



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 05:39 am BST

PDB ID : 3G7F  
Title : Crystal structure of Blastochloris viridis heterodimer mutant reaction center  
Authors : Ponomarenko, N.S.; Li, L.; Tereshko, V.; Ismagilov, R.F.; Norris Jr., J.R.  
Deposited on : 2009-02-09  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

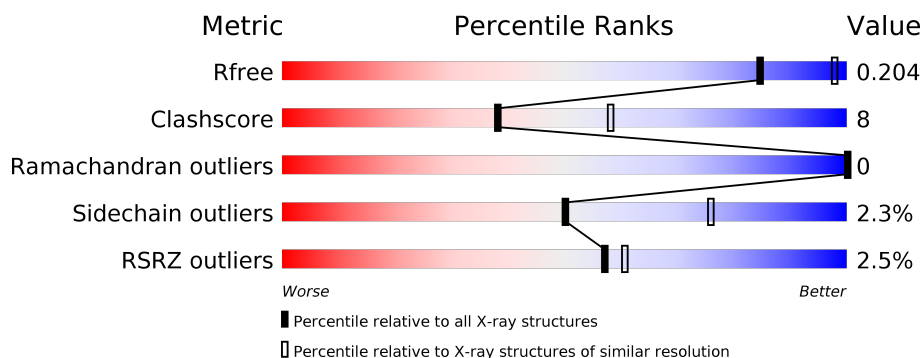
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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>92%</div> <div>7%</div> </div>
2	H	258	<div> <div>6%</div> <div>88%</div> <div>9%</div> </div>
3	L	273	<div> <div>%</div> <div>92%</div> <div>7%</div> </div>
4	M	323	<div> <div>2%</div> <div>86%</div> <div>14%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	BPB	M	401	-	-	X	-
11	UQ1	M	503	-	-	-	X
6	SO4	C	815	-	-	-	X
6	SO4	C	817	-	-	-	X
6	SO4	L	814	-	-	-	X
6	SO4	M	816	-	-	-	X
6	SO4	M	818	-	-	-	X
6	SO4	M	819	-	-	-	X
7	HTO	L	708	-	-	-	X
7	HTO	L	709	-	-	-	X

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 10922 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 Photosynthetic reaction center H subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	250	Total	C	N	O	S	0	0	0
			1956	1250	335	369	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	216	ASP	GLU	variant	UNP P06008
H	256	ALA	SER	variant	UNP P06008

- Molecule 3 is a protein called Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	1	0
			2172	1460	350	355	7			

- Molecule 4 is a protein called Photosynthetic reaction center M subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	2	0
			2557	1704	417	424	12			

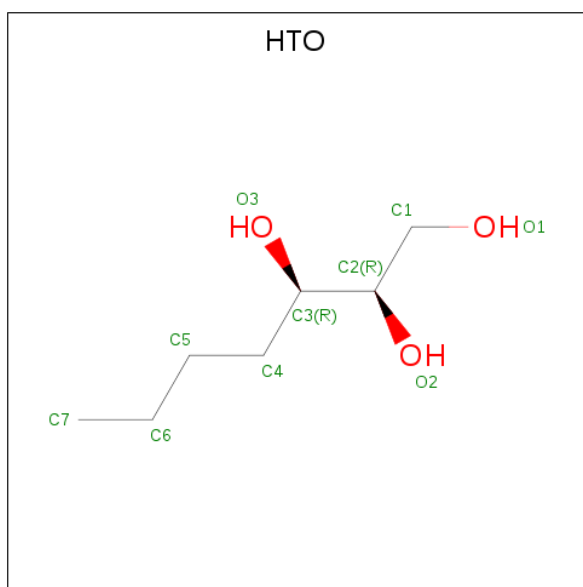
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	200	LEU	HIS	variant	UNP P06010

- # HEC

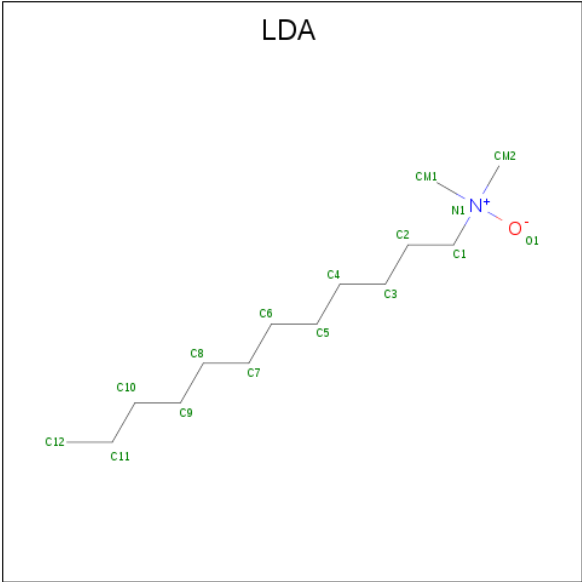
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0
6	H	1	Total O S 5 4 1	0	0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

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



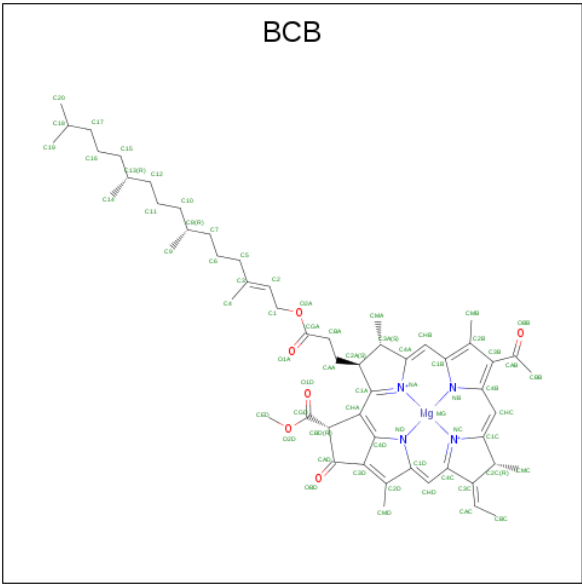
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			10	7	3		
7	C	1	Total	C	O	0	0
			10	7	3		
7	H	1	Total	C	O	0	0
			10	7	3		
7	L	1	Total	C	O	0	0
			10	7	3		
7	L	1	Total	C	O	0	0
			10	7	3		

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



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

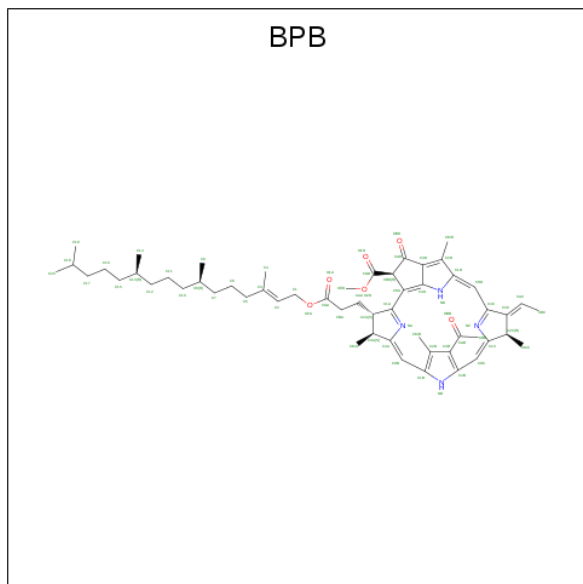
- Molecule 9 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).





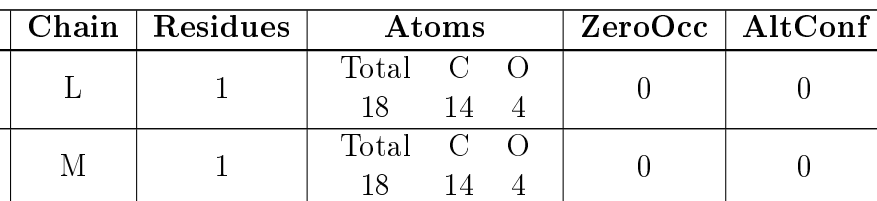
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
9	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 10 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula:  $C_{55}H_{74}N_4O_6$ ).



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

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

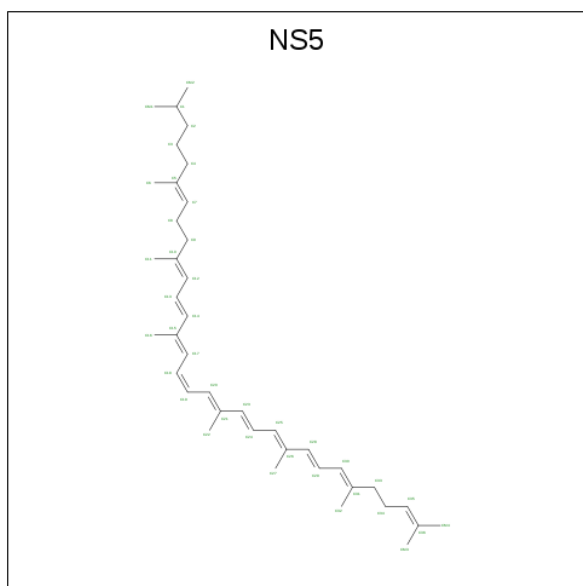


- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 12  | M     | 1        | Total Fe<br>1 1 | 0       | 0       |

- MQ9

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

- Molecule 14 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: C<sub>40</sub>H<sub>60</sub>).



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

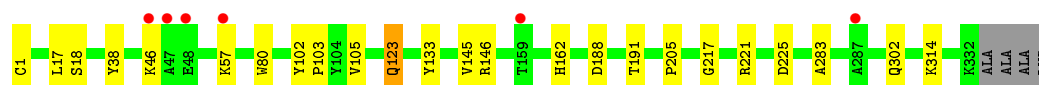
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	292	Total	O	0	0
			292	292		
15	H	172	Total	O	1	0
			172	172		
15	L	94	Total	O	0	0
			94	94		
15	M	172	Total	O	2	0
			172	172		

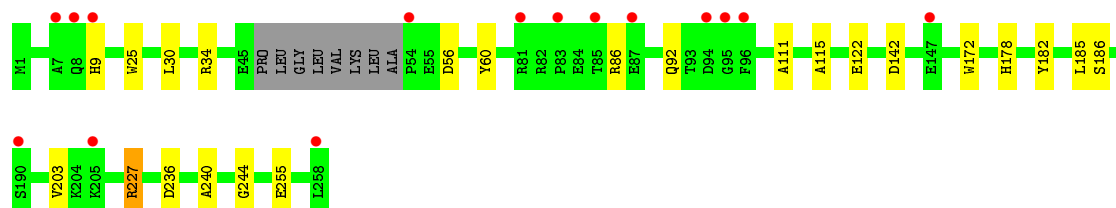
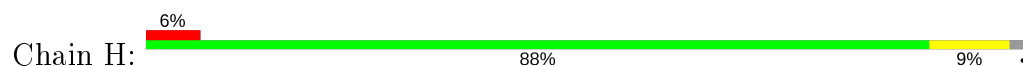
### 3 Residue-property plots [i](#)

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



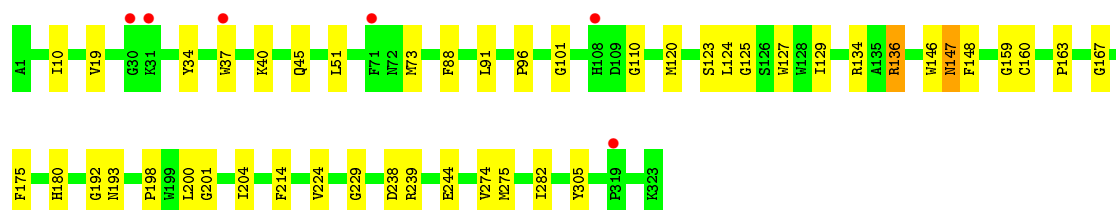
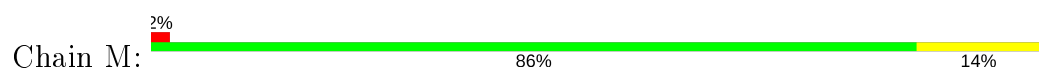
- Molecule 2: Photosynthetic reaction center H subunit



- Molecule 3: Photosynthetic reaction center L subunit



- Molecule 4: Photosynthetic reaction center M subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	220.13 Å   220.13 Å   112.74 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.50) 99.2 (19.99-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 2.50 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.176   ,   0.206 0.175   ,   0.204	Depositor DCC
$R_{free}$ test set	4765 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 60.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10922	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, BPB, HTO, BCB, MQ9, FE2, SO4, HEC, UQ1, FME, NS5

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	C	0.62	0/2665	0.66	0/3633
2	H	0.65	0/1991	0.65	0/2718
3	L	0.72	0/2267	0.68	2/3095 (0.1%)
4	M	0.71	0/2670	0.63	0/3651
All	All	0.67	0/9593	0.65	2/13097 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	12	ARG	NE-CZ-NH2	-6.70	116.95	120.30
3	L	12	ARG	CG-CD-NE	-5.23	100.82	111.80

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2598	0	2568	16	0
2	H	1956	0	1944	14	0
3	L	2172	0	2097	22	0
4	M	2557	0	2462	48	0
5	C	172	0	120	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	35	0	0	1	0
6	H	20	0	0	0	0
6	L	5	0	0	0	0
6	M	35	0	0	1	0
7	C	20	0	32	2	0
7	H	10	0	16	1	0
7	L	20	0	32	0	0
8	H	32	0	62	0	0
8	M	32	0	62	3	0
9	L	132	0	144	27	0
9	M	66	0	72	7	0
10	L	65	0	74	6	0
10	M	130	0	148	40	0
11	L	18	0	18	4	0
11	M	18	0	18	0	0
12	M	1	0	0	0	0
13	M	58	0	80	4	0
14	M	40	0	60	4	0
15	C	292	0	0	2	0
15	H	172	0	0	4	0
15	L	94	0	0	0	0
15	M	172	0	0	3	0
All	All	10922	0	10009	152	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 8.

The worst 5 of 152 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)
10:M:401:BPB:H4A	10:M:402:BPB:CBB	1.98	0.92
10:M:401:BPB:H4A	10:M:402:BPB:HBBB	1.53	0.90
10:M:402:BPB:CBB	10:M:402:BPB:HHC	2.04	0.88
4:M:204:ILE:HG12	10:M:401:BPB:CHB	2.03	0.87
4:M:200:LEU:HD13	4:M:204:ILE:HD12	1.60	0.81

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	246/258 (95%)	240 (98%)	6 (2%)	0	100	100
3	L	272/273 (100%)	267 (98%)	5 (2%)	0	100	100
4	M	323/323 (100%)	314 (97%)	9 (3%)	0	100	100
All	All	1171/1190 (98%)	1139 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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%)	275 (98%)	5 (2%)	59	81
2	H	204/211 (97%)	198 (97%)	6 (3%)	42	69
3	L	219/218 (100%)	215 (98%)	4 (2%)	59	81
4	M	251/249 (101%)	244 (97%)	7 (3%)	43	70
All	All	954/960 (99%)	932 (98%)	22 (2%)	50	76

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	227	ARG
3	L	80	LEU
4	M	180	HIS

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Mol	Chain	Res	Type
2	H	236	ASP
3	L	12	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	58	GLN
2	H	220	ASN
3	L	214	GLN
1	C	302	GLN
3	L	183	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FME	H	1	2	8,9,10	0.83	0	7,9,11	3.29	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	H	1	2	-	3/7/9/11	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-7.98	110.55	122.82
2	H	1	FME	CE-SD-CG	2.42	108.73	100.40

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-CG-SD-CE
2	H	1	FME	CB-CA-N-CN

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 43 ligands modelled in this entry, 1 is monoatomic - leaving 42 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	$\# Z  > 2$
7	HTO	L	708	-	9,9,9	0.22	0	10,10,10	0.78	0
6	SO4	M	802	-	4,4,4	0.14	0	6,6,6	0.34	0
6	SO4	C	808	-	4,4,4	0.24	0	6,6,6	0.36	0
5	HEC	C	401	1	26,50,50	1.99	2 (7%)	18,82,82	1.38	2 (11%)
6	SO4	L	814	-	4,4,4	0.14	0	6,6,6	0.05	0
9	BCB	L	401	3	60,74,74	3.72	20 (33%)	48,115,115	2.19	15 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	LDA	M	704	-	12,15,15	2.07	1 (8%)	14,17,17	0.60	0
9	BCB	L	400	3	60,74,74	3.80	21 (35%)	48,115,115	2.40	17 (35%)
8	LDA	H	701	-	12,15,15	1.84	1 (8%)	14,17,17	0.74	0
6	SO4	H	806	-	4,4,4	0.18	0	6,6,6	0.28	0
13	MQ9	M	501	-	59,59,59	1.84	16 (27%)	72,75,75	1.40	16 (22%)
6	SO4	C	810	-	4,4,4	0.14	0	6,6,6	0.18	0
6	SO4	M	801	-	4,4,4	0.21	0	6,6,6	0.36	0
6	SO4	H	807	-	4,4,4	0.10	0	6,6,6	0.24	0
8	LDA	H	703	-	12,15,15	1.79	1 (8%)	14,17,17	0.68	0
6	SO4	M	805	-	4,4,4	0.12	0	6,6,6	0.32	0
5	HEC	C	402	1	26,50,50	1.85	3 (11%)	18,82,82	1.37	3 (16%)
7	HTO	H	705	-	9,9,9	0.41	0	10,10,10	0.84	0
10	BPB	L	402	-	64,70,70	1.55	10 (15%)	64,101,101	1.85	15 (23%)
6	SO4	C	815	-	4,4,4	0.14	0	6,6,6	0.05	0
10	BPB	M	401	-	64,70,70	1.68	10 (15%)	64,101,101	1.98	17 (26%)
10	BPB	M	402	-	64,70,70	1.60	8 (12%)	64,101,101	1.86	15 (23%)
7	HTO	C	707	-	9,9,9	0.77	0	10,10,10	0.97	0
6	SO4	C	811	-	4,4,4	0.16	0	6,6,6	0.28	0
9	BCB	M	400	4	60,74,74	3.77	21 (35%)	48,115,115	2.17	15 (31%)
6	SO4	M	804	-	4,4,4	0.15	0	6,6,6	0.18	0
6	SO4	H	812	-	4,4,4	0.11	0	6,6,6	0.15	0
6	SO4	C	817	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	C	813	-	4,4,4	0.20	0	6,6,6	0.45	0
7	HTO	C	706	-	9,9,9	0.43	0	10,10,10	0.61	0
7	HTO	L	709	-	9,9,9	0.22	0	10,10,10	0.74	0
6	SO4	M	816	-	4,4,4	0.15	0	6,6,6	0.05	0
6	SO4	H	803	-	4,4,4	0.12	0	6,6,6	0.25	0
6	SO4	M	818	-	4,4,4	0.14	0	6,6,6	0.05	0
11	UQ1	M	503	-	18,18,18	2.31	2 (11%)	22,25,25	1.19	2 (9%)
11	UQ1	L	502	-	18,18,18	2.26	2 (11%)	22,25,25	1.16	2 (9%)
5	HEC	C	404	1	26,50,50	1.54	2 (7%)	18,82,82	1.63	4 (22%)
14	NS5	M	600	-	39,39,39	1.51	3 (7%)	44,46,46	1.88	10 (22%)
5	HEC	C	403	1	26,50,50	1.69	3 (11%)	18,82,82	1.39	2 (11%)
6	SO4	M	819	-	4,4,4	0.14	0	6,6,6	0.07	0
6	SO4	C	809	-	4,4,4	0.15	0	6,6,6	0.23	0
8	LDA	M	702	-	12,15,15	1.95	1 (8%)	14,17,17	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HTO	L	708	-	-	6/10/10/10	-
5	HEC	C	401	1	-	0/6/54/54	-
9	BCB	L	401	3	-	8/41/177/177	-
8	LDA	M	704	-	-	9/13/13/13	-
9	BCB	L	400	3	-	14/41/177/177	-
8	LDA	H	701	-	-	8/13/13/13	-
10	BPB	M	401	-	-	17/47/105/105	0/5/6/6
13	MQ9	M	501	-	-	13/53/73/73	0/2/2/2
11	UQ1	L	502	-	-	2/9/33/33	0/1/1/1
8	LDA	H	703	-	-	8/13/13/13	-
5	HEC	C	402	1	-	1/6/54/54	-
7	HTO	H	705	-	-	7/10/10/10	-
10	BPB	L	402	-	-	7/47/105/105	0/5/6/6
10	BPB	M	402	-	-	20/47/105/105	0/5/6/6
7	HTO	C	707	-	-	7/10/10/10	-
9	BCB	M	400	4	-	12/41/177/177	-
7	HTO	C	706	-	-	3/10/10/10	-
7	HTO	L	709	-	-	5/10/10/10	-
11	UQ1	M	503	-	-	0/9/33/33	0/1/1/1
5	HEC	C	404	1	-	0/6/54/54	-
14	NS5	M	600	-	-	9/43/43/43	-
5	HEC	C	403	1	-	0/6/54/54	-
8	LDA	M	702	-	-	5/13/13/13	-

The worst 5 of 127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	400	BCB	C1A-CHA	-10.50	1.37	1.54
9	L	400	BCB	CHD-C1D	-9.70	1.38	1.53
9	L	400	BCB	C1A-CHA	-9.39	1.39	1.54
9	L	401	BCB	C1A-CHA	-9.14	1.39	1.54
9	L	401	BCB	CHD-C1D	-9.10	1.39	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	L	402	BPB	C3D-C2D-C1D	-6.95	95.75	105.87
10	M	401	BPB	C3D-C2D-C1D	-6.92	95.79	105.87
10	M	402	BPB	C3D-C2D-C1D	-6.65	96.18	105.87
9	L	400	BCB	CBB-CAB-C3B	5.53	122.44	116.80
10	M	402	BPB	O2D-CGD-CBD	5.49	121.03	111.27

There are no chirality outliers.

5 of 161 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	708	HTO	O1-C1-C2-O2
7	L	708	HTO	O1-C1-C2-C3
9	L	401	BCB	C2B-C3B-CAB-OB
9	L	401	BCB	C2B-C3B-CAB-CBB
8	M	704	LDA	C2-C1-N1-O1

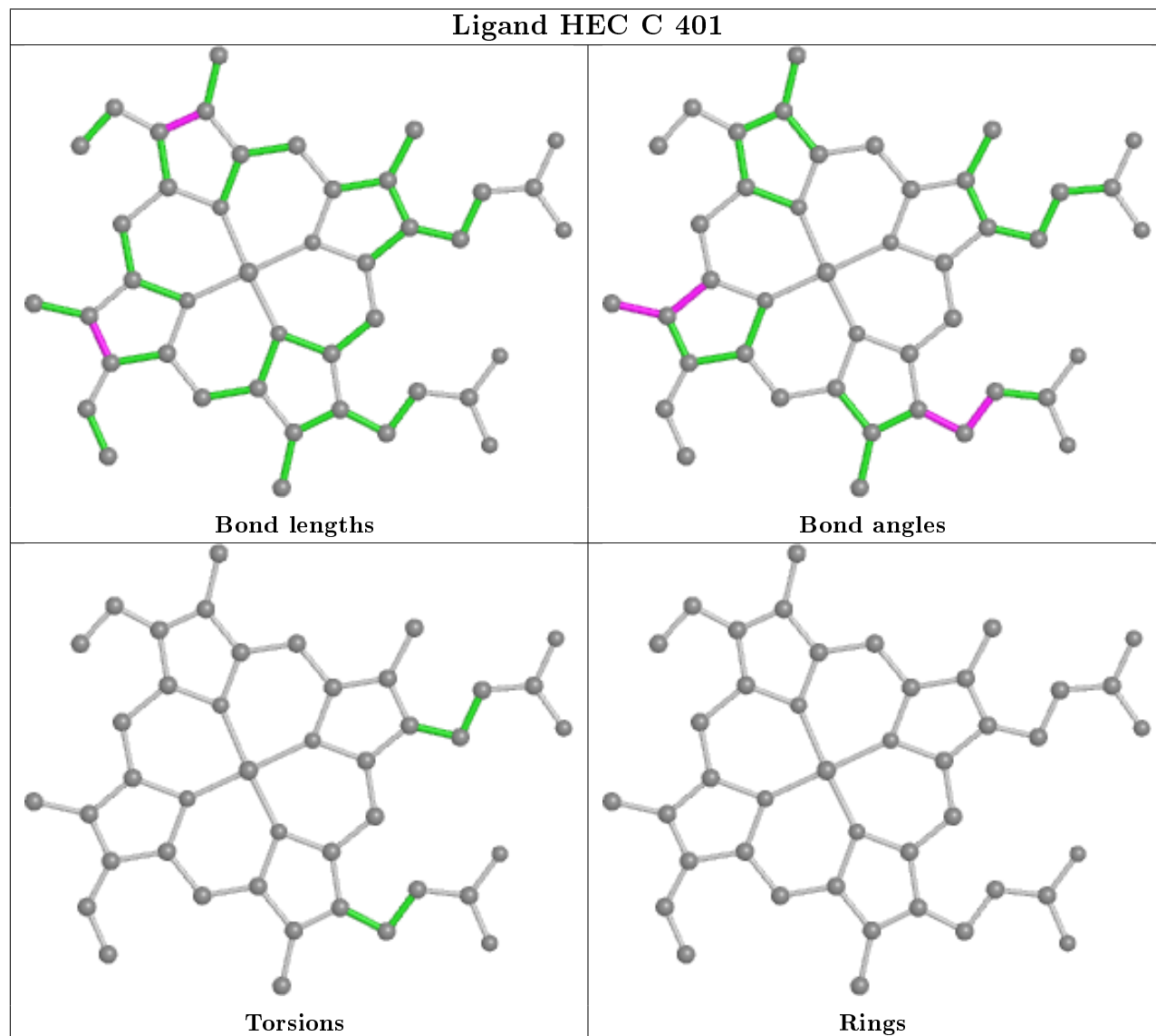
There are no ring outliers.

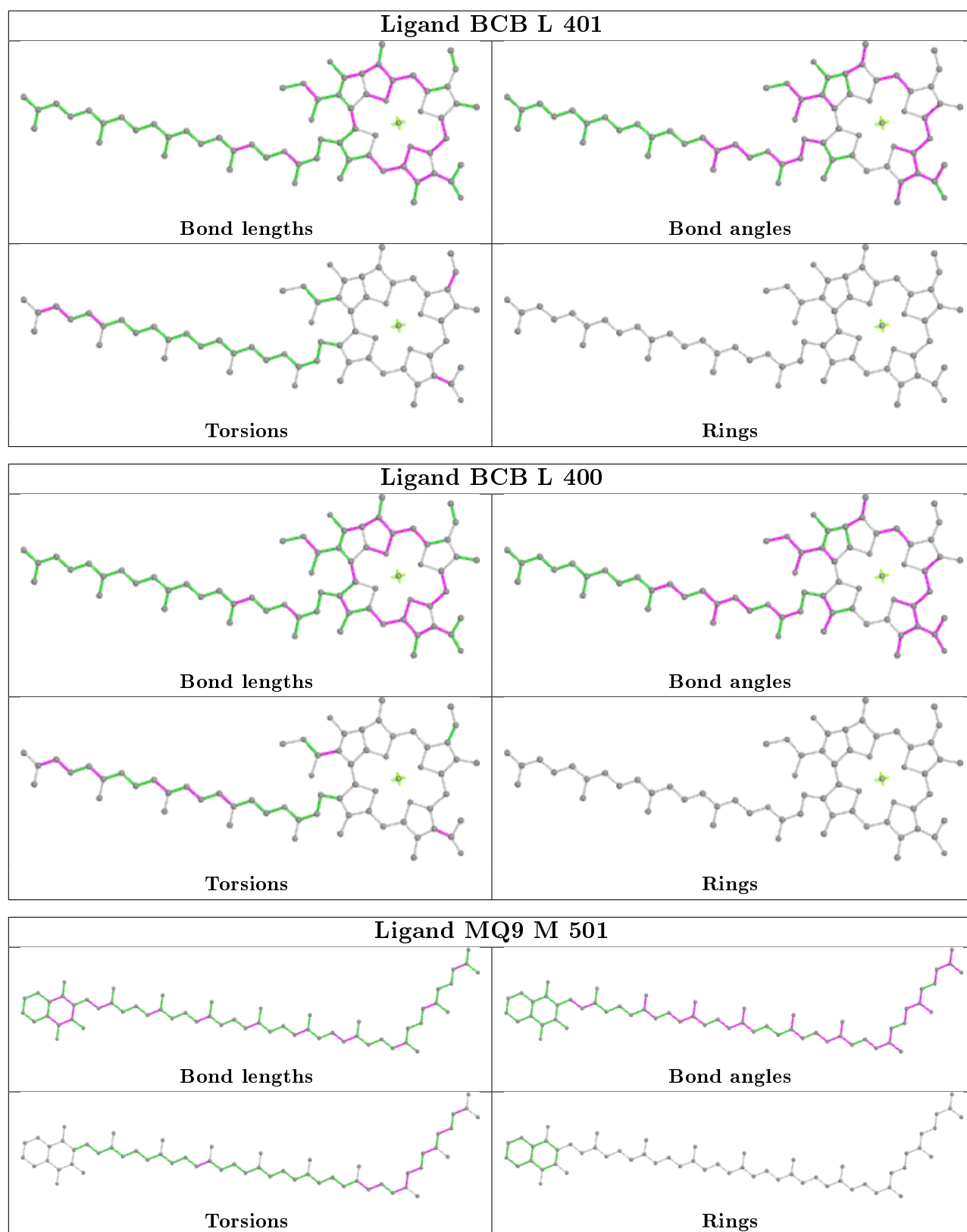
18 monomers are involved in 89 short contacts:

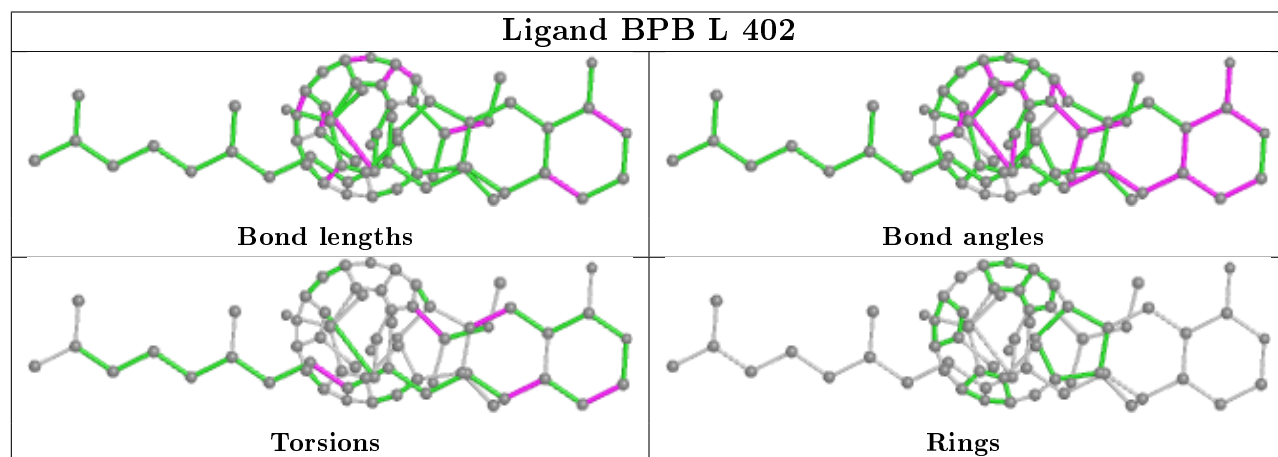
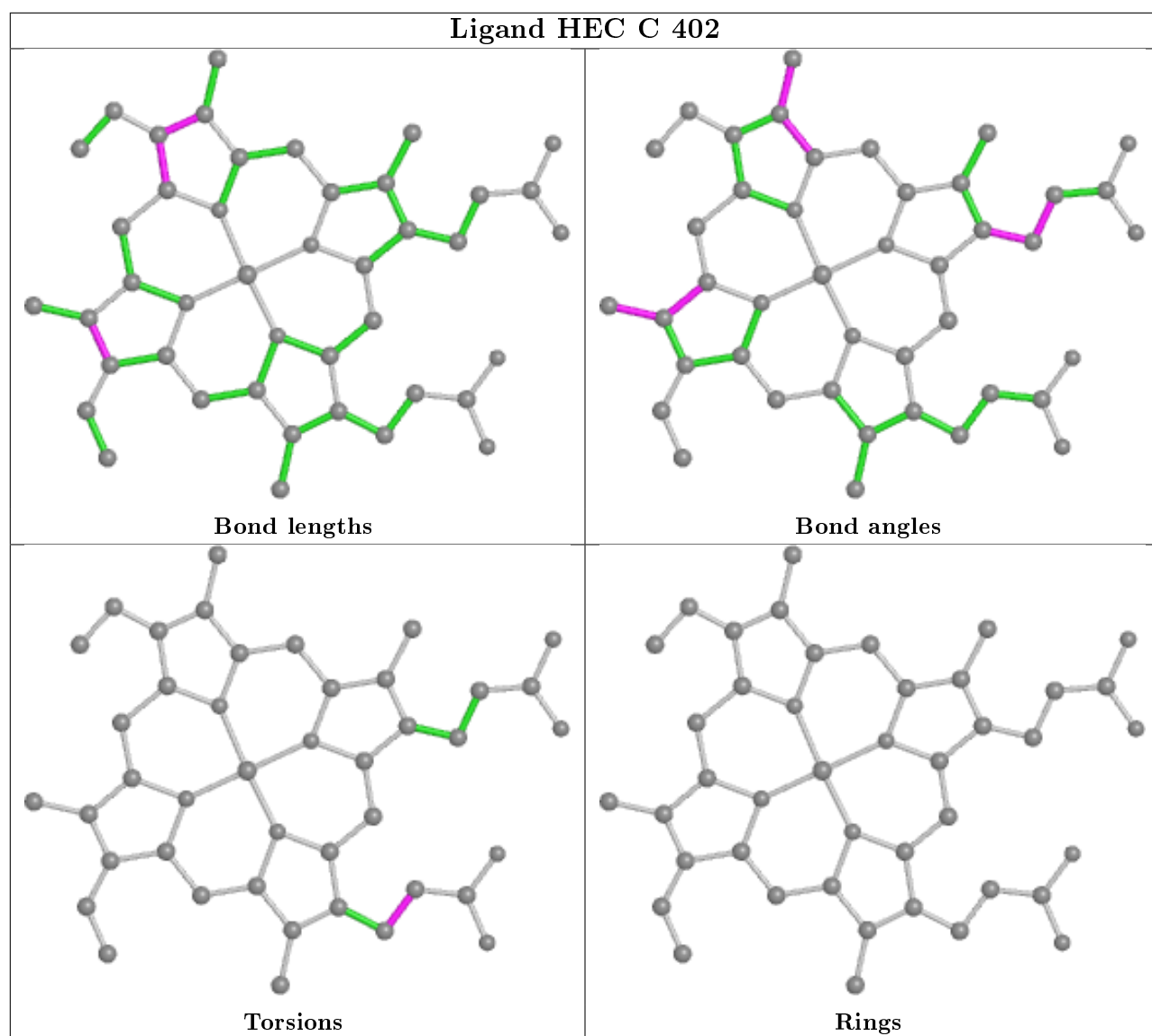
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	L	401	BCB	8	0
8	M	704	LDA	1	0
9	L	400	BCB	20	0
13	M	501	MQ9	4	0
6	M	805	SO4	1	0
7	H	705	HTO	1	0
10	L	402	BPB	6	0
10	M	401	BPB	27	0
10	M	402	BPB	17	0
7	C	707	HTO	1	0
9	M	400	BCB	7	0
6	C	813	SO4	1	0
7	C	706	HTO	1	0
11	L	502	UQ1	4	0
5	C	404	HEC	1	0
14	M	600	NS5	4	0
5	C	403	HEC	2	0
8	M	702	LDA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

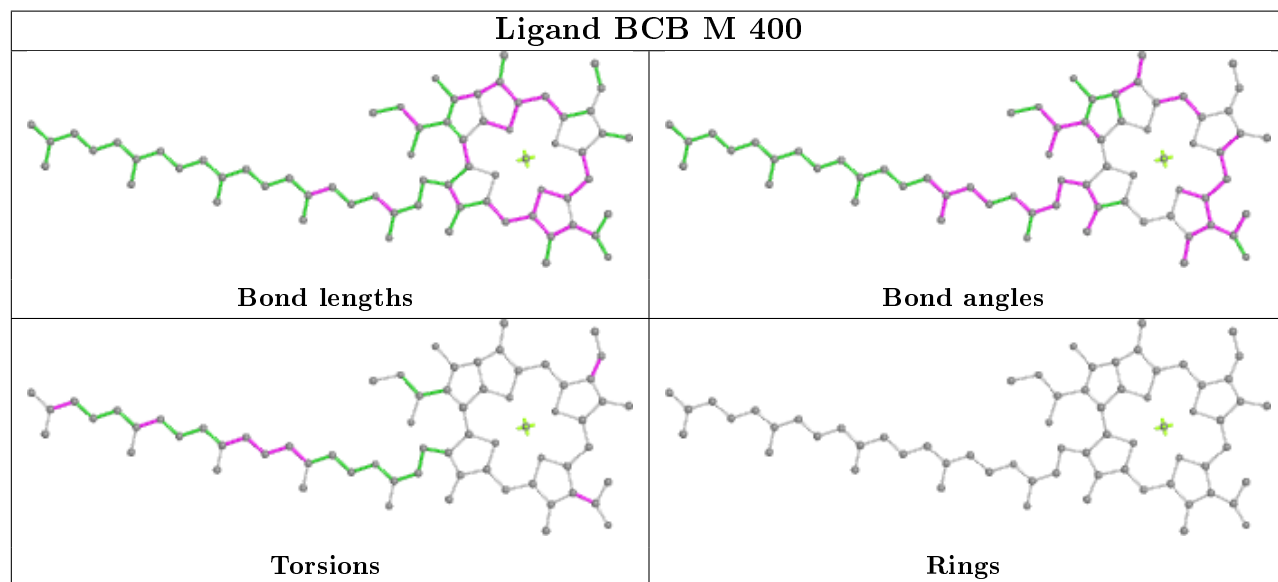
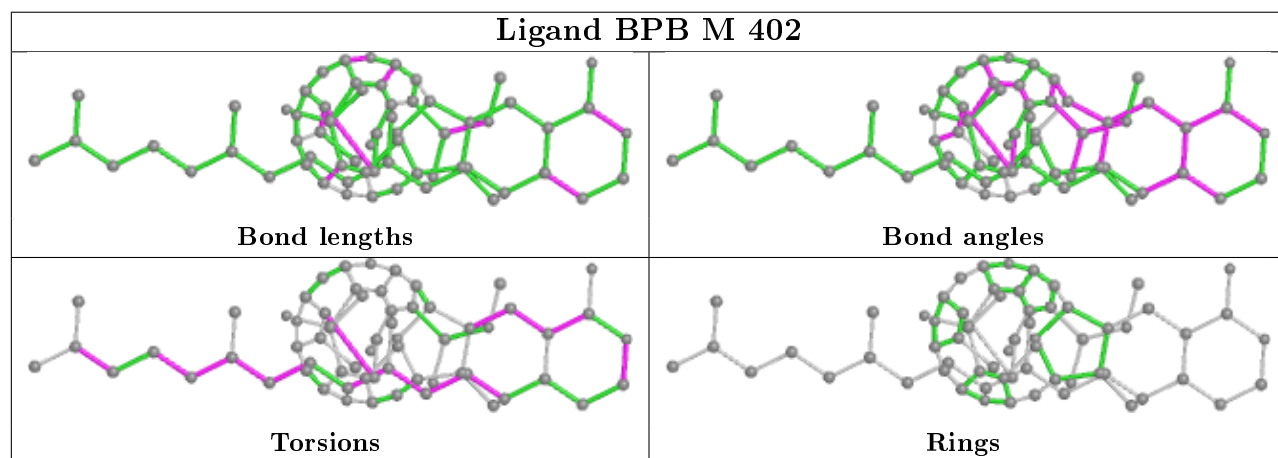
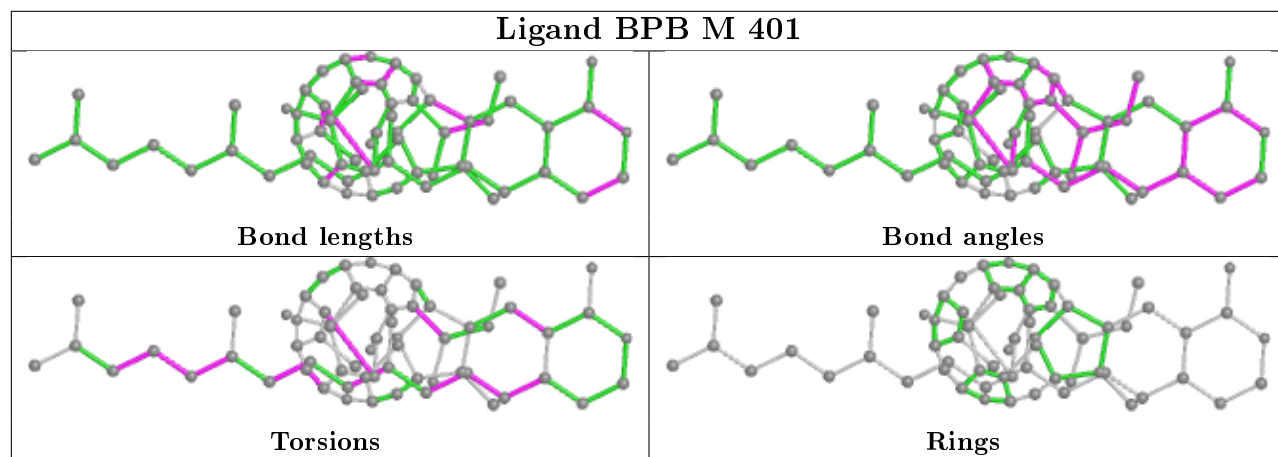
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

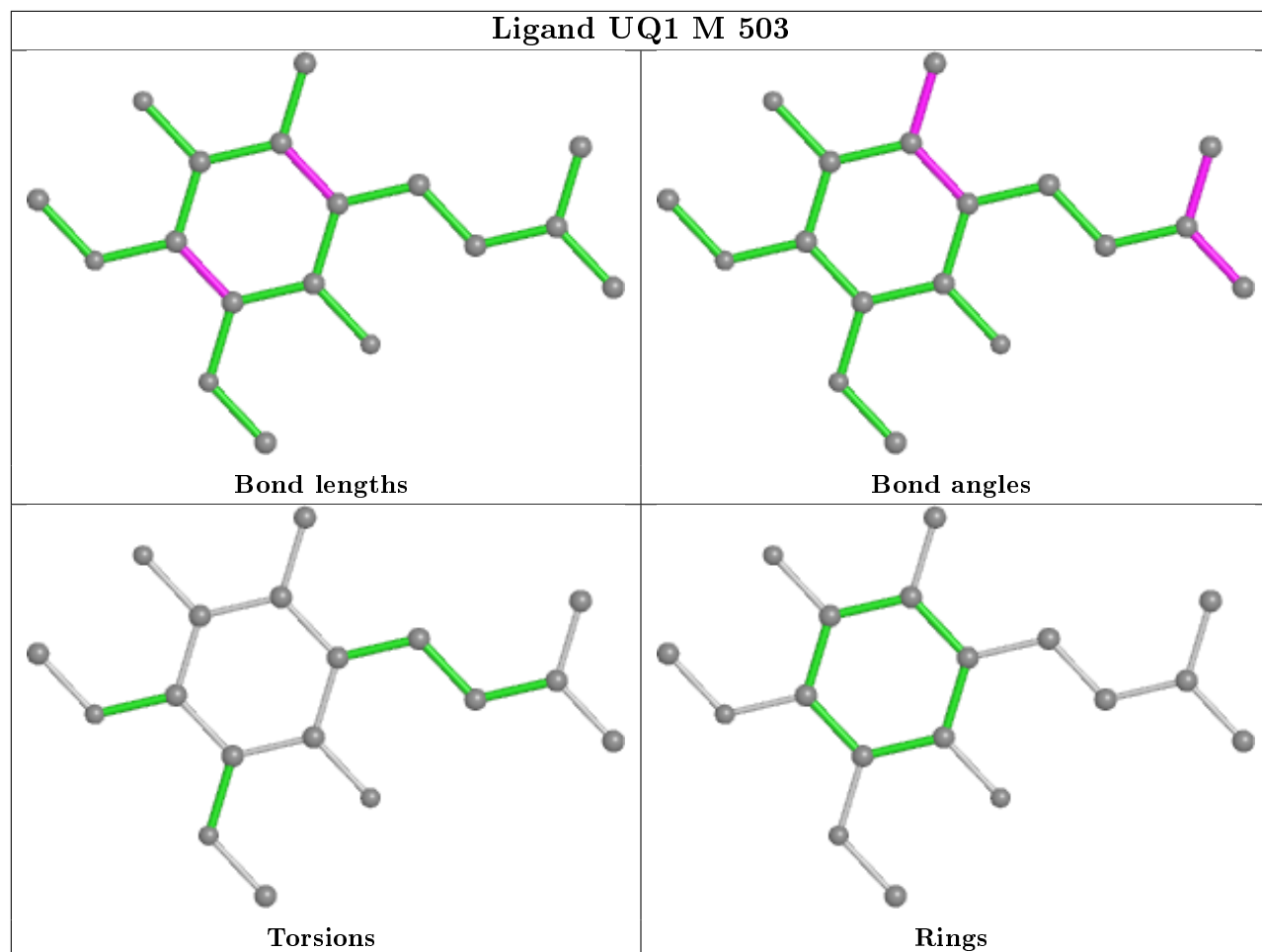




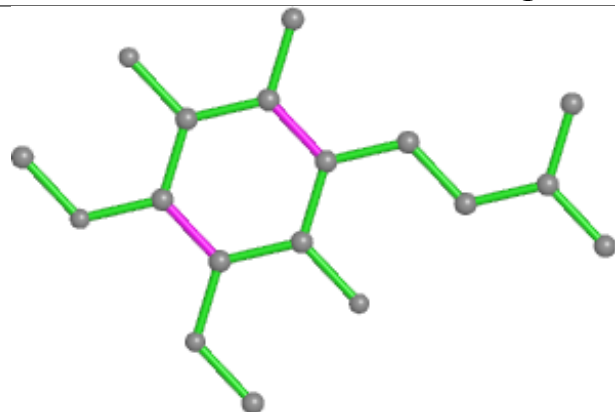




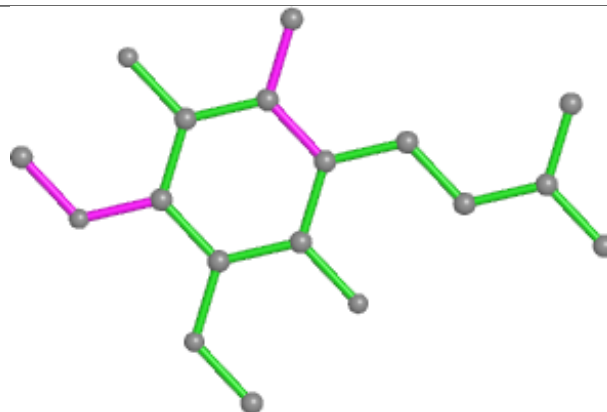




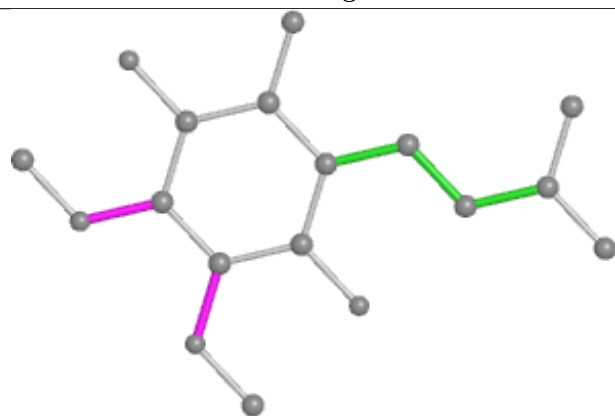
## Ligand UQ1 L 502



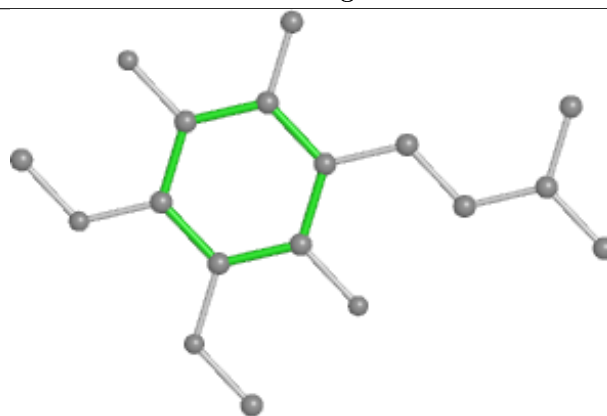
Bond lengths



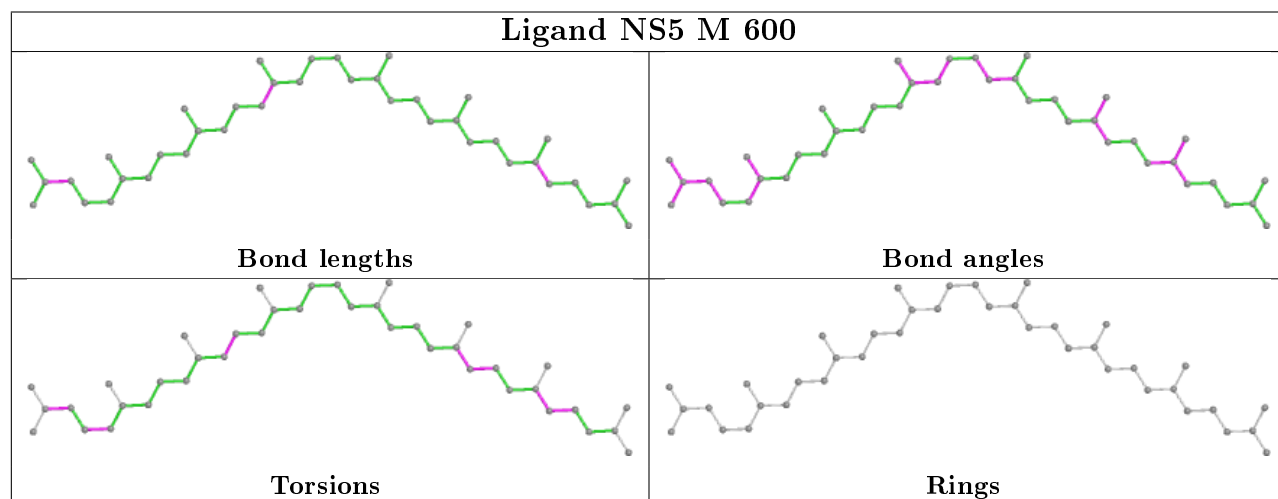
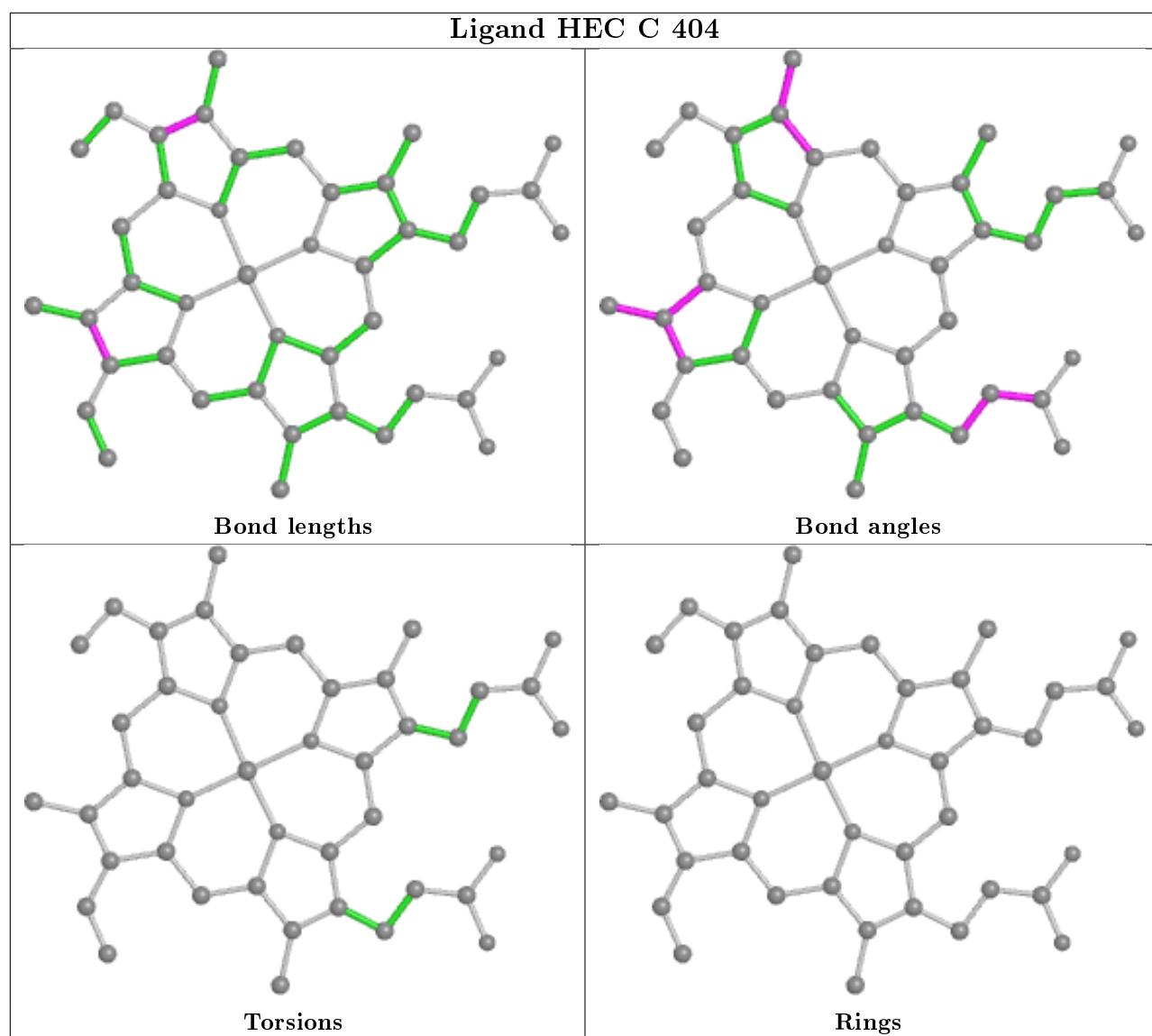
Bond angles

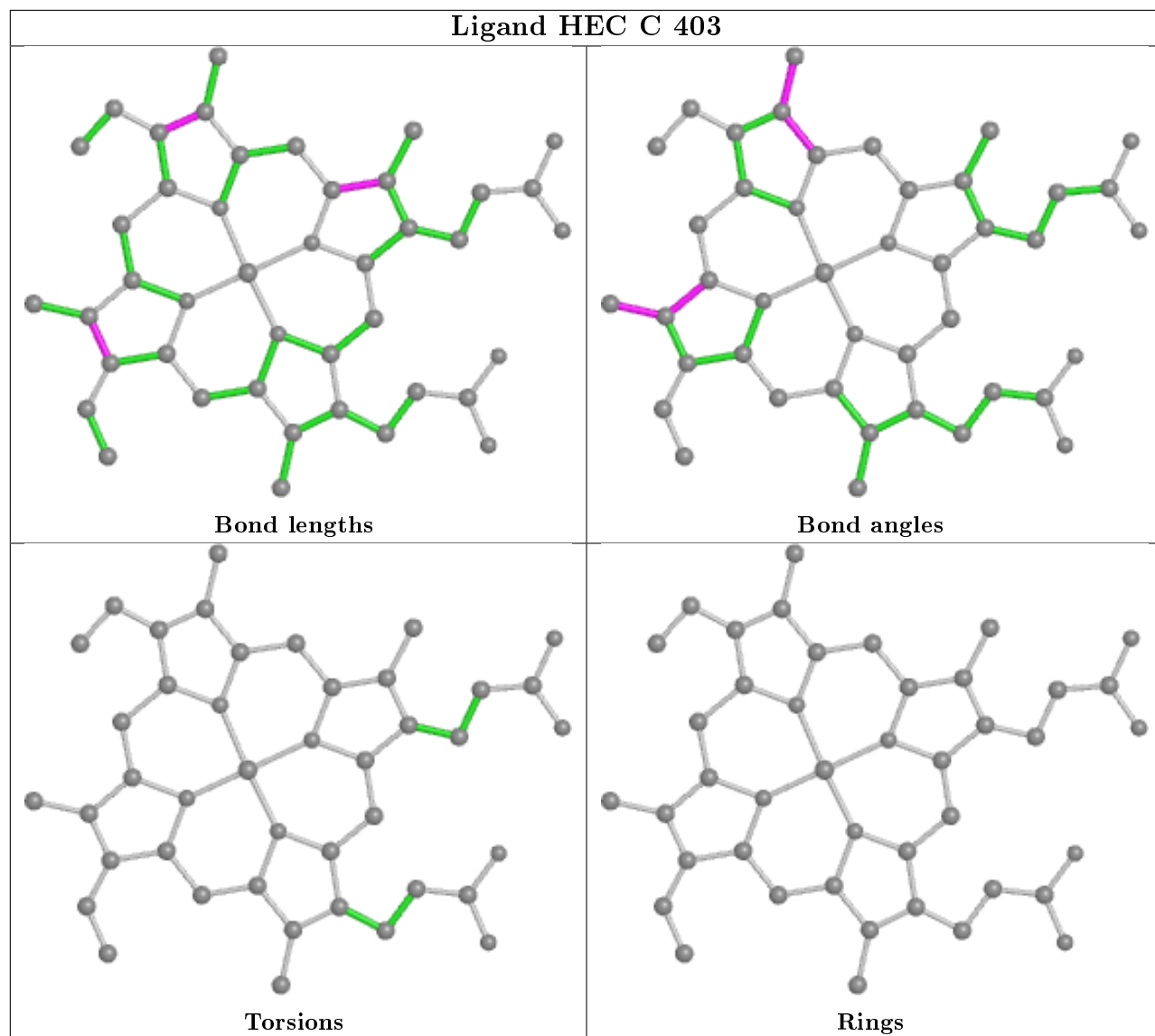


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.55	6 (1%) 68 71	21, 31, 49, 61	0
2	H	249/258 (96%)	-0.41	15 (6%) 21 22	18, 32, 50, 60	0
3	L	273/273 (100%)	-0.78	2 (0%) 87 89	20, 26, 41, 47	0
4	M	323/323 (100%)	-0.68	6 (1%) 66 69	17, 28, 45, 50	0
All	All	1177/1190 (98%)	-0.61	29 (2%) 57 61	17, 29, 46, 61	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	5.4
4	M	319	PRO	3.7
2	H	8	GLN	3.7
2	H	83	PRO	3.7
1	C	47	ALA	3.4

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	0.97	0.10	36,38,49,53	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, 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
7	HTO	L	709	10/10	-0.18	1.79	2,2,2,2	10
6	SO4	M	816	5/5	-0.13	1.86	2,2,2,2	5
6	SO4	M	819	5/5	0.01	1.41	2,2,2,2	5
6	SO4	L	814	5/5	0.08	1.95	2,2,2,2	5
6	SO4	C	815	5/5	0.11	1.75	2,2,2,2	5
6	SO4	M	818	5/5	0.20	1.57	2,2,2,2	5
7	HTO	L	708	10/10	0.22	1.90	2,2,2,2	10
6	SO4	C	817	5/5	0.22	1.95	2,2,2,2	5
11	UQ1	M	503	18/18	0.33	0.48	93,94,95,95	0
8	LDA	M	702	16/16	0.76	0.32	47,57,67,67	0
10	BPB	M	401	65/65	0.77	0.34	28,39,45,47	65
8	LDA	M	704	16/16	0.81	0.26	55,58,68,69	0
14	NS5	M	600	40/40	0.81	0.23	35,45,74,74	4
7	HTO	C	707	10/10	0.85	0.22	50,54,57,57	0
7	HTO	C	706	10/10	0.87	0.21	45,50,51,51	0
10	BPB	M	402	65/65	0.87	0.21	21,27,97,99	0
8	LDA	H	703	16/16	0.90	0.22	47,53,60,62	0
6	SO4	C	809	5/5	0.91	0.36	66,67,67,68	5
11	UQ1	L	502	18/18	0.91	0.14	45,46,49,50	0
6	SO4	C	808	5/5	0.92	0.15	55,56,57,58	5
6	SO4	C	813	5/5	0.92	0.29	39,39,41,41	5
6	SO4	M	805	5/5	0.93	0.23	48,49,49,50	5
6	SO4	C	811	5/5	0.93	0.24	42,43,44,44	5
9	BCB	M	400	66/66	0.93	0.14	23,27,85,86	0
13	MQ9	M	501	58/58	0.94	0.13	16,22,74,75	0
6	SO4	H	807	5/5	0.94	0.34	64,65,66,66	5
7	HTO	H	705	10/10	0.94	0.13	41,42,44,45	0
6	SO4	H	812	5/5	0.94	0.17	47,47,48,48	5
6	SO4	C	810	5/5	0.95	0.16	46,47,47,47	5
8	LDA	H	701	16/16	0.95	0.12	36,41,47,48	0
6	SO4	H	803	5/5	0.96	0.26	67,68,68,69	0
9	BCB	L	401	66/66	0.97	0.08	18,24,40,44	0
9	BCB	L	400	66/66	0.97	0.11	23,26,33,38	0
5	HEC	C	402	43/43	0.97	0.12	26,30,37,39	0
5	HEC	C	404	43/43	0.98	0.09	21,24,34,41	0
10	BPB	L	402	65/65	0.98	0.09	14,20,28,29	0

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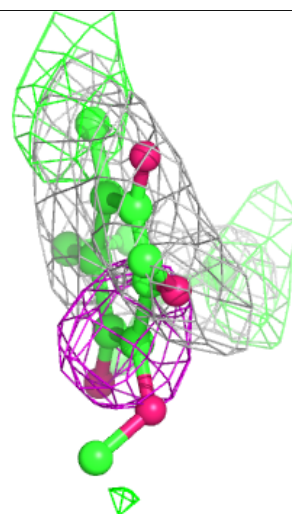
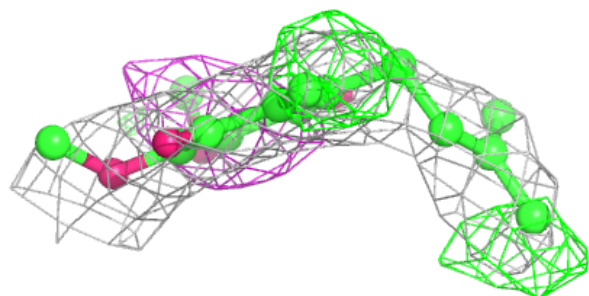
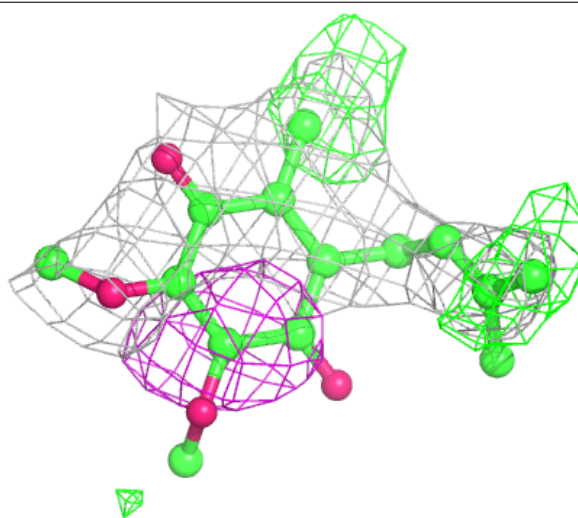
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	M	804	5/5	0.98	0.18	53,54,55,56	0
6	SO4	H	806	5/5	0.98	0.07	48,49,50,50	5
5	HEC	C	401	43/43	0.98	0.12	30,33,45,51	0
6	SO4	M	801	5/5	0.99	0.13	29,29,32,32	0
6	SO4	M	802	5/5	0.99	0.07	47,48,49,50	0
5	HEC	C	403	43/43	0.99	0.09	14,21,27,31	0
12	FE2	M	500	1/1	1.00	0.03	21,21,21,21	0

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

**Electron density around UQ1 M 503:**

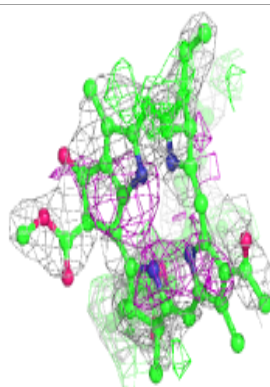
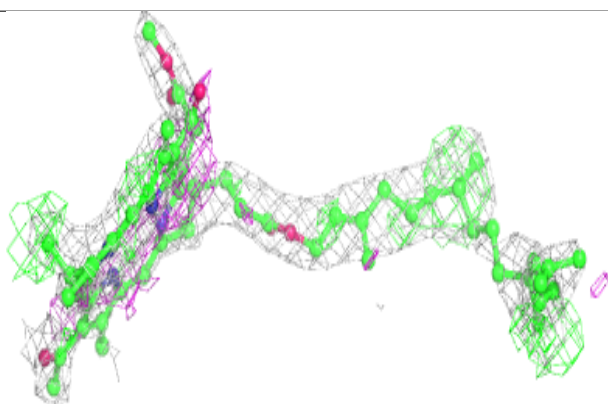
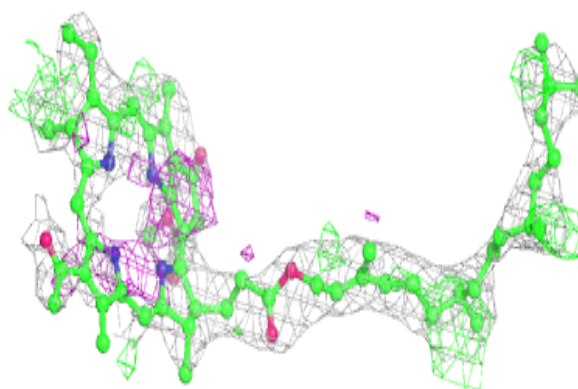
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



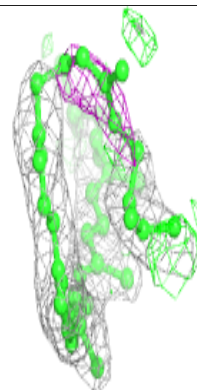
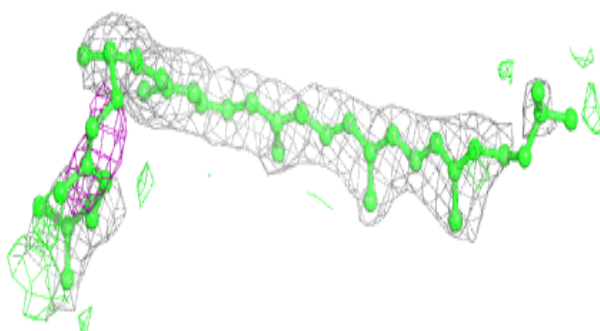
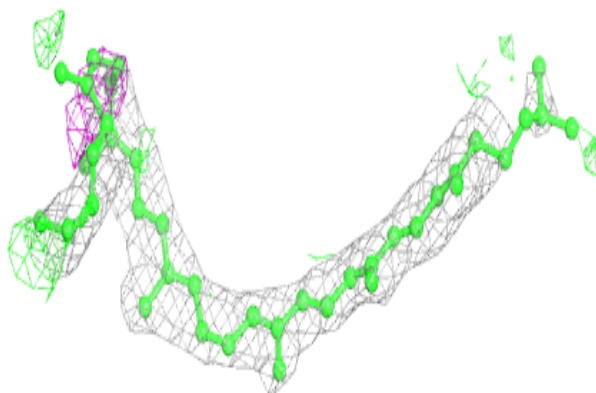


**Electron density around BPB M 401:**

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

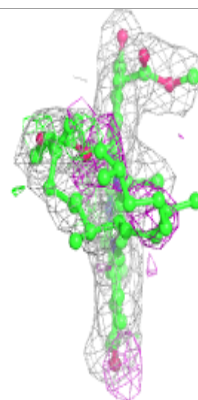
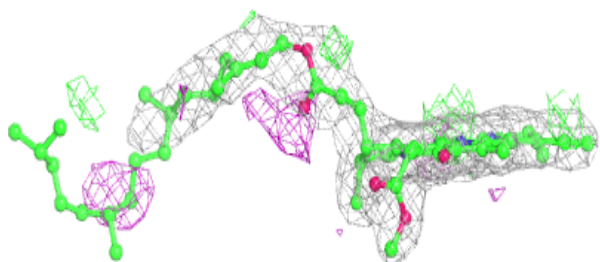
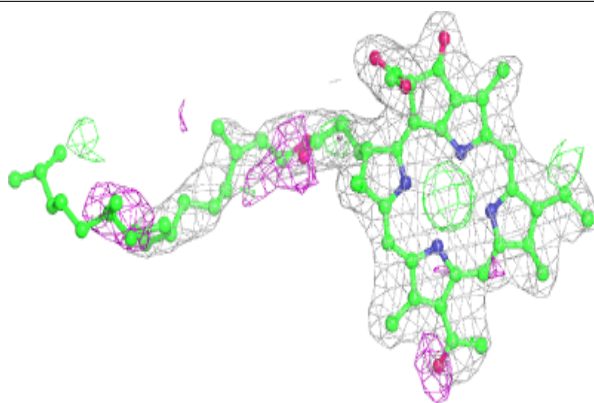
**Electron density around NS5 M 600:**

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and green (positive)

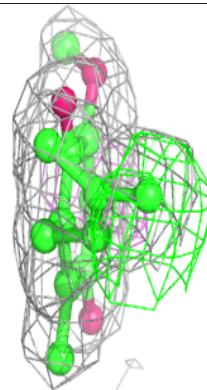
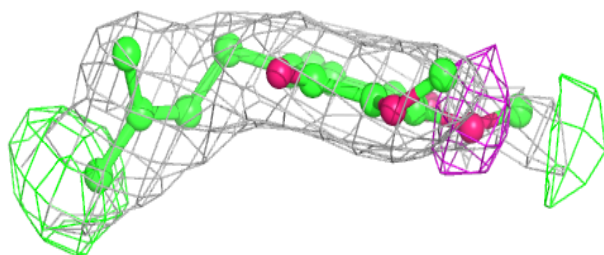
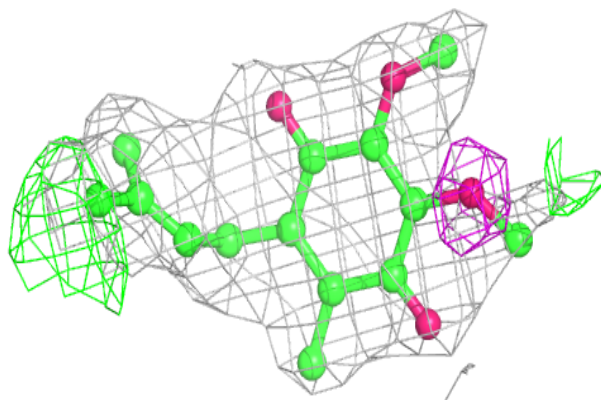


**Electron density around BPB M 402:**

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

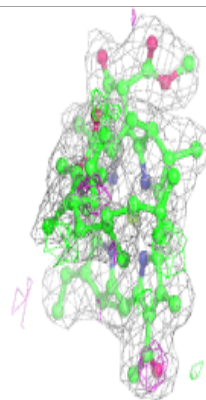
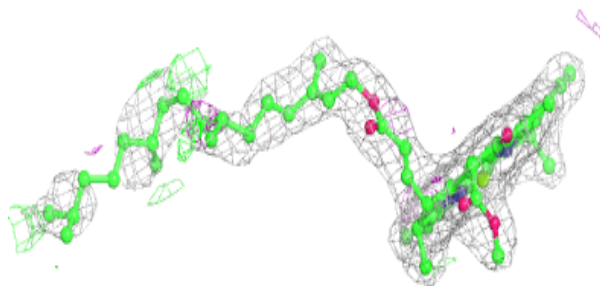
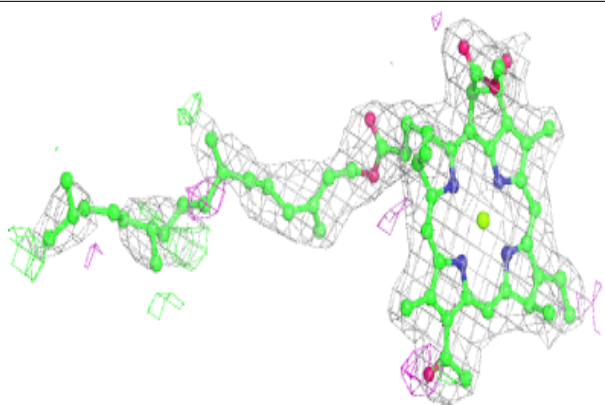
**Electron density around UQ1 L 502:**

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

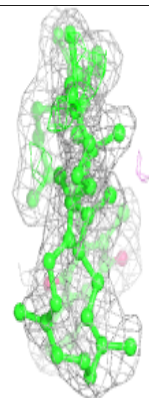
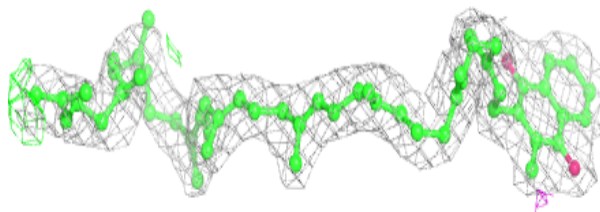
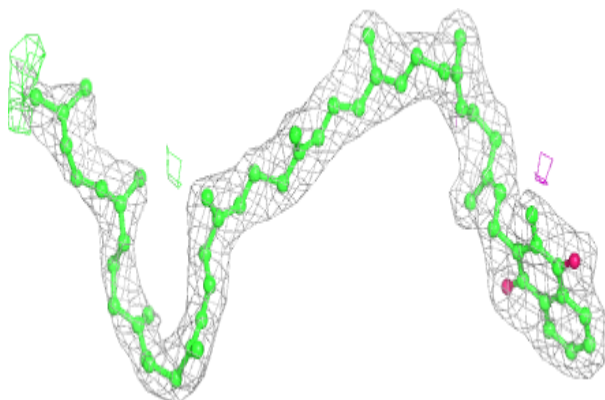


**Electron density around BCB M 400:**

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

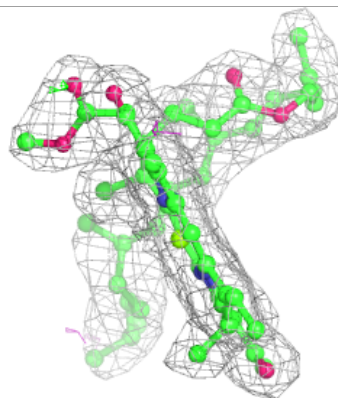
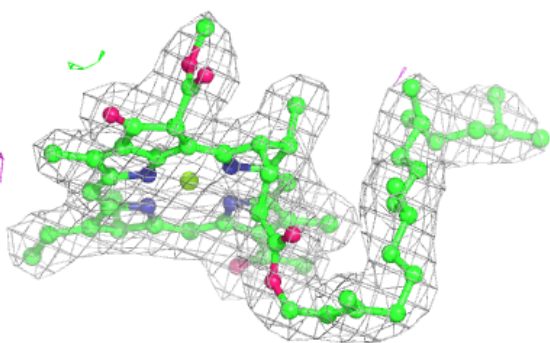
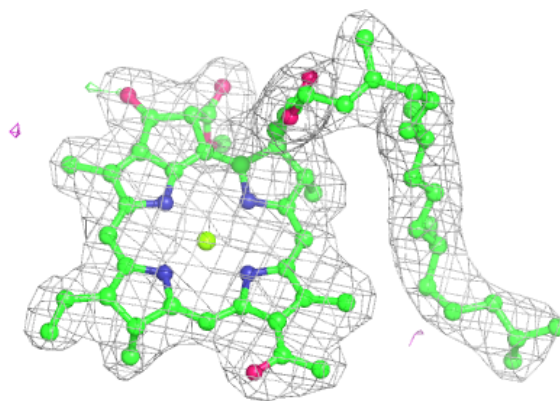
**Electron density around MQ9 M 501:**

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

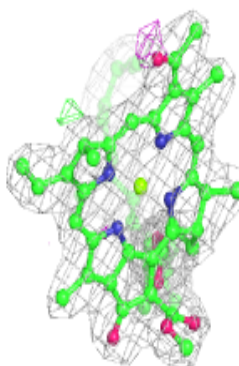
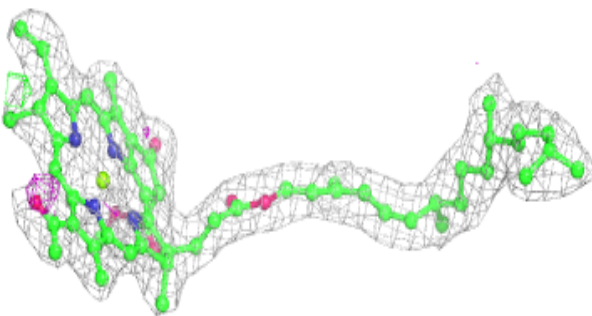
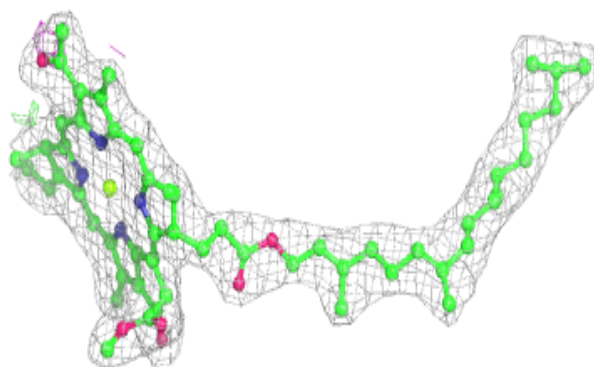


**Electron density around BCB L 401:**

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

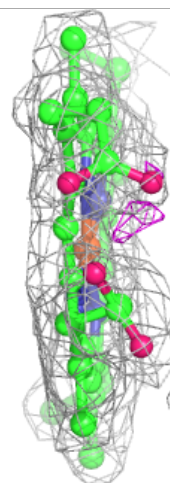
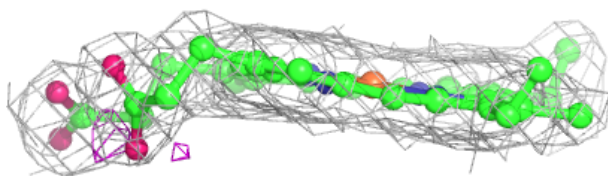
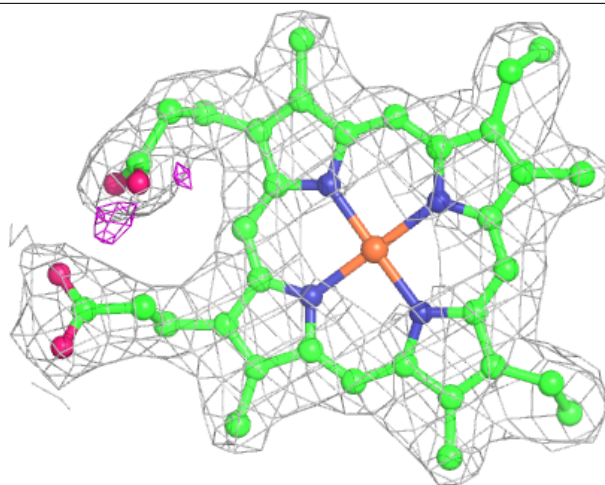
**Electron density around BCB L 400:**

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



**Electron density around HEC C 402:**

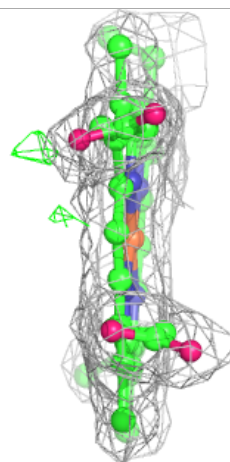
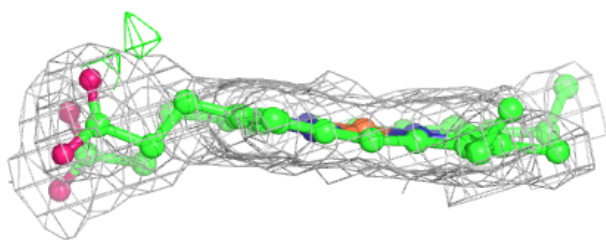
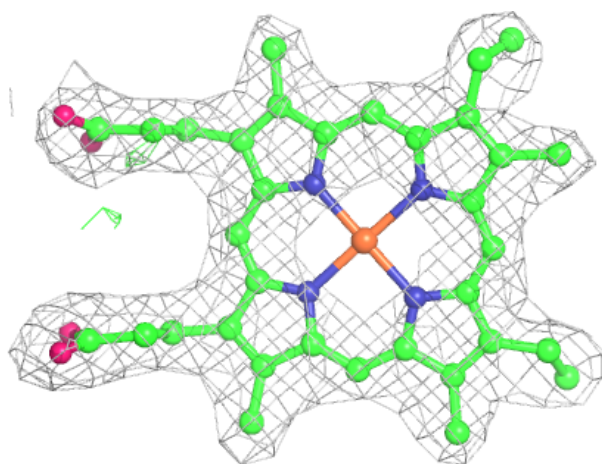
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





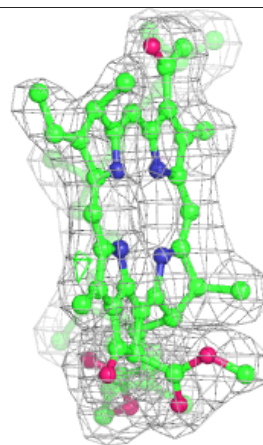
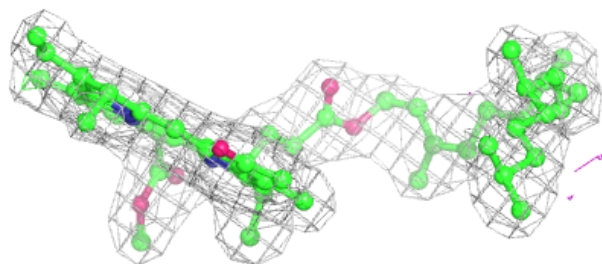
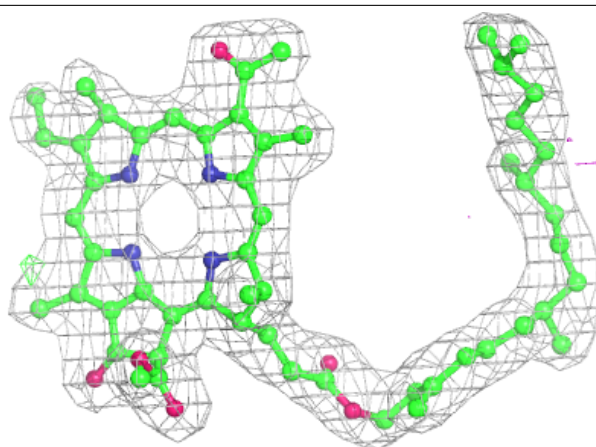
**Electron density around HEC C 404:**

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



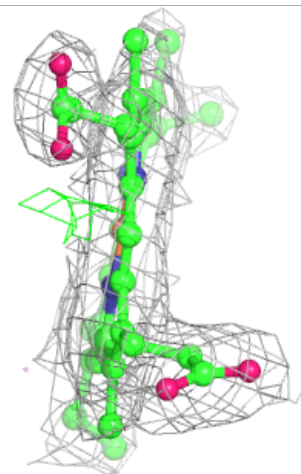
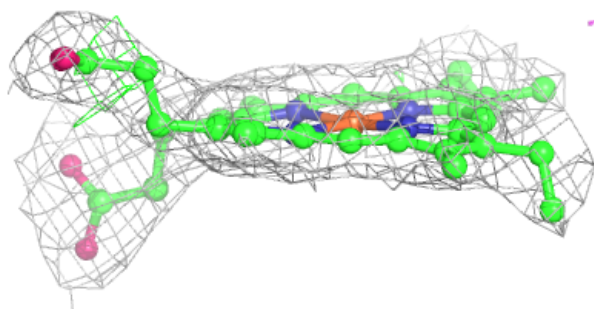
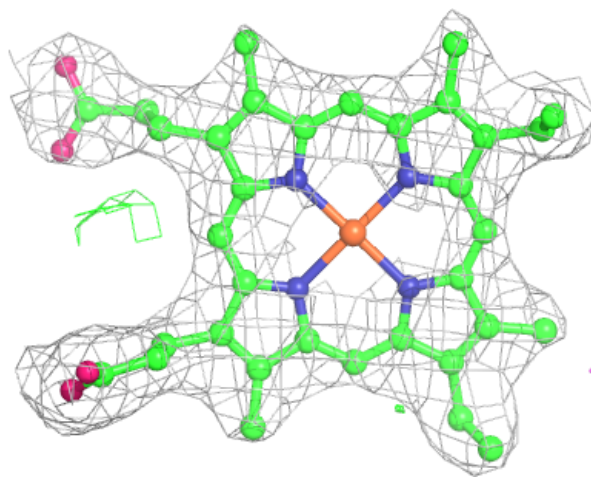
**Electron density around BPB L 402:**

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

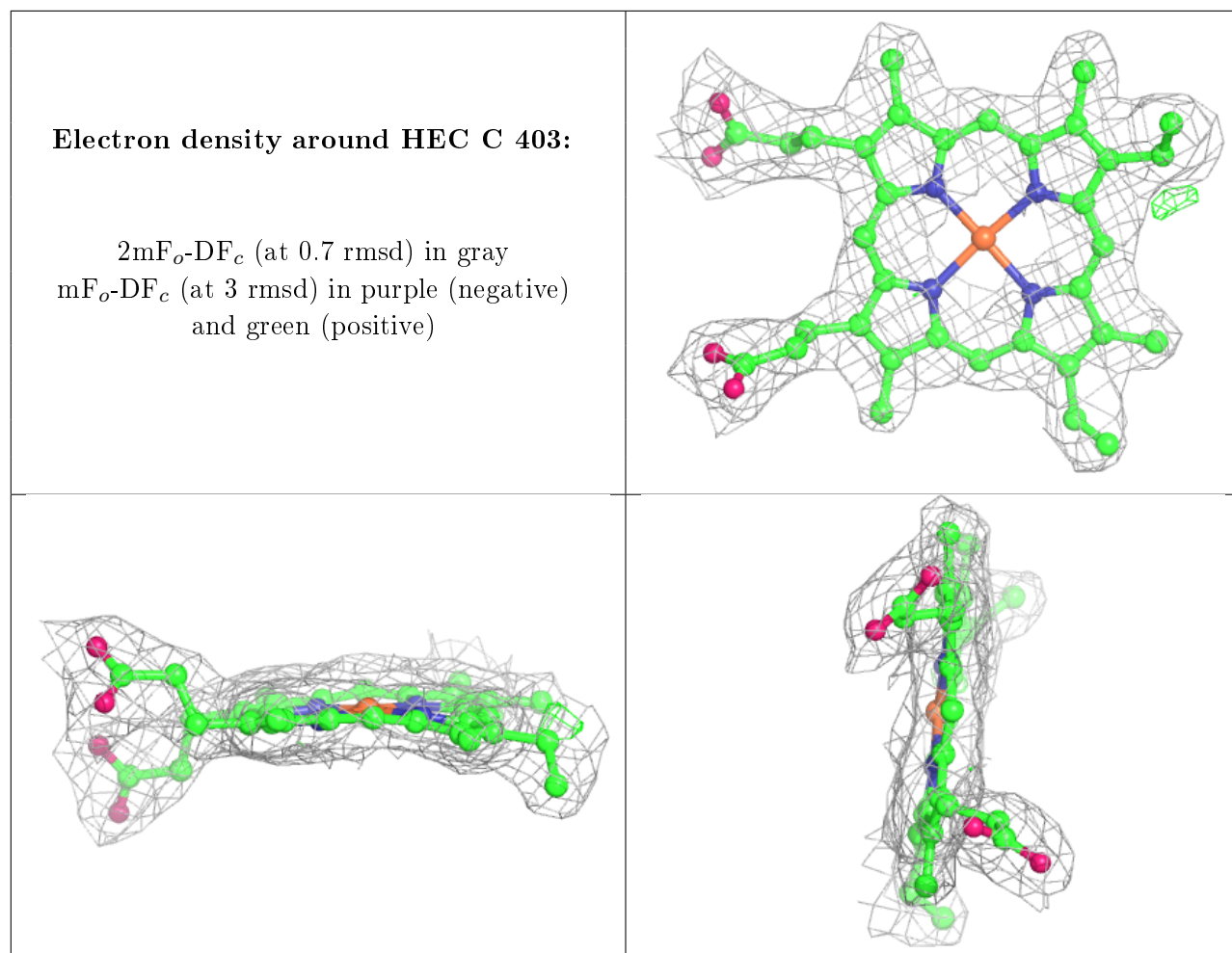


**Electron density around HEC C 401:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.