



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 10:01 am BST

PDB ID : 3T6E  
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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

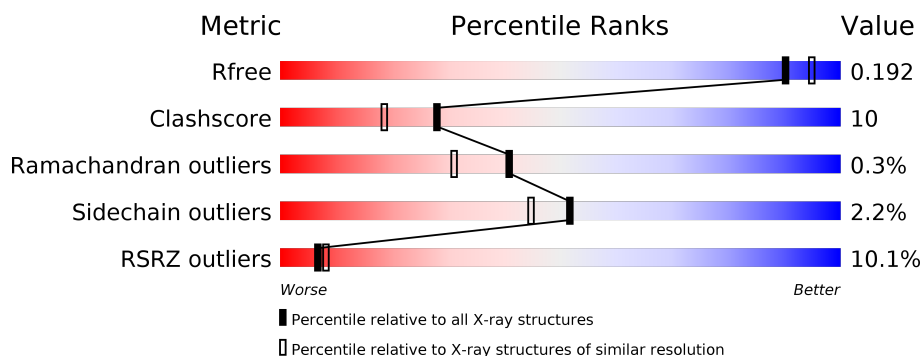
# 1 Overall quality at a glance

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))
$R_{free}$	130704	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>7%</div> <div>86%</div> <div>8%</div> <div>6%</div> </div>
2	H	258	<div> <div>11%</div> <div>91%</div> <div>9%</div> <div>•</div> </div>
3	L	273	<div> <div>6%</div> <div>92%</div> <div>7%</div> <div>•</div> </div>
4	M	323	<div> <div>15%</div> <div>93%</div> <div>7%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	C	359	-	-	X	-
10	GOL	C	361	-	-	-	X
10	GOL	H	272	-	-	-	X
10	GOL	L	279	-	-	X	-
10	GOL	M	334	-	-	-	X
10	GOL	M	335	-	-	-	X
13	UQ9	L	502	-	-	X	X
6	LDA	H	707	-	-	-	X
6	LDA	L	703	-	-	-	X
6	LDA	L	720	-	-	-	X
6	LDA	M	702	-	-	X	X
6	LDA	M	706	-	-	-	X
6	LDA	M	715	-	-	-	X
7	DGA	M	732	-	-	X	-
8	SO4	C	337	-	-	X	-
8	SO4	C	338	-	-	X	-
8	SO4	C	342	-	-	X	-
8	SO4	C	344	-	-	X	-
8	SO4	H	261	-	-	X	-
8	SO4	M	329	-	-	X	-
8	SO4	M	330	-	-	-	X
9	HTO	C	348	-	-	X	X
9	HTO	H	268	-	-	-	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			

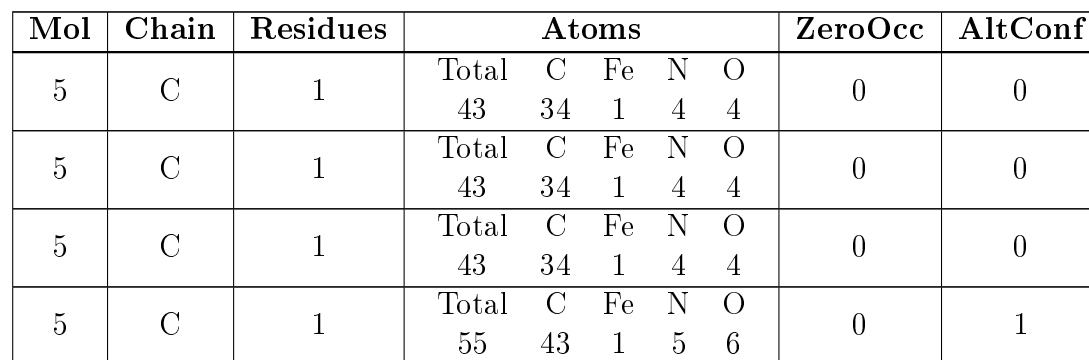
- Molecule 3 is a protein called Reaction center protein L chain.

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			

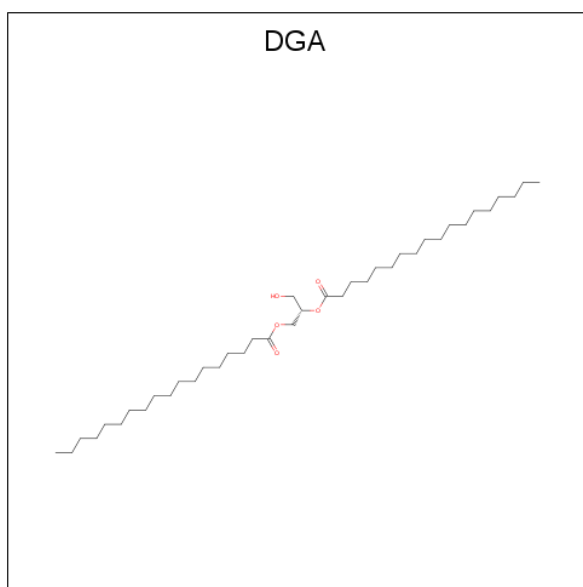
- Molecule 5 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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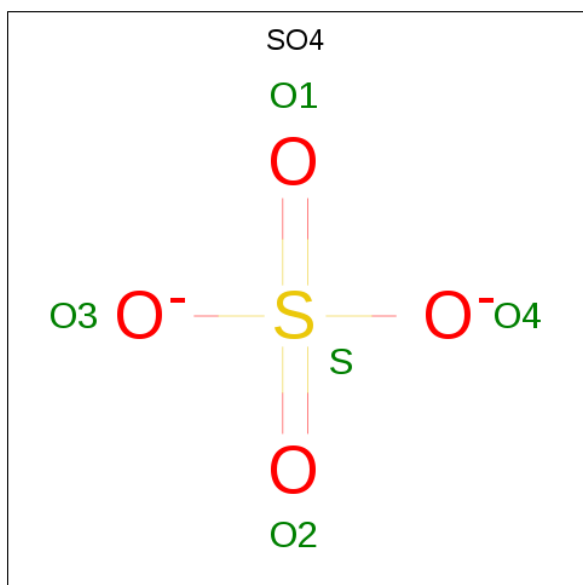
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			16	14	1	1		
6	C	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			13	11	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
6	H	1	Total	C	N	O	0	0
			16	14	1	1		
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 (three-letter code: DGA) (formula: C<sub>39</sub>H<sub>76</sub>O<sub>5</sub>).



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 (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

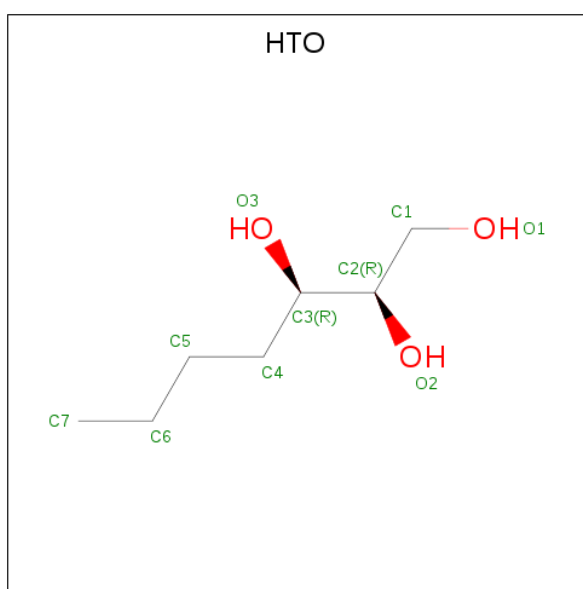
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



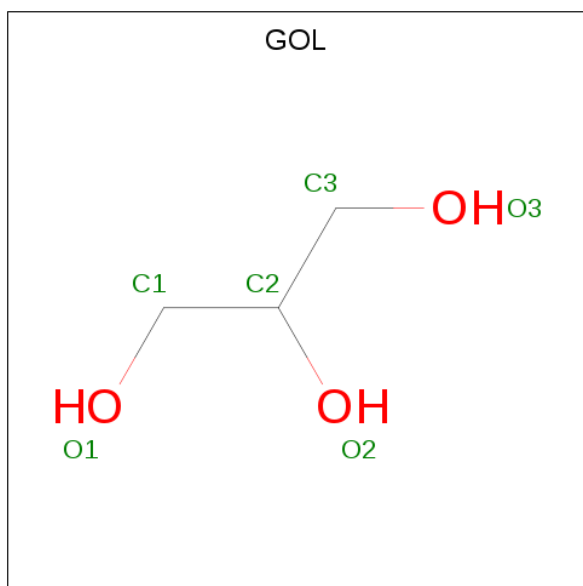
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			10	7	3		
9	C	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	H	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		

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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 (three-letter code: 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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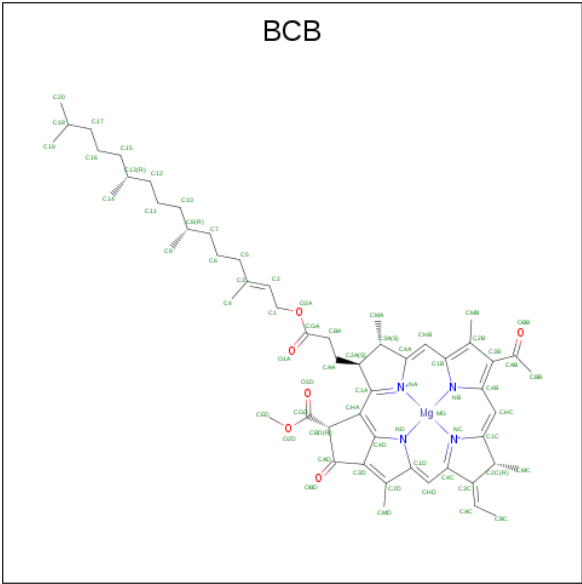
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	H	1	Total	C	O	0	0
			6	3	3		
10	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		

- Molecule 11 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).



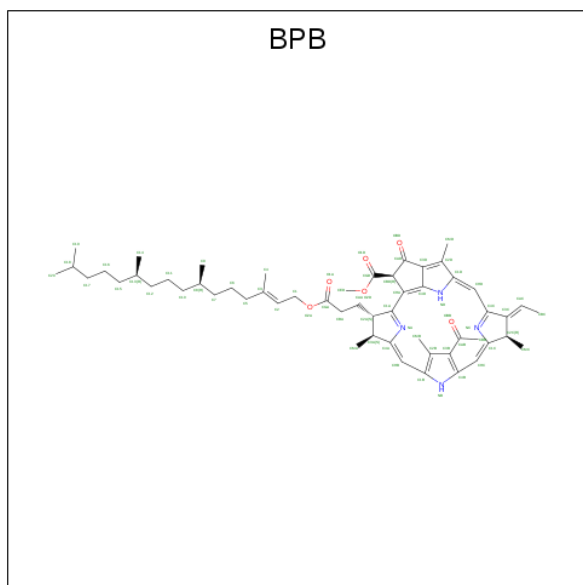
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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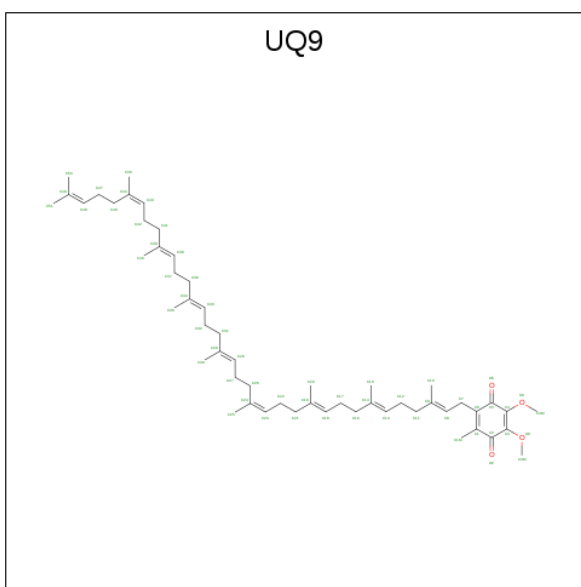
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	L	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
11	M	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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



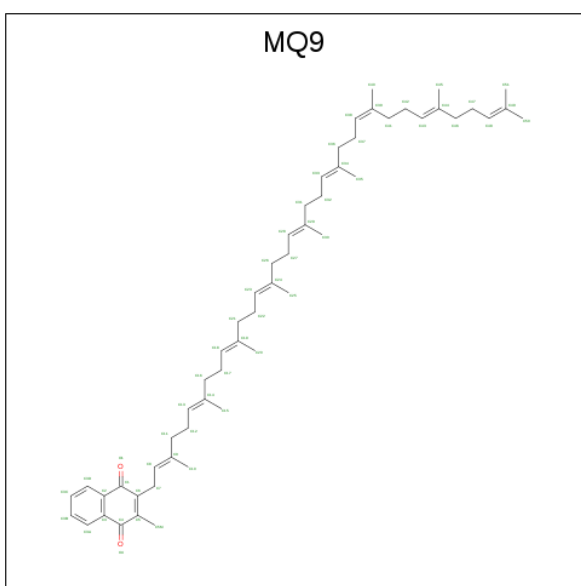
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 13 is Ubiquinone-9 (three-letter code: 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 (three-letter code: MQ9) (formula:  $C_{56}H_{80}O_2$ ).

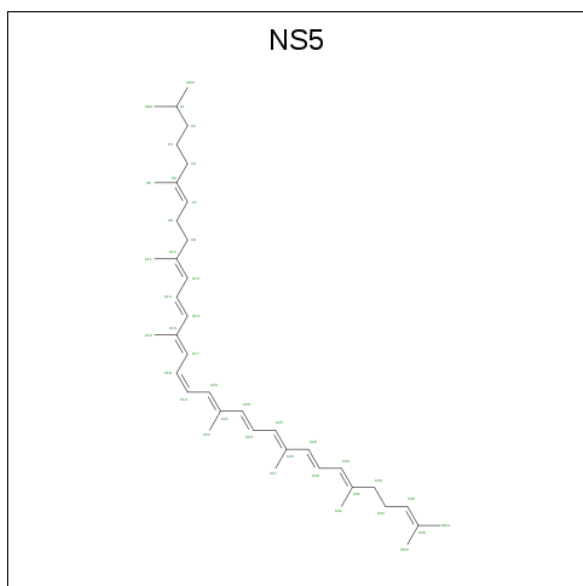


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	M	1	Total	C	O	0	0
			58	56	2		

- Molecule 15 is FE (II) ION (three-letter code: 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 (three-letter code: NS5) (formula: C<sub>40</sub>H<sub>60</sub>).



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

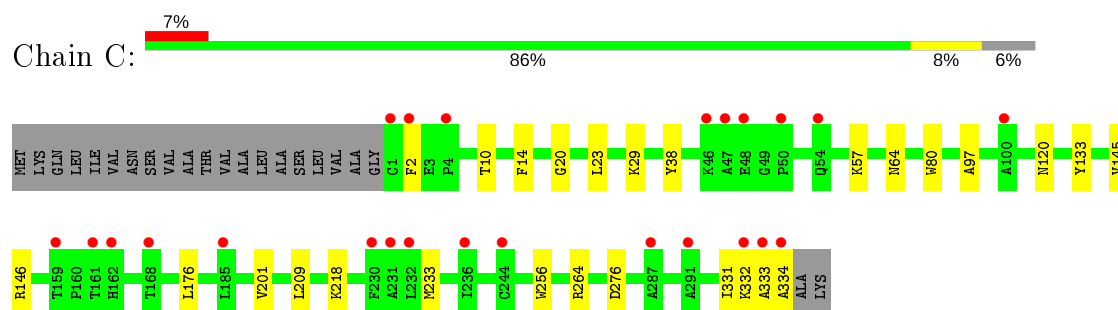
- Molecule 17 is water.

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		

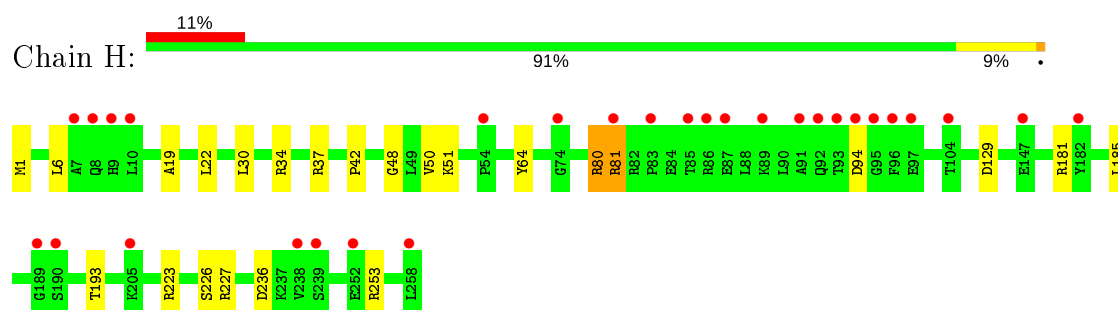
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

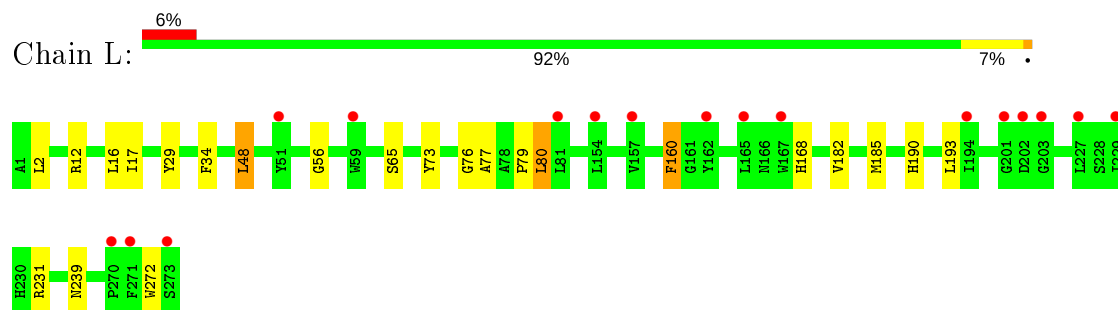
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



- Molecule 2: Reaction center protein H chain



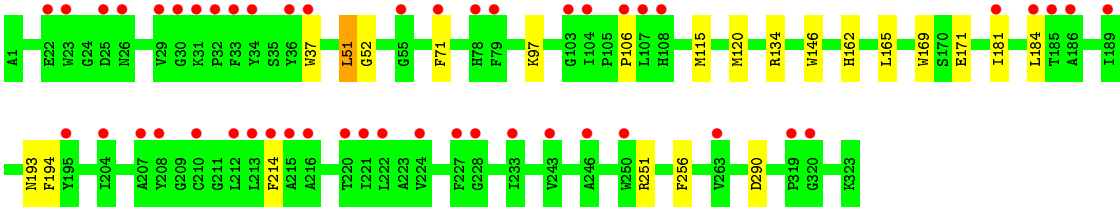
- Molecule 3: Reaction center protein L chain



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.92Å)	Xtriage
Refinement program	REFMAC 5.6.0101	Depositor
R, $R_{free}$	0.155 , 0.178 0.170 , 0.192	Depositor DCC
$R_{free}$ test set	10655 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 79.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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

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	0.90	1/2718 (0.0%)	0.78	1/3702 (0.0%)
2	H	0.85	0/2064	0.81	2/2820 (0.1%)
3	L	0.90	0/2298	0.77	3/3135 (0.1%)
4	M	0.86	0/2689	0.75	1/3676 (0.0%)
All	All	0.88	1/9769 (0.0%)	0.77	7/13333 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	201	VAL	CB-CG2	5.07	1.63	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	160	PHE	CB-CG-CD1	5.77	124.84	120.80
4	M	251	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	H	181	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	C	264	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	H	80	ARG	NE-CZ-NH1	5.25	122.93	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	21	0
2	H	2034	0	2011	18	0
3	L	2207	0	2134	22	0
4	M	2591	0	2478	32	0
5	C	184	0	108	2	0
6	C	32	0	62	5	0
6	H	77	0	146	25	0
6	L	64	0	124	10	0
6	M	80	0	155	22	0
7	C	37	0	58	1	0
7	H	31	0	44	6	0
7	L	33	0	48	7	0
7	M	34	0	50	23	0
8	C	55	0	0	9	0
8	H	40	0	0	8	0
8	M	40	0	0	2	0
9	C	20	0	32	13	0
9	H	30	0	48	3	0
9	L	20	0	32	0	0
9	M	10	0	16	0	0
10	C	102	0	136	15	0
10	H	66	0	88	4	0
10	L	42	0	56	7	0
10	M	42	0	56	5	0
11	L	132	0	144	7	0
11	M	132	0	144	12	0
12	L	65	0	74	2	0
12	M	65	0	74	3	0
13	L	77	0	99	37	0
14	M	58	0	80	0	0
15	M	1	0	0	0	0
16	M	40	0	60	2	0
17	C	441	0	0	3	0
17	H	233	0	0	3	0
17	L	125	0	0	1	0
17	M	175	0	0	3	0
All	All	12066	0	11181	219	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 10.

The worst 5 of 219 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)
4:M:71[B]:PHE:CD2	7:M:732:DGA:HA72	1.43	1.50
6:H:718:LDA:H31	6:H:718:LDA:CM1	1.39	1.38
4:M:71[B]:PHE:CE2	7:M:732:DGA:HA52	1.61	1.35
6:M:706:LDA:HM13	8:M:329:SO4:O4	1.10	1.27
6:H:718:LDA:C3	6:H:718:LDA:HM13	1.49	1.27

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%)	13	4
3	L	276/273 (101%)	272 (99%)	4 (1%)	0	100	100
4	M	324/323 (100%)	318 (98%)	5 (2%)	1 (0%)	41	31
All	All	1195/1210 (99%)	1165 (98%)	26 (2%)	4 (0%)	41	31

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%)	73	72
2	H	210/212 (99%)	204 (97%)	6 (3%)	42	33
3	L	223/218 (102%)	217 (97%)	6 (3%)	44	36
4	M	252/248 (102%)	246 (98%)	6 (2%)	49	41
All	All	970/975 (100%)	949 (98%)	21 (2%)	52	45

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	2	LEU
3	L	48	LEU
4	M	181	ILE
2	H	236	ASP
4	M	194	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	178	HIS
3	L	239	ASN
2	H	220	ASN
1	C	302	GLN
3	L	183	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	7,9,11	2.63	2 (28%)
2	FME	H	1[A]	2	8,9,10	0.78	0	7,9,11	2.27	1 (14%)
4	CSO	M	160	4	3,6,7	0.65	0	0,6,8	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	H	1[B]	2	-	4/7/9/11	-
2	FME	H	1[A]	2	-	5/7/9/11	-
4	CSO	M	160	4	-	0/1/5/7	-

There are no bond length outliers.

All (3) 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[B]	FME	O-C-CA	-2.00	119.53	124.78

There are no chirality outliers.

5 of 9 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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	$\# Z  > 2$
9	HTO	C	349	-	9,9,9	0.59	0	10,10,10	0.92	0
10	GOL	H	277	-	5,5,5	0.34	0	5,5,5	0.33	0
7	DGA	C	730	1	36,36,43	0.82	2 (5%)	38,38,45	1.43	3 (7%)
6	LDA	M	715	-	12,15,15	1.96	1 (8%)	14,17,17	0.47	0
10	GOL	C	358	-	5,5,5	0.51	0	5,5,5	0.55	0
7	DGA	L	731	-	32,32,43	0.67	0	34,34,45	1.59	6 (17%)
10	GOL	C	360	-	5,5,5	0.21	0	5,5,5	0.32	0
7	DGA	M	732	-	33,33,43	0.64	0	35,35,45	1.60	4 (11%)
8	SO4	C	341	-	4,4,4	0.36	0	6,6,6	0.28	0
10	GOL	H	270	-	5,5,5	0.34	0	5,5,5	0.58	0
12	BPB	M	402	-	64,70,70	1.17	3 (4%)	64,101,101	1.42	12 (18%)
10	GOL	C	353[B]	-	5,5,5	0.51	0	5,5,5	0.39	0
10	GOL	M	334	-	5,5,5	0.32	0	5,5,5	1.14	0
8	SO4	M	330	-	4,4,4	0.40	0	6,6,6	0.39	0
11	BCB	L	401	3	60,74,74	3.48	18 (30%)	48,115,115	2.11	9 (18%)
8	SO4	C	339	-	4,4,4	0.30	0	6,6,6	0.23	0
10	GOL	C	363	-	5,5,5	0.32	0	5,5,5	0.50	0
10	GOL	M	337	-	5,5,5	0.27	0	5,5,5	0.39	0
6	LDA	M	706	-	12,15,15	2.07	1 (8%)	14,17,17	0.57	0
8	SO4	M	326	-	4,4,4	0.15	0	6,6,6	0.39	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	HTO	L	274	-	9,9,9	0.69	0	10,10,10	1.60	4 (40%)
10	GOL	C	364	-	5,5,5	0.65	0	5,5,5	2.21	2 (40%)
5	HEC	C	401	1	26,50,50	0.97	0	18,82,82	2.00	5 (27%)
10	GOL	C	359	-	5,5,5	0.43	0	5,5,5	0.37	0
10	GOL	L	277	-	5,5,5	0.25	0	5,5,5	1.06	0
5	HEC	C	403	1	26,50,50	0.99	1 (3%)	18,82,82	1.26	3 (16%)
8	SO4	H	260	-	4,4,4	0.30	0	6,6,6	0.25	0
7	DGA	H	733	-	30,30,43	0.63	1 (3%)	32,32,45	1.81	8 (25%)
8	SO4	M	324	-	4,4,4	0.46	0	6,6,6	1.00	0
11	BCB	L	400	3	60,74,74	3.59	20 (33%)	48,115,115	2.43	14 (29%)
8	SO4	M	329	-	4,4,4	0.23	0	6,6,6	0.35	0
8	SO4	C	347	-	4,4,4	0.32	0	6,6,6	0.08	0
10	GOL	H	269	-	5,5,5	0.21	0	5,5,5	0.65	0
10	GOL	L	279	-	5,5,5	0.79	0	5,5,5	1.07	0
10	GOL	M	336	-	5,5,5	0.19	0	5,5,5	0.62	0
6	LDA	C	722	-	12,15,15	1.98	1 (8%)	14,17,17	0.50	0
14	MQ9	M	501	-	59,59,59	2.15	26 (44%)	72,75,75	1.28	9 (12%)
8	SO4	C	342	-	4,4,4	0.51	0	6,6,6	0.23	0
5	HEC	C	404[A]	-	26,50,50	1.02	1 (3%)	18,82,82	2.00	6 (33%)
10	GOL	C	356	-	5,5,5	0.85	0	5,5,5	1.54	1 (20%)
10	GOL	C	351	-	5,5,5	0.63	0	5,5,5	1.22	0
6	LDA	H	707	-	12,15,15	1.97	1 (8%)	14,17,17	0.55	0
8	SO4	C	346	-	4,4,4	0.41	0	6,6,6	0.27	0
6	LDA	M	704	-	12,15,15	2.01	1 (8%)	14,17,17	0.55	0
6	LDA	M	702	-	12,15,15	1.99	1 (8%)	14,17,17	0.80	0
6	LDA	H	721	-	12,15,15	1.82	1 (8%)	14,17,17	1.05	1 (7%)
10	GOL	C	350	-	5,5,5	1.04	1 (20%)	5,5,5	1.18	1 (20%)
10	GOL	M	333	-	5,5,5	0.27	0	5,5,5	0.30	0
10	GOL	L	278	-	5,5,5	0.87	0	5,5,5	1.39	1 (20%)
10	GOL	L	282	-	5,5,5	0.34	0	5,5,5	0.24	0
10	GOL	C	352	-	5,5,5	0.35	0	5,5,5	0.54	0
9	HTO	C	348	-	9,9,9	0.42	0	10,10,10	1.85	2 (20%)
10	GOL	H	273	-	5,5,5	0.24	0	5,5,5	0.67	0
12	BPB	L	402	-	64,70,70	0.88	1 (1%)	64,101,101	1.26	7 (10%)
10	GOL	C	355	-	5,5,5	0.27	0	5,5,5	0.40	0
6	LDA	H	718	-	9,12,15	2.45	1 (11%)	11,14,17	0.60	0
10	GOL	C	362	-	5,5,5	0.26	0	5,5,5	0.54	0
8	SO4	M	327	-	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	259	-	4,4,4	0.28	0	6,6,6	0.26	0
5	HEC	C	402	1	26,50,50	1.19	3 (11%)	18,82,82	1.45	4 (22%)
13	UQ9	L	503	-	19,19,58	2.38	7 (36%)	23,26,73	1.66	4 (17%)
6	LDA	H	719	-	12,15,15	2.03	1 (8%)	14,17,17	0.68	0
10	GOL	M	338	-	5,5,5	0.29	0	5,5,5	1.46	1 (20%)
8	SO4	H	265	-	4,4,4	0.35	0	6,6,6	0.07	0
8	SO4	H	263	-	4,4,4	0.39	0	6,6,6	0.36	0
8	SO4	C	337	-	4,4,4	0.33	0	6,6,6	0.16	0
10	GOL	C	354	-	5,5,5	0.73	0	5,5,5	0.54	0
6	LDA	L	720	-	12,15,15	1.95	1 (8%)	14,17,17	1.12	2 (14%)
10	GOL	C	353[A]	-	5,5,5	0.56	0	5,5,5	0.75	0
8	SO4	C	338	-	4,4,4	0.30	0	6,6,6	0.27	0
8	SO4	C	343	-	4,4,4	0.22	0	6,6,6	0.40	0
16	NS5	M	600	-	39,39,39	2.21	19 (48%)	44,46,46	2.11	11 (25%)
6	LDA	M	705	-	12,15,15	1.77	1 (8%)	14,17,17	0.65	0
8	SO4	H	261	-	4,4,4	0.40	0	6,6,6	1.07	1 (16%)
8	SO4	H	264	-	4,4,4	0.41	0	6,6,6	0.27	0
10	GOL	L	281	-	5,5,5	0.26	0	5,5,5	0.36	0
11	BCB	M	401	4	60,74,74	3.65	22 (36%)	48,115,115	2.50	15 (31%)
8	SO4	M	331	-	4,4,4	0.32	0	6,6,6	0.81	0
6	LDA	L	709	-	12,15,15	2.01	1 (8%)	14,17,17	0.28	0
9	HTO	L	275	-	9,9,9	0.90	0	10,10,10	3.27	4 (40%)
9	HTO	H	268	-	9,9,9	0.34	0	10,10,10	1.83	2 (20%)
6	LDA	L	703	-	12,15,15	2.10	1 (8%)	14,17,17	0.62	0
8	SO4	M	328	-	4,4,4	0.28	0	6,6,6	0.62	0
11	BCB	M	400	4	60,74,74	3.40	18 (30%)	48,115,115	2.00	12 (25%)
5	HEC	C	404[B]	-	26,50,50	0.96	1 (3%)	18,82,82	1.77	5 (27%)
13	UQ9	L	502	-	58,58,58	2.25	23 (39%)	70,73,73	1.48	14 (20%)
6	LDA	C	712	-	12,15,15	2.19	1 (8%)	14,17,17	0.54	0
10	GOL	C	365	-	5,5,5	0.22	0	5,5,5	0.48	0
10	GOL	H	272	-	5,5,5	0.25	0	5,5,5	0.63	0
10	GOL	H	275	-	5,5,5	0.31	0	5,5,5	0.35	0
8	SO4	H	262[A]	-	4,4,4	0.44	0	6,6,6	0.48	0
10	GOL	H	279	-	5,5,5	0.25	0	5,5,5	0.51	0
10	GOL	L	280	-	5,5,5	0.28	0	5,5,5	0.19	0
8	SO4	H	262[B]	-	4,4,4	0.40	0	6,6,6	0.54	0
10	GOL	H	274	-	5,5,5	0.23	0	5,5,5	0.44	0
10	GOL	M	335	-	5,5,5	0.60	0	5,5,5	1.81	2 (40%)
8	SO4	C	344	-	4,4,4	0.54	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	GOL	L	276	-	5,5,5	0.37	0	5,5,5	0.53	0
6	LDA	H	701	-	12,15,15	1.47	1 (8%)	14,17,17	1.12	1 (7%)
10	GOL	H	276	-	5,5,5	0.19	0	5,5,5	0.44	0
10	GOL	C	357	-	5,5,5	0.52	0	5,5,5	0.39	0
9	HTO	M	332	-	9,9,9	0.56	0	10,10,10	3.41	6 (60%)
10	GOL	M	339	-	5,5,5	0.32	0	5,5,5	0.48	0
8	SO4	C	340	-	4,4,4	0.30	0	6,6,6	0.37	0
6	LDA	L	708	-	12,15,15	1.64	1 (8%)	14,17,17	0.84	1 (7%)
10	GOL	H	278	-	5,5,5	0.18	0	5,5,5	0.69	0
10	GOL	H	271	-	5,5,5	0.51	0	5,5,5	1.23	1 (20%)
10	GOL	C	361	-	5,5,5	0.25	0	5,5,5	0.35	0
9	HTO	H	267	-	9,9,9	0.54	0	10,10,10	1.01	0
8	SO4	M	325	-	4,4,4	0.24	0	6,6,6	0.28	0
8	SO4	C	345	-	4,4,4	0.58	0	6,6,6	0.45	0
9	HTO	H	266	-	9,9,9	0.38	0	10,10,10	1.38	2 (20%)

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	402	1	-	1/6/54/54	-
9	HTO	H	268	-	-	8/10/10/10	-
10	GOL	H	269	-	-	4/4/4/4	-
10	GOL	L	279	-	-	2/4/4/4	-
13	UQ9	L	503	-	-	6/11/35/81	0/1/1/1
9	HTO	C	349	-	-	7/10/10/10	-
11	BCB	M	400	4	-	15/41/177/177	-
5	HEC	C	404[B]	-	-	1/6/54/54	-
14	MQ9	M	501	-	-	2/53/73/73	0/2/2/2
7	DGA	C	730	1	-	18/37/37/45	-
13	UQ9	L	502	-	-	24/57/81/81	0/1/1/1
6	LDA	M	715	-	-	9/13/13/13	-
6	LDA	H	719	-	-	5/13/13/13	-
6	LDA	C	712	-	-	9/13/13/13	-
10	GOL	C	355	-	-	2/4/4/4	-
5	HEC	C	404[A]	-	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	C	365	-	-	2/4/4/4	-
9	HTO	C	348	-	-	7/10/10/10	-
10	GOL	C	358	-	-	2/4/4/4	-
10	GOL	C	356	-	-	0/4/4/4	-
10	GOL	M	335	-	-	2/4/4/4	-
10	GOL	H	270	-	-	4/4/4/4	-
7	DGA	L	731	-	-	12/34/34/45	-
10	GOL	H	279	-	-	2/4/4/4	-
6	LDA	L	703	-	-	7/13/13/13	-
6	LDA	H	707	-	-	6/13/13/13	-
10	GOL	C	360	-	-	2/4/4/4	-
6	LDA	M	704	-	-	6/13/13/13	-
10	GOL	L	281	-	-	4/4/4/4	-
7	DGA	M	732	-	-	16/35/35/45	-
6	LDA	M	702	-	-	10/13/13/13	-
10	GOL	C	354	-	-	2/4/4/4	-
6	LDA	H	721	-	-	8/13/13/13	-
10	GOL	H	274	-	-	2/4/4/4	-
10	GOL	H	272	-	-	0/4/4/4	-
12	BPB	M	402	-	-	11/47/105/105	0/5/6/6
10	GOL	M	333	-	-	2/4/4/4	-
10	GOL	C	350	-	-	0/4/4/4	-
10	GOL	C	351	-	-	2/4/4/4	-
10	GOL	C	353[A]	-	-	4/4/4/4	-
10	GOL	L	276	-	-	2/4/4/4	-
10	GOL	L	282	-	-	2/4/4/4	-
6	LDA	H	701	-	-	5/13/13/13	-
10	GOL	H	276	-	-	2/4/4/4	-
16	NS5	M	600	-	-	9/43/43/43	-
11	BCB	L	401	3	-	7/41/177/177	-
6	LDA	L	708	-	-	1/13/13/13	-
10	GOL	C	352	-	-	2/4/4/4	-
10	GOL	H	273	-	-	2/4/4/4	-
10	GOL	C	363	-	-	2/4/4/4	-
6	LDA	M	705	-	-	5/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	BPB	L	402	-	-	4/47/105/105	0/5/6/6
6	LDA	L	720	-	-	6/13/13/13	-
10	GOL	H	277	-	-	3/4/4/4	-
10	GOL	H	275	-	-	2/4/4/4	-
6	LDA	M	706	-	-	8/13/13/13	-
10	GOL	M	339	-	-	2/4/4/4	-
11	BCB	L	400	3	-	9/41/177/177	-
10	GOL	C	353[B]	-	-	4/4/4/4	-
10	GOL	M	334	-	-	2/4/4/4	-
9	HTO	M	332	-	-	7/10/10/10	-
10	GOL	C	361	-	-	4/4/4/4	-
9	HTO	L	275	-	-	7/10/10/10	-
10	GOL	H	271	-	-	4/4/4/4	-
5	HEC	C	401	1	-	0/6/54/54	-
10	GOL	M	336	-	-	2/4/4/4	-
9	HTO	L	274	-	-	0/10/10/10	-
11	BCB	M	401	4	-	10/41/177/177	-
10	GOL	C	364	-	-	1/4/4/4	-
10	GOL	H	278	-	-	4/4/4/4	-
9	HTO	H	267	-	-	4/10/10/10	-
10	GOL	C	359	-	-	2/4/4/4	-
10	GOL	L	278	-	-	4/4/4/4	-
10	GOL	L	280	-	-	4/4/4/4	-
10	GOL	M	337	-	-	4/4/4/4	-
6	LDA	C	722	-	-	9/13/13/13	-
9	HTO	H	266	-	-	7/10/10/10	-
7	DGA	H	733	-	-	19/32/32/45	-
10	GOL	C	357	-	-	2/4/4/4	-
5	HEC	C	403	1	-	0/6/54/54	-
6	LDA	L	709	-	-	4/13/13/13	-
10	GOL	C	362	-	-	2/4/4/4	-
10	GOL	L	277	-	-	0/4/4/4	-
6	LDA	H	718	-	-	6/10/10/13	-
10	GOL	M	338	-	-	2/4/4/4	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	400	BCB	CHD-C1D	-9.59	1.38	1.53
11	L	400	BCB	CHD-C1D	-9.36	1.38	1.53
11	L	401	BCB	CHD-C1D	-9.14	1.39	1.53
11	L	400	BCB	CHC-C4B	-9.06	1.39	1.53
11	M	401	BCB	C1A-CHA	-8.91	1.40	1.54

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	400	BCB	C1D-CHD-C4C	7.14	127.58	112.37
11	L	401	BCB	C1D-CHD-C4C	7.09	127.48	112.37
11	M	401	BCB	CMB-C2B-C3B	7.04	131.77	114.29
9	L	275	HTO	O2-C2-C3	-6.93	95.50	109.72
11	L	400	BCB	C1D-CHD-C4C	6.92	127.11	112.37

There are no chirality outliers.

5 of 413 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	349	HTO	C1-C2-C3-O3
9	C	349	HTO	C1-C2-C3-C4
9	C	349	HTO	O2-C2-C3-O3
9	C	349	HTO	O2-C2-C3-C4
9	C	349	HTO	C2-C3-C4-C5

There are no ring outliers.

56 monomers are involved in 199 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	349	HTO	4	0
7	C	730	DGA	1	0
6	M	715	LDA	1	0
10	C	358	GOL	1	0
7	L	731	DGA	7	0
7	M	732	DGA	23	0
10	H	270	GOL	1	0
12	M	402	BPB	3	0
10	C	353[B]	GOL	1	0
11	L	401	BCB	4	0
10	M	337	GOL	2	0
6	M	706	LDA	3	0
10	C	359	GOL	9	0

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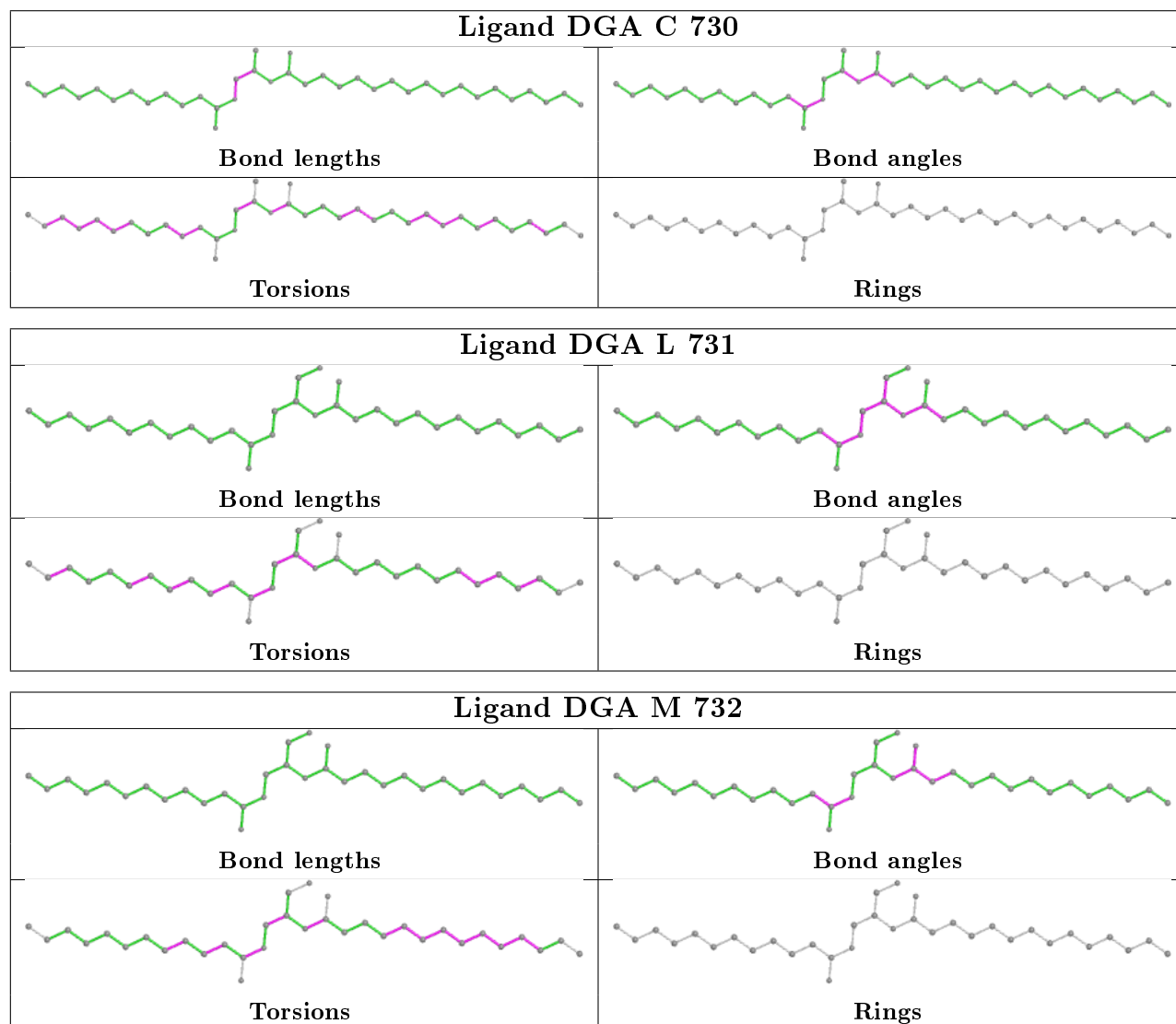
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	403	HEC	2	0
7	H	733	DGA	6	0
11	L	400	BCB	3	0
8	M	329	SO4	2	0
10	L	279	GOL	5	0
6	C	722	LDA	5	0
8	C	342	SO4	3	0
6	H	707	LDA	6	0
8	C	346	SO4	1	0
6	M	704	LDA	7	0
6	M	702	LDA	11	0
6	H	721	LDA	5	0
10	M	333	GOL	1	0
10	L	278	GOL	1	0
10	C	352	GOL	2	0
9	C	348	HTO	9	0
10	H	273	GOL	1	0
12	L	402	BPB	2	0
6	H	718	LDA	8	0
13	L	503	UQ9	6	0
6	H	719	LDA	2	0
8	C	337	SO4	3	0
10	C	354	GOL	1	0
6	L	720	LDA	5	0
8	C	338	SO4	3	0
16	M	600	NS5	2	0
8	H	261	SO4	6	0
8	H	264	SO4	1	0
11	M	401	BCB	3	0
9	H	268	HTO	2	0
6	L	703	LDA	5	0
11	M	400	BCB	9	0
13	L	502	UQ9	31	0
6	C	712	LDA	3	0
8	H	262[A]	SO4	1	0
8	H	262[B]	SO4	1	0
10	H	274	GOL	2	0
10	M	335	GOL	2	0
8	C	344	SO4	2	0
10	L	276	GOL	3	0
6	H	701	LDA	4	0
10	C	361	GOL	1	0

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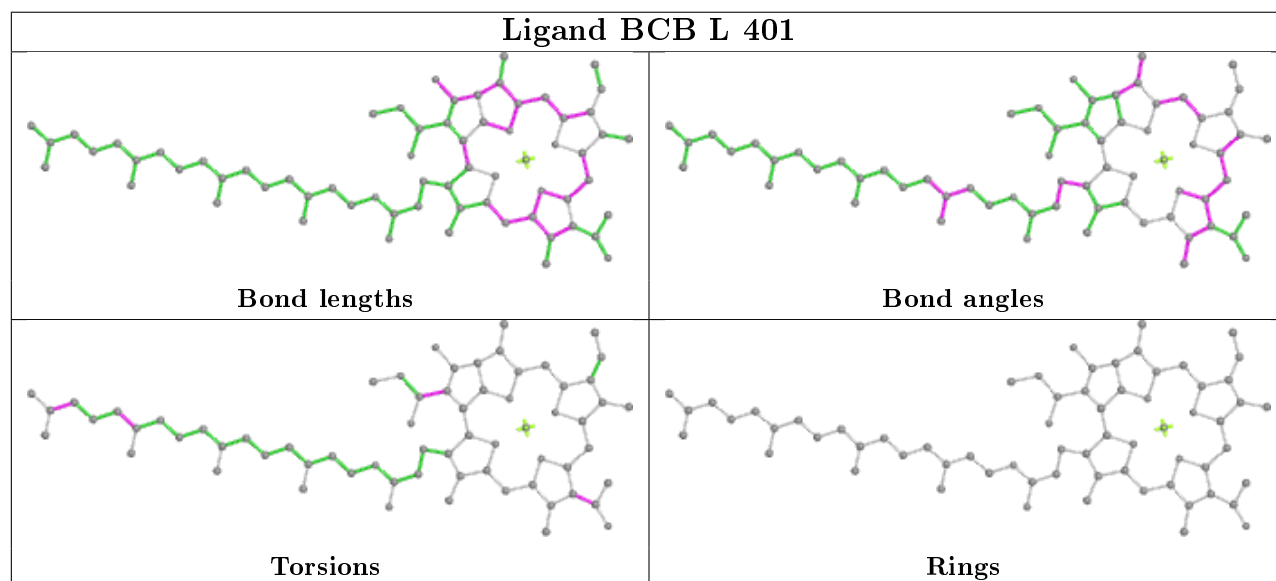
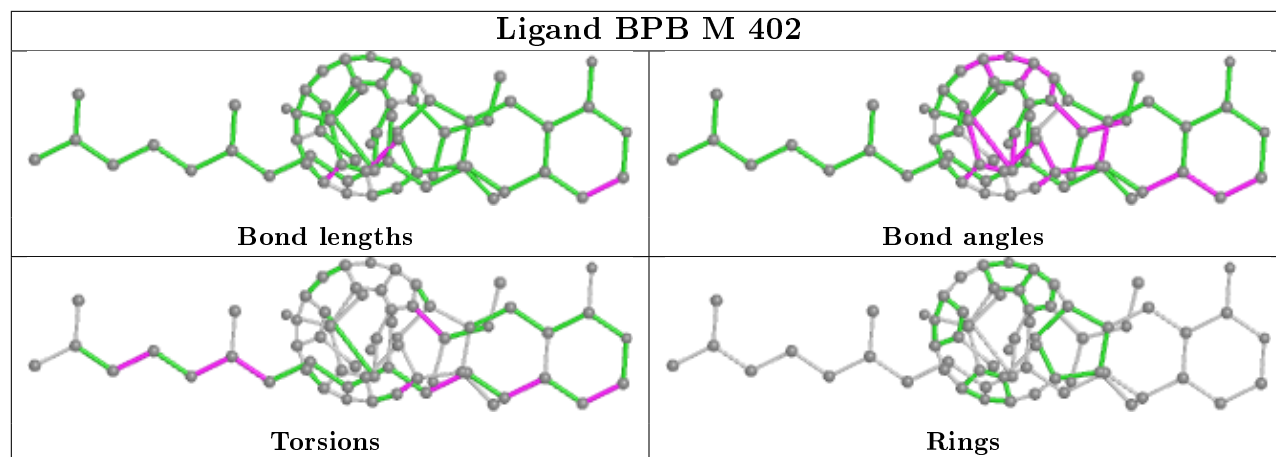
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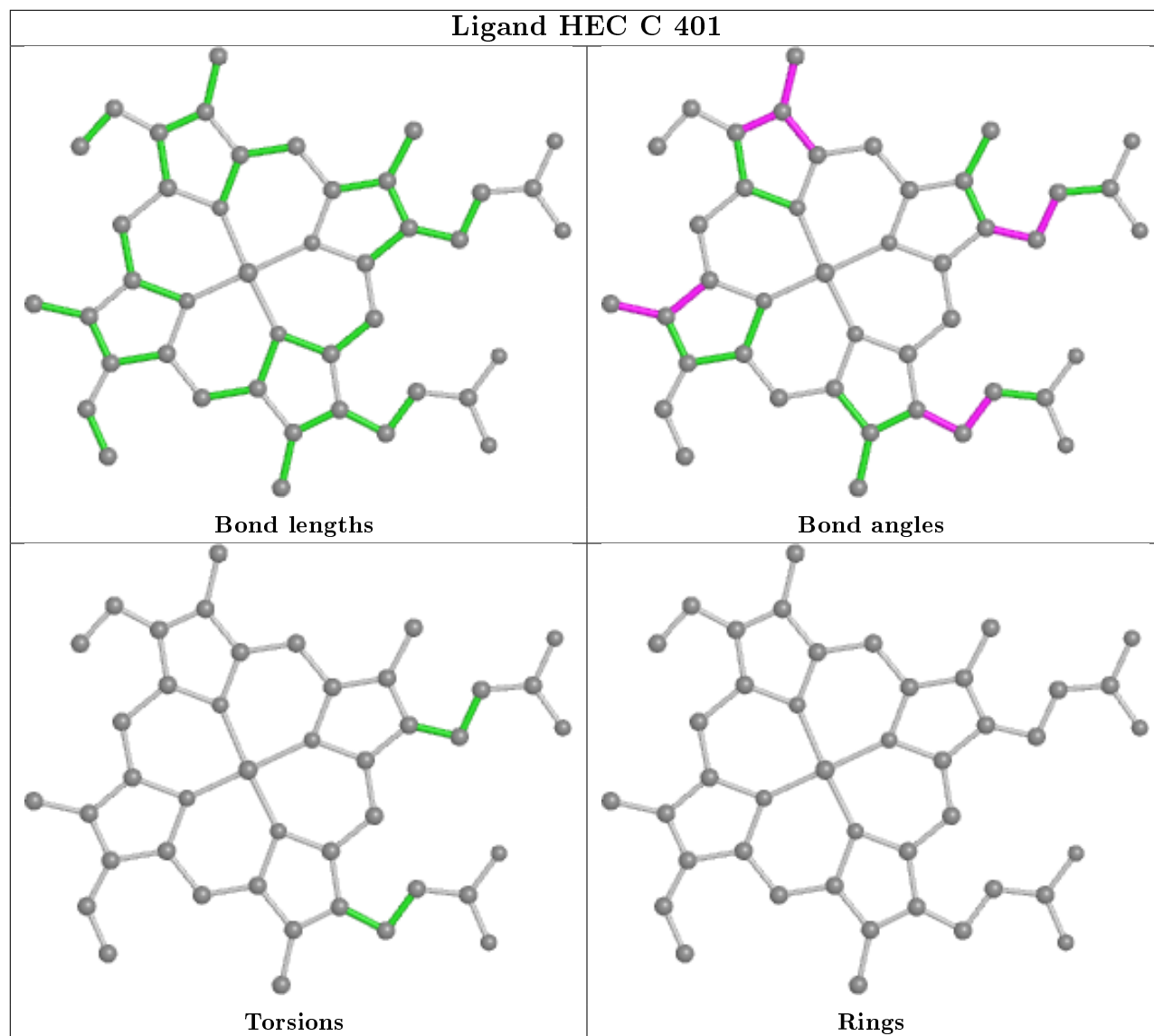
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	H	267	HTO	1	0

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 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.

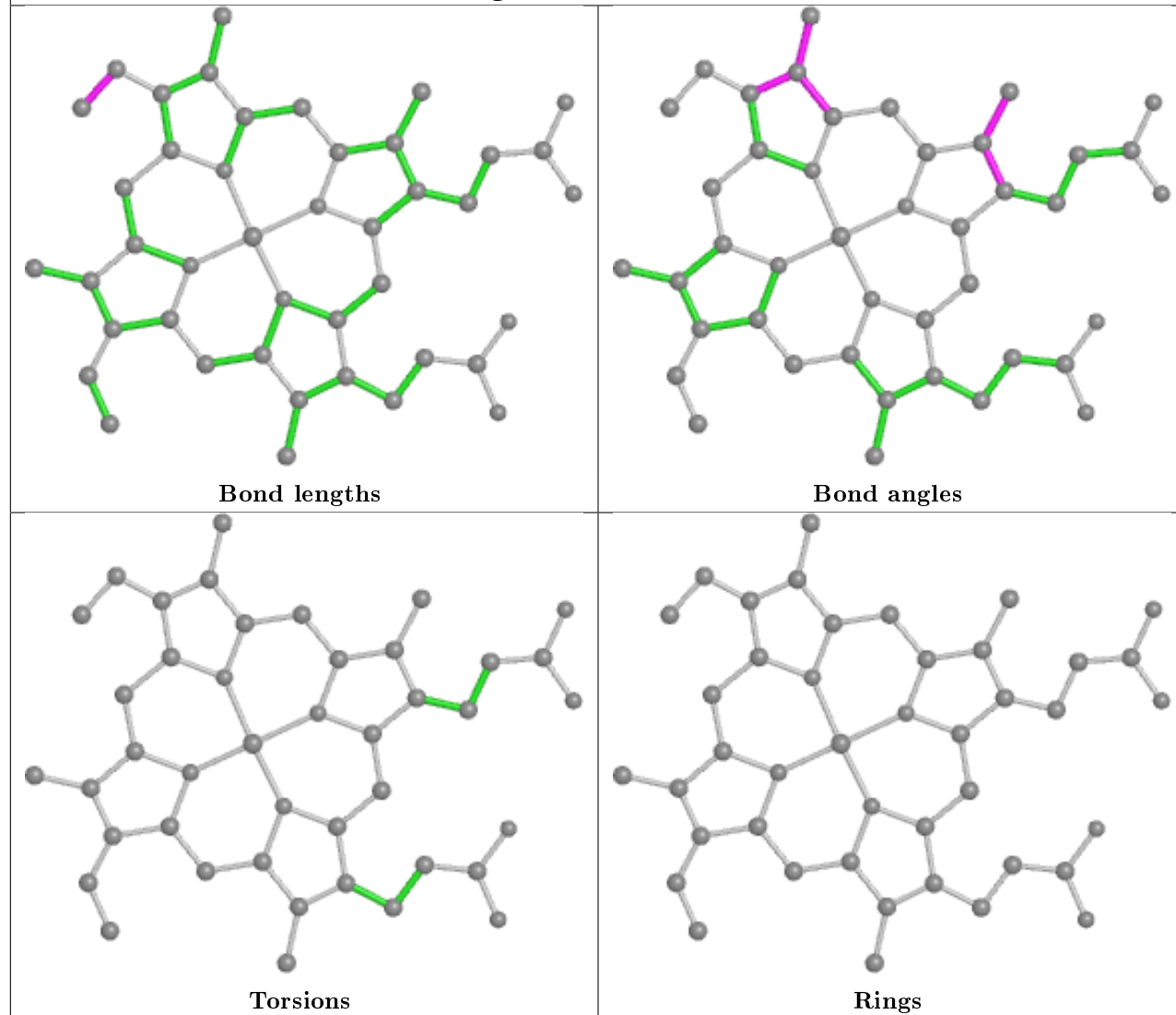




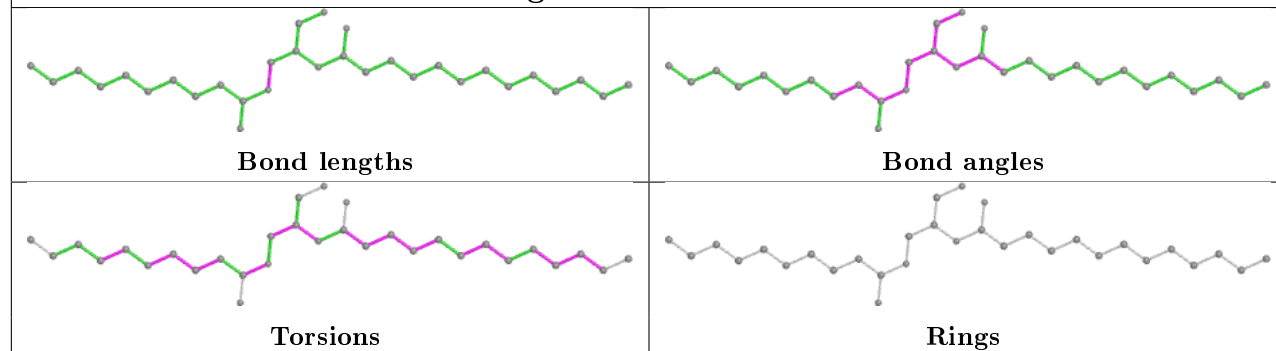


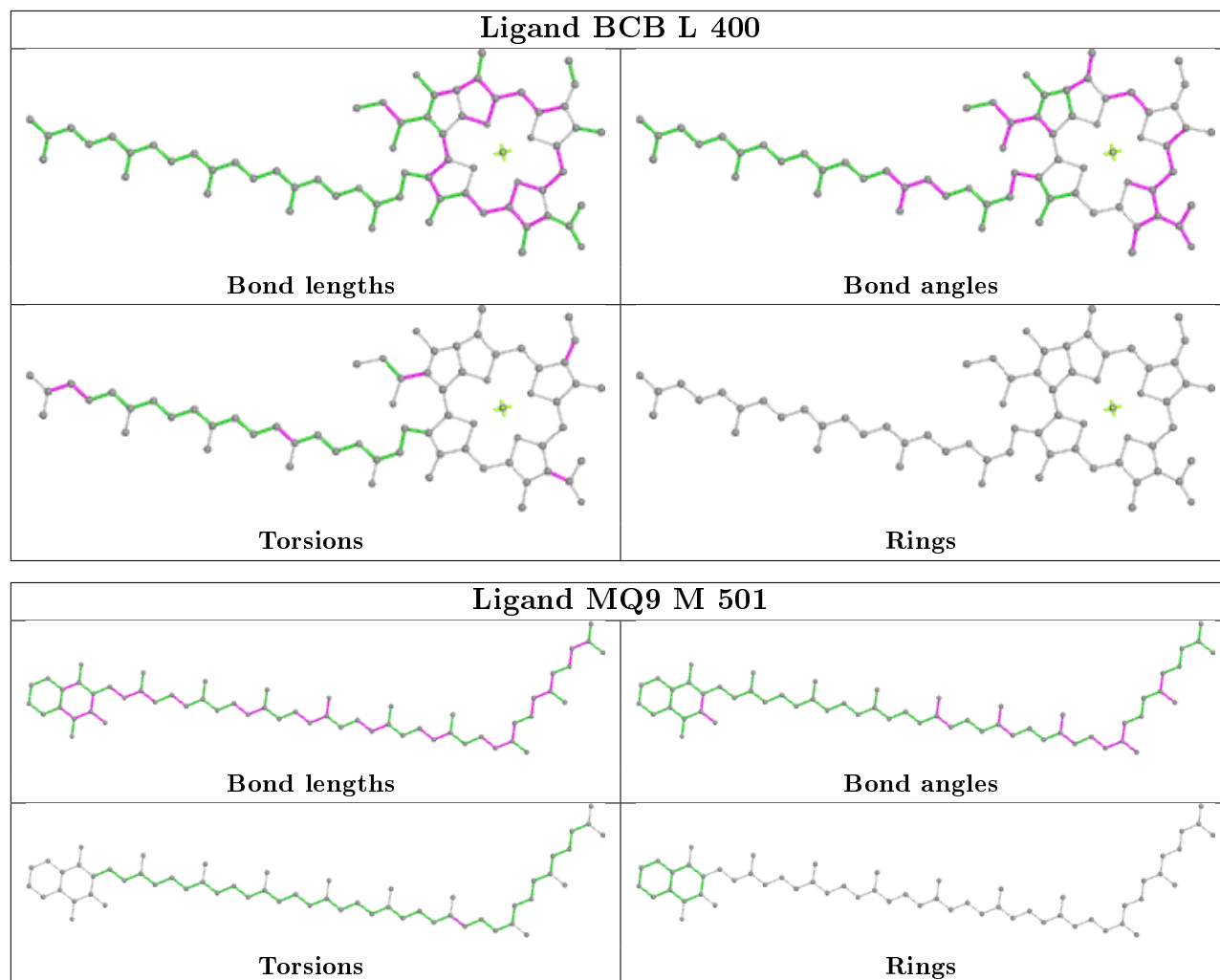


## Ligand HEC C 403

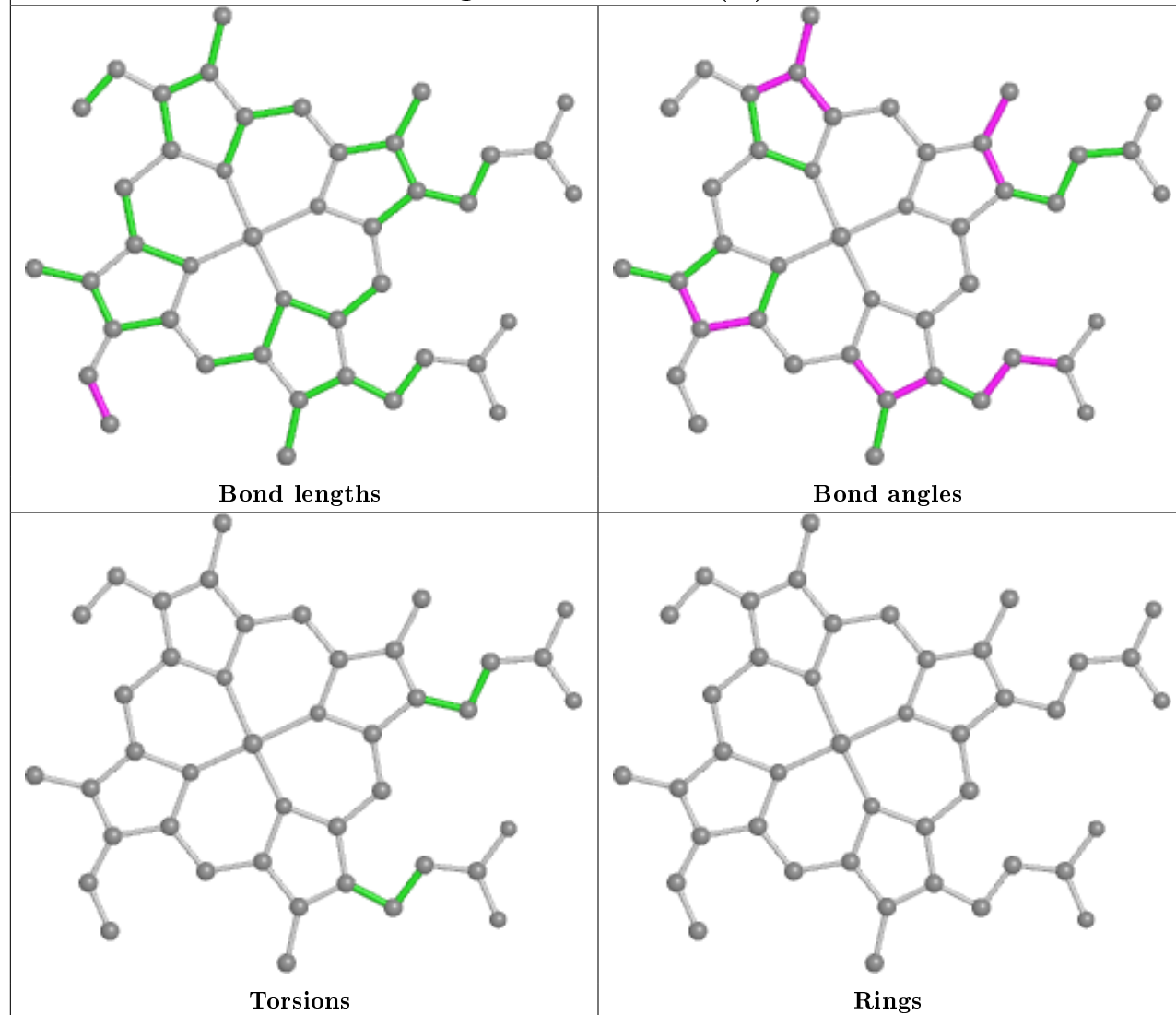


## Ligand DGA H 733

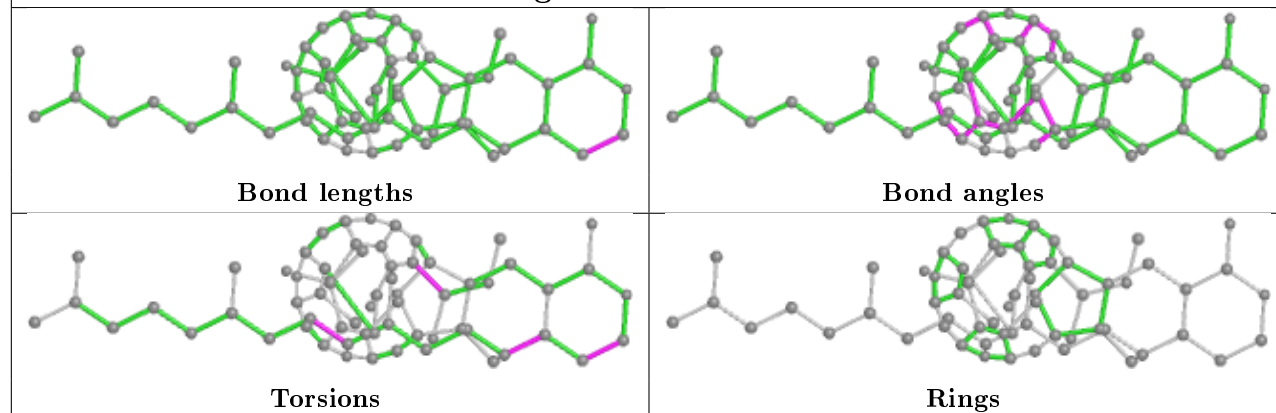


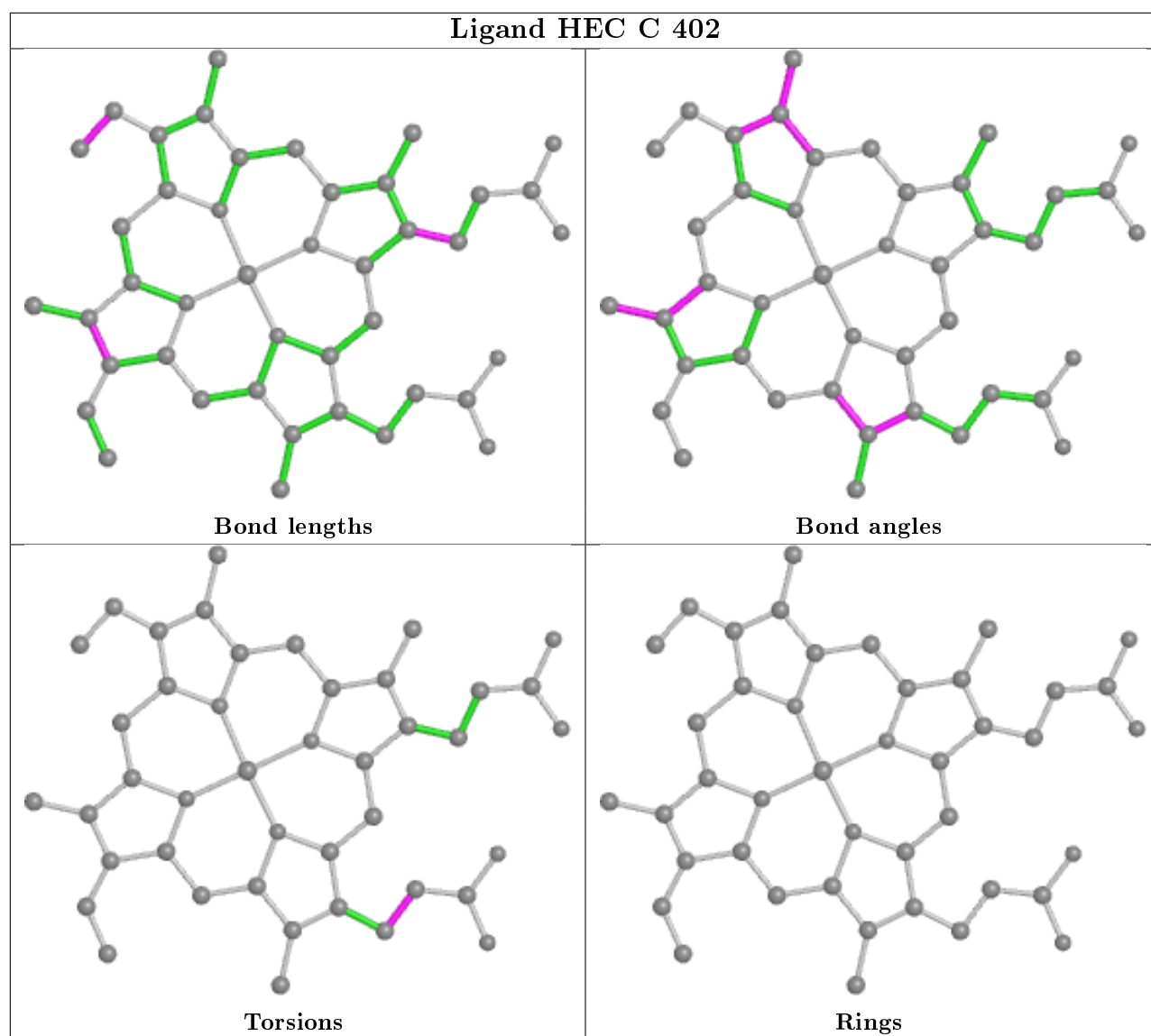


## Ligand HEC C 404 (A)

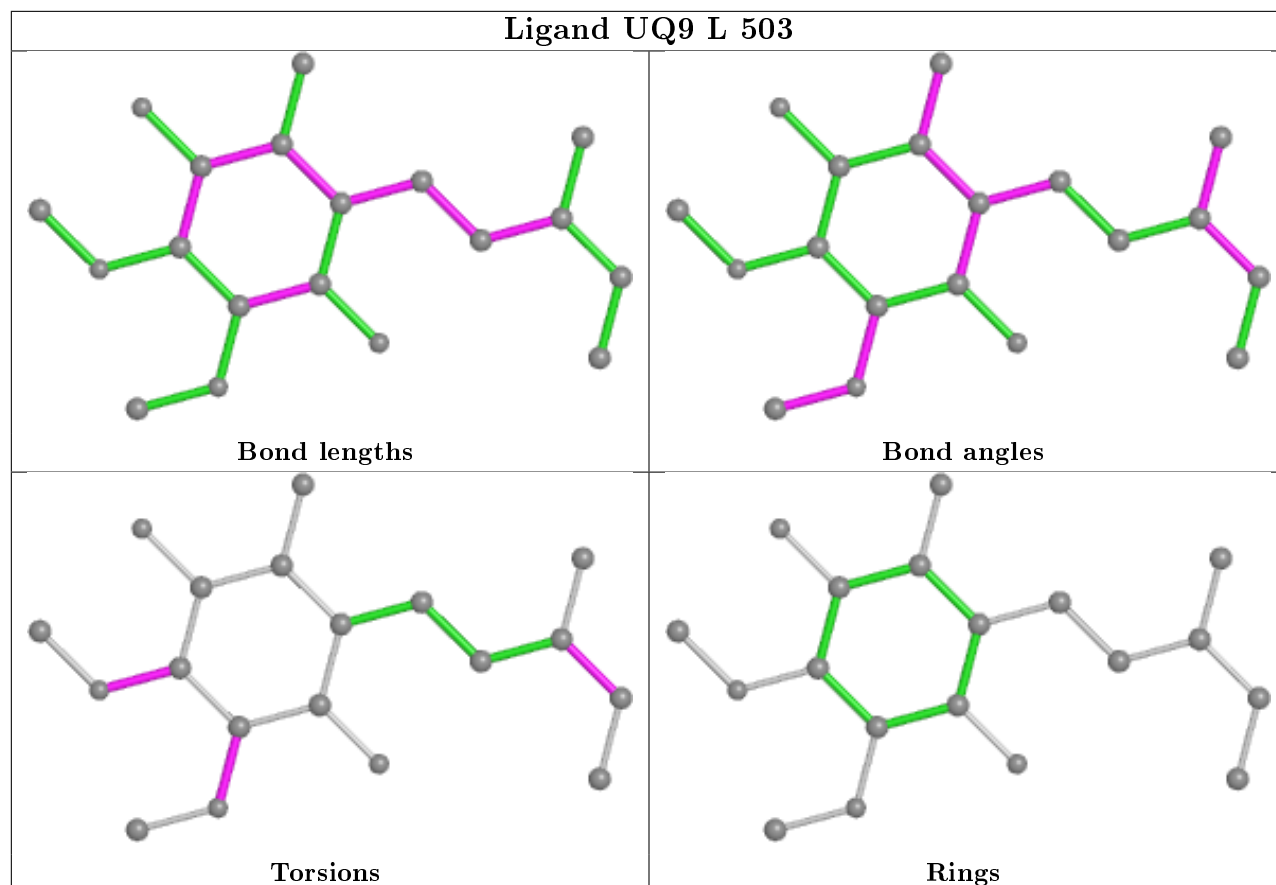


## Ligand BPB L 402

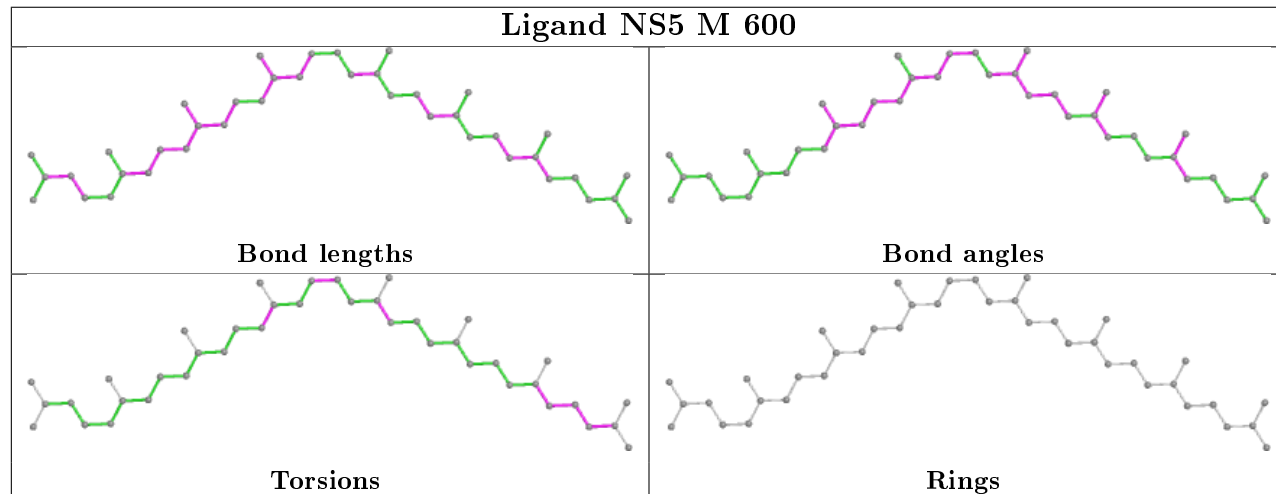


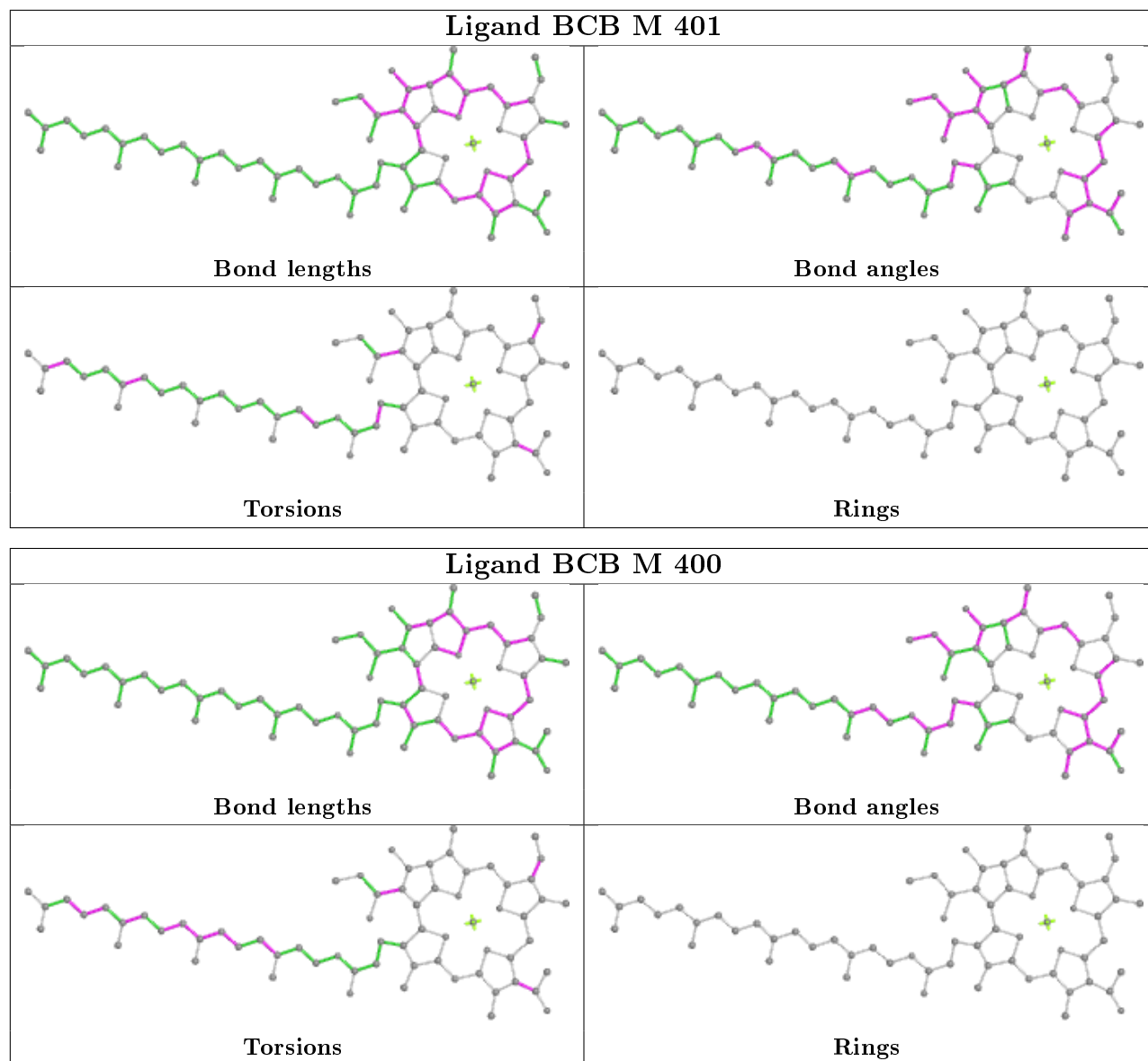


## Ligand UQ9 L 503



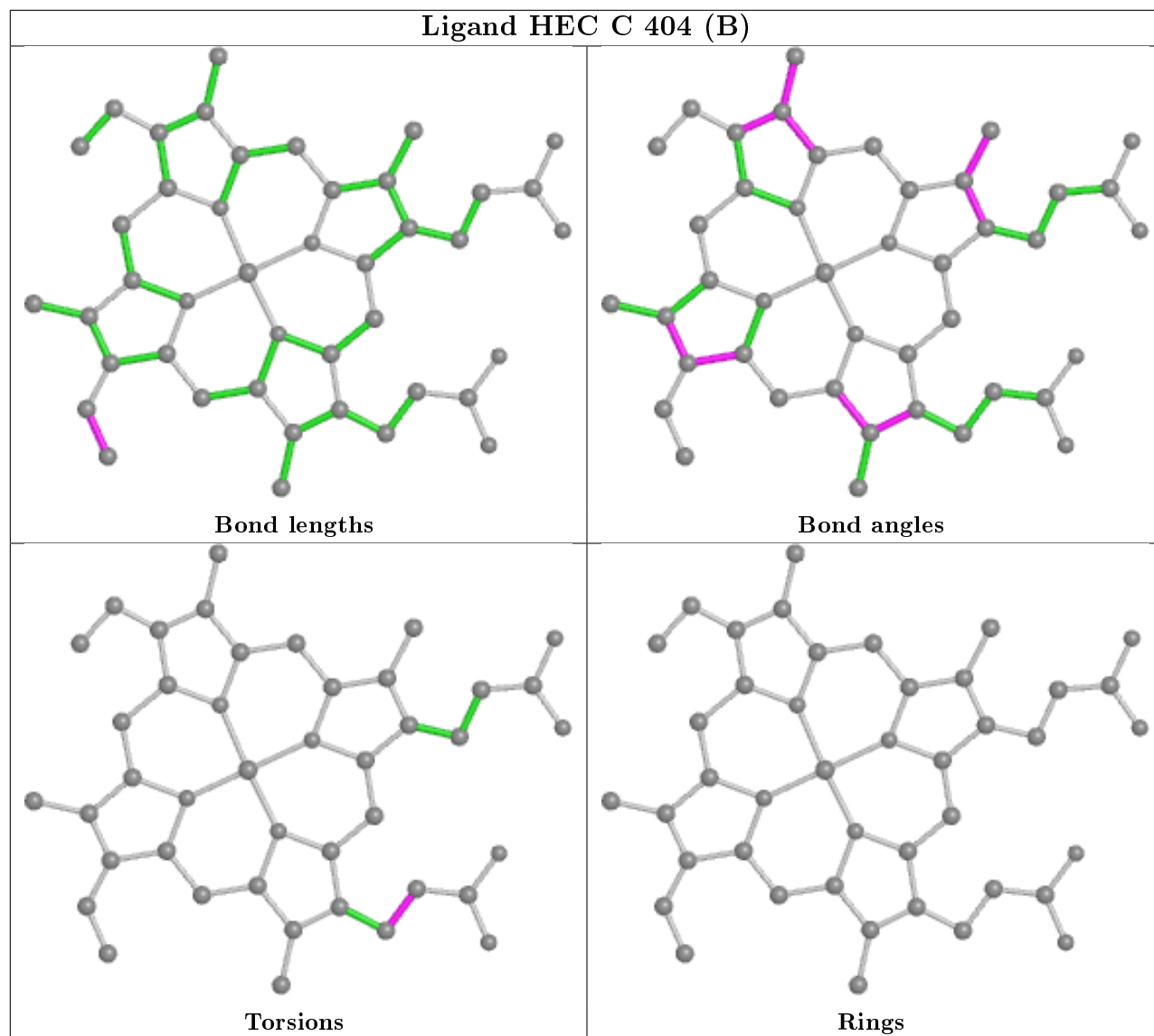
## Ligand NS5 M 600

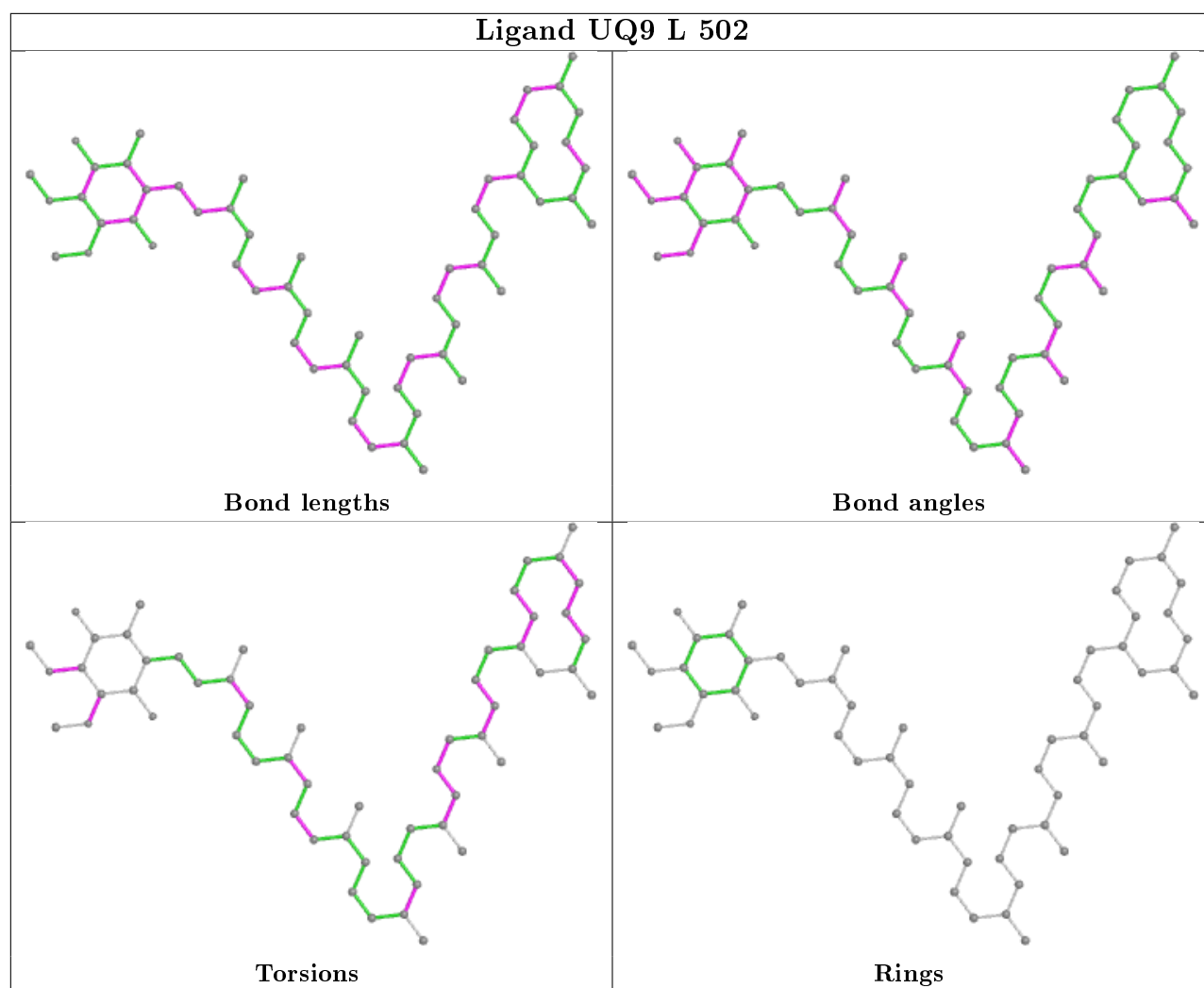






## Ligand HEC C 404 (B)





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	334/356 (93%)	0.30	24 (7%) 15 17	38, 49, 70, 123	0
2	H	249/258 (96%)	0.43	29 (11%) 4 5	42, 58, 85, 120	1 (0%)
3	L	273/273 (100%)	0.28	17 (6%) 20 23	37, 47, 62, 88	0
4	M	322/323 (99%)	0.52	49 (15%) 2 2	38, 49, 70, 91	0
All	All	1178/1210 (97%)	0.38	119 (10%) 7 8	37, 50, 73, 123	1 (0%)

The worst 5 of 119 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	333	ALA	8.1
1	C	334	ALA	7.9
4	M	37	TRP	7.8
3	L	51	TYR	5.9
2	H	7	ALA	5.7

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	CSO	M	160	7/8	0.90	0.13	46,49,73,77	0
2	FME	H	1[A]	10/11	0.93	0.13	50,54,59,61	10
2	FME	H	1[B]	10/11	0.93	0.13	49,52,54,64	10

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	LDA	M	715	16/16	-0.06	0.47	63,77,84,85	16
10	GOL	M	333	6/6	0.36	0.30	70,70,73,78	6
7	DGA	L	731	33/44	0.42	0.33	47,69,78,82	33
6	LDA	L	709	16/16	0.45	0.36	49,67,91,92	16
6	LDA	L	720	16/16	0.48	0.41	58,70,76,78	16
13	UQ9	L	503	19/58	0.48	0.38	49,70,84,86	19
6	LDA	M	706	16/16	0.49	0.53	61,65,73,73	16
8	SO4	H	264	5/5	0.52	0.36	63,65,67,73	5
13	UQ9	L	502	58/58	0.52	1.40	38,58,69,73	58
6	LDA	M	702	16/16	0.53	0.79	52,56,62,65	16
6	LDA	M	704	16/16	0.56	0.39	64,67,86,88	16
9	HTO	C	348	10/10	0.57	0.61	52,62,68,74	10
10	GOL	H	277	6/6	0.58	0.35	65,69,71,72	6
7	DGA	M	732	34/44	0.59	0.27	58,72,80,84	34
10	GOL	H	279	6/6	0.59	0.25	80,86,88,91	6
6	LDA	C	712	16/16	0.60	0.31	56,62,74,74	16
7	DGA	C	730	37/44	0.64	0.31	58,76,94,99	37
10	GOL	H	270	6/6	0.66	0.32	63,69,69,71	6
6	LDA	H	707	16/16	0.67	0.45	53,67,77,85	16
10	GOL	M	337	6/6	0.67	0.29	56,64,66,69	6
9	HTO	H	268	10/10	0.69	0.41	71,76,80,80	10
6	LDA	H	718	13/16	0.69	0.27	55,61,79,84	13
10	GOL	M	338	6/6	0.70	0.26	67,71,72,73	6
10	GOL	H	273	6/6	0.70	0.32	71,75,79,80	6
8	SO4	C	345	5/5	0.70	0.37	71,79,83,86	5
8	SO4	M	327	5/5	0.71	0.26	79,82,83,86	5
10	GOL	H	272	6/6	0.71	0.40	66,72,75,76	6
10	GOL	C	360	6/6	0.72	0.26	71,73,75,78	6
8	SO4	H	265	5/5	0.72	0.38	71,74,75,76	5
9	HTO	C	349	10/10	0.72	0.22	59,68,74,75	10
9	HTO	H	267	10/10	0.72	0.26	74,77,89,91	10
6	LDA	M	705	16/16	0.72	0.22	63,70,77,78	16

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	SO4	C	346	5/5	0.73	0.32	73,73,82,82	5
7	DGA	H	733	31/44	0.74	0.32	45,62,78,79	31
6	LDA	C	722	16/16	0.74	0.40	54,61,65,65	16
10	GOL	C	354	6/6	0.74	0.21	57,68,78,86	6
10	GOL	C	353[B]	6/6	0.74	0.33	42,56,71,73	6
10	GOL	C	353[A]	6/6	0.74	0.33	44,55,59,61	6
10	GOL	H	276	6/6	0.75	0.20	71,79,85,85	6
8	SO4	M	330	5/5	0.75	0.67	58,64,67,70	5
6	LDA	L	703	16/16	0.75	0.68	56,61,69,72	16
10	GOL	C	365	6/6	0.76	0.27	59,60,61,65	6
16	NS5	M	600	40/40	0.76	0.24	53,76,118,126	0
10	GOL	M	335	6/6	0.77	0.46	50,57,62,64	6
10	GOL	C	362	6/6	0.78	0.22	70,75,75,75	6
10	GOL	C	361	6/6	0.79	0.46	66,71,76,80	6
10	GOL	M	334	6/6	0.79	0.53	63,65,67,68	6
8	SO4	C	340	5/5	0.79	0.17	72,73,77,79	5
10	GOL	C	363	6/6	0.80	0.30	72,75,78,78	6
10	GOL	M	336	6/6	0.81	0.17	81,82,84,87	6
8	SO4	C	347	5/5	0.82	0.15	71,73,76,77	5
10	GOL	H	269	6/6	0.82	0.20	68,76,79,83	6
10	GOL	C	359	6/6	0.82	0.72	47,54,60,68	6
10	GOL	C	355	6/6	0.82	0.22	67,70,71,71	6
9	HTO	L	274	10/10	0.82	0.28	58,67,76,80	10
10	GOL	C	351	6/6	0.83	0.29	51,58,65,67	6
9	HTO	H	266	10/10	0.83	0.19	60,68,76,78	0
10	GOL	L	281	6/6	0.84	0.22	60,62,66,67	6
10	GOL	M	339	6/6	0.84	0.21	37,53,62,67	6
6	LDA	H	719	16/16	0.84	0.20	55,61,81,83	16
6	LDA	L	708	16/16	0.84	0.18	47,58,66,76	0
10	GOL	C	357	6/6	0.85	0.15	69,69,76,78	6
10	GOL	H	271	6/6	0.86	0.28	54,63,65,75	6
10	GOL	L	279	6/6	0.86	0.39	48,50,60,61	6
14	MQ9	M	501	58/58	0.86	0.20	38,46,92,98	0
6	LDA	H	701	16/16	0.86	0.25	47,57,69,70	0
9	HTO	L	275	10/10	0.86	0.23	64,69,72,74	10
10	GOL	L	280	6/6	0.87	0.34	60,65,70,74	6
10	GOL	H	274	6/6	0.87	0.32	59,71,78,81	6
10	GOL	L	282	6/6	0.88	0.20	60,67,75,75	6
8	SO4	C	338	5/5	0.88	0.17	66,66,73,74	5
10	GOL	H	278	6/6	0.88	0.16	75,77,78,79	6
8	SO4	H	261	5/5	0.88	0.21	46,55,72,75	5
10	GOL	L	278	6/6	0.89	0.27	46,54,56,58	6

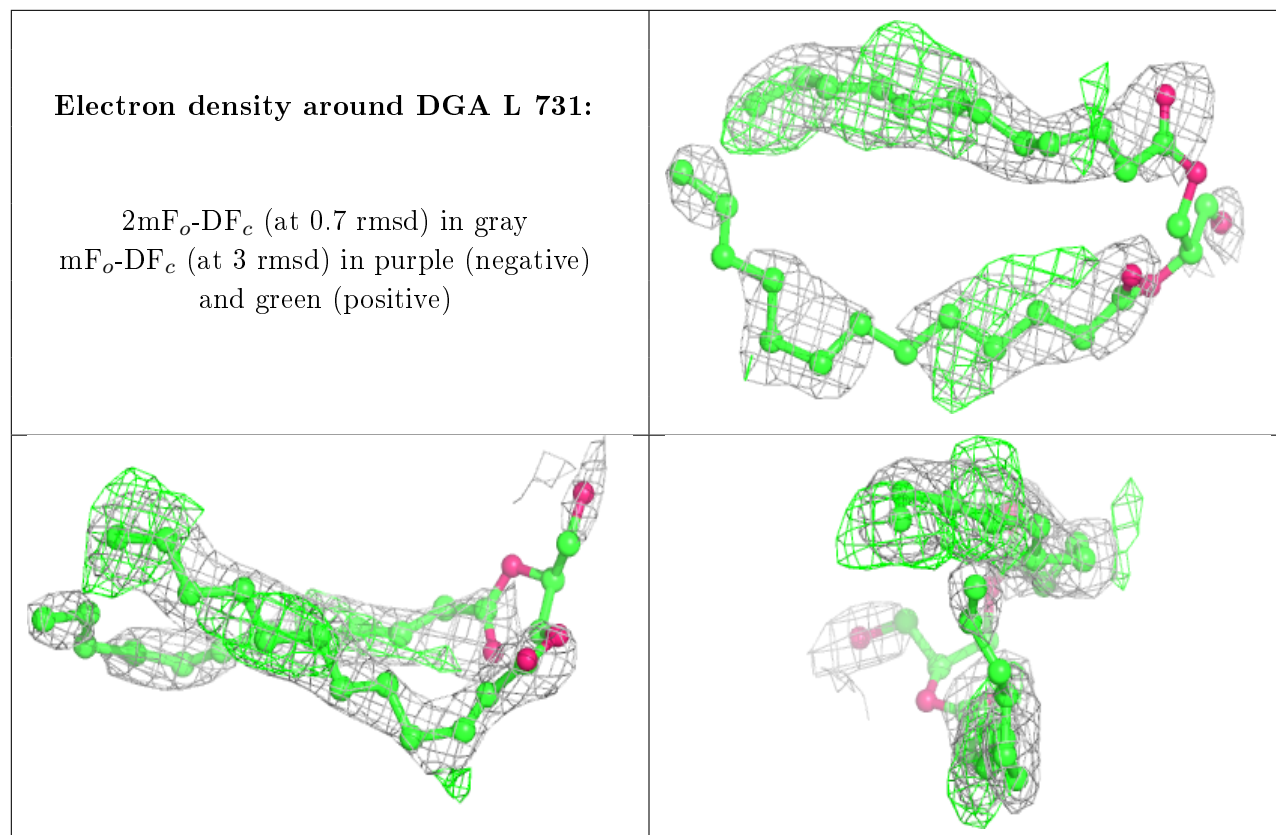
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	GOL	C	364	6/6	0.89	0.17	53,55,61,62	6
9	HTO	M	332	10/10	0.89	0.85	52,59,68,70	10
10	GOL	C	358	6/6	0.90	0.14	48,64,67,68	6
10	GOL	H	275	6/6	0.91	0.18	51,66,74,75	6
8	SO4	H	262[B]	5/5	0.92	0.20	58,63,71,72	5
10	GOL	C	352	6/6	0.92	0.21	37,56,61,61	6
10	GOL	L	277	6/6	0.92	0.41	55,61,63,65	6
8	SO4	C	344	5/5	0.92	0.22	61,69,77,79	5
10	GOL	L	276	6/6	0.92	0.14	55,56,58,60	0
8	SO4	C	337	5/5	0.92	0.16	70,73,78,84	5
8	SO4	H	262[A]	5/5	0.92	0.20	55,56,67,71	5
8	SO4	C	343	5/5	0.92	0.20	66,66,70,74	5
8	SO4	C	342	5/5	0.92	0.23	47,56,60,62	5
8	SO4	M	329	5/5	0.93	0.15	62,73,75,76	5
10	GOL	C	350	6/6	0.93	0.38	49,56,58,60	0
10	GOL	C	356	6/6	0.93	0.26	60,69,74,75	0
8	SO4	H	260	5/5	0.94	0.13	82,82,83,88	5
8	SO4	C	341	5/5	0.94	0.24	62,70,77,79	5
8	SO4	M	331	5/5	0.94	0.27	75,77,81,85	5
8	SO4	C	339	5/5	0.95	0.15	62,67,67,69	5
11	BCB	M	400	66/66	0.95	0.15	37,46,109,115	0
6	LDA	H	721	16/16	0.95	0.13	53,63,80,87	16
11	BCB	M	401	66/66	0.95	0.17	33,39,62,67	0
12	BPB	L	402	65/65	0.96	0.15	37,41,51,53	0
5	HEC	C	402	43/43	0.96	0.10	41,46,55,61	0
8	SO4	M	328	5/5	0.96	0.19	59,65,67,71	5
12	BPB	M	402	65/65	0.96	0.11	39,46,101,105	0
11	BCB	L	400	66/66	0.96	0.18	34,39,49,57	0
11	BCB	L	401	66/66	0.96	0.17	35,39,69,79	0
5	HEC	C	403	43/43	0.97	0.15	36,40,43,49	0
5	HEC	C	404[B]	43/43	0.97	0.12	38,41,46,49	12
5	HEC	C	401	43/43	0.97	0.09	46,52,61,67	0
5	HEC	C	404[A]	43/43	0.97	0.12	38,41,49,51	12
8	SO4	H	259	5/5	0.98	0.08	64,65,69,71	5
8	SO4	M	326	5/5	0.98	0.24	57,65,67,67	5
8	SO4	M	325	5/5	0.99	0.18	69,70,77,82	0
15	FE2	M	500	1/1	0.99	0.12	42,42,42,42	0
8	SO4	H	263	5/5	0.99	0.15	47,50,52,52	5
8	SO4	M	324	5/5	1.00	0.11	54,54,60,71	0

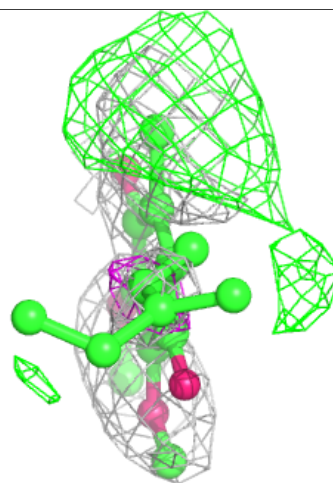
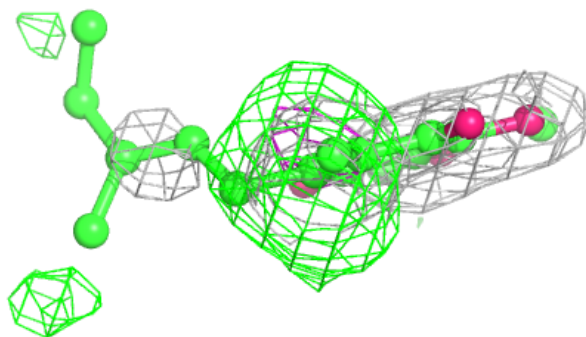
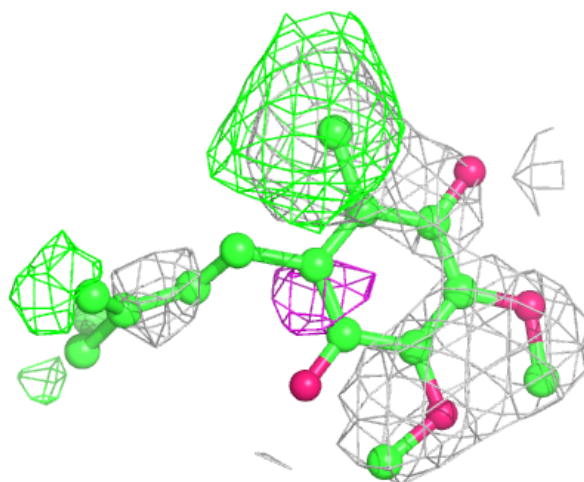
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.



**Electron density around UQ9 L 503:**

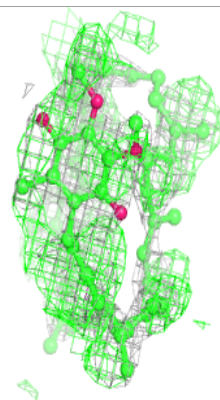
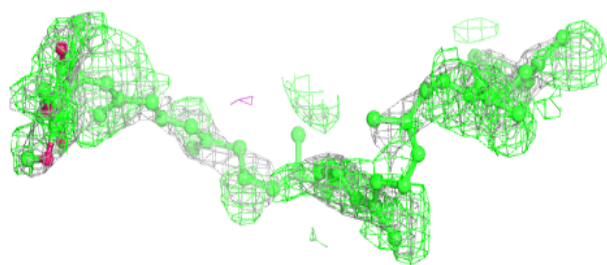
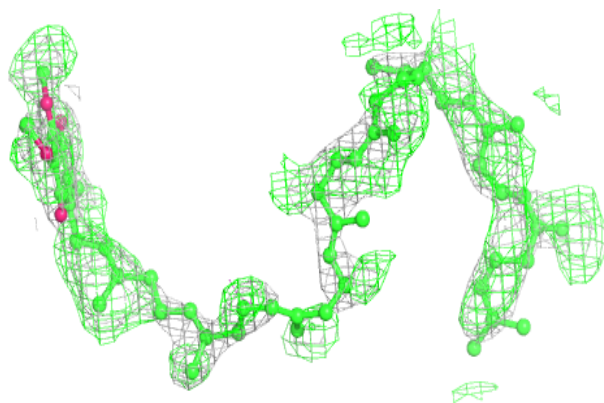
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





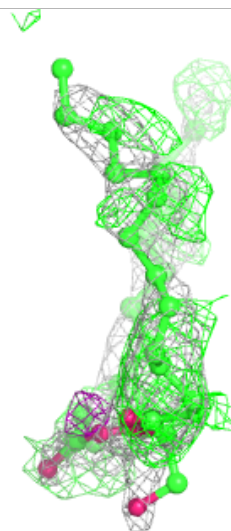
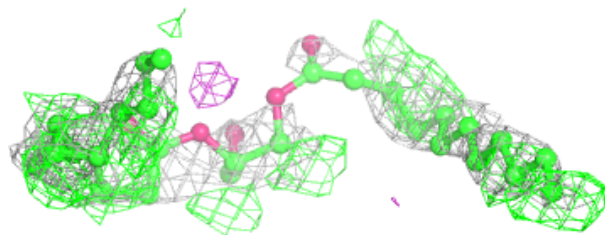
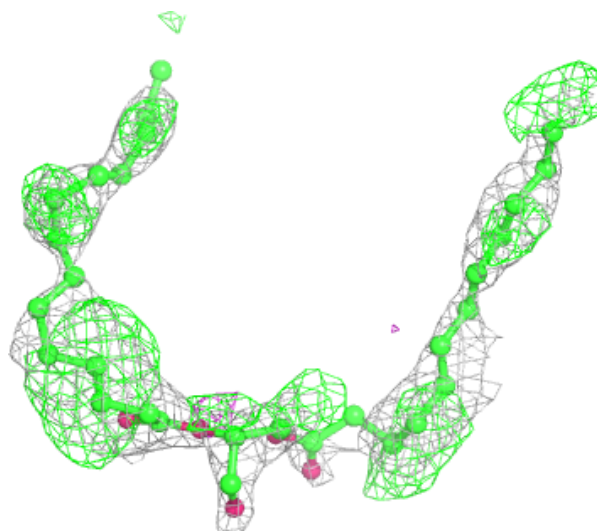
**Electron density around UQ9 L 502:**

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



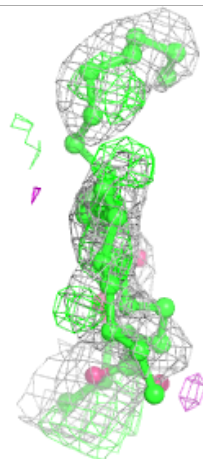
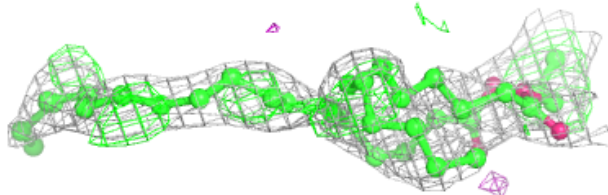
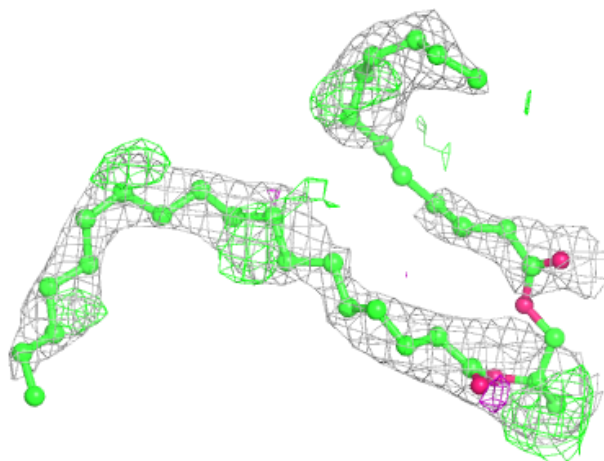
**Electron density around DGA M 732:**

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



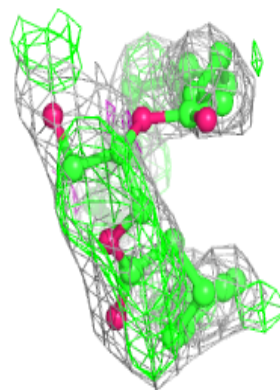
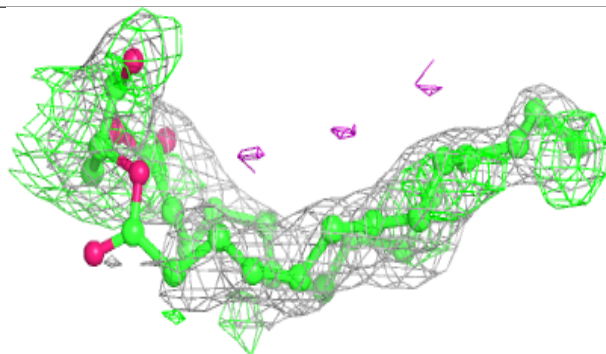
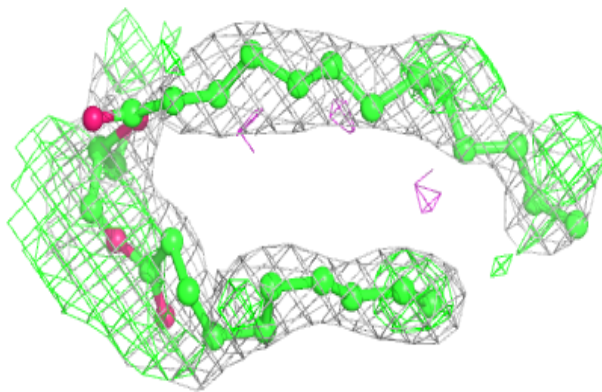
**Electron density around DGA C 730:**

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

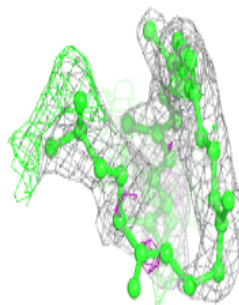
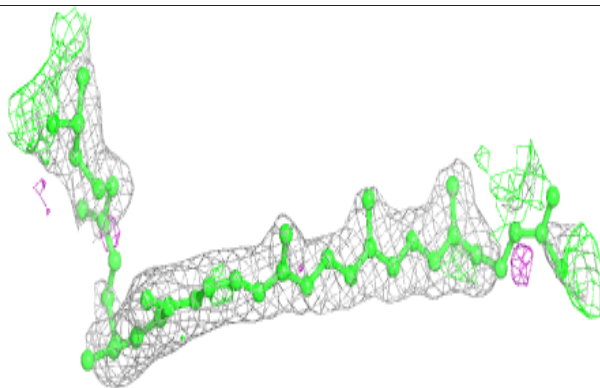
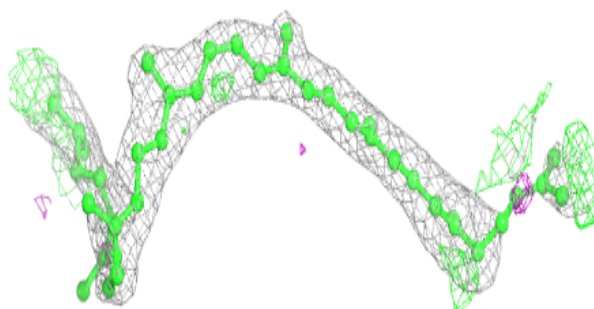


**Electron density around DGA H 733:**

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

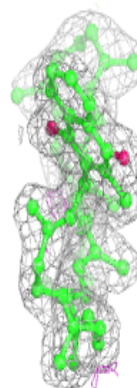
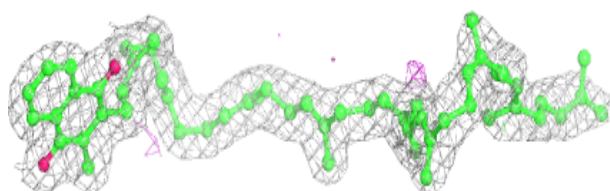
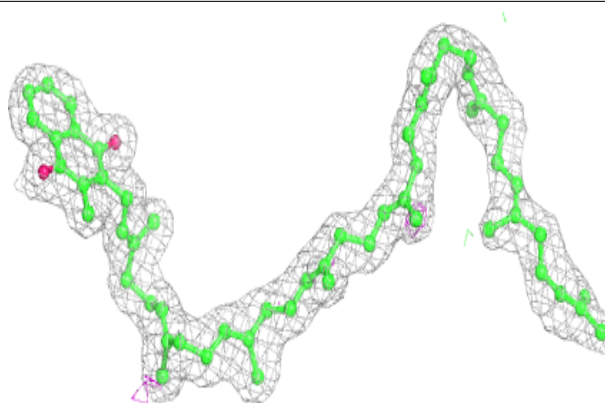
**Electron density around NS5 M 600:**

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

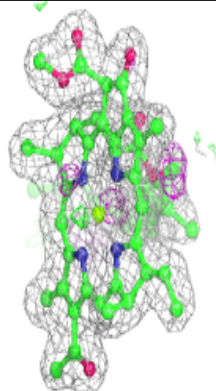
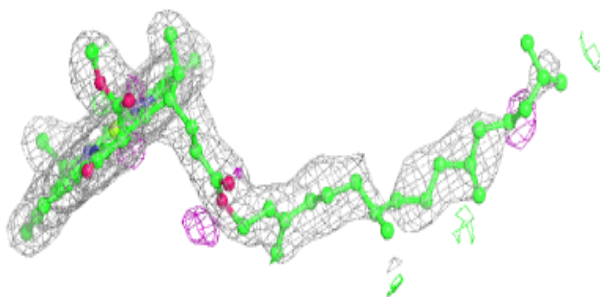
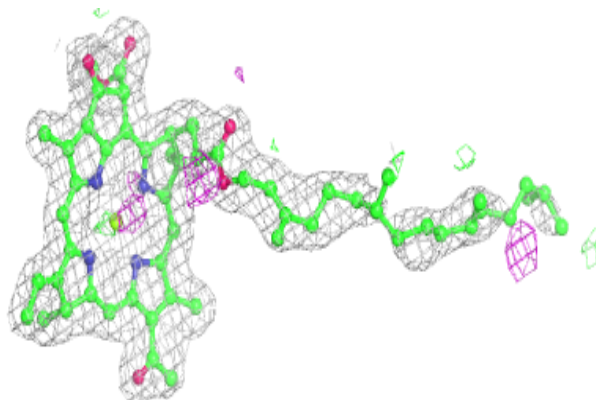


**Electron density around MQ9 M 501:**

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

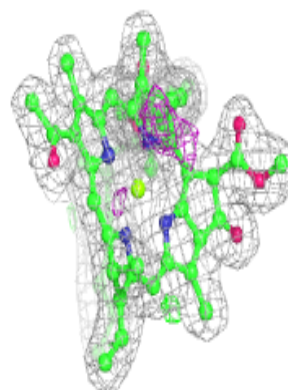
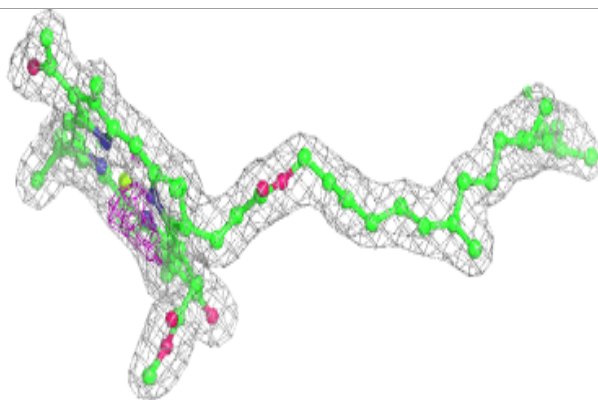
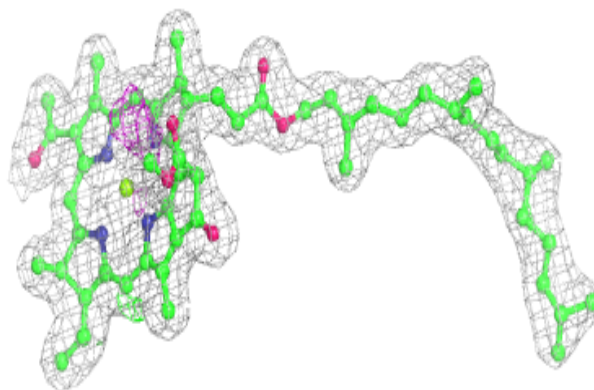
**Electron density around BCB M 400:**

$2mF_o-DF_c$  (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:**

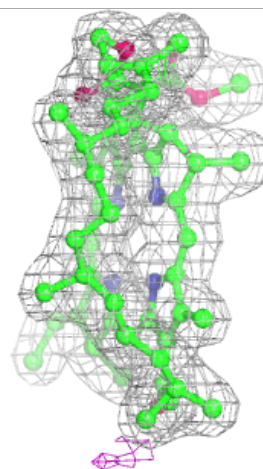
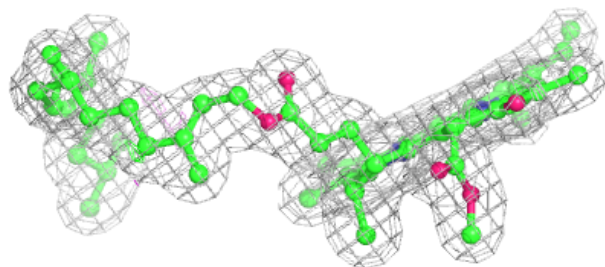
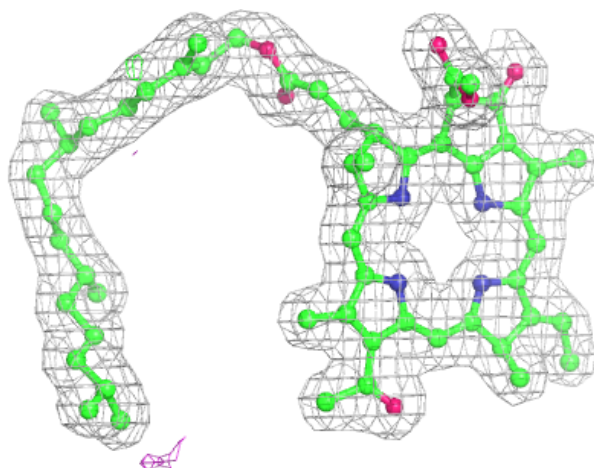
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





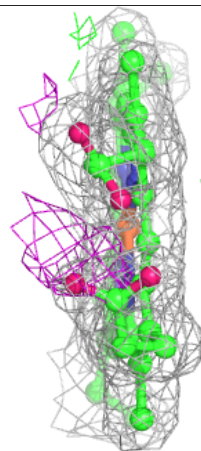
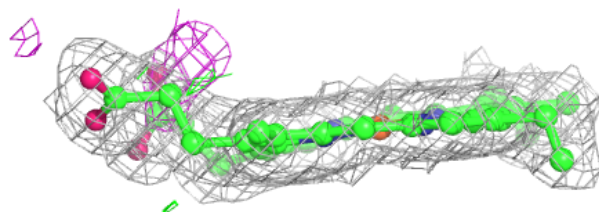
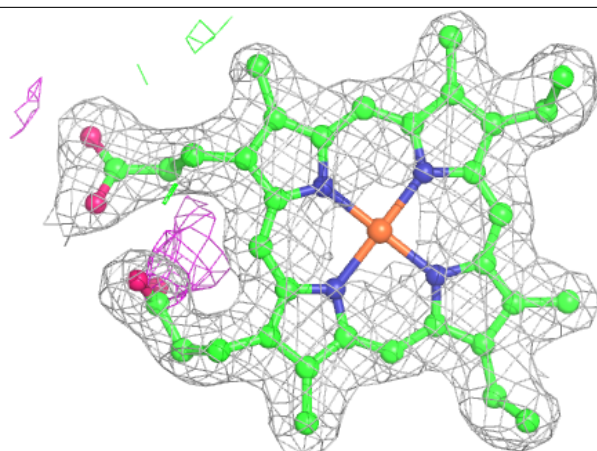
**Electron density around BPB L 402:**

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

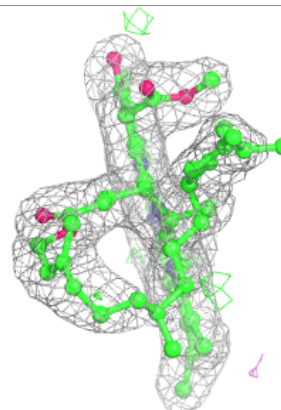
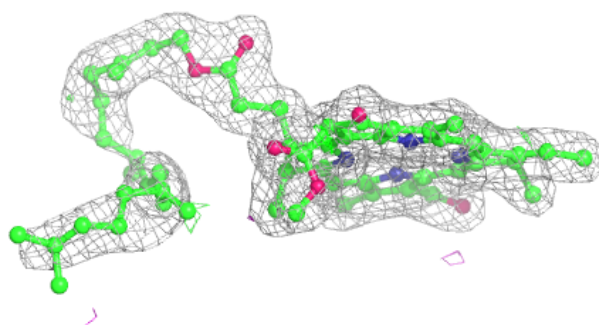
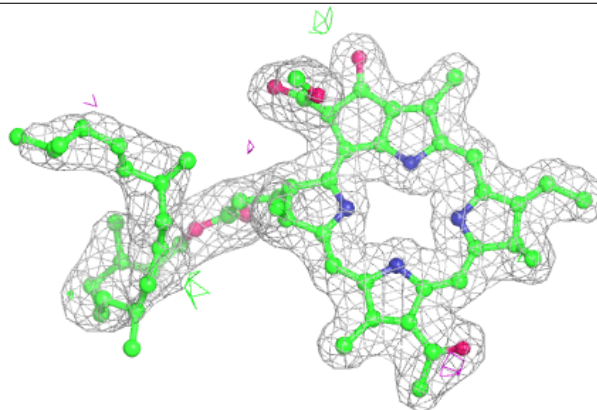


**Electron density around HEC C 402:**

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

**Electron density around BPB M 402:**

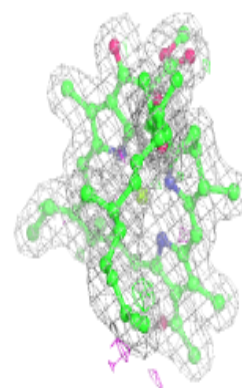
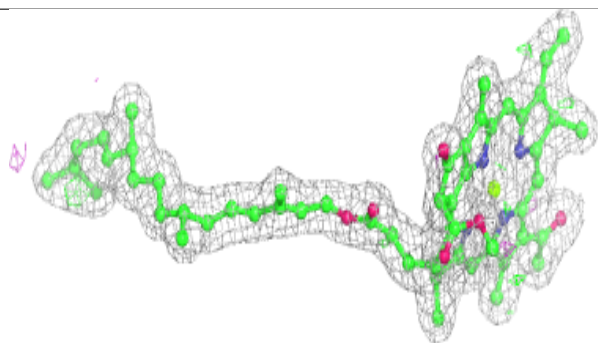
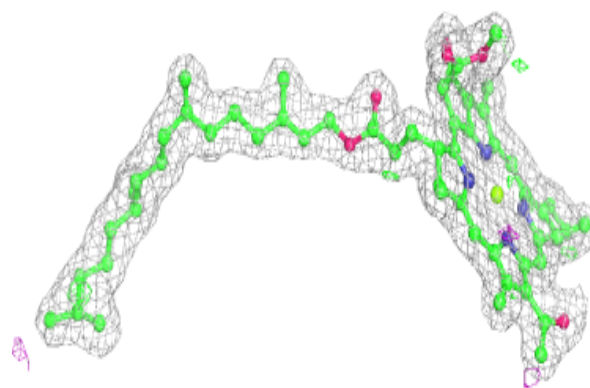
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



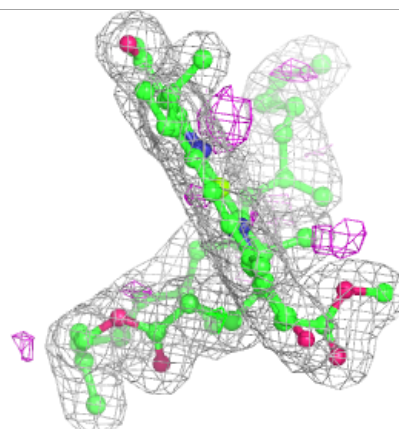
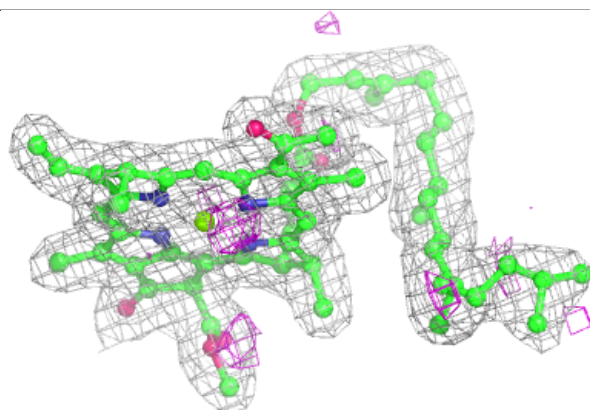
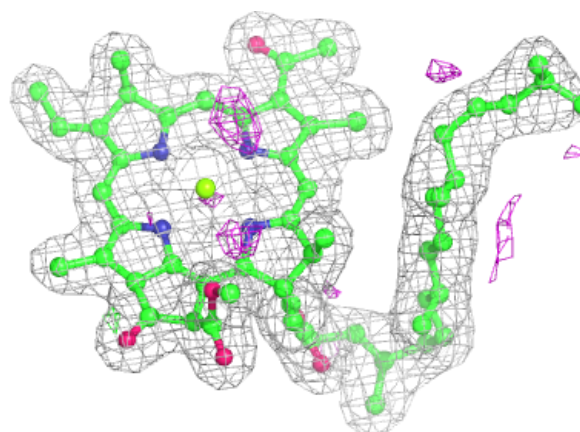


**Electron density around BCB L 400:**

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

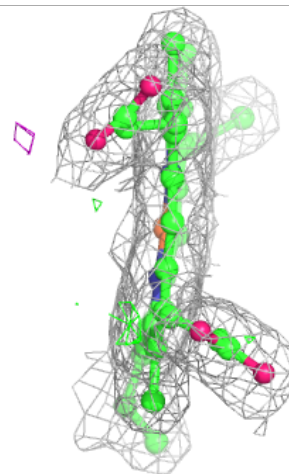
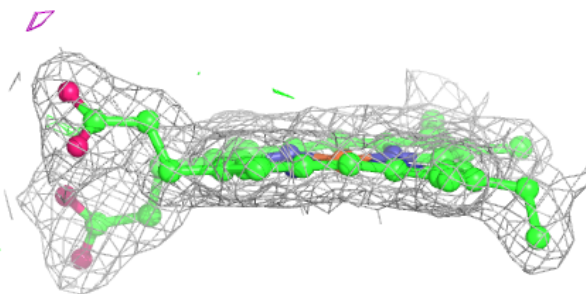
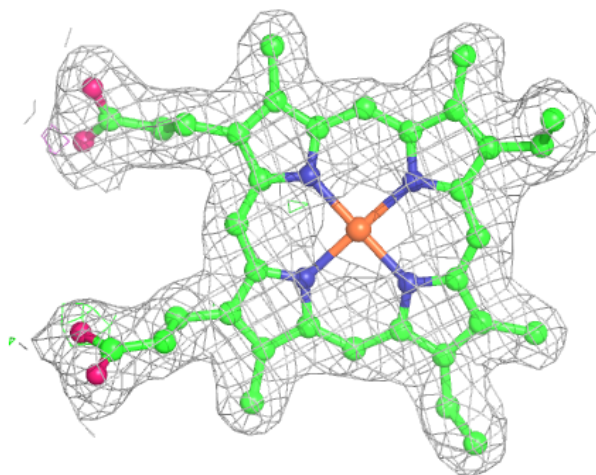
**Electron density around BCB L 401:**

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



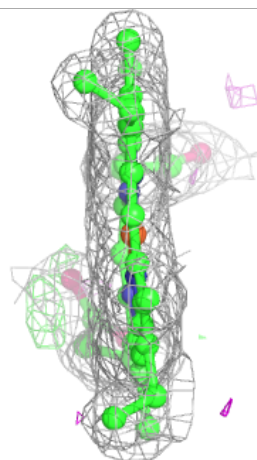
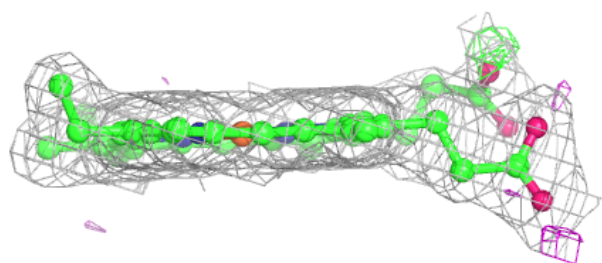
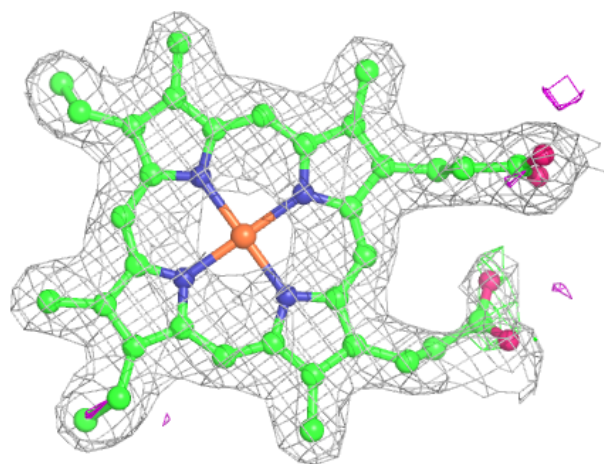
**Electron density around HEC C 403:**

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



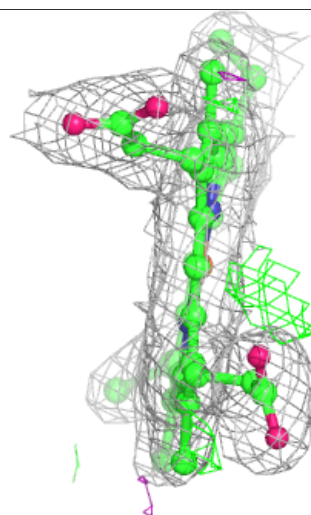
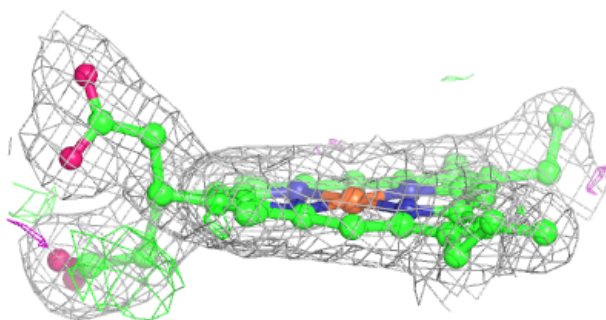
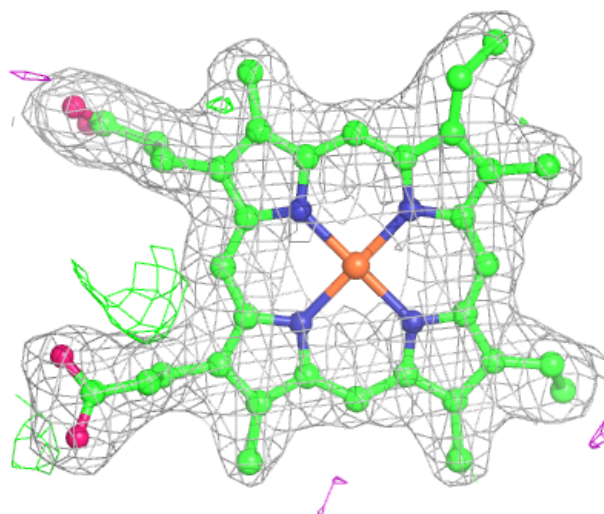
**Electron density around HEC C 404 (B):**

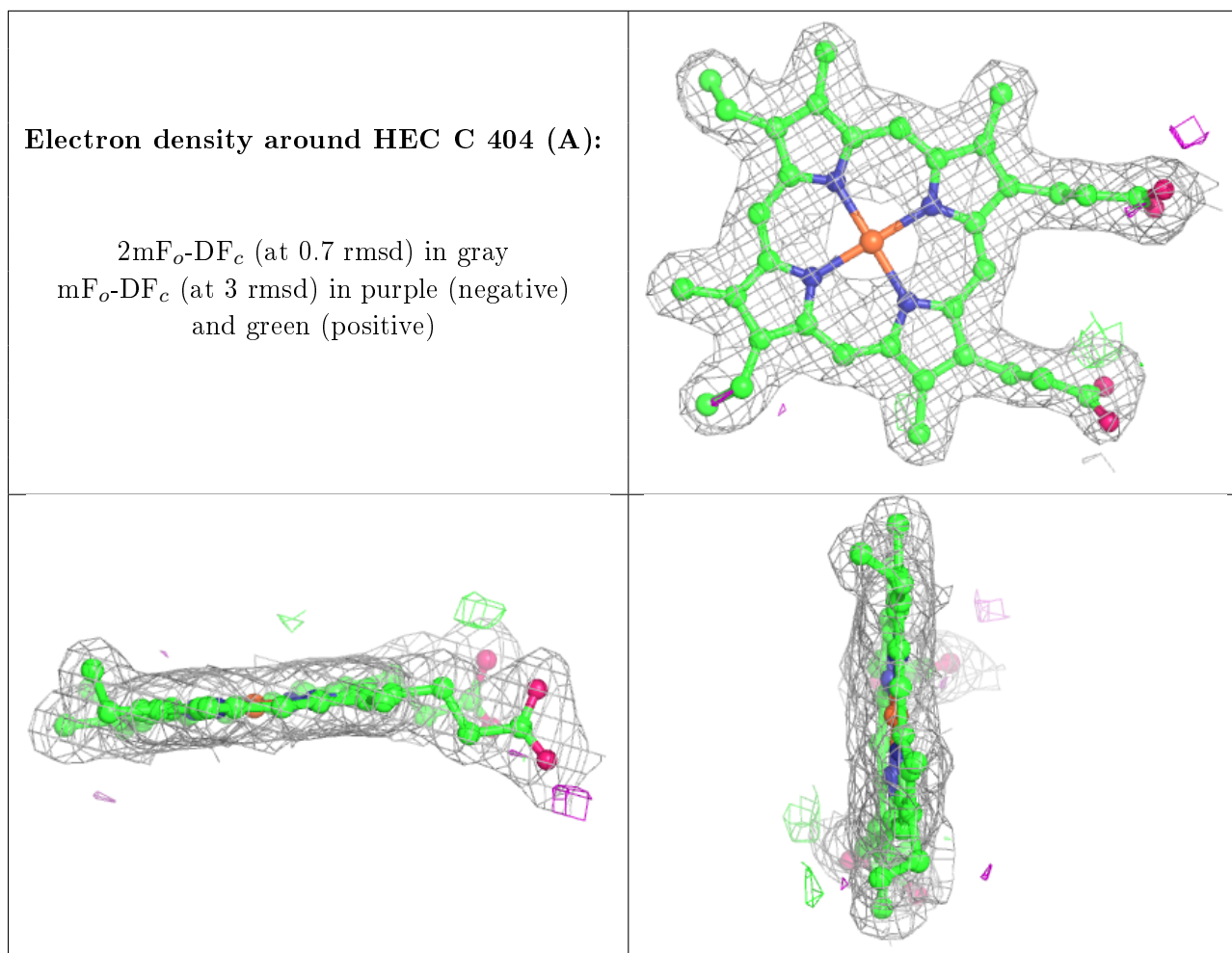
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.