



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation 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

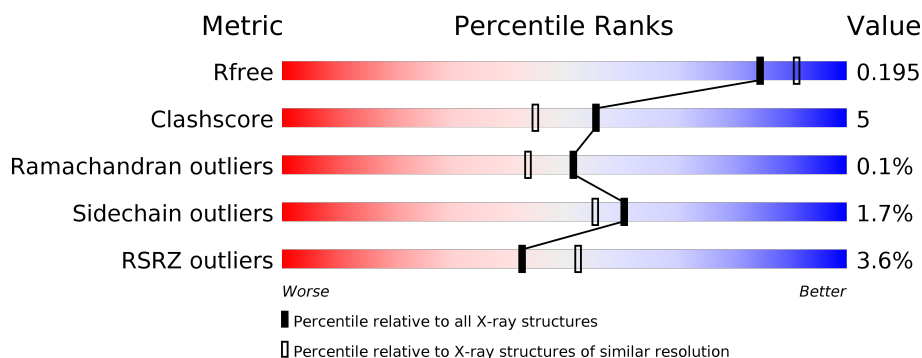
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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  $\geq 3$ , 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	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: O<sub>4</sub>S).



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		

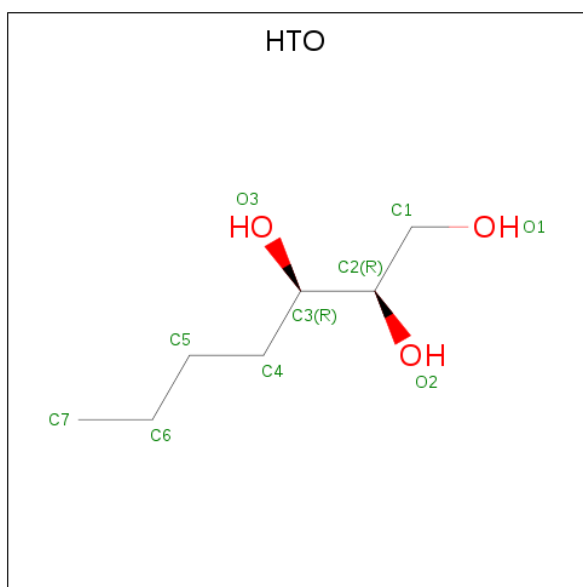
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	M	1	Total 5	O 4	S 1	0	0
5	M	1	Total 5	O 4	S 1	0	0
5	M	1	Total 5	O 4	S 1	5	0
5	M	1	Total 5	O 4	S 1	5	0
5	M	1	Total 5	O 4	S 1	5	0

- 
- The chemical structure of HEC (Hydroxyethylchlorin) is shown. It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The structure is labeled with various atoms and bonds, including C1A, C2A, C3A, C4A, C1B, C2B, C3B, C4B, C1C, C2C, C3C, C4C, C1D, C2D, C3D, C4D, C1E, C2E, C3E, C4E, C1F, C2F, C3F, C4F, C1G, C2G, C3G, C4G, C1H, C2H, C3H, C4H, C1I, C2I, C3I, C4I, C1J, C2J, C3J, C4J, C1K, C2K, C3K, C4K, C1L, C2L, C3L, C4L, C1M, C2M, C3M, C4M, C1N, C2N, C3N, C4N, C1O, C2O, C3O, C4O, C1P, C2P, C3P, C4P, C1Q, C2Q, C3Q, C4Q, C1R, C2R, C3R, C4R, C1S, C2S, C3S, C4S, C1T, C2T, C3T, C4T, C1U, C2U, C3U, C4U, C1V, C2V, C3V, C4V, C1W, C2W, C3W, C4W, C1X, C2X, C3X, C4X, C1Y, C2Y, C3Y, C4Y, C1Z, C2Z, C3Z, C4Z, C1AA, C2AA, C3AA, C4AA, C1AB, C2AB, C3AB, C4AB, C1AC, C2AC, C3AC, C4AC, C1AD, C2AD, C3AD, C4AD, C1AE, C2AE, C3AE, C4AE, C1AF, C2AF, C3AF, C4AF, C1AG, C2AG, C3AG, C4AG, C1AH, C2AH, C3AH, C4AH, C1AI, C2AI, C3AI, C4AI, C1AJ, C2AJ, C3AJ, C4AJ, C1AK, C2AK, C3AK, C4AK, C1AL, C2AL, C3AL, C4AL, C1AM, C2AM, C3AM, C4AM, C1AN, C2AN, C3AN, C4AN, C1AO, C2AO, C3AO, C4AO, C1AP, C2AP, C3AP, C4AP, C1AQ, C2AQ, C3AQ, C4AQ, C1AR, 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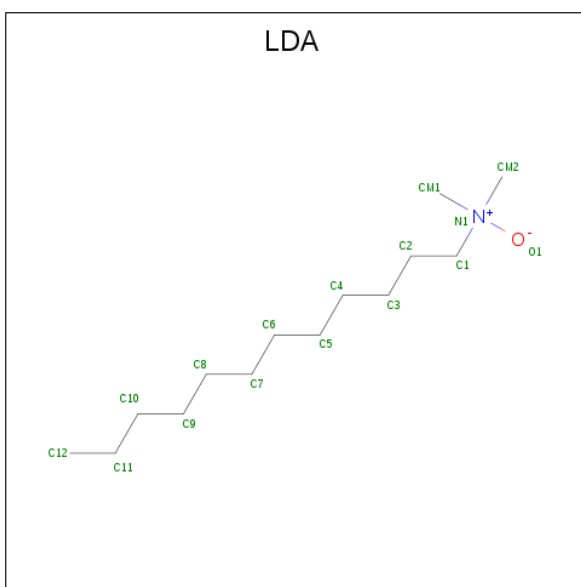
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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- WORLD WIDE  
PDB  
PROTEIN DATA BANK



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

- 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: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).



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

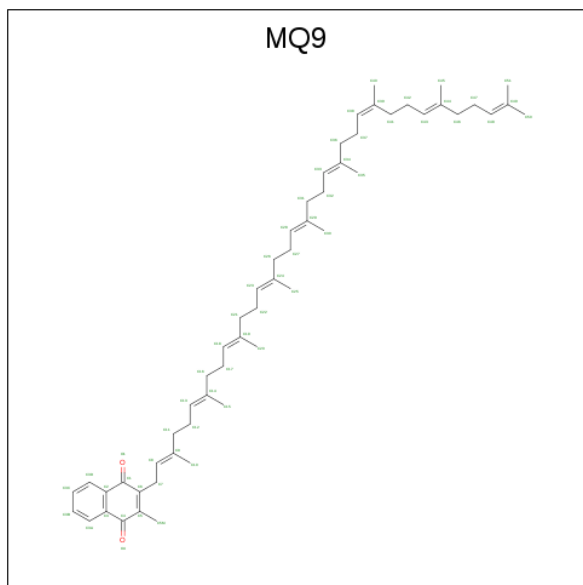
- Molecule 12 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula:  $C_{55}H_{74}N_4O_6$ ).





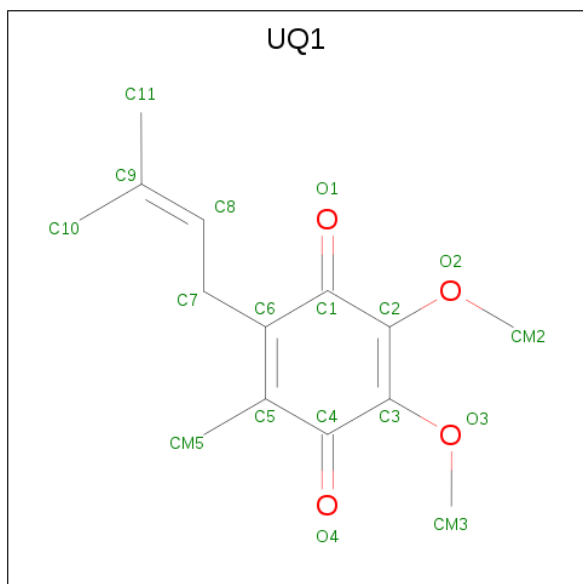
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	L	1	Total	C	N	O	0	0
			65	55	4	6		
12	M	1	Total	C	N	O	0	0
			65	55	4	6		

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



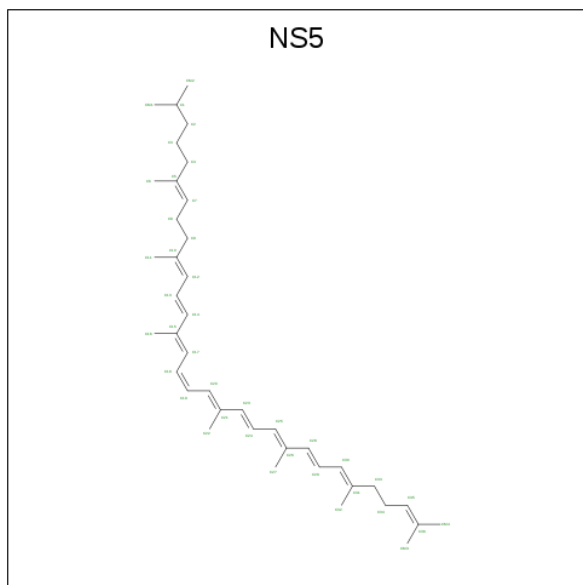
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	L	1	Total	C	O	0	0
			58	56	2		

- 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: C<sub>40</sub>H<sub>60</sub>).



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

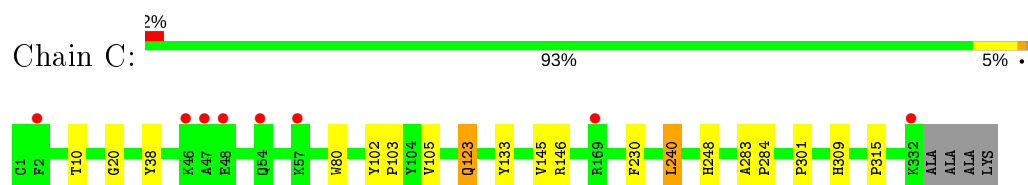
- Molecule 16 is water.

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		

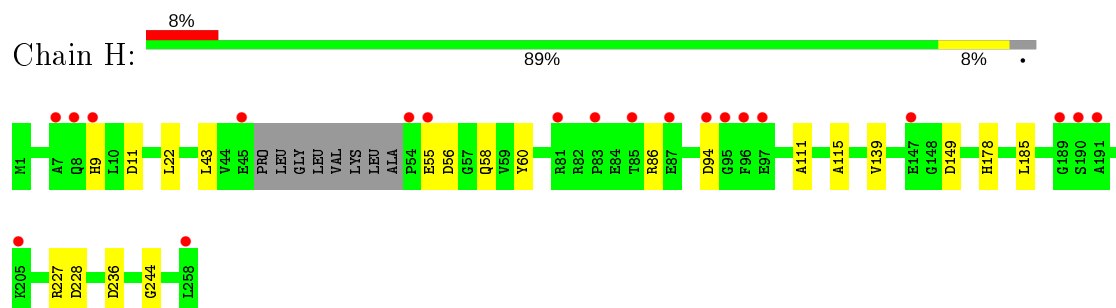
### 3 Residue-property plots [i](#)

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.

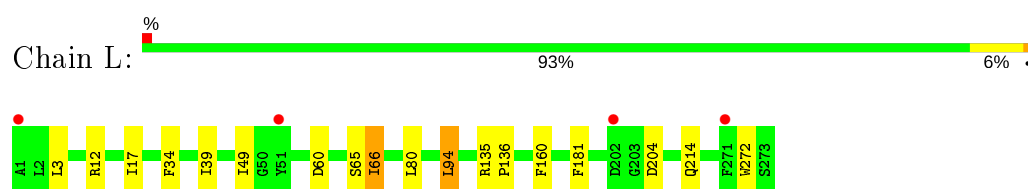
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



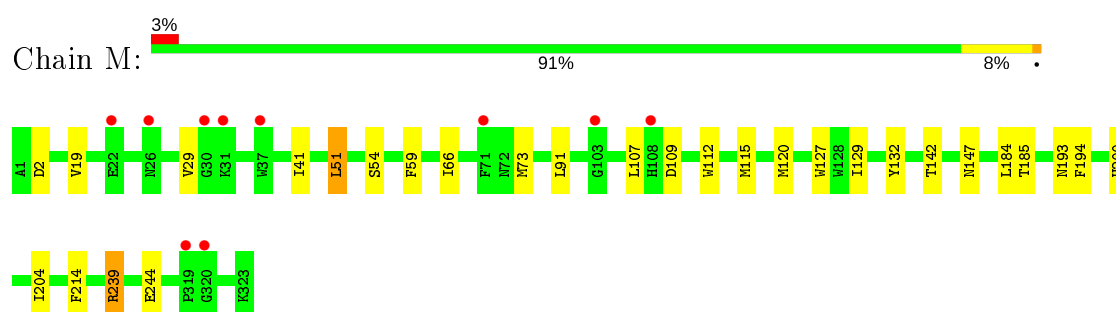
- Molecule 2: Reaction center protein H chain



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 63.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<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: 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.

All (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
4	M	109	ASP	CB-CG-OD2	5.78	123.50	118.30
3	L	204	ASP	CB-CG-OD2	5.64	123.38	118.30
3	L	66[A]	ILE	CB-CG1-CD1	-5.55	98.36	113.90
3	L	66[B]	ILE	CB-CG1-CD1	-5.55	98.36	113.90
3	L	60	ASP	CB-CG-OD2	5.44	123.20	118.30
2	H	94	ASP	CB-CG-OD2	5.35	123.12	118.30
2	H	11	ASP	CB-CG-OD2	5.12	122.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	149	ASP	CB-CG-OD2	5.07	122.86	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 [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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
12:M:402:BPB:CBB	12:M:402:BPB:HHC	2.11	0.80
11:M:401:BCB:C2	12:M:402:BPB:HBBB	2.13	0.78
4:M:73:MET:HE3	4:M:91:LEU:HB2	1.67	0.77
12:M:402:BPB:HBBB	12:M:402:BPB:HHC	1.70	0.73
11:M:400:BCB:CBB	11:M:400:BCB:HHC	2.20	0.71
5:M:802:SO4:O4	8:M:704:LDA:HM11	1.90	0.71
11:M:401:BCB:CBB	11:M:401:BCB:HMB1	2.21	0.70
4:M:107:LEU:CD2	4:M:115[B]:MET:CE	2.72	0.68
1:C:123:GLN:HE21	1:C:123:GLN:H	1.40	0.68
4:M:120:MET:HE2	11:M:401:BCB:H171	1.75	0.68
11:L:401:BCB:HMB1	11:L:401:BCB:CBB	2.25	0.67
12:L:402:BPB:HMB	12:L:402:BPB:CBB	2.24	0.67
4:M:107:LEU:HD21	4:M:115[B]:MET:HE2	1.77	0.65
11:L:400:BCB:CBB	11:L:400:BCB:HMB1	2.27	0.65
4:M:66:ILE:HD12	12:M:402:BPB:H9A	1.78	0.65
11:M:400:BCB:HBB2	11:M:400:BCB:HHC	1.79	0.65
4:M:107:LEU:HD21	4:M:115[B]:MET:CE	2.26	0.64
4:M:120:MET:HE3	11:M:401:BCB:C19	2.25	0.64
4:M:59:PHE:HA	12:M:402:BPB:C4	2.26	0.61
6:C:403:HEC:HBB3	6:C:403:HEC:HMB1	1.82	0.61
4:M:107:LEU:CD2	4:M:115[B]:MET:HE2	2.31	0.60
3:L:49:ILE:HG23	3:L:66[B]:ILE:HD11	1.83	0.60
4:M:239:ARG:HD3	4:M:244:GLU:CG	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:239:ARG:HD3	4:M:244:GLU:HG2	1.86	0.57
1:C:123:GLN:H	1:C:123:GLN:NE2	2.02	0.57
2:H:22:LEU:HD23	2:H:22:LEU:O	2.04	0.57
4:M:120:MET:HE2	11:M:401:BCB:C17	2.35	0.56
7:C:707:HTO:H41	16:C:1062:HOH:O	2.05	0.56
3:L:39:ILE:HD12	13:L:501:MQ9:C43	2.26	0.56
11:M:401:BCB:HMB1	11:M:401:BCB:HBB3	1.90	0.53
2:H:22:LEU:HD23	2:H:22:LEU:C	2.29	0.52
3:L:65:SER:C	3:L:66[A]:ILE:HD13	2.30	0.52
11:M:401:BCB:H12	12:M:402:BPB:HBB	1.92	0.51
3:L:135:ARG:HB3	3:L:136:PRO:HD3	1.92	0.51
12:L:402:BPB:HHC	12:L:402:BPB:OBB	2.11	0.50
12:L:402:BPB:HMB	12:L:402:BPB:HBBB	1.92	0.50
1:C:105:VAL:HG22	16:C:1106:HOH:O	2.12	0.49
11:L:400:BCB:HBB3	11:L:400:BCB:HMB1	1.93	0.49
12:M:402:BPB:CBB	12:M:402:BPB:CHC	2.86	0.49
11:L:401:BCB:HMB1	11:L:401:BCB:HBB2	1.95	0.49
11:M:401:BCB:C1	12:M:402:BPB:CBB	2.91	0.49
12:M:402:BPB:HHC	12:M:402:BPB:HBBA	1.91	0.48
12:M:402:BPB:HMB	12:M:402:BPB:OBB	2.13	0.48
11:M:400:BCB:HMB1	11:M:400:BCB:OBB	2.14	0.48
11:M:401:BCB:H12	12:M:402:BPB:CBB	2.44	0.48
6:C:401:HEC:HMC1	6:C:401:HEC:HBC3	1.94	0.48
2:H:55:GLU:H	2:H:58:GLN:HE21	1.60	0.48
2:H:86:ARG:NH2	2:H:111:ALA:HB3	2.29	0.48
6:C:403:HEC:HBC3	6:C:403:HEC:HMC1	1.96	0.47
4:M:184:LEU:HD21	11:M:400:BCB:CAC	2.44	0.47
1:C:105:VAL:HG13	16:C:1106:HOH:O	2.14	0.47
3:L:65:SER:O	3:L:66[A]:ILE:HD13	2.15	0.47
3:L:214:GLN:NE2	4:M:19:VAL:H	2.13	0.47
11:M:401:BCB:C1	12:M:402:BPB:HBBB	2.45	0.47
11:L:401:BCB:HBB3	11:L:401:BCB:HMB1	1.96	0.46
1:C:145:VAL:O	1:C:146:ARG:HD2	2.16	0.46
11:L:401:BCB:HBA1	11:L:401:BCB:C4A	2.45	0.46
11:M:401:BCB:HBB2	11:M:401:BCB:HMB1	1.94	0.46
1:C:301:PRO:HG2	6:C:402:HEC:HBD1	1.99	0.45
1:C:309:HIS:CE1	1:C:315:PRO:HD3	2.51	0.45
4:M:132:TYR:CE1	4:M:142:THR:HG21	2.51	0.44
4:M:112:TRP:CE3	4:M:115[B]:MET:HE3	2.52	0.44
4:M:29:VAL:HG22	4:M:51:LEU:HD13	1.99	0.44
1:C:102:TYR:N	1:C:103:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:THR:O	1:C:20:GLY:HA3	2.19	0.43
4:M:41:ILE:HD12	4:M:41:ILE:C	2.40	0.43
4:M:120:MET:CE	11:M:401:BCB:C17	2.96	0.42
1:C:230:PHE:CE2	4:M:185:THR:HG21	2.54	0.42
12:L:402:BPB:HMB	12:L:402:BPB:HBBA	1.98	0.42
3:L:17:ILE:HD12	3:L:34:PHE:CZ	2.54	0.42
11:L:400:BCB:HBB2	11:L:400:BCB:HMB1	2.01	0.42
1:C:240:LEU:HD22	1:C:309:HIS:CG	2.55	0.42
3:L:17:ILE:HD12	3:L:34:PHE:HZ	1.84	0.42
6:C:402:HEC:HMB1	6:C:402:HEC:HBB3	2.02	0.41
4:M:127:TRP:CD1	12:M:402:BPB:HBA	2.56	0.41
4:M:200:HIS:CE1	4:M:204:ILE:HD11	2.55	0.41
4:M:107:LEU:HD21	4:M:115[B]:MET:HE1	2.02	0.41
4:M:54[B]:SER:OG	4:M:129:ILE:CG2	2.68	0.41
11:M:400:BCB:HHC	11:M:400:BCB:HBB3	2.00	0.41
11:M:400:BCB:HBC1	11:M:401:BCB:CAD	2.50	0.41
3:L:181:PHE:HB3	12:M:402:BPB:HBBA	2.02	0.41
3:L:94:LEU:HD23	3:L:94:LEU:HA	1.91	0.41
4:M:120:MET:CE	11:M:401:BCB:H171	2.47	0.41
2:H:139:VAL:HG21	2:H:228:ASP:HB3	2.02	0.41
1:C:283:ALA:N	1:C:284:PRO:CD	2.83	0.41
2:H:43:LEU:CD2	3:L:3:LEU:HD23	2.50	0.41
11:L:400:BCB:H193	13:L:501:MQ9:H252	2.03	0.41
4:M:107:LEU:CD2	4:M:115[B]:MET:HE1	2.50	0.41
1:C:80:TRP:CD1	1:C:133:TYR:HB2	2.56	0.40
11:L:401:BCB:OBB	11:L:401:BCB:HHC	2.21	0.40
2:H:56:ASP:HB3	2:H:60:TYR:CE2	2.57	0.40
4:M:112:TRP:CE3	4:M:115[B]:MET:CE	3.04	0.40
2:H:115:ALA:HB2	2:H:244:GLY:HA3	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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 ⓘ

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

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	38	TYR
1	C	123	GLN
1	C	240	LEU
2	H	9	HIS
2	H	178	HIS
2	H	185	LEU
2	H	227	ARG
2	H	236	ASP
3	L	80	LEU
3	L	94	LEU

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Mol	Chain	Res	Type
3	L	160	PHE
3	L	272	TRP
4	M	51	LEU
4	M	147	ASN
4	M	194	PHE
4	M	214	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	123	GLN
2	H	58	GLN
2	H	102	GLN
2	H	220	ASN
2	H	225	GLN
3	L	183	ASN
3	L	213	ASN
3	L	214	GLN
4	M	147	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
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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	-
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	-

All (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
11	L	400	BCB	CHC-C4B	-8.87	1.39	1.53
11	M	400	BCB	CHD-C1D	-8.81	1.39	1.53
11	L	400	BCB	CHD-C1D	-8.73	1.39	1.53
11	M	400	BCB	CHC-C4B	-8.63	1.40	1.53
11	L	401	BCB	CHD-C1D	-8.52	1.40	1.53
11	L	400	BCB	C1A-CHA	-8.45	1.40	1.54
11	M	400	BCB	CHB-C1B	-8.26	1.40	1.53
11	L	401	BCB	CHB-C1B	-8.19	1.40	1.53
11	L	401	BCB	CHC-C4B	-8.13	1.40	1.53
11	L	400	BCB	CHB-C1B	-8.13	1.40	1.53
11	M	401	BCB	CHD-C1D	-8.11	1.40	1.53
14	L	503	UQ1	C6-C5	8.06	1.49	1.35
14	L	502	UQ1	C6-C5	7.70	1.49	1.35
11	M	400	BCB	CHD-C4C	-7.60	1.40	1.53
11	M	401	BCB	CHD-C4C	-7.48	1.40	1.53
15	M	600[B]	NS5	C35-C36	7.30	1.53	1.32
11	M	400	BCB	C3B-C2B	-7.28	1.36	1.55
11	L	400	BCB	CHD-C4C	-7.24	1.41	1.53
12	M	402	BPB	CAC-C3C	7.22	1.53	1.33
15	M	600[A]	NS5	C35-C36	7.20	1.53	1.32
11	M	401	BCB	C3B-C2B	-7.14	1.36	1.55
11	L	401	BCB	C4D-ND	-7.14	1.35	1.50
12	L	402	BPB	CAC-C3C	7.06	1.52	1.33
11	L	401	BCB	CHD-C4C	-6.98	1.41	1.53
8	M	704	LDA	O1-N1	-6.97	1.25	1.42
11	M	400	BCB	C4D-ND	-6.80	1.36	1.50
11	M	401	BCB	C4D-ND	-6.78	1.36	1.50
11	L	400	BCB	C1D-ND	-6.77	1.36	1.50
11	L	400	BCB	C4D-ND	-6.75	1.36	1.50
8	L	702	LDA	O1-N1	-6.73	1.26	1.42
11	L	400	BCB	C3B-C2B	-6.60	1.38	1.55
11	M	400	BCB	C1D-ND	-6.54	1.36	1.50
11	L	401	BCB	C3D-C2D	-6.53	1.38	1.55
11	L	400	BCB	C3D-C2D	-6.52	1.38	1.55
8	H	703	LDA	O1-N1	-6.46	1.27	1.42
11	L	401	BCB	C3B-C2B	-6.43	1.38	1.55
11	M	401	BCB	C1D-ND	-6.41	1.36	1.50
11	M	400	BCB	C3D-C2D	-6.36	1.38	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	M	401	BCB	C3D-C2D	-6.35	1.38	1.55
8	H	701	LDA	O1-N1	-6.32	1.27	1.42
11	L	401	BCB	C1D-ND	-6.13	1.37	1.50
11	M	401	BCB	C1B-NB	-6.11	1.37	1.50
11	L	400	BCB	C1B-NB	-6.03	1.37	1.50
11	M	401	BCB	CHB-C4A	-5.93	1.39	1.52
11	M	401	BCB	C4B-NB	-5.88	1.37	1.50
11	M	400	BCB	CHB-C4A	-5.84	1.39	1.52
11	M	400	BCB	CHC-C1C	-5.80	1.39	1.52
11	L	400	BCB	CHB-C4A	-5.71	1.39	1.52
11	L	400	BCB	C4B-NB	-5.70	1.38	1.50
11	L	401	BCB	C1B-NB	-5.64	1.38	1.50
11	M	401	BCB	CHC-C1C	-5.61	1.40	1.52
11	L	401	BCB	C4B-NB	-5.46	1.38	1.50
11	M	401	BCB	C2B-C1B	-5.41	1.43	1.53
11	M	400	BCB	C4B-NB	-5.39	1.38	1.50
11	L	401	BCB	CHB-C4A	-5.38	1.40	1.52
11	M	400	BCB	C1B-NB	-5.37	1.38	1.50
11	L	400	BCB	CHC-C1C	-5.29	1.40	1.52
11	L	401	BCB	CHC-C1C	-5.18	1.40	1.52
11	L	401	BCB	C2D-C1D	-5.08	1.44	1.53
11	M	400	BCB	C2B-C1B	-5.04	1.44	1.53
11	L	401	BCB	C2B-C1B	-5.03	1.44	1.53
6	C	401	HEC	C3B-C2B	-5.01	1.35	1.40
6	C	403	HEC	C3B-C2B	-4.97	1.35	1.40
11	L	400	BCB	C2B-C1B	-4.86	1.44	1.53
6	C	402	HEC	C3B-C2B	-4.82	1.35	1.40
6	C	404	HEC	C3B-C2B	-4.72	1.35	1.40
11	L	400	BCB	C2D-C1D	-4.70	1.44	1.53
6	C	402	HEC	C3C-C2C	-4.60	1.35	1.40
11	M	400	BCB	C2D-C1D	-4.56	1.45	1.53
11	M	401	BCB	C2D-C1D	-4.50	1.45	1.53
6	C	401	HEC	C3C-C2C	-4.31	1.36	1.40
6	C	404	HEC	C3C-C2C	-4.30	1.36	1.40
11	M	401	BCB	O2D-CGD	4.21	1.43	1.33
11	M	400	BCB	C3B-CAB	-4.17	1.47	1.52
13	L	501	MQ9	C3-C4	-4.12	1.40	1.48
11	L	400	BCB	O2D-CGD	4.06	1.43	1.33
12	L	402	BPB	O2A-CGA	4.03	1.45	1.33
11	M	400	BCB	O2A-CGA	4.01	1.45	1.33
12	L	402	BPB	O2D-CGD	3.96	1.42	1.33
11	L	401	BCB	O2D-CGD	3.95	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	402	BPB	O2D-CGD	3.90	1.42	1.33
12	M	402	BPB	O2A-CGA	3.89	1.44	1.33
11	L	400	BCB	C3B-CAB	-3.89	1.47	1.52
13	L	501	MQ9	C6-C5	3.82	1.42	1.35
11	L	401	BCB	O2A-CGA	3.72	1.44	1.33
13	L	501	MQ9	C2-C1	-3.70	1.41	1.48
11	M	401	BCB	O2A-CGA	3.64	1.44	1.33
6	C	403	HEC	C3C-C2C	-3.64	1.37	1.40
11	M	400	BCB	O2D-CGD	3.63	1.42	1.33
11	M	401	BCB	C3B-CAB	-3.56	1.48	1.52
11	L	401	BCB	C3D-CAD	-3.52	1.44	1.51
13	L	501	MQ9	C8-C9	3.47	1.41	1.33
11	L	400	BCB	O2A-CGA	3.27	1.42	1.33
13	L	501	MQ9	C5-C4	-3.26	1.41	1.48
14	L	503	UQ1	C3-C2	3.24	1.49	1.36
11	L	401	BCB	C3B-CAB	-3.23	1.48	1.52
11	L	400	BCB	C3D-CAD	-3.22	1.45	1.51
14	L	502	UQ1	C3-C2	3.10	1.49	1.36
12	L	402	BPB	C3B-C4B	3.07	1.45	1.41
12	M	402	BPB	C3B-C4B	3.04	1.45	1.41
12	L	402	BPB	C2-C3	2.90	1.39	1.33
13	L	501	MQ9	C33-C34	2.89	1.39	1.33
13	L	501	MQ9	C28-C29	2.83	1.39	1.33
11	M	401	BCB	C3D-CAD	-2.80	1.46	1.51
13	L	501	MQ9	C18-C19	2.79	1.39	1.33
13	L	501	MQ9	C13-C14	2.77	1.39	1.33
13	L	501	MQ9	C43-C44	2.75	1.39	1.33
12	M	402	BPB	C2-C3	2.73	1.39	1.33
13	L	501	MQ9	C38-C39	2.68	1.39	1.33
13	L	501	MQ9	C6-C1	-2.68	1.40	1.47
11	L	401	BCB	C2-C3	2.68	1.39	1.33
6	C	404	HEC	C3C-C4C	2.57	1.47	1.43
11	M	400	BCB	C3D-CAD	-2.55	1.46	1.51
11	L	400	BCB	C2A-C3A	-2.54	1.50	1.54
13	L	501	MQ9	C23-C24	2.50	1.39	1.33
13	L	501	MQ9	C7-C8	-2.50	1.47	1.50
11	M	401	BCB	C2A-C3A	-2.48	1.50	1.54
6	C	402	HEC	C3C-C4C	2.44	1.47	1.43
11	M	401	BCB	C2-C3	2.42	1.38	1.33
11	M	400	BCB	C2-C3	2.39	1.38	1.33
12	L	402	BPB	C4D-CHA	-2.37	1.36	1.43
11	M	400	BCB	C2A-C3A	-2.28	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	402	BPB	C1D-ND	2.25	1.43	1.38
13	L	501	MQ9	C48-C49	2.25	1.38	1.32
12	L	402	BPB	C2C-C3C	-2.23	1.48	1.51
12	M	402	BPB	C1D-ND	2.21	1.43	1.38
12	M	402	BPB	C4D-CHA	-2.18	1.37	1.43
12	L	402	BPB	C3D-C4D	-2.14	1.36	1.43
11	M	400	BCB	CAA-C2A	2.12	1.57	1.53
6	C	403	HEC	C3C-C4C	2.12	1.46	1.43
11	L	400	BCB	C1-C2	-2.11	1.42	1.49
11	M	401	BCB	CBD-CGD	2.09	1.55	1.52
12	M	402	BPB	C3D-C4D	-2.07	1.37	1.43
6	C	402	HEC	CAD-C3D	2.04	1.55	1.52
13	L	501	MQ9	O1-C1	2.03	1.27	1.23
13	L	501	MQ9	C47-C48	-2.03	1.43	1.50
13	L	501	MQ9	C37-C38	-2.02	1.43	1.50
11	M	401	BCB	C4A-C3A	-2.01	1.51	1.53

All (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
11	M	401	BCB	CMB-C2B-C3B	5.63	128.26	114.29
11	L	401	BCB	CMB-C2B-C3B	5.60	128.19	114.29
15	M	600[A]	NS5	C19-C20-C21	-5.55	119.39	127.31
15	M	600[B]	NS5	C19-C20-C21	-5.55	119.39	127.31
11	M	400	BCB	CMD-C2D-C3D	5.35	127.57	114.29
11	L	400	BCB	C1D-CHD-C4C	5.33	123.73	112.37
11	M	401	BCB	C1D-CHD-C4C	5.33	123.72	112.37
11	M	401	BCB	CMD-C2D-C3D	5.26	127.35	114.29
11	L	401	BCB	C1D-CHD-C4C	5.26	123.57	112.37
11	M	400	BCB	CBA-CAA-C2A	-5.18	108.68	115.72
11	L	401	BCB	CBA-CAA-C2A	-5.16	108.71	115.72
11	L	400	BCB	CMD-C2D-C3D	5.15	127.08	114.29
11	L	400	BCB	CHA-CBD-CGD	-5.14	103.39	115.02
12	M	402	BPB	O2D-CGD-CBD	5.12	120.37	111.27
11	L	401	BCB	CMD-C2D-C3D	5.07	126.89	114.29
11	M	400	BCB	CMB-C2B-C3B	5.05	126.83	114.29
15	M	600[A]	NS5	C34-C35-C36	-4.78	111.40	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	400	BCB	CBB-CAB-C3B	4.71	121.61	116.80
11	M	401	BCB	CBB-CAB-C3B	4.70	121.60	116.80
11	L	401	BCB	CBB-CAB-C3B	4.69	121.59	116.80
12	L	402	BPB	O2D-CGD-CBD	4.61	119.46	111.27
15	M	600[B]	NS5	C34-C35-C36	-4.60	112.04	127.75
15	M	600[B]	NS5	CM4-C36-C35	-4.08	110.86	122.65
15	M	600[A]	NS5	CM3-C36-C35	-4.02	111.02	122.65
15	M	600[A]	NS5	CM4-C36-C35	-4.01	111.07	122.65
11	M	401	BCB	O2D-CGD-CBD	3.95	120.39	111.11
11	L	400	BCB	C4-C3-C5	3.91	121.85	115.27
15	M	600[B]	NS5	CM3-C36-C35	-3.91	111.34	122.65
11	M	400	BCB	O2D-CGD-CBD	3.82	120.08	111.11
11	L	401	BCB	O2D-CGD-CBD	3.72	119.84	111.11
11	M	400	BCB	CBB-CAB-C3B	3.68	120.56	116.80
6	C	403	HEC	CMC-C2C-C1C	-3.63	122.89	128.46
11	M	401	BCB	CHC-C4B-C3B	3.53	126.84	118.17
11	L	400	BCB	CBA-CAA-C2A	-3.51	110.95	115.72
11	L	400	BCB	O2D-CGD-CBD	3.48	119.28	111.11
12	M	402	BPB	CMD-C2D-C3D	3.29	135.19	127.61
11	L	400	BCB	CHC-C4B-C3B	3.27	126.18	118.17
6	C	402	HEC	CMC-C2C-C1C	-3.24	123.49	128.46
11	L	401	BCB	CHC-C4B-C3B	3.20	126.02	118.17
12	L	402	BPB	C3C-C2C-C1C	3.18	105.05	100.72
12	L	402	BPB	CMD-C2D-C3D	3.16	134.88	127.61
11	M	400	BCB	C1-C2-C3	-3.15	120.60	126.04
6	C	404	HEC	CMC-C2C-C1C	-3.13	123.65	128.46
12	M	402	BPB	CAD-C3D-C2D	-3.13	125.69	140.80
12	L	402	BPB	CAD-C3D-C2D	-3.03	126.15	140.80
11	M	400	BCB	CHC-C4B-C3B	3.02	125.57	118.17
11	L	400	BCB	C1-C2-C3	-3.01	120.84	126.04
6	C	401	HEC	CMC-C2C-C1C	-2.88	124.03	128.46
12	M	402	BPB	C1-O2A-CGA	2.88	124.01	116.44
11	M	401	BCB	O2D-CGD-O1D	-2.87	118.22	123.84
15	M	600[A]	NS5	C6-C5-C4	2.84	120.05	115.27
15	M	600[B]	NS5	C6-C5-C4	2.84	120.05	115.27
11	L	400	BCB	C3B-C4B-NB	2.81	108.87	103.75
11	L	401	BCB	O1D-CGD-CBD	-2.76	119.07	124.54
12	M	402	BPB	CBD-CHA-C1A	2.74	131.21	126.84
12	L	402	BPB	CMD-C2D-C1D	2.69	129.20	125.06
6	C	404	HEC	CMB-C2B-C1B	-2.67	124.36	128.46
12	M	402	BPB	C4-C3-C2	-2.61	116.98	123.68
11	M	400	BCB	O1D-CGD-CBD	-2.60	119.38	124.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	M	400	BCB	C4-C3-C5	2.60	119.64	115.27
13	L	501	MQ9	C20-C19-C21	2.60	119.64	115.27
6	C	401	HEC	CBD-CAD-C3D	-2.59	107.70	112.49
15	M	600[A]	NS5	C12-C13-C14	-2.59	115.13	123.22
15	M	600[B]	NS5	C12-C13-C14	-2.59	115.13	123.22
13	L	501	MQ9	C37-C38-C39	-2.58	121.45	127.66
11	L	401	BCB	C3B-C4B-NB	2.58	108.45	103.75
11	M	401	BCB	C3B-C4B-NB	2.58	108.45	103.75
11	L	401	BCB	C4-C3-C5	2.55	119.56	115.27
14	L	503	UQ1	CM5-C5-C6	-2.55	120.24	124.40
11	M	401	BCB	C4-C3-C5	2.54	119.55	115.27
12	L	402	BPB	CED-O2D-CGD	2.54	121.68	115.94
15	M	600[A]	NS5	C32-C31-C33	2.52	119.51	115.27
15	M	600[B]	NS5	C32-C31-C33	2.52	119.51	115.27
15	M	600[A]	NS5	C18-C17-C15	-2.51	123.73	127.31
15	M	600[B]	NS5	C18-C17-C15	-2.51	123.73	127.31
11	M	400	BCB	C3B-C4B-NB	2.50	108.31	103.75
12	M	402	BPB	C3C-C2C-C1C	2.49	104.10	100.72
13	L	501	MQ9	C40-C39-C41	2.46	119.42	115.27
11	L	400	BCB	O2A-CGA-CBA	2.46	119.61	111.91
6	C	403	HEC	CMB-C2B-C1B	-2.45	124.69	128.46
11	L	401	BCB	CHC-C1C-C2C	2.43	124.52	117.19
13	L	501	MQ9	C35-C34-C36	2.42	119.34	115.27
6	C	401	HEC	CMB-C2B-C1B	-2.41	124.75	128.46
11	M	401	BCB	CHC-C1C-C2C	2.41	124.48	117.19
11	M	401	BCB	CED-O2D-CGD	2.41	121.38	115.94
11	M	401	BCB	CMA-C3A-C2A	-2.40	108.88	115.73
13	L	501	MQ9	C22-C23-C24	-2.40	121.88	127.66
12	M	402	BPB	O1D-CGD-CBD	-2.39	119.60	124.48
12	L	402	BPB	CBC-CAC-C3C	-2.38	119.75	126.72
6	C	404	HEC	CAD-CBD-CGD	-2.38	108.67	112.67
13	L	501	MQ9	C42-C43-C44	-2.38	121.93	127.66
15	M	600[A]	NS5	C11-C10-C9	2.37	119.26	115.27
15	M	600[B]	NS5	C11-C10-C9	2.37	119.26	115.27
11	M	400	BCB	CHC-C1C-C2C	2.37	124.35	117.19
11	L	400	BCB	CHC-C1C-C2C	2.36	124.33	117.19
15	M	600[A]	NS5	C24-C25-C26	-2.35	123.96	127.31
15	M	600[B]	NS5	C24-C25-C26	-2.35	123.96	127.31
13	L	501	MQ9	C17-C18-C19	-2.33	122.06	127.66
12	M	402	BPB	CMD-C2D-C1D	2.27	128.57	125.06
13	L	501	MQ9	C25-C24-C26	2.27	119.09	115.27
12	L	402	BPB	CBD-CHA-C1A	2.27	130.46	126.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	402	BPB	O1D-CGD-CBD	-2.26	119.86	124.48
14	L	503	UQ1	C11-C9-C10	2.26	119.59	114.60
11	M	400	BCB	CED-O2D-CGD	2.26	121.04	115.94
13	L	501	MQ9	C40-C39-C38	-2.24	117.93	123.68
14	L	502	UQ1	C11-C9-C10	2.23	119.53	114.60
13	L	501	MQ9	C5M-C5-C6	-2.23	120.77	124.40
11	L	400	BCB	C6-C7-C8	-2.21	108.77	115.92
15	M	600[A]	NS5	C22-C21-C20	-2.21	119.83	122.92
15	M	600[B]	NS5	C22-C21-C20	-2.21	119.83	122.92
12	M	402	BPB	C4-C3-C5	2.19	118.96	115.27
14	L	502	UQ1	CM5-C5-C6	-2.18	120.85	124.40
11	L	401	BCB	O2A-CGA-CBA	2.16	118.69	111.91
11	M	400	BCB	O2A-CGA-CBA	2.16	118.68	111.91
13	L	501	MQ9	C51-C49-C50	2.14	119.33	114.60
13	L	501	MQ9	C47-C48-C49	-2.13	120.48	127.75
13	L	501	MQ9	C30-C29-C31	2.12	118.83	115.27
12	M	402	BPB	C3A-C2A-C1A	2.10	104.48	101.34
11	M	401	BCB	CBA-CAA-C2A	-2.09	112.88	115.72
12	M	402	BPB	CAA-C2A-C1A	-2.08	105.33	112.19
6	C	403	HEC	CMD-C2D-C1D	-2.08	125.26	128.46
11	L	400	BCB	O1D-CGD-CBD	-2.08	120.43	124.54
12	L	402	BPB	CHD-C1D-ND	-2.08	120.26	124.58
11	M	400	BCB	C6-C7-C8	-2.07	109.22	115.92
6	C	402	HEC	CAA-CBA-CGA	-2.07	109.20	112.67
13	L	501	MQ9	C10-C9-C11	2.06	118.74	115.27
6	C	401	HEC	CMD-C2D-C1D	-2.05	125.31	128.46
11	M	400	BCB	CHA-CBD-CGD	-2.05	110.39	115.02
11	L	401	BCB	CHA-CBD-CGD	-2.03	110.44	115.02
6	C	403	HEC	CBA-CAA-C2A	-2.01	108.77	112.48

There are no chirality outliers.

All (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
12	L	402	BPB	O2A-C1-C2-C3
11	L	401	BCB	C2B-C3B-CAB-OBB
11	L	401	BCB	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	M	400	BCB	C4B-C3B-CAB-OBB
11	M	400	BCB	C4B-C3B-CAB-CBB
11	M	401	BCB	C2B-C3B-CAB-OBB
11	M	401	BCB	C2B-C3B-CAB-CBB
11	M	401	BCB	C2C-C3C-CAC-CBC
11	M	401	BCB	CAD-CBD-CGD-O1D
11	M	401	BCB	CAD-CBD-CGD-O2D
13	L	501	MQ9	C34-C36-C37-C38
13	L	501	MQ9	C37-C38-C39-C40
13	L	501	MQ9	C37-C38-C39-C41
13	L	501	MQ9	C38-C39-C41-C42
13	L	501	MQ9	C39-C41-C42-C43
13	L	501	MQ9	C42-C43-C44-C46
13	L	501	MQ9	C47-C48-C49-C50
7	C	707	HTO	O1-C1-C2-O2
7	C	707	HTO	O1-C1-C2-C3
7	C	707	HTO	C1-C2-C3-O3
11	L	400	BCB	C2B-C3B-CAB-OBB
11	L	400	BCB	C2B-C3B-CAB-CBB
15	M	600[B]	NS5	C34-C35-C36-CM3
15	M	600[B]	NS5	C34-C35-C36-CM4
15	M	600[A]	NS5	C34-C35-C36-CM3
15	M	600[A]	NS5	C34-C35-C36-CM4
13	L	501	MQ9	C47-C48-C49-C51
15	M	600[A]	NS5	C2-C3-C4-C5
15	M	600[B]	NS5	C2-C3-C4-C5
12	M	402	BPB	C4-C3-C5-C6
12	M	402	BPB	C2-C3-C5-C6
11	M	401	BCB	C2A-CAA-CBA-CGA
13	L	501	MQ9	C42-C43-C44-C45
11	L	400	BCB	C4-C3-C5-C6
11	L	400	BCB	C2-C3-C5-C6
15	M	600[A]	NS5	C31-C33-C34-C35
15	M	600[B]	NS5	C31-C33-C34-C35
12	M	402	BPB	C8-C10-C11-C12
11	M	400	BCB	C5-C6-C7-C8
11	M	400	BCB	C13-C15-C16-C17
12	M	402	BPB	C10-C11-C12-C13
11	L	400	BCB	C15-C16-C17-C18
12	M	402	BPB	C15-C16-C17-C18
12	M	402	BPB	C13-C15-C16-C17
8	H	701	LDA	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
8	H	703	LDA	C5-C6-C7-C8
8	H	701	LDA	C6-C7-C8-C9
11	M	401	BCB	C13-C15-C16-C17
12	M	402	BPB	C16-C17-C18-C19
12	M	402	BPB	C16-C17-C18-C20
8	H	703	LDA	C4-C5-C6-C7
8	M	704	LDA	C7-C8-C9-C10
15	M	600[A]	NS5	C1-C2-C3-C4
15	M	600[B]	NS5	C1-C2-C3-C4
8	H	703	LDA	C11-C10-C9-C8
8	H	701	LDA	C4-C5-C6-C7
11	L	401	BCB	C16-C17-C18-C19
12	M	402	BPB	C11-C12-C13-C14
11	L	401	BCB	C16-C17-C18-C20
8	H	703	LDA	C1-C2-C3-C4
12	L	402	BPB	C4-C3-C5-C6
11	M	400	BCB	C4-C3-C5-C6
7	L	709	HTO	C4-C5-C6-C7
7	C	706	HTO	O2-C2-C3-O3
7	L	708	HTO	O2-C2-C3-O3
7	C	707	HTO	O2-C2-C3-O3
7	H	705	HTO	C4-C5-C6-C7
12	M	402	BPB	C11-C10-C8-C7
12	M	402	BPB	C11-C12-C13-C15
11	M	400	BCB	C2-C3-C5-C6
11	M	400	BCB	C6-C7-C8-C10
11	M	400	BCB	C11-C12-C13-C15
11	M	400	BCB	C6-C7-C8-C9
11	M	400	BCB	C11-C12-C13-C14
15	M	600[A]	NS5	C7-C8-C9-C10
15	M	600[B]	NS5	C7-C8-C9-C10
12	L	402	BPB	C2-C3-C5-C6
7	C	706	HTO	C1-C2-C3-C4
7	H	705	HTO	C1-C2-C3-C4
7	C	707	HTO	O2-C2-C3-C4
11	M	400	BCB	C11-C10-C8-C7
12	L	402	BPB	CAD-CBD-CGD-O2D
11	L	401	BCB	C2C-C3C-CAC-CBC
11	M	400	BCB	C2C-C3C-CAC-CBC
11	M	400	BCB	C11-C10-C8-C9
11	M	400	BCB	C3-C5-C6-C7
11	L	400	BCB	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
12	M	402	BPB	C12-C13-C15-C16
8	L	702	LDA	C11-C10-C9-C8
7	L	709	HTO	C3-C4-C5-C6
14	L	502	UQ1	C1-C2-O2-CM2
12	L	402	BPB	C8-C10-C11-C12
8	H	703	LDA	C7-C8-C9-C10
11	M	400	BCB	C16-C17-C18-C19
11	L	400	BCB	CAD-CBD-CGD-O1D
11	L	401	BCB	C12-C13-C15-C16
12	M	402	BPB	C14-C13-C15-C16
11	M	400	BCB	C16-C17-C18-C20
11	M	401	BCB	C16-C17-C18-C20
13	L	501	MQ9	C40-C39-C41-C42
8	L	702	LDA	C2-C3-C4-C5
7	C	706	HTO	C1-C2-C3-O3
11	M	400	BCB	C1A-C2A-CAA-CBA
11	M	401	BCB	C11-C12-C13-C15
11	M	401	BCB	C16-C17-C18-C19
13	L	501	MQ9	C45-C44-C46-C47
11	L	401	BCB	C14-C13-C15-C16
7	C	706	HTO	O3-C3-C4-C5
15	M	600[A]	NS5	C11-C10-C9-C8
15	M	600[B]	NS5	C11-C10-C9-C8
6	C	402	HEC	C3D-CAD-CBD-CGD
15	M	600[A]	NS5	C12-C10-C9-C8
12	M	402	BPB	C6-C7-C8-C10
15	M	600[B]	NS5	C12-C10-C9-C8
11	M	401	BCB	C11-C12-C13-C14
11	M	401	BCB	O2A-C1-C2-C3
7	H	705	HTO	O2-C2-C3-O3
8	L	702	LDA	C2-C1-N1-CM1
8	L	702	LDA	C2-C1-N1-CM2
11	L	400	BCB	CAD-CBD-CGD-O2D
12	M	402	BPB	C6-C7-C8-C9
7	H	705	HTO	C2-C3-C4-C5
13	L	501	MQ9	C33-C34-C36-C37
8	M	704	LDA	C11-C10-C9-C8
13	L	501	MQ9	C41-C42-C43-C44
8	M	704	LDA	C2-C1-N1-O1
7	C	707	HTO	C3-C4-C5-C6
14	L	502	UQ1	C3-C2-O2-CM2

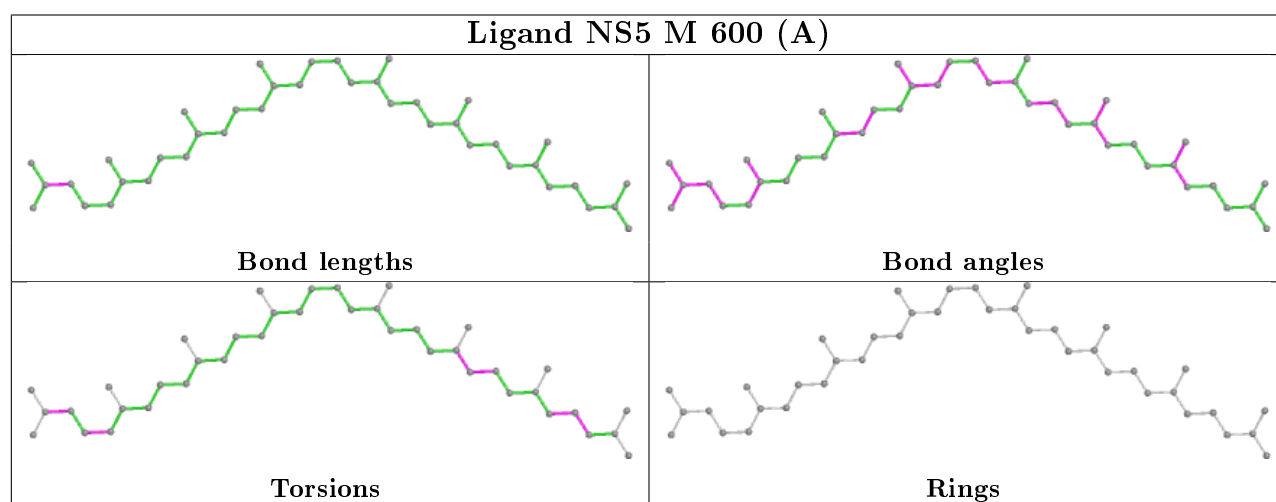
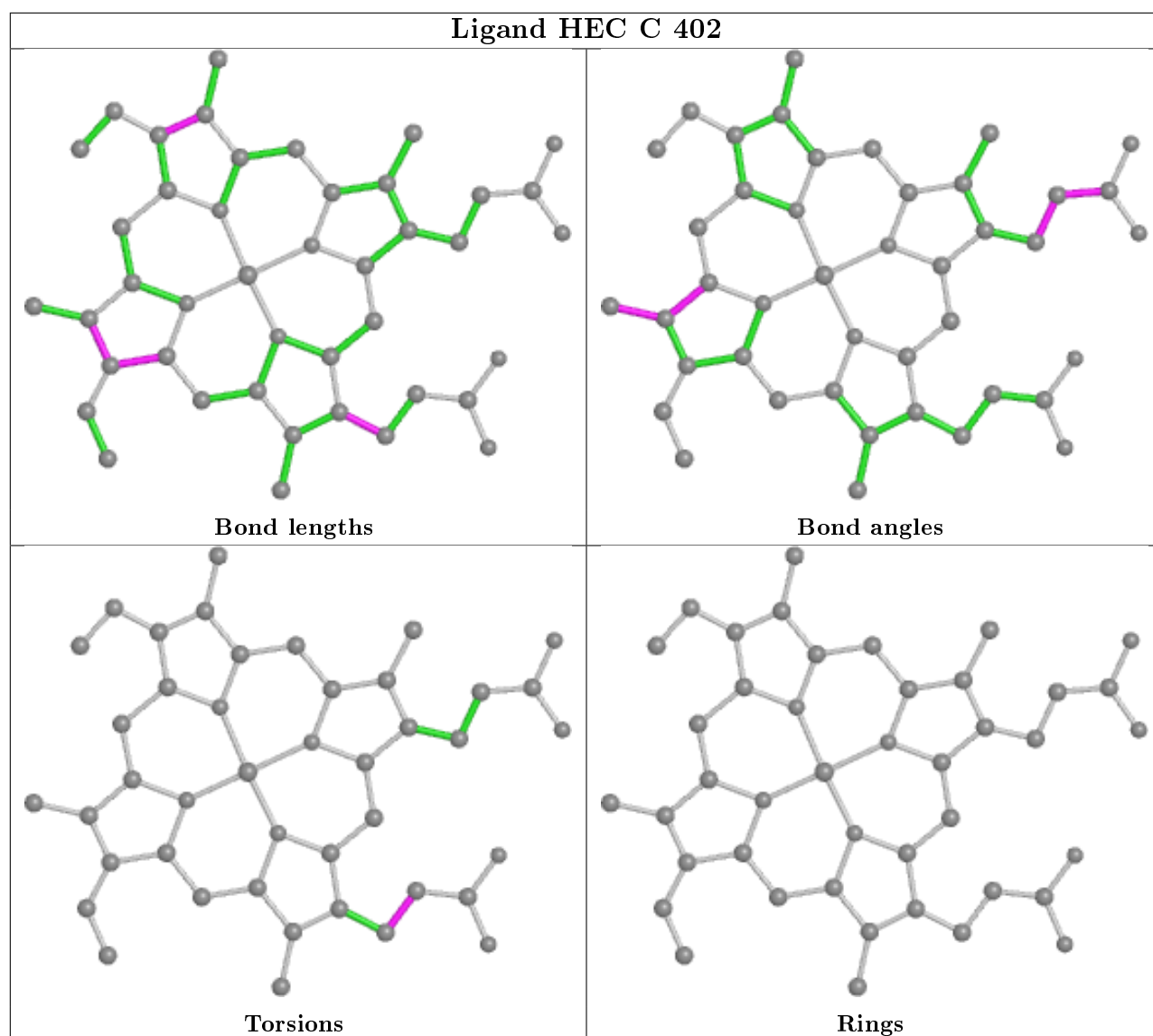
There are no ring outliers.



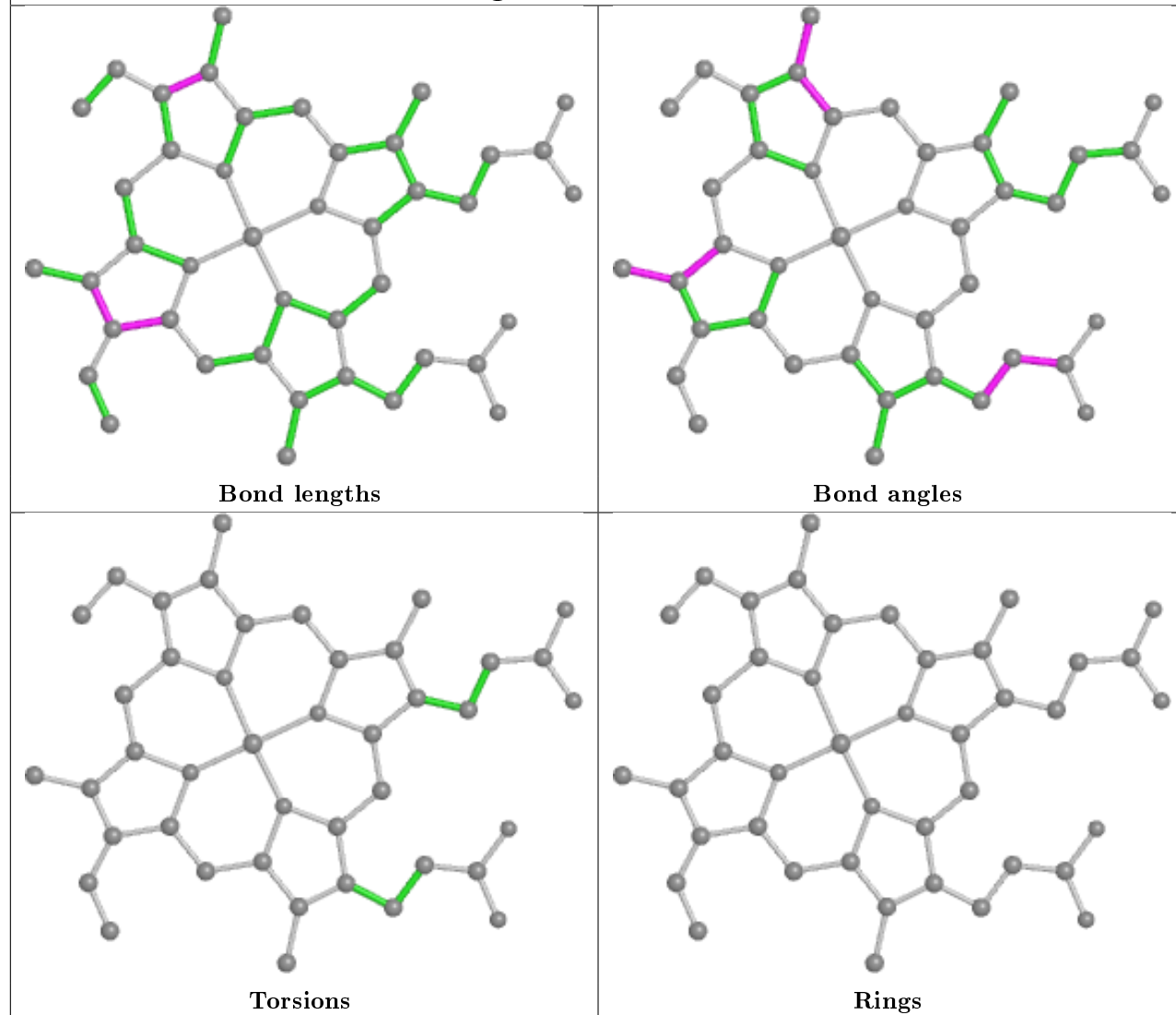
13 monomers are involved in 57 short contacts:

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
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

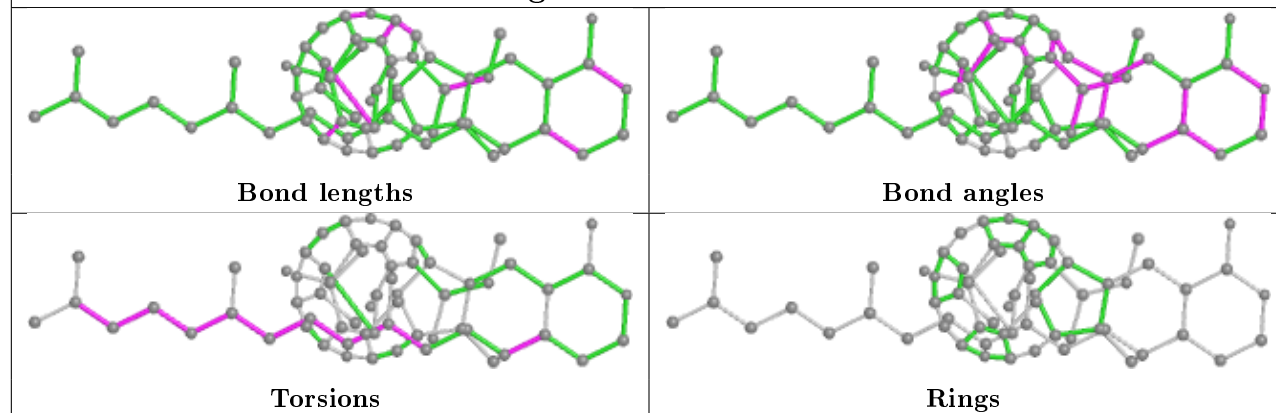
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



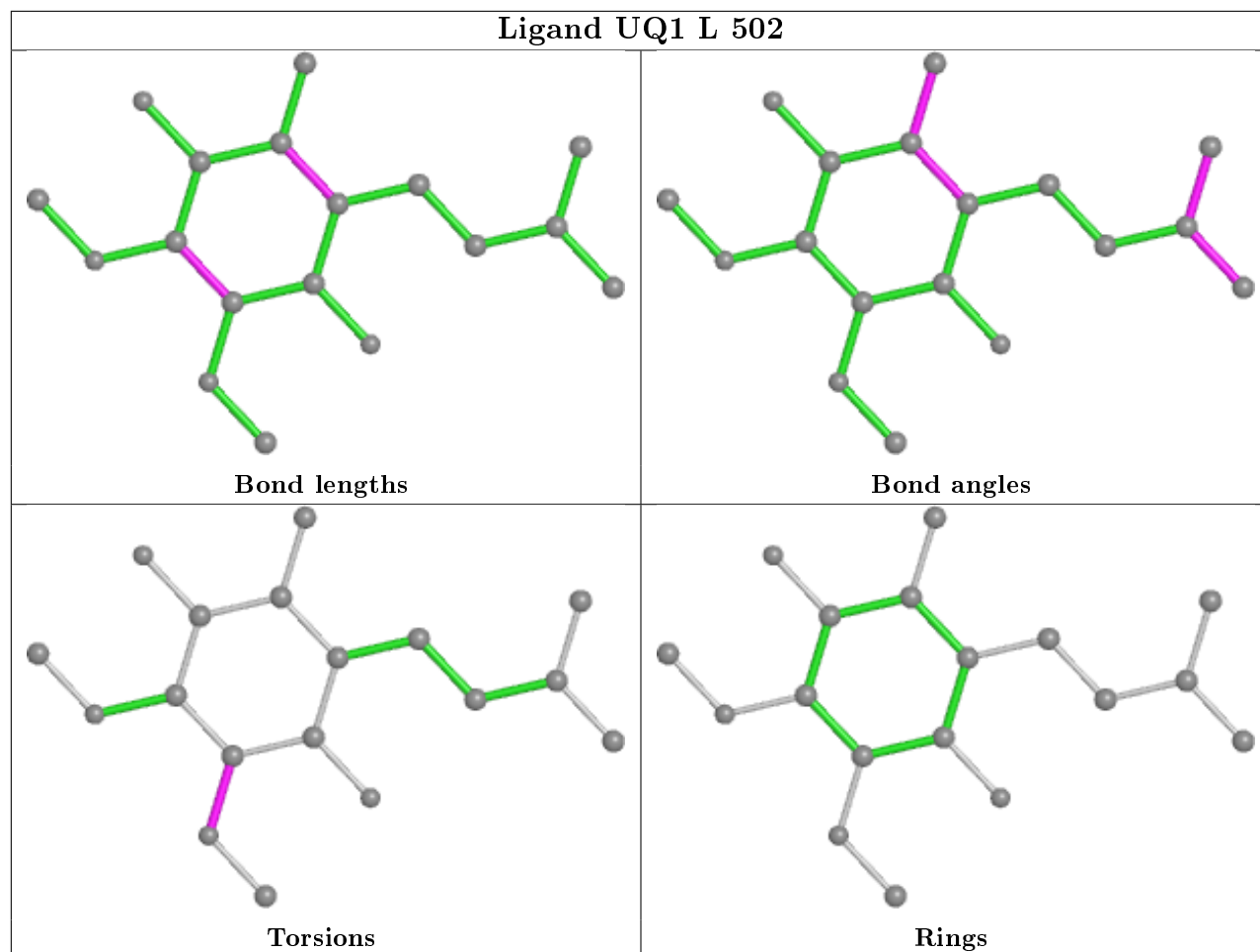
## Ligand HEC C 404



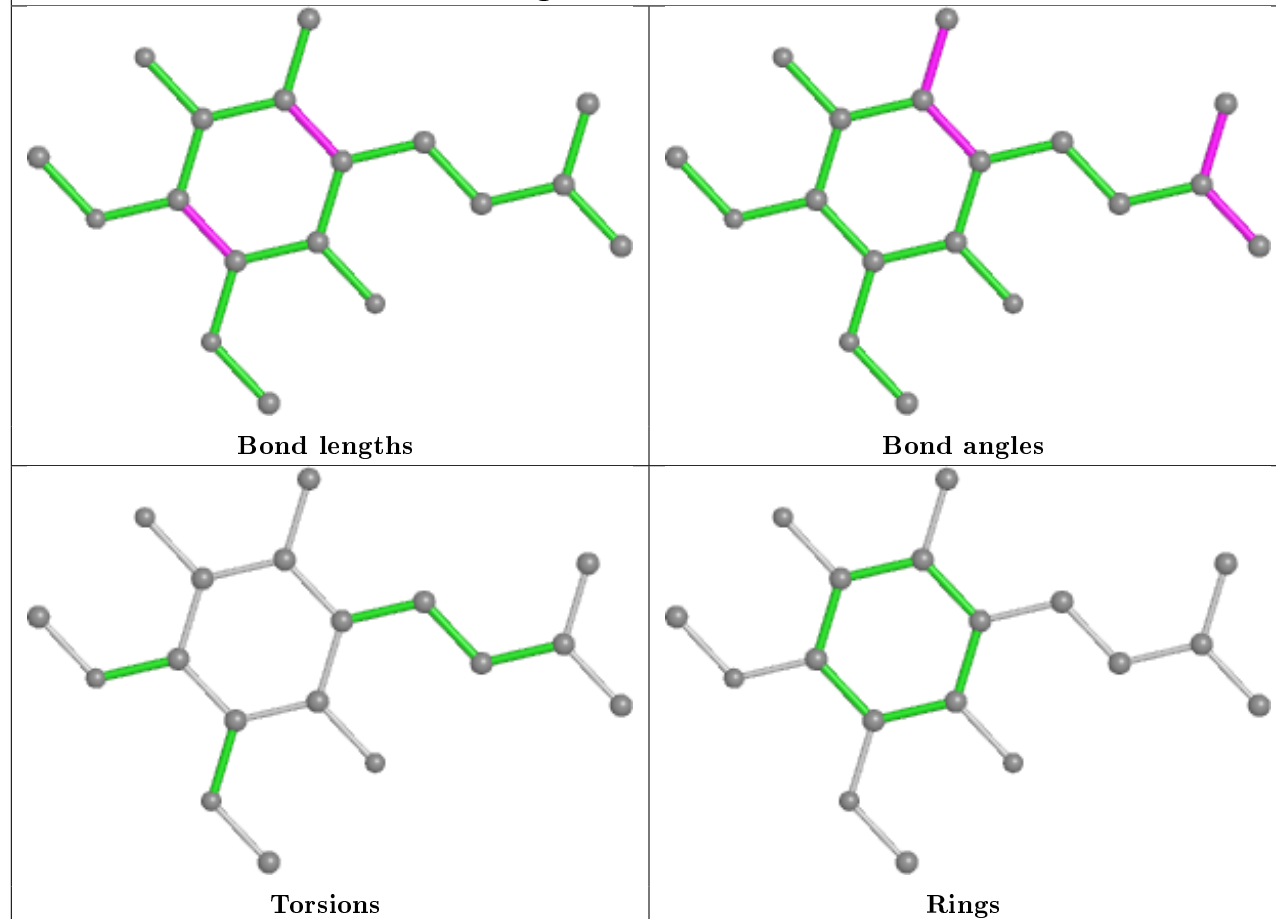
## Ligand BPB M 402



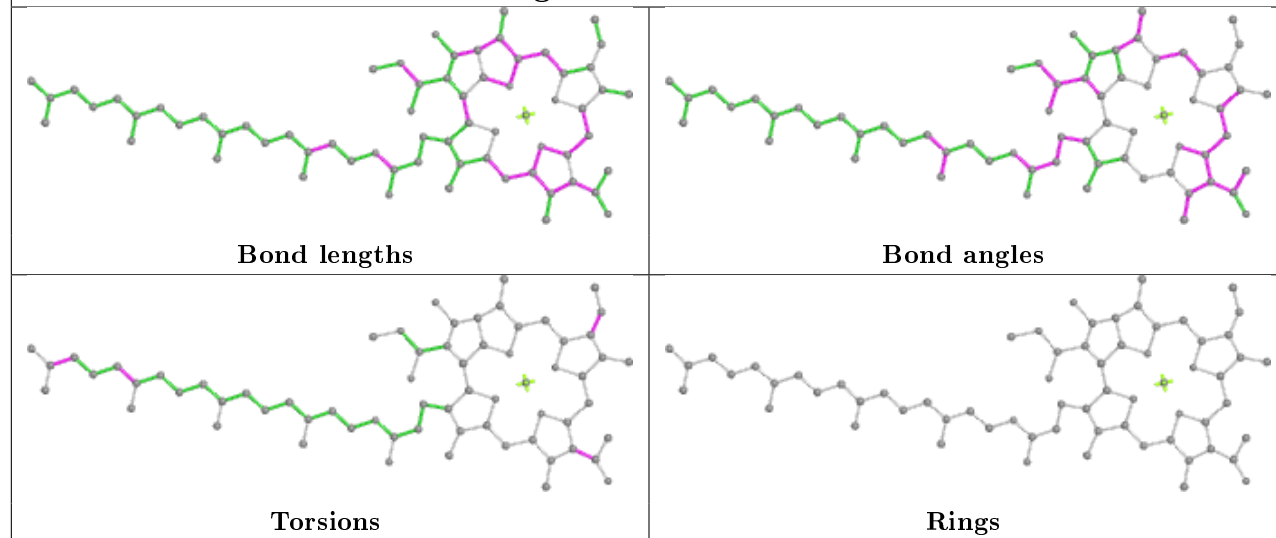
## Ligand UQ1 L 502

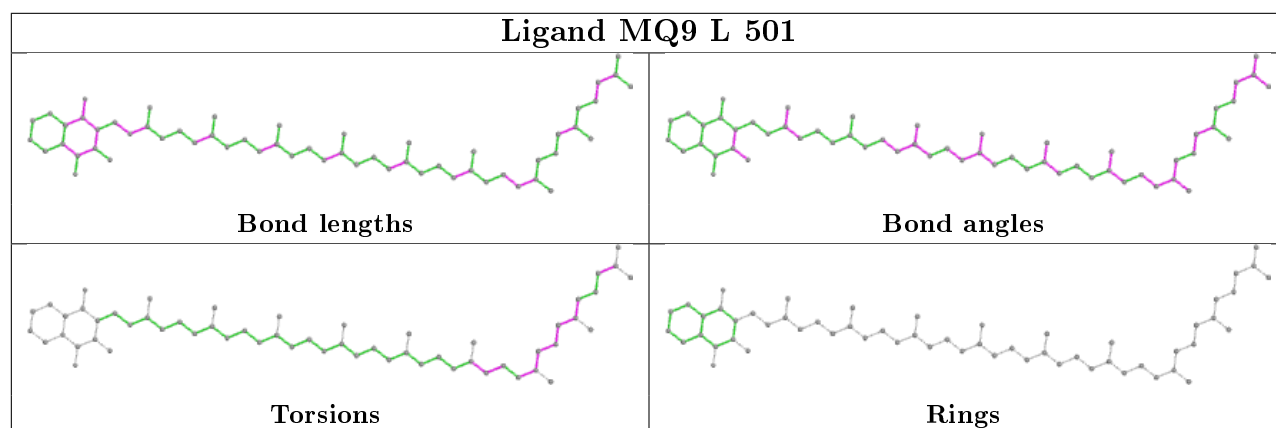
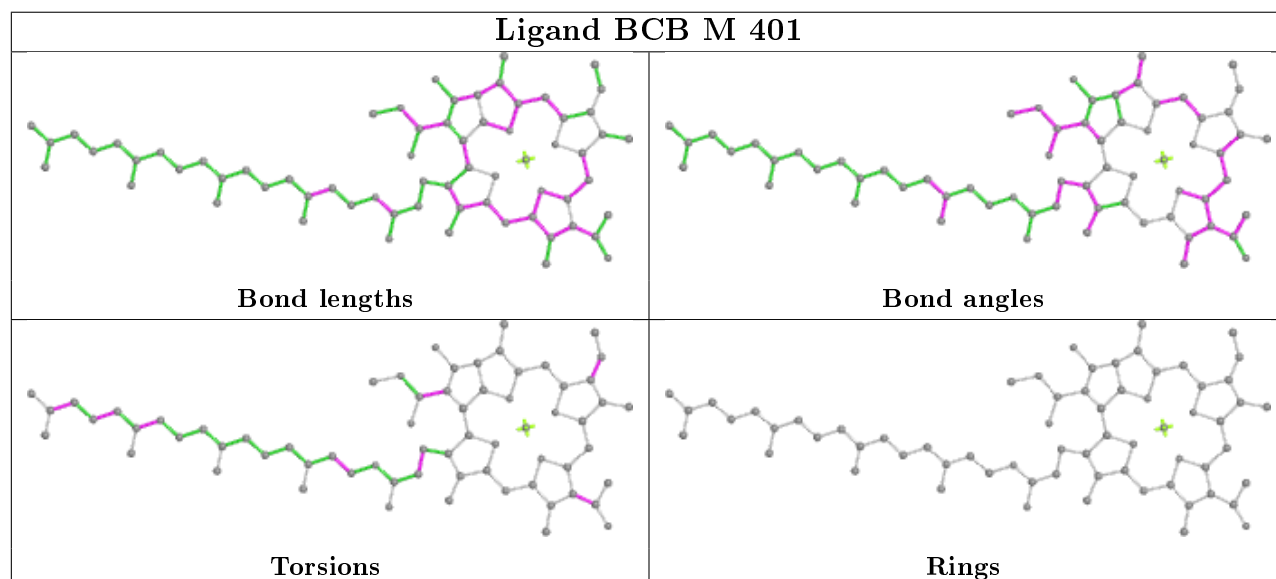
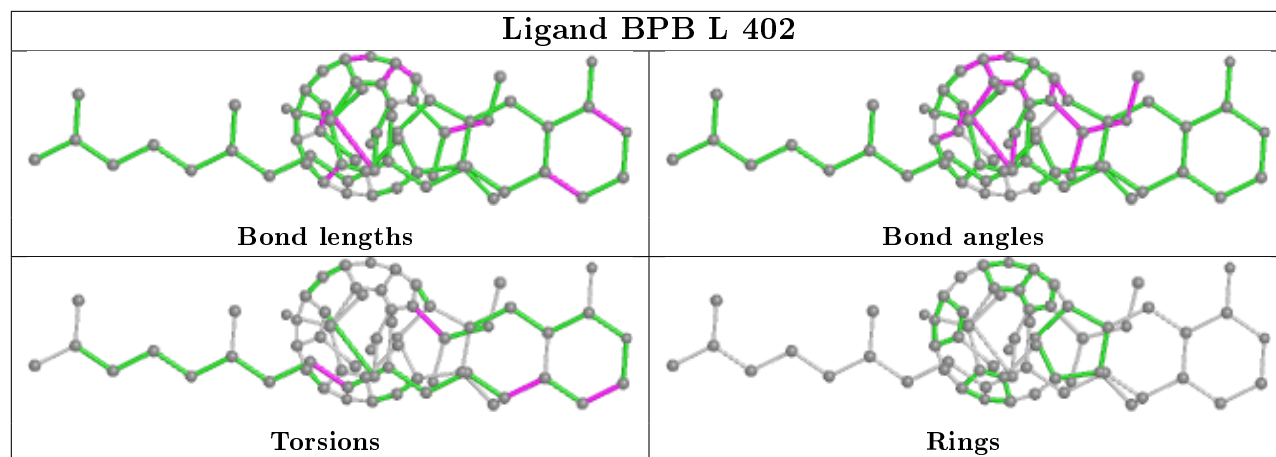


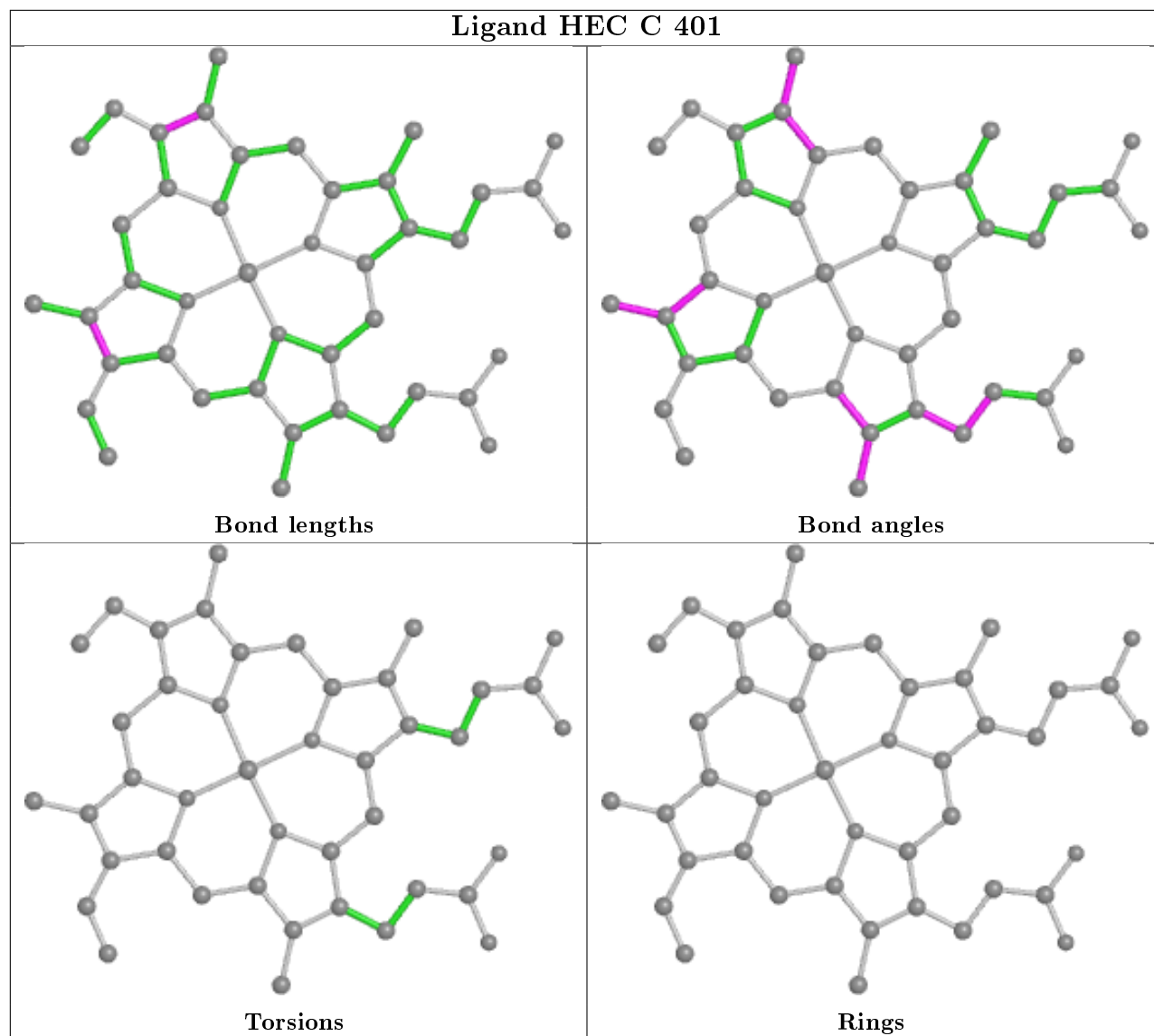
## Ligand UQ1 L 503



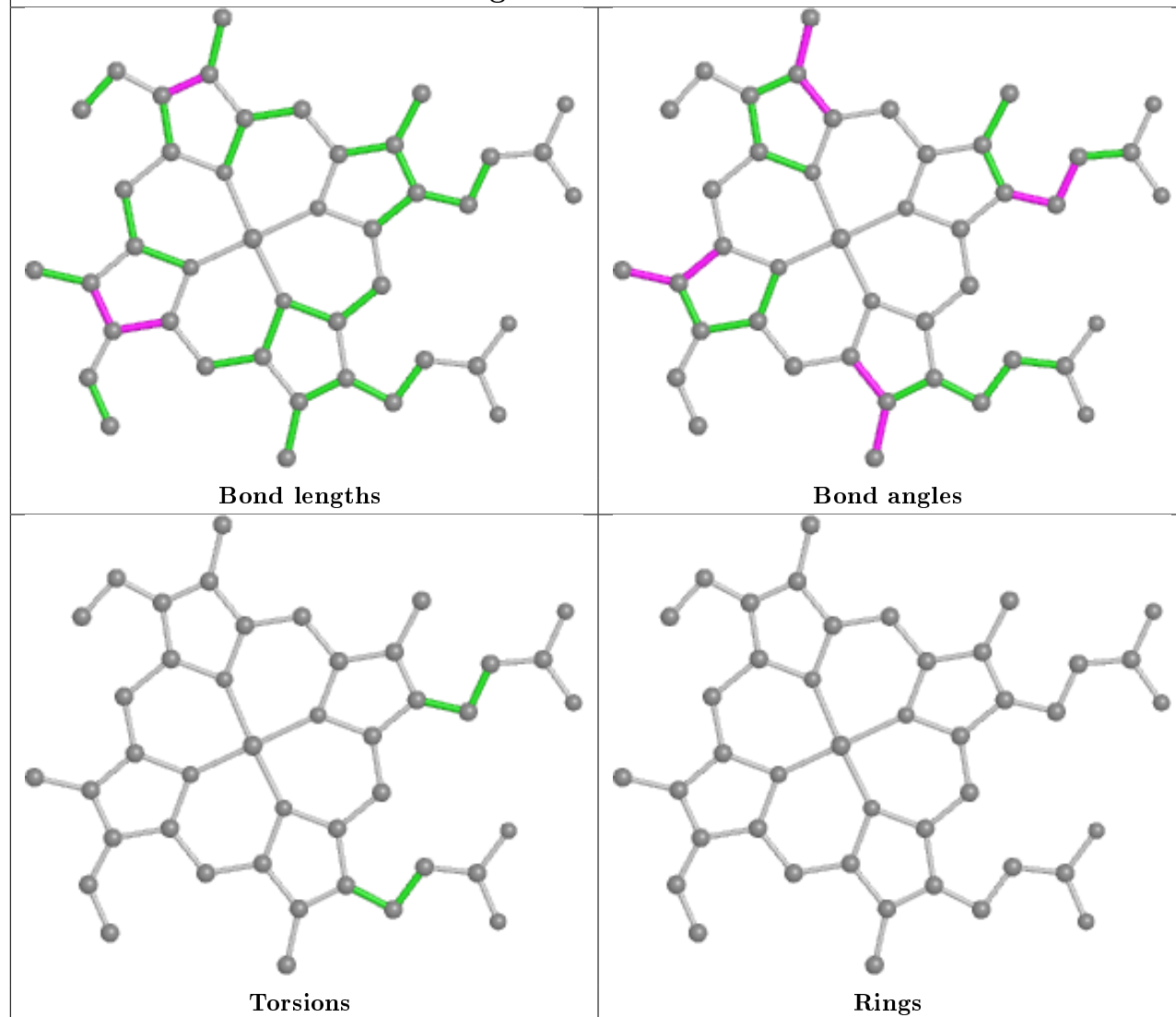
## Ligand BCB L 401



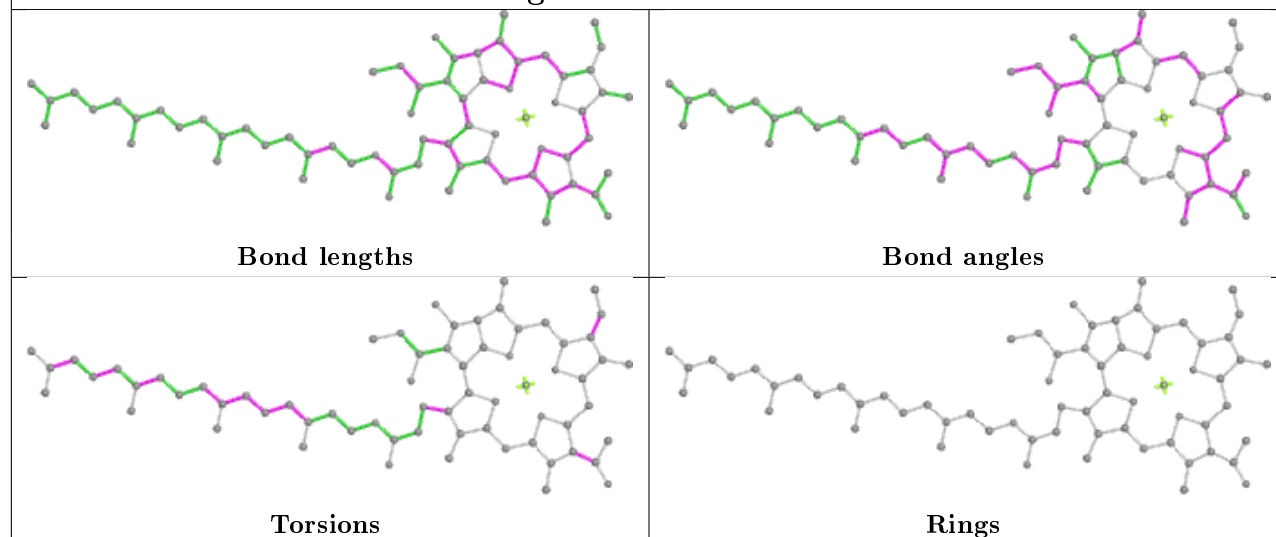




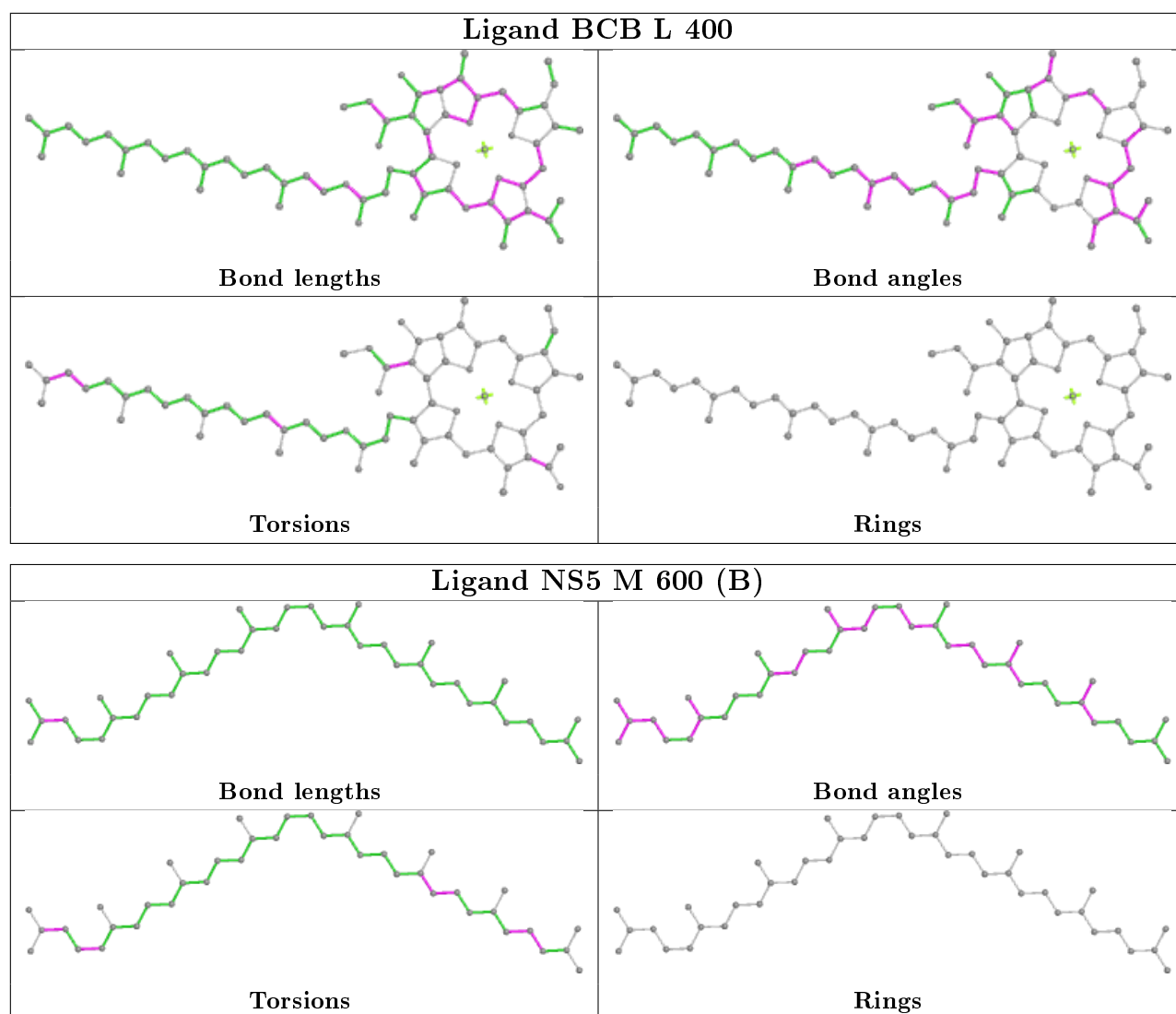
## Ligand HEC C 403



## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	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

All (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
2	H	81	ARG	4.1
2	H	96	PHE	3.8
2	H	9	HIS	3.5
4	M	319	PRO	3.4
3	L	202	ASP	3.3
3	L	271	PHE	3.2
2	H	94	ASP	3.2
3	L	51	TYR	3.2
1	C	48	GLU	3.1
4	M	31	LYS	3.1
1	C	57	LYS	3.0
2	H	45	GLU	2.9
4	M	108	HIS	2.8
4	M	71	PHE	2.8
4	M	37	TRP	2.8
2	H	87	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
4	M	26	ASN	2.6
1	C	47	ALA	2.5
4	M	320	GLY	2.4
2	H	147	GLU	2.4
3	L	1	ALA	2.4
2	H	205	LYS	2.4
4	M	30	GLY	2.4
2	H	191	ALA	2.3
2	H	95	GLY	2.3
1	C	332	LYS	2.3
4	M	22	GLU	2.3
2	H	258	LEU	2.3
2	H	55	GLU	2.1
1	C	46	LYS	2.1
1	C	2	PHE	2.1
2	H	190	SER	2.1
2	H	189	GLY	2.1
1	C	54	GLN	2.0
4	M	103	GLY	2.0
1	C	169	ARG	2.0
2	H	97	GLU	2.0

## 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
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 [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
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
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

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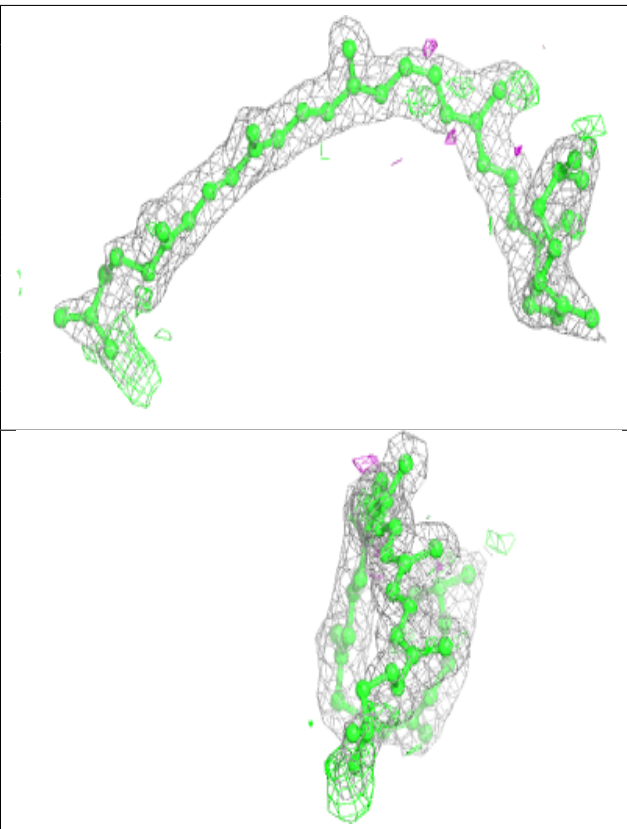
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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.

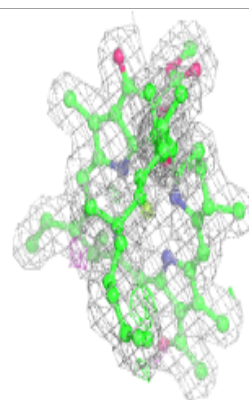
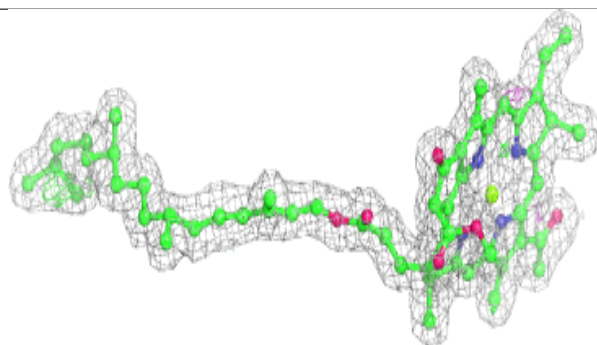
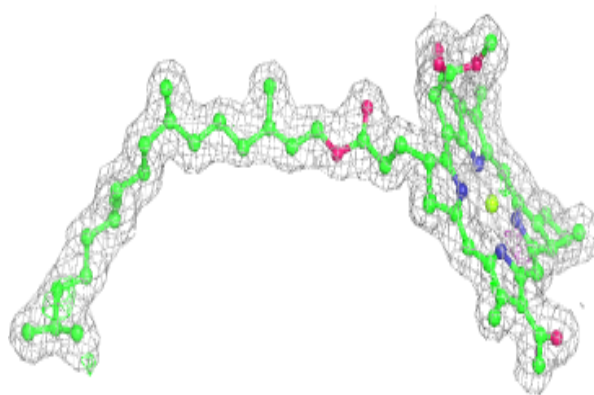
**Electron density around NS5 M 600 (B):**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

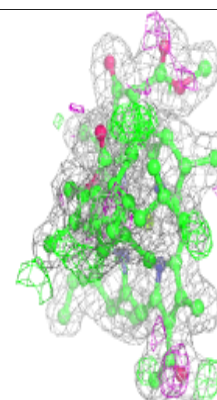
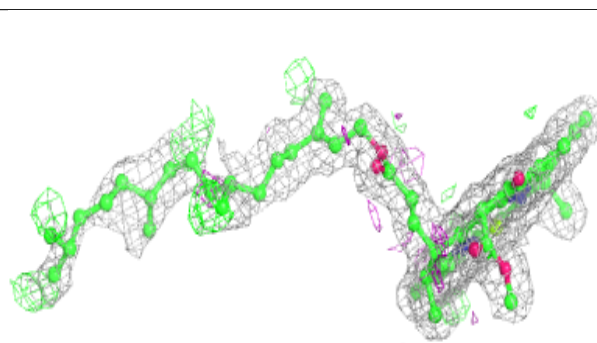
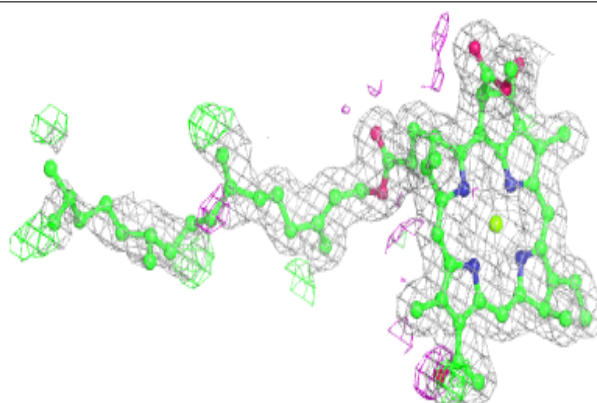


**Electron density around BCB L 400:**

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

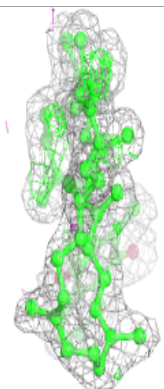
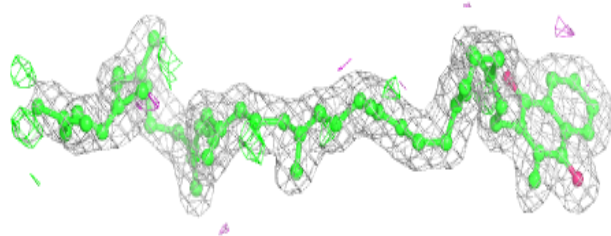
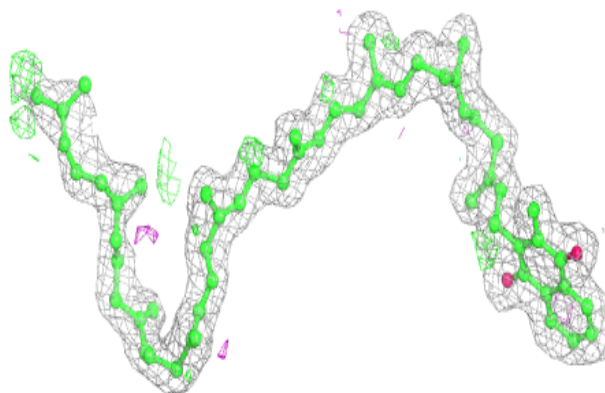
**Electron density around BCB M 400:**

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

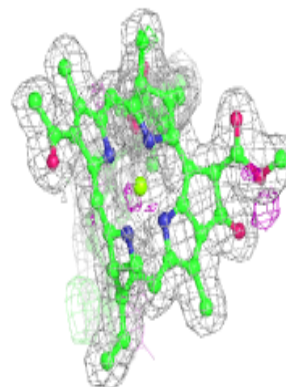
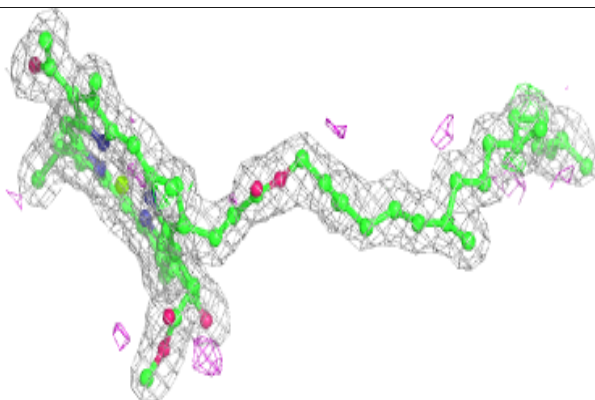
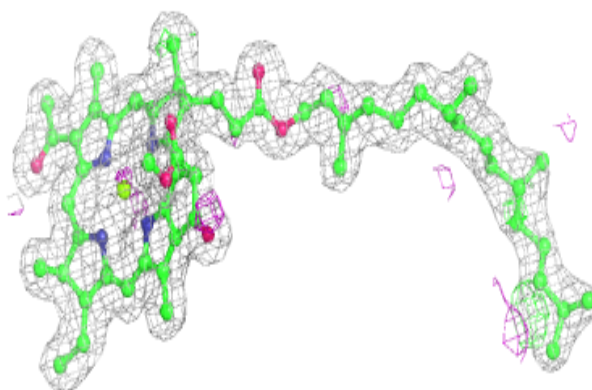


**Electron density around MQ9 L 501:**

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and green (positive)

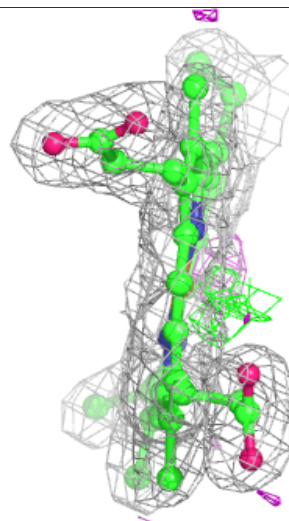
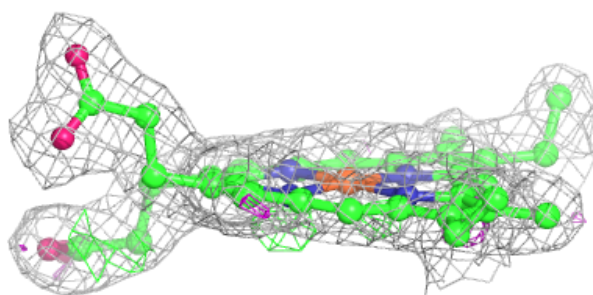
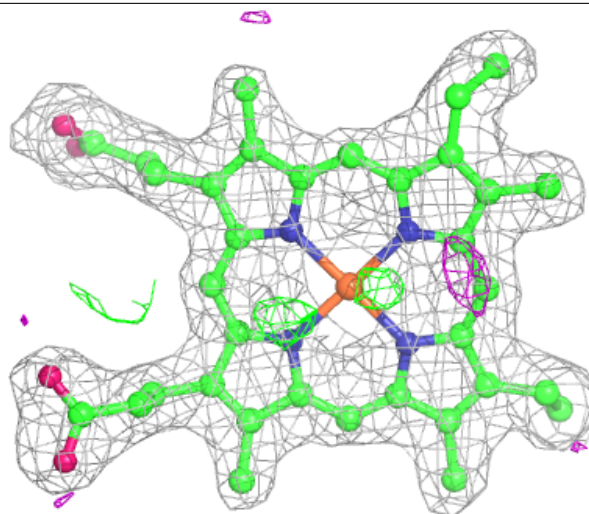
**Electron density around BCB M 401:**

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and green (positive)



**Electron density around HEC C 401:**

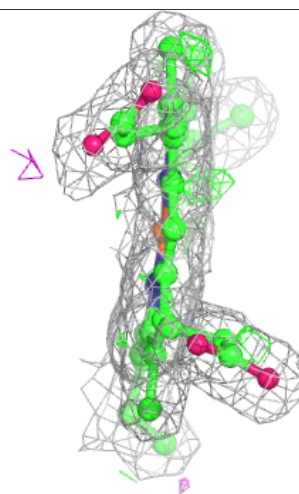
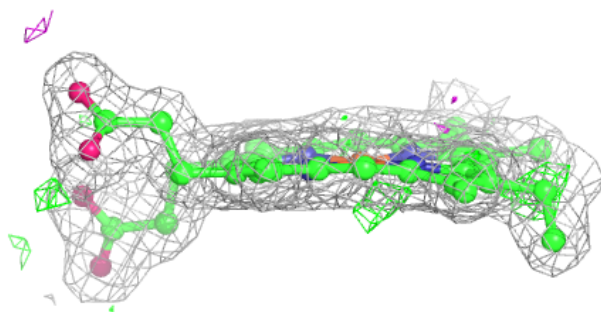
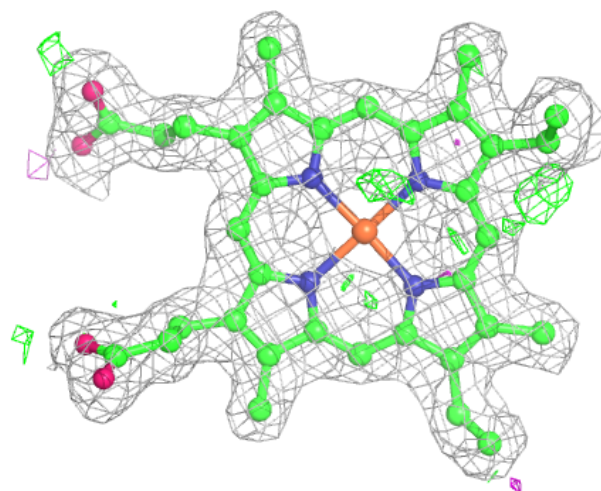
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





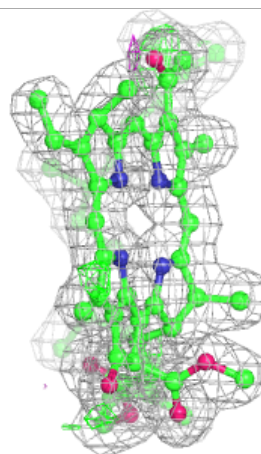
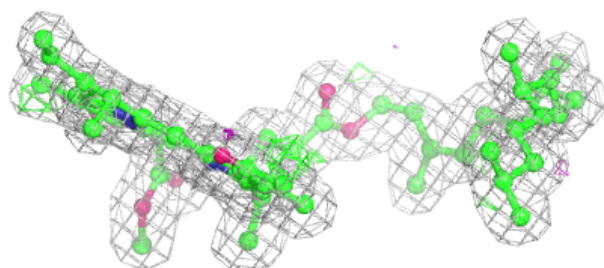
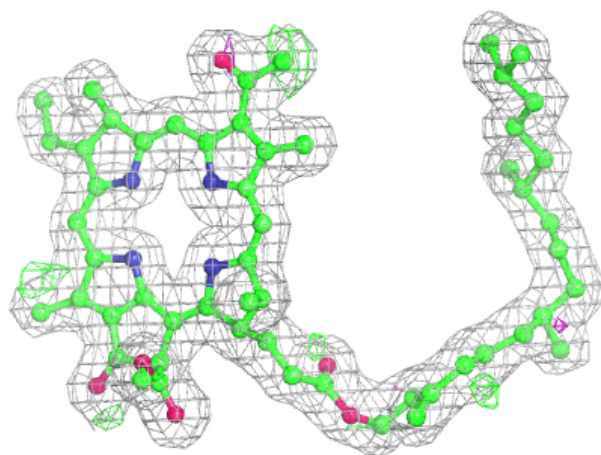
**Electron density around HEC C 403:**

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



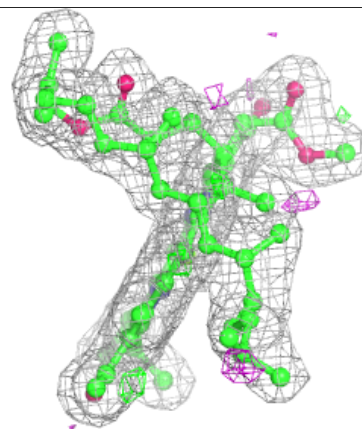
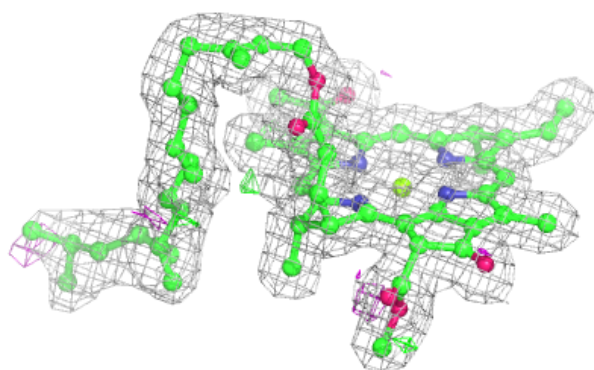
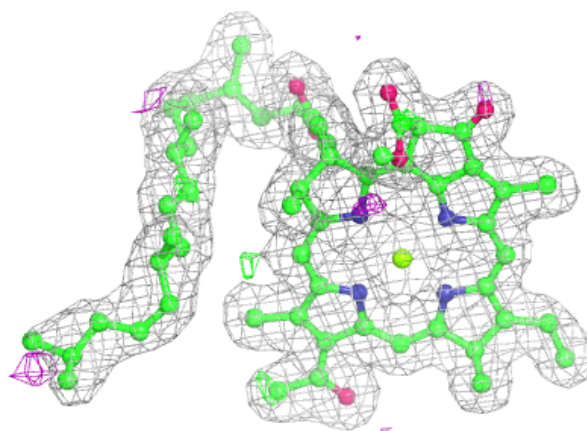
**Electron density around BPB L 402:**

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and green (positive)

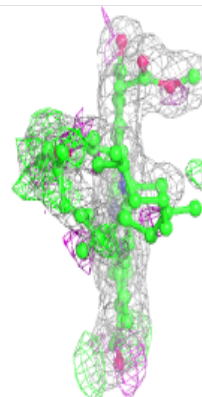
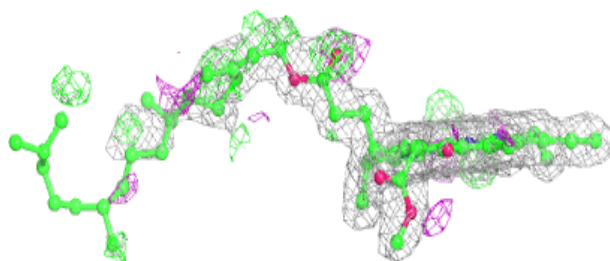
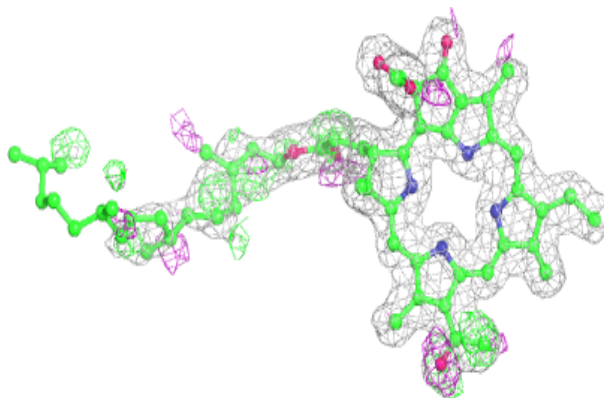


**Electron density around BCB L 401:**

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

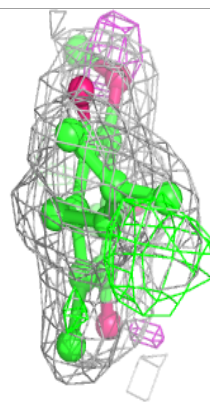
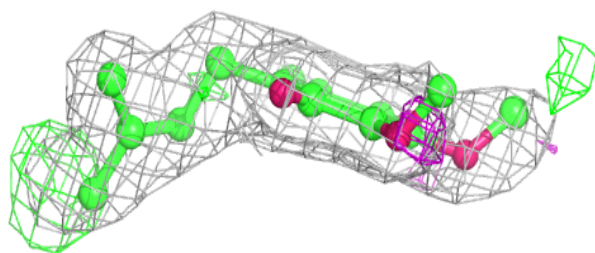
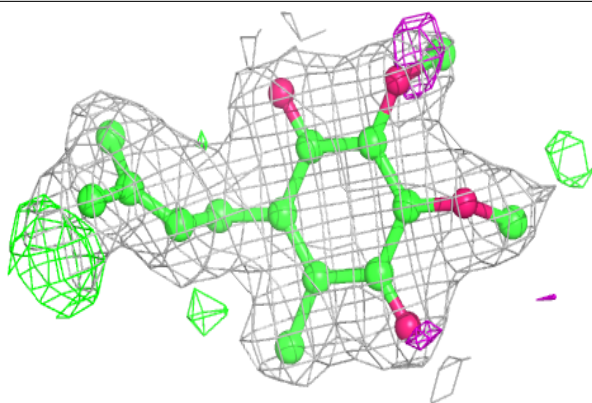
**Electron density around BPB M 402:**

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



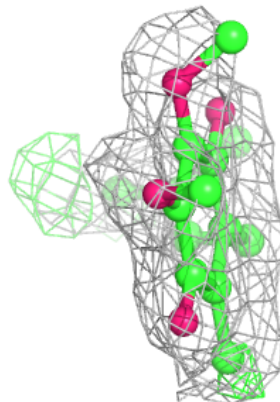
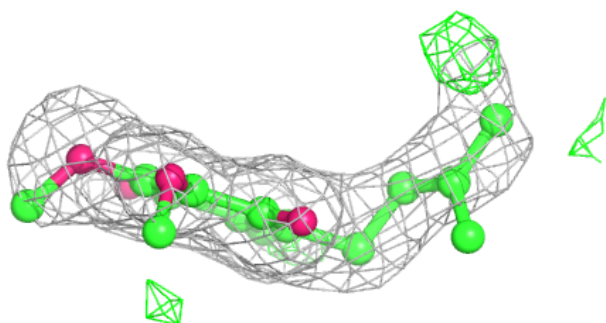
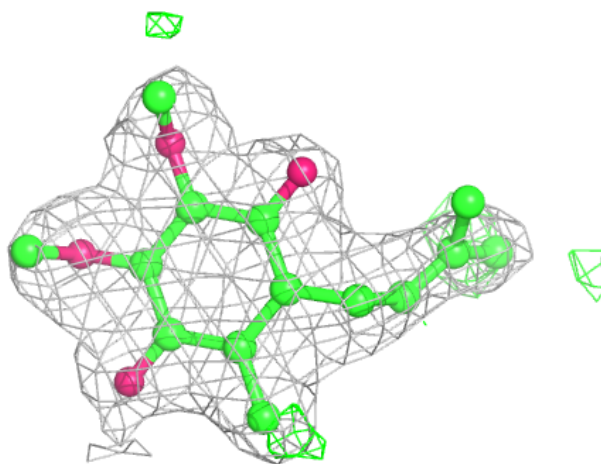
**Electron density around UQ1 L 502:**

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



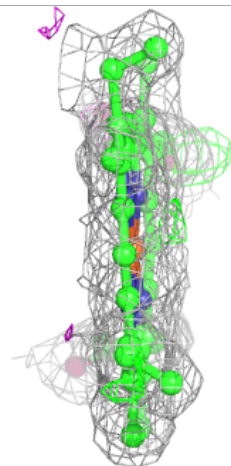
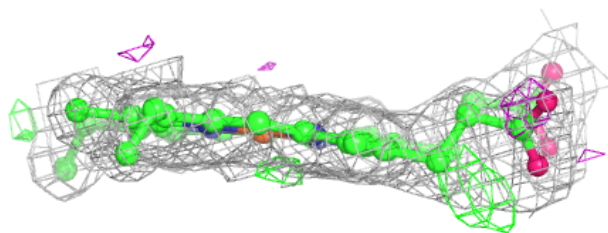
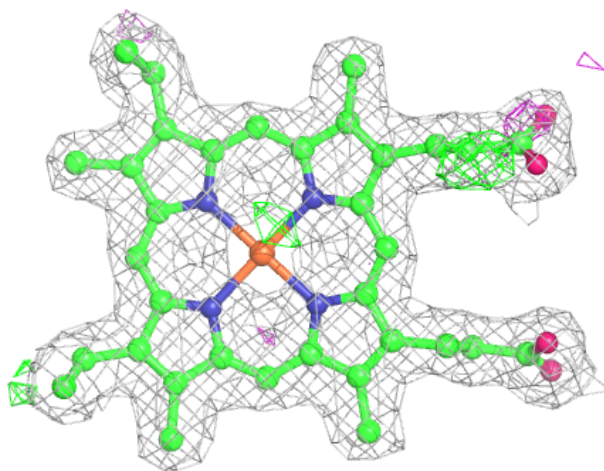
**Electron density around UQ1 L 503:**

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and green (positive)



**Electron density around HEC C 404:**

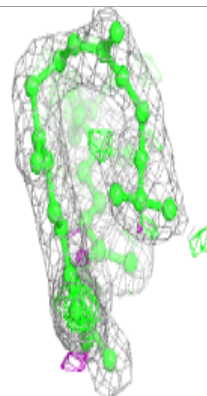
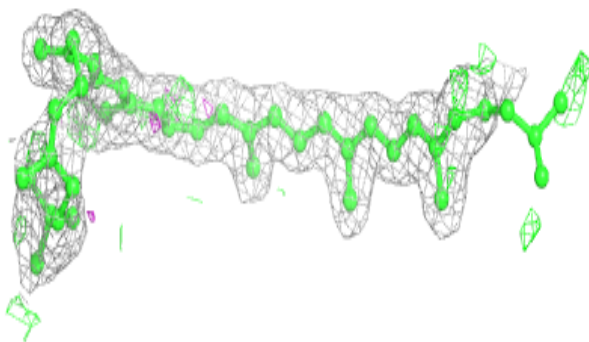
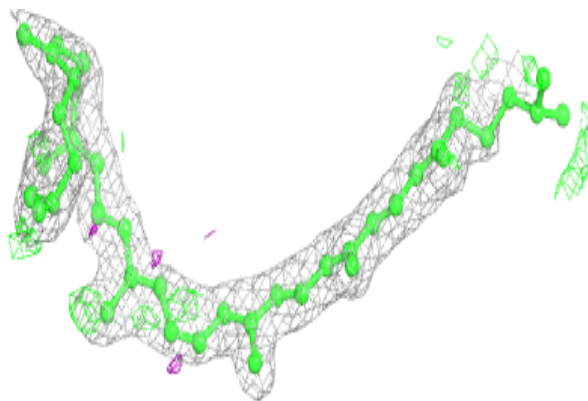
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

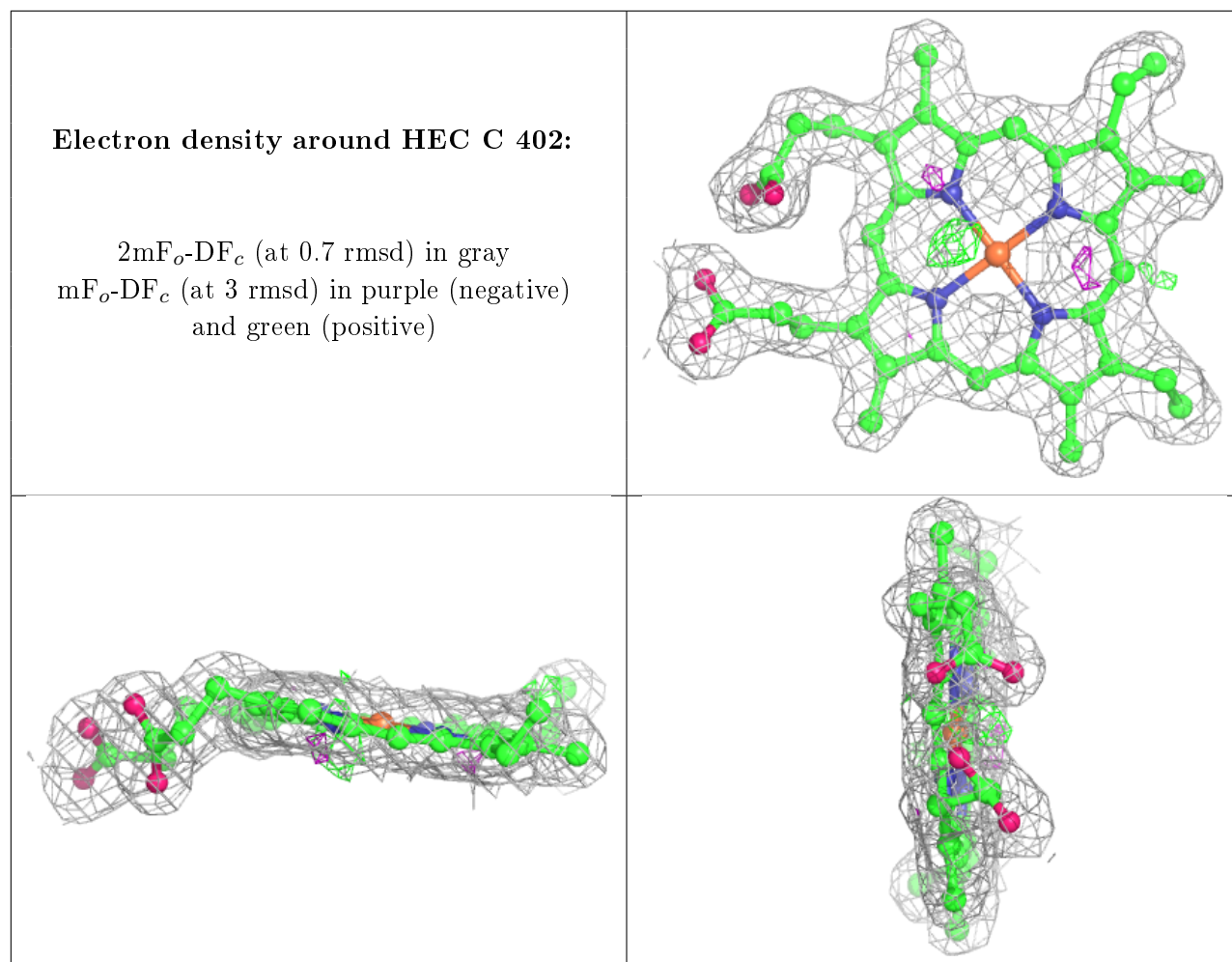




**Electron density around NS5 M 600 (A):**

$2mF_o-DF_c$  (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.