



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 14, 2020 – 03:19 pm BST

PDB ID : 2I5N
Title : 1.96 Å X-ray structure of photosynthetic reaction center from Rhodospseudomonas viridis: Crystals grown by microfluidic technique
Authors : Li, L.; Mustafi, D.; Fu, Q.; Tereshko, V.; Chen, D.L.; Tice, J.D.; Ismagilov, R.F.
Deposited on : 2006-08-25
Resolution : 1.96 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

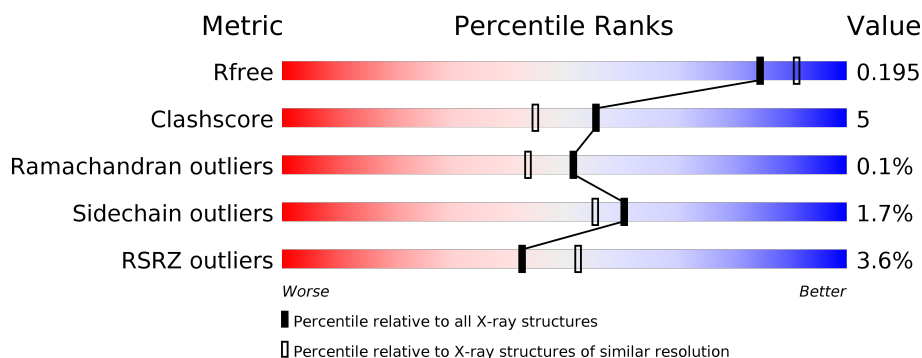
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>93%</div> <div>5% ..</div> </div> </div>
2	H	258	<div> <div>8%</div> <div> <div></div> <div>89%</div> <div>8% .</div> </div> </div>
3	L	273	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6% .</div> </div> </div>
4	M	323	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>8% .</div> </div> </div>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 11035 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	1	0
			1959	1251	335	371	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	1	FME	MET	MODIFIED RESIDUE	UNP P06008

- 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	2	0
			2174	1462	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	2	0
			2559	1704	419	424	12			

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



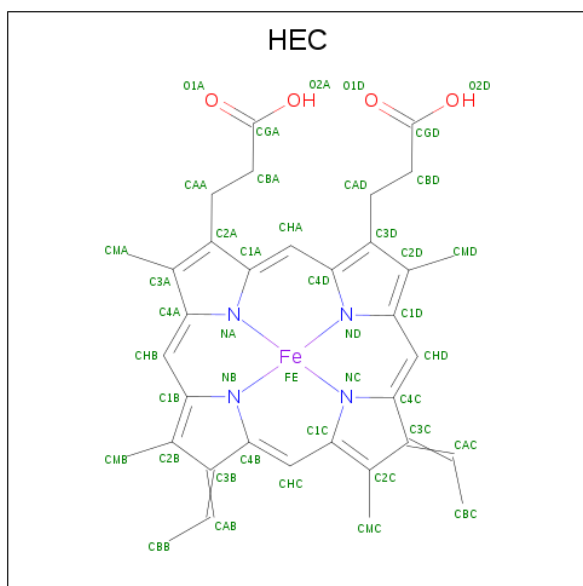
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	5	0
			5	4	1		
5	C	1	Total	O	S	5	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total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

Continued on next page...

Continued from previous page...

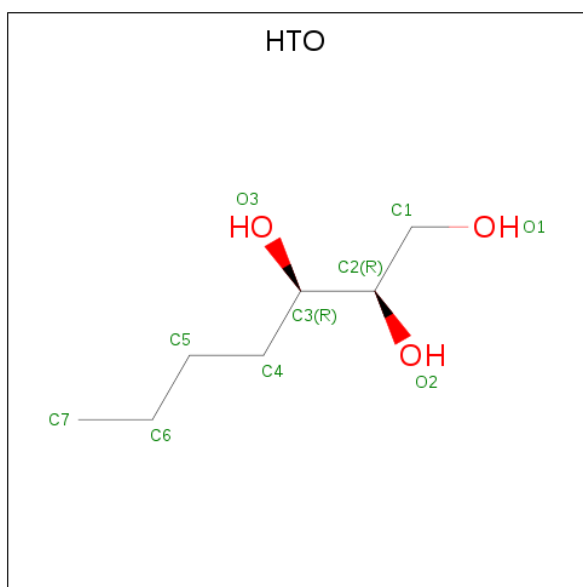
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	1	Total	O	S	0	0
			5	4	1		
5	M	1	Total	O	S	0	0
			5	4	1		
5	M	1	Total	O	S	5	0
			5	4	1		
5	M	1	Total	O	S	5	0
			5	4	1		
5	M	1	Total	O	S	5	0
			5	4	1		

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



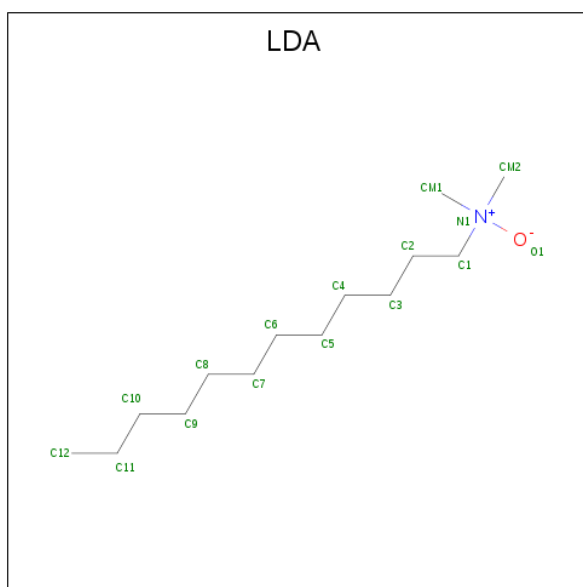
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
6	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
6	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
6	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- 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		
7	L	1	Total	C	O	10	0
			10	7	3		
7	L	1	Total	C	O	10	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 UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	1	Total	C	10	0
			10	10		
9	L	3	Total	C	30	0
			30	30		
9	M	2	Total	C	20	0
			20	20		

- Molecule 10 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	1	Total	Fe	0	0
			1	1		

- Molecule 11 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C₅₅H₇₂MgN₄O₆).



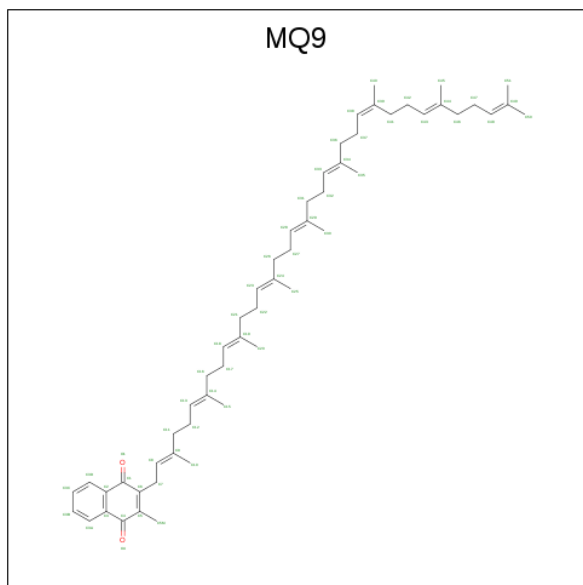
Mol	Chain	Residues	Atoms				ZeroOcc	AltCon	
11	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
11	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
11	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
11	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

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



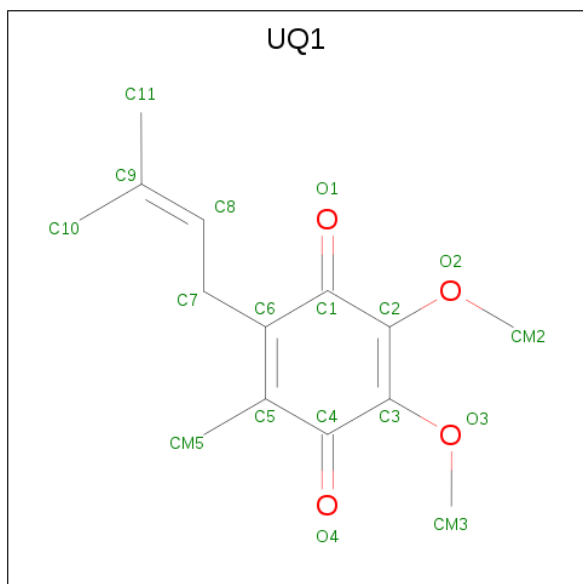
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



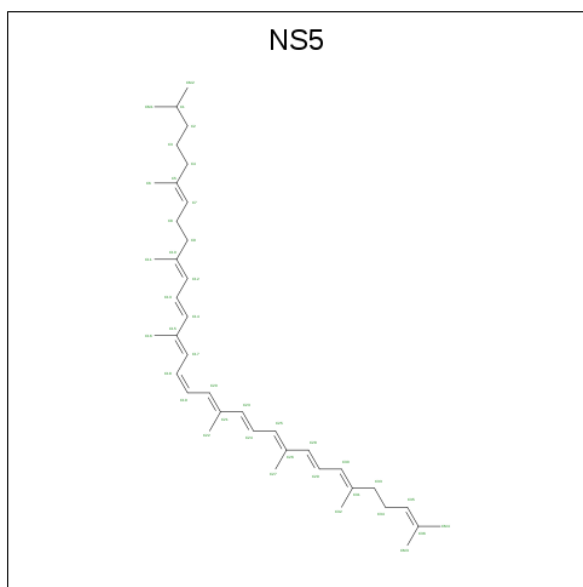
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	L	1	Total	C	O	0	0
			58	56	2		

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



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

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



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	M	1	Total	C	0	1
			44	44		

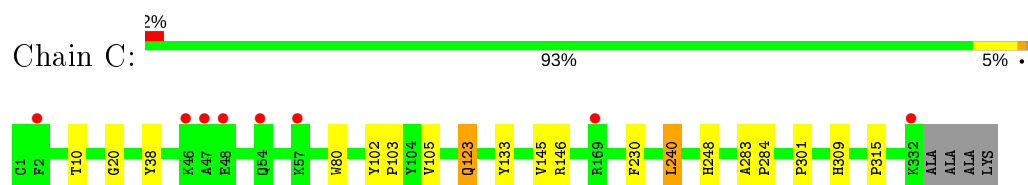
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	C	327	Total	O	0	0
			327	327		
16	H	179	Total	O	0	0
			179	179		
16	L	100	Total	O	0	0
			100	100		
16	M	165	Total	O	0	0
			165	165		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	220.40 Å 220.40 Å 113.01 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.96 19.97 – 1.96	Depositor EDS
% Data completeness (in resolution range)	96.5 (20.00-1.96) 96.5 (19.97-1.96)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.96 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.190 0.178 , 0.195	Depositor DCC
R_{free} test set	9533 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11035	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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

5.1 Standard geometry

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, UNL, 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	0.37	0/2665	0.82	0/3633
2	H	0.37	0/1999	0.88	3/2728 (0.1%)
3	L	0.41	0/2274	0.87	6/3105 (0.2%)
4	M	0.38	0/2673	0.85	4/3655 (0.1%)
All	All	0.38	0/9611	0.85	13/13121 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	239	ARG	NE-CZ-NH1	7.97	124.29	120.30
3	L	12	ARG	NE-CZ-NH2	-7.55	116.52	120.30
4	M	239	ARG	NE-CZ-NH2	-7.33	116.64	120.30
3	L	12	ARG	NE-CZ-NH1	6.46	123.53	120.30
4	M	2	ASP	CB-CG-OD2	6.36	124.02	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	248	HIS	Peptide

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	2598	0	2568	13	0
2	H	1959	0	1947	8	0
3	L	2174	0	2102	13	0
4	M	2559	0	2458	29	0
5	C	35	0	0	0	0
5	H	20	0	0	0	0
5	L	5	0	0	0	0
5	M	35	0	0	1	0
6	C	172	0	120	5	0
7	C	20	0	32	1	0
7	H	10	0	16	0	0
7	L	20	0	32	0	0
8	H	32	0	62	0	0
8	L	16	0	31	0	0
8	M	16	0	31	1	0
9	H	10	0	0	0	0
9	L	30	0	0	0	0
9	M	20	0	0	0	0
10	L	1	0	0	0	0
11	L	132	0	144	9	0
11	M	132	0	144	23	0
12	L	65	0	74	4	0
12	M	65	0	74	17	0
13	L	58	0	80	3	0
14	L	36	0	36	0	0
15	M	44	0	18	0	0
16	C	327	0	0	3	0
16	H	179	0	0	0	0
16	L	100	0	0	0	0
16	M	165	0	0	0	0
All	All	11035	0	9969	102	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 102 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)
12:M:402:BPB:H4	12:M:402:BPB:H7A	1.29	1.14
3:L:39:ILE:HD12	13:L:501:MQ9:H43	1.42	0.99
4:M:120:MET:HE3	11:M:401:BCB:H193	1.47	0.96
12:M:402:BPB:C7	12:M:402:BPB:H4	1.97	0.91
4:M:59:PHE:HA	12:M:402:BPB:H4A	1.54	0.86

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%)	318 (96%)	12 (4%)	0	100	100
2	H	247/258 (96%)	246 (100%)	1 (0%)	0	100	100
3	L	273/273 (100%)	268 (98%)	5 (2%)	0	100	100
4	M	323/323 (100%)	315 (98%)	7 (2%)	1 (0%)	41	30
All	All	1173/1190 (99%)	1147 (98%)	25 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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%)	277 (99%)	3 (1%)	73	71
2	H	206/212 (97%)	201 (98%)	5 (2%)	49	40
3	L	220/218 (101%)	216 (98%)	4 (2%)	59	53
4	M	251/249 (101%)	247 (98%)	4 (2%)	62	58
All	All	957/961 (100%)	941 (98%)	16 (2%)	60	55

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	236	ASP
3	L	80	LEU
4	M	51	LEU
2	H	227	ARG
4	M	147	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	225	GLN
4	M	147	ASN
3	L	213	ASN
2	H	102	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 ⓘ

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	0.84	0	7,9,11	2.68	3 (42%)

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	-	3/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-6.18	113.32	122.82
2	H	1	FME	CE-SD-CG	2.40	108.63	100.40
2	H	1	FME	O-C-CA	-2.03	119.46	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

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 50 ligands modelled in this entry, 6 are unknown and 1 is monoatomic - leaving 43 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$
6	HEC	C	402	1	26,50,50	1.74	4 (15%)	18,82,82	1.47	2 (11%)
7	HTO	C	706	-	9,9,9	0.38	0	10,10,10	0.62	0
5	SO4	M	818	-	4,4,4	0.13	0	6,6,6	0.15	0
15	NS5	M	600[A]	-	39,39,39	1.47	1 (2%)	44,46,46	1.96	11 (25%)
5	SO4	H	807	-	4,4,4	0.13	0	6,6,6	0.11	0
5	SO4	C	813	-	4,4,4	0.20	0	6,6,6	0.08	0
5	SO4	H	803	-	4,4,4	0.13	0	6,6,6	0.22	0
5	SO4	M	805	-	4,4,4	0.14	0	6,6,6	0.31	0
6	HEC	C	404	1	26,50,50	1.64	3 (11%)	18,82,82	1.58	3 (16%)
5	SO4	C	815	-	4,4,4	0.13	0	6,6,6	0.18	0
5	SO4	C	811	-	4,4,4	0.15	0	6,6,6	0.12	0
7	HTO	H	705	-	9,9,9	0.43	0	10,10,10	0.86	0
5	SO4	C	810	-	4,4,4	0.15	0	6,6,6	0.08	0
8	LDA	L	702	-	12,15,15	1.96	1 (8%)	14,17,17	0.67	0
5	SO4	C	817	-	4,4,4	0.14	0	6,6,6	0.16	0
5	SO4	L	814	-	4,4,4	0.18	0	6,6,6	0.24	0
7	HTO	L	708	-	9,9,9	0.33	0	10,10,10	0.61	0
12	BPB	M	402	-	64,70,70	1.55	8 (12%)	64,101,101	1.79	13 (20%)
14	UQ1	L	502	-	18,18,18	2.03	2 (11%)	22,25,25	1.09	2 (9%)
5	SO4	M	819	-	4,4,4	0.11	0	6,6,6	0.27	0
5	SO4	H	812	-	4,4,4	0.15	0	6,6,6	0.09	0
8	LDA	H	701	-	12,15,15	1.85	1 (8%)	14,17,17	0.68	0
14	UQ1	L	503	-	18,18,18	2.16	2 (11%)	22,25,25	1.12	2 (9%)
5	SO4	C	808	-	4,4,4	0.13	0	6,6,6	0.26	0
11	BCB	L	401	3	60,74,74	3.56	20 (33%)	48,115,115	2.22	13 (27%)
5	SO4	M	801	-	4,4,4	0.17	0	6,6,6	0.33	0
7	HTO	L	709	-	9,9,9	0.32	0	10,10,10	0.68	0
12	BPB	L	402	-	64,70,70	1.57	9 (14%)	64,101,101	1.76	11 (17%)
5	SO4	M	816	-	4,4,4	0.14	0	6,6,6	0.12	0
5	SO4	M	802	-	4,4,4	0.19	0	6,6,6	0.18	0
11	BCB	M	401	4	60,74,74	3.72	23 (38%)	48,115,115	2.35	14 (29%)
13	MQ9	L	501	-	59,59,59	1.77	18 (30%)	72,75,75	1.35	14 (19%)
5	SO4	M	804	-	4,4,4	0.16	0	6,6,6	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HEC	C	401	1	26,50,50	1.67	2 (7%)	18,82,82	1.61	4 (22%)
5	SO4	C	809	-	4,4,4	0.11	0	6,6,6	0.16	0
7	HTO	C	707	-	9,9,9	0.46	0	10,10,10	0.74	0
8	LDA	H	703	-	12,15,15	1.88	1 (8%)	14,17,17	0.61	0
6	HEC	C	403	1	26,50,50	1.61	3 (11%)	18,82,82	1.59	4 (22%)
8	LDA	M	704	-	12,15,15	2.03	1 (8%)	14,17,17	0.44	0
11	BCB	M	400	4	60,74,74	3.69	22 (36%)	48,115,115	2.24	16 (33%)
11	BCB	L	400	3	60,74,74	3.62	21 (35%)	48,115,115	2.36	15 (31%)
5	SO4	H	806	-	4,4,4	0.22	0	6,6,6	0.16	0
15	NS5	M	600[B]	-	39,39,39	1.49	1 (2%)	44,46,46	1.95	11 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEC	C	402	1	-	1/6/54/54	-
7	HTO	C	706	-	-	5/10/10/10	-
15	NS5	M	600[A]	-	-	8/43/43/43	-
15	NS5	M	600[B]	-	-	8/43/43/43	-
11	BCB	M	400	4	-	17/41/177/177	-
6	HEC	C	404	1	-	0/6/54/54	-
7	HTO	H	705	-	-	5/10/10/10	-
8	LDA	L	702	-	-	4/13/13/13	-
8	LDA	M	704	-	-	3/13/13/13	-
7	HTO	L	708	-	-	3/10/10/10	-
12	BPB	M	402	-	-	16/47/105/105	0/5/6/6
8	LDA	H	701	-	-	3/13/13/13	-
14	UQ1	L	503	-	-	0/9/33/33	0/1/1/1
11	BCB	L	401	3	-	7/41/177/177	-
14	UQ1	L	502	-	-	2/9/33/33	0/1/1/1
7	HTO	L	709	-	-	2/10/10/10	-
12	BPB	L	402	-	-	5/47/105/105	0/5/6/6
13	MQ9	L	501	-	-	13/53/73/73	0/2/2/2
11	BCB	M	401	4	-	12/41/177/177	-
6	HEC	C	401	1	-	0/6/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEC	C	403	1	-	0/6/54/54	-
7	HTO	C	707	-	-	6/10/10/10	-
8	LDA	H	703	-	-	5/13/13/13	-
11	BCB	L	400	3	-	8/41/177/177	-

The worst 5 of 143 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	400	BCB	C1A-CHA	-9.82	1.38	1.54
11	M	401	BCB	C1A-CHA	-9.35	1.39	1.54
11	L	401	BCB	C1A-CHA	-9.03	1.39	1.54
11	M	401	BCB	CHC-C4B	-8.92	1.39	1.53
11	M	401	BCB	CHB-C1B	-8.89	1.39	1.53

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	402	BPB	C3D-C2D-C1D	-6.84	95.91	105.87
12	M	402	BPB	C3D-C2D-C1D	-6.61	96.23	105.87
11	M	401	BCB	CHA-CBD-CGD	-6.01	101.42	115.02
11	M	400	BCB	C1D-CHD-C4C	5.80	124.74	112.37
11	L	400	BCB	CMB-C2B-C3B	5.67	128.38	114.29

There are no chirality outliers.

5 of 133 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	706	HTO	O2-C2-C3-C4
7	H	705	HTO	O2-C2-C3-C4
7	L	708	HTO	C1-C2-C3-O3
7	L	708	HTO	C1-C2-C3-C4
12	M	402	BPB	C11-C10-C8-C9

There are no ring outliers.

13 monomers are involved in 57 short contacts:

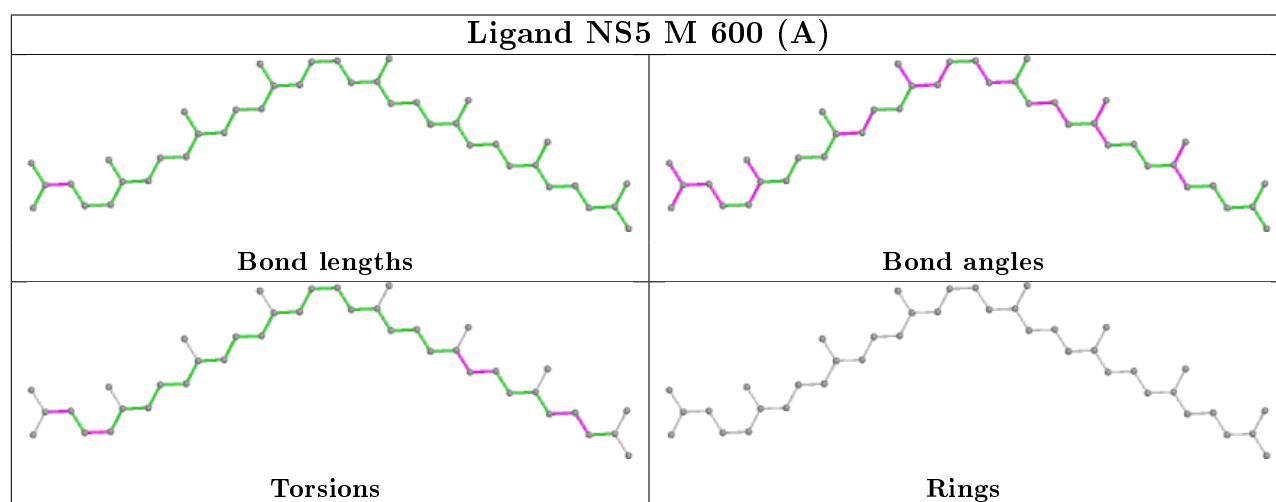
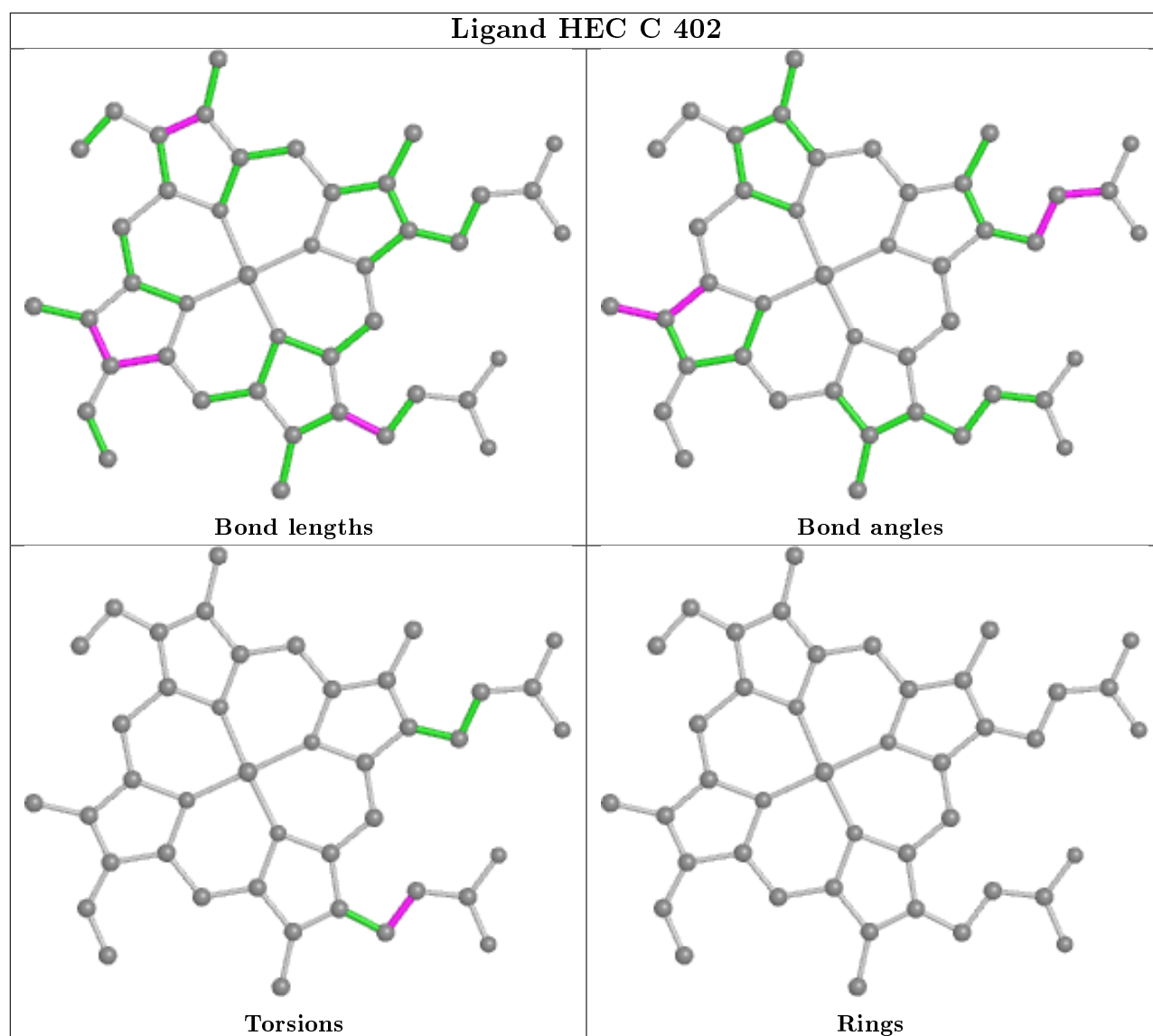
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	402	HEC	2	0
12	M	402	BPB	17	0
11	L	401	BCB	5	0

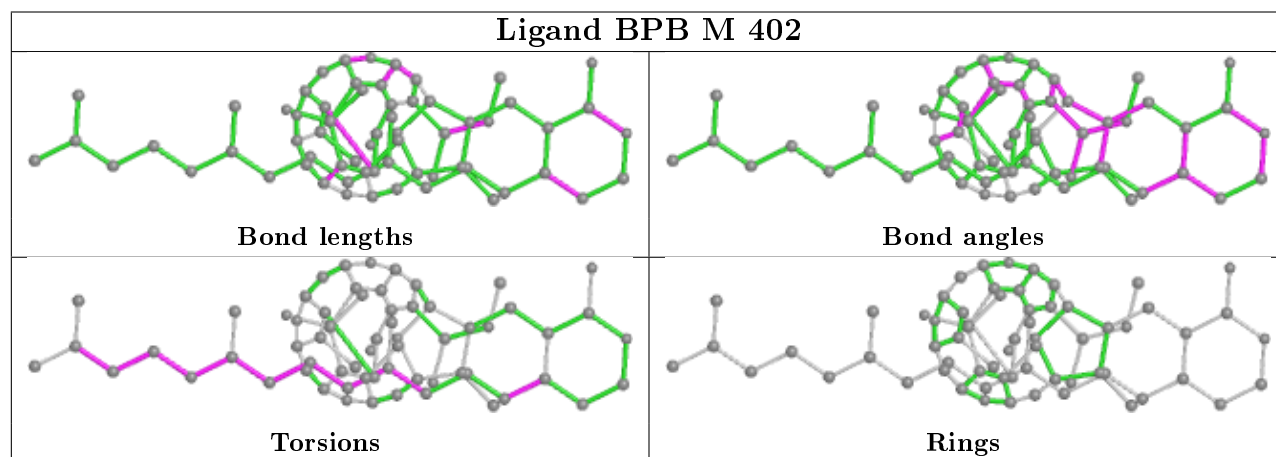
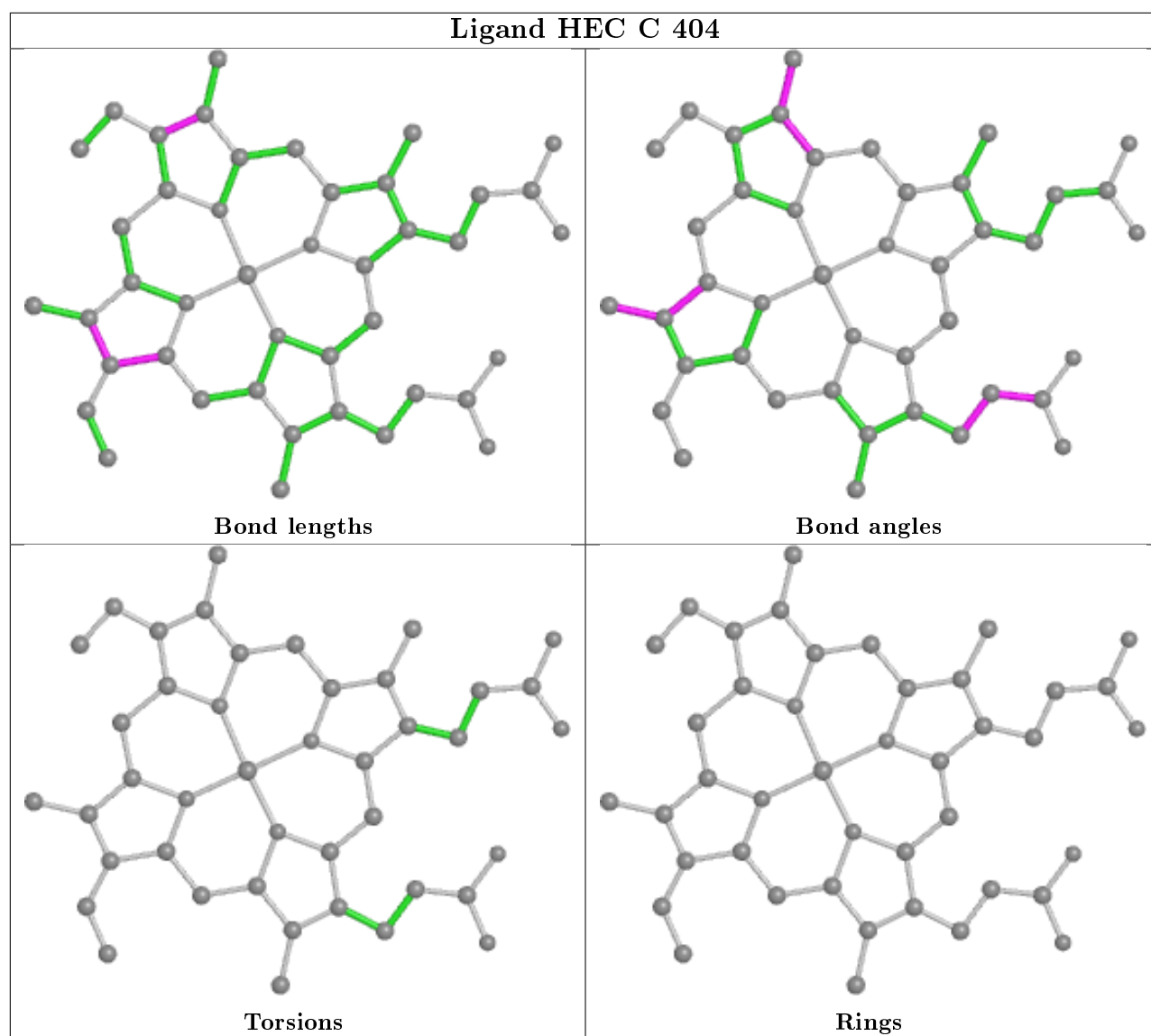
Continued on next page...

Continued from previous page...

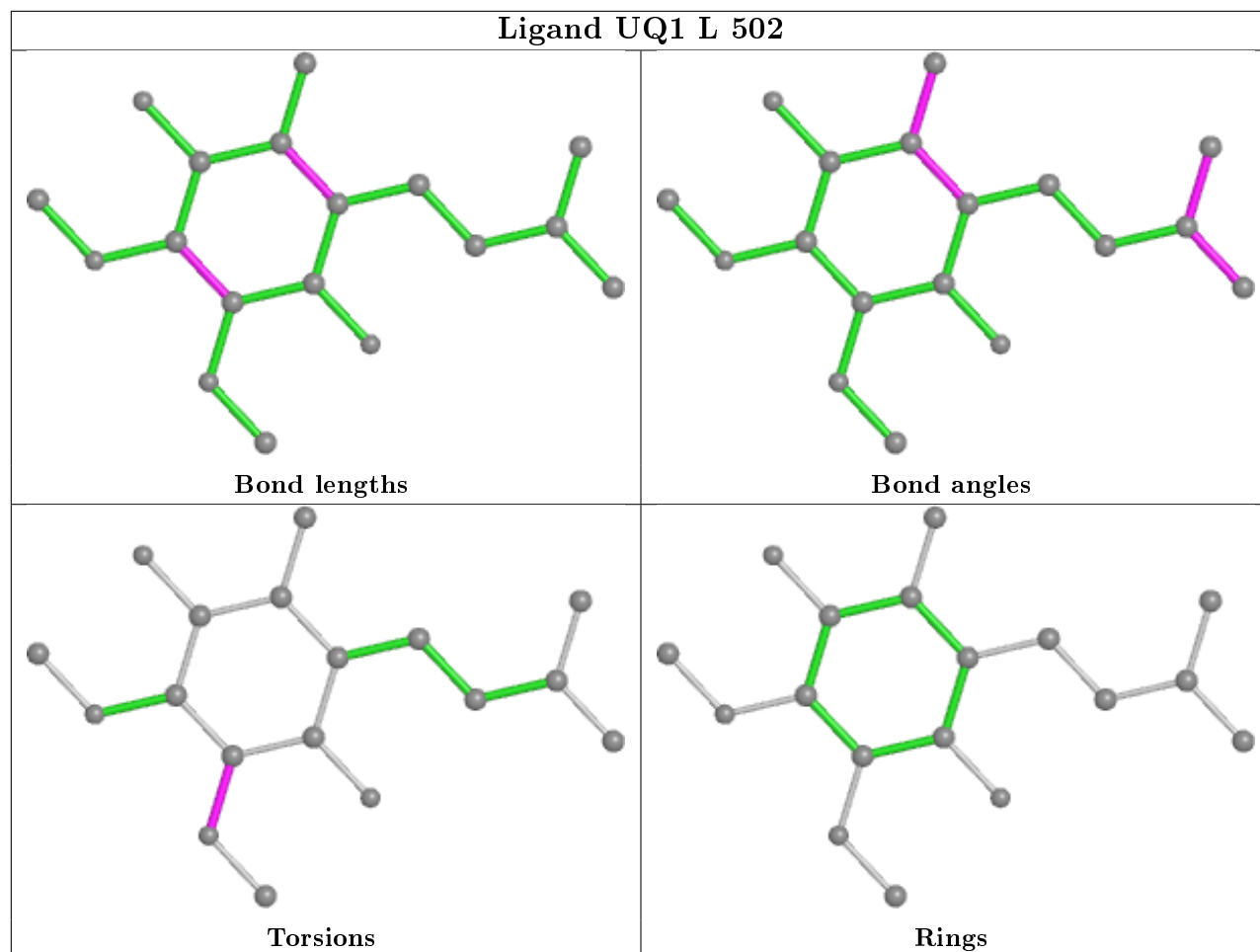
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	L	402	BPB	4	0
5	M	802	SO4	1	0
11	M	401	BCB	15	0
13	L	501	MQ9	3	0
6	C	401	HEC	1	0
7	C	707	HTO	1	0
6	C	403	HEC	2	0
8	M	704	LDA	1	0
11	M	400	BCB	9	0
11	L	400	BCB	4	0

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.

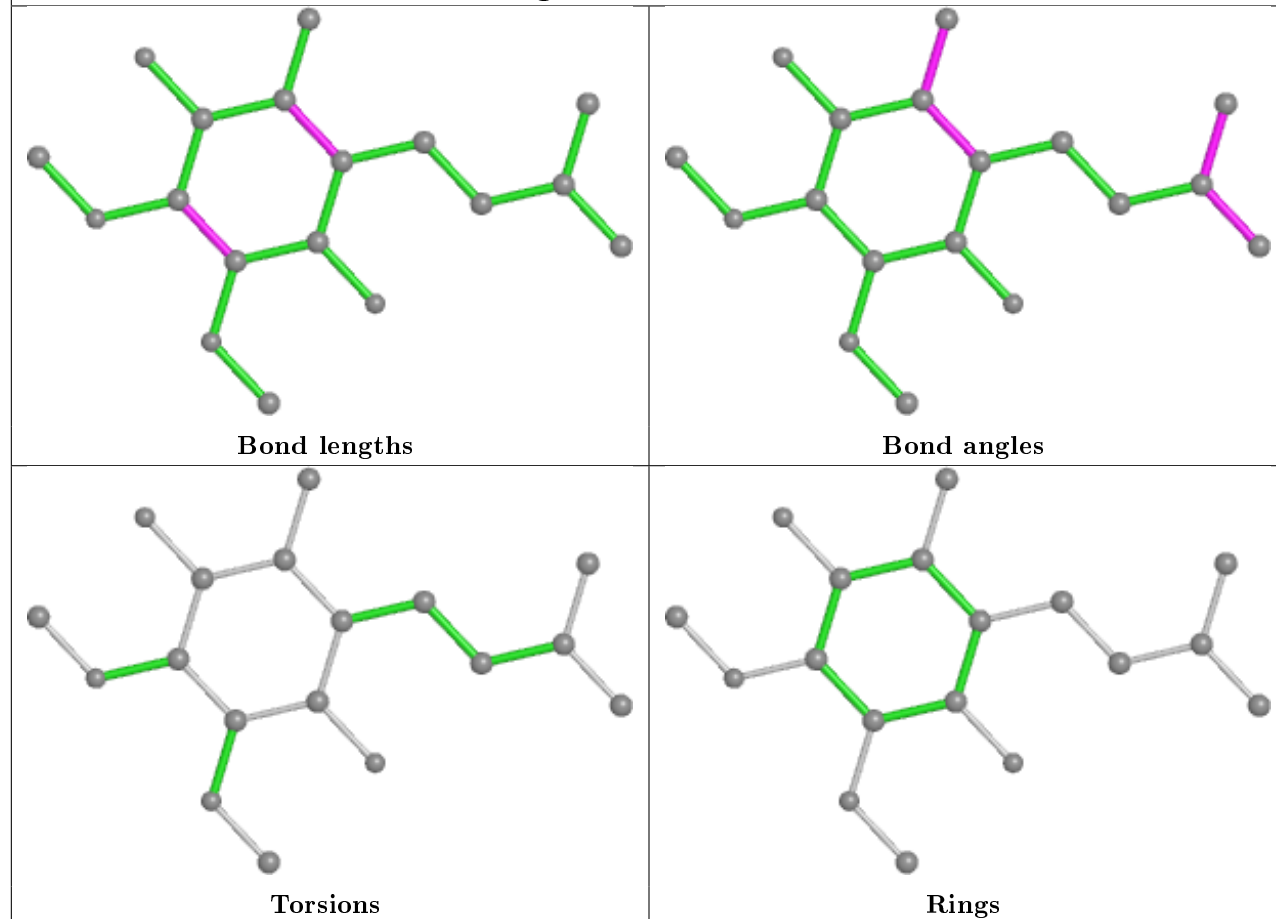




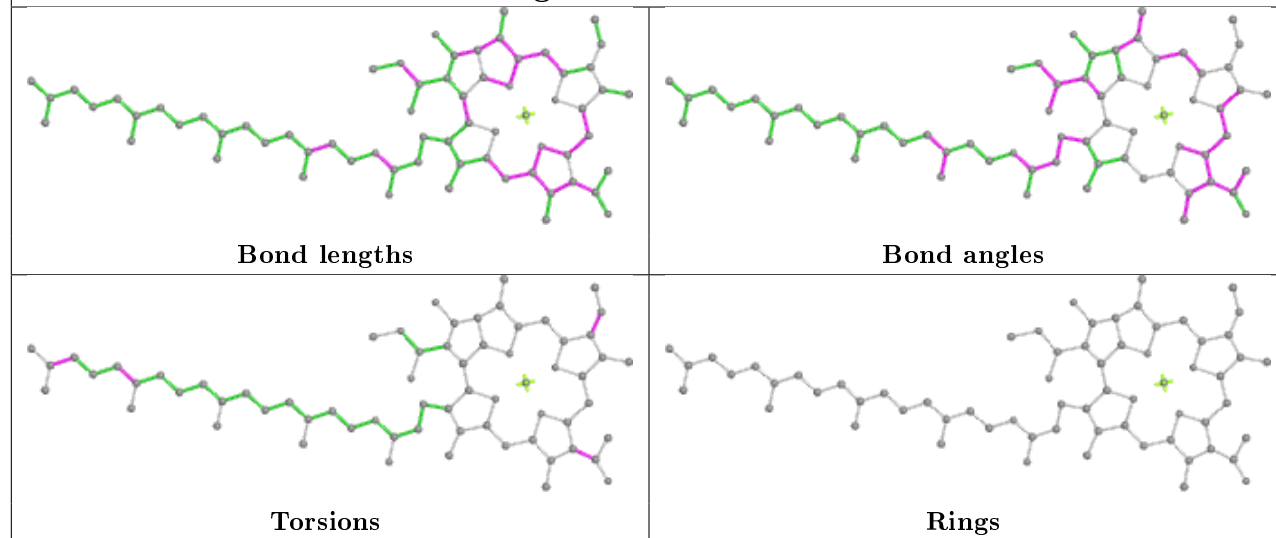
Ligand UQ1 L 502

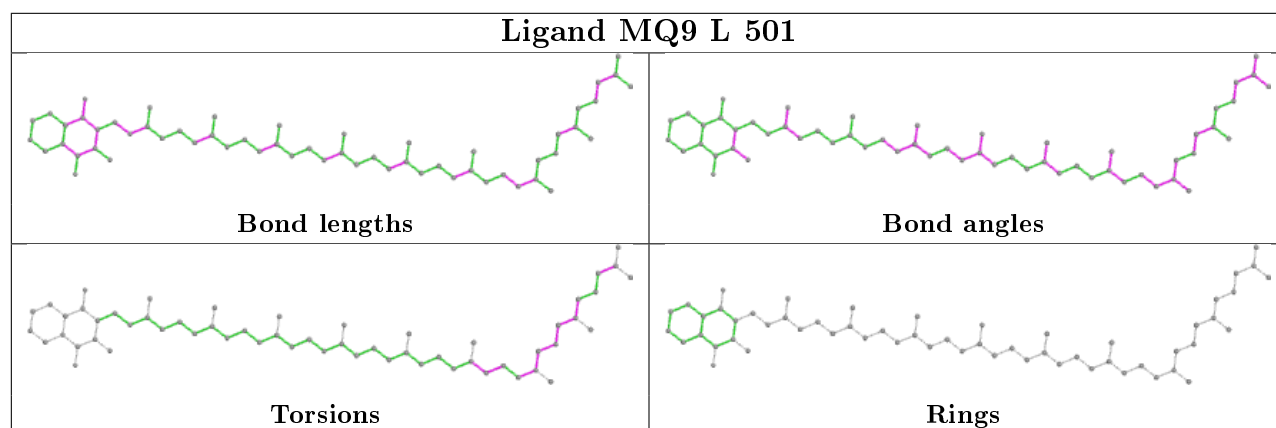
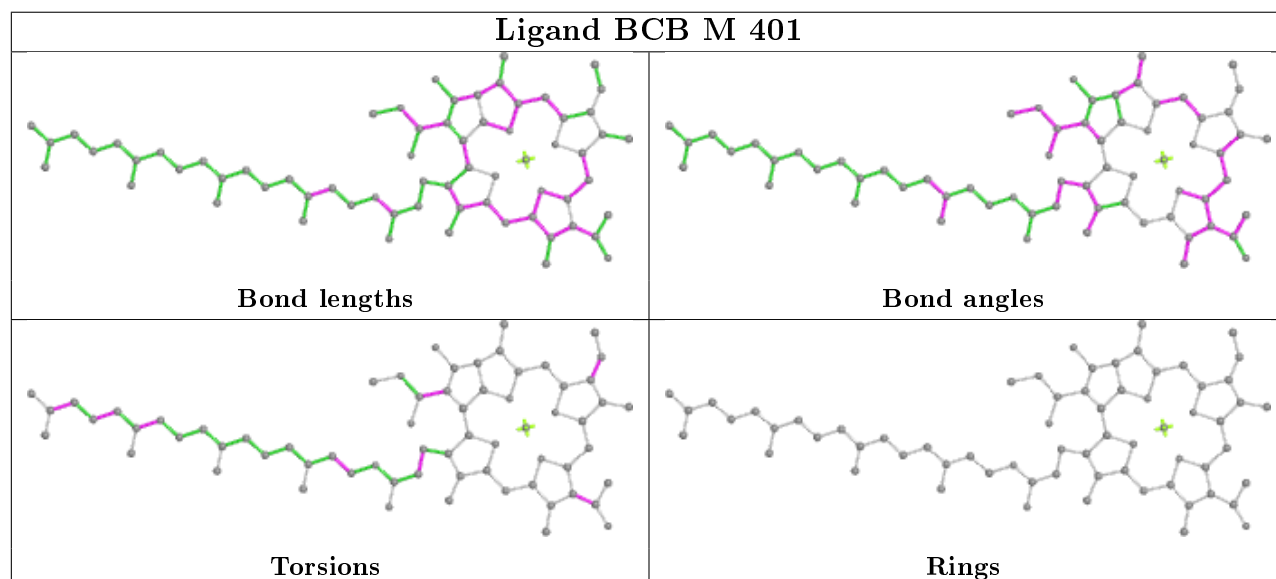
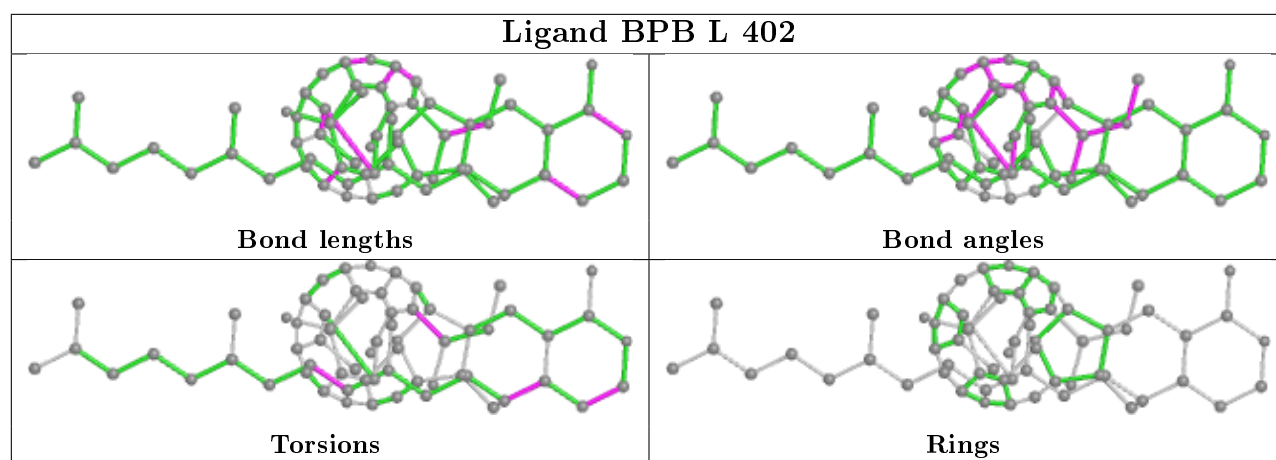


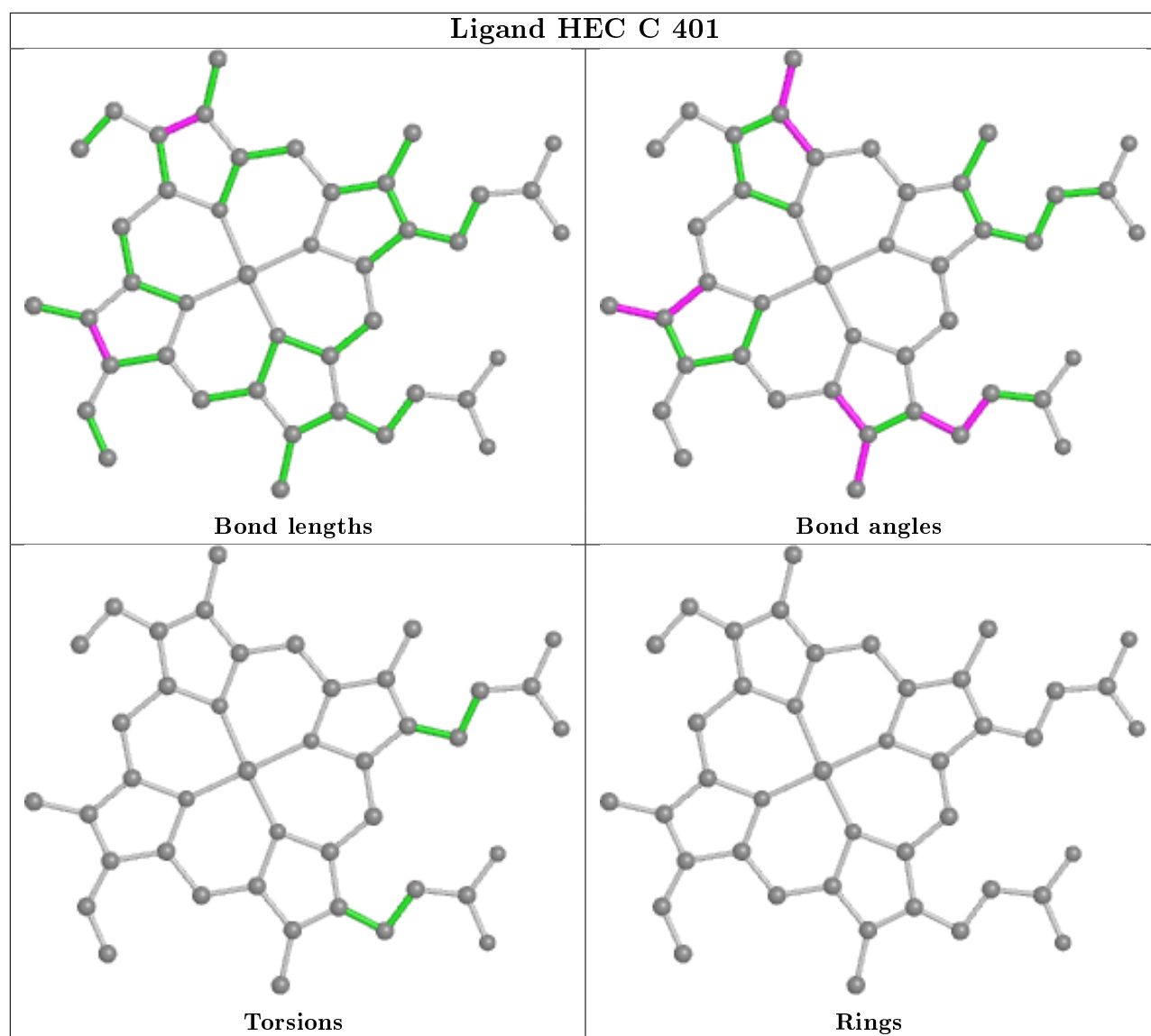
Ligand UQ1 L 503



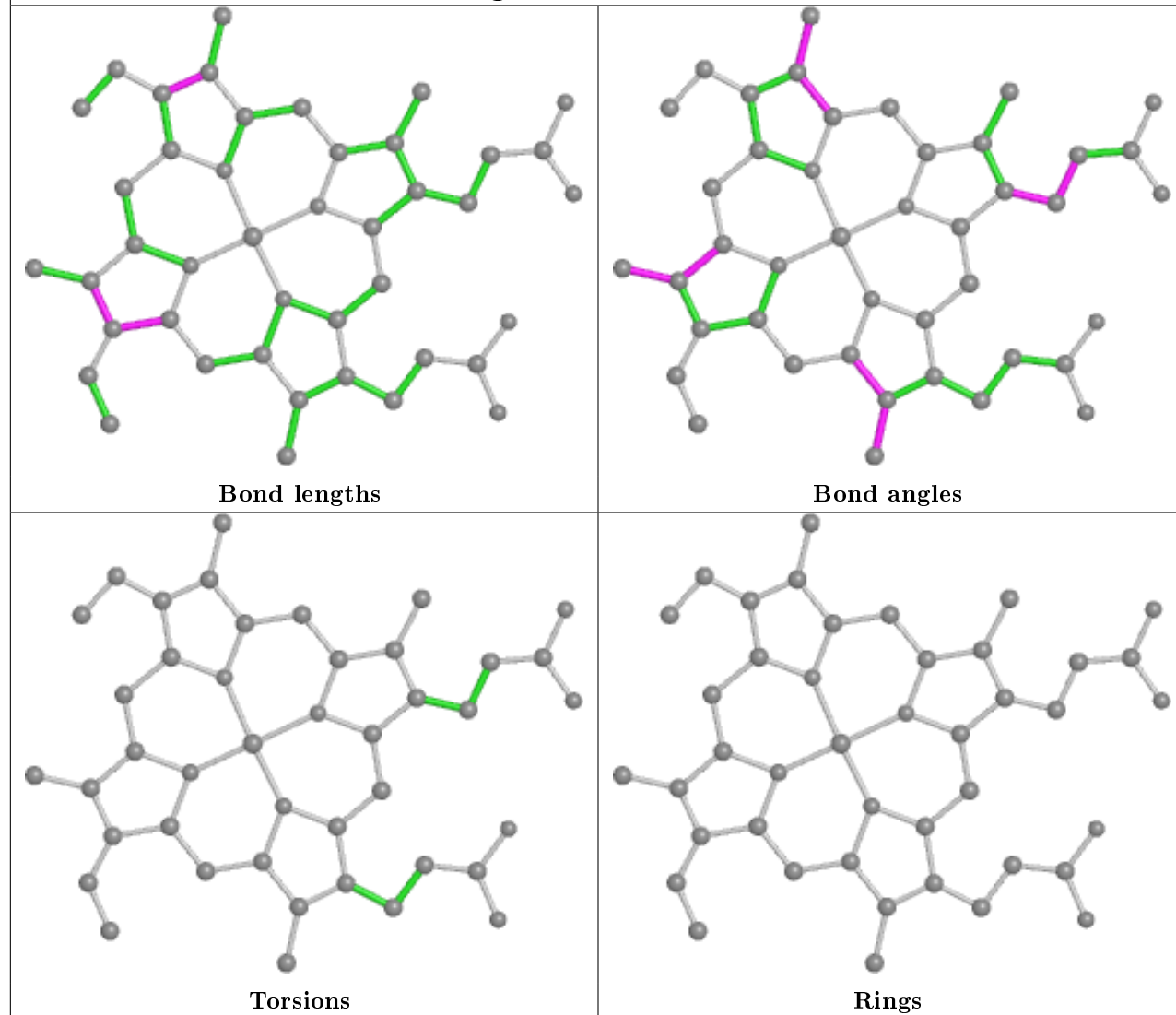
Ligand BCB L 401



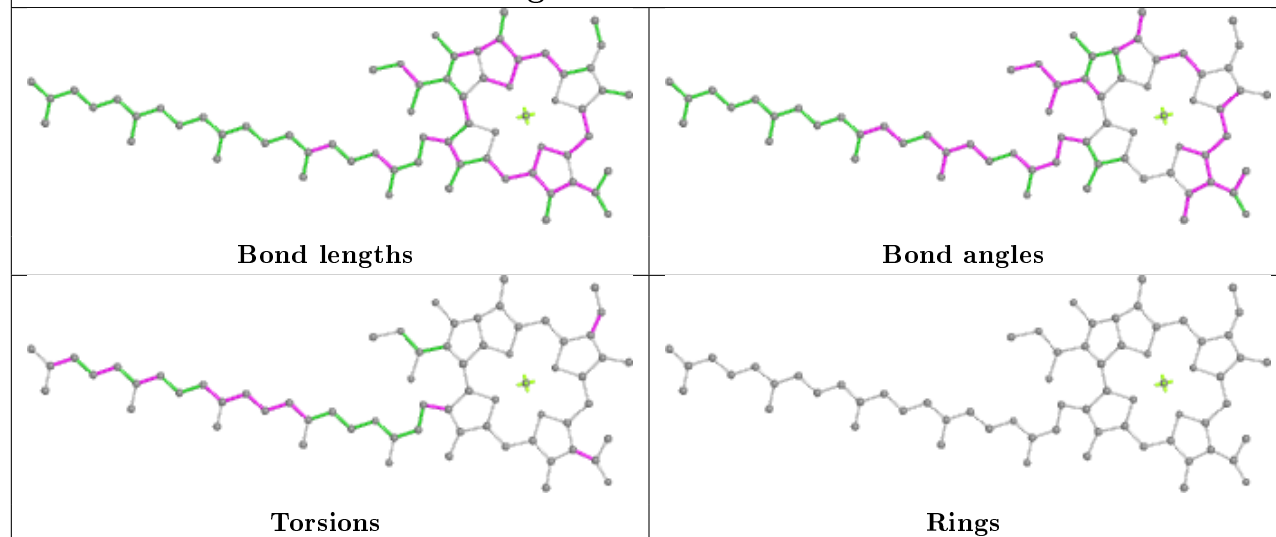


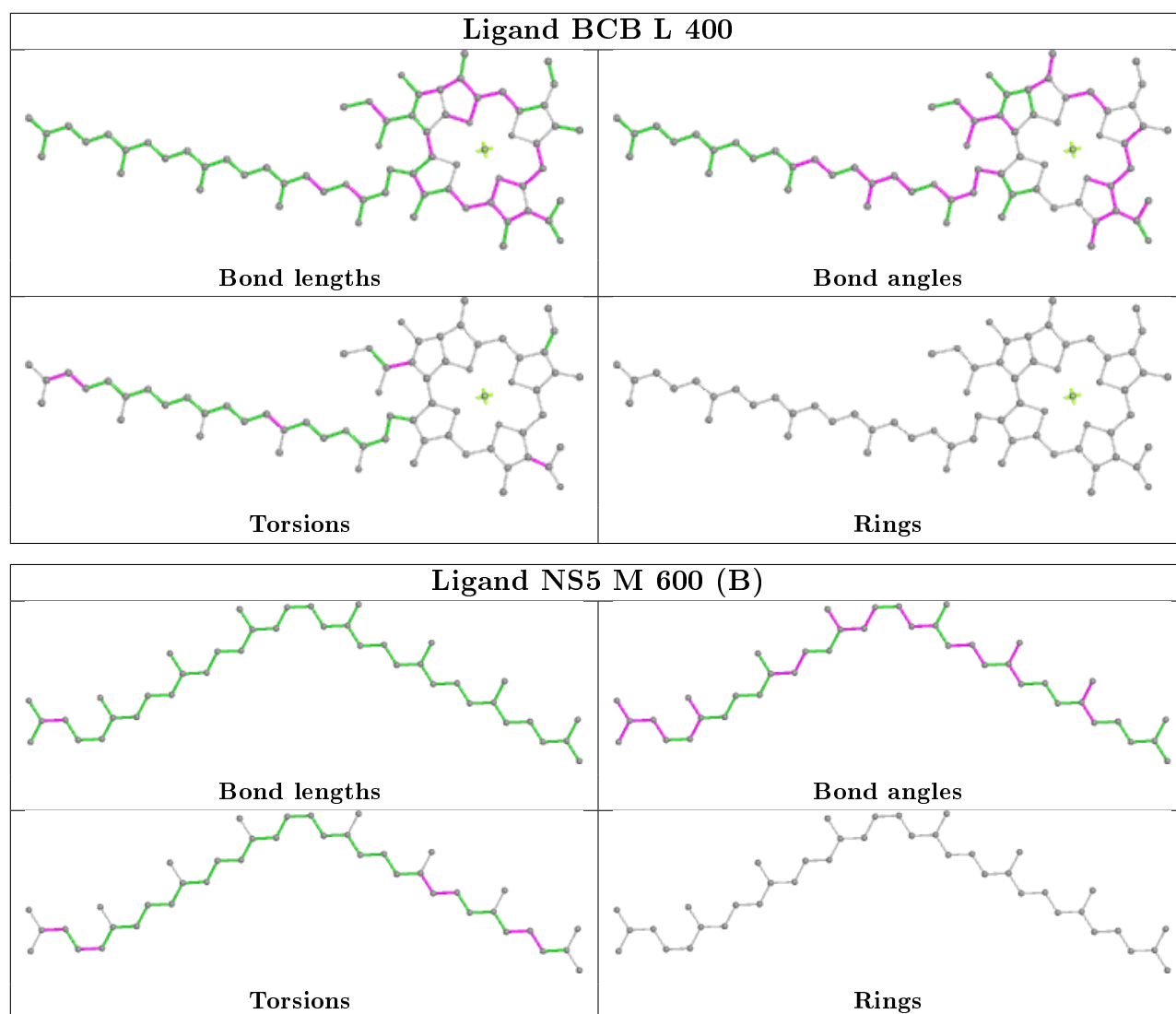


Ligand HEC C 403



Ligand BCB M 400





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%)	-0.28	8 (2%) 59 68	16, 24, 40, 54	0
2	H	249/258 (96%)	-0.05	20 (8%) 12 19	16, 25, 44, 60	0
3	L	273/273 (100%)	-0.51	4 (1%) 73 81	15, 20, 31, 41	0
4	M	323/323 (100%)	-0.37	10 (3%) 49 58	14, 22, 37, 47	0
All	All	1177/1190 (98%)	-0.31	42 (3%) 42 52	14, 23, 39, 60	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	8.5
2	H	8	GLN	5.6
2	H	54	PRO	5.5
2	H	7	ALA	5.5
2	H	83	PRO	4.7

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	0.94	0.09	24,27,40,48	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
9	UNL	M	714	10/-	-	-	48,52,60,60	10
15	NS5	M	600[B]	40/40	0.89	0.17	20,29,57,58	4
9	UNL	L	713	10/-	-	-	38,43,54,54	10
5	SO4	H	806	5/5	0.94	0.12	45,46,50,50	5
11	BCB	L	400	66/66	0.97	0.10	12,15,25,32	0
9	UNL	M	715	10/-	-	-	41,53,63,64	10
8	LDA	M	704	16/16	0.78	0.23	56,59,67,68	0
7	HTO	C	707	10/10	0.86	0.19	27,38,44,45	0
5	SO4	C	809	5/5	0.87	0.25	37,46,48,50	5
8	LDA	H	703	16/16	0.92	0.19	35,49,60,62	0
11	BCB	M	400	66/66	0.94	0.11	14,18,69,71	0
13	MQ9	L	501	58/58	0.94	0.11	13,20,66,68	0
11	BCB	M	401	66/66	0.96	0.09	12,16,36,38	0
6	HEC	C	401	43/43	0.98	0.10	19,25,34,39	0
6	HEC	C	403	43/43	0.98	0.09	12,16,19,24	0
5	SO4	M	802	5/5	0.98	0.09	38,41,45,46	0
5	SO4	M	804	5/5	0.98	0.16	43,45,48,49	0
10	FE2	L	500	1/1	1.00	0.03	16,16,16,16	0
7	HTO	L	709	10/10	-	-	20,36,41,42	10
5	SO4	M	816	5/5	-	-	35,36,38,39	5
5	SO4	C	808	5/5	0.92	0.16	39,39,45,46	5
8	LDA	H	701	16/16	0.94	0.10	24,33,42,44	0
5	SO4	H	812	5/5	0.94	0.15	45,46,46,47	5
12	BPB	L	402	65/65	0.97	0.09	13,16,22,25	0
11	BCB	L	401	66/66	0.97	0.07	12,16,35,43	0
5	SO4	M	801	5/5	0.99	0.08	23,30,32,37	0
5	SO4	M	819	5/5	-	-	38,40,42,42	5
12	BPB	M	402	65/65	0.89	0.17	14,19,91,92	0
14	UQ1	L	502	18/18	0.94	0.11	33,34,38,40	0
7	HTO	L	708	10/10	-	-	25,33,35,35	10
5	SO4	C	817	5/5	-	-	32,32,39,39	5
5	SO4	L	814	5/5	-	-	29,30,35,37	5
14	UQ1	L	503	18/18	0.82	0.23	44,46,52,53	0
8	LDA	L	702	16/16	0.86	0.17	29,34,38,39	0
7	HTO	H	705	10/10	0.94	0.12	26,32,35,37	0
5	SO4	C	811	5/5	0.94	0.14	41,42,42,45	5
5	SO4	C	810	5/5	0.97	0.08	36,38,38,39	5

Continued on next page...

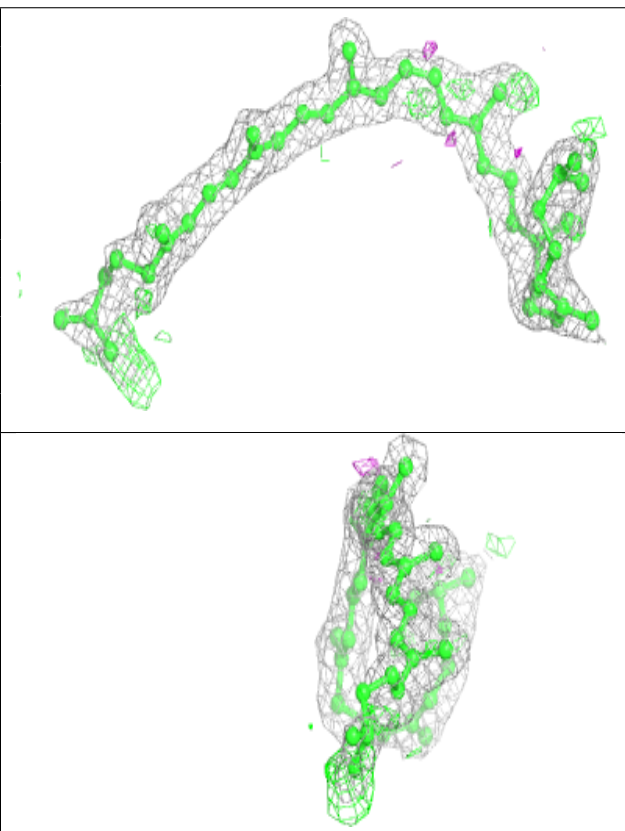
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	C	815	5/5	-	-	27,31,34,37	5
6	HEC	C	404	43/43	0.98	0.08	15,18,27,37	0
9	UNL	L	712	10/-	-	-	44,49,53,55	10
5	SO4	M	805	5/5	0.94	0.17	38,39,45,47	5
5	SO4	H	803	5/5	0.98	0.20	40,41,44,44	0
9	UNL	L	711	10/-	-	-	35,45,52,53	10
15	NS5	M	600[A]	40/40	0.89	0.17	20,29,57,58	4
5	SO4	C	813	5/5	0.91	0.23	41,41,42,44	5
5	SO4	H	807	5/5	0.94	0.24	44,49,51,51	5
5	SO4	M	818	5/5	-	-	50,52,52,54	5
7	HTO	C	706	10/10	0.82	0.22	28,40,44,45	0
9	UNL	H	710	10/-	-	-	30,42,49,49	10
6	HEC	C	402	43/43	0.98	0.09	18,21,26,28	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.

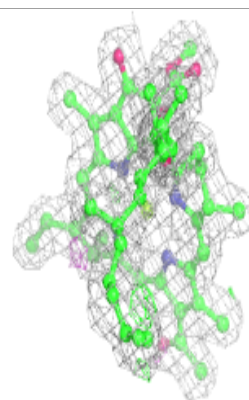
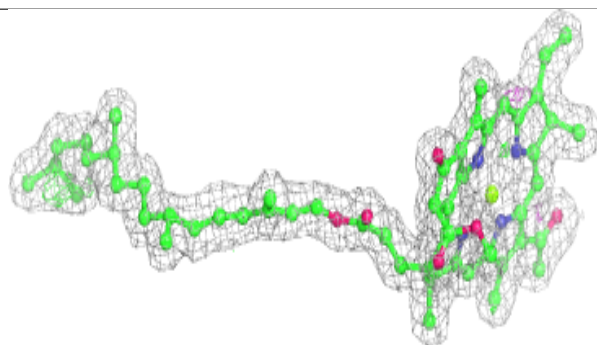
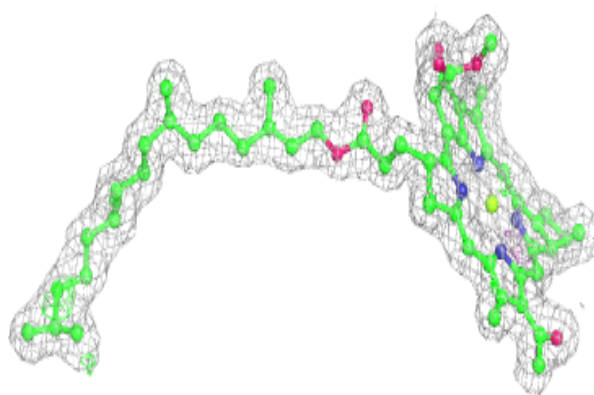
Electron density around NS5 M 600 (B):

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

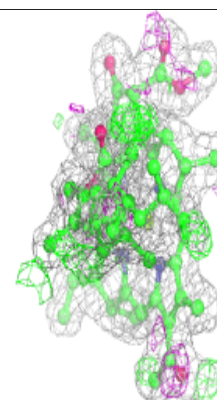
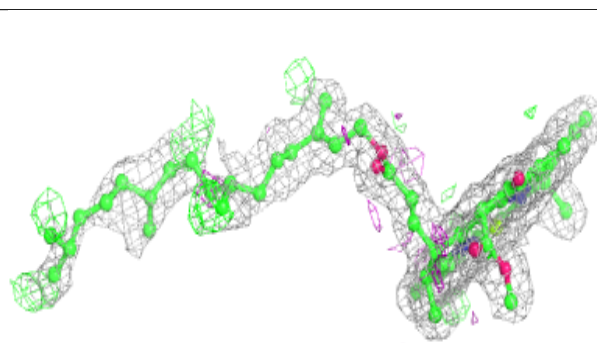
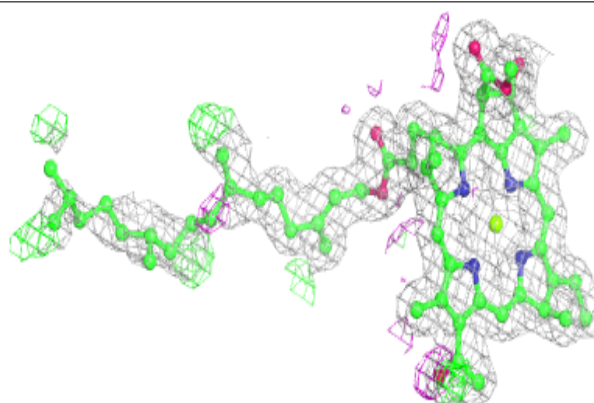


Electron density around BCB L 400:

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

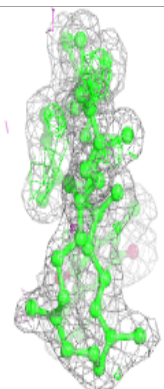
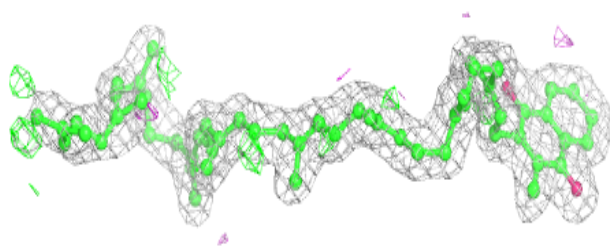
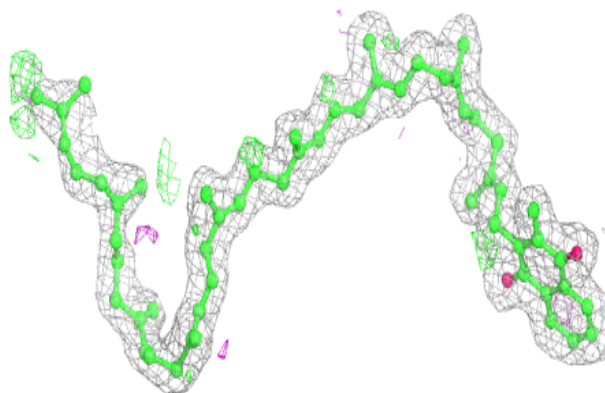
**Electron density around BCB M 400:**

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

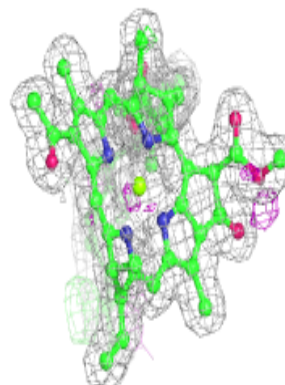
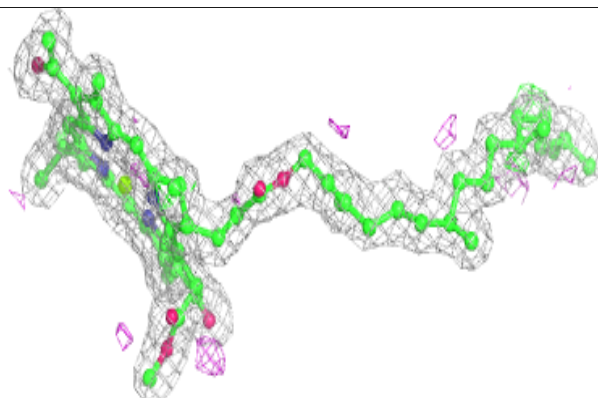
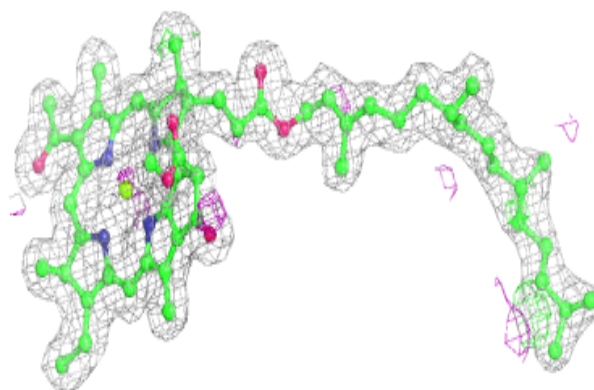


Electron density around MQ9 L 501:

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

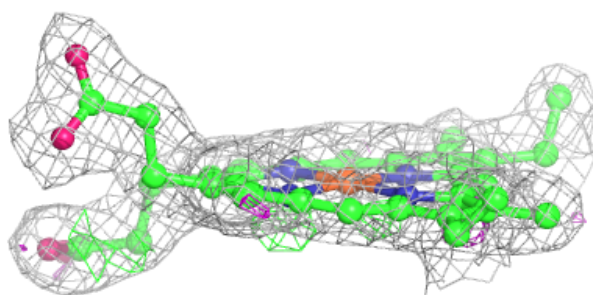
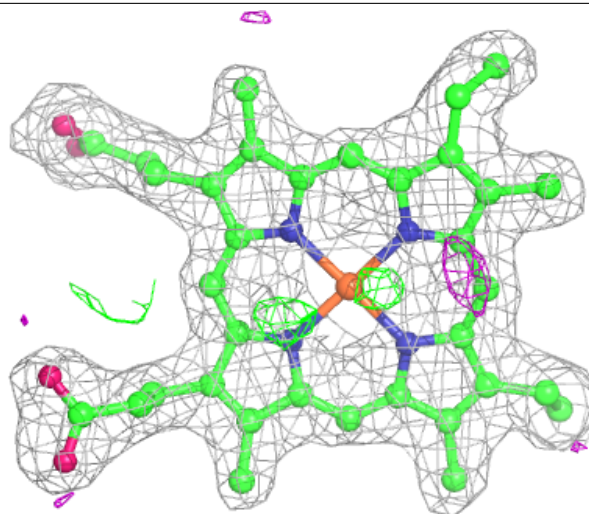
**Electron density around BCB M 401:**

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



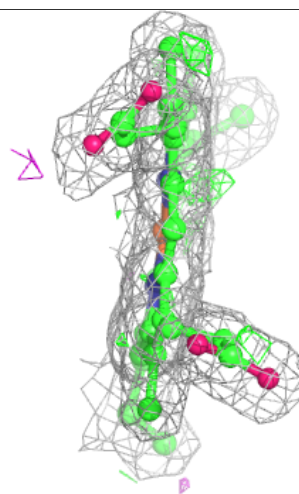
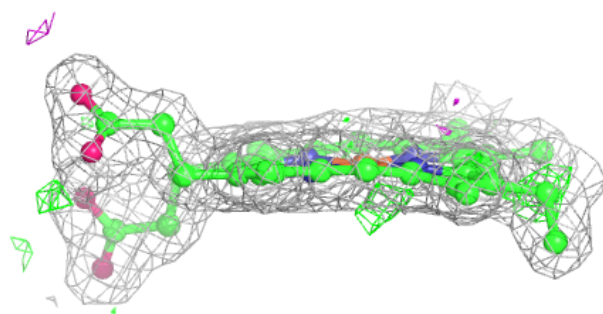
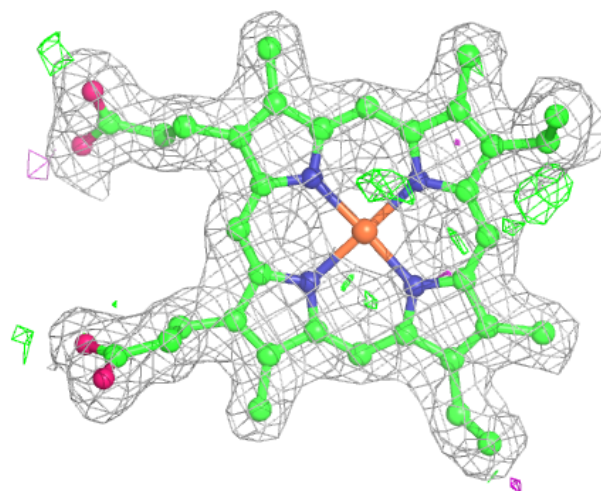
Electron density around HEC C 401:

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



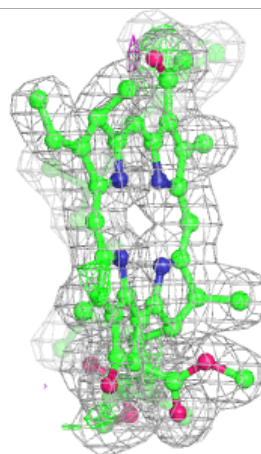
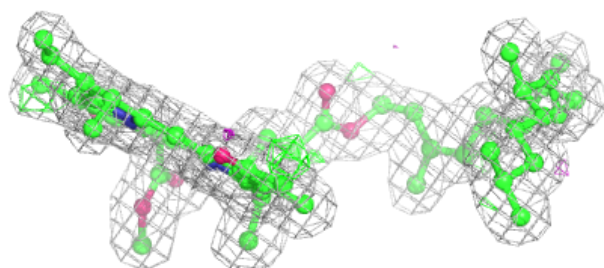
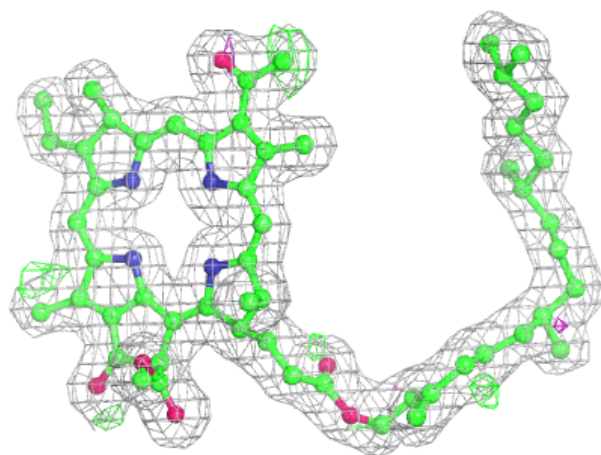
Electron density around HEC C 403:

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



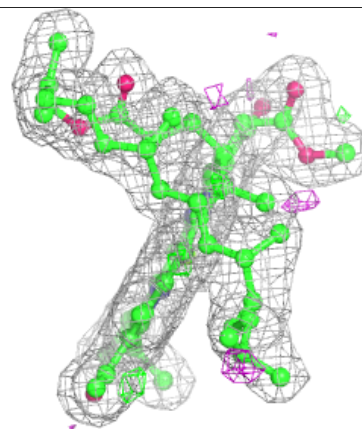
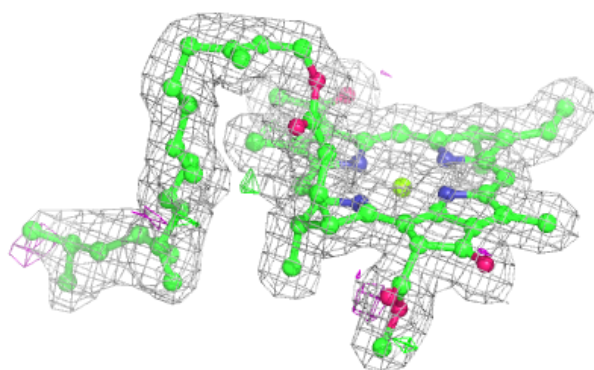
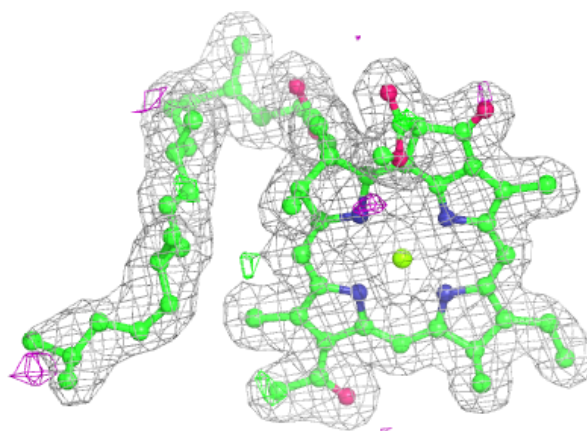
Electron density around BPB L 402:

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

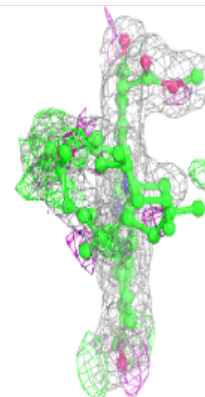
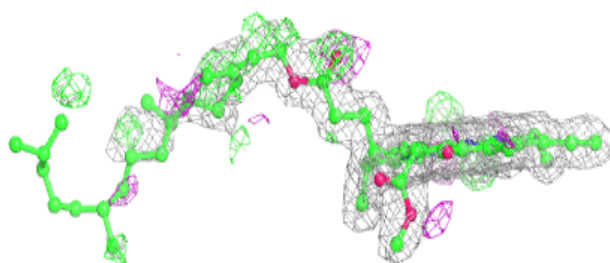
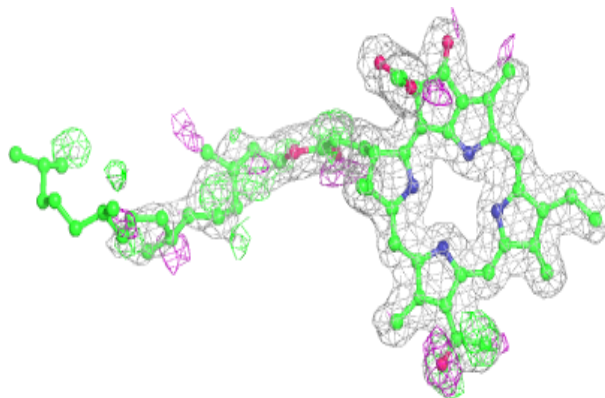


Electron density around BCB L 401:

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

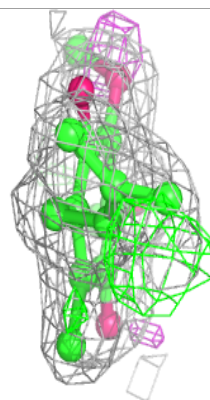
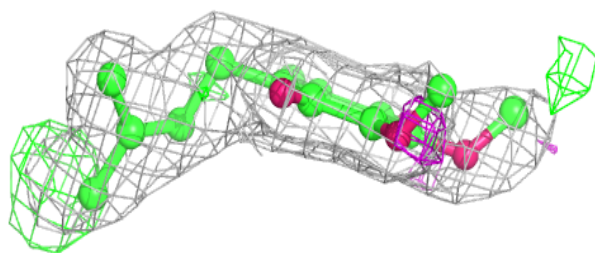
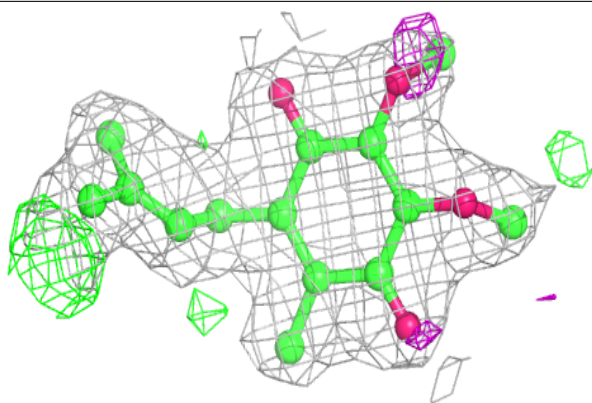
**Electron density around BPB M 402:**

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



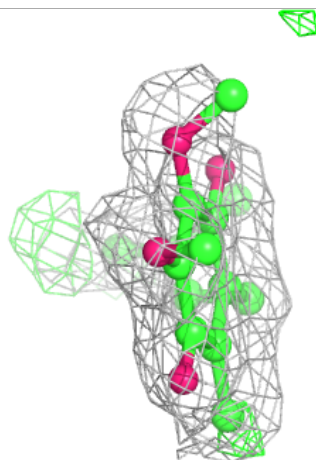
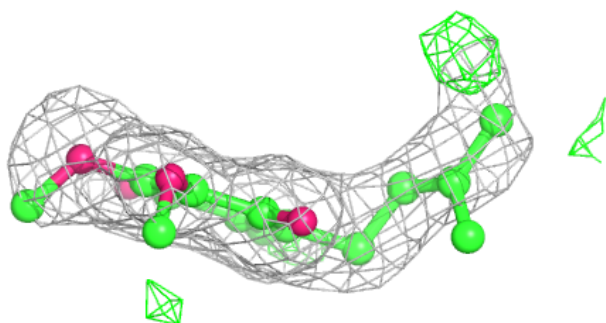
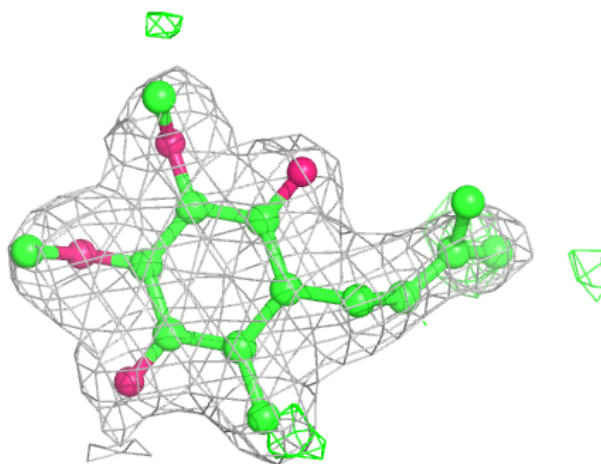
Electron density around UQ1 L 502:

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



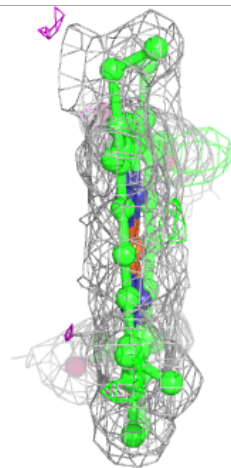
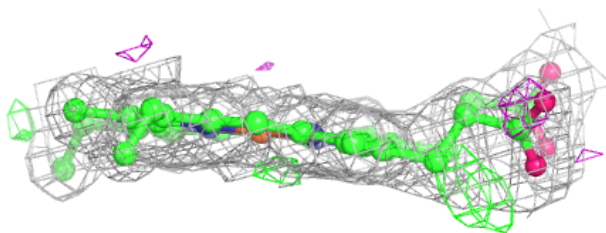
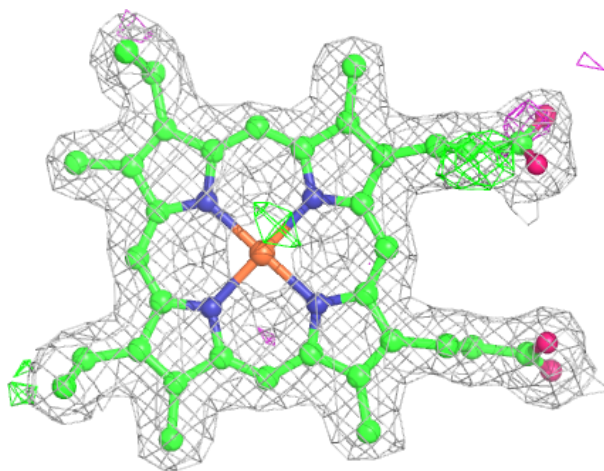
Electron density around UQ1 L 503:

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



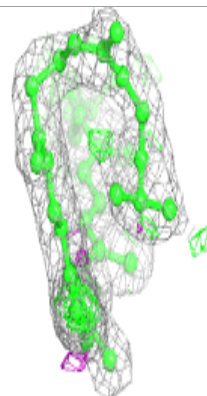
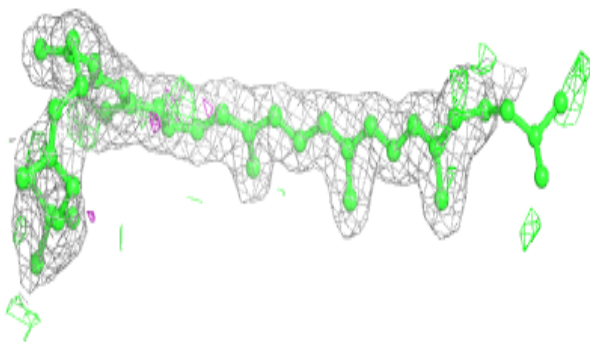
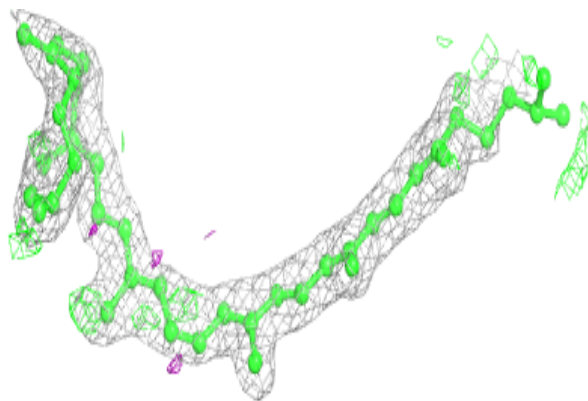
Electron density around HEC C 404:

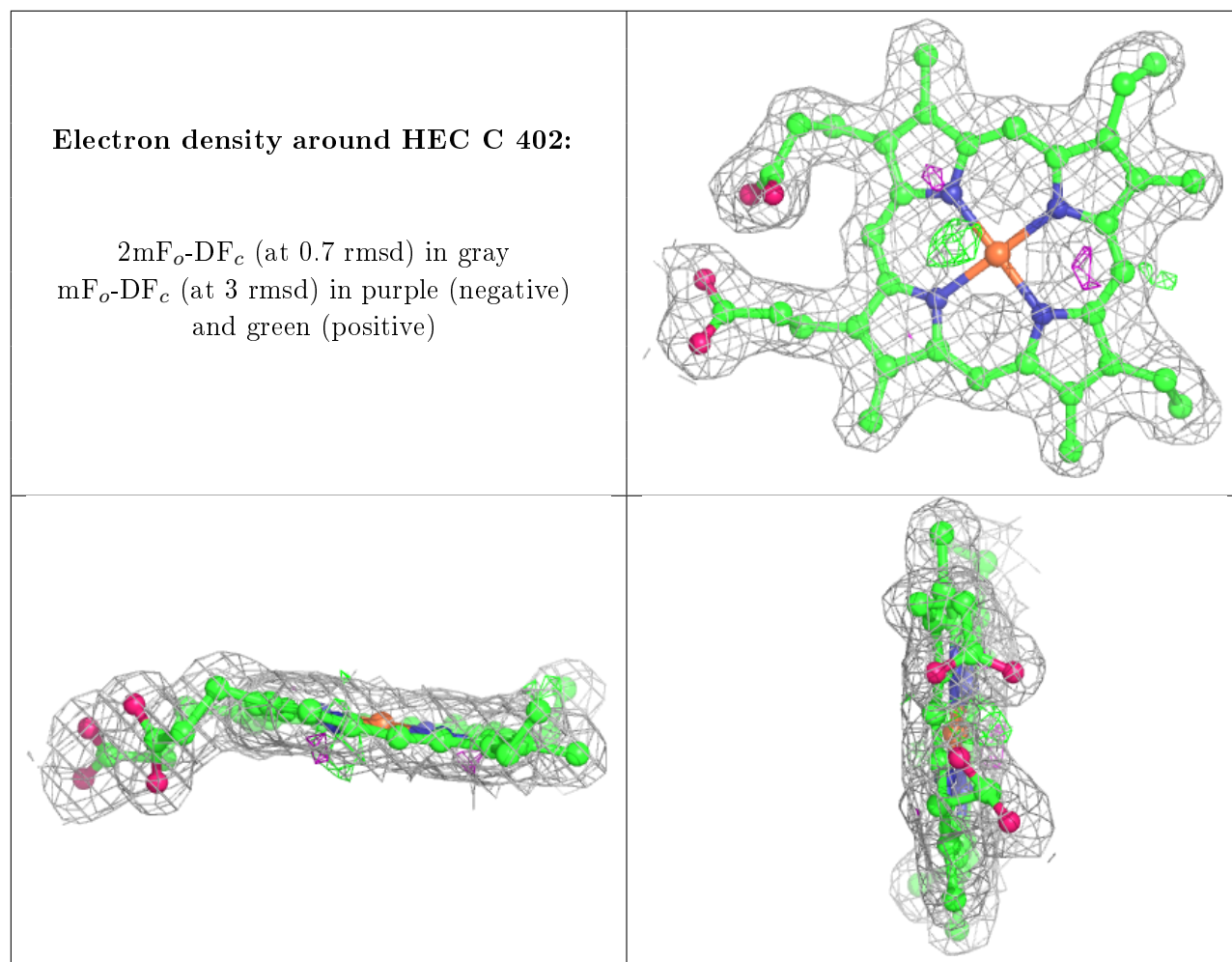
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NS5 M 600 (A):

$2mF_o-DF_c$ (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.