



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:25 PM UTC

PDB ID : 3T6E / pdb_00003t6e
Title : Crystal Structure of the Reaction Centre from Blastochloris viridis strain DSM 133 (ATCC 19567) substrain-94
Authors : Roszak, A.W.; Gardiner, A.T.; Isaacs, N.W.; Cogdell, R.J.
Deposited on : 2011-07-28
Resolution : 1.92 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

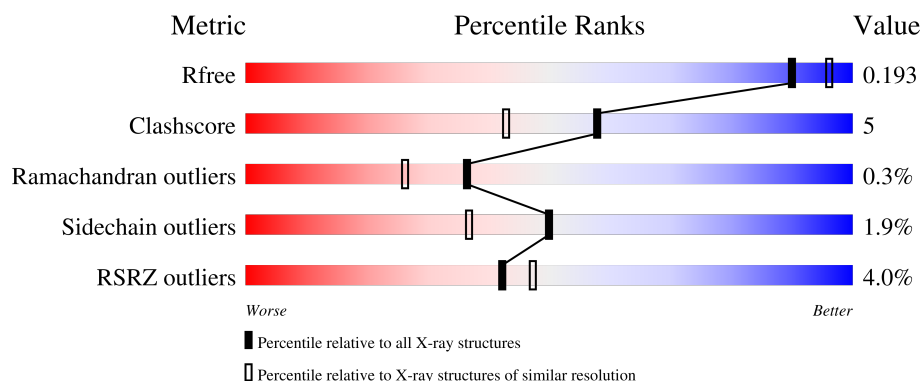
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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}	180053	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 $\leq 5\%$. 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	6% 86% 8% 6%
2	H	258	6% 90% 9% .
3	L	273	3% 93% 7%
4	M	323	6% 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	H	270	-	-	-	X
10	GOL	H	279	-	-	-	X
10	GOL	L	279	-	-	X	-
11	BCB	L	400	X	-	-	-
11	BCB	L	401	X	-	-	-
11	BCB	M	400	X	-	-	-
11	BCB	M	401	X	-	-	-
6	LDA	H	718	-	-	-	X
6	LDA	M	715	-	-	-	X
8	SO4	C	344	-	-	X	-
9	HTO	M	332	-	X	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 12066 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
1	C	334	Total	C	N	O	S	0	4	0
			2651	1667	480	486	18			

- Molecule 2 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	258	Total	C	N	O	S	45	4	0
			2034	1298	349	384	3			

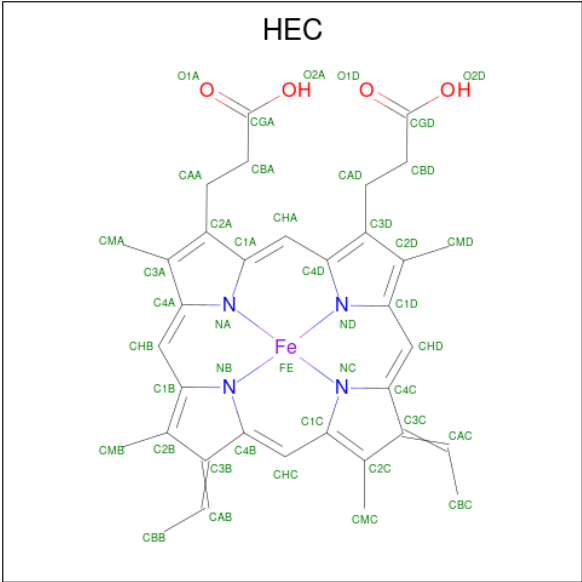
- Molecule 3 is a protein called Reaction center protein L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	5	0
			2207	1482	354	361	10			

- Molecule 4 is a protein called Reaction center protein M chain.

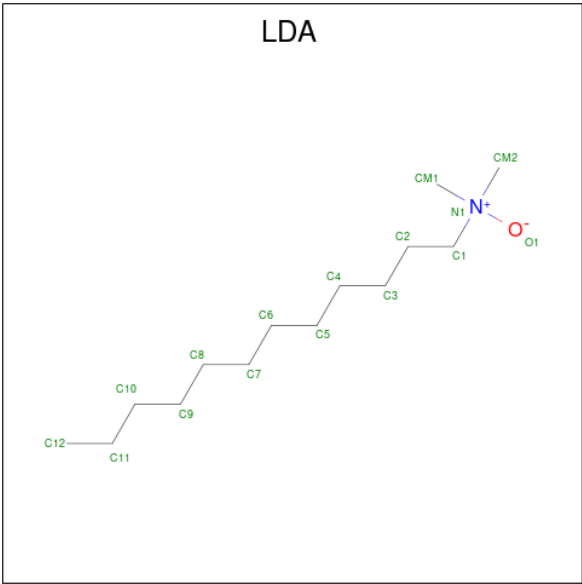
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	4	0
			2591	1725	425	429	12			

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



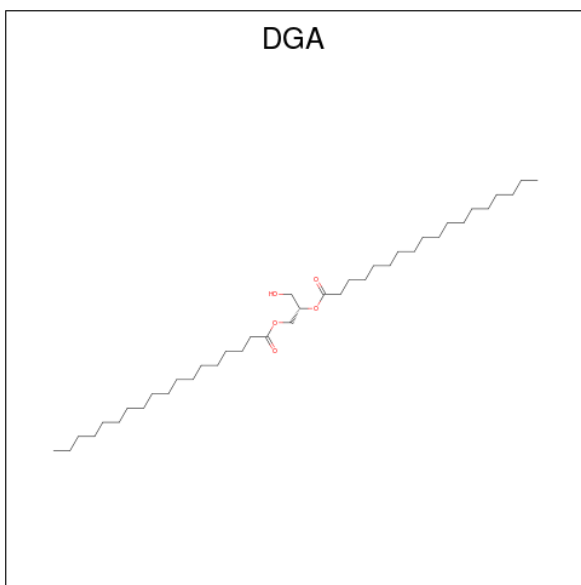
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 55	C 43	Fe 1	N 5	O 6	0	1

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).



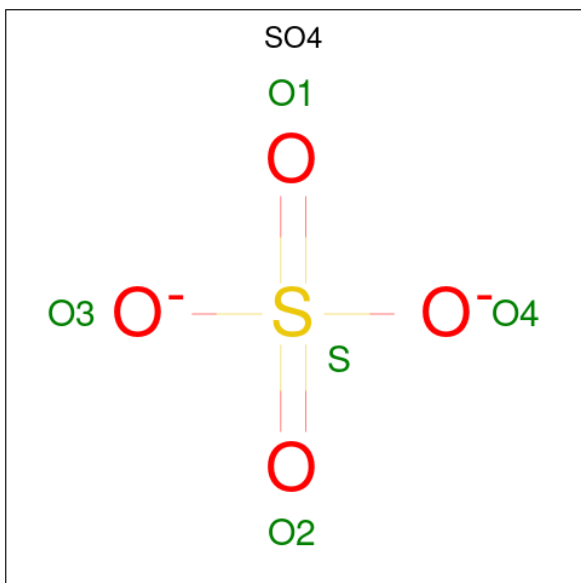
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			16	14	1	1		
6	C	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			13	11	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	L	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		
6	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 7 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			37	33	4		
7	H	1	Total	C	O	0	0
			31	26	5		
7	L	1	Total	C	O	0	0
			33	28	5		
7	M	1	Total	C	O	0	0
			34	29	5		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



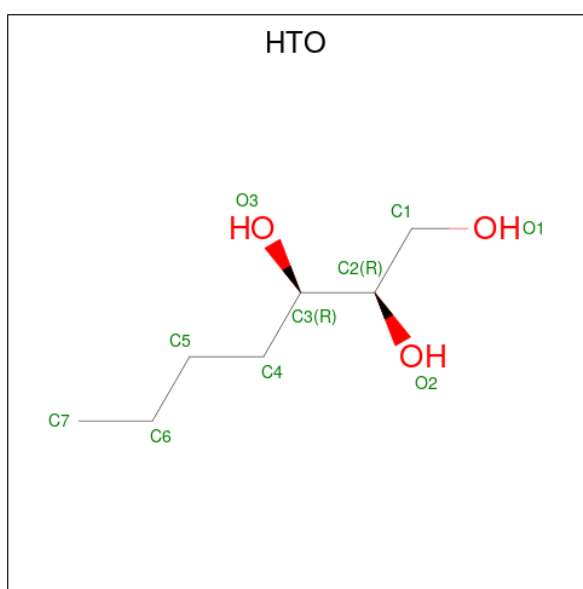
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total	O	S	0	0
			5	4	1		
8	C	1	Total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

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

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



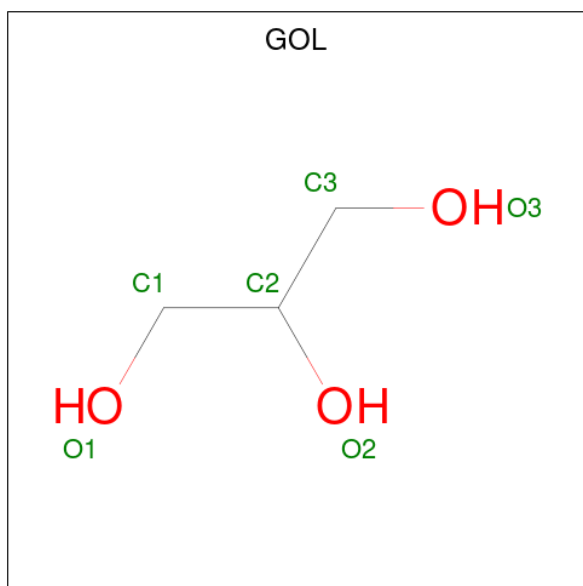
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		

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

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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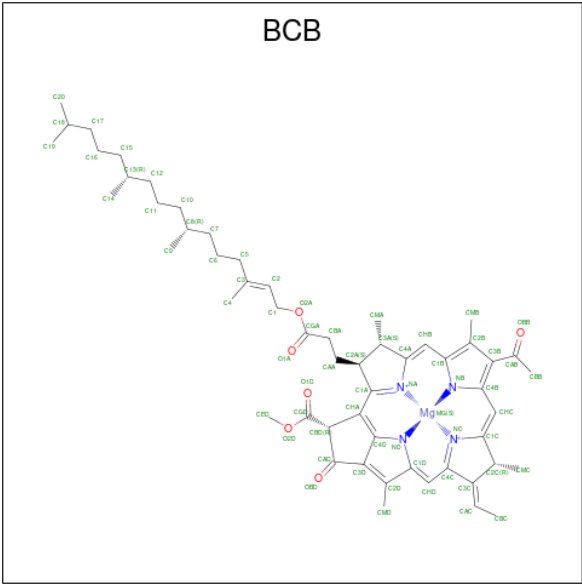
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10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

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

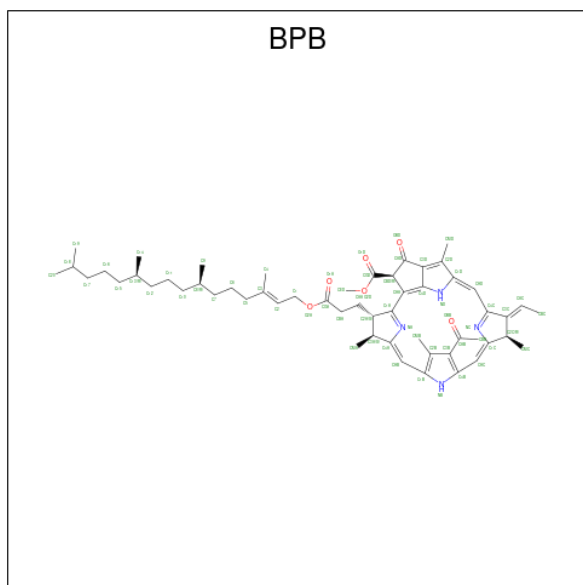
- Molecule 11 is BACTERIOCHLOROPHYLL B (CCD ID: BCB) (formula: C₅₅H₇₂MgN₄O₆).



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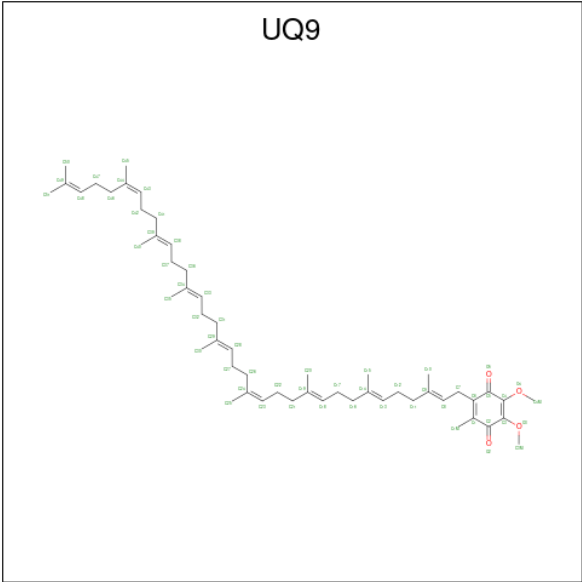
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



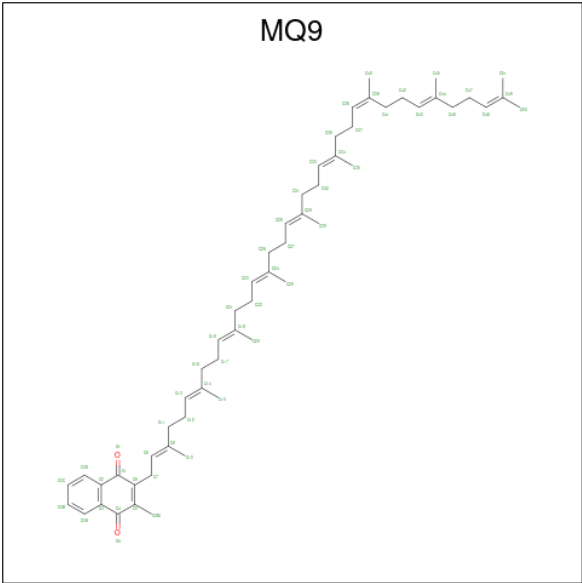
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	L	1	Total	C	O	0	0
			58	54	4		
13	L	1	Total	C	O	0	0
			19	15	4		

- Molecule 14 is MENAQUINONE-9 (CCD ID: MQ9) (formula: C₅₆H₈₀O₂).

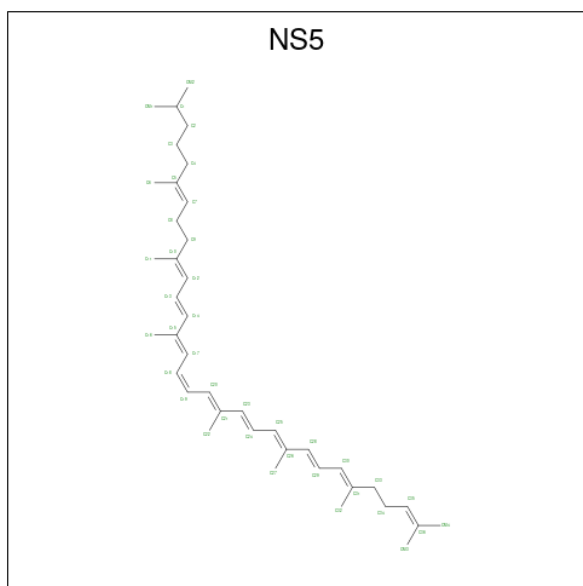


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	M	1	Total	C	O	0	0
			58	56	2		

- Molecule 15 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 16 is 15-cis-1,2-dihydroneurosporene (CCD ID: NS5) (formula: C₄₀H₆₀).



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

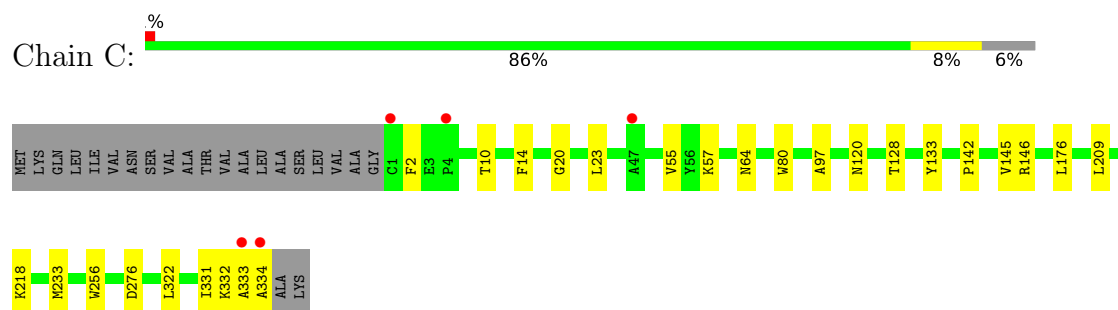
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	C	441	Total	O	0	0
			441	441		
17	H	233	Total	O	0	0
			233	233		
17	L	125	Total	O	0	0
			125	125		
17	M	175	Total	O	0	0
			175	175		

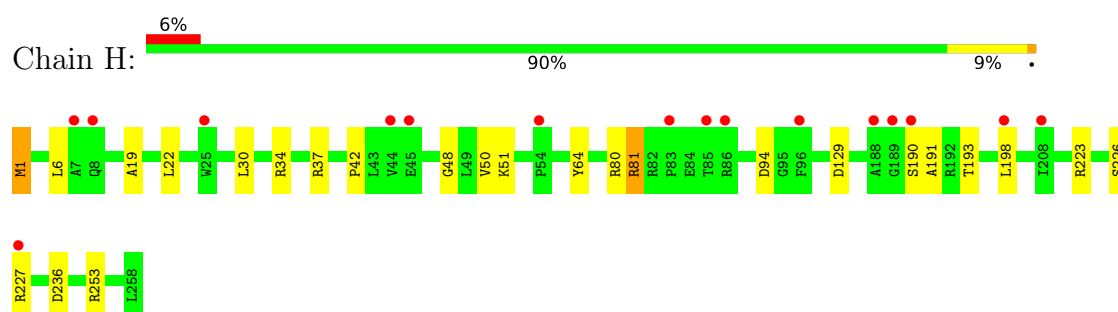
3 Residue-property plots [i](#)

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.

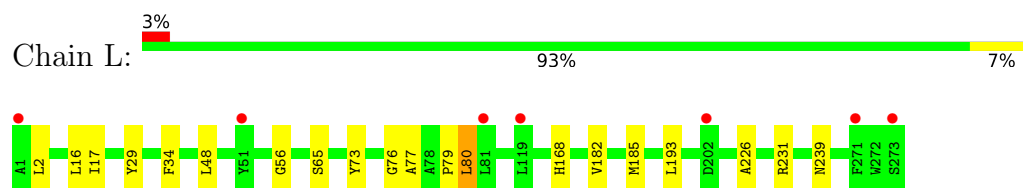
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



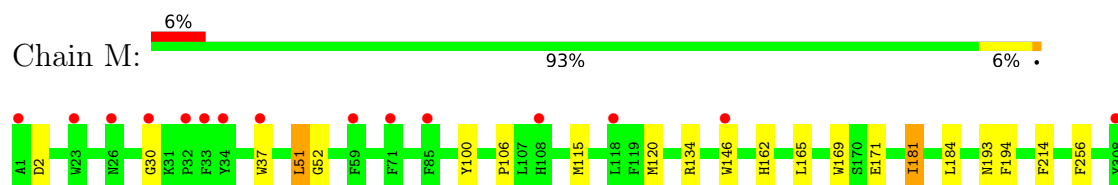
- Molecule 2: Reaction center protein H chain

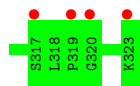


- Molecule 3: Reaction center protein L chain



- Molecule 4: Reaction center protein M chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	221.58Å 221.58Å 113.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.46 – 1.92 43.46 – 1.92	Depositor EDS
% Data completeness (in resolution range)	99.4 (43.46-1.92) 99.4 (43.46-1.92)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.6.0101	Depositor
R, R_{free}	0.155 , 0.178 (Not available) , 0.193	Depositor DCC
R_{free} test set	10655 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 76.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12066	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: MQ9, NS5, GOL, BPB, HTO, SO4, FME, BCB, HEC, FE2, LDA, DGA, CSO, UQ9

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	1.05	0/2718	0.94	3/3702 (0.1%)
2	H	1.03	0/2064	0.90	2/2820 (0.1%)
3	L	1.03	1/2298 (0.0%)	0.92	0/3135
4	M	1.03	1/2689 (0.0%)	0.92	2/3676 (0.1%)
All	All	1.04	2/9769 (0.0%)	0.92	7/13333 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	181	ILE	CA-CB	5.82	1.61	1.54
3	L	226	ALA	CA-CB	5.63	1.62	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	142	PRO	O-C-N	6.63	124.36	121.31
4	M	30	GLY	N-CA-C	-6.63	105.28	112.04
1	C	55	VAL	CB-CA-C	-5.27	105.30	111.94
2	H	190	SER	N-CA-C	-5.26	102.26	110.42
1	C	128	THR	N-CA-C	-5.21	105.65	111.27

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	2651	0	2624	19	0
2	H	2034	0	2011	18	0
3	L	2207	0	2134	22	0
4	M	2591	0	2478	14	0
5	C	184	0	108	1	0
6	C	32	0	62	2	0
6	H	77	0	146	11	0
6	L	64	0	124	5	0
6	M	80	0	155	7	0
7	C	37	0	58	1	0
7	H	31	0	44	2	0
7	L	33	0	48	2	0
7	M	34	0	50	2	0
8	C	55	0	0	2	0
8	H	40	0	0	1	0
8	M	40	0	0	0	0
9	C	20	0	32	4	0
9	H	30	0	48	2	0
9	L	20	0	32	0	0
9	M	10	0	16	0	0
10	C	102	0	136	4	0
10	H	66	0	88	3	0
10	L	42	0	56	6	0
10	M	42	0	56	1	0
11	L	132	0	144	7	0
11	M	132	0	144	11	0
12	L	65	0	74	2	0
12	M	65	0	74	3	0
13	L	77	0	99	8	0
14	M	58	0	80	0	0
15	M	1	0	0	0	0
16	M	40	0	60	3	0
17	C	441	0	0	1	0
17	H	233	0	0	3	0
17	L	125	0	0	0	0
17	M	175	0	0	2	0
All	All	12066	0	11181	101	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 5.

The worst 5 of 101 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)
3:L:185[B]:MET:SD	11:M:400:BCB:H41	1.94	1.08
1:C:332:LYS:H	9:C:349:HTO:H71	1.27	0.96
7:H:733:DGA:HA42	17:M:960:HOH:O	1.78	0.82
6:H:701:LDA:CM2	6:M:702:LDA:HM11	2.11	0.80
1:C:333:ALA:HB1	1:C:334:ALA:HB2	1.65	0.76

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	336/356 (94%)	326 (97%)	10 (3%)	0	100	100
2	H	259/258 (100%)	249 (96%)	7 (3%)	3 (1%)	10	3
3	L	276/273 (101%)	272 (99%)	4 (1%)	0	100	100
4	M	324/323 (100%)	318 (98%)	5 (2%)	1 (0%)	36	26
All	All	1195/1210 (99%)	1165 (98%)	26 (2%)	4 (0%)	36	26

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	50	VAL
4	M	193	ASN
2	H	51	LYS
2	H	48	GLY

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	285/297 (96%)	282 (99%)	3 (1%)	65	60
2	H	210/212 (99%)	204 (97%)	6 (3%)	37	21
3	L	223/218 (102%)	219 (98%)	4 (2%)	51	39
4	M	252/248 (102%)	247 (98%)	5 (2%)	48	35
All	All	970/975 (100%)	952 (98%)	18 (2%)	50	37

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	M	134	ARG
4	M	214	PHE
4	M	194	PHE
2	H	236	ASP
4	M	51	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	302	GLN
2	H	58	GLN
2	H	220	ASN
3	L	239	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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[B]	2	8,9,10	0.87	0	8,9,11	2.43	2 (25%)
4	CSO	M	160	4	3,6,7	0.67	0	1,6,8	0.23	0
2	FME	H	1[A]	2	8,9,10	0.78	0	8,9,11	2.13	2 (25%)

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[B]	2	-	3/7/9/11	-
4	CSO	M	160	4	-	0/1/5/7	-
2	FME	H	1[A]	2	-	5/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	H	1[B]	FME	CA-N-CN	-6.06	113.50	122.82
2	H	1[A]	FME	CA-N-CN	-5.04	115.06	122.82
2	H	1[A]	FME	O1-CN-N	-2.05	120.03	125.32
2	H	1[B]	FME	O-C-CA	-2.04	119.53	124.77

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1[B]	FME	1	0
2	H	1[A]	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 113 ligands modelled in this entry, 1 is monoatomic - leaving 112 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	$\# Z > 2$
5	HEC	C	403	1	46,50,50	1.75	9 (19%)	58,82,82	1.78	9 (15%)
6	LDA	H	718	-	10,12,15	2.56	2 (20%)	11,14,17	0.60	0
8	SO4	H	261	-	4,4,4	0.43	0	6,6,6	1.06	1 (16%)
8	SO4	C	338	-	4,4,4	0.41	0	6,6,6	0.27	0
6	LDA	H	701	-	13,15,15	1.61	2 (15%)	14,17,17	1.12	1 (7%)
6	LDA	L	709	-	13,15,15	1.95	2 (15%)	14,17,17	0.28	0
9	HTO	H	268	-	9,9,9	0.34	0	10,10,10	1.85	3 (30%)
8	SO4	H	260	-	4,4,4	0.41	0	6,6,6	0.18	0
10	GOL	H	269	-	5,5,5	0.21	0	5,5,5	0.71	0
8	SO4	H	259	-	4,4,4	0.39	0	6,6,6	0.25	0
5	HEC	C	404[A]	-	46,50,50	1.74	9 (19%)	58,82,82	1.76	9 (15%)
8	SO4	M	325	-	4,4,4	0.34	0	6,6,6	0.26	0
10	GOL	M	336	-	5,5,5	0.18	0	5,5,5	0.69	0
6	LDA	H	707	-	13,15,15	2.16	2 (15%)	14,17,17	0.55	0
8	SO4	M	331	-	4,4,4	0.42	0	6,6,6	0.72	0
9	HTO	L	274	-	9,9,9	0.70	0	10,10,10	1.67	4 (40%)
10	GOL	M	338	-	5,5,5	0.31	0	5,5,5	1.57	1 (20%)
8	SO4	C	343	-	4,4,4	0.32	0	6,6,6	0.38	0
6	LDA	M	715	-	13,15,15	2.01	2 (15%)	14,17,17	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GOL	C	350	-	5,5,5	1.06	1 (20%)	5,5,5	1.23	1 (20%)
10	GOL	H	272	-	5,5,5	0.25	0	5,5,5	0.69	0
13	UQ9	L	502	-	58,58,58	2.29	22 (37%)	72,73,73	1.46	14 (19%)
6	LDA	L	708	-	13,15,15	1.56	1 (7%)	14,17,17	0.84	1 (7%)
6	LDA	L	703	-	13,15,15	2.38	2 (15%)	14,17,17	0.61	0
10	GOL	H	270	-	5,5,5	0.35	0	5,5,5	0.64	0
11	BCB	M	401	4	60,74,74	1.13	4 (6%)	59,115,115	3.40	17 (28%)
10	GOL	C	358	-	5,5,5	0.52	0	5,5,5	0.57	0
9	HTO	H	266	-	9,9,9	0.39	0	10,10,10	1.41	2 (20%)
8	SO4	C	337	-	4,4,4	0.44	0	6,6,6	0.15	0
8	SO4	M	327	-	4,4,4	0.42	0	6,6,6	0.12	0
8	SO4	M	330	-	4,4,4	0.50	0	6,6,6	0.42	0
11	BCB	L	401	3	60,74,74	1.34	9 (15%)	59,115,115	3.03	15 (25%)
5	HEC	C	404[B]	-	46,50,50	1.75	10 (21%)	58,82,82	1.64	6 (10%)
6	LDA	M	706	-	13,15,15	1.97	1 (7%)	14,17,17	0.57	0
6	LDA	M	704	-	13,15,15	2.09	2 (15%)	14,17,17	0.54	0
10	GOL	C	357	-	5,5,5	0.52	0	5,5,5	0.43	0
8	SO4	C	339	-	4,4,4	0.39	0	6,6,6	0.22	0
6	LDA	H	719	-	13,15,15	2.21	2 (15%)	14,17,17	0.68	0
8	SO4	H	265	-	4,4,4	0.45	0	6,6,6	0.11	0
10	GOL	C	365	-	5,5,5	0.22	0	5,5,5	0.52	0
10	GOL	C	360	-	5,5,5	0.21	0	5,5,5	0.35	0
10	GOL	L	280	-	5,5,5	0.28	0	5,5,5	0.22	0
10	GOL	L	279	-	5,5,5	0.81	0	5,5,5	1.14	0
12	BPB	M	402	-	57,70,70	1.47	8 (14%)	55,101,101	1.62	7 (12%)
10	GOL	L	277	-	5,5,5	0.27	0	5,5,5	1.13	0
6	LDA	M	705	-	13,15,15	1.95	2 (15%)	14,17,17	0.65	0
10	GOL	M	337	-	5,5,5	0.28	0	5,5,5	0.43	0
11	BCB	M	400	4	60,74,74	1.35	6 (10%)	59,115,115	2.61	16 (27%)
8	SO4	H	262[A]	-	4,4,4	0.51	0	6,6,6	0.48	0
13	UQ9	L	503	-	19,19,58	2.29	6 (31%)	24,26,73	1.75	5 (20%)
8	SO4	C	340	-	4,4,4	0.40	0	6,6,6	0.34	0
6	LDA	C	712	-	13,15,15	2.07	1 (7%)	14,17,17	0.52	0
10	GOL	C	363	-	5,5,5	0.33	0	5,5,5	0.55	0
10	GOL	H	278	-	5,5,5	0.18	0	5,5,5	0.75	0
6	LDA	L	720	-	13,15,15	1.83	1 (7%)	14,17,17	1.11	2 (14%)
10	GOL	C	364	-	5,5,5	0.69	0	5,5,5	2.37	2 (40%)
9	HTO	L	275	-	9,9,9	0.93	0	10,10,10	3.23	4 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GOL	C	354	-	5,5,5	0.75	0	5,5,5	0.56	0
10	GOL	L	276	-	5,5,5	0.38	0	5,5,5	0.57	0
9	HTO	C	348	-	9,9,9	0.44	0	10,10,10	1.88	2 (20%)
8	SO4	C	342	-	4,4,4	0.43	0	6,6,6	0.26	0
9	HTO	C	349	-	9,9,9	0.61	0	10,10,10	0.89	0
10	GOL	M	335	-	5,5,5	0.61	0	5,5,5	1.91	2 (40%)
10	GOL	L	281	-	5,5,5	0.26	0	5,5,5	0.39	0
9	HTO	H	267	-	9,9,9	0.56	0	10,10,10	1.02	0
10	GOL	C	359	-	5,5,5	0.44	0	5,5,5	0.39	0
10	GOL	C	352	-	5,5,5	0.35	0	5,5,5	0.57	0
6	LDA	M	702	-	13,15,15	2.17	2 (15%)	14,17,17	0.80	0
10	GOL	H	274	-	5,5,5	0.22	0	5,5,5	0.46	0
10	GOL	C	356	-	5,5,5	0.87	0	5,5,5	1.64	1 (20%)
10	GOL	H	275	-	5,5,5	0.31	0	5,5,5	0.35	0
10	GOL	M	339	-	5,5,5	0.32	0	5,5,5	0.50	0
8	SO4	M	328	-	4,4,4	0.37	0	6,6,6	0.56	0
10	GOL	M	334	-	5,5,5	0.33	0	5,5,5	1.22	0
7	DGA	M	732	-	33,33,43	0.65	0	35,35,45	1.60	4 (11%)
10	GOL	H	273	-	5,5,5	0.25	0	5,5,5	0.73	0
8	SO4	H	262[B]	-	4,4,4	0.47	0	6,6,6	0.48	0
8	SO4	M	324	-	4,4,4	0.51	0	6,6,6	0.96	0
10	GOL	C	351	-	5,5,5	0.66	0	5,5,5	1.29	1 (20%)
8	SO4	M	329	-	4,4,4	0.31	0	6,6,6	0.36	0
8	SO4	C	341	-	4,4,4	0.46	0	6,6,6	0.28	0
14	MQ9	M	501	-	59,59,59	2.20	26 (44%)	73,75,75	1.26	10 (13%)
10	GOL	H	279	-	5,5,5	0.26	0	5,5,5	0.56	0
10	GOL	M	333	-	5,5,5	0.27	0	5,5,5	0.34	0
10	GOL	H	271	-	5,5,5	0.53	0	5,5,5	1.32	1 (20%)
8	SO4	C	347	-	4,4,4	0.42	0	6,6,6	0.10	0
7	DGA	C	730	1	36,36,43	0.84	2 (5%)	38,38,45	1.39	4 (10%)
10	GOL	L	278	-	5,5,5	0.91	0	5,5,5	1.49	1 (20%)
10	GOL	C	355	-	5,5,5	0.27	0	5,5,5	0.44	0
8	SO4	C	345	-	4,4,4	0.66	0	6,6,6	0.34	0
8	SO4	C	346	-	4,4,4	0.50	0	6,6,6	0.19	0
10	GOL	C	362	-	5,5,5	0.26	0	5,5,5	0.59	0
5	HEC	C	401	1	46,50,50	1.66	5 (10%)	58,82,82	1.98	12 (20%)
5	HEC	C	402	1	46,50,50	1.64	8 (17%)	58,82,82	1.82	10 (17%)
6	LDA	C	722	-	13,15,15	2.16	2 (15%)	14,17,17	0.50	0
11	BCB	L	400	3	60,74,74	1.41	9 (15%)	59,115,115	3.29	15 (25%)
8	SO4	C	344	-	4,4,4	0.38	0	6,6,6	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	DGA	L	731	-	32,32,43	0.67	0	34,34,45	1.61	6 (17%)
7	DGA	H	733	-	30,30,43	0.64	1 (3%)	32,32,45	1.83	8 (25%)
10	GOL	C	353[B]	-	5,5,5	0.53	0	5,5,5	0.41	0
10	GOL	H	277	-	5,5,5	0.34	0	5,5,5	0.34	0
10	GOL	H	276	-	5,5,5	0.19	0	5,5,5	0.49	0
8	SO4	H	263	-	4,4,4	0.45	0	6,6,6	0.36	0
10	GOL	C	361	-	5,5,5	0.25	0	5,5,5	0.40	0
8	SO4	M	326	-	4,4,4	0.25	0	6,6,6	0.29	0
8	SO4	H	264	-	4,4,4	0.50	0	6,6,6	0.23	0
10	GOL	L	282	-	5,5,5	0.34	0	5,5,5	0.27	0
10	GOL	C	353[A]	-	5,5,5	0.58	0	5,5,5	0.80	0
6	LDA	H	721	-	13,15,15	2.20	2 (15%)	14,17,17	1.05	1 (7%)
9	HTO	M	332	-	9,9,9	0.60	0	10,10,10	3.44	5 (50%)
16	NS5	M	600	-	39,39,39	1.82	13 (33%)	46,46,46	2.24	13 (28%)
12	BPB	L	402	-	57,70,70	1.45	7 (12%)	55,101,101	1.91	8 (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
5	HEC	C	403	1	-	4/14/54/54	-
6	LDA	H	718	-	-	6/10/10/13	-
6	LDA	H	701	-	-	5/13/13/13	-
6	LDA	L	709	-	-	4/13/13/13	-
9	HTO	H	268	-	-	8/10/10/10	-
10	GOL	H	269	-	-	4/4/4/4	-
5	HEC	C	404[A]	-	-	4/14/54/54	-
10	GOL	M	336	-	-	2/4/4/4	-
6	LDA	H	707	-	-	6/13/13/13	-
9	HTO	L	274	-	-	0/10/10/10	-
10	GOL	M	338	-	-	1/4/4/4	-
6	LDA	M	715	-	-	9/13/13/13	-
10	GOL	C	350	-	-	0/4/4/4	-
10	GOL	H	272	-	-	0/4/4/4	-
13	UQ9	L	502	-	-	24/57/81/81	0/1/1/1
6	LDA	L	708	-	-	1/13/13/13	-
6	LDA	L	703	-	-	7/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	H	270	-	-	4/4/4/4	-
11	BCB	M	401	4	3/3/21/26	8/37/137/137	-
10	GOL	C	358	-	-	2/4/4/4	-
9	HTO	H	266	-	-	7/10/10/10	-
11	BCB	L	401	3	3/3/21/26	6/37/137/137	-
5	HEC	C	404[B]	-	-	9/14/54/54	-
6	LDA	M	706	-	-	7/13/13/13	-
6	LDA	M	704	-	-	6/13/13/13	-
10	GOL	C	357	-	-	2/4/4/4	-
6	LDA	H	719	-	-	5/13/13/13	-
10	GOL	C	365	-	-	2/4/4/4	-
10	GOL	C	360	-	-	1/4/4/4	-
10	GOL	L	280	-	-	3/4/4/4	-
10	GOL	L	279	-	-	2/4/4/4	-
12	BPB	M	402	-	-	9/37/105/105	0/5/6/6
10	GOL	L	277	-	-	0/4/4/4	-
6	LDA	M	705	-	-	5/13/13/13	-
10	GOL	M	337	-	-	4/4/4/4	-
11	BCB	M	400	4	3/3/21/26	13/37/137/137	-
13	UQ9	L	503	-	-	6/11/35/81	0/1/1/1
6	LDA	C	712	-	-	9/13/13/13	-
10	GOL	C	363	-	-	2/4/4/4	-
10	GOL	H	278	-	-	4/4/4/4	-
6	LDA	L	720	-	-	6/13/13/13	-
10	GOL	C	364	-	-	1/4/4/4	-
9	HTO	L	275	-	-	7/10/10/10	-
10	GOL	C	354	-	-	2/4/4/4	-
10	GOL	L	276	-	-	2/4/4/4	-
9	HTO	C	348	-	-	7/10/10/10	-
9	HTO	C	349	-	-	7/10/10/10	-
10	GOL	M	335	-	-	2/4/4/4	-
10	GOL	L	281	-	-	3/4/4/4	-
9	HTO	H	267	-	-	5/10/10/10	-
10	GOL	C	359	-	-	2/4/4/4	-
10	GOL	C	352	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	M	702	-	-	10/13/13/13	-
10	GOL	H	274	-	-	2/4/4/4	-
10	GOL	C	356	-	-	0/4/4/4	-
10	GOL	H	275	-	-	2/4/4/4	-
10	GOL	M	339	-	-	2/4/4/4	-
10	GOL	M	334	-	-	2/4/4/4	-
7	DGA	M	732	-	-	16/35/35/45	-
10	GOL	H	273	-	-	2/4/4/4	-
10	GOL	C	351	-	-	2/4/4/4	-
14	MQ9	M	501	-	-	2/53/73/73	0/2/2/2
10	GOL	H	279	-	-	2/4/4/4	-
10	GOL	M	333	-	-	2/4/4/4	-
10	GOL	H	271	-	-	4/4/4/4	-
7	DGA	C	730	1	-	19/37/37/45	-
10	GOL	L	278	-	-	4/4/4/4	-
10	GOL	C	355	-	-	1/4/4/4	-
10	GOL	C	362	-	-	2/4/4/4	-
5	HEC	C	401	1	-	6/14/54/54	-
5	HEC	C	402	1	-	9/14/54/54	-
6	LDA	C	722	-	-	9/13/13/13	-
11	BCB	L	400	3	3/3/21/26	7/37/137/137	-
7	DGA	L	731	-	-	12/34/34/45	-
7	DGA	H	733	-	-	19/32/32/45	-
10	GOL	C	353[B]	-	-	4/4/4/4	-
10	GOL	H	277	-	-	4/4/4/4	-
10	GOL	H	276	-	-	2/4/4/4	-
10	GOL	C	361	-	-	3/4/4/4	-
10	GOL	L	282	-	-	2/4/4/4	-
10	GOL	C	353[A]	-	-	4/4/4/4	-
6	LDA	H	721	-	-	8/13/13/13	-
9	HTO	M	332	-	-	7/10/10/10	-
16	NS5	M	600	-	-	10/43/43/43	-
12	BPB	L	402	-	-	2/37/105/105	0/5/6/6

The worst 5 of 183 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	712	LDA	O1-N1	-7.17	1.24	1.42
6	H	718	LDA	O1-N1	-6.98	1.25	1.42
12	M	402	BPB	C1B-C2B	6.92	1.47	1.39
6	L	703	LDA	O1-N1	-6.89	1.25	1.42
13	L	503	UQ9	C7-C8	-6.84	1.39	1.50

The worst 5 of 224 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	400	BCB	C1B-CHB-C4A	13.44	129.97	121.32
11	L	400	BCB	C4B-CHC-C1C	13.26	129.85	121.32
11	L	401	BCB	C4B-CHC-C1C	13.22	129.83	121.32
11	M	401	BCB	C4B-CHC-C1C	13.19	129.81	121.32
11	L	401	BCB	C1B-CHB-C4A	11.76	128.88	121.32

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	L	400	BCB	NC
11	L	400	BCB	NA
11	L	400	BCB	ND
11	L	401	BCB	NC
11	L	401	BCB	NA

5 of 429 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	401	HEC	C2B-C3B-CAB-CBB
5	C	401	HEC	C4B-C3B-CAB-CBB
5	C	401	HEC	C2C-C3C-CAC-CBC
5	C	401	HEC	C4C-C3C-CAC-CBC
5	C	402	HEC	C2B-C3B-CAB-CBB

There are no ring outliers.

35 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	403	HEC	1	0
6	H	718	LDA	1	0
6	H	701	LDA	4	0
9	H	268	HTO	1	0
13	L	502	UQ9	8	0

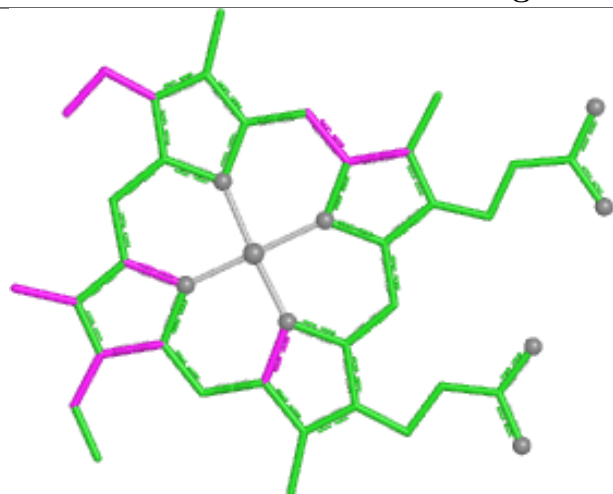
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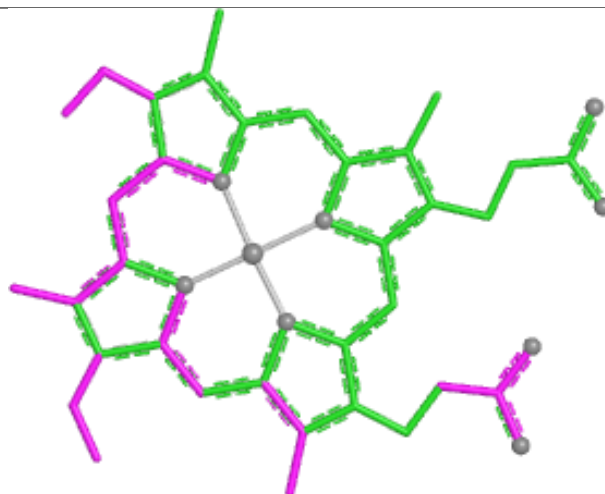
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	H	270	GOL	1	0
11	M	401	BCB	2	0
10	C	358	GOL	1	0
11	L	401	BCB	4	0
6	M	704	LDA	1	0
6	H	719	LDA	1	0
10	L	279	GOL	5	0
12	M	402	BPB	3	0
11	M	400	BCB	9	0
6	L	720	LDA	5	0
10	C	354	GOL	1	0
10	L	276	GOL	3	0
9	C	349	HTO	4	0
9	H	267	HTO	1	0
10	C	352	GOL	1	0
6	M	702	LDA	6	0
10	H	274	GOL	2	0
7	M	732	DGA	2	0
8	H	262[B]	SO4	1	0
10	M	333	GOL	1	0
7	C	730	DGA	1	0
6	C	722	LDA	2	0
11	L	400	BCB	3	0
8	C	344	SO4	2	0
7	L	731	DGA	2	0
7	H	733	DGA	2	0
10	C	353[B]	GOL	1	0
6	H	721	LDA	5	0
16	M	600	NS5	3	0
12	L	402	BPB	2	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 than 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.

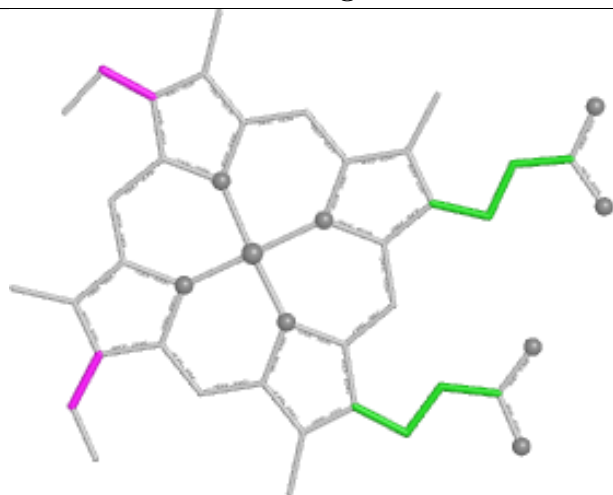
Ligand HEC C 403



Bond lengths



Bond angles

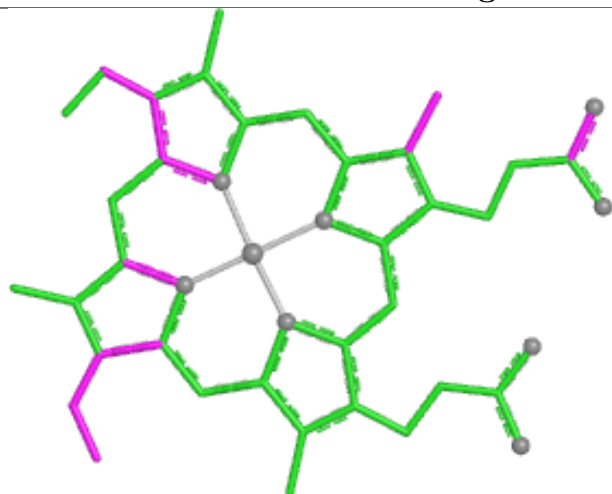


Torsions

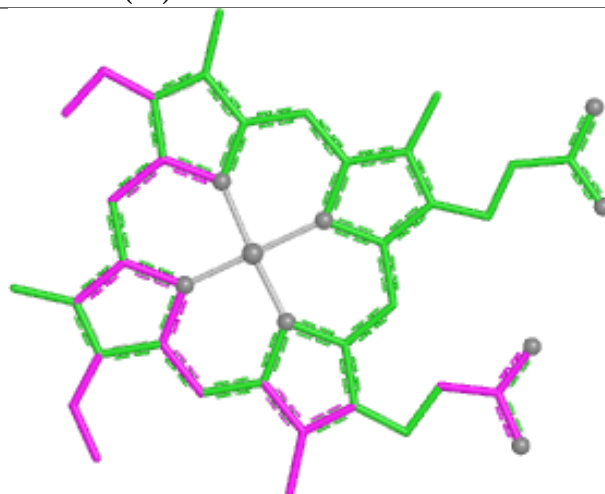


Rings

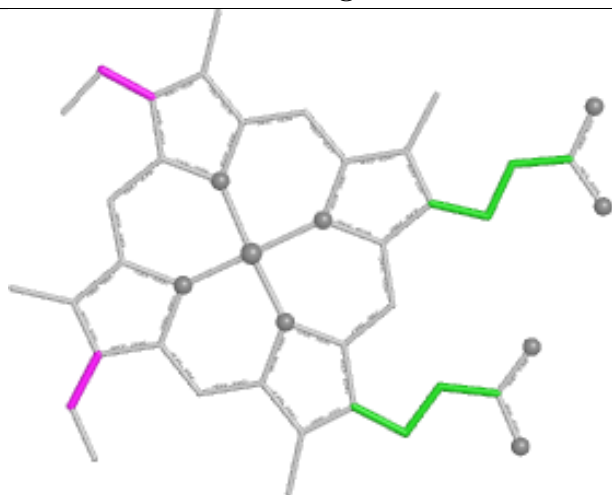
Ligand HEC C 404 (A)



Bond lengths



Bond angles

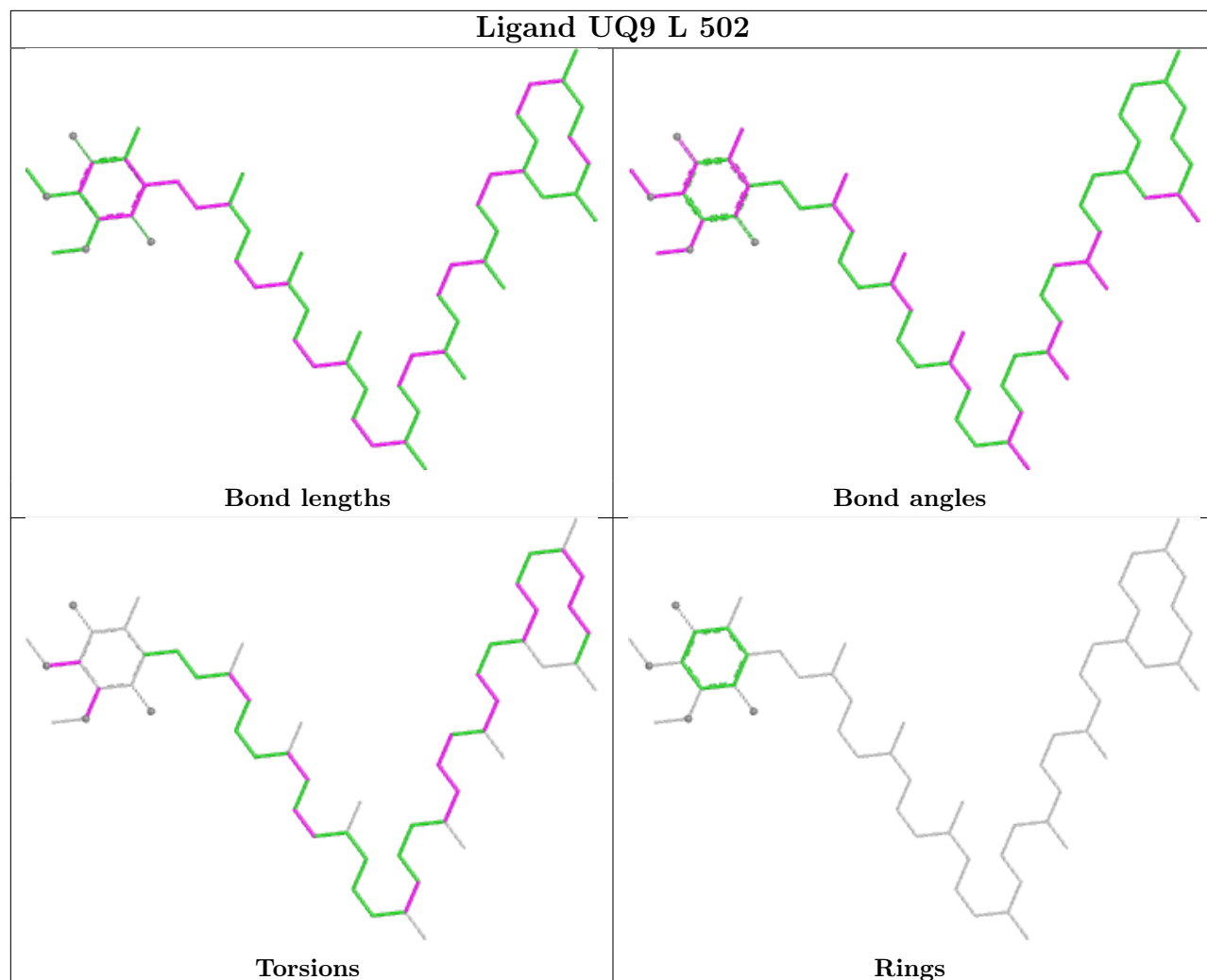


Torsions

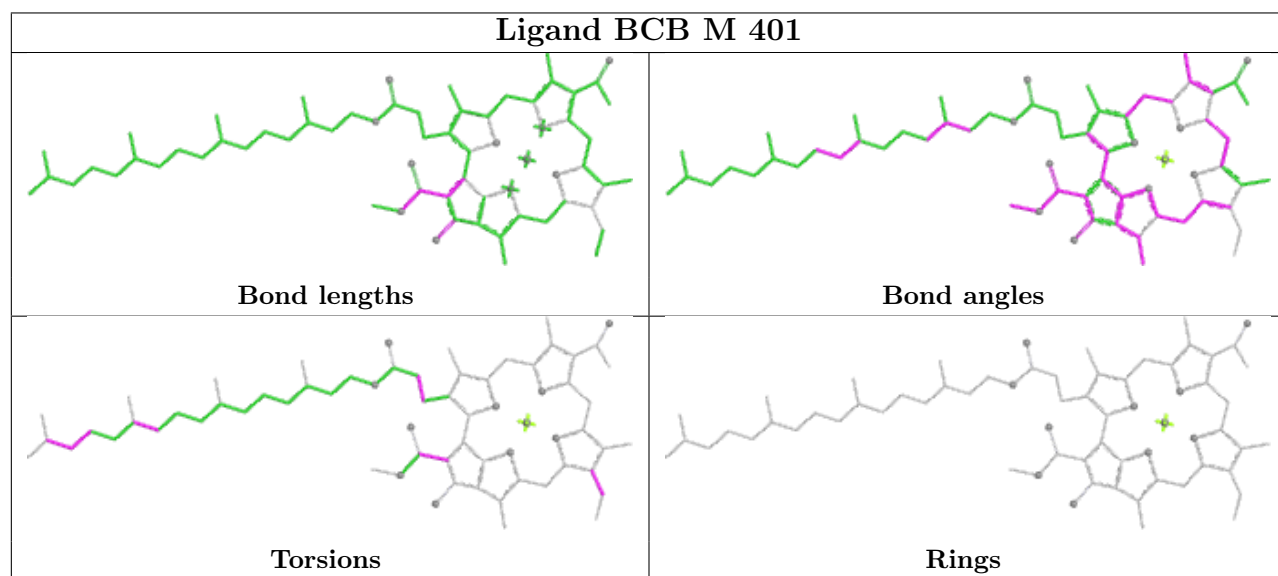


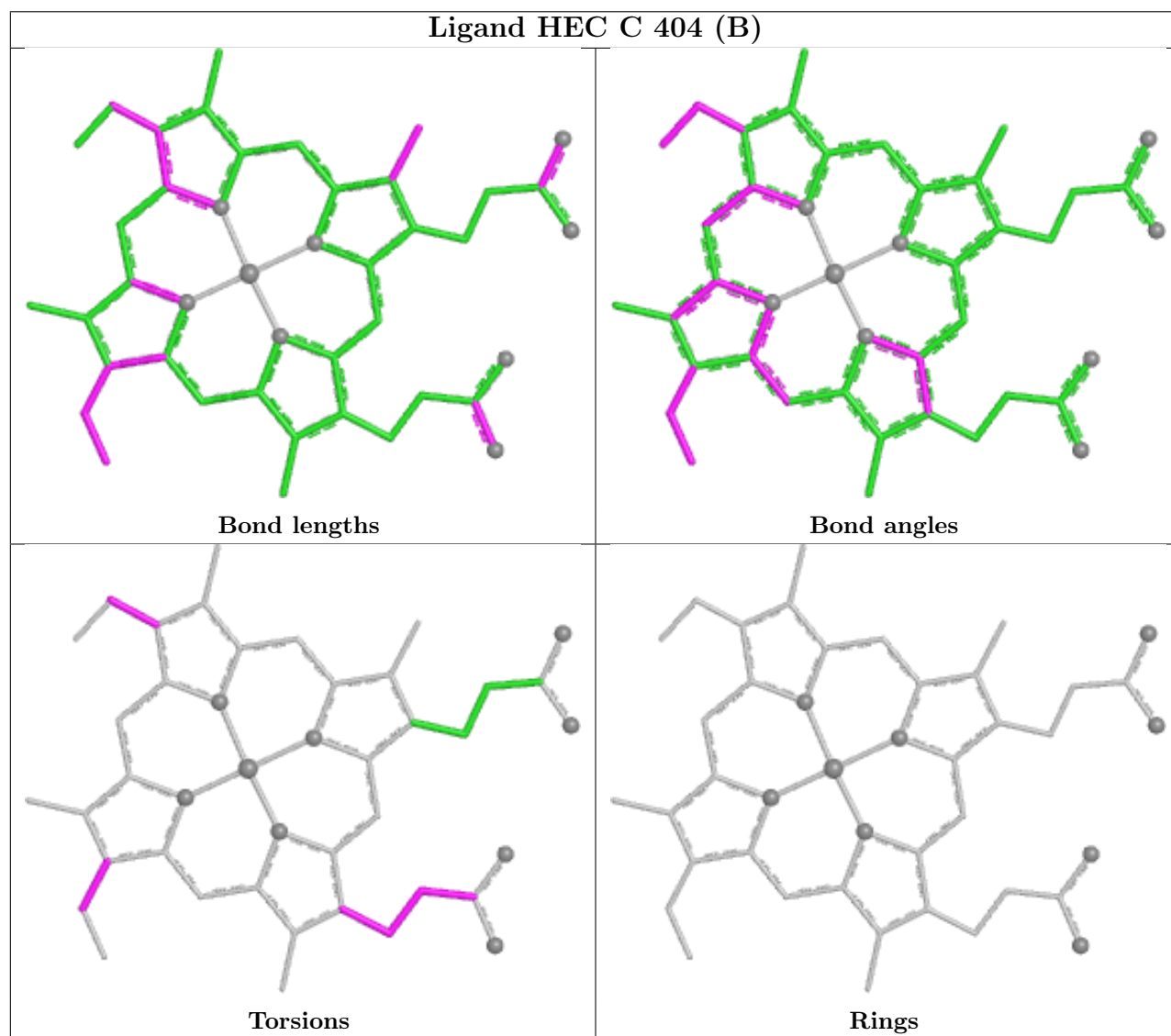
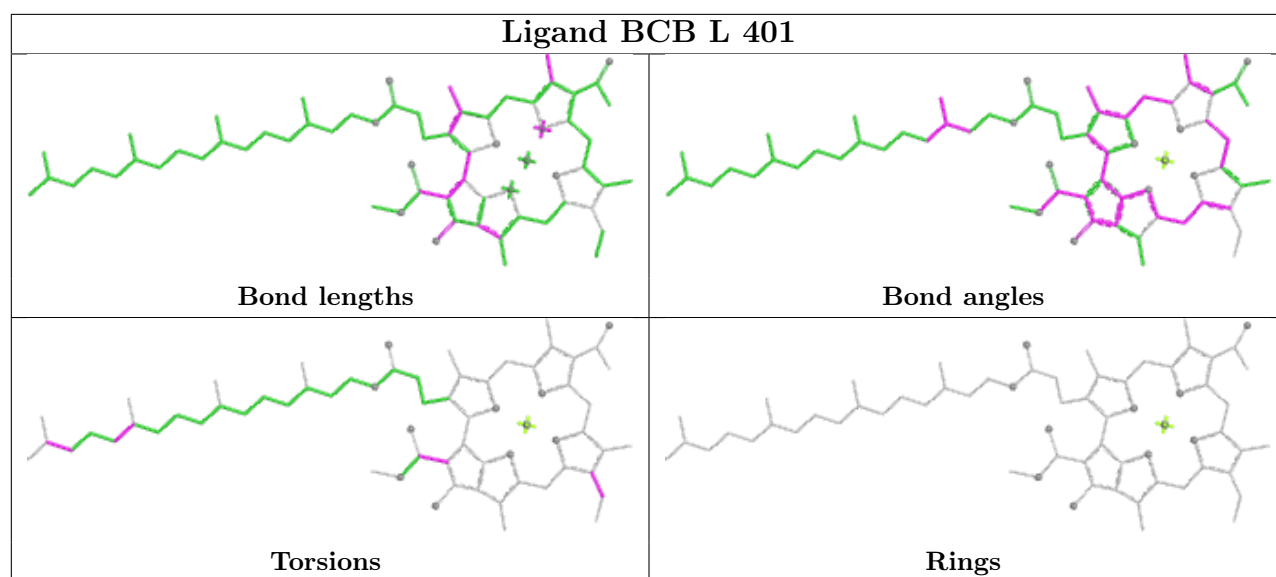
Rings

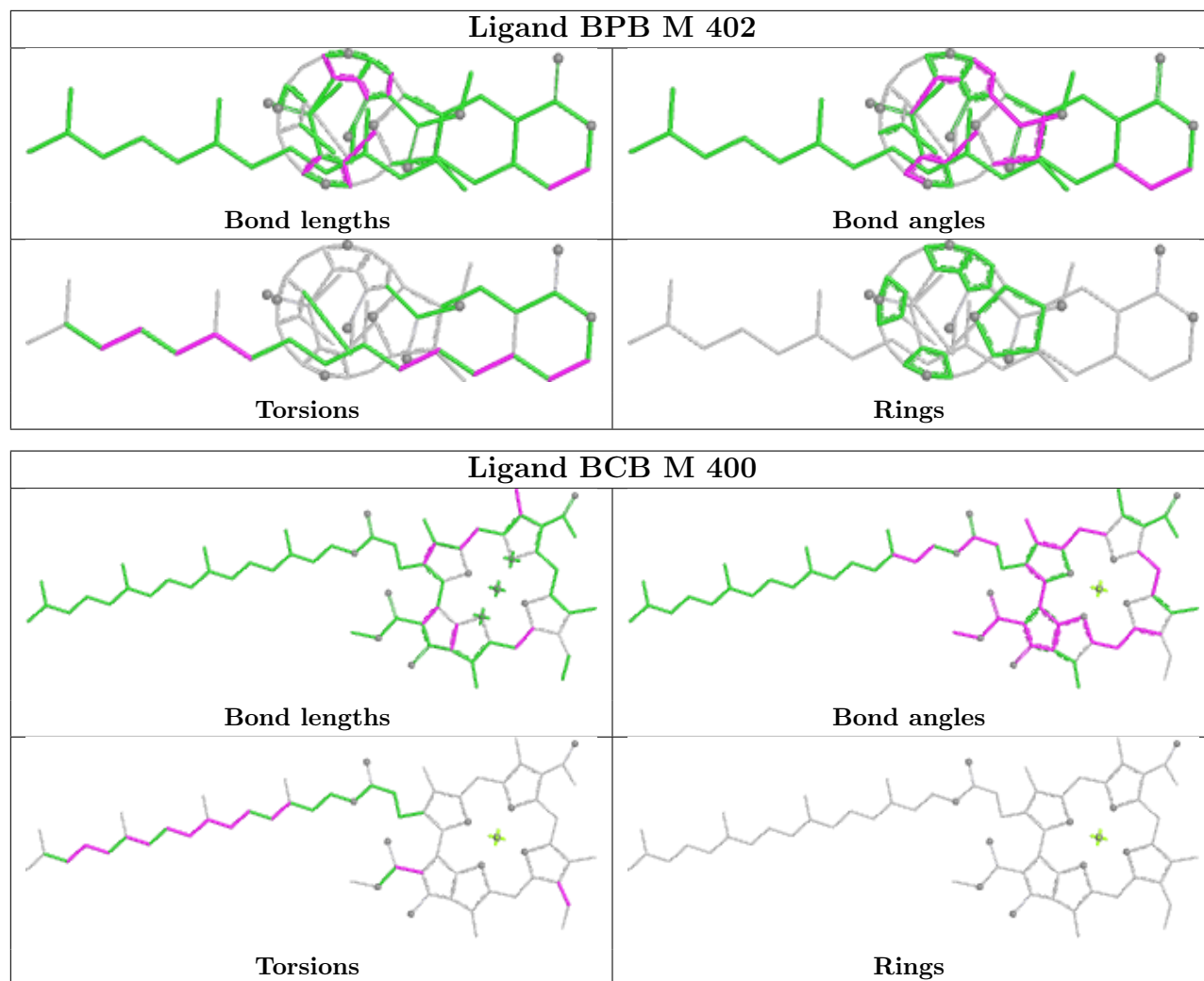
Ligand UQ9 L 502



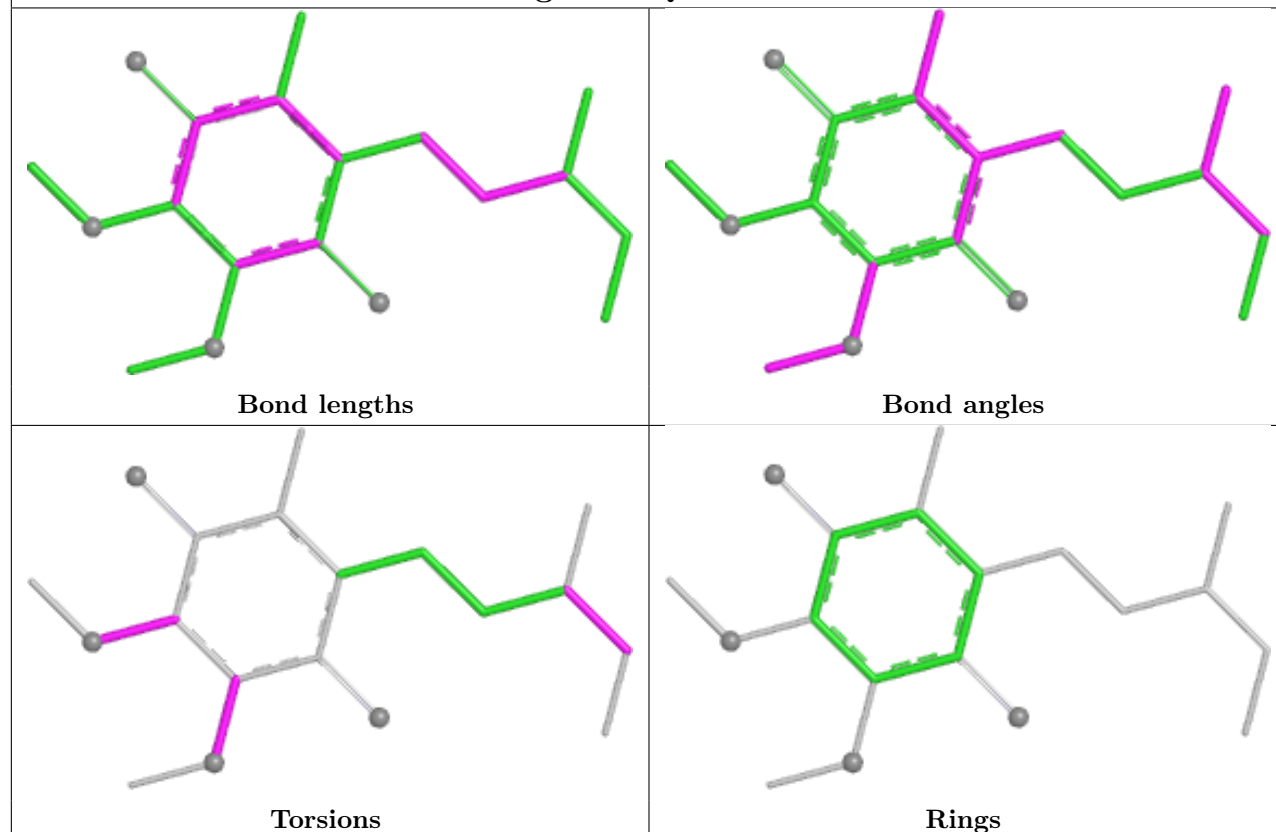
Ligand BCB M 401



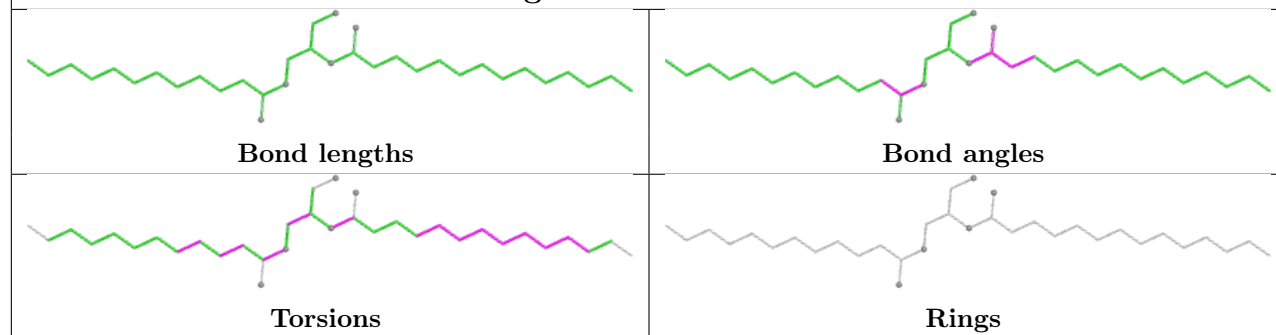




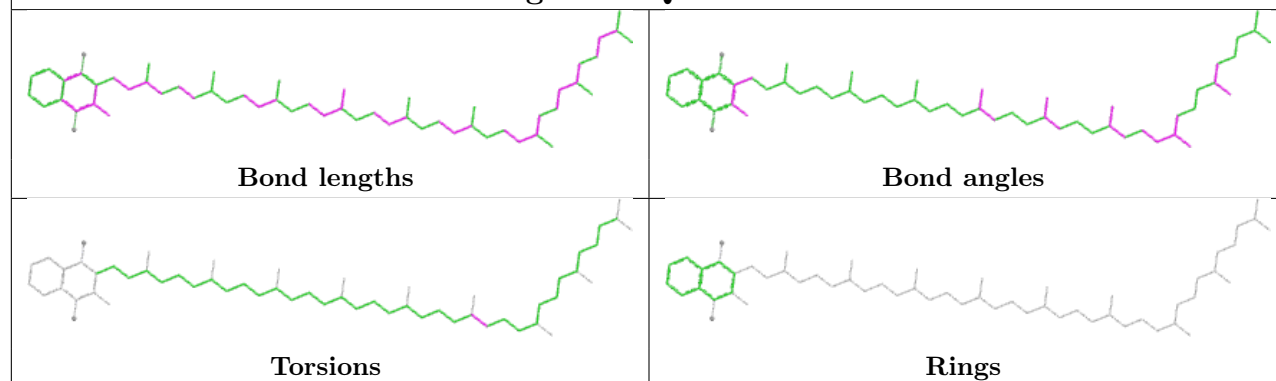
Ligand UQ9 L 503

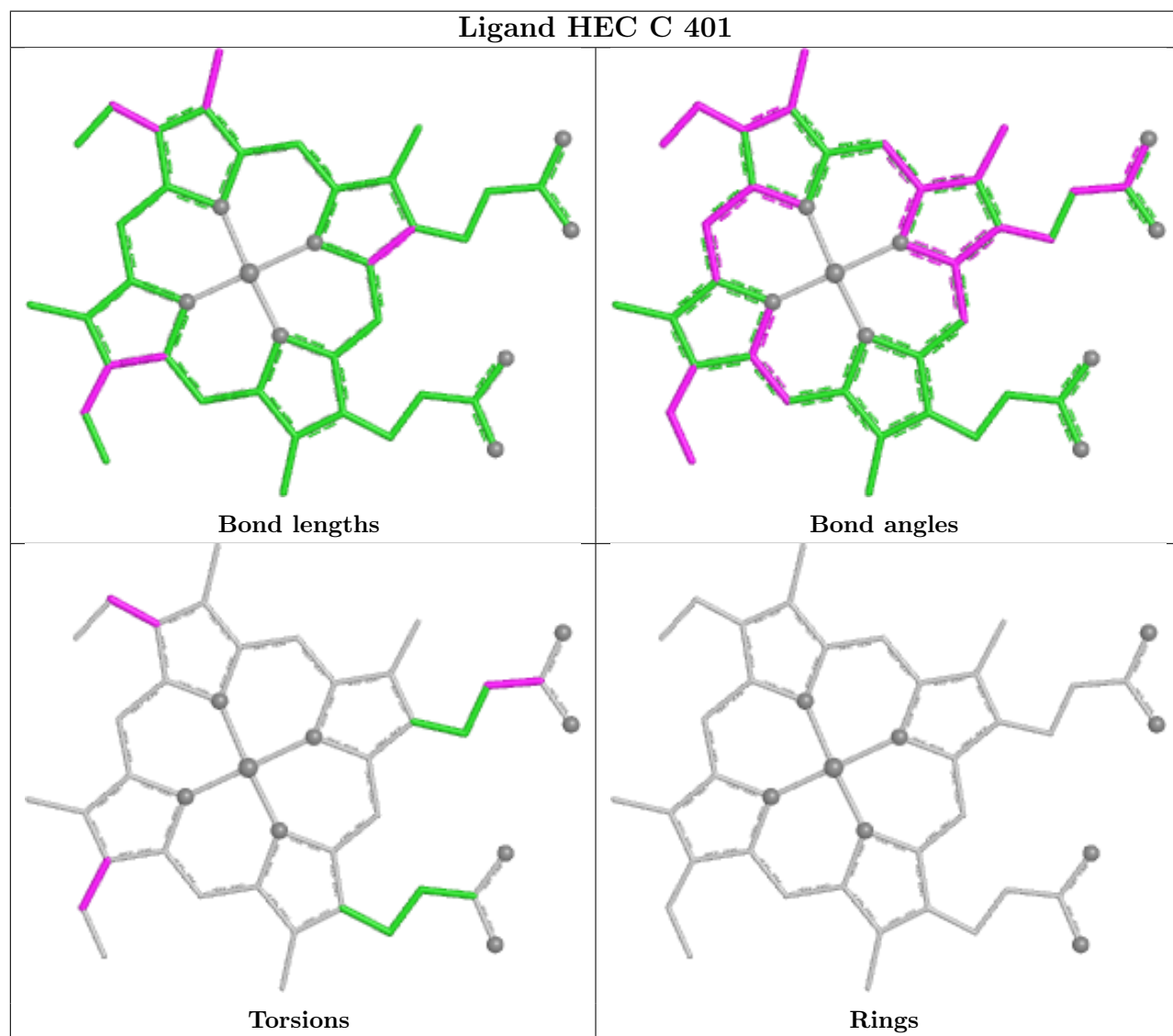
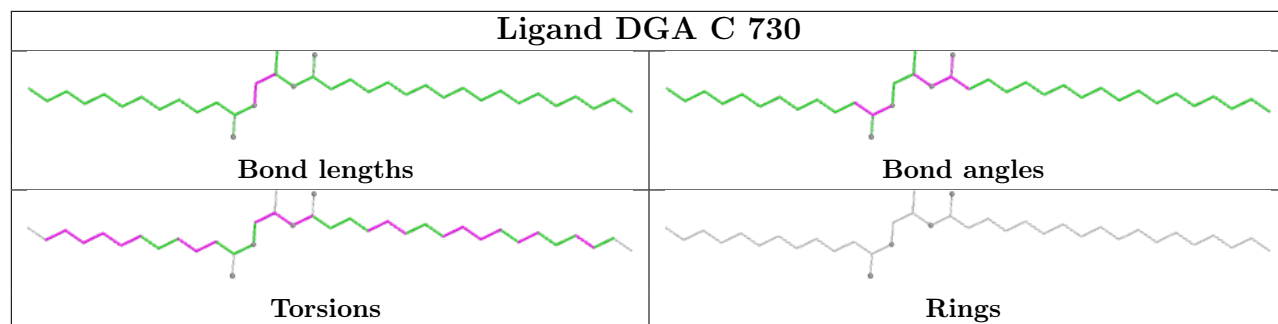


Ligand DGA M 732

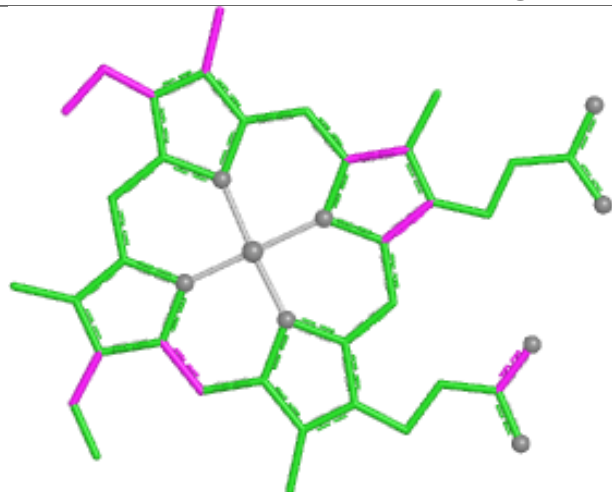


Ligand MQ9 M 501

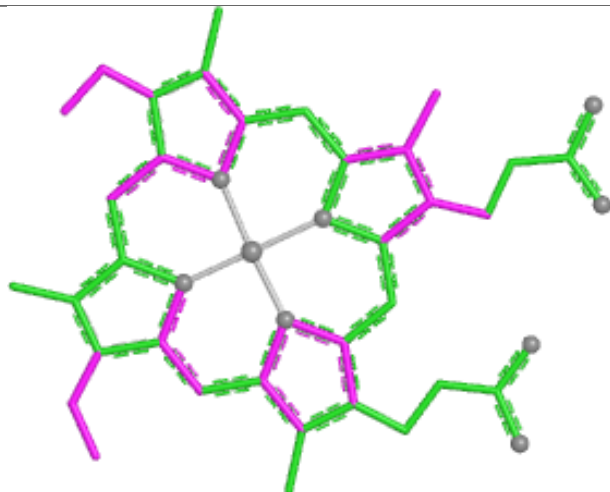




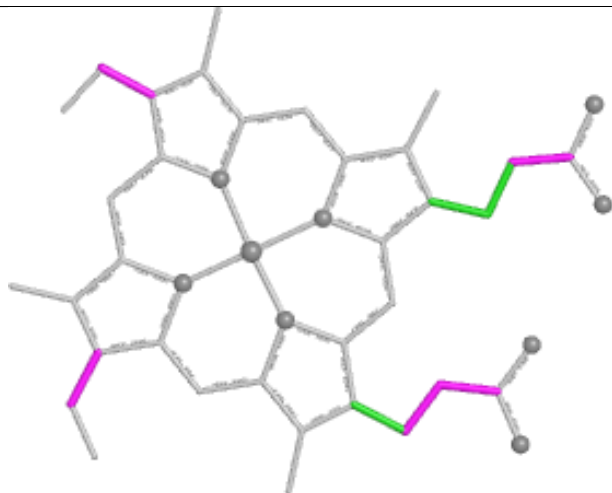
Ligand HEC C 402



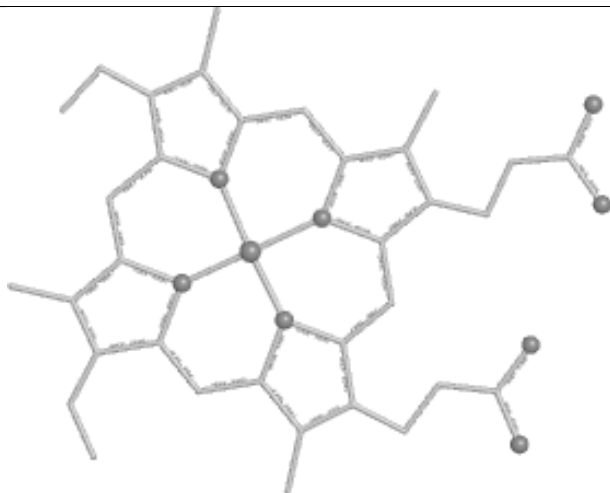
Bond lengths



Bond angles

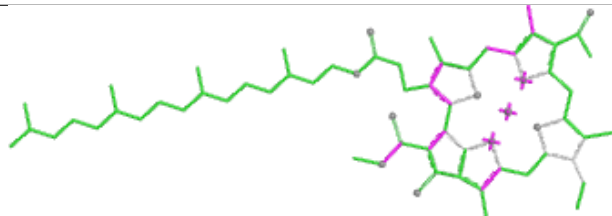


Torsions

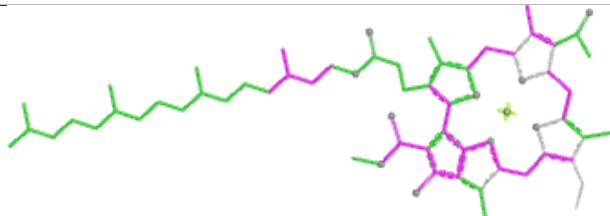


Rings

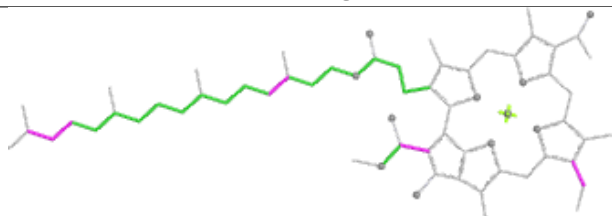
Ligand BCB L 400



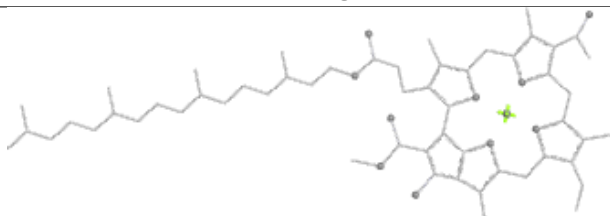
Bond lengths



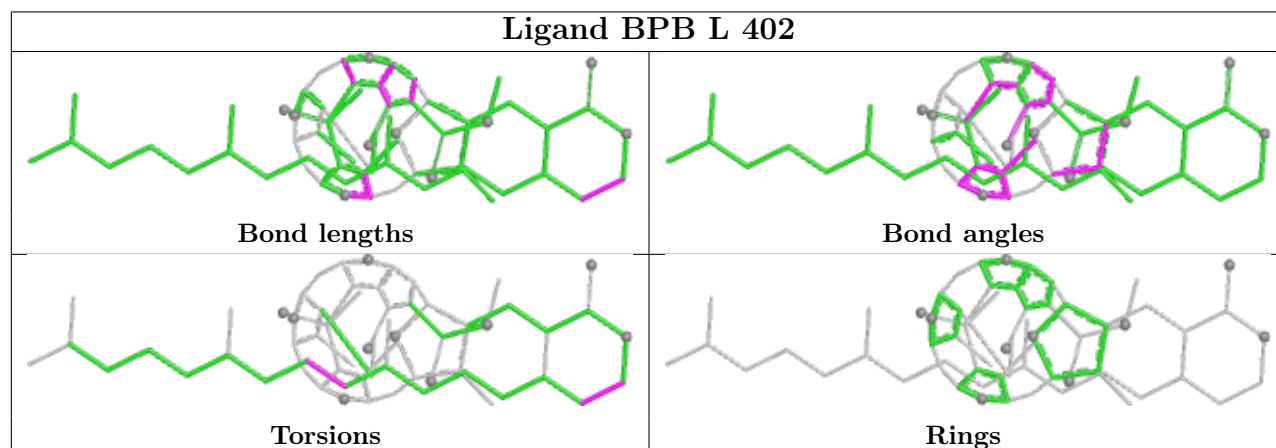
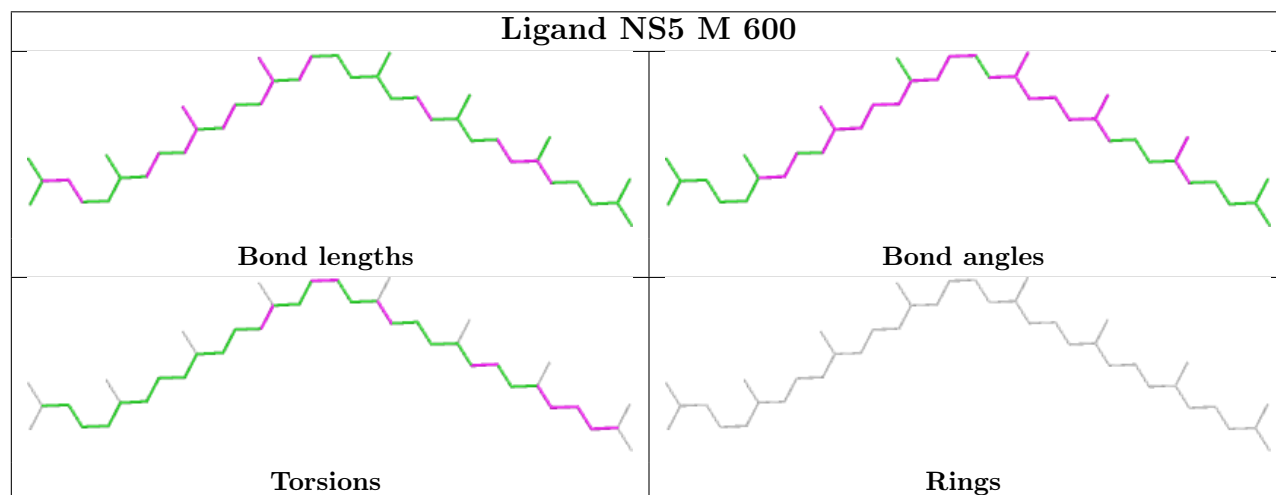
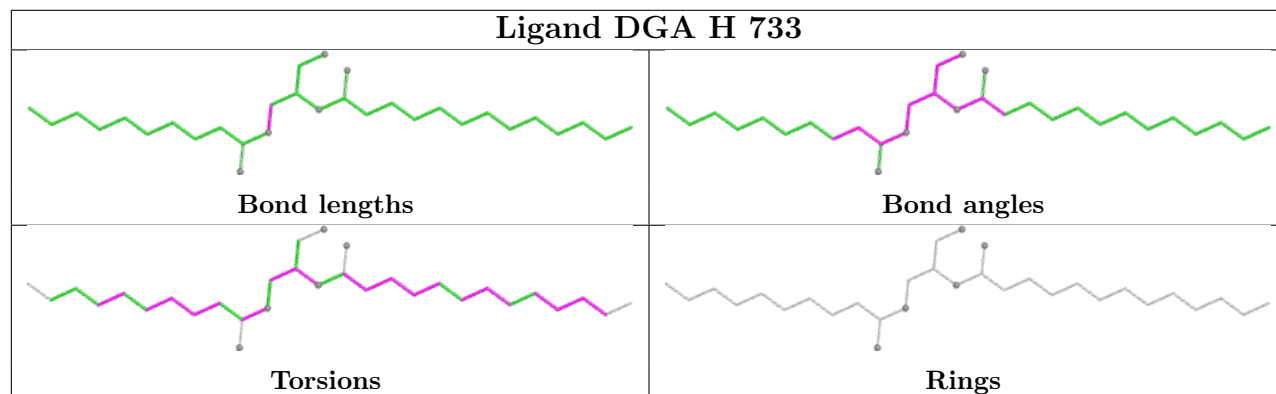
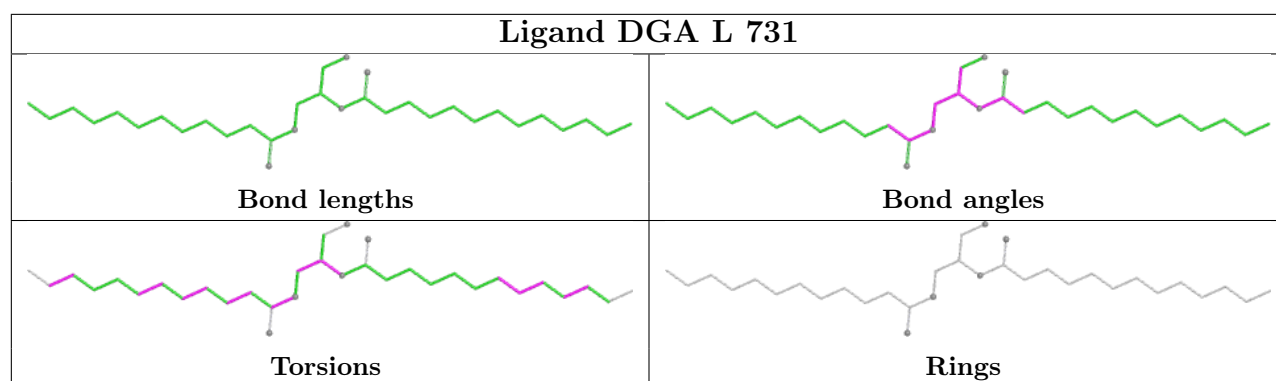
Bond angles



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%)	0.26	5 (1%) 72 79	22, 49, 70, 122	4 (1%)
2	H	249/258 (96%)	0.71	16 (6%) 25 29	28, 58, 85, 120	4 (1%)
3	L	273/273 (100%)	0.24	7 (2%) 57 63	22, 47, 62, 88	5 (1%)
4	M	322/323 (99%)	0.41	19 (5%) 28 32	21, 49, 70, 91	4 (1%)
All	All	1178/1210 (97%)	0.39	47 (3%) 42 47	21, 50, 73, 122	17 (1%)

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	M	37	TRP	6.6
2	H	54	PRO	6.1
2	H	83	PRO	5.6
2	H	227[A]	ARG	5.1
1	C	334	ALA	4.4

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	0.86	0.19	50,54,59,61	10
2	FME	H	1[B]	10/11	0.86	0.19	49,52,54,64	10
4	CSO	M	160	7/8	0.90	0.13	46,49,73,77	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
10	GOL	H	279	6/6	0.58	0.46	80,86,88,91	6
10	GOL	H	270	6/6	0.69	0.40	63,69,69,71	6
8	SO4	H	265	5/5	0.69	0.35	71,74,75,76	5
13	UQ9	L	503	19/58	0.72	0.39	49,70,84,86	19
6	LDA	H	718	13/16	0.76	0.45	55,61,79,84	13
8	SO4	H	264	5/5	0.77	0.35	63,65,67,73	5
8	SO4	C	345	5/5	0.78	0.27	71,79,83,86	5
6	LDA	M	715	16/16	0.78	0.58	63,77,84,85	16
10	GOL	C	361	6/6	0.79	0.35	66,71,76,80	6
10	GOL	M	334	6/6	0.80	0.53	63,65,67,68	6
9	HTO	H	267	10/10	0.80	0.28	74,77,89,91	10
8	SO4	C	347	5/5	0.81	0.32	71,73,76,77	5
10	GOL	H	273	6/6	0.81	0.48	71,75,79,80	6
10	GOL	H	277	6/6	0.81	0.27	65,69,71,72	6
6	LDA	H	707	16/16	0.82	0.39	53,67,77,85	16
8	SO4	C	340	5/5	0.82	0.23	72,73,77,79	5
8	SO4	C	343	5/5	0.82	0.23	66,66,70,74	5
10	GOL	M	333	6/6	0.83	0.47	70,70,73,78	6
9	HTO	C	348	10/10	0.83	0.35	52,62,68,74	10
10	GOL	C	364	6/6	0.83	0.34	53,55,61,62	6
6	LDA	M	702	16/16	0.84	0.38	52,56,62,65	16
10	GOL	H	276	6/6	0.84	0.34	71,79,85,85	6
6	LDA	M	704	16/16	0.84	0.44	64,67,86,88	16
6	LDA	C	712	16/16	0.84	0.42	56,62,74,74	16
10	GOL	C	363	6/6	0.84	0.27	72,75,78,78	6
7	DGA	C	730	37/44	0.84	0.28	58,76,94,99	37
10	GOL	M	337	6/6	0.84	0.34	56,64,66,69	6
13	UQ9	L	502	58/58	0.84	0.47	38,58,69,73	58
6	LDA	L	720	16/16	0.84	0.37	58,70,76,78	16
6	LDA	M	706	16/16	0.85	0.39	61,65,73,73	16
10	GOL	C	365	6/6	0.85	0.31	59,60,61,65	6
10	GOL	H	269	6/6	0.85	0.27	68,76,79,83	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	SO4	C	346	5/5	0.85	0.18	73,73,82,82	5
7	DGA	L	731	33/44	0.85	0.36	47,69,78,82	33
9	HTO	C	349	10/10	0.85	0.30	59,68,74,75	10
8	SO4	H	261	5/5	0.85	0.23	46,55,72,75	5
10	GOL	C	351	6/6	0.85	0.24	51,58,65,67	6
10	GOL	C	353[A]	6/6	0.85	0.26	44,55,59,61	6
10	GOL	C	353[B]	6/6	0.85	0.26	42,56,71,73	6
10	GOL	M	335	6/6	0.85	0.30	50,57,62,64	6
10	GOL	M	336	6/6	0.85	0.40	81,82,84,87	6
10	GOL	C	354	6/6	0.85	0.26	57,68,78,86	6
10	GOL	M	338	6/6	0.85	0.30	67,71,72,73	6
8	SO4	H	262[A]	5/5	0.85	0.13	55,56,67,71	5
8	SO4	H	262[B]	5/5	0.85	0.13	58,63,71,72	5
7	DGA	M	732	34/44	0.86	0.37	58,72,80,84	34
10	GOL	H	272	6/6	0.86	0.40	66,72,75,76	6
8	SO4	C	339	5/5	0.87	0.15	62,67,67,69	5
6	LDA	L	703	16/16	0.87	0.38	56,61,69,72	16
9	HTO	H	268	10/10	0.87	0.38	71,76,80,80	10
10	GOL	H	274	6/6	0.87	0.30	59,71,78,81	6
7	DGA	H	733	31/44	0.87	0.36	45,62,78,79	31
16	NS5	M	600	40/40	0.87	0.23	53,76,118,126	0
8	SO4	M	330	5/5	0.88	0.36	58,64,67,70	5
10	GOL	H	271	6/6	0.88	0.39	54,63,65,75	6
10	GOL	L	281	6/6	0.88	0.35	60,62,66,67	6
6	LDA	H	719	16/16	0.89	0.30	55,61,81,83	16
6	LDA	C	722	16/16	0.89	0.41	54,61,65,65	16
9	HTO	L	275	10/10	0.89	0.32	64,69,72,74	10
10	GOL	C	358	6/6	0.89	0.17	48,64,67,68	6
10	GOL	H	278	6/6	0.89	0.39	75,77,78,79	6
9	HTO	M	332	10/10	0.89	0.33	52,59,68,70	10
10	GOL	L	279	6/6	0.89	0.33	48,50,60,61	6
8	SO4	M	327	5/5	0.89	0.18	79,82,83,86	5
10	GOL	L	282	6/6	0.89	0.25	60,67,75,75	6
10	GOL	C	356	6/6	0.90	0.20	60,69,74,75	0
8	SO4	C	342	5/5	0.91	0.22	47,56,60,62	5
10	GOL	C	357	6/6	0.91	0.26	69,69,76,78	6
8	SO4	C	337	5/5	0.91	0.16	70,73,78,84	5
10	GOL	C	355	6/6	0.91	0.24	67,70,71,71	6
10	GOL	C	362	6/6	0.91	0.39	70,75,75,75	6
10	GOL	C	360	6/6	0.92	0.27	71,73,75,78	6
6	LDA	M	705	16/16	0.92	0.27	63,70,77,78	16
9	HTO	L	274	10/10	0.92	0.18	58,67,76,80	10

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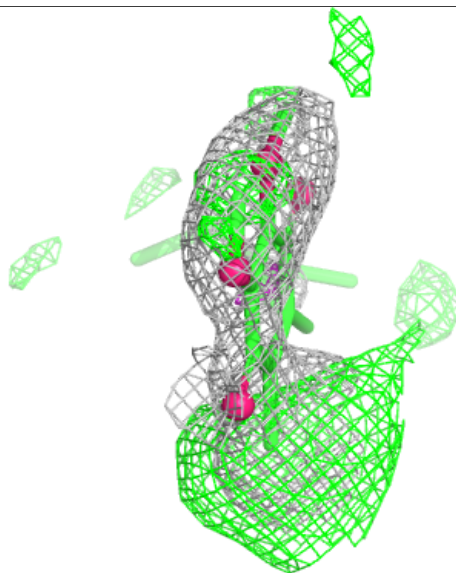
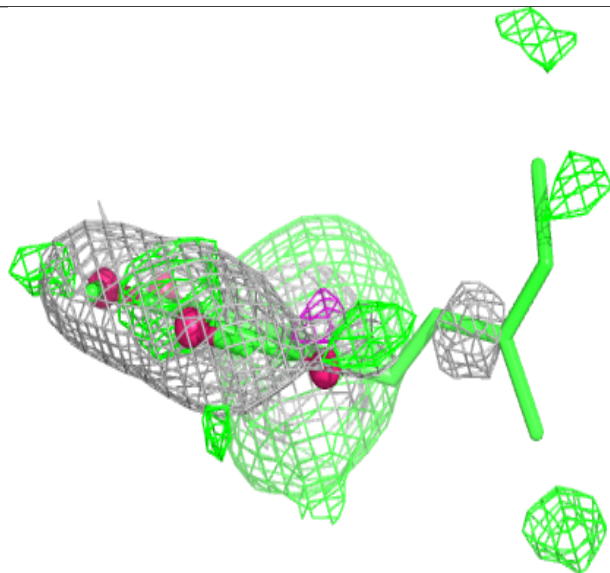
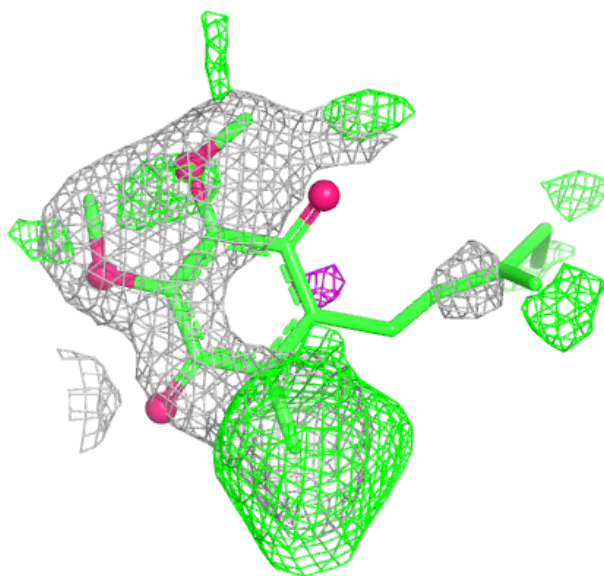
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	M	331	5/5	0.92	0.13	75,77,81,85	5
10	GOL	M	339	6/6	0.92	0.21	37,53,62,67	6
6	LDA	L	709	16/16	0.92	0.25	49,67,91,92	16
8	SO4	C	344	5/5	0.92	0.18	61,69,77,79	5
8	SO4	C	341	5/5	0.92	0.13	62,70,77,79	5
10	GOL	L	276	6/6	0.93	0.15	55,56,58,60	0
10	GOL	L	277	6/6	0.93	0.18	55,61,63,65	6
10	GOL	L	278	6/6	0.93	0.28	46,54,56,58	6
8	SO4	C	338	5/5	0.93	0.17	66,66,73,74	5
8	SO4	M	329	5/5	0.93	0.16	62,73,75,76	5
9	HTO	H	266	10/10	0.93	0.16	60,68,76,78	0
10	GOL	C	359	6/6	0.93	0.21	47,54,60,68	6
10	GOL	C	352	6/6	0.93	0.22	37,56,61,61	6
10	GOL	H	275	6/6	0.94	0.22	51,66,74,75	6
8	SO4	H	260	5/5	0.94	0.10	82,82,83,88	5
6	LDA	H	701	16/16	0.94	0.12	47,57,69,70	0
8	SO4	M	326	5/5	0.95	0.18	57,65,67,67	5
10	GOL	C	350	6/6	0.95	0.12	49,56,58,60	0
6	LDA	H	721	16/16	0.95	0.19	53,63,80,87	16
10	GOL	L	280	6/6	0.95	0.27	60,65,70,74	6
11	BCB	M	400	66/66	0.96	0.11	37,46,109,115	0
12	BPB	M	402	65/65	0.96	0.10	39,46,101,105	0
8	SO4	M	328	5/5	0.96	0.09	59,65,67,71	5
6	LDA	L	708	16/16	0.96	0.11	47,58,66,76	0
8	SO4	H	259	5/5	0.96	0.10	64,65,69,71	5
14	MQ9	M	501	58/58	0.97	0.10	38,46,92,98	0
11	BCB	M	401	66/66	0.97	0.08	33,39,62,67	0
11	BCB	L	400	66/66	0.98	0.07	34,39,49,57	0
11	BCB	L	401	66/66	0.98	0.07	35,39,69,79	0
8	SO4	M	324	5/5	0.98	0.08	54,54,60,71	0
8	SO4	M	325	5/5	0.98	0.07	69,70,77,82	0
12	BPB	L	402	65/65	0.98	0.06	37,41,51,53	0
5	HEC	C	401	43/43	0.99	0.07	46,52,61,67	0
8	SO4	H	263	5/5	0.99	0.10	47,50,52,52	5
5	HEC	C	402	43/43	0.99	0.07	41,46,55,61	0
5	HEC	C	403	43/43	0.99	0.06	36,40,43,49	0
5	HEC	C	404[A]	43/43	0.99	0.07	38,41,49,51	12
5	HEC	C	404[B]	43/43	0.99	0.07	38,41,46,49	12
15	FE2	M	500	1/1	1.00	0.02	42,42,42,42	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.

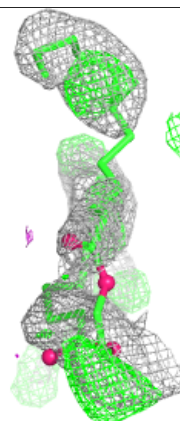
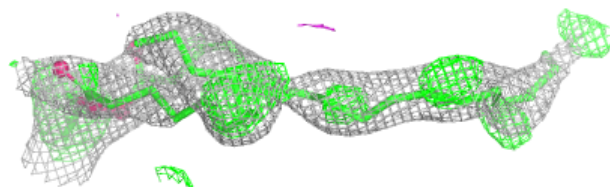
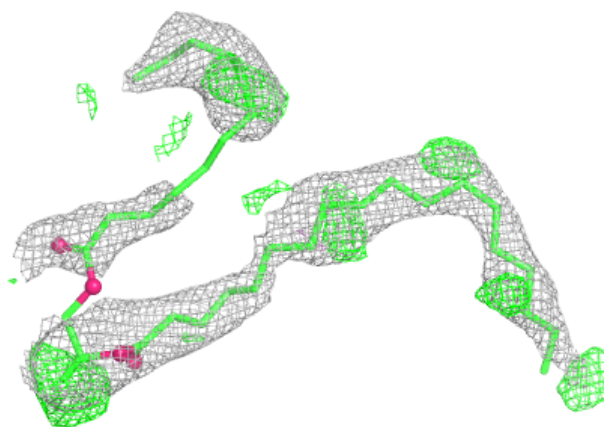
Electron density around UQ9 L 503:

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

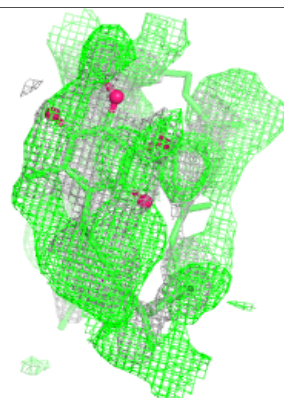
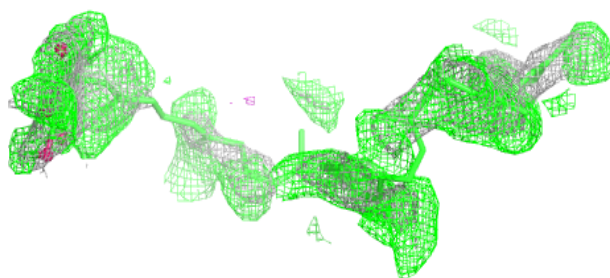
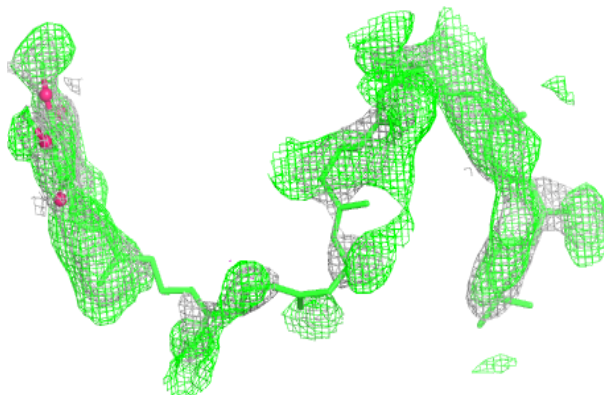


Electron density around DGA C 730:

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

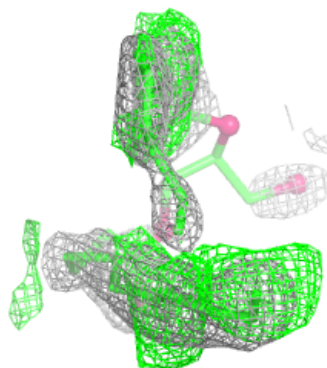
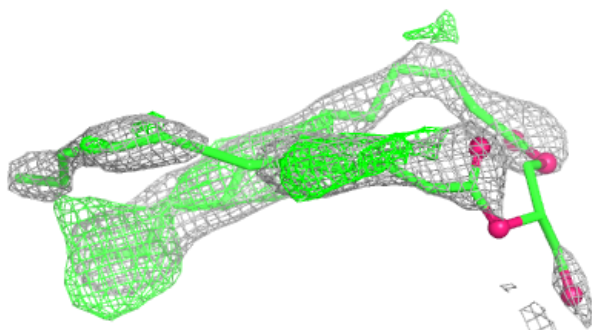
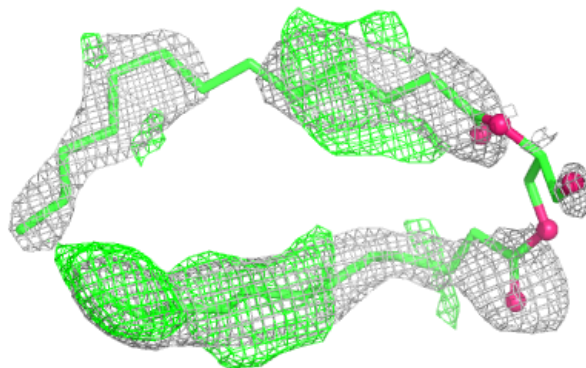
**Electron density around UQ9 L 502:**

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



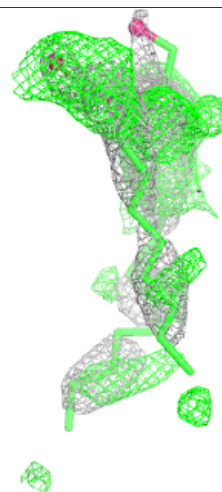
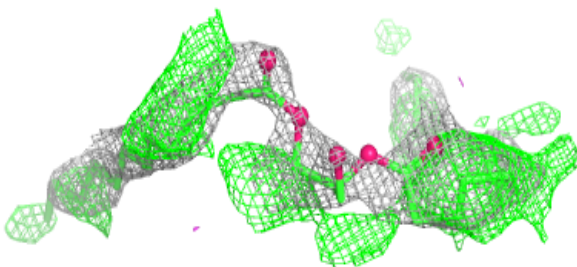
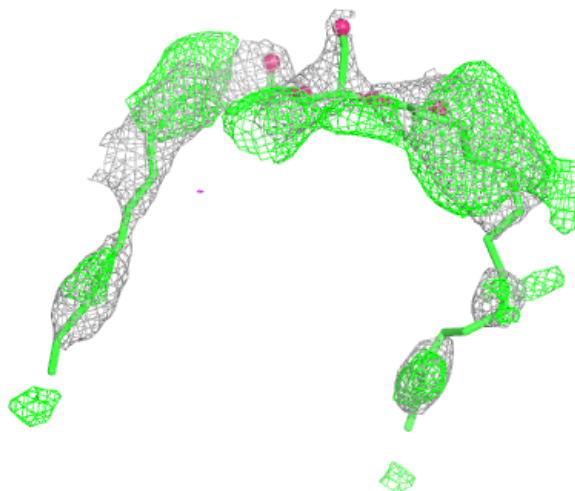
Electron density around DGA L 731:

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



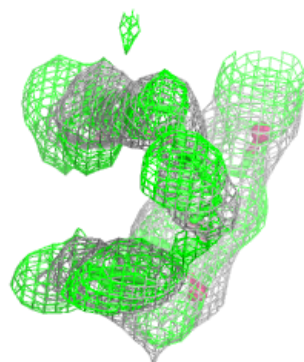
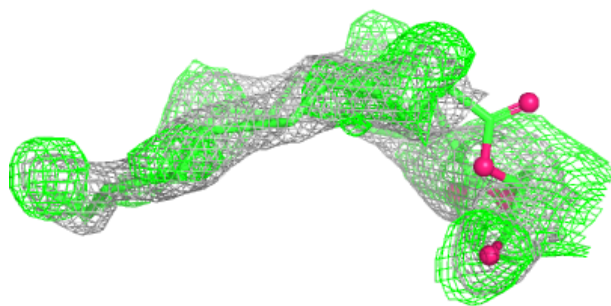
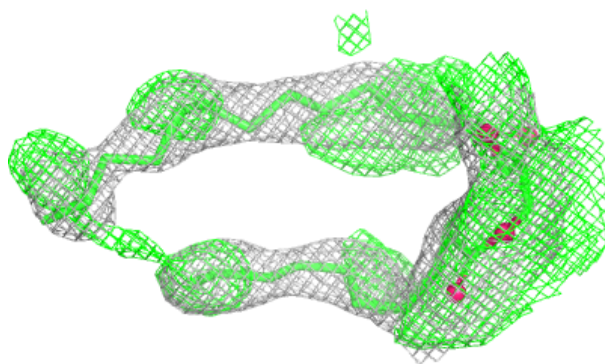
Electron density around DGA M 732:

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

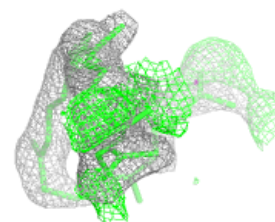
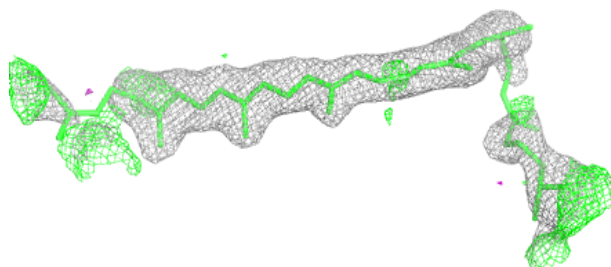
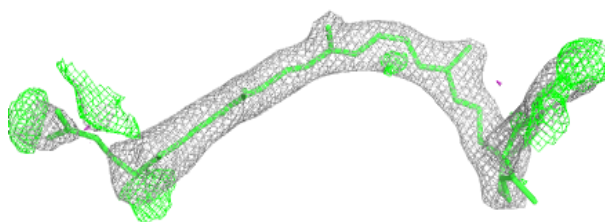


Electron density around DGA H 733:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

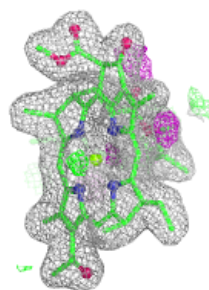
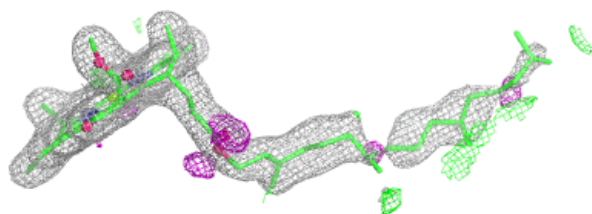
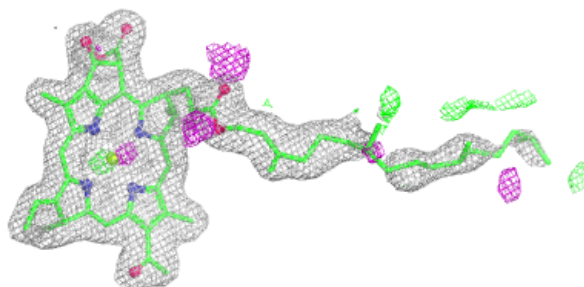
**Electron density around NS5 M 600:**

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

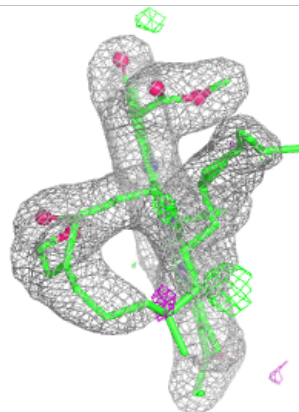
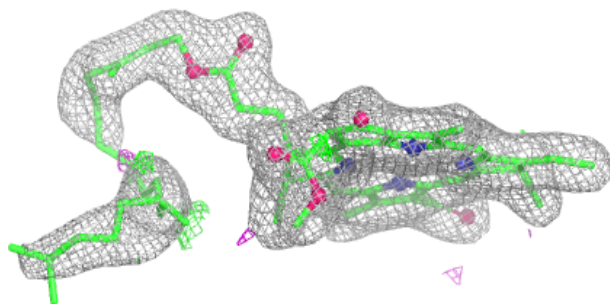
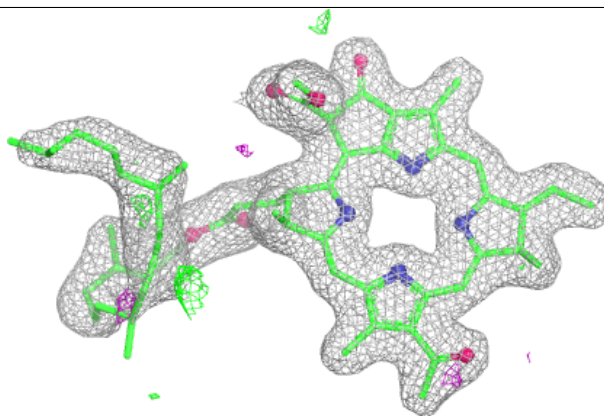


Electron density around BCB M 400:

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

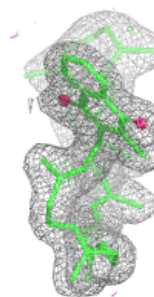
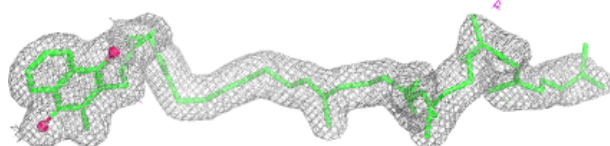
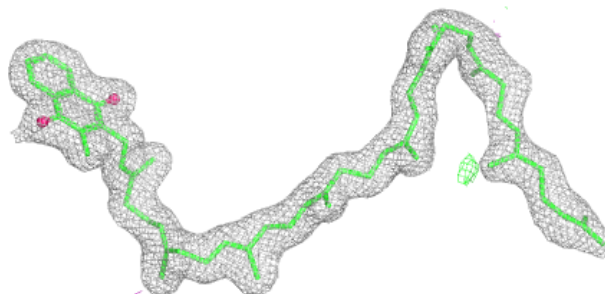
**Electron density around BPB M 402:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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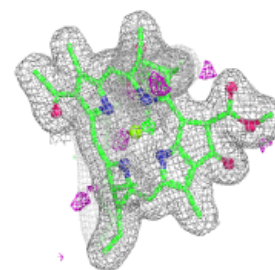
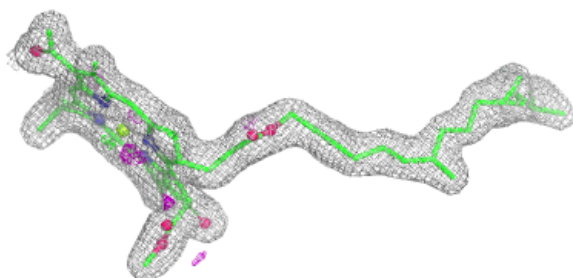
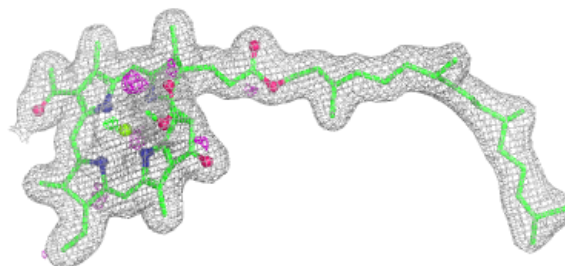


Electron density around MQ9 M 501:

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

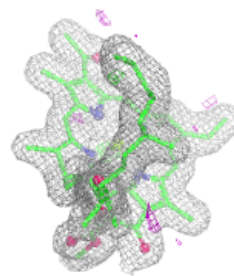
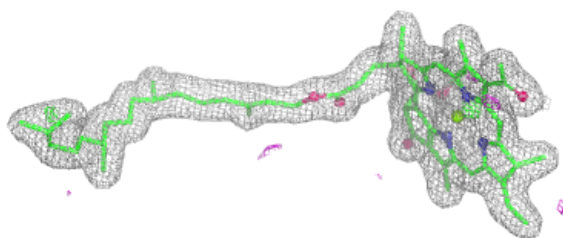
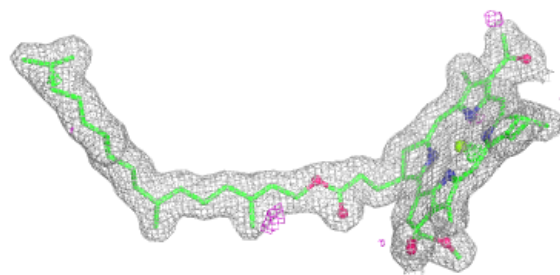
**Electron density around BCB M 401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

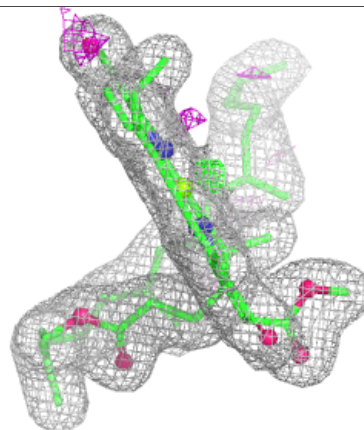
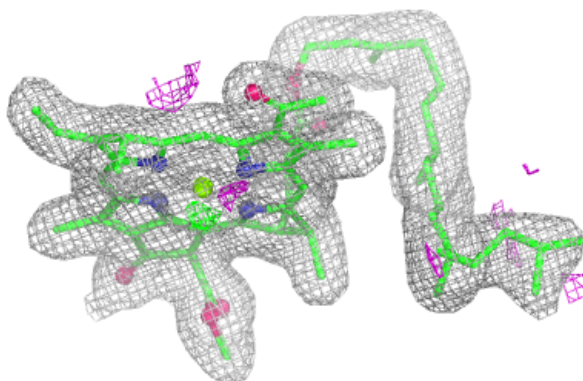
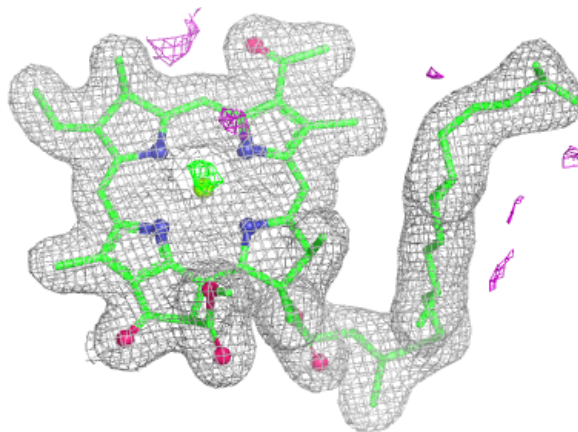


Electron density around BCB L 400:

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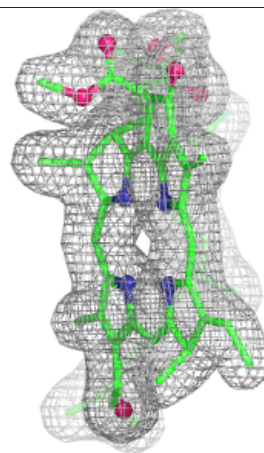
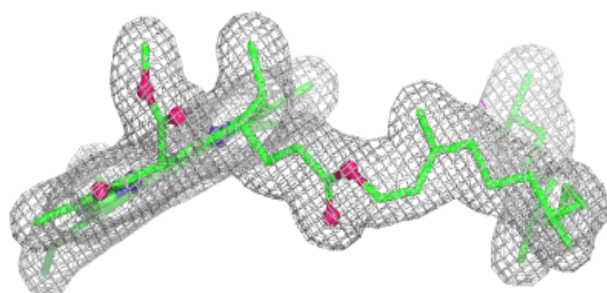
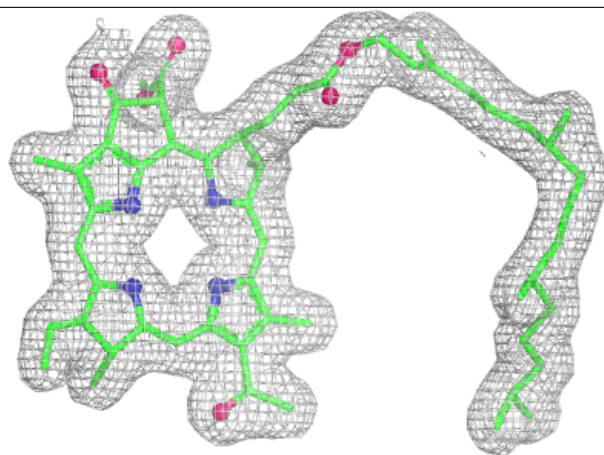
**Electron density around BCB L 401:**

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



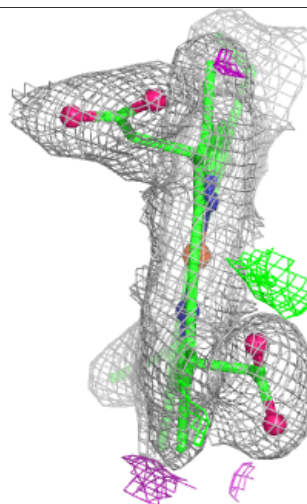
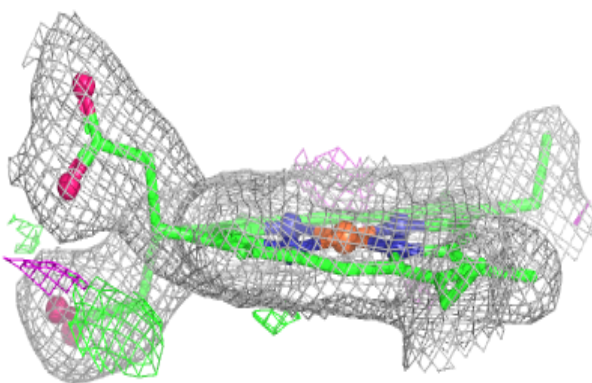
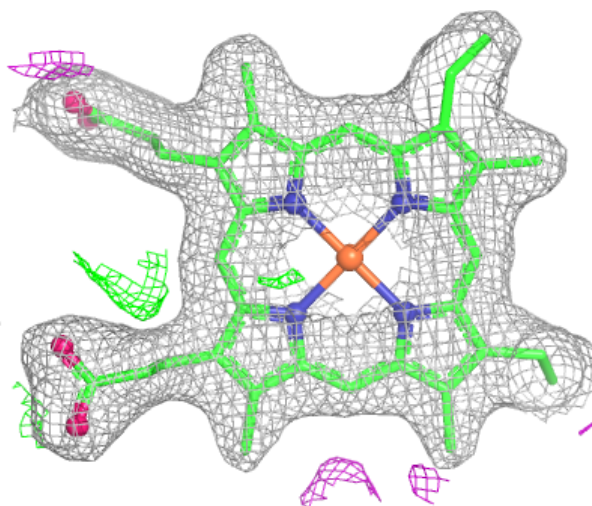
Electron density around BPB L 402:

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



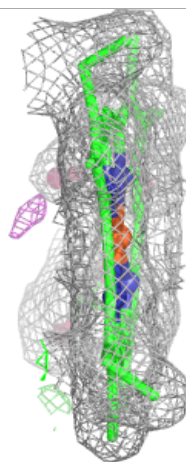
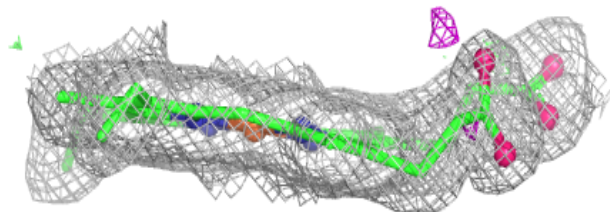
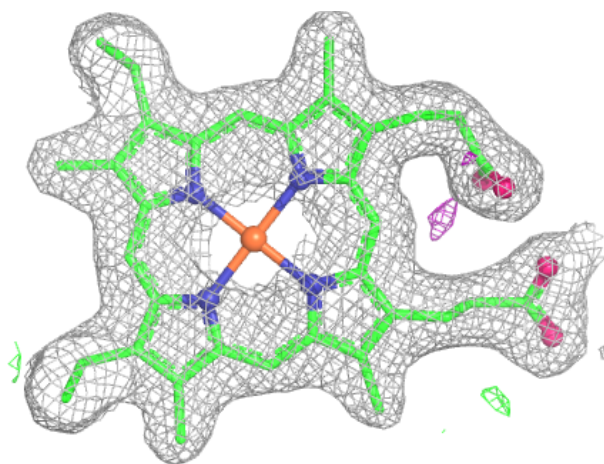
Electron density around HEC C 401:

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and green (positive)



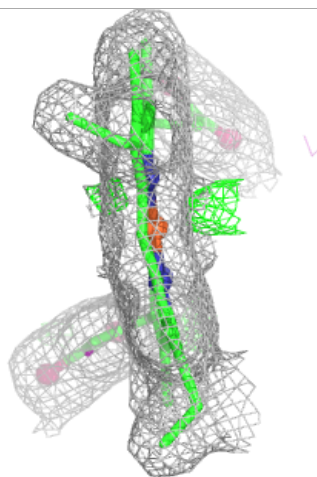
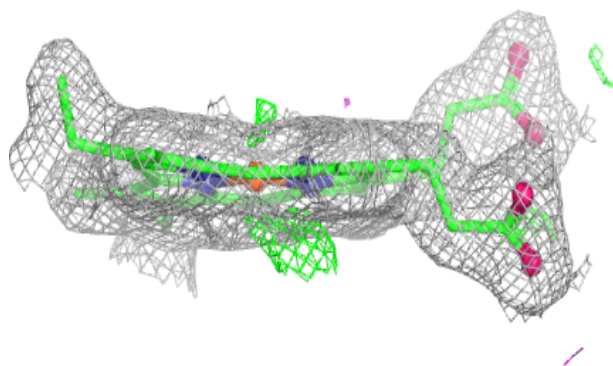
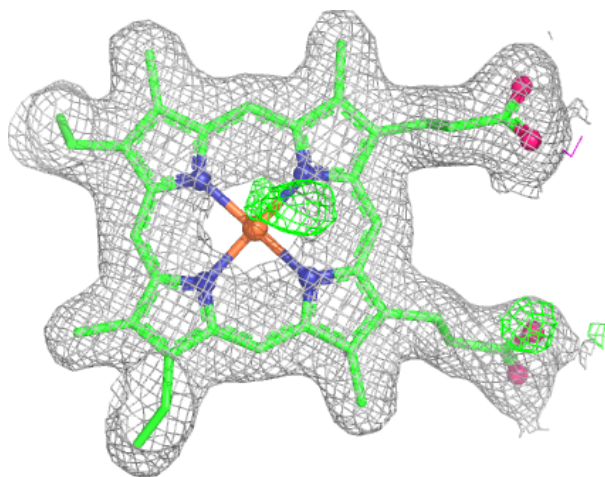
Electron density around HEC C 402:

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and green (positive)



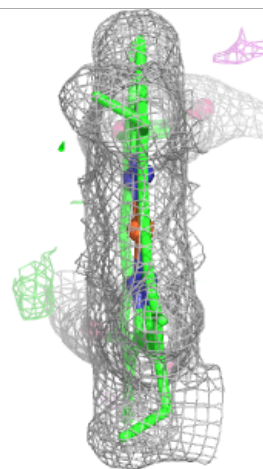
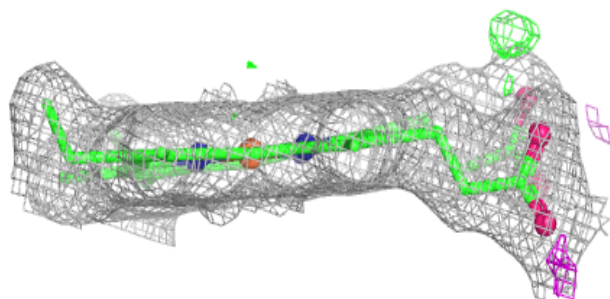
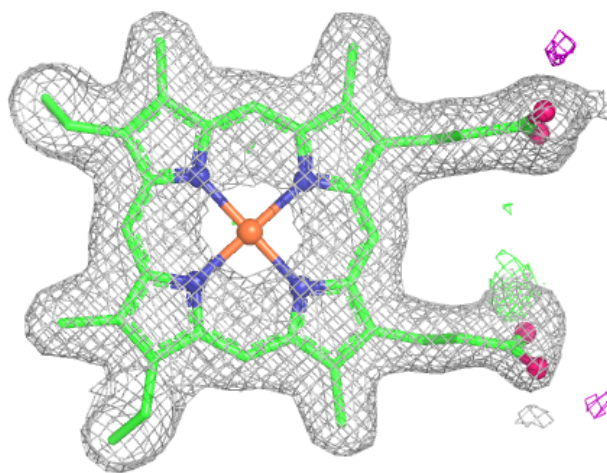
Electron density around HEC C 403:

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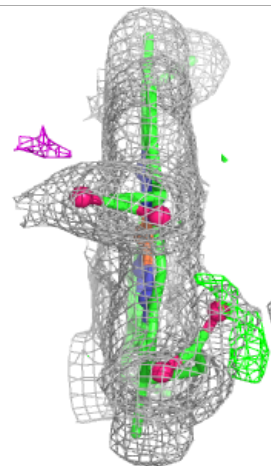
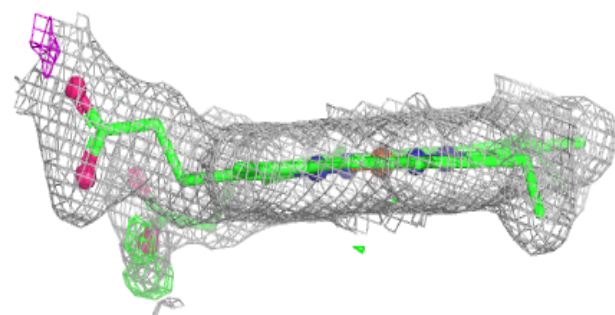
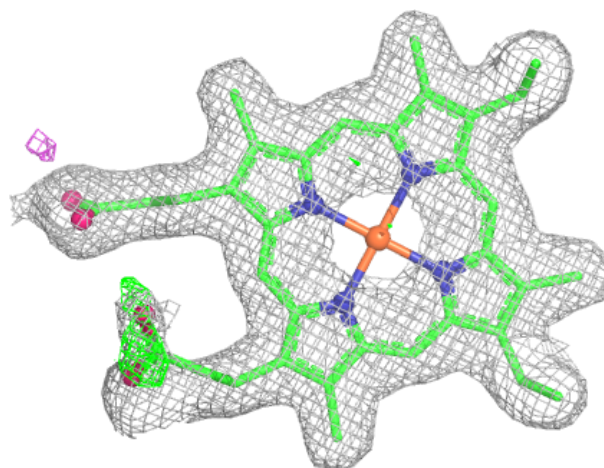
Electron density around HEC C 404 (A):

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



Electron density around HEC C 404 (B):

$2mF_o-DF_c$ (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.