



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 06:44 pm BST

PDB ID : 3D38
Title : Crystal structure of new trigonal form of photosynthetic reaction center from *Blastochloris viridis*. Crystals grown in microfluidics by detergent capture.
Authors : Li, L.; Nachtergaele, S.H.M.; Seddon, A.M.; Tereshko, V.; Ponomarenko, N.; Ismagilov, R.F.; Accelerated Technologies Center for Gene to 3D Structure (ATCG3D)
Deposited on : 2008-05-09
Resolution : 3.21 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 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

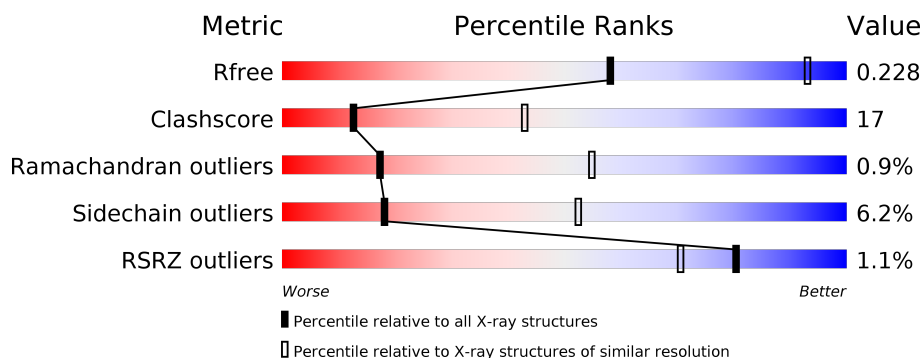
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	336	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>••</div> </div> </div>
2	H	258	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>••</div> </div> </div>
3	L	273	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>•</div> </div> </div>
4	M	323	<div> <div></div> <div> <div></div> <div>72%</div> <div>25%</div> <div>•</div> </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
11	UQ1	L	503	-	-	-	X
5	SO4	C	809	-	-	-	X
7	HTO	H	705	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 10311 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	332	Total	C	N	O	S	0	0	0
			2598	1637	465	478	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	250	Total	C	N	O	S	0	0	0
			1958	1251	335	370	2			

- 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	0	0
			2171	1459	350	355	7			

- 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	0	0
			2555	1702	419	423	11			

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



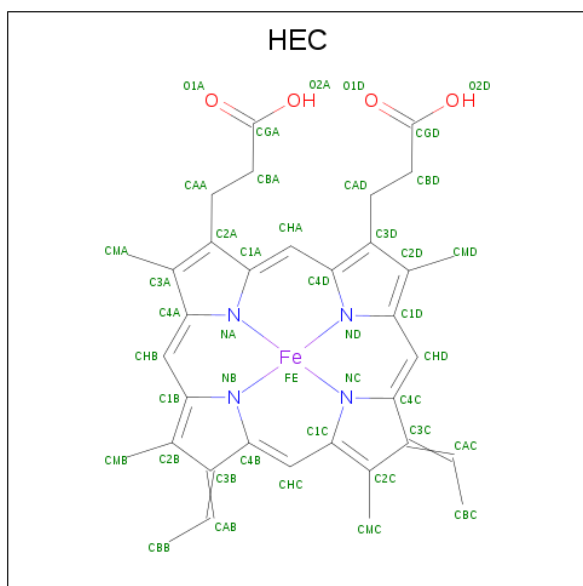
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total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

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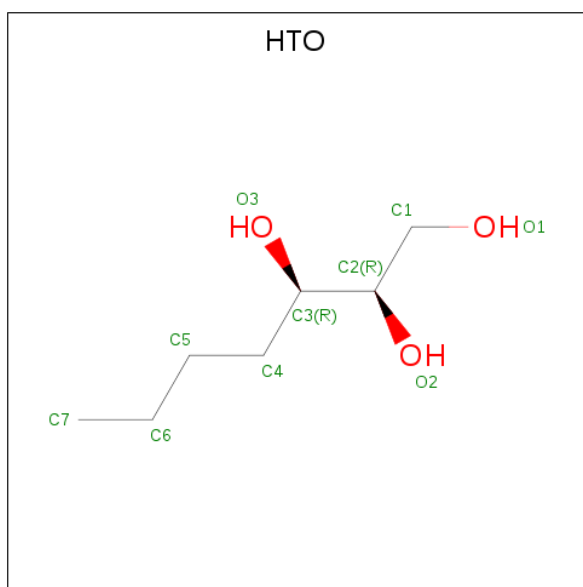
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



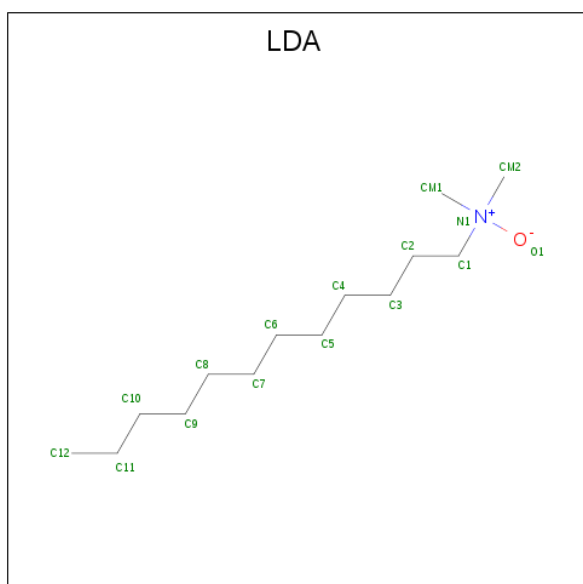
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 7 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



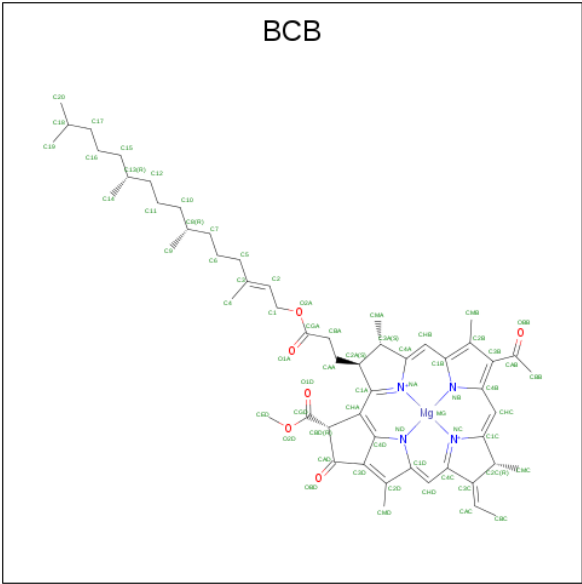
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			10	7	3		
7	C	1	Total	C	O	0	0
			10	7	3		
7	H	1	Total	C	O	0	0
			10	7	3		

- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



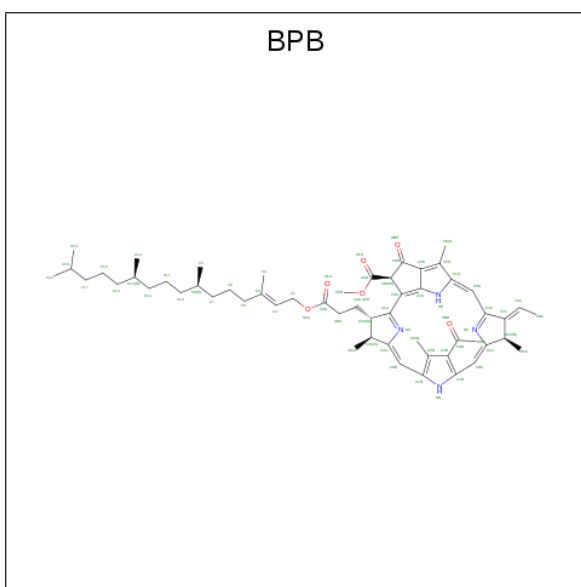
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	L	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C₅₅H₇₂MgN₄O₆).



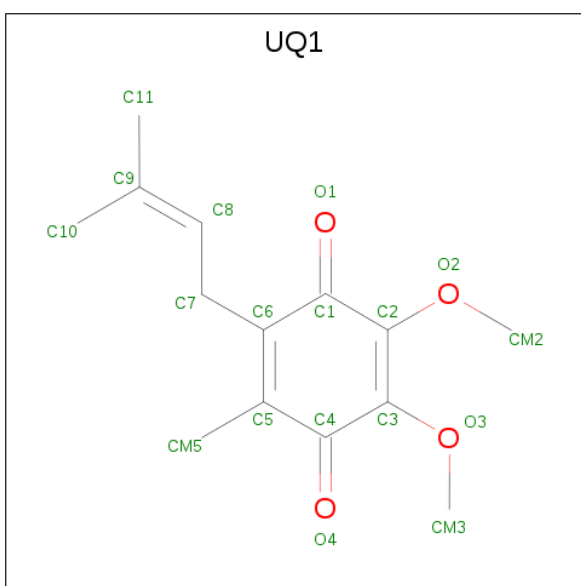
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
9	M	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 10 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: C₅₅H₇₄N₄O₆).



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

- Molecule 11 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).

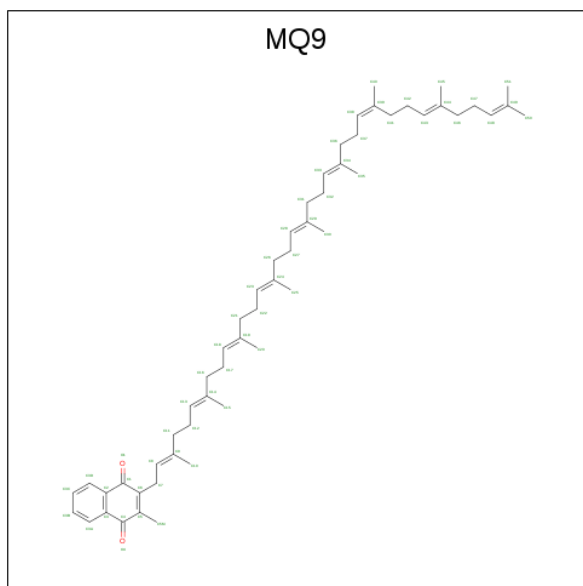


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	L	1	Total	C	O	0	0
			18	14	4		
11	L	1	Total	C	O	0	0
			18	14	4		

- Molecule 12 is FE (II) ION (three-letter code: FE2) (formula: Fe).

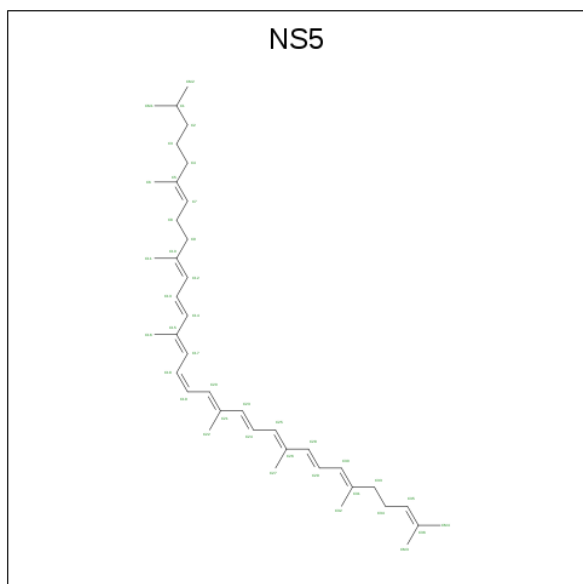
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	0
			1	1		

- Molecule 13 is MENAQUINONE-9 (three-letter code: MQ9) (formula: C₅₆H₈₀O₂).



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

- Molecule 14 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: C₄₀H₆₀).



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

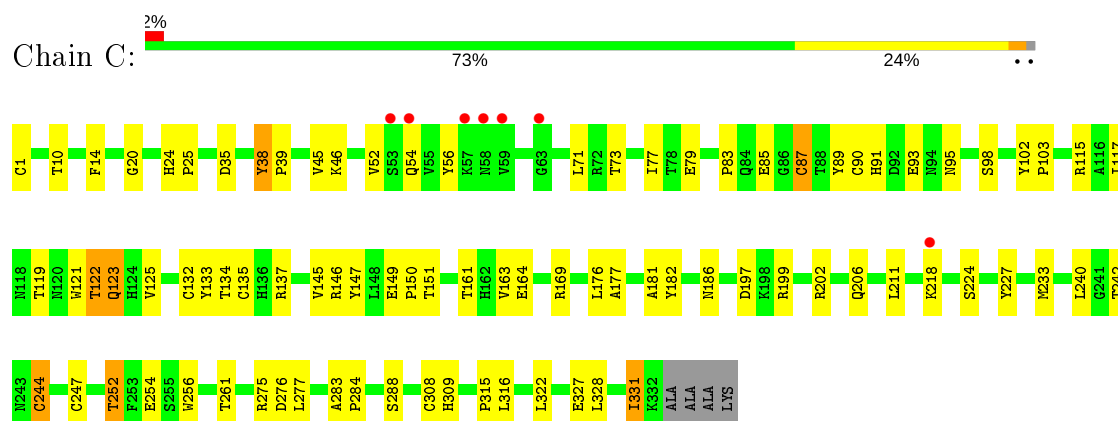
- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	47	Total O 47 47	0	0
15	H	28	Total O 28 28	0	0
15	L	38	Total O 38 38	0	0
15	M	46	Total O 46 46	0	0

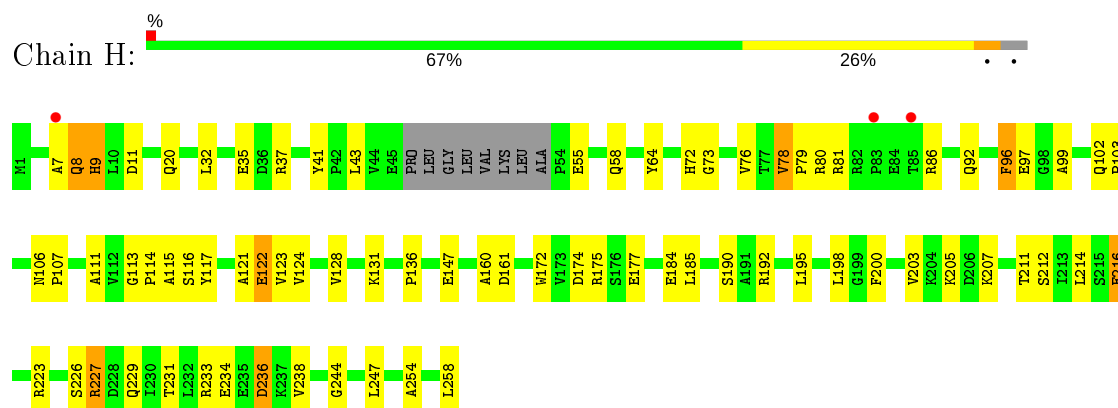
3 Residue-property plots

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.

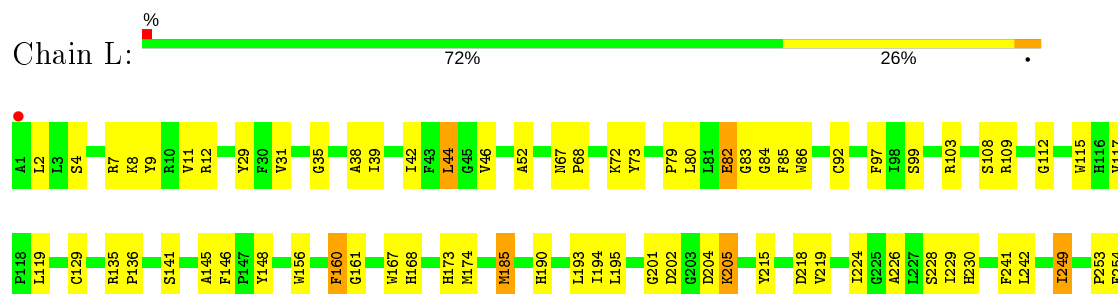
- Molecule 1: Photosynthetic reaction center cytochrome c subunit

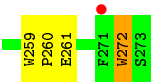


- Molecule 2: Reaction center protein H chain

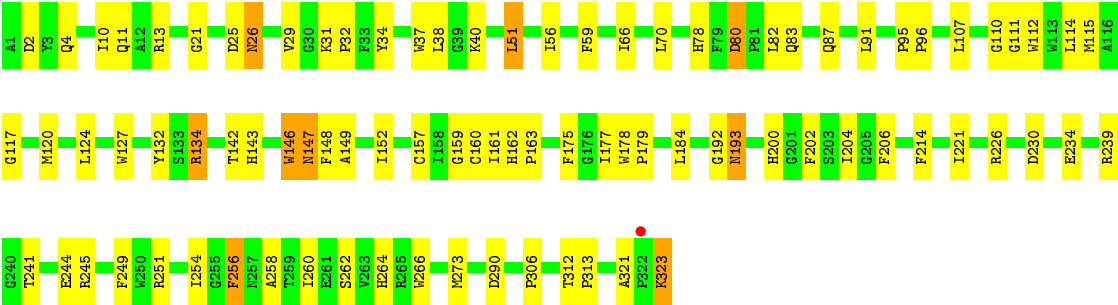


- Molecule 3: Reaction center protein L chain





● Molecule 4: Reaction center protein M chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	241.17Å 241.17Å 113.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.21 47.92 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.21) 99.6 (47.92-3.21)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.4.0073	Depositor
R, R_{free}	0.192 , 0.224 0.196 , 0.228	Depositor DCC
R_{free} test set	3145 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10311	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: LDA, BPB, HTO, BCB, MQ9, FE2, SO4, HEC, UQ1, 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	0.53	1/2665 (0.0%)	0.64	0/3633
2	H	0.59	0/1993	0.68	0/2720
3	L	0.60	1/2259 (0.0%)	0.66	0/3084
4	M	0.57	0/2659	0.65	1/3637 (0.0%)
All	All	0.57	2/9576 (0.0%)	0.66	1/13074 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	CYS	CB-SG	-5.84	1.72	1.81
3	L	129	CYS	CB-SG	-5.38	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	70	LEU	CA-CB-CG	7.57	132.71	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2598	0	2573	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1958	0	1946	65	0
3	L	2171	0	2098	64	0
4	M	2555	0	2452	76	0
5	C	35	0	0	0	0
5	H	20	0	0	1	0
5	M	20	0	0	1	0
6	C	172	0	125	31	0
7	C	20	0	32	1	0
7	H	10	0	16	2	0
8	H	32	0	62	6	0
8	L	16	0	31	2	0
8	M	16	0	31	0	0
9	L	132	0	144	24	0
9	M	132	0	144	27	0
10	L	65	0	74	9	0
10	M	65	0	74	20	0
11	L	36	0	36	4	0
12	M	1	0	0	0	0
13	M	58	0	80	3	0
14	M	40	0	60	11	0
15	C	47	0	0	9	0
15	H	28	0	0	5	0
15	L	38	0	0	3	0
15	M	46	0	0	7	0
All	All	10311	0	9978	337	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 17.

The worst 5 of 337 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:CYS:SG	6:C:401:HEC:HAC	1.31	1.69
1:C:132:CYS:SG	6:C:402:HEC:HAB	1.48	1.52
1:C:244:CYS:SG	6:C:403:HEC:HAB	1.54	1.47
1:C:132:CYS:SG	6:C:402:HEC:CAB	2.08	1.39
1:C:135:CYS:SG	6:C:402:HEC:CAC	2.12	1.37

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	330/336 (98%)	294 (89%)	35 (11%)	1 (0%)	41	74
2	H	246/258 (95%)	220 (89%)	22 (9%)	4 (2%)	9	42
3	L	271/273 (99%)	246 (91%)	24 (9%)	1 (0%)	34	69
4	M	321/323 (99%)	290 (90%)	26 (8%)	5 (2%)	9	42
All	All	1168/1190 (98%)	1050 (90%)	107 (9%)	11 (1%)	17	55

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	147	GLU
2	H	73	GLY
4	M	32	PRO
4	M	51	LEU
4	M	193	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	280/282 (99%)	266 (95%)	14 (5%)	24	59
2	H	205/212 (97%)	188 (92%)	17 (8%)	11	40
3	L	218/218 (100%)	203 (93%)	15 (7%)	15	48
4	M	249/249 (100%)	236 (95%)	13 (5%)	23	58
All	All	952/961 (99%)	893 (94%)	59 (6%)	18	52

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	216	GLU
3	L	7	ARG
4	M	214	PHE
2	H	223	ARG
2	H	236	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	106	ASN
2	H	225	GLN
4	M	4	GLN
2	H	58	GLN
2	H	102	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	2	8,9,10	0.83	0	7,9,11	3.72	2 (28%)

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	2	-	4/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-9.15	108.76	122.82
2	H	1	FME	CE-SD-CG	2.39	108.62	100.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	O1-CN-N-CA
2	H	1	FME	C-CA-CB-CG
2	H	1	FME	CB-CG-SD-CE
2	H	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 1 is monoatomic - leaving 36 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	SO4	C	815	-	4,4,4	0.15	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	BCB	M	400	4	60,74,74	3.79	22 (36%)	48,115,115	2.25	17 (35%)
8	LDA	L	702	-	12,15,15	2.10	1 (8%)	14,17,17	0.63	0
11	UQ1	L	503	-	18,18,18	2.23	2 (11%)	22,25,25	1.23	2 (9%)
5	SO4	M	801	-	4,4,4	0.21	0	6,6,6	0.63	0
11	UQ1	L	502	-	18,18,18	2.19	2 (11%)	22,25,25	1.37	4 (18%)
9	BCB	M	401	4	60,74,74	3.71	22 (36%)	48,115,115	2.28	19 (39%)
5	SO4	C	813	-	4,4,4	0.09	0	6,6,6	0.27	0
5	SO4	H	812	-	4,4,4	0.16	0	6,6,6	0.19	0
6	HEC	C	402	1	26,50,50	1.90	2 (7%)	18,82,82	1.54	3 (16%)
5	SO4	C	808	-	4,4,4	0.11	0	6,6,6	0.19	0
5	SO4	M	804	-	4,4,4	0.16	0	6,6,6	0.29	0
5	SO4	C	809	-	4,4,4	0.14	0	6,6,6	0.10	0
7	HTO	H	705	-	9,9,9	0.69	0	10,10,10	0.83	0
6	HEC	C	404	1	26,50,50	1.85	2 (7%)	18,82,82	1.68	4 (22%)
10	BPB	L	402	-	64,70,70	1.65	8 (12%)	64,101,101	1.88	19 (29%)
9	BCB	L	400	3	60,74,74	3.64	22 (36%)	48,115,115	2.27	18 (37%)
9	BCB	L	401	3	60,74,74	3.85	22 (36%)	48,115,115	2.26	18 (37%)
5	SO4	H	807	-	4,4,4	0.13	0	6,6,6	0.33	0
10	BPB	M	402	-	64,70,70	1.57	10 (15%)	64,101,101	1.82	13 (20%)
5	SO4	C	811	-	4,4,4	0.17	0	6,6,6	0.23	0
5	SO4	M	802	-	4,4,4	0.18	0	6,6,6	0.19	0
5	SO4	H	806	-	4,4,4	0.17	0	6,6,6	0.26	0
6	HEC	C	403	1	26,50,50	1.86	3 (11%)	18,82,82	1.30	3 (16%)
6	HEC	C	401	1	26,50,50	2.07	3 (11%)	18,82,82	1.31	2 (11%)
8	LDA	H	701	-	12,15,15	2.03	1 (8%)	14,17,17	0.47	0
5	SO4	C	814	-	4,4,4	0.12	0	6,6,6	0.36	0
7	HTO	C	706	-	9,9,9	0.27	0	10,10,10	0.75	0
13	MQ9	M	501	-	59,59,59	1.80	18 (30%)	72,75,75	1.56	20 (27%)
14	NS5	M	600	-	39,39,39	1.57	3 (7%)	44,46,46	1.93	13 (29%)
5	SO4	H	803	-	4,4,4	0.17	0	6,6,6	0.24	0
5	SO4	C	810	-	4,4,4	0.15	0	6,6,6	0.09	0
8	LDA	H	703	-	12,15,15	1.92	1 (8%)	14,17,17	0.53	0
8	LDA	M	704	-	12,15,15	2.16	1 (8%)	14,17,17	0.44	0
5	SO4	M	805	-	4,4,4	0.18	0	6,6,6	0.42	0
7	HTO	C	707	-	9,9,9	0.66	0	10,10,10	0.55	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BPB	M	402	-	-	17/47/105/105	0/5/6/6
10	BPB	L	402	-	-	16/47/105/105	0/5/6/6
9	BCB	M	400	4	-	17/41/177/177	-
6	HEC	C	402	1	-	0/6/54/54	-
8	LDA	L	702	-	-	11/13/13/13	-
11	UQ1	L	503	-	-	0/9/33/33	0/1/1/1
6	HEC	C	404	1	-	2/6/54/54	-
6	HEC	C	403	1	-	0/6/54/54	-
11	UQ1	L	502	-	-	4/9/33/33	0/1/1/1
9	BCB	L	400	3	-	16/41/177/177	-
7	HTO	H	705	-	-	8/10/10/10	-
8	LDA	H	701	-	-	8/13/13/13	-
9	BCB	M	401	4	-	19/41/177/177	-
8	LDA	H	703	-	-	6/13/13/13	-
6	HEC	C	401	1	-	0/6/54/54	-
7	HTO	C	706	-	-	5/10/10/10	-
13	MQ9	M	501	-	-	16/53/73/73	0/2/2/2
14	NS5	M	600	-	-	14/43/43/43	-
9	BCB	L	401	3	-	12/41/177/177	-
8	LDA	M	704	-	-	9/13/13/13	-
7	HTO	C	707	-	-	8/10/10/10	-

The worst 5 of 145 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	L	401	BCB	C1A-CHA	-10.29	1.37	1.54
9	M	400	BCB	C1A-CHA	-10.26	1.38	1.54
9	L	400	BCB	C1A-CHA	-10.25	1.38	1.54
9	L	401	BCB	CHB-C1B	-9.37	1.38	1.53
9	L	401	BCB	CHD-C1D	-9.02	1.39	1.53

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	402	BPB	C3D-C2D-C1D	-6.79	95.98	105.87
10	L	402	BPB	C3D-C2D-C1D	-6.49	96.42	105.87
9	M	400	BCB	C1D-CHD-C4C	6.10	125.37	112.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	M	401	BCB	CHA-CBD-CGD	-5.98	101.48	115.02
10	M	402	BPB	O2D-CGD-CBD	5.68	121.37	111.27

There are no chirality outliers.

5 of 188 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	M	400	BCB	C4B-C3B-CAB-OBB
9	M	400	BCB	C4B-C3B-CAB-CBB
8	L	702	LDA	C2-C1-N1-O1
8	L	702	LDA	C2-C1-N1-CM1
8	L	702	LDA	N1-C1-C2-C3

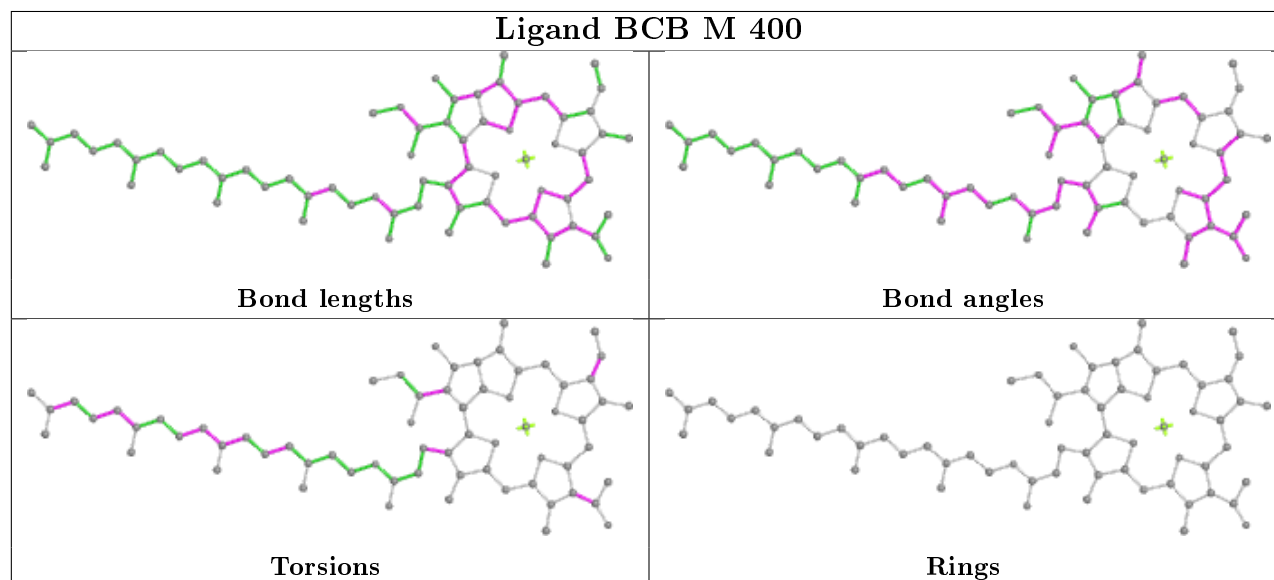
There are no ring outliers.

19 monomers are involved in 129 short contacts:

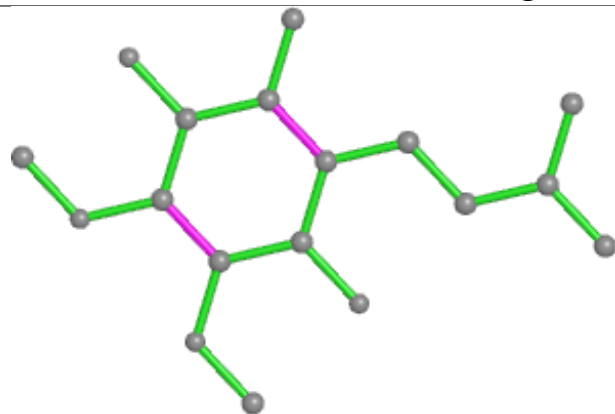
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	M	400	BCB	11	0
8	L	702	LDA	2	0
11	L	502	UQ1	4	0
9	M	401	BCB	17	0
6	C	402	HEC	10	0
7	H	705	HTO	2	0
6	C	404	HEC	2	0
10	L	402	BPB	9	0
9	L	400	BCB	17	0
9	L	401	BCB	10	0
5	H	807	SO4	1	0
10	M	402	BPB	20	0
6	C	403	HEC	6	0
6	C	401	HEC	13	0
7	C	706	HTO	1	0
13	M	501	MQ9	3	0
14	M	600	NS5	11	0
8	H	703	LDA	6	0
5	M	805	SO4	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.

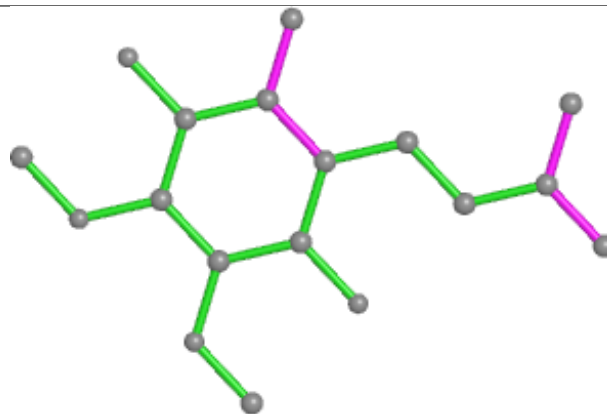
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



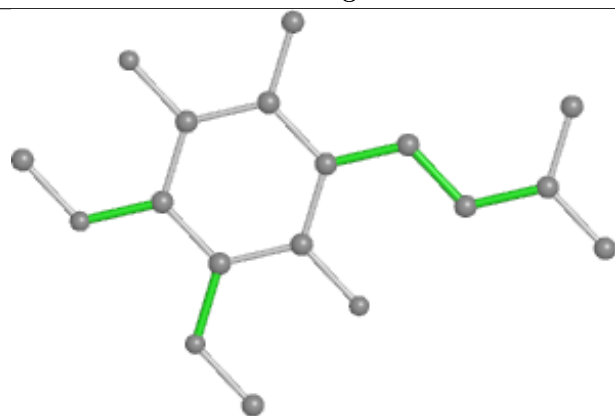
Ligand UQ1 L 503



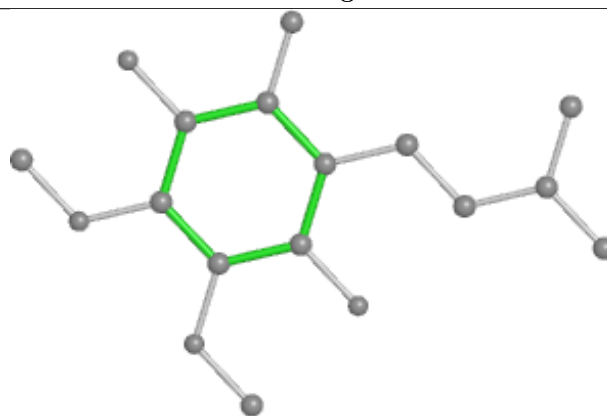
Bond lengths



Bond angles

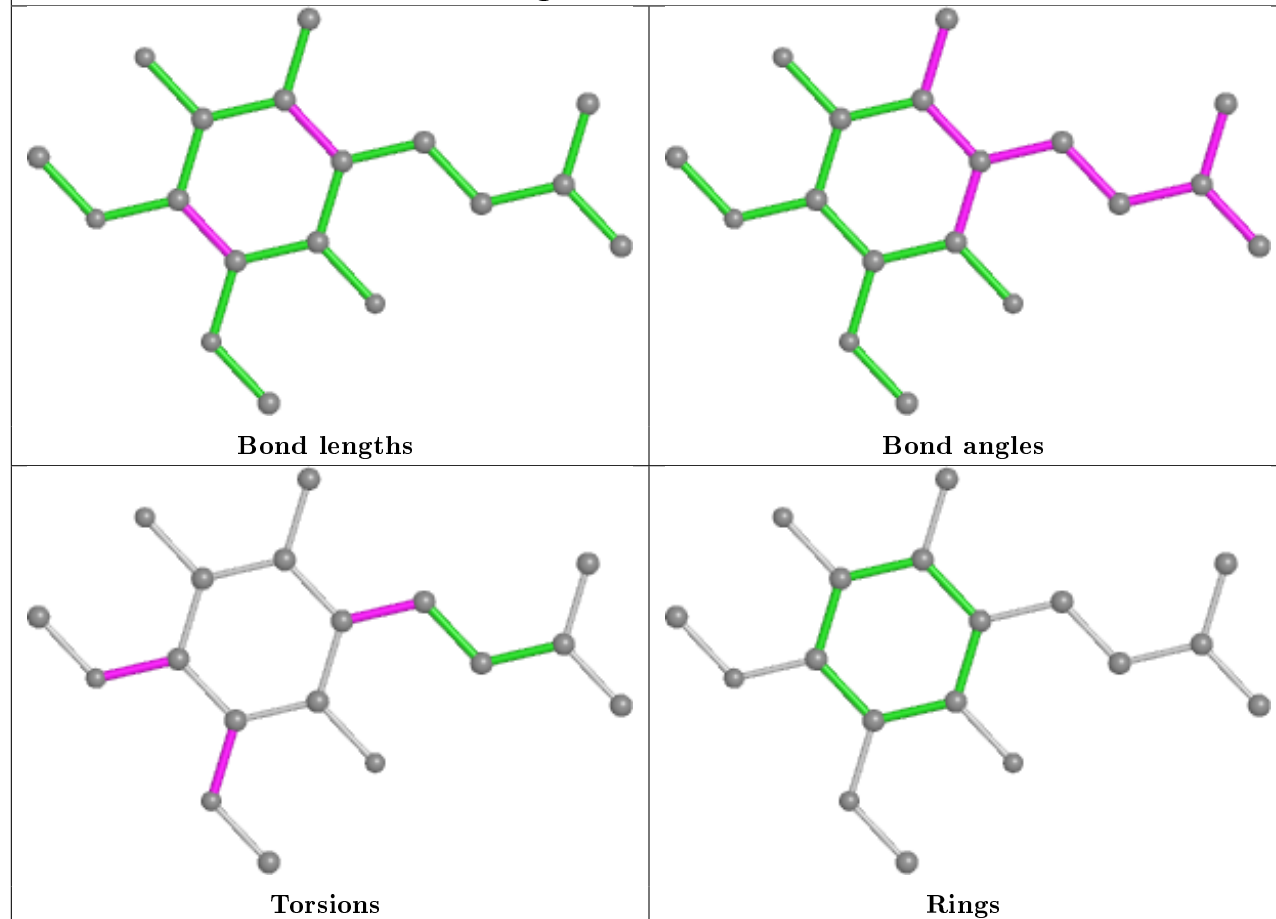


Torsions

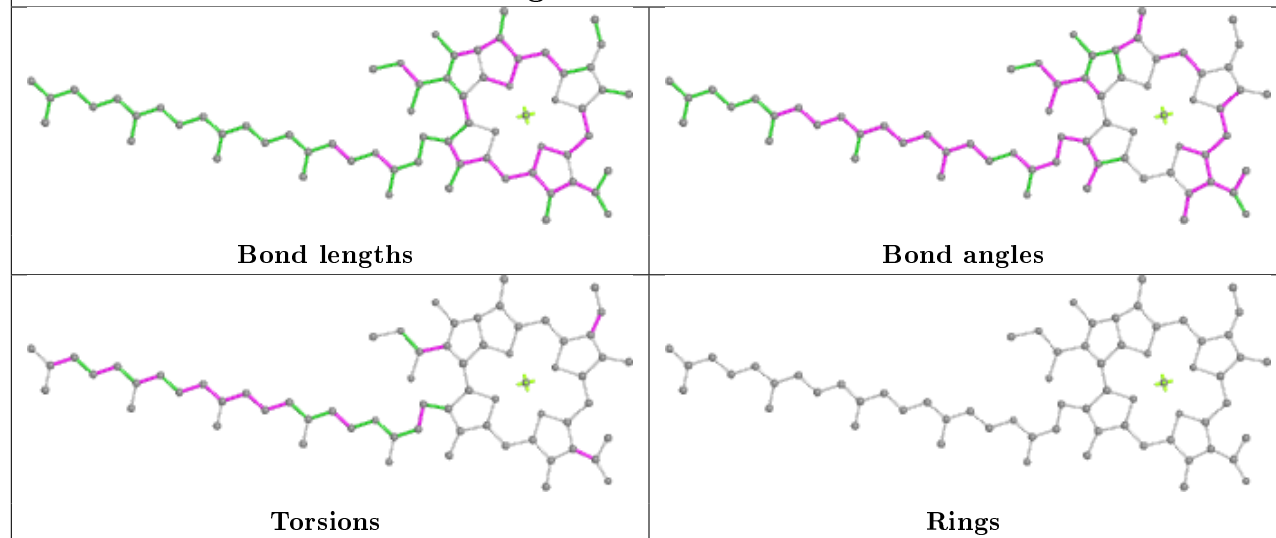


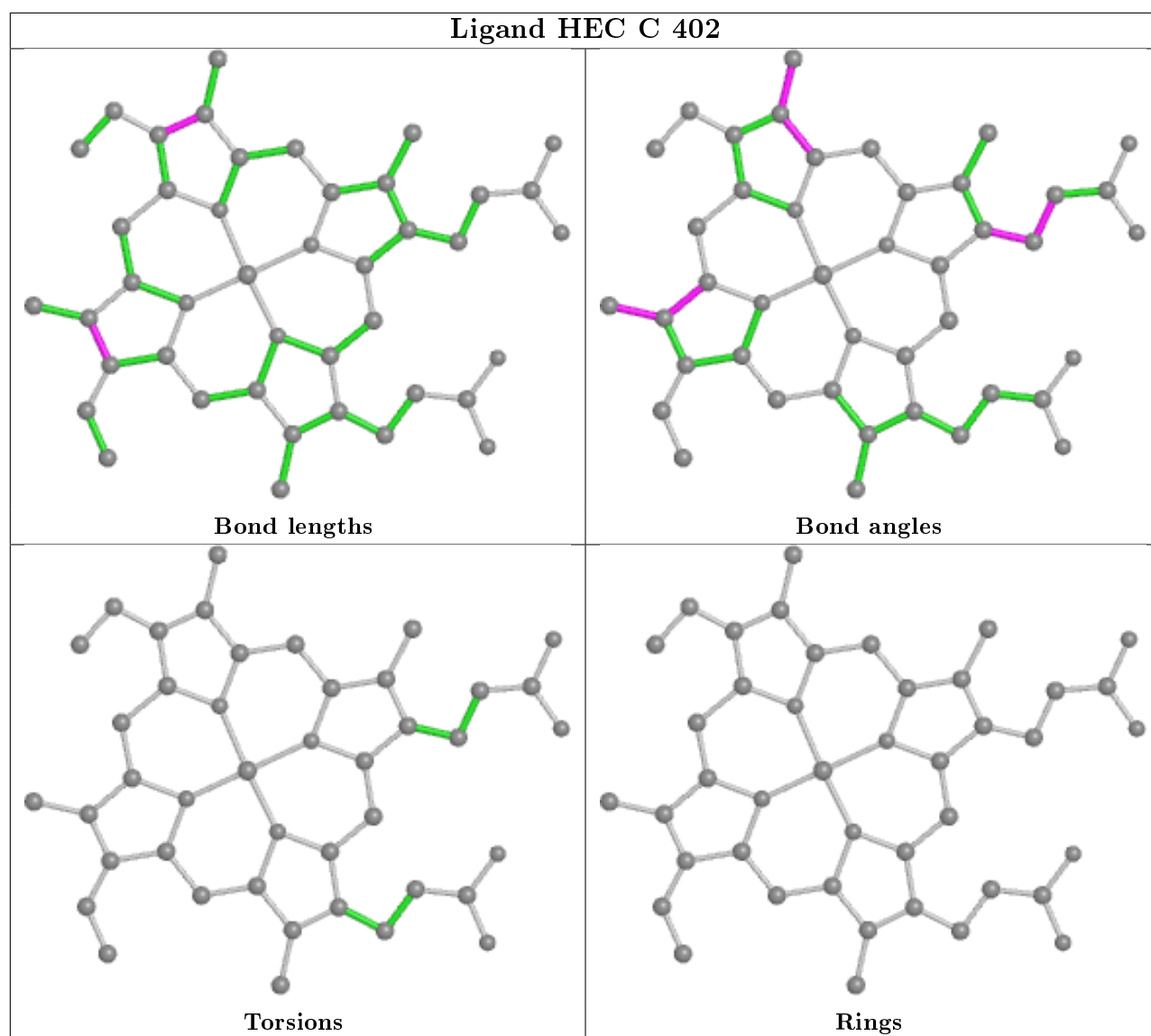
Rings

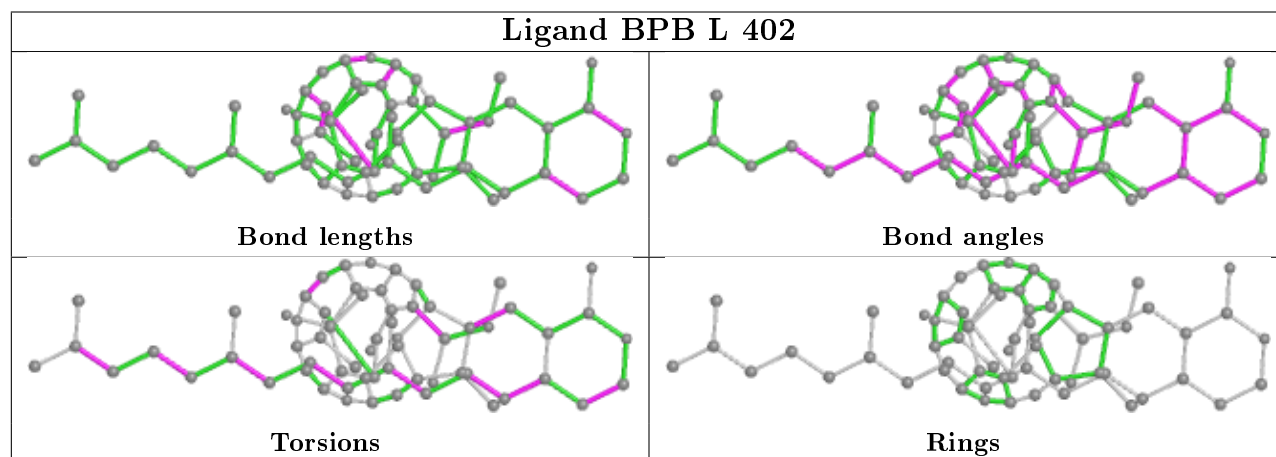
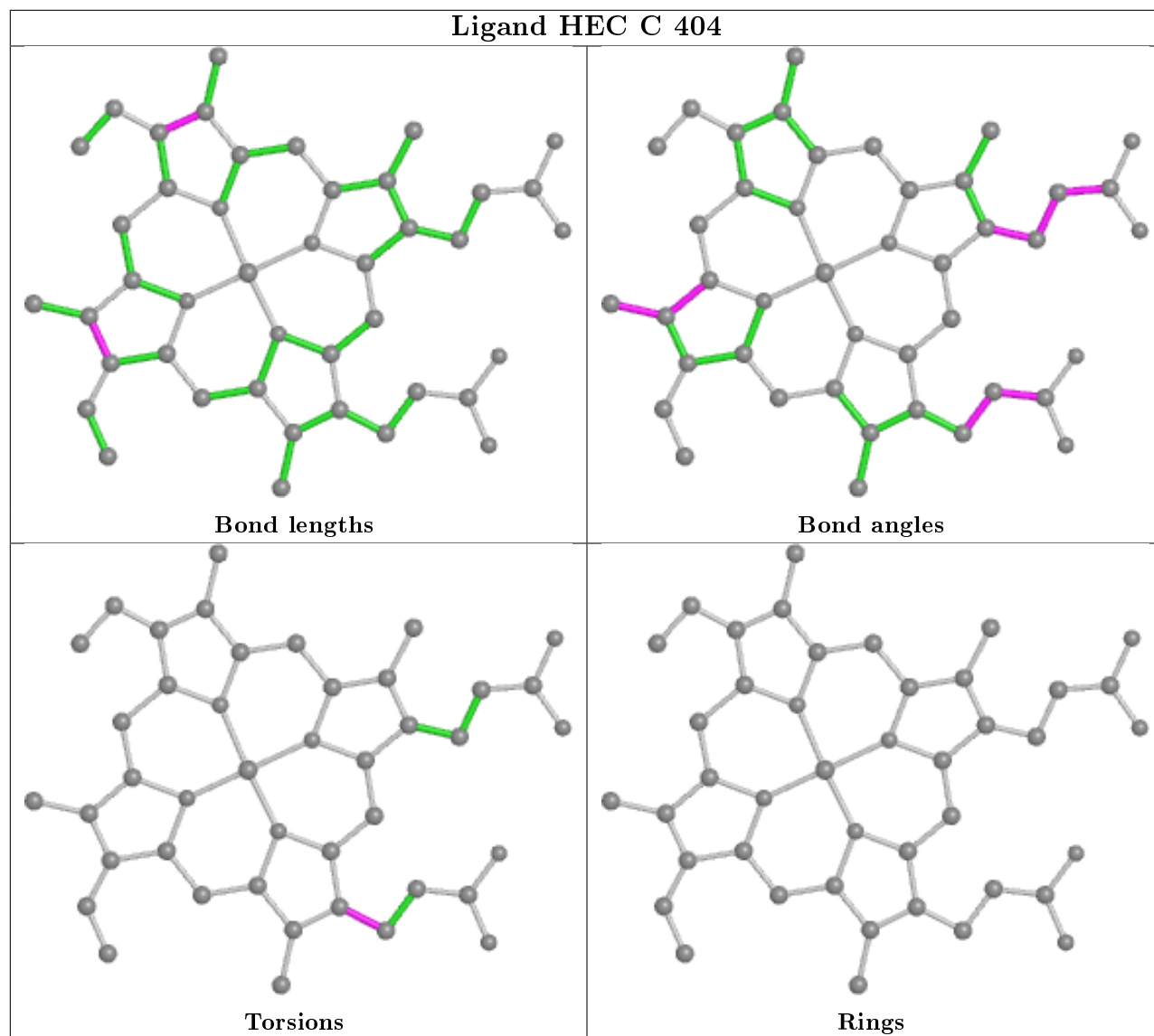
Ligand UQ1 L 502

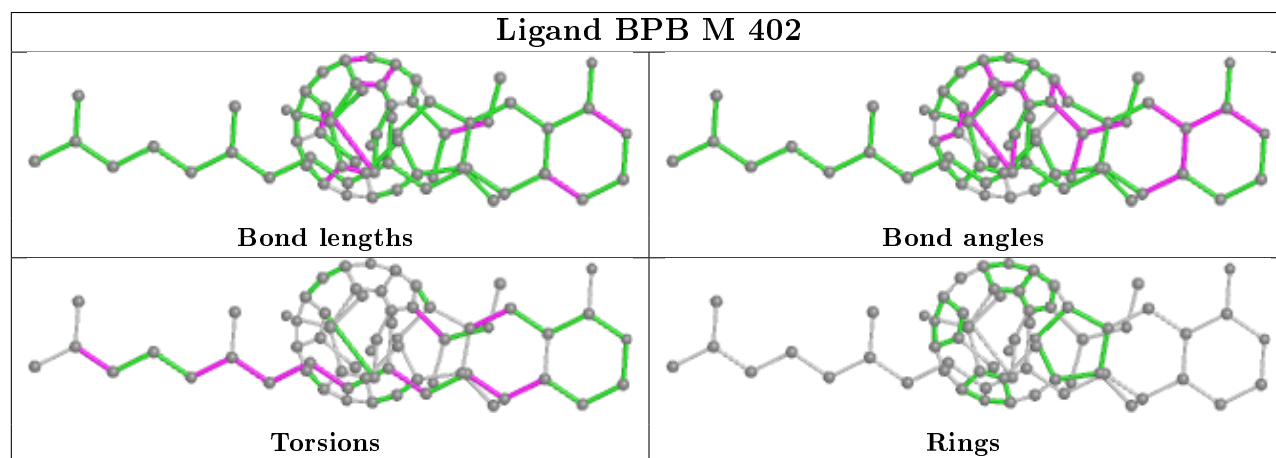
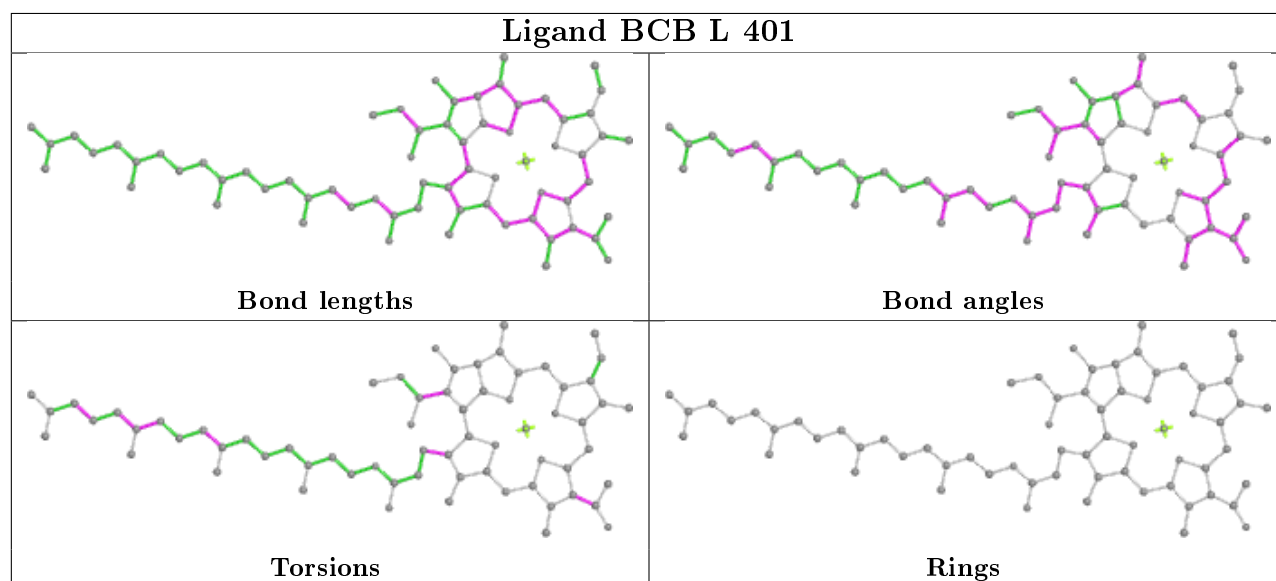
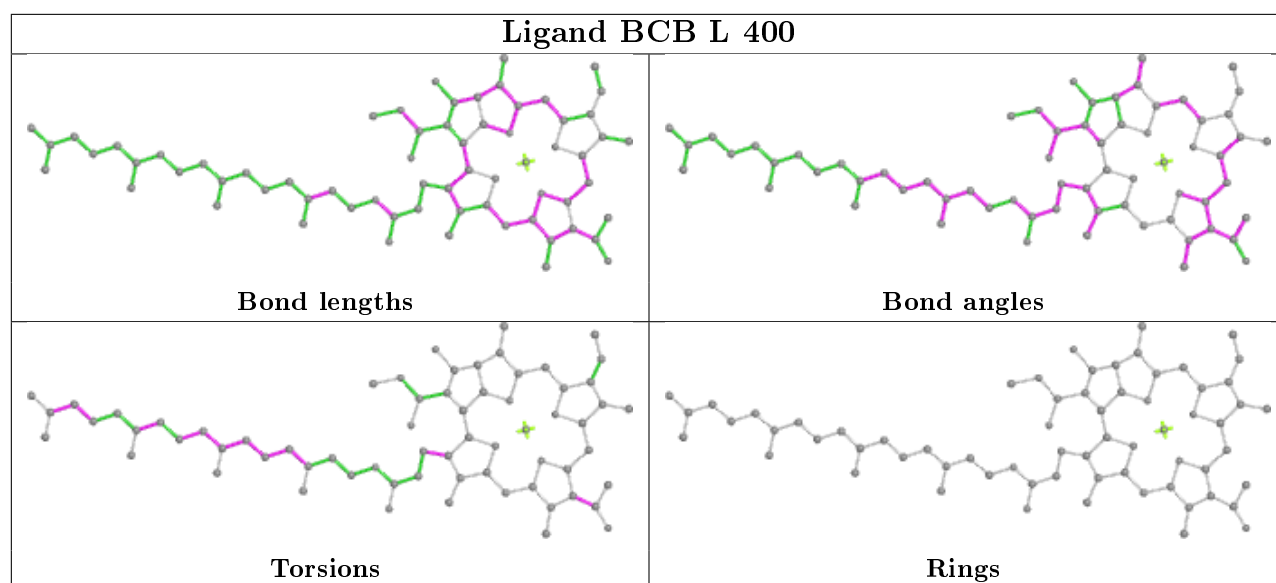


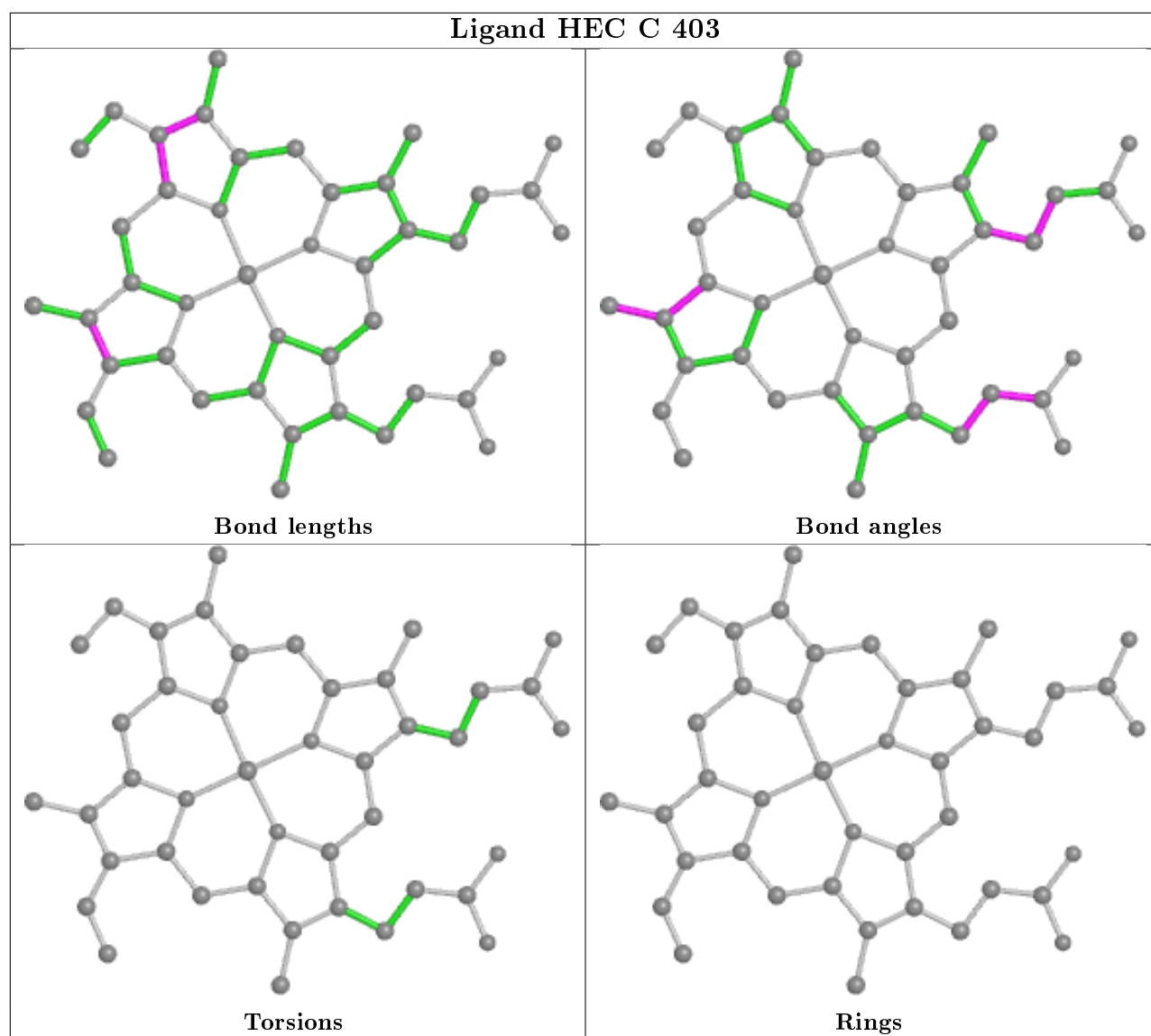
Ligand BCB M 401

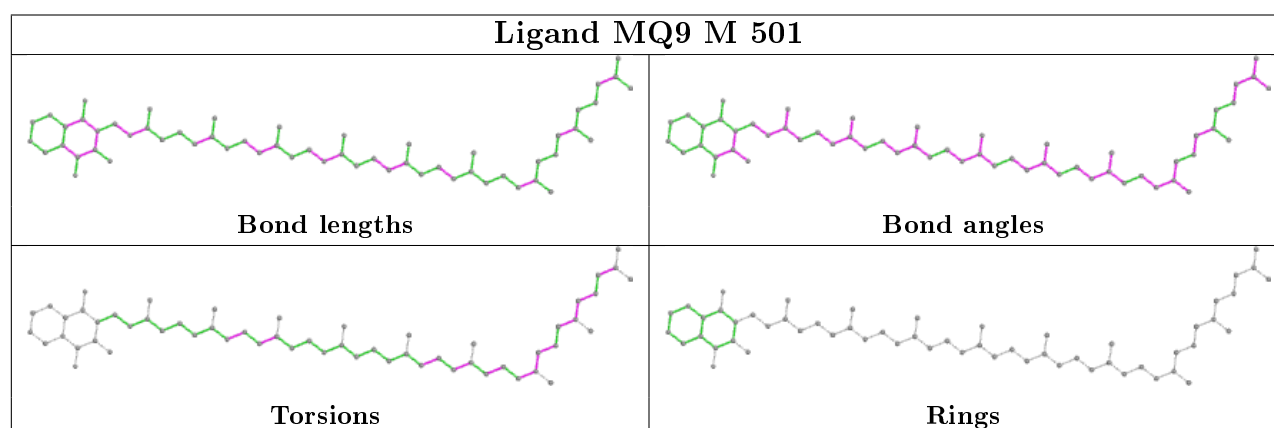
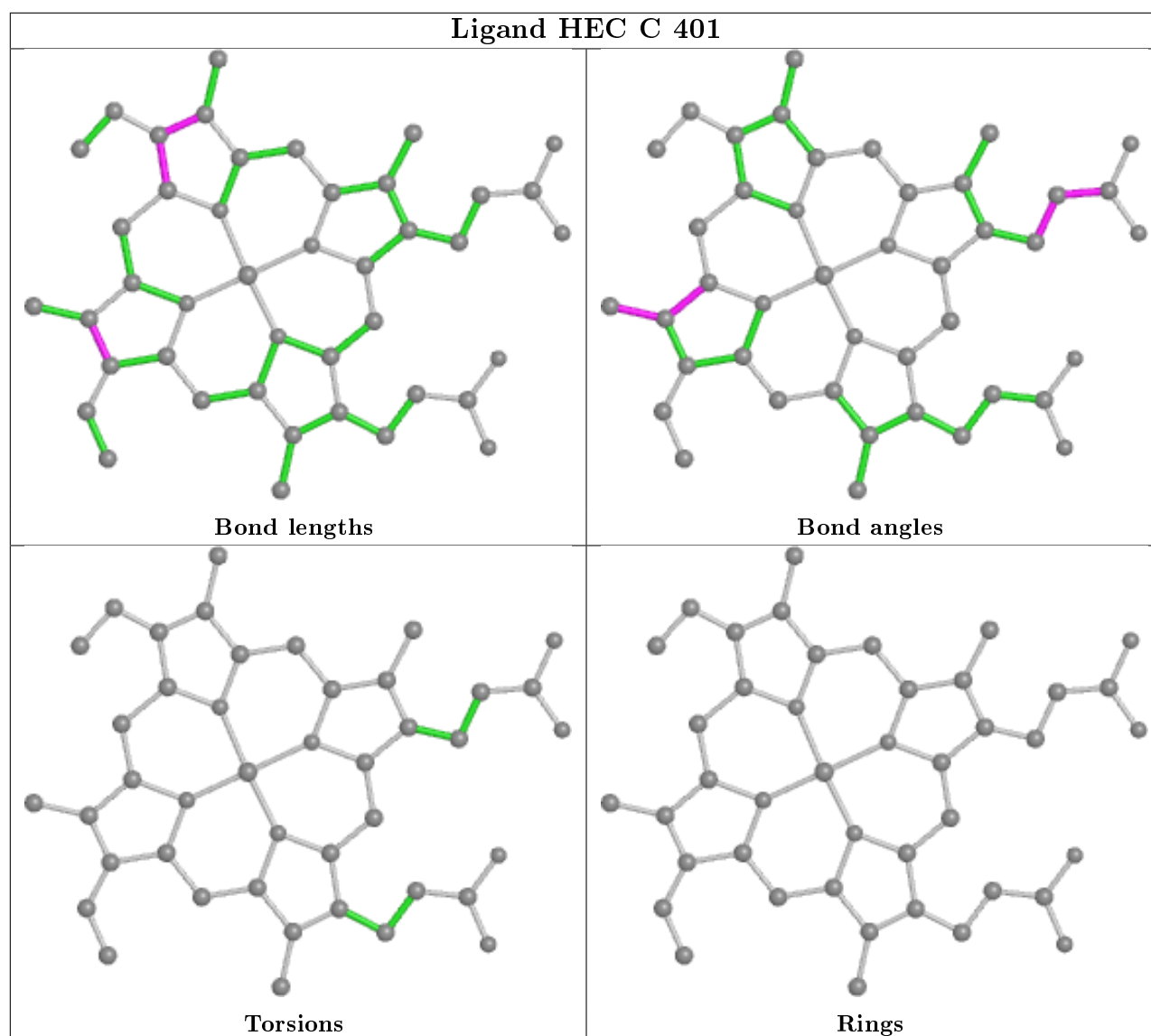


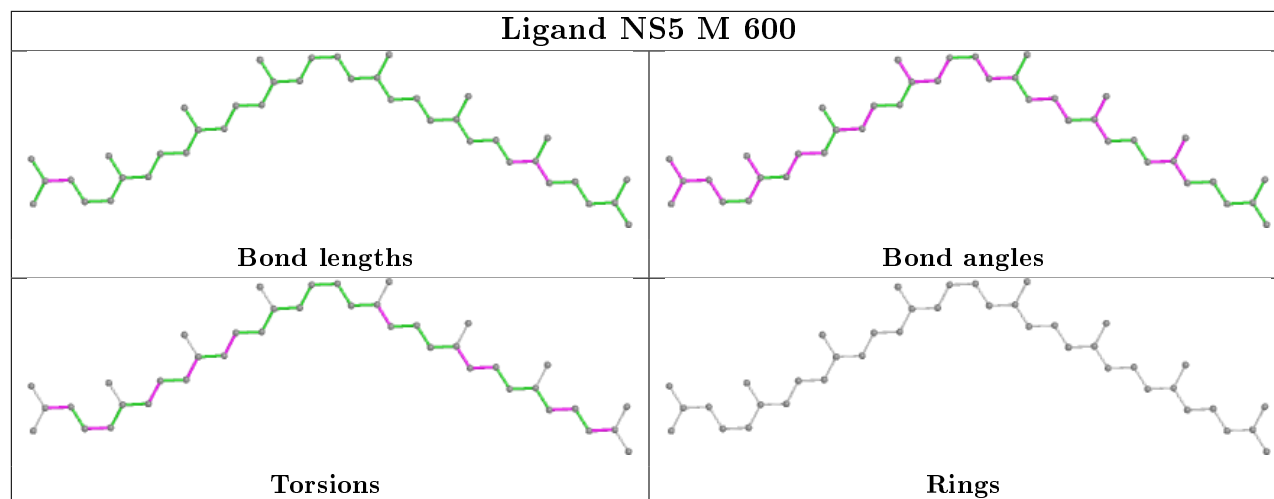












5.7 Other polymers [i](#)

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	332/336 (98%)	-0.24	7 (2%) 63 50	46, 74, 113, 124	0
2	H	249/258 (96%)	-0.19	3 (1%) 79 68	50, 73, 99, 105	0
3	L	273/273 (100%)	-0.58	2 (0%) 87 82	37, 54, 74, 85	0
4	M	323/323 (100%)	-0.51	1 (0%) 94 92	42, 60, 89, 117	0
All	All	1177/1190 (98%)	-0.38	13 (1%) 80 70	37, 66, 102, 124	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	3.7
1	C	59	VAL	3.6
1	C	54	GLN	3.0
1	C	53	SER	2.8
2	H	83	PRO	2.7

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, 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	10/11	0.77	0.37	104,105,115,117	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

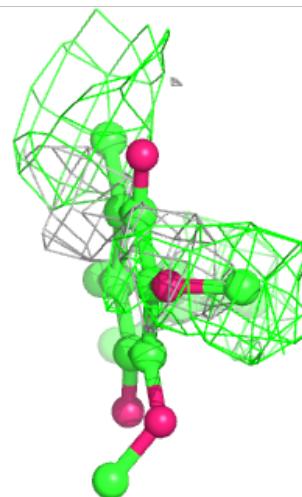
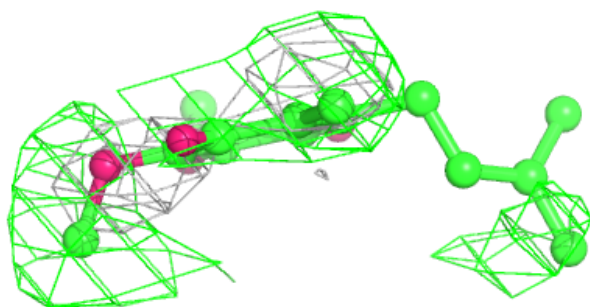
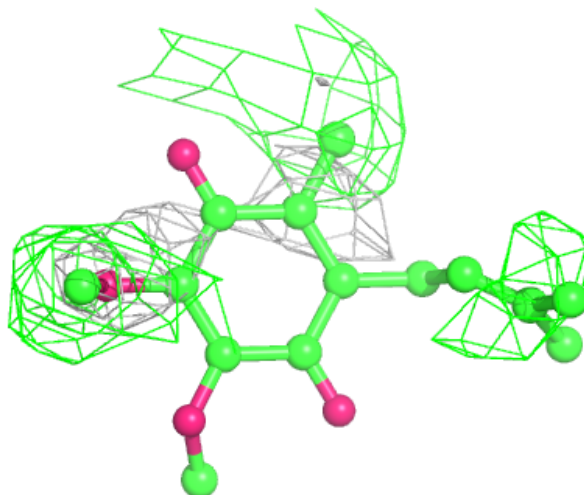
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	C	808	5/5	0.47	0.40	104,104,104,104	5
5	SO4	C	809	5/5	0.48	0.54	109,110,110,110	5
7	HTO	H	705	10/10	0.55	0.59	56,59,61,61	10
11	UQ1	L	503	18/18	0.62	0.59	73,76,78,78	18
5	SO4	H	812	5/5	0.76	0.33	92,92,93,93	5
5	SO4	H	803	5/5	0.77	0.34	82,82,83,83	5
7	HTO	C	707	10/10	0.77	0.39	44,48,49,49	10
5	SO4	C	810	5/5	0.80	0.42	88,88,88,88	5
5	SO4	H	807	5/5	0.81	0.42	108,108,108,109	5
5	SO4	C	813	5/5	0.82	0.43	79,79,80,80	5
5	SO4	C	811	5/5	0.85	0.60	76,76,76,77	5
14	NS5	M	600	40/40	0.87	0.28	65,71,100,101	4
7	HTO	C	706	10/10	0.88	0.71	56,57,58,58	10
11	UQ1	L	502	18/18	0.89	0.40	63,65,66,66	18
10	BPB	M	402	65/65	0.89	0.28	61,67,123,124	0
8	LDA	M	704	16/16	0.91	0.41	68,70,73,73	16
13	MQ9	M	501	58/58	0.91	0.25	40,64,102,103	0
5	SO4	C	814	5/5	0.92	0.37	48,48,49,50	5
5	SO4	C	815	5/5	0.92	0.25	40,40,41,41	5
8	LDA	H	703	16/16	0.94	0.39	54,58,60,61	16
5	SO4	M	804	5/5	0.95	0.18	94,95,96,96	0
8	LDA	L	702	16/16	0.95	0.36	67,73,79,80	0
5	SO4	H	806	5/5	0.95	0.14	72,72,73,73	5
10	BPB	L	402	65/65	0.96	0.19	38,51,60,60	0
6	HEC	C	401	43/43	0.96	0.27	99,110,118,120	0
8	LDA	H	701	16/16	0.96	0.17	54,57,68,68	0
5	SO4	M	805	5/5	0.96	0.09	64,65,65,67	5
5	SO4	M	801	5/5	0.96	0.11	61,62,63,63	0
9	BCB	M	400	66/66	0.97	0.18	37,48,107,108	0
9	BCB	L	401	66/66	0.97	0.19	41,44,59,64	0
9	BCB	L	400	66/66	0.98	0.18	37,40,45,49	0
6	HEC	C	402	43/43	0.98	0.19	73,76,80,81	0
6	HEC	C	403	43/43	0.98	0.19	46,48,52,54	0
6	HEC	C	404	43/43	0.98	0.16	52,55,68,73	0
9	BCB	M	401	66/66	0.98	0.18	36,41,63,68	0
5	SO4	M	802	5/5	0.99	0.09	89,89,90,90	0
12	FE2	M	500	1/1	1.00	0.16	50,50,50,50	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.

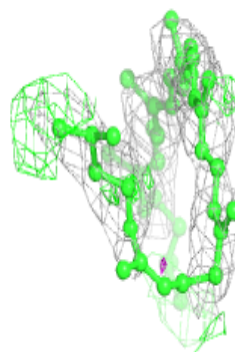
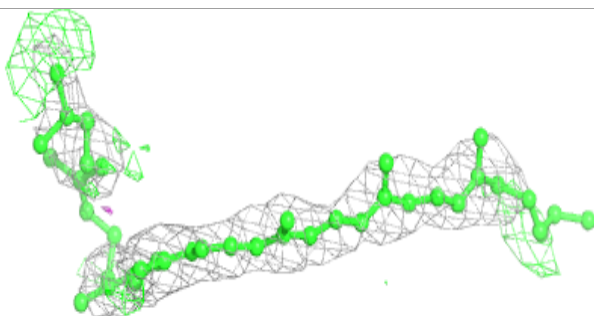
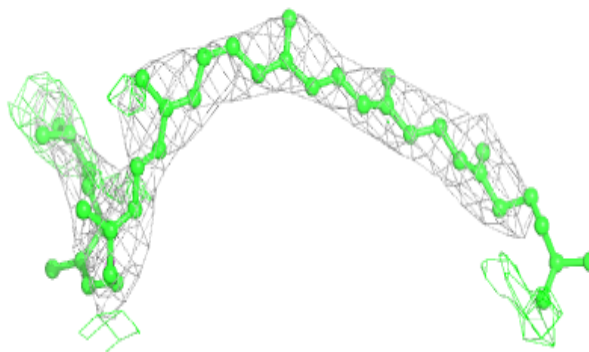
Electron density around UQ1 L 503:

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

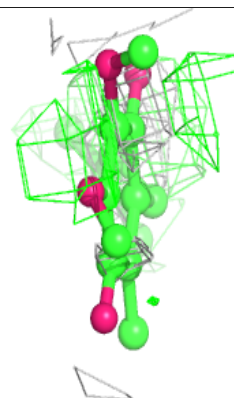
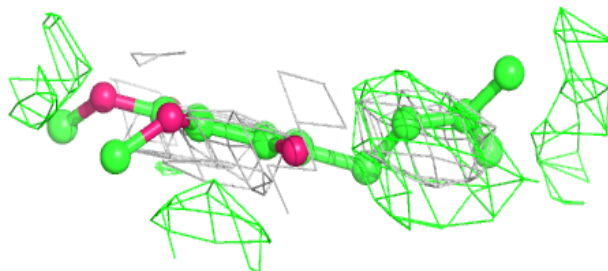
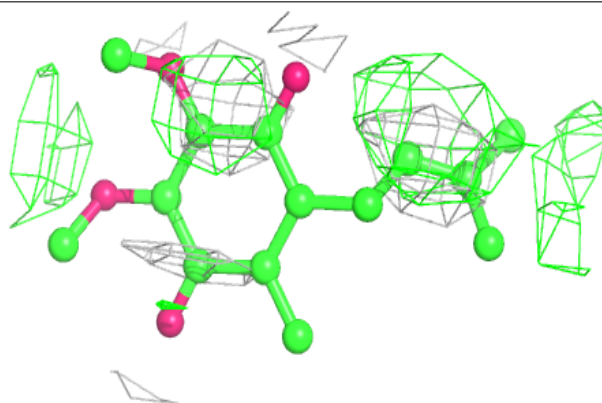


Electron density around NS5 M 600:

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

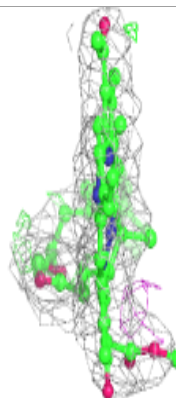
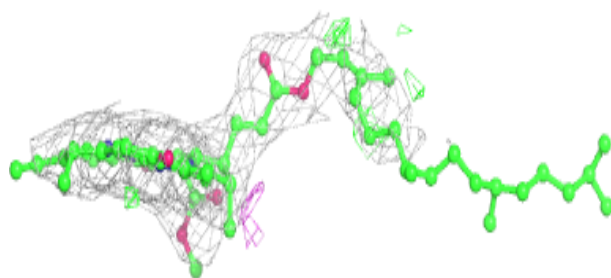
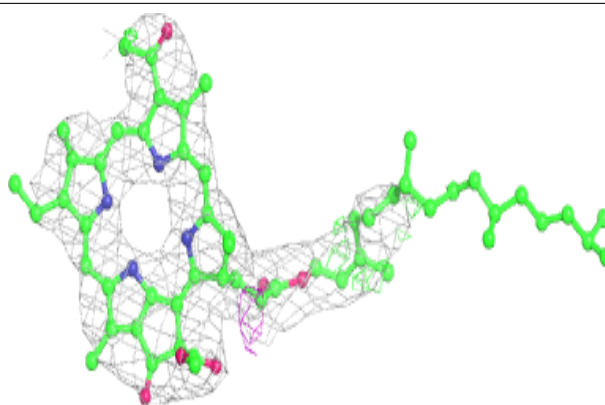
**Electron density around UQ1 L 502:**

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

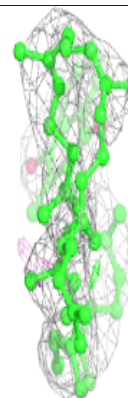
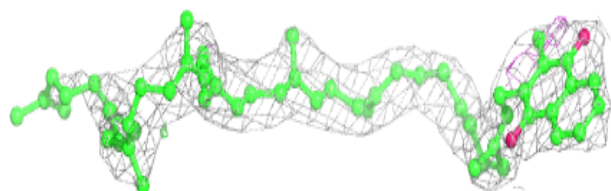
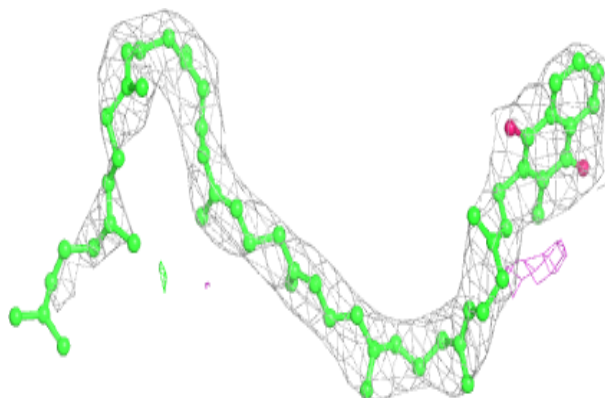


Electron density around BPB M 402:

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

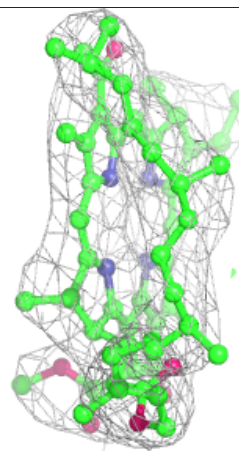
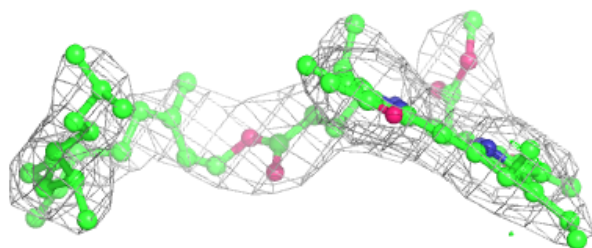
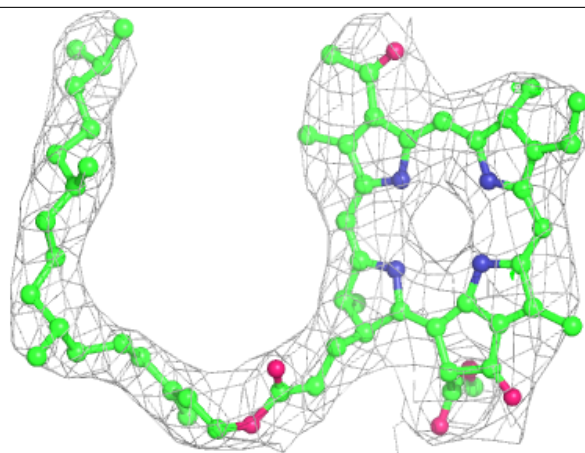
**Electron density around MQ9 M 501:**

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



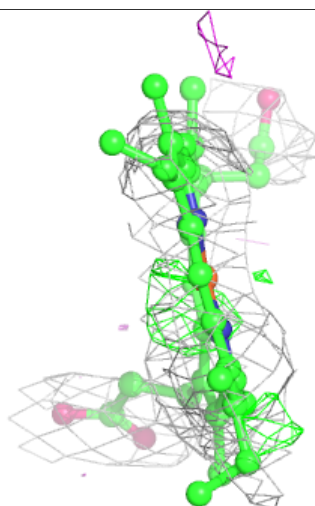
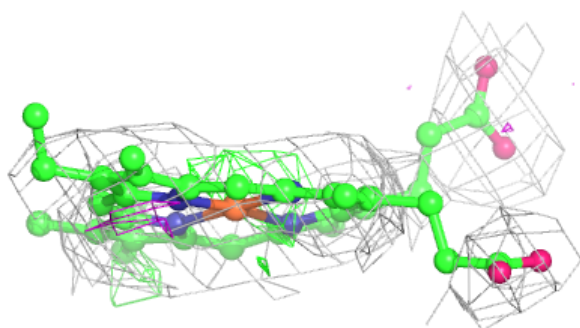
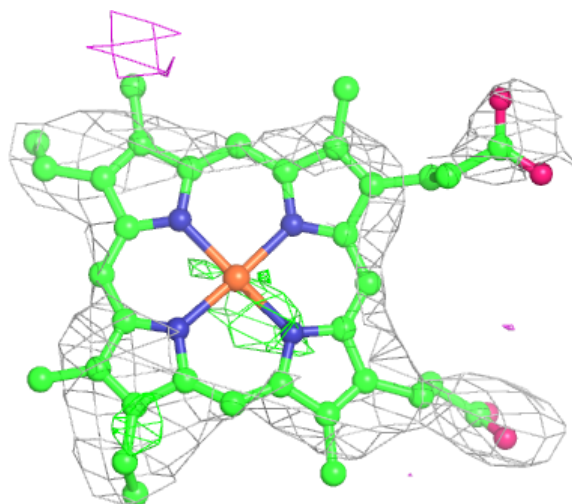
Electron density around BPB L 402:

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



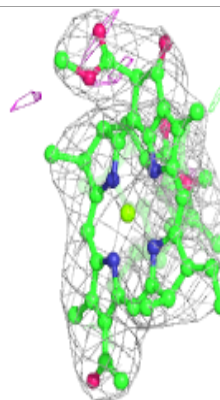
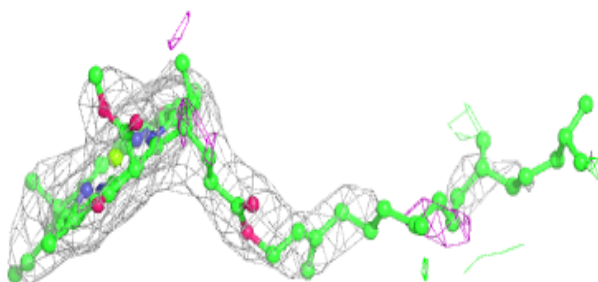
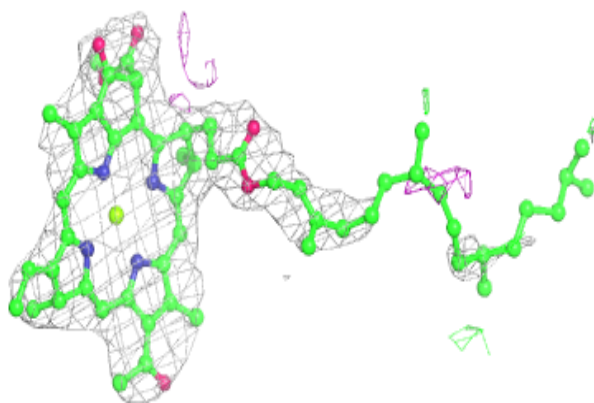
Electron density around HEC C 401:

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

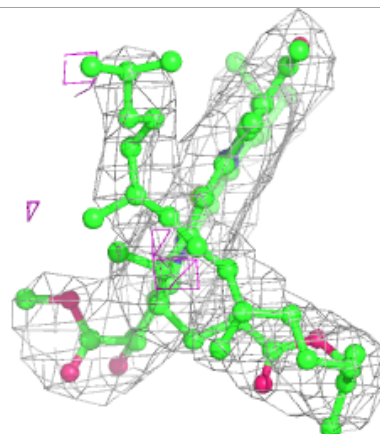
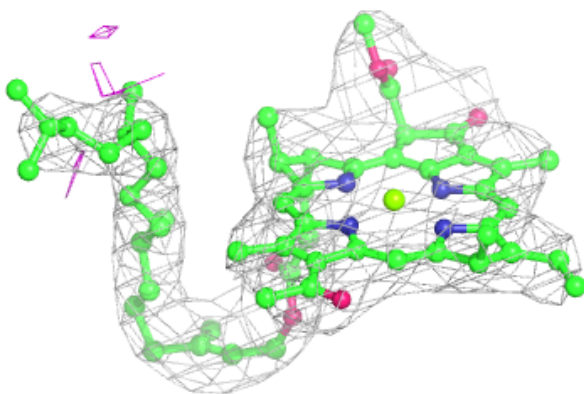
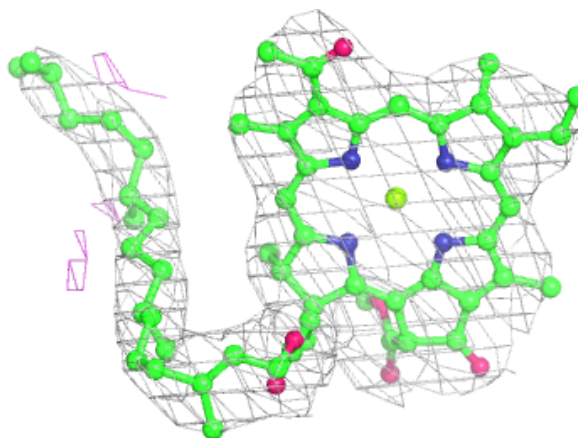


Electron density around BCB M 400:

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

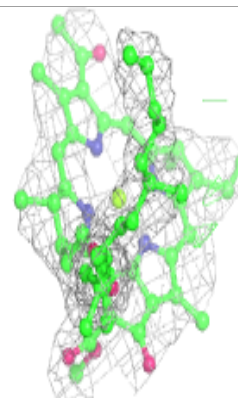
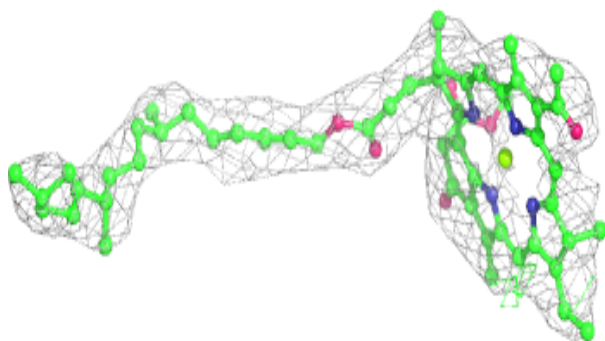
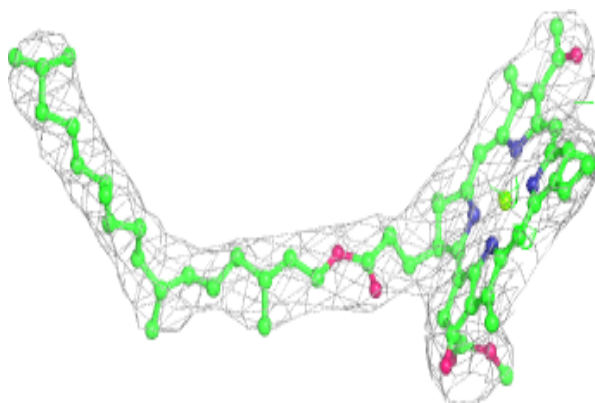
**Electron density around BCB L 401:**

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

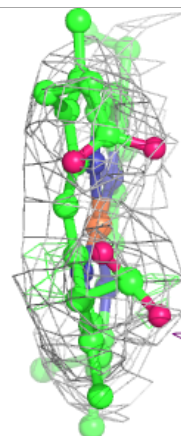
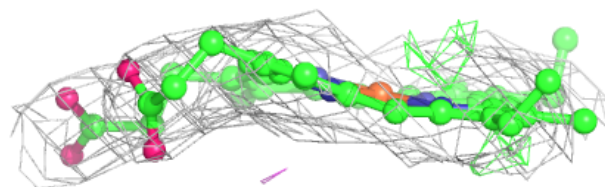
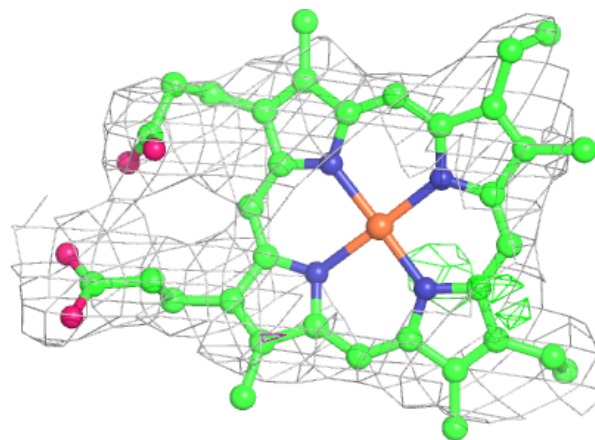


Electron density around BCB L 400:

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

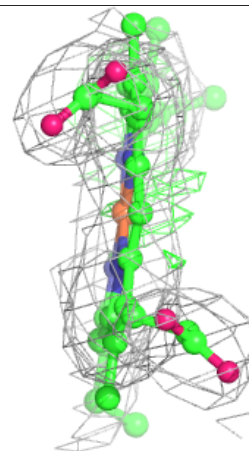
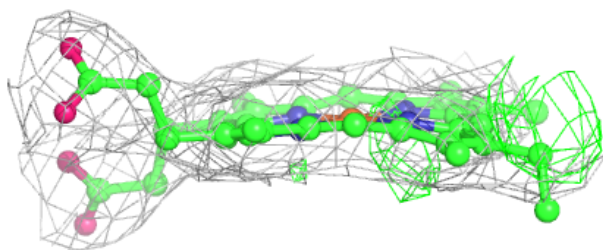
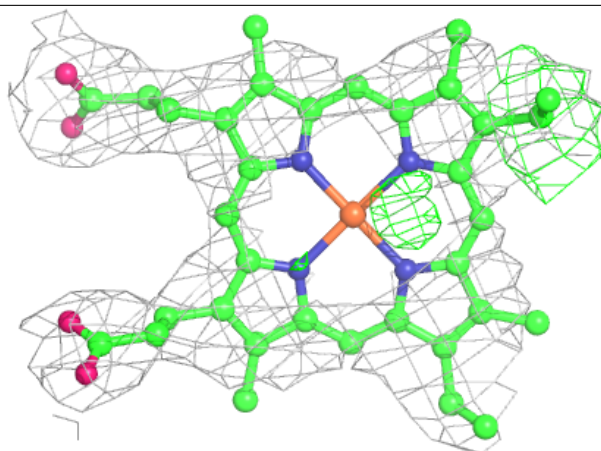
**Electron density around HEC C 402:**

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



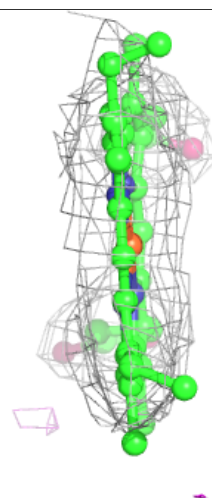
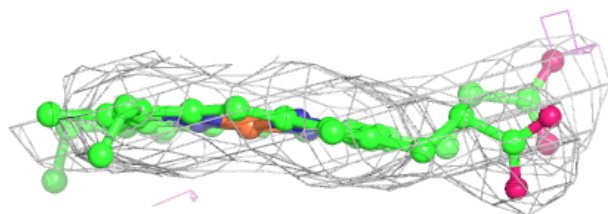
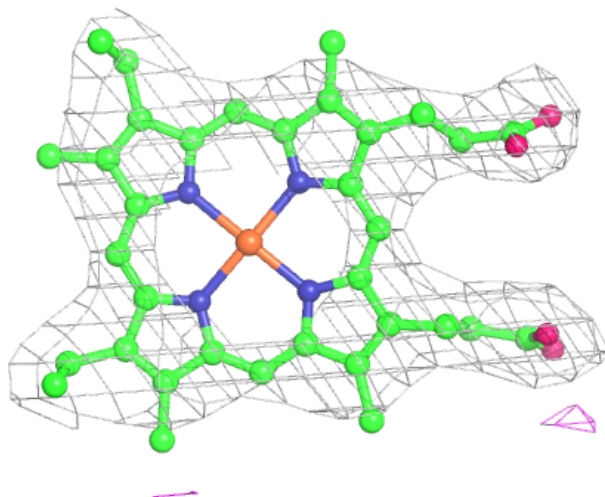
Electron density around HEC C 403:

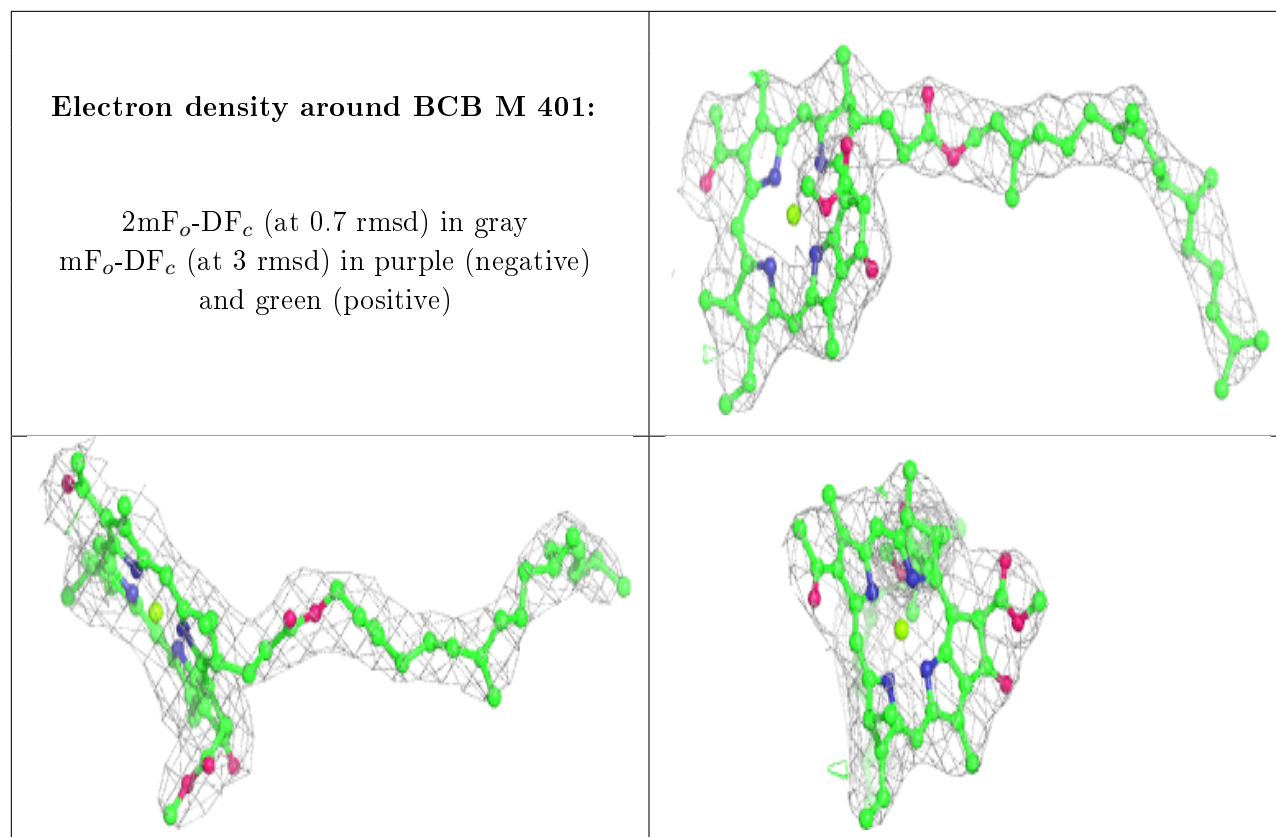
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 404:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.