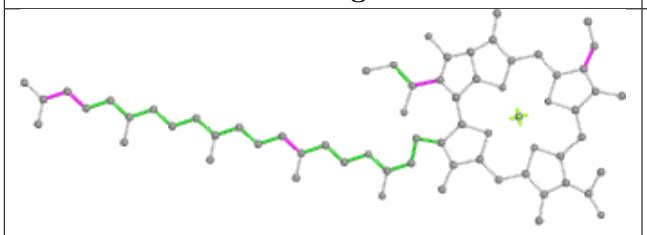
Ligand BCB L 400



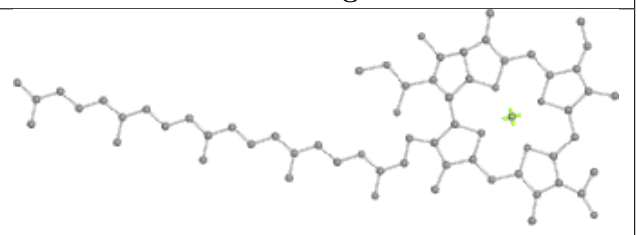
Bond lengths



Bond angles

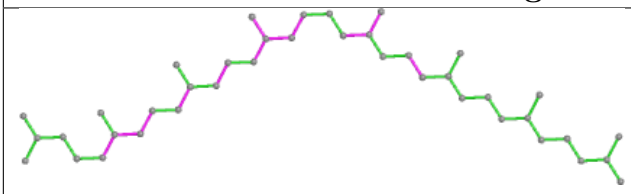


Torsions

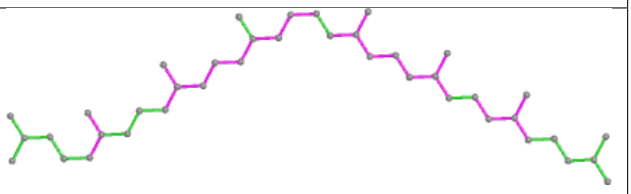


Rings

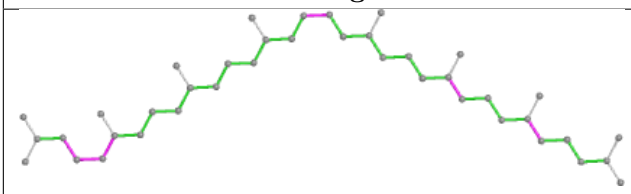
Ligand NS5 M 600



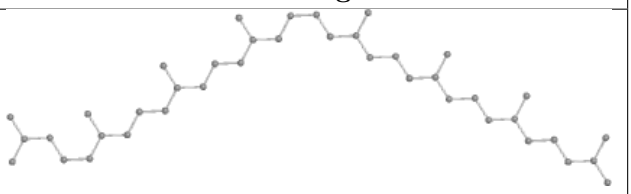
Bond lengths



Bond angles

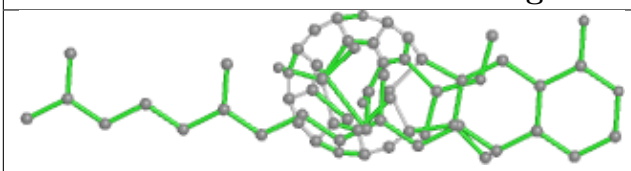


Torsions

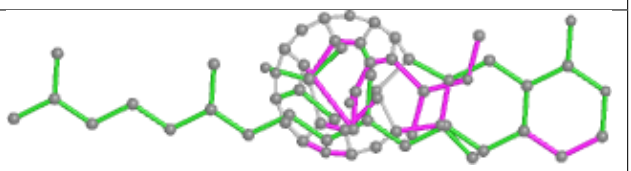


Rings

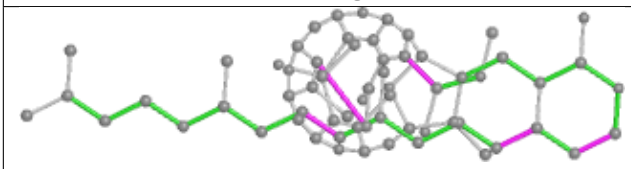
Ligand BPB L 402



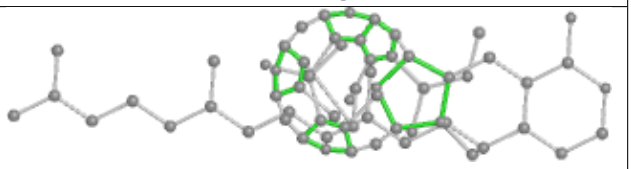
Bond lengths



Bond angles

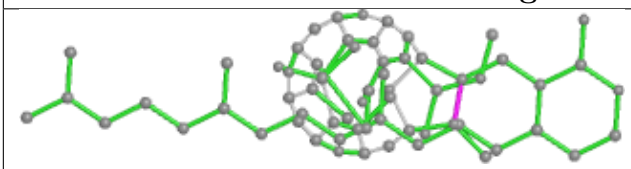


Torsions



Rings

Ligand BPB M 402



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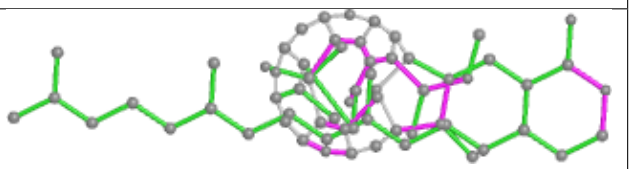
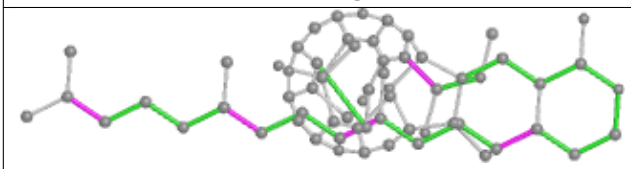


Bond angles



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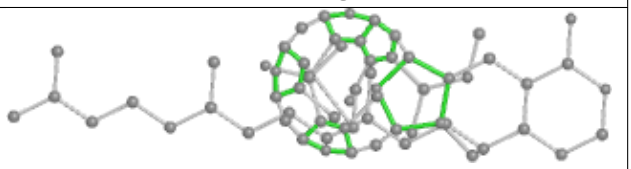
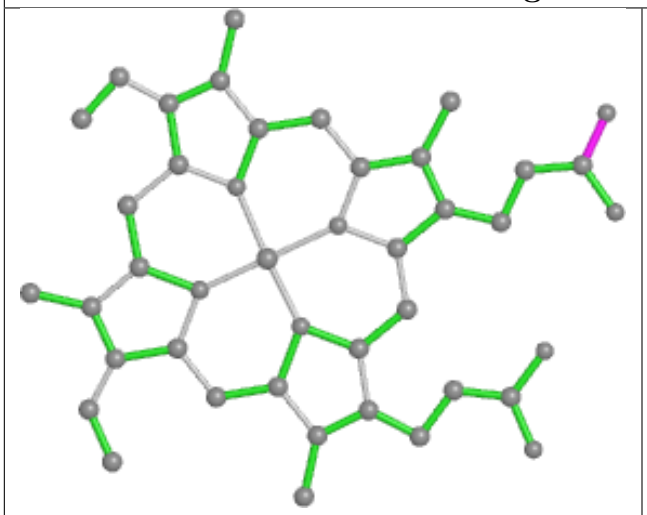
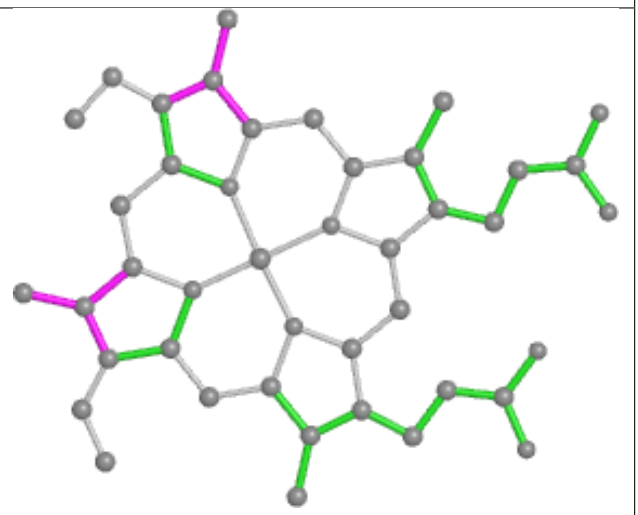


Rings

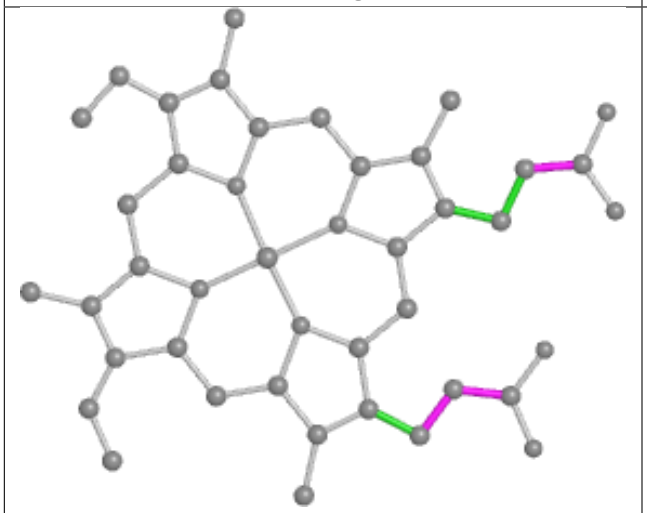
Ligand HEC C 402



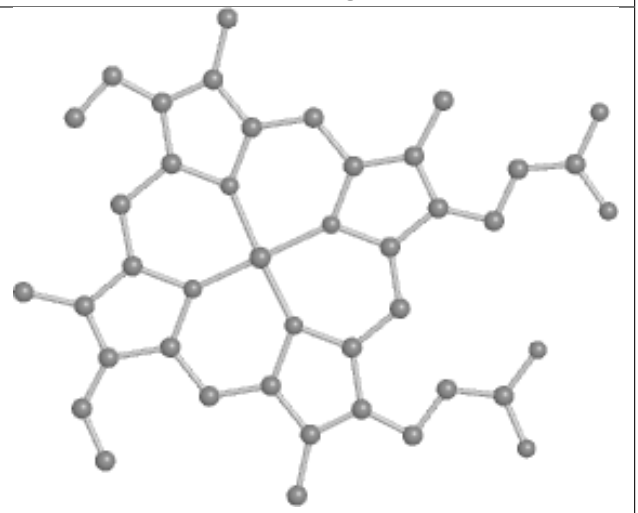
Bond lengths



Bond angles

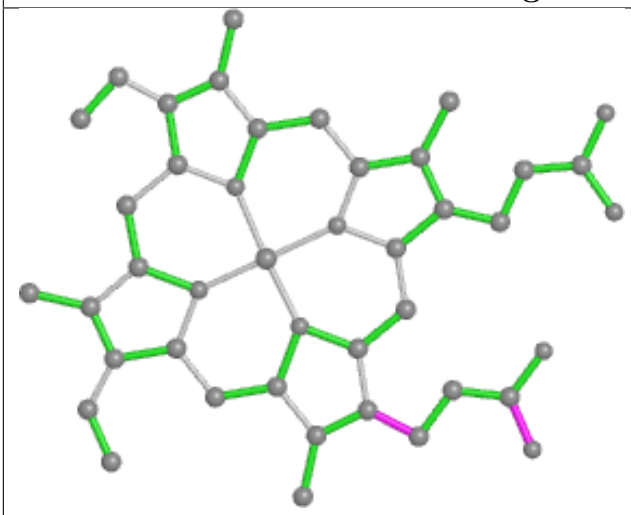


Torsions



Rings

Ligand HEC C 401



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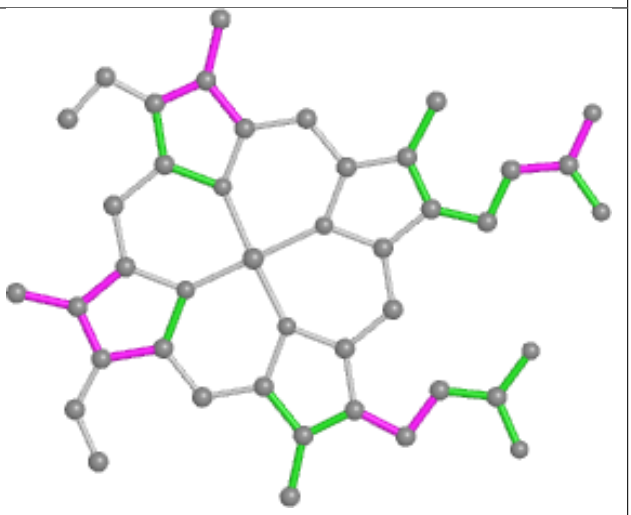
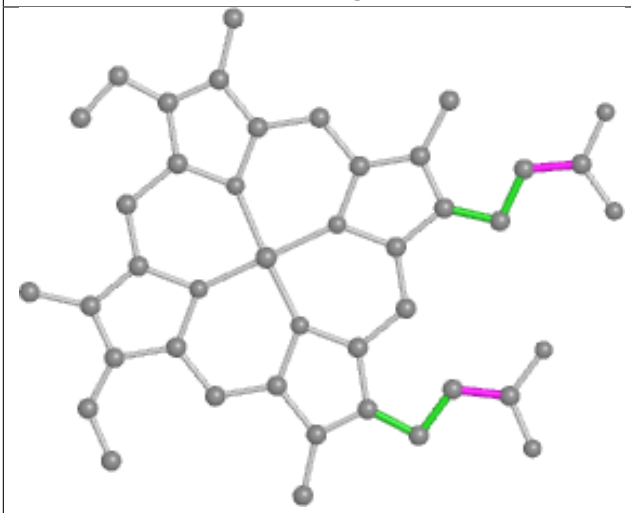
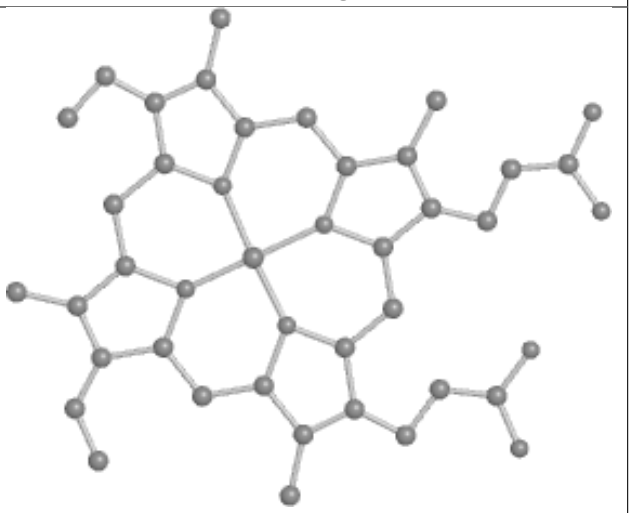


Bond angles

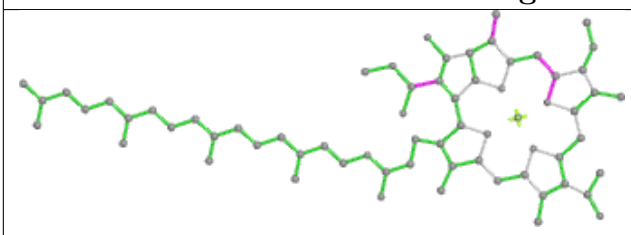


Torsions



Rings

Ligand BCB M 400



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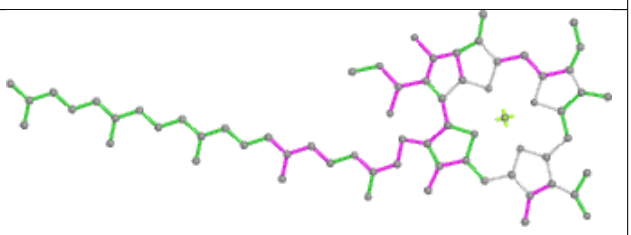
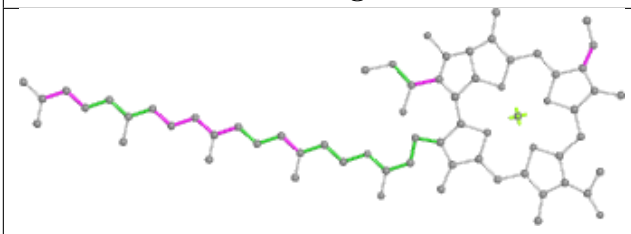
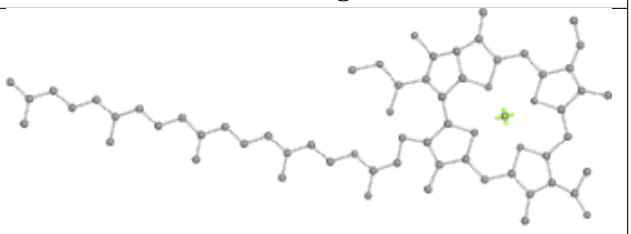


Bond angles

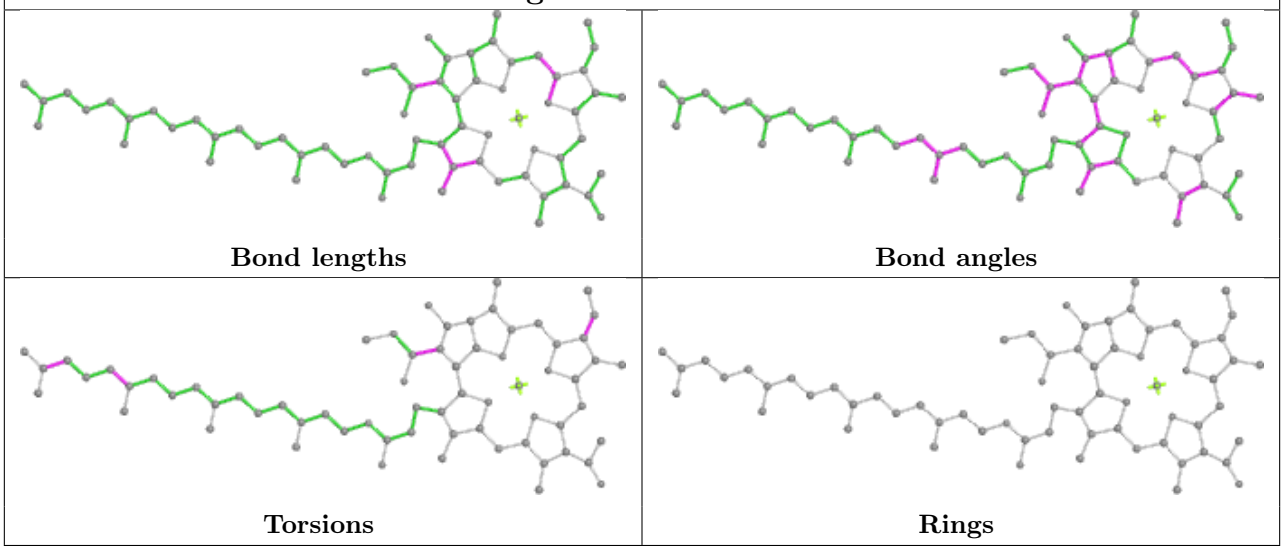


Torsions

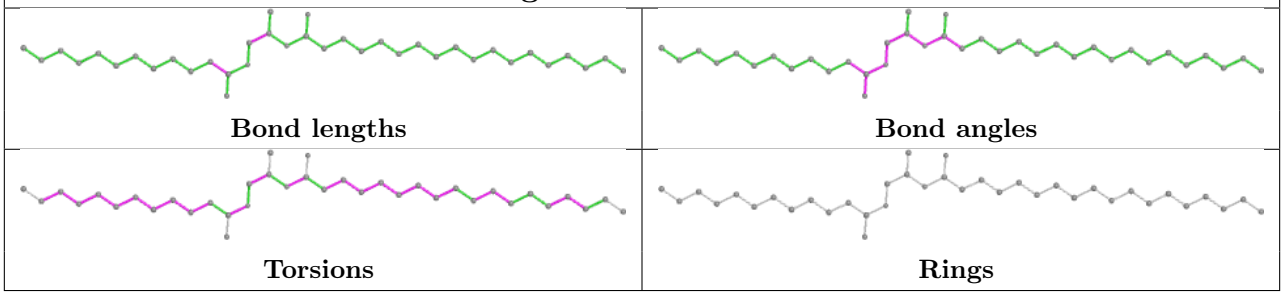


Rings

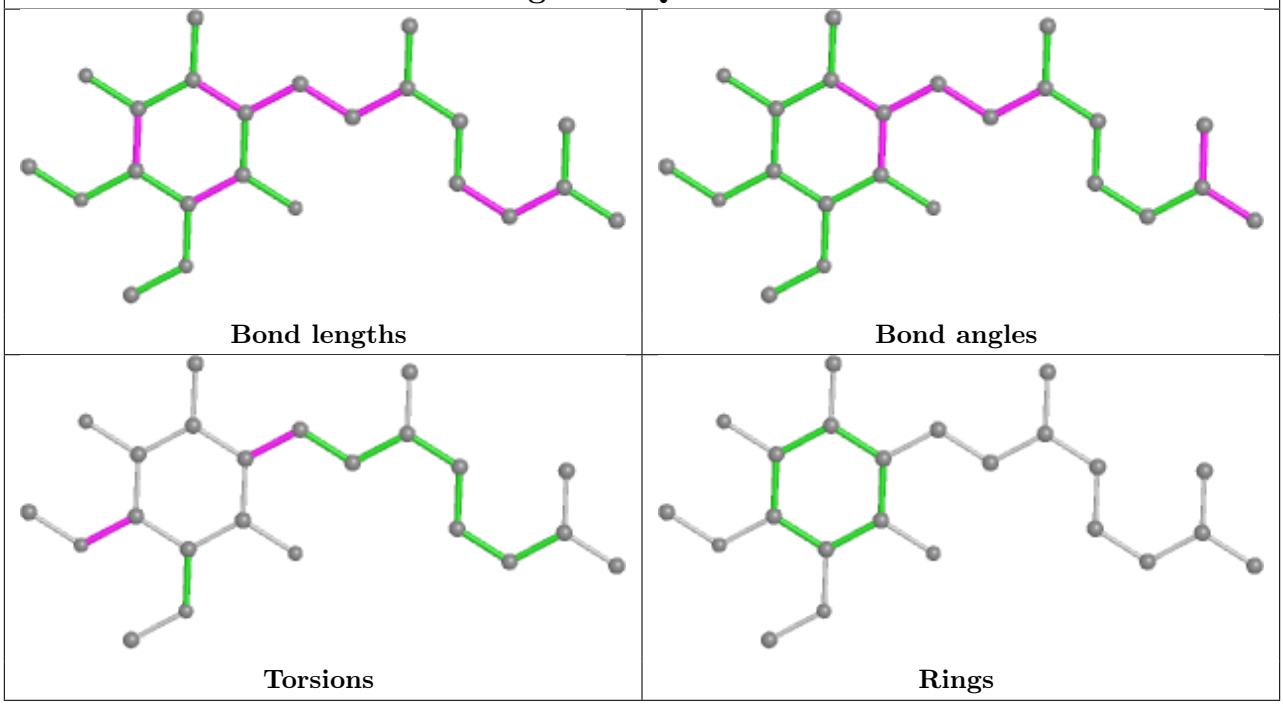
Ligand BCB L 401



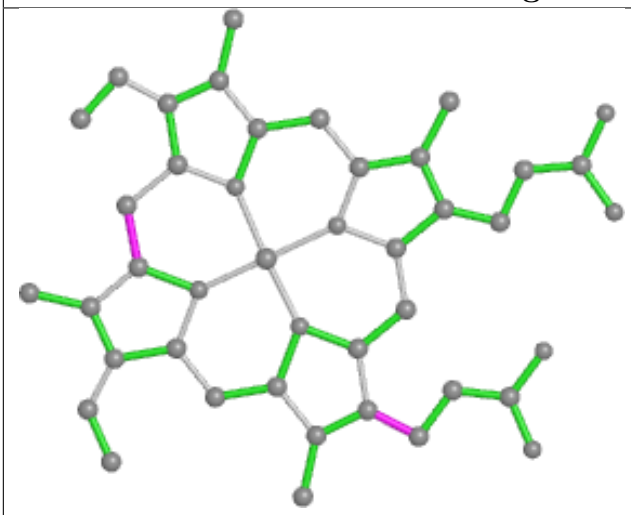
Ligand DGA C 730



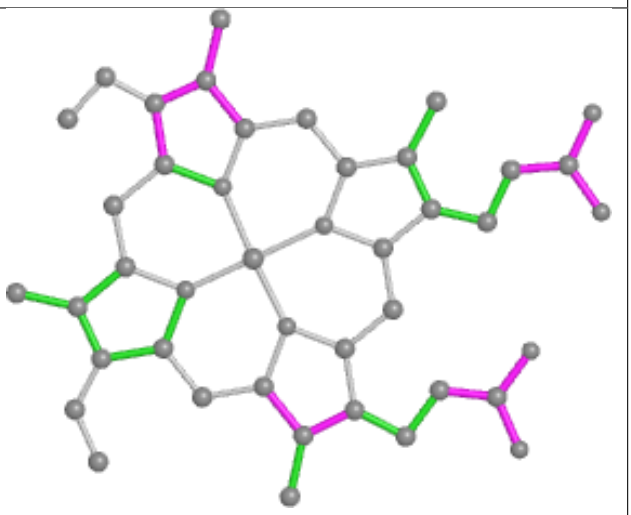
Ligand UQ9 L 503



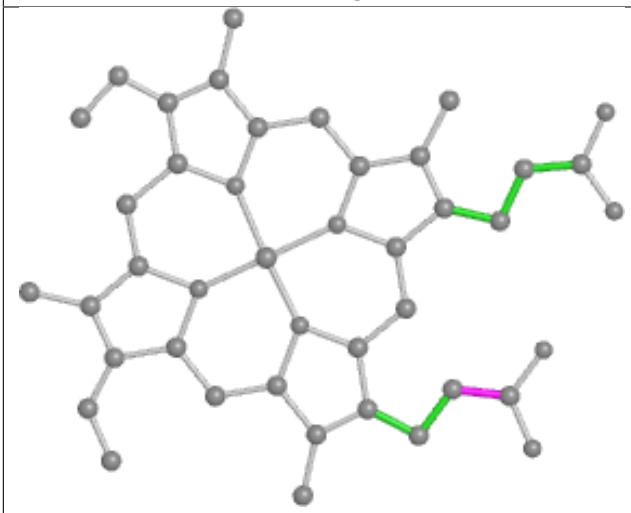
Ligand HEC C 404



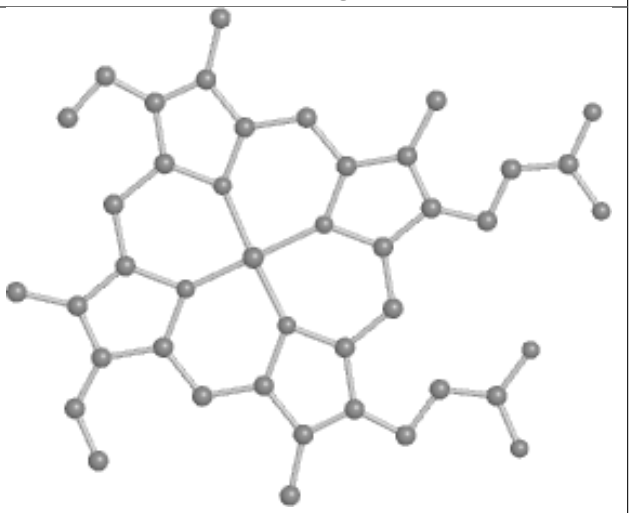
Bond lengths



Bond angles

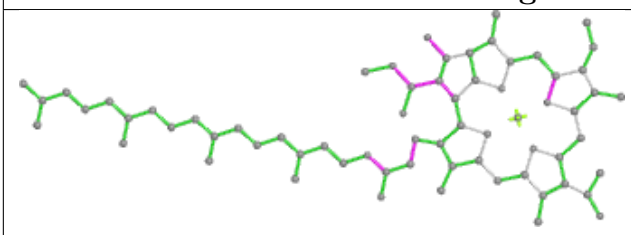


Torsions

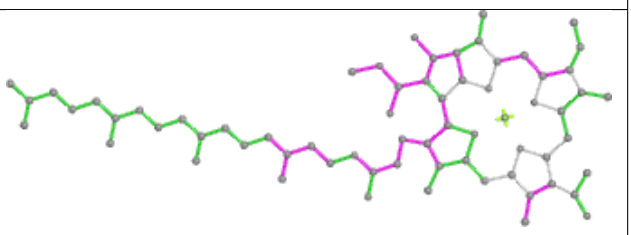


Rings

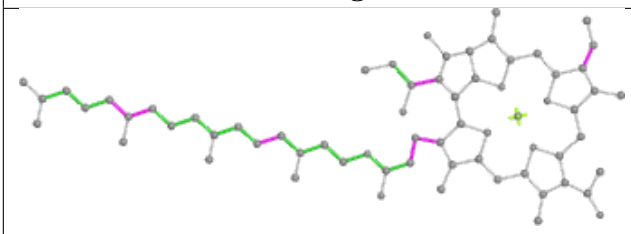
Ligand BCB M 401



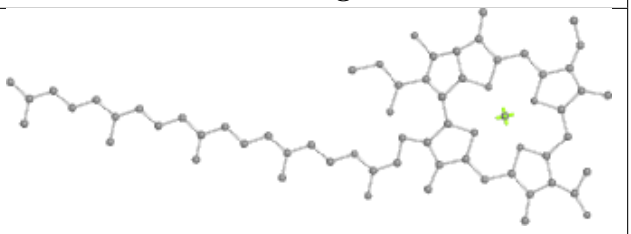
Bond lengths



Bond angles

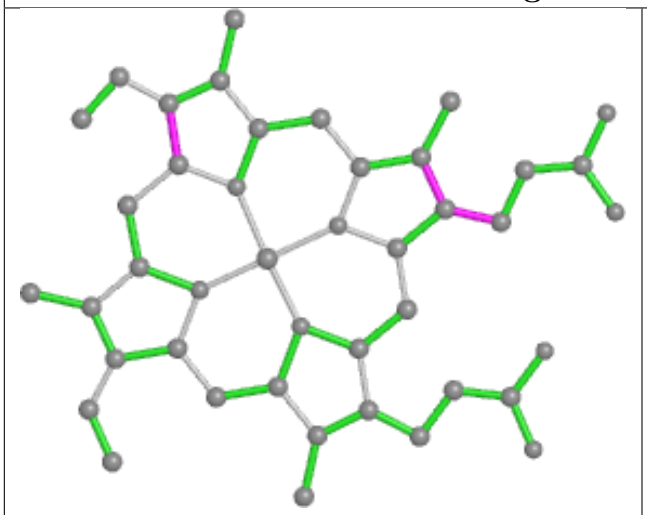


Torsions

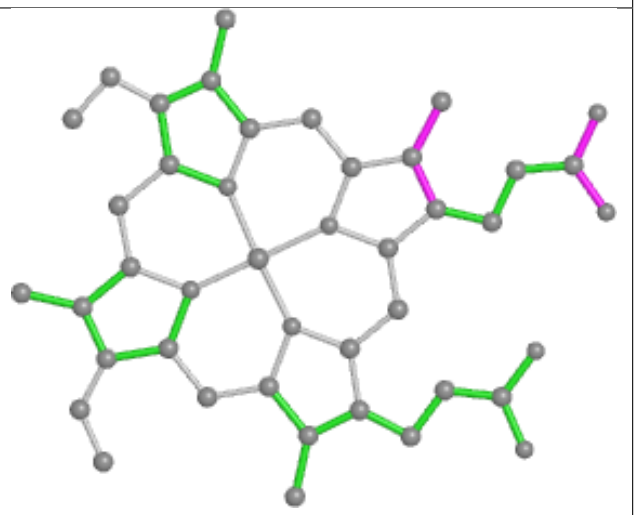


Rings

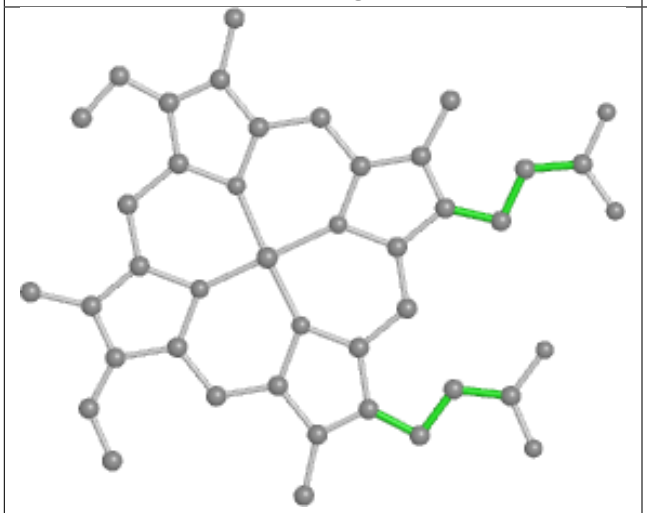
Ligand HEC C 403



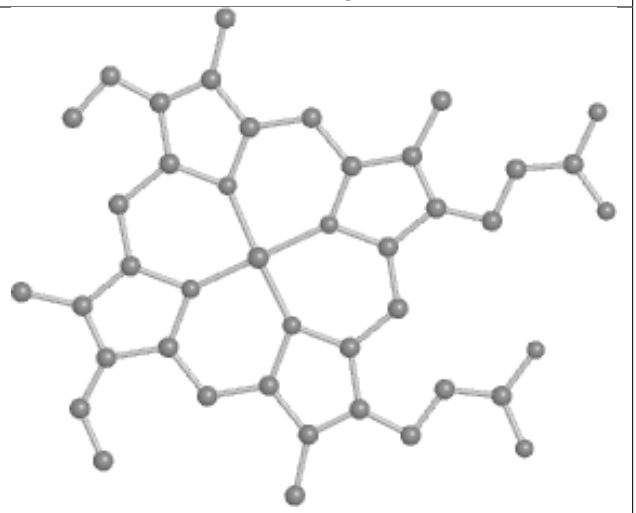
Bond lengths



Bond angles

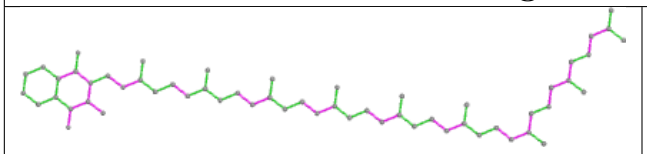


Torsions

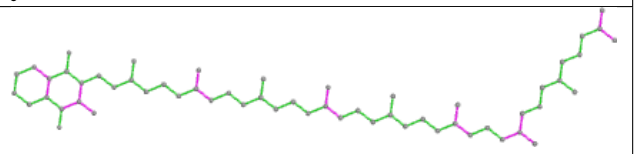


Rings

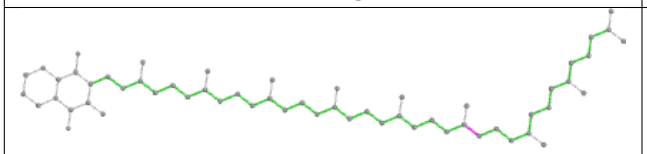
Ligand MQ9 M 501



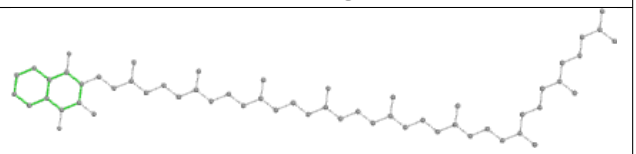
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	C	334/356 (93%)	0.38	39 (11%)	4	7	34, 46, 68, 125	0
2	H	249/258 (96%)	-0.02	13 (5%)	27	37	35, 51, 81, 119	0
3	L	273/273 (100%)	0.08	19 (6%)	16	24	33, 42, 58, 82	0
4	M	323/323 (100%)	0.27	26 (8%)	12	19	32, 43, 65, 83	0
All	All	1179/1210 (97%)	0.19	97 (8%)	11	18	32, 45, 69, 125	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	333	ALA	9.1
1	C	334	ALA	8.5
1	C	47	ALA	5.6
3	L	273	SER	5.1
1	C	332	LYS	4.9

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95th 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
2	FME	H	1[A]	10/11	0.97	0.10	47,50,54,56	7
2	FME	H	1[B]	10/11	0.97	0.10	47,53,59,61	7

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, 95th 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
6	LDA	H	718[B]	16/16	0.29	0.54	50,80,89,90	16
7	DGA	C	730	37/44	0.33	0.41	112,125,144,151	0
6	LDA	M	706	16/16	0.34	0.59	49,55,65,68	16
10	GOL	M	341	6/6	0.36	0.44	68,71,74,75	6
17	HTH	M	332	10/10	0.37	0.31	58,68,76,77	10
8	SO4	H	271	5/5	0.44	0.34	64,64,65,68	5
9	HTO	L	280	10/10	0.47	0.39	63,69,71,72	10
6	LDA	L	712	16/16	0.54	0.43	51,64,70,71	16
6	LDA	L	709	16/16	0.54	0.28	39,63,93,97	16
9	HTO	H	274[A]	10/10	0.54	0.57	53,69,72,75	10
6	LDA	L	711	16/16	0.55	0.31	60,68,76,77	16
6	LDA	L	702	16/16	0.56	0.80	51,53,57,57	16
10	GOL	M	338	6/6	0.56	0.36	57,60,62,63	6
6	LDA	M	717	16/16	0.59	0.39	50,59,89,91	16
10	GOL	C	374[B]	6/6	0.60	0.49	66,67,68,68	6
9	HTO	L	279	10/10	0.60	0.32	65,66,69,75	10
10	GOL	H	288	6/6	0.61	0.19	60,68,68,73	6
6	LDA	C	716	16/16	0.61	0.34	50,65,72,74	16
9	HTO	C	357	10/10	0.65	0.61	59,65,73,80	10
10	GOL	C	376	6/6	0.65	0.33	63,74,77,83	6
10	GOL	C	371	6/6	0.65	0.43	55,62,62,63	6
8	SO4	M	330	5/5	0.66	0.46	67,68,68,69	5
9	HTO	C	358[A]	10/10	0.66	0.30	58,62,67,68	10
10	GOL	C	370	6/6	0.67	0.42	64,66,68,68	6
10	GOL	M	342	6/6	0.67	0.24	66,67,69,70	6
8	SO4	C	351	5/5	0.67	0.40	60,60,63,67	5
10	GOL	C	363	6/6	0.68	0.29	46,59,65,69	6
6	LDA	M	707	16/16	0.69	0.31	42,58,72,81	16
8	SO4	L	275	5/5	0.69	0.44	66,66,67,68	5
6	LDA	C	722	16/16	0.70	0.24	53,63,66,66	16
10	GOL	L	288	6/6	0.70	0.52	54,57,58,60	6
8	SO4	H	270	5/5	0.71	0.33	60,61,63,63	5
6	LDA	M	715	16/16	0.71	0.39	58,71,77,79	16
10	GOL	H	281	6/6	0.71	0.39	64,67,72,76	6
10	GOL	H	287	6/6	0.72	0.17	65,71,72,73	6
10	GOL	H	277	6/6	0.73	0.31	55,59,62,62	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	SO4	M	329	5/5	0.73	0.41	57,58,63,67	5
6	LDA	L	710	16/16	0.73	0.28	52,60,81,82	16
8	SO4	C	354	5/5	0.74	0.37	66,69,70,71	5
10	GOL	H	279	6/6	0.74	0.28	63,68,71,72	6
10	GOL	H	289	6/6	0.74	0.35	62,66,66,67	6
10	GOL	C	378	6/6	0.74	0.43	78,80,81,81	6
8	SO4	C	347	5/5	0.75	0.40	78,82,83,90	5
10	GOL	H	283	6/6	0.75	0.21	59,60,61,61	6
10	GOL	M	340	6/6	0.75	0.29	60,64,65,66	6
6	LDA	H	719	16/16	0.75	0.22	58,63,71,72	16
10	GOL	C	372	6/6	0.75	0.22	56,62,65,65	6
9	HTO	C	355	10/10	0.75	0.24	62,66,71,72	10
8	SO4	C	350	5/5	0.76	0.39	64,67,69,72	5
10	GOL	C	375	6/6	0.76	0.38	66,69,70,72	6
9	HTO	H	273	10/10	0.76	0.34	48,51,60,62	10
10	GOL	L	287	6/6	0.76	0.25	54,55,57,57	6
6	LDA	M	705	16/16	0.76	0.25	61,69,87,87	16
13	UQ9	L	503	23/58	0.77	0.30	59,73,85,87	23
6	LDA	L	724	16/16	0.77	0.47	53,63,68,69	16
9	HTO	M	333	10/10	0.78	0.72	44,51,55,55	10
10	GOL	M	339	6/6	0.79	0.39	60,65,66,66	6
8	SO4	H	265	5/5	0.79	0.21	69,74,75,81	5
10	GOL	H	280	6/6	0.79	0.23	52,60,65,66	6
10	GOL	H	276[A]	6/6	0.79	0.26	50,60,62,62	2
10	GOL	H	276[B]	6/6	0.79	0.26	50,59,60,62	2
9	HTO	L	278	10/10	0.79	0.20	57,65,67,69	10
8	SO4	H	269	5/5	0.80	0.30	71,72,75,76	5
10	GOL	C	367	6/6	0.81	1.39	50,58,59,60	6
10	GOL	C	369	6/6	0.81	1.19	49,56,61,61	6
13	UQ9	L	502	58/58	0.81	0.52	44,80,97,99	58
9	HTO	L	277	10/10	0.81	0.17	57,64,69,76	10
8	SO4	L	274	5/5	0.81	0.26	62,62,65,68	5
10	GOL	H	284	6/6	0.82	0.21	58,63,65,68	6
9	HTO	C	356	10/10	0.82	0.27	59,72,76,77	10
6	LDA	L	708	16/16	0.82	0.21	40,56,68,76	0
8	SO4	M	331	5/5	0.82	0.21	60,60,61,62	5
10	GOL	L	284	6/6	0.82	0.21	52,65,67,67	6
10	GOL	L	285	6/6	0.82	0.21	51,67,70,71	6
10	GOL	C	366	6/6	0.82	0.22	56,62,63,71	6
8	SO4	C	348	5/5	0.82	0.20	70,73,77,80	5
8	SO4	C	343	5/5	0.83	0.40	52,62,65,66	5
8	SO4	C	353	5/5	0.83	0.38	66,69,72,76	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	GOL	H	285	6/6	0.83	0.28	68,70,71,71	6
6	LDA	L	703	16/16	0.83	0.40	52,57,61,63	16
10	GOL	C	364	6/6	0.83	0.24	52,67,67,68	6
8	SO4	M	328	5/5	0.83	0.34	61,62,64,69	5
8	SO4	H	266	5/5	0.84	0.33	65,66,68,71	5
8	SO4	C	349	5/5	0.84	0.42	63,64,71,71	5
6	LDA	H	720	16/16	0.84	0.24	55,69,73,73	16
10	GOL	M	337	6/6	0.84	0.13	68,69,69,70	6
6	LDA	L	723	16/16	0.84	1.01	55,58,64,68	16
10	GOL	H	278	6/6	0.84	0.20	63,67,68,71	6
10	GOL	H	291	6/6	0.85	0.26	74,78,80,81	6
9	HTO	L	276	10/10	0.85	0.48	50,67,70,71	10
10	GOL	M	336	6/6	0.86	0.17	68,69,70,71	6
8	SO4	C	337[A]	5/5	0.86	0.23	59,62,67,67	5
10	GOL	C	373	6/6	0.86	1.85	60,63,64,65	6
8	SO4	C	337[B]	5/5	0.86	0.23	59,64,69,70	5
8	SO4	H	264	5/5	0.86	0.18	61,67,72,73	5
10	GOL	C	360	6/6	0.87	0.22	44,56,62,71	6
10	GOL	L	286	6/6	0.87	0.65	58,63,64,68	6
6	LDA	M	713	16/16	0.87	0.18	63,69,84,86	16
8	SO4	C	352	5/5	0.87	0.35	78,78,81,82	5
10	GOL	C	365	6/6	0.87	0.18	60,67,69,72	6
10	GOL	L	282	6/6	0.87	0.15	53,59,59,63	6
8	SO4	H	263	5/5	0.87	0.49	75,76,78,79	5
8	SO4	C	340	5/5	0.88	0.29	57,71,76,82	5
6	LDA	M	714	16/16	0.88	0.20	70,75,81,82	16
10	GOL	H	282	6/6	0.88	0.37	59,66,68,69	6
10	GOL	H	290	6/6	0.88	0.19	49,59,63,67	6
8	SO4	C	344	5/5	0.88	0.38	74,76,79,82	5
10	GOL	C	377	6/6	0.88	0.12	63,65,67,67	6
8	SO4	H	267	5/5	0.88	0.26	56,64,65,65	5
10	GOL	C	368	6/6	0.89	0.19	62,63,68,70	6
9	HTO	H	272	10/10	0.89	0.17	61,67,75,80	10
10	GOL	L	283	6/6	0.89	0.13	59,63,68,70	6
8	SO4	H	261[B]	5/5	0.90	0.19	47,54,61,61	5
10	GOL	C	362	6/6	0.90	0.38	51,57,63,63	6
6	LDA	M	704	16/16	0.90	0.22	49,80,87,87	16
8	SO4	H	268	5/5	0.90	0.54	63,66,70,72	5
8	SO4	C	342	5/5	0.90	0.24	63,68,71,75	5
10	GOL	H	286	6/6	0.90	0.33	67,67,69,70	6
16	NS5	M	600	40/40	0.90	0.14	42,54,95,96	0
8	SO4	H	261[A]	5/5	0.90	0.19	52,58,64,65	5

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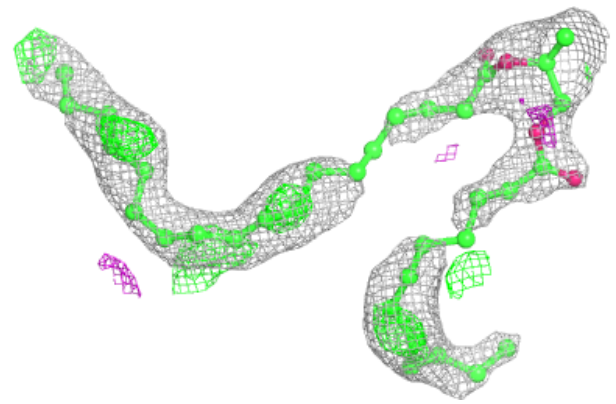
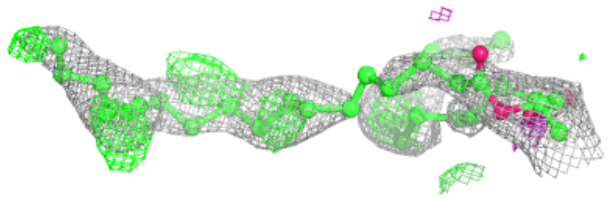
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MQ9	M	501	58/58	0.91	0.17	31,41,92,98	0
6	LDA	H	701	16/16	0.91	0.26	43,57,71,73	0
10	GOL	C	361	6/6	0.91	0.24	60,64,72,75	6
8	SO4	C	346	5/5	0.93	0.25	57,65,71,72	5
8	SO4	C	339	5/5	0.93	0.36	69,71,75,80	5
10	GOL	M	335	6/6	0.93	0.10	44,54,60,68	6
10	GOL	L	281	6/6	0.94	0.41	54,58,66,68	6
8	SO4	M	327	5/5	0.94	0.22	53,58,68,75	5
10	GOL	M	334	6/6	0.94	0.18	40,56,66,69	6
8	SO4	C	345	5/5	0.94	0.23	66,68,72,72	5
6	LDA	H	721	16/16	0.95	0.14	50,66,69,69	0
10	GOL	H	275	6/6	0.95	0.27	59,62,64,67	0
8	SO4	C	341	5/5	0.95	0.17	67,74,80,81	5
11	BCB	M	400	66/66	0.95	0.18	34,40,109,121	0
11	BCB	M	401	66/66	0.95	0.17	28,34,58,66	0
12	BPB	M	402	65/65	0.96	0.13	33,41,124,132	0
10	GOL	C	359	6/6	0.96	0.44	44,50,54,55	6
11	BCB	L	401	66/66	0.96	0.14	27,35,64,75	0
8	SO4	H	260	5/5	0.96	0.09	59,63,68,71	5
8	SO4	C	338	5/5	0.96	0.19	53,57,60,64	5
12	BPB	L	402	65/65	0.96	0.13	32,39,48,51	0
8	SO4	H	259	5/5	0.97	0.13	60,62,67,69	5
11	BCB	L	400	66/66	0.97	0.18	28,36,48,52	0
8	SO4	M	326	5/5	0.97	0.18	56,61,62,62	5
5	HEC	C	401	43/43	0.98	0.10	41,46,55,58	0
5	HEC	C	402	43/43	0.98	0.09	39,44,52,60	0
5	HEC	C	403	43/43	0.98	0.15	32,36,41,42	0
5	HEC	C	404	43/43	0.98	0.09	32,38,51,64	0
8	SO4	M	324	5/5	0.99	0.11	47,52,61,63	0
8	SO4	M	325	5/5	0.99	0.17	64,67,78,79	0
8	SO4	H	262	5/5	0.99	0.12	41,43,45,47	5
14	FE2	M	500	1/1	1.00	0.14	37,37,37,37	0

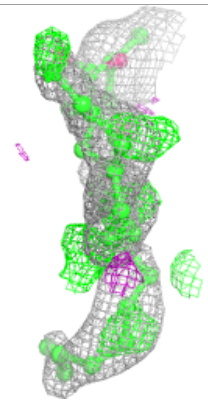
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGA C 730:

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

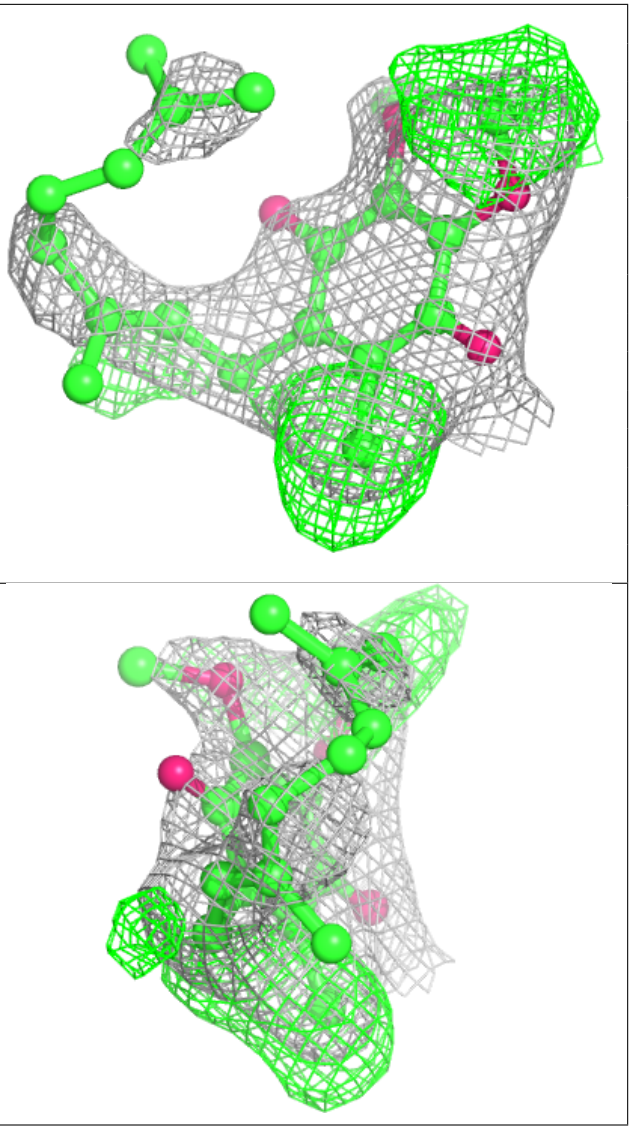






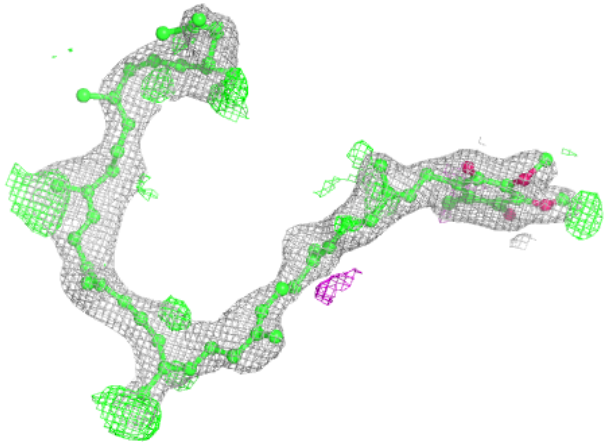
Electron density around UQ9 L 503:

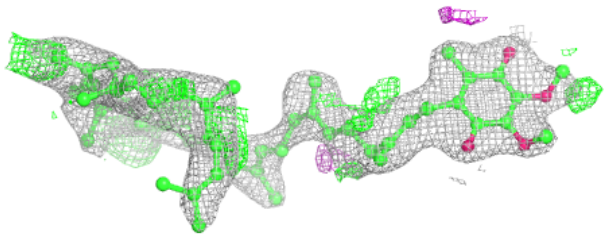
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UQ9 L 502:

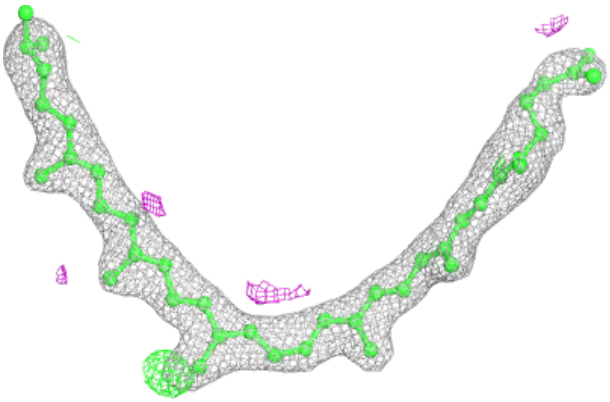
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

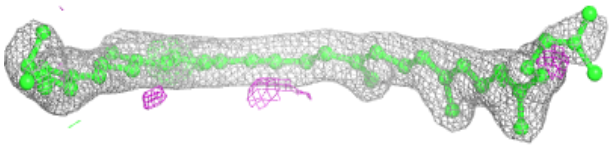


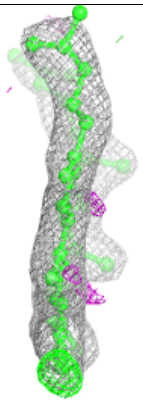


Electron density around NS5 M 600:

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

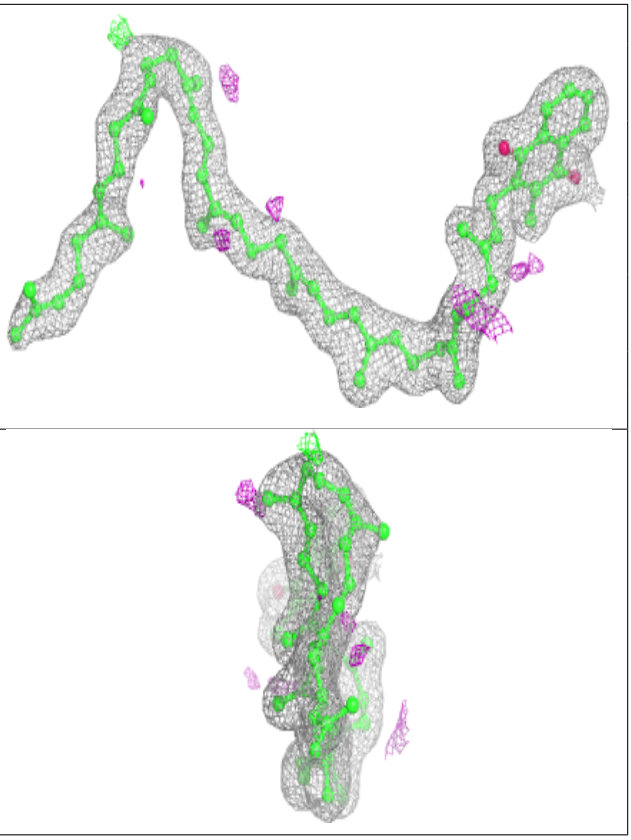






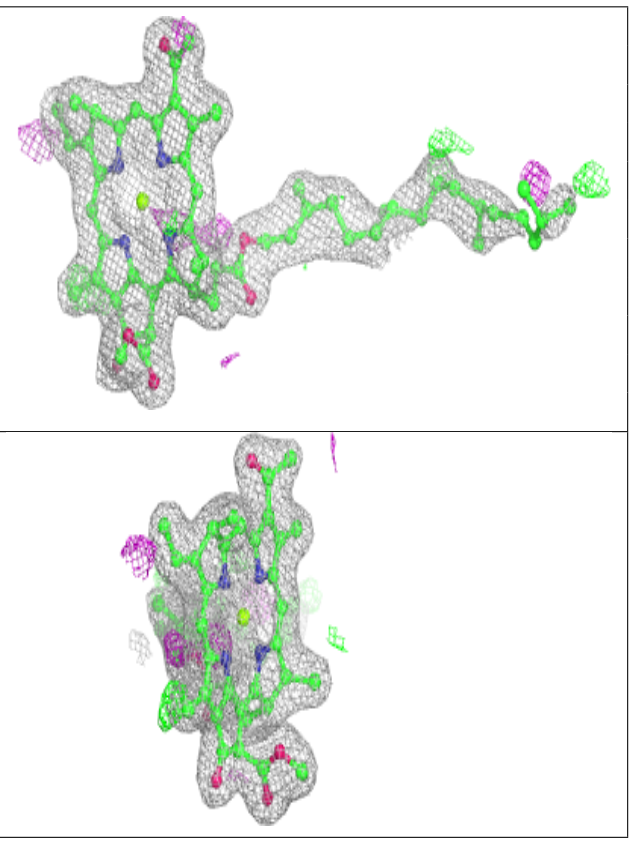
Electron density around MQ9 M 501:

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



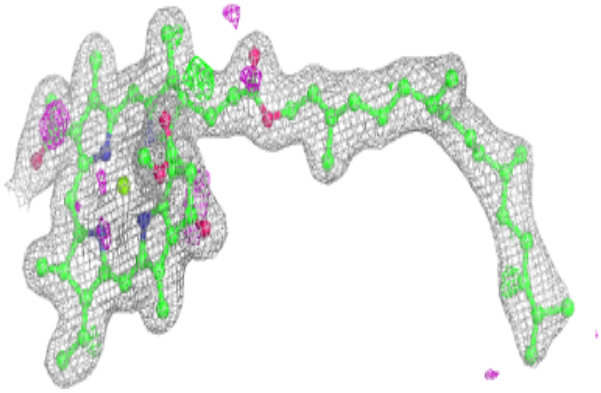
Electron density around BCB M 400:

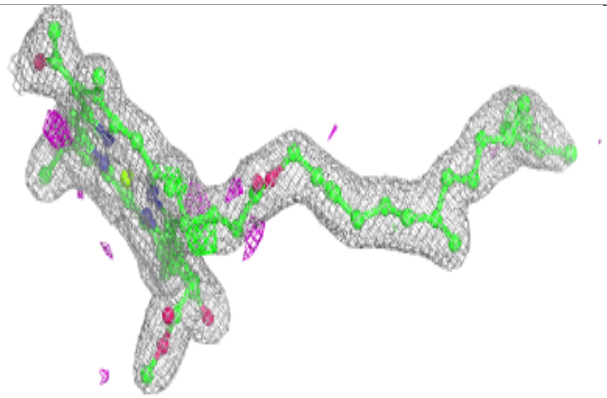
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

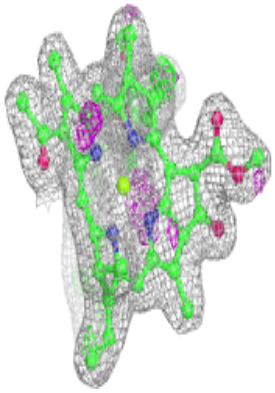


Electron density around BCB M 401:

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

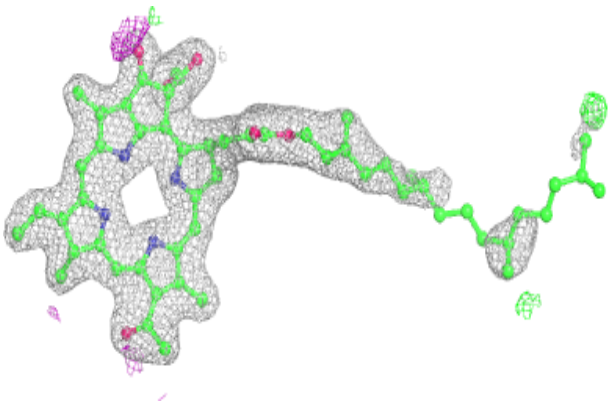


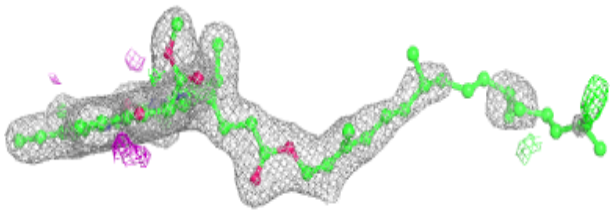


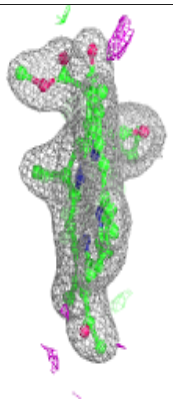


Electron density around BPB M 402:

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

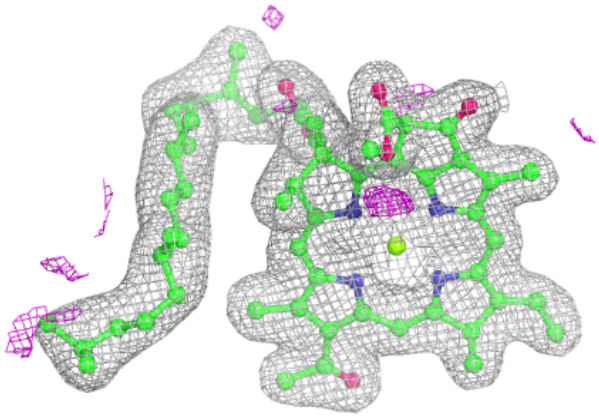


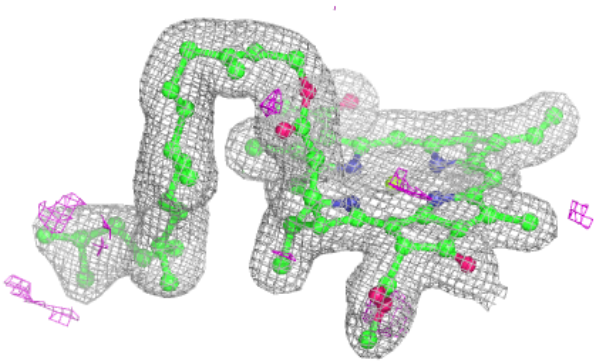


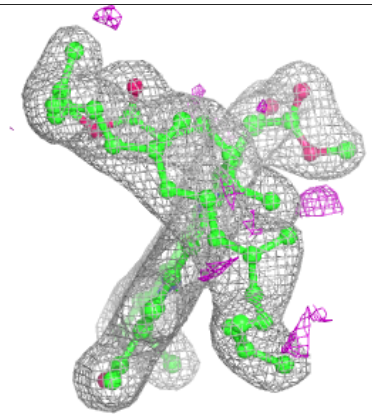


Electron density around BCB L 401:

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

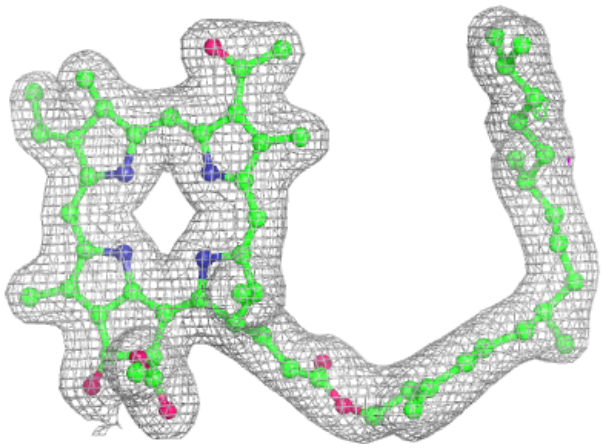


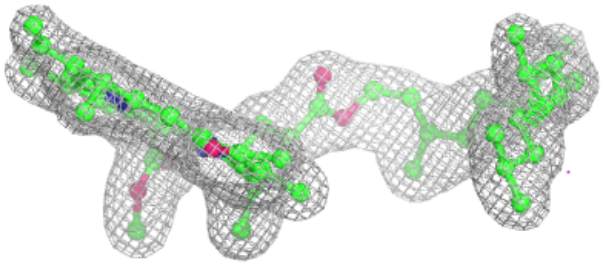


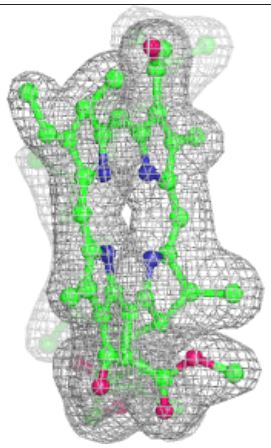


Electron density around BPB L 402:

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

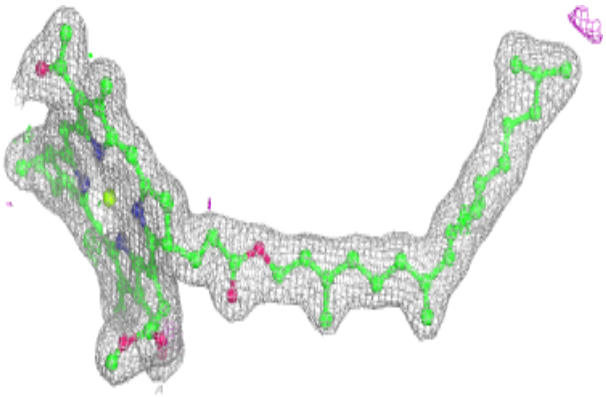


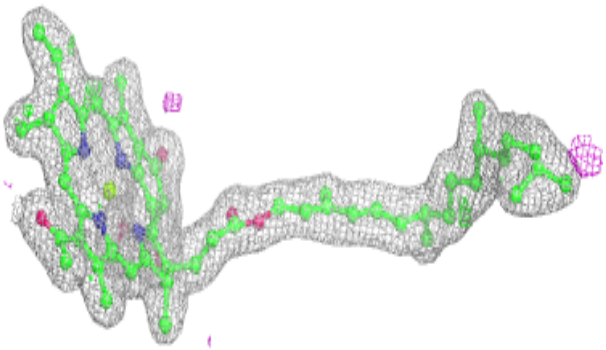


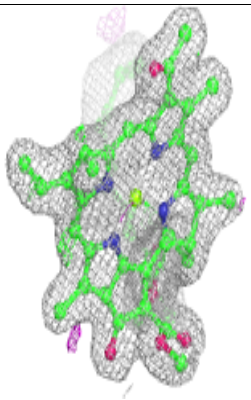


Electron density around BCB L 400:

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

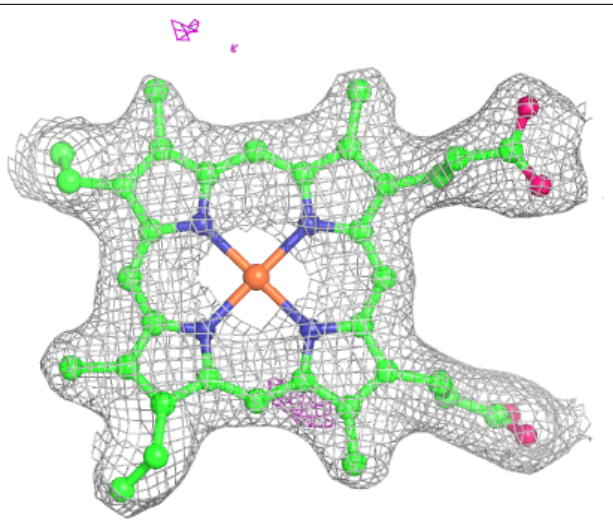


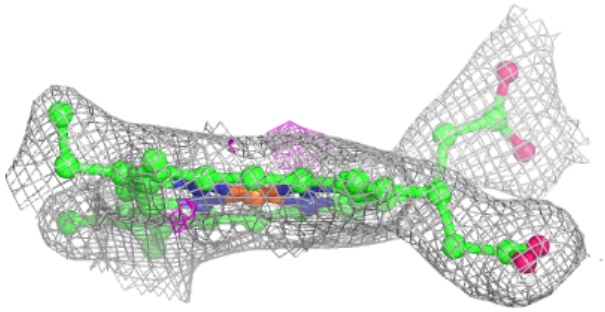


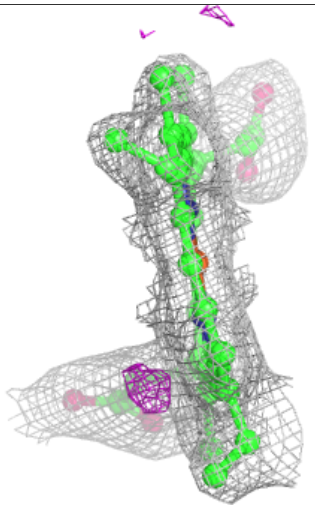


Electron density around HEC C 401:

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

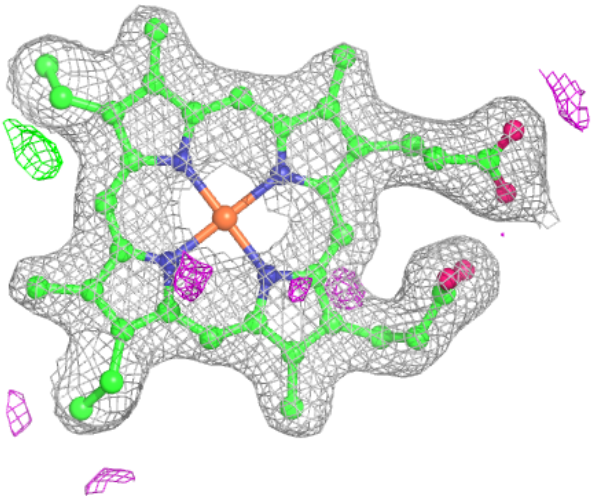


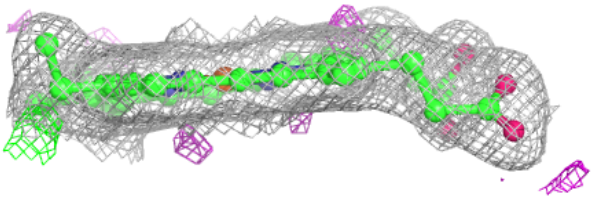


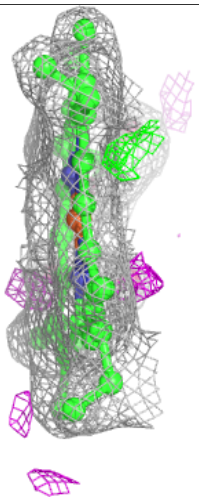


Electron density around HEC C 402:

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

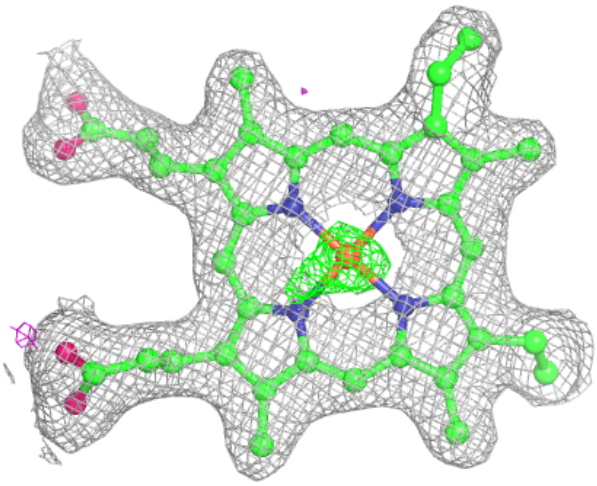


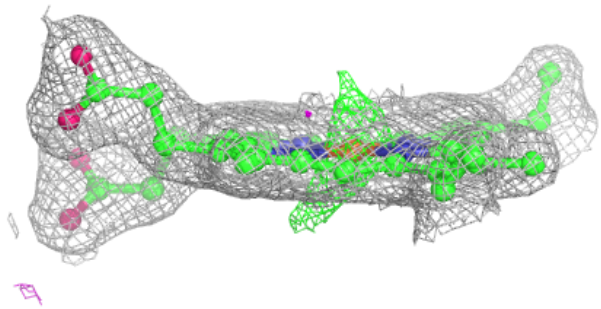




Electron density around HEC C 403:

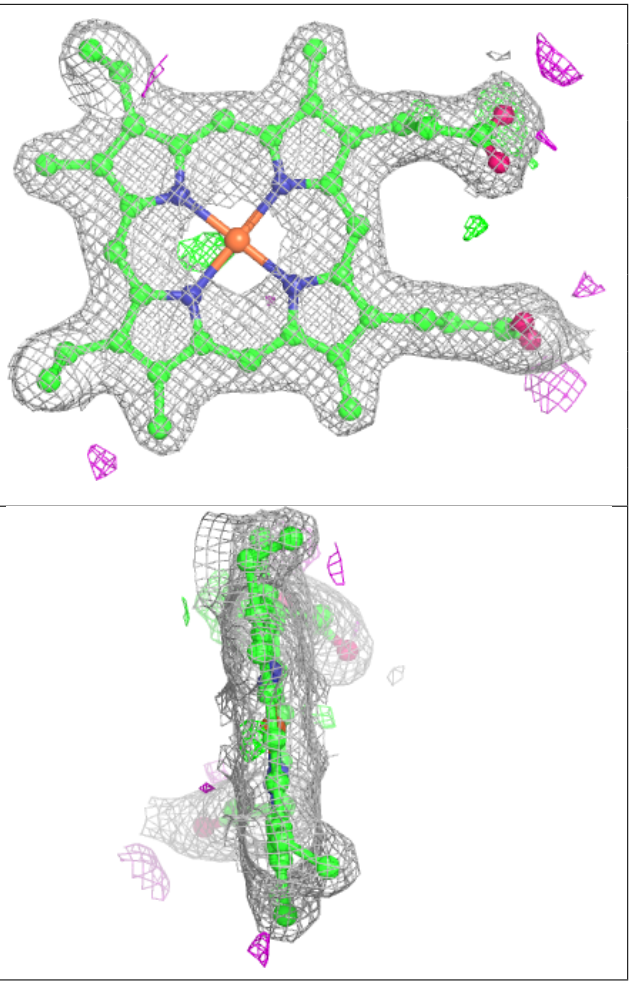
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEC C 404:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.