



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2020 – 11:48 AM BST

PDB ID : 2WJM  
Title : Lipidic sponge phase crystal structure of the photosynthetic reaction centre from *Blastochloris viridis* (low dose)  
Authors : Woehri, A.B.; Wahlgren, W.Y.; Malmerberg, E.; Johansson, L.C.; Neutze, R.; Katona, G.  
Deposited on : 2009-05-27  
Resolution : 1.95 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.

---

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 : 2.13  
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) : 2.13

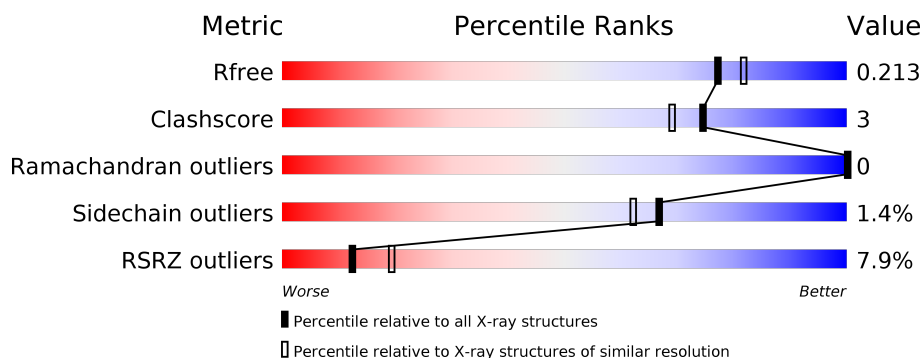
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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>4%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
2	H	258	<div> <div>11%</div> <div> <div></div> <div>90%</div> <div>6%</div> </div> </div>
3	L	274	<div> <div>11%</div> <div> <div></div> <div>92%</div> <div>7%</div> </div> </div>
4	M	324	<div> <div>6%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10671 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	243	Total	C	N	O	S	0	0	0
			1880	1205	326	347	2			

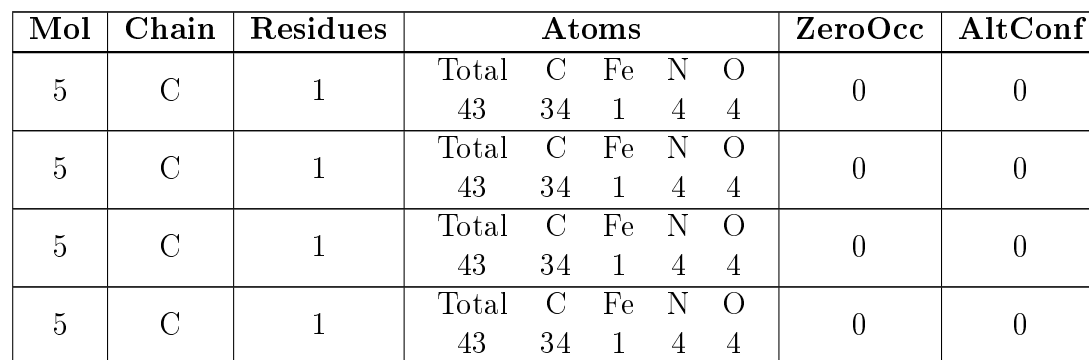
- Molecule 3 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	273	Total	C	N	O	S	0	2	0
			2170	1458	350	355	7			

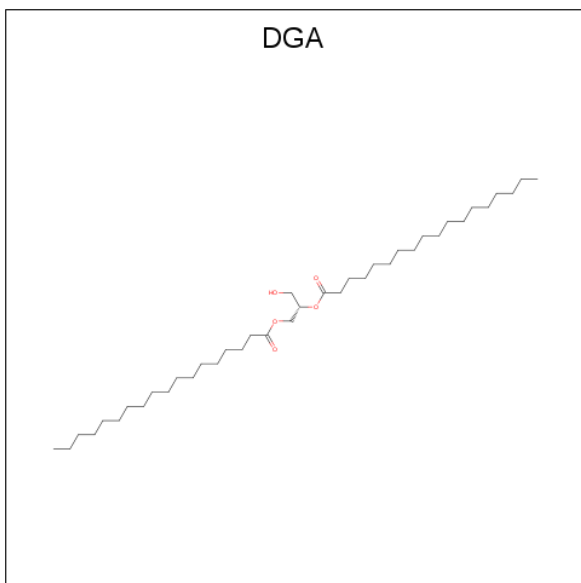
- Molecule 4 is a protein called REACTION CENTER PROTEIN M CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2548	1697	417	423	11			

- Molecule 5 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).

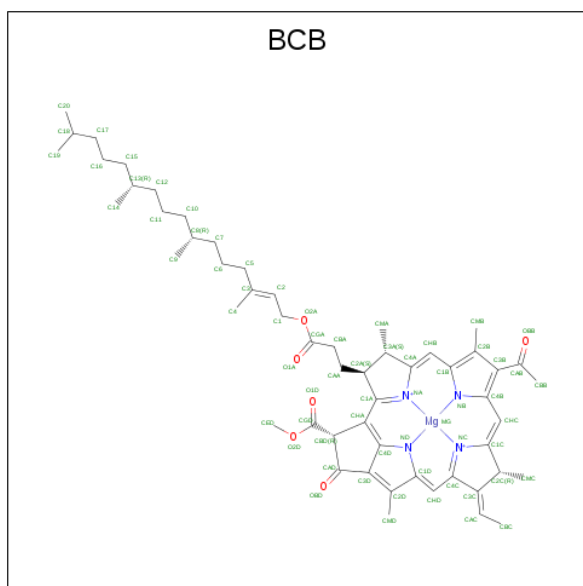


- Molecule 6 is DIACYL GLYCEROL (three-letter code: DGA) (formula:  $\text{C}_{39}\text{H}_{76}\text{O}_5$ ).



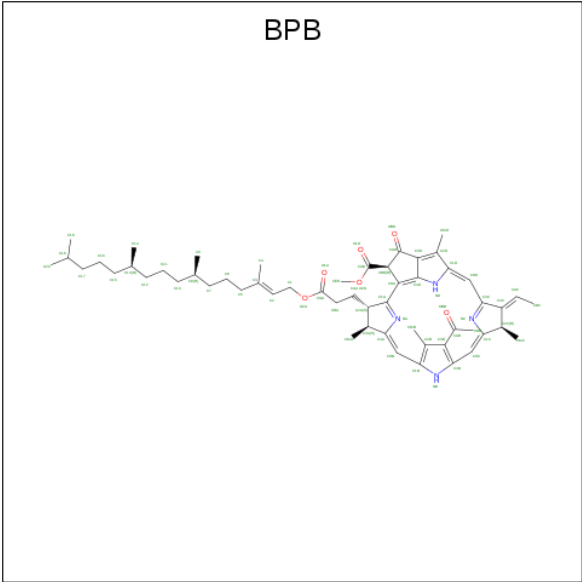
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			37	33	4		

- Molecule 7 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula:  $C_{55}H_{72}MgN_4O_6$ ).



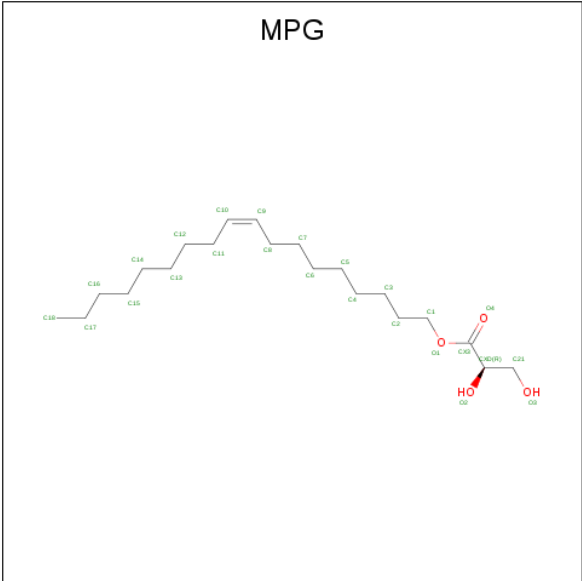
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	L	1	Total 66	C 55	Mg 1	N 4	O 6	0	0
7	M	1	Total 65	C 54	Mg 1	N 4	O 6	0	0
7	M	1	Total 66	C 55	Mg 1	N 4	O 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula:  $\text{C}_{55}\text{H}_{74}\text{N}_4\text{O}_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	L	1	Total	C	N	O	0	0
			65	55	4	6		
8	M	1	Total	C	N	O	0	0
			61	51	4	6		

- Molecule 9 is [(Z)-octadec-9-enyl] (2R)-2,3-bis(oxidanyl)propanoate (three-letter code: MPG) (formula: C<sub>21</sub>H<sub>40</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	L	1	Total	C	O	0	0
			25	21	4		

Continued on next page...

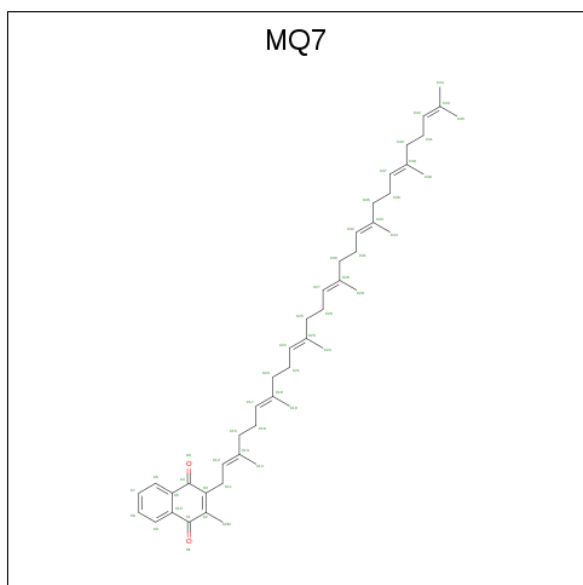
*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	L	1	Total C O 25 21 4	0	0
9	M	1	Total C 17 17	0	0

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

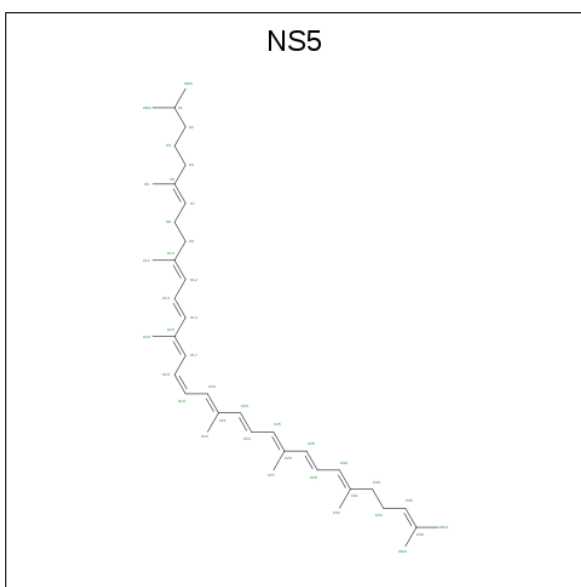
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	L	1	Total Fe 1 1	0	0

- Molecule 11 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C<sub>46</sub>H<sub>64</sub>O<sub>2</sub>).



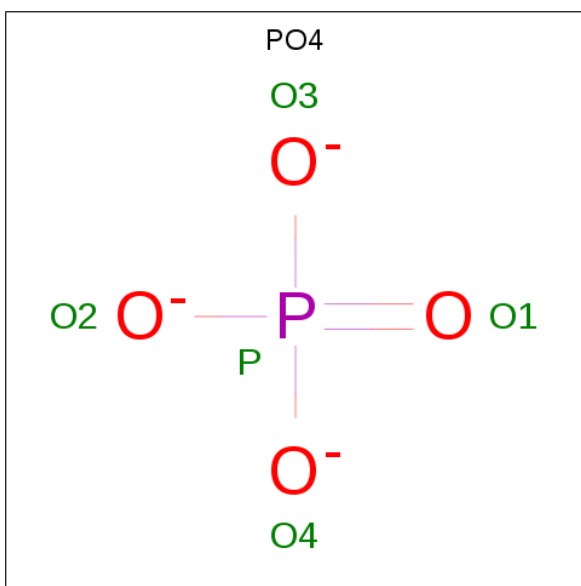
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total C O 48 46 2	0	0

- Molecule 12 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
12	M	1	Total	C	0	0
			40	40		

- Molecule 13 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

- Molecule 14 is water.

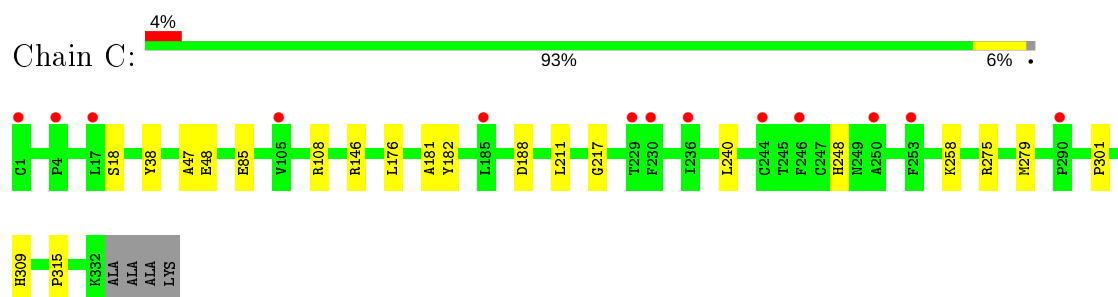


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	C	311	Total 311	O 311	0	0
14	H	146	Total 146	O 146	0	0
14	L	92	Total 92	O 92	0	0
14	M	162	Total 162	O 162	0	0

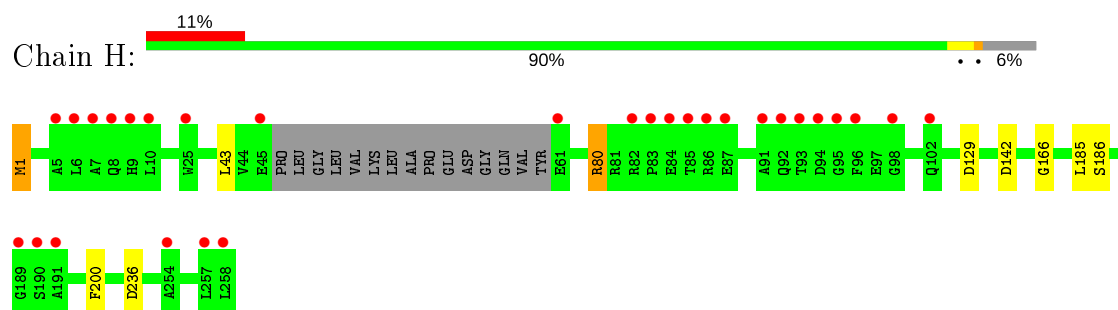
### 3 Residue-property plots [i](#)

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

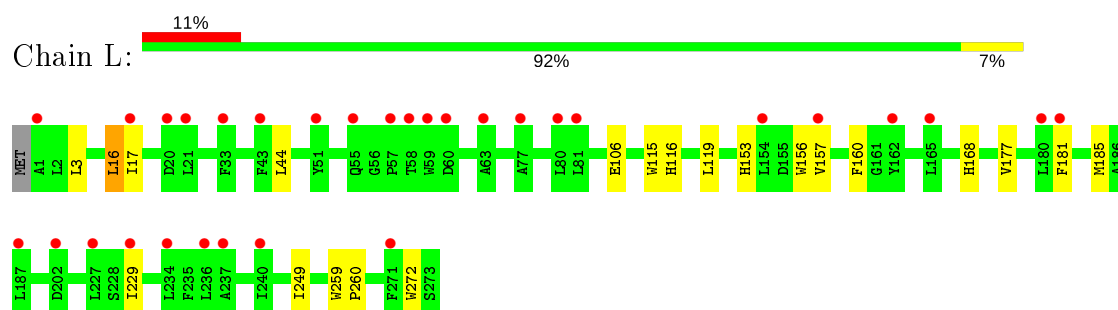
#### • Molecule 1: PHOTOSYNTHETIC REACTION CENTER CYTOCHROME C SUBUNIT



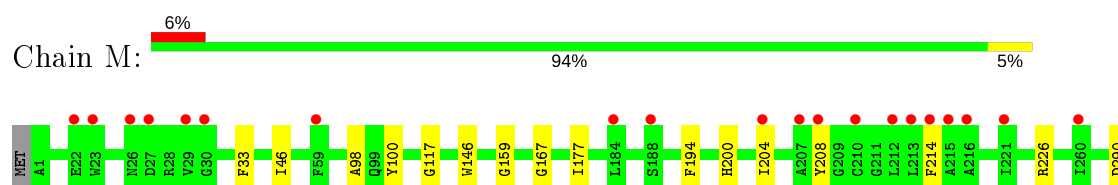
#### • Molecule 2: REACTION CENTER PROTEIN H CHAIN



#### • 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 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.45Å 138.50Å 177.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	176.78 – 1.95 45.87 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.8 (176.78-1.95) 95.9 (45.87-1.95)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.173 , 0.201 0.186 , 0.213	Depositor DCC
$R_{free}$ test set	7313 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.3	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	10671	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: MPG, BPB, PO4, BCB, DGA, FE2, MQ7, HEC, 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	0.70	1/2665 (0.0%)	0.76	5/3633 (0.1%)
2	H	0.61	0/1913	0.73	3/2613 (0.1%)
3	L	0.65	0/2263	0.66	0/3089
4	M	0.68	0/2652	0.66	0/3630
All	All	0.66	1/9493 (0.0%)	0.70	8/12965 (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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	85	GLU	CG-CD	5.87	1.60	1.51

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	80	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	C	108	ARG	NE-CZ-NH2	-8.12	116.24	120.30
2	H	80	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	C	108	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	C	146	ARG	NE-CZ-NH2	-6.47	117.06	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	248	HIS	Peptide
1	C	47	ALA	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2598	0	2567	10	0
2	H	1880	0	1869	6	0
3	L	2170	0	2100	13	0
4	M	2548	0	2432	14	0
5	C	172	0	120	5	0
6	C	37	0	58	0	0
7	L	132	0	144	11	0
7	M	131	0	140	6	0
8	L	65	0	74	8	0
8	M	61	0	63	6	0
9	L	50	0	80	3	0
9	M	17	0	31	0	0
10	L	1	0	0	0	0
11	M	48	0	64	0	0
12	M	40	0	60	7	0
13	M	10	0	0	0	0
14	C	311	0	0	1	0
14	H	146	0	0	2	0
14	L	92	0	0	0	0
14	M	162	0	0	0	0
All	All	10671	0	9802	63	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 3.

The worst 5 of 63 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)
8:M:403:BPB:HHC	8:M:403:BPB:HBBB	1.44	0.98
7:M:401:BCB:HBB2	7:M:401:BCB:HHC	1.53	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:303:BPB:HHC	8:L:303:BPB:HBBB	1.55	0.88
2:H:142:ASP:OD1	14:H:301:HOH:O	2.04	0.73
7:M:401:BCB:HHC	7:M:401:BCB:CBB	2.19	0.73

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%)	321 (97%)	9 (3%)	0	100	100
2	H	239/258 (93%)	235 (98%)	4 (2%)	0	100	100
3	L	273/274 (100%)	266 (97%)	7 (3%)	0	100	100
4	M	321/324 (99%)	312 (97%)	9 (3%)	0	100	100
All	All	1163/1192 (98%)	1134 (98%)	29 (2%)	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%)	279 (100%)	1 (0%)	91	90
2	H	192/212 (91%)	190 (99%)	2 (1%)	76	74

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	218/219 (100%)	211 (97%)	7 (3%)	39	27
4	M	247/250 (99%)	244 (99%)	3 (1%)	71	68
All	All	937/963 (97%)	924 (99%)	13 (1%)	67	62

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	44	LEU
3	L	160	PHE
4	M	194	PHE
3	L	17	ILE
3	L	272	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	302	GLN
3	L	183	ASN
3	L	239	ASN
4	M	16	HIS

### 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	1 (12%)	7,9,11	3.07	2 (28%)



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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	H	1	2	-	4/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	FME	CN-N	2.05	1.40	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	FME	CA-N-CN	-7.35	111.52	122.82
2	H	1	FME	CE-SD-CG	2.25	108.13	100.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	HEC	C	402	1	26,50,50	2.30	7 (26%)	18,82,82	1.78	6 (33%)
11	MQ7	M	404	-	49,49,49	1.44	2 (4%)	60,63,63	1.18	6 (10%)
7	BCB	M	401	-	59,73,74	3.02	24 (40%)	46,113,115	2.09	10 (21%)
9	MPG	L	305	-	24,24,24	1.50	2 (8%)	24,25,25	1.64	3 (12%)
5	HEC	C	401	1	26,50,50	2.47	6 (23%)	18,82,82	1.97	5 (27%)
5	HEC	C	403	1	26,50,50	2.42	7 (26%)	18,82,82	1.61	3 (16%)
9	MPG	L	304	-	24,24,24	1.40	2 (8%)	24,25,25	1.51	2 (8%)
7	BCB	L	302	-	60,74,74	2.90	22 (36%)	48,115,115	2.01	12 (25%)
9	MPG	M	406	-	16,16,24	0.27	0	15,15,25	0.62	0
6	DGA	C	405	1	36,36,43	1.28	2 (5%)	38,38,45	1.20	2 (5%)
7	BCB	L	301	-	60,74,74	2.92	19 (31%)	48,115,115	2.38	17 (35%)
13	PO4	M	407	-	4,4,4	0.64	0	6,6,6	1.50	2 (33%)
5	HEC	C	404	1	26,50,50	2.45	5 (19%)	18,82,82	1.65	5 (27%)
8	BPB	L	303	-	64,70,70	2.00	14 (21%)	64,101,101	1.66	13 (20%)
13	PO4	M	408	-	4,4,4	0.61	0	6,6,6	1.85	2 (33%)
12	NS5	M	405	-	39,39,39	2.17	5 (12%)	44,46,46	2.16	15 (34%)
7	BCB	M	402	-	60,74,74	2.96	22 (36%)	48,115,115	2.32	13 (27%)
8	BPB	M	403	-	60,66,70	2.01	15 (25%)	59,96,101	1.88	13 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	C	402	1	-	1/6/54/54	-
11	MQ7	M	404	-	-	3/41/61/61	0/2/2/2
7	BCB	M	401	-	-	10/40/176/177	-
9	MPG	L	305	-	-	13/25/25/25	-
5	HEC	C	401	1	-	0/6/54/54	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEC	C	403	1	-	0/6/54/54	-
9	MPG	L	304	-	-	16/25/25/25	-
7	BCB	L	302	-	-	12/41/177/177	-
9	MPG	M	406	-	-	3/14/14/25	-
6	DGA	C	405	1	-	15/37/37/45	-
7	BCB	L	301	-	-	7/41/177/177	-
5	HEC	C	404	1	-	0/6/54/54	-
8	BPB	L	303	-	-	7/47/105/105	0/5/6/6
12	NS5	M	405	-	-	13/43/43/43	-
7	BCB	M	402	-	-	8/41/177/177	-
8	BPB	M	403	-	-	17/43/101/105	0/5/6/6

The worst 5 of 154 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	401	BCB	C1D-ND	-8.76	1.31	1.50
7	L	301	BCB	CHB-C4A	-8.07	1.34	1.52
7	M	401	BCB	CHB-C4A	-8.03	1.34	1.52
7	L	302	BCB	CHB-C4A	-7.96	1.34	1.52
7	L	301	BCB	C1D-ND	-7.91	1.33	1.50

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	302	BCB	CMB-C2B-C3B	7.85	133.79	114.29
7	M	402	BCB	CMB-C2B-C3B	7.58	133.12	114.29
8	M	403	BPB	CMD-C2D-C1D	6.62	135.26	125.06
7	L	301	BCB	CMB-C2B-C3B	6.40	130.19	114.29
7	M	401	BCB	CMB-C2B-C3B	6.30	129.94	114.29

There are no chirality outliers.

5 of 125 torsion outliers are listed below:

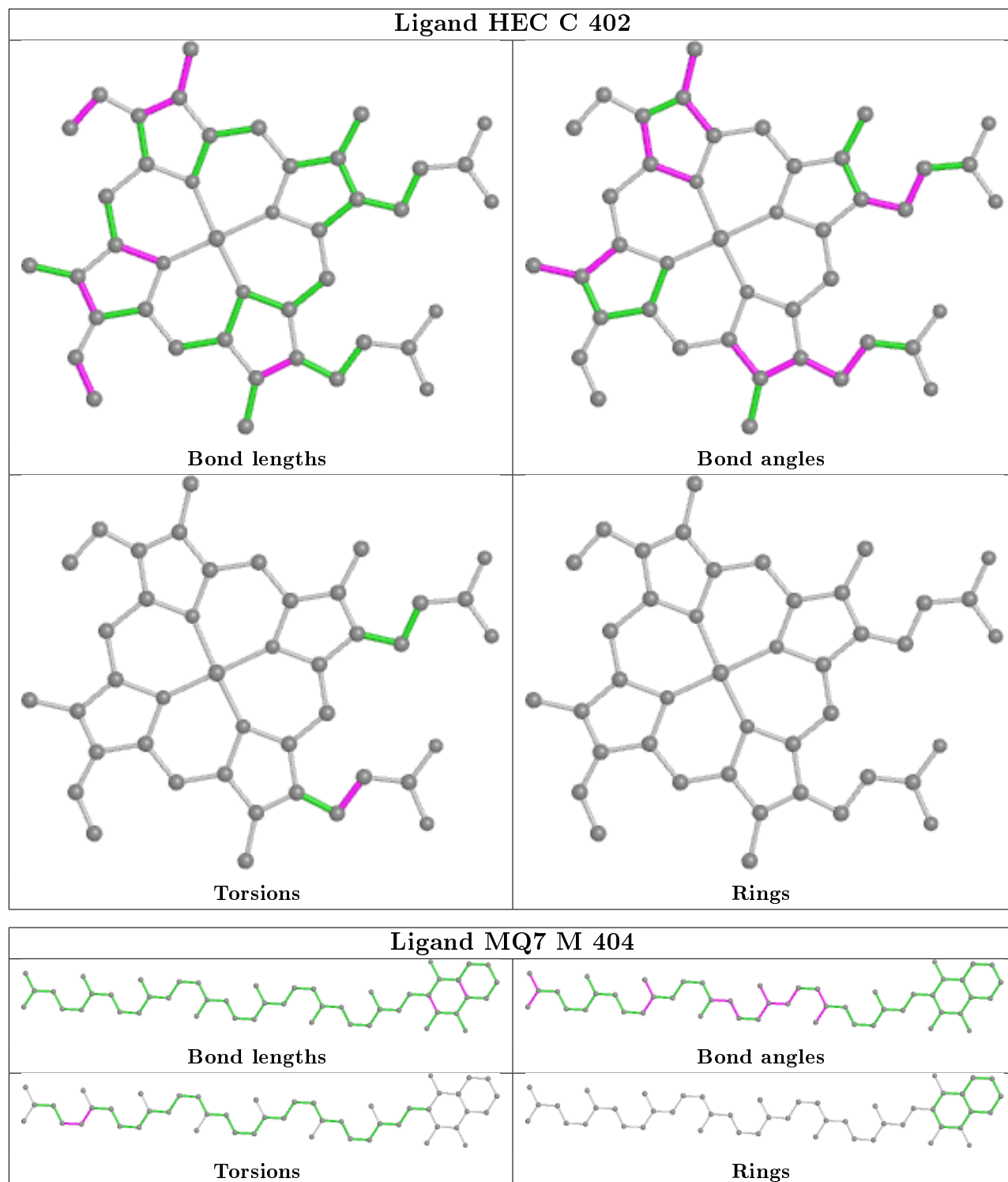
Mol	Chain	Res	Type	Atoms
9	L	305	MPG	O3-C21-CXD-O2
9	L	305	MPG	O1-CX3-CXD-C21
7	M	401	BCB	C4B-C3B-CAB-CBB
9	L	304	MPG	CXD-CX3-O1-C1
9	L	304	MPG	O4-CX3-O1-C1

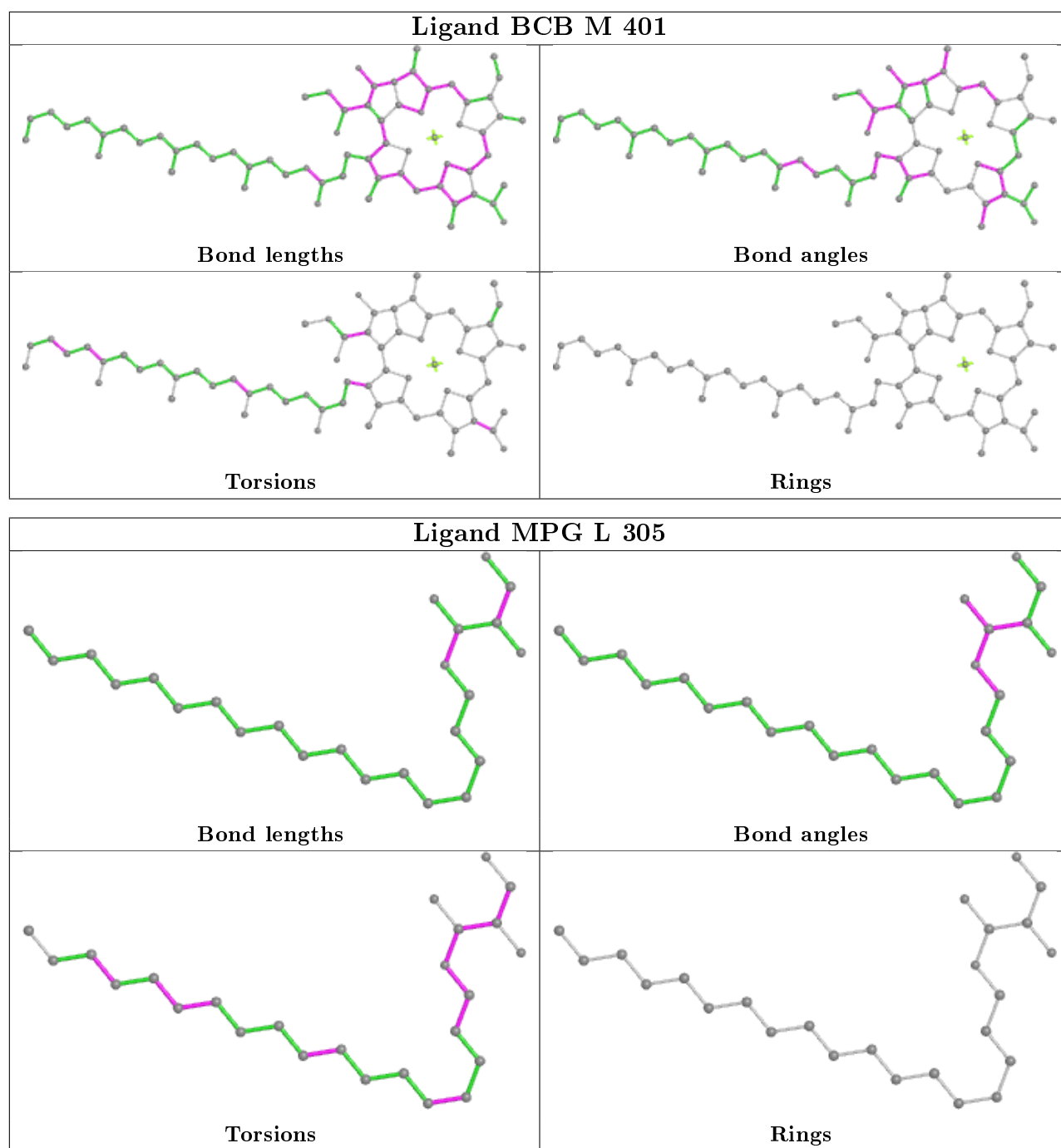
There are no ring outliers.

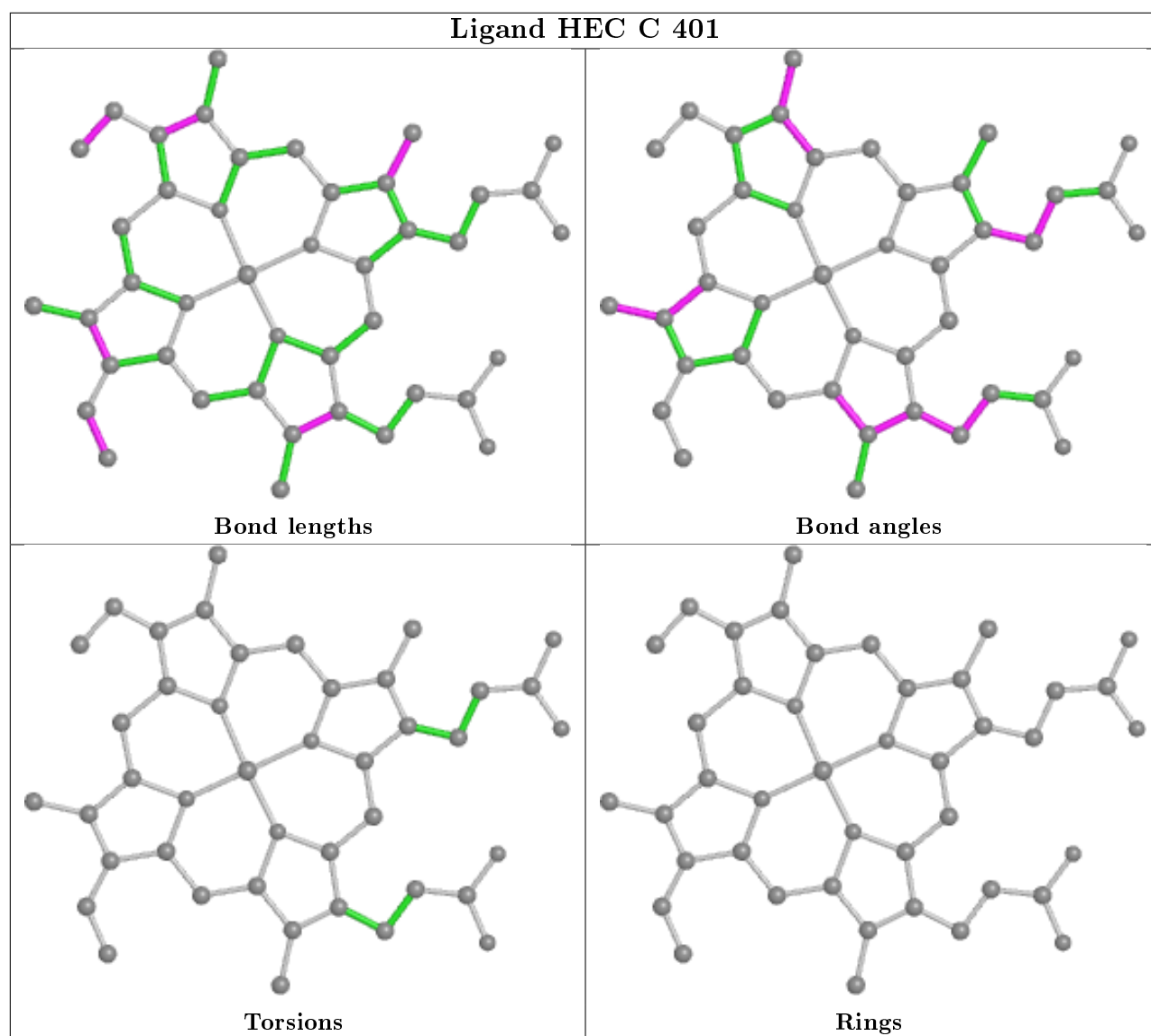
12 monomers are involved in 41 short contacts:

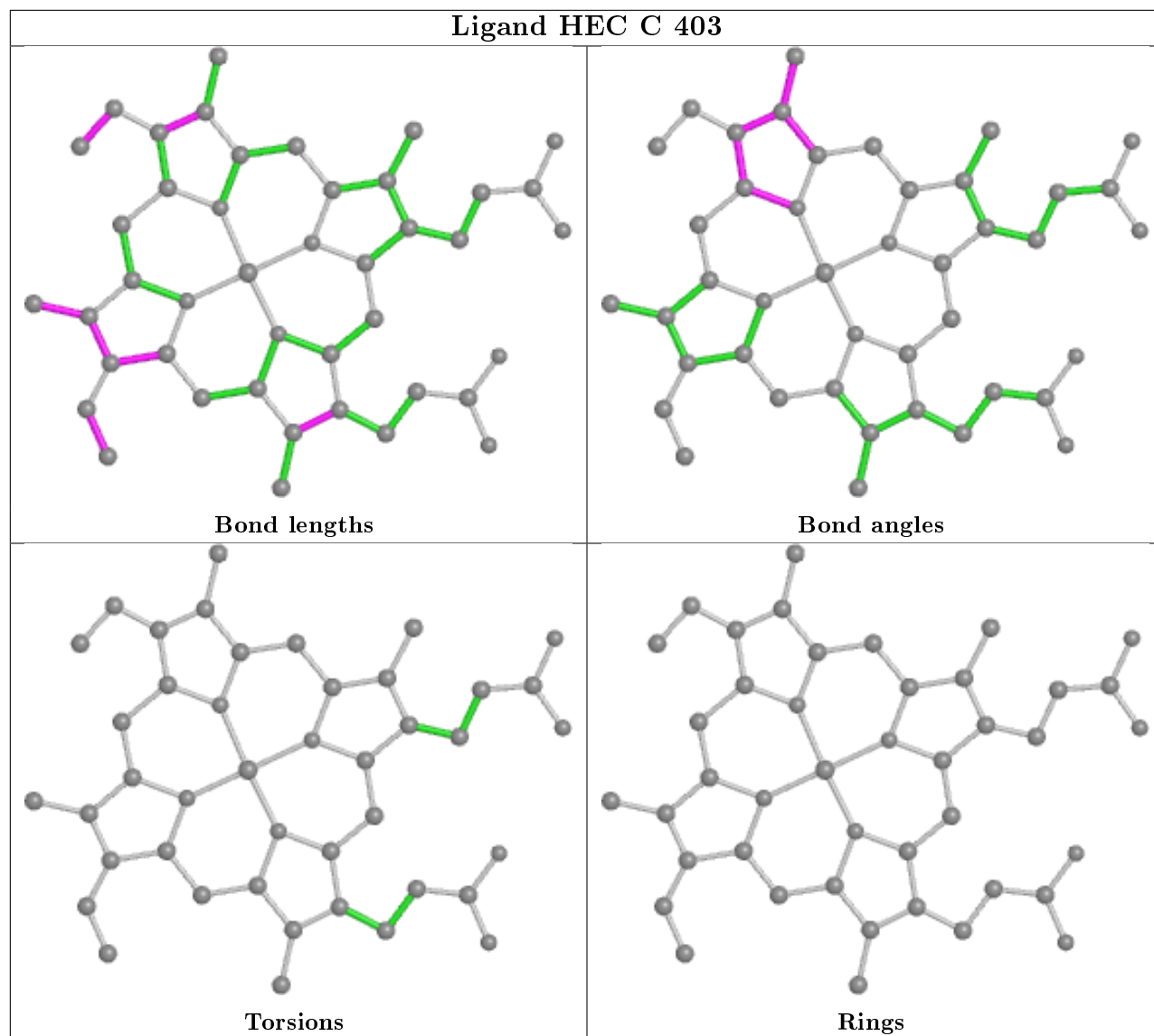
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	402	HEC	1	0
7	M	401	BCB	4	0
5	C	401	HEC	2	0
5	C	403	HEC	1	0
9	L	304	MPG	3	0
7	L	302	BCB	6	0
7	L	301	BCB	5	0
5	C	404	HEC	1	0
8	L	303	BPB	8	0
12	M	405	NS5	7	0
7	M	402	BCB	3	0
8	M	403	BPB	6	0

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.

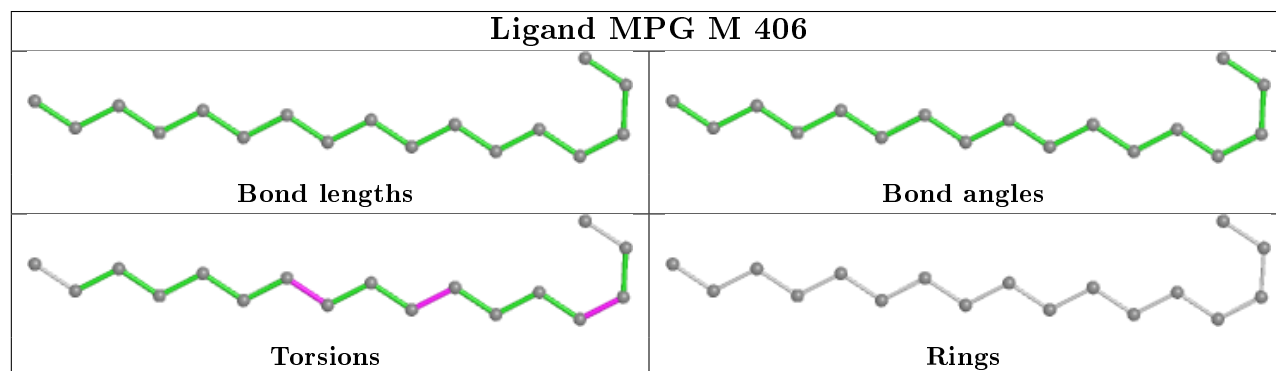
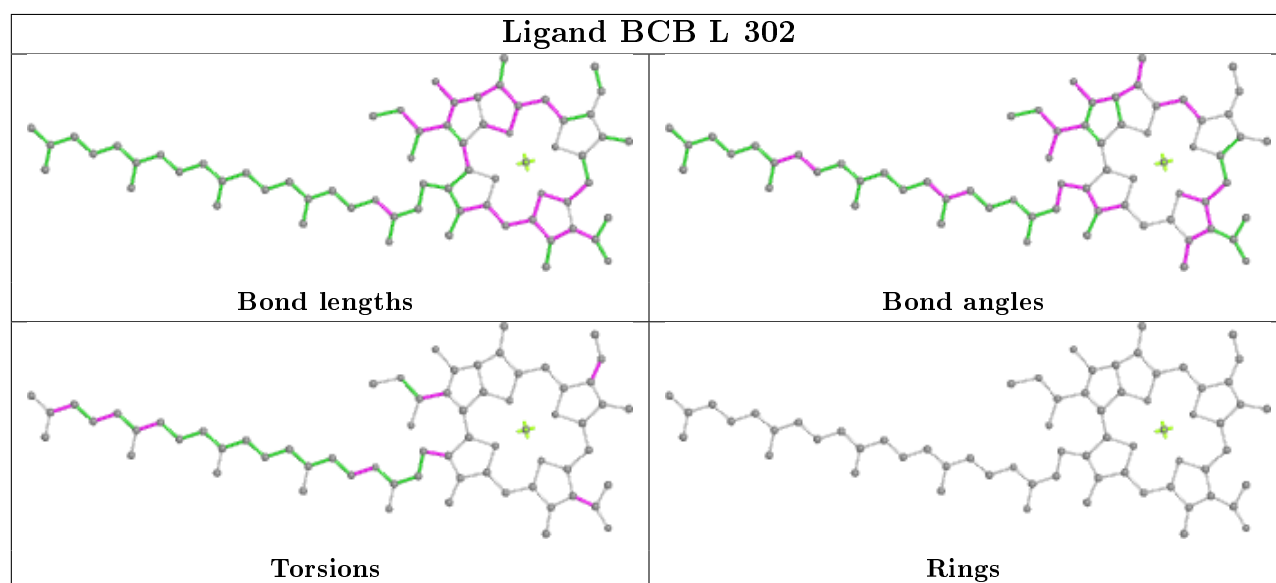
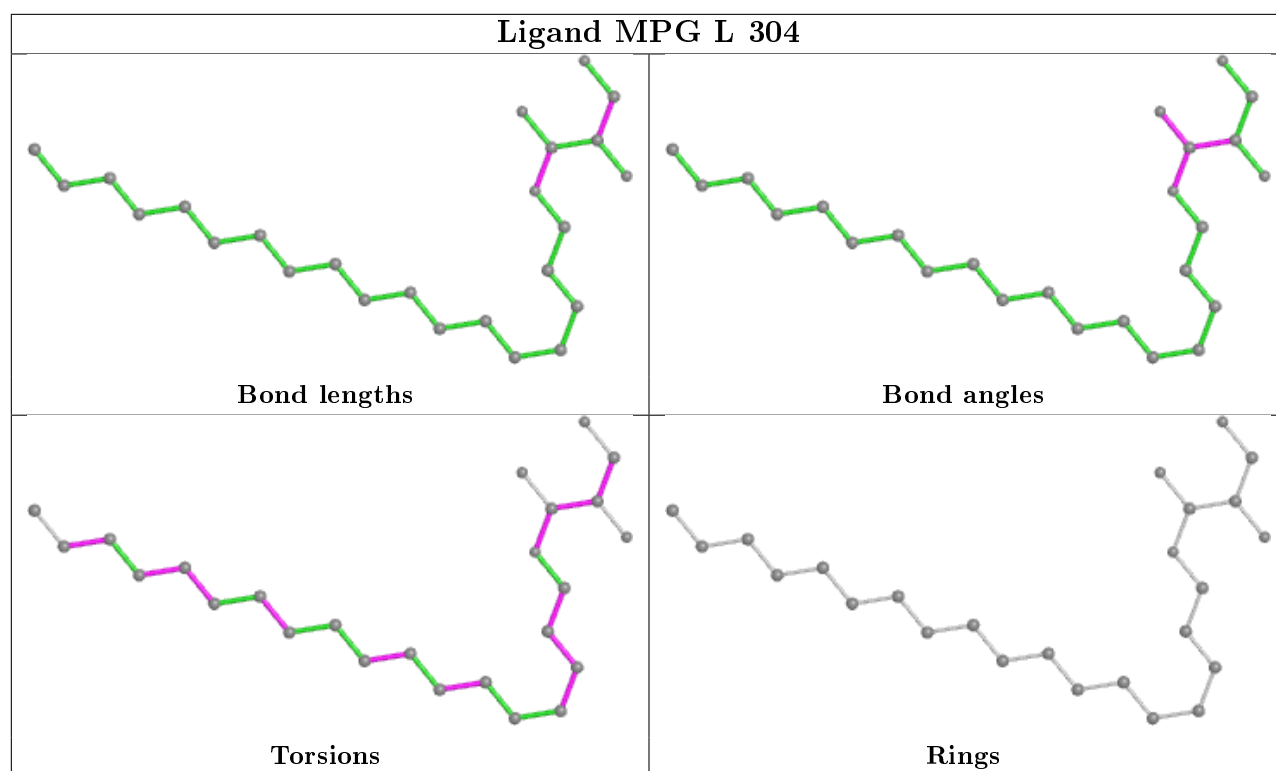


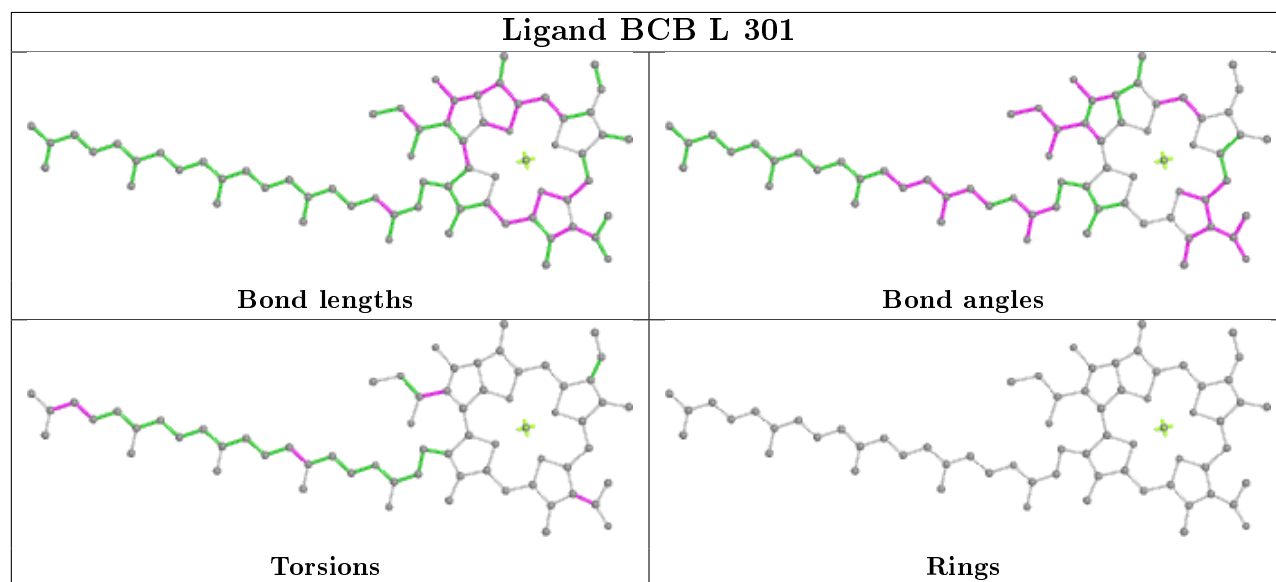
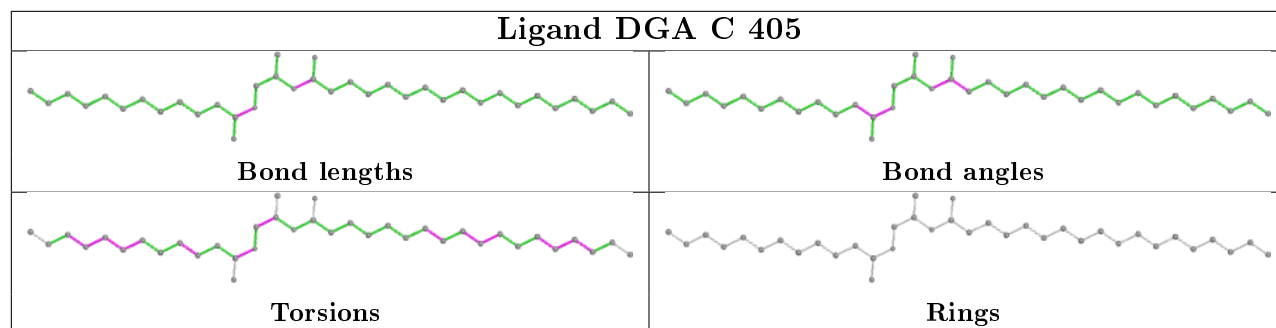


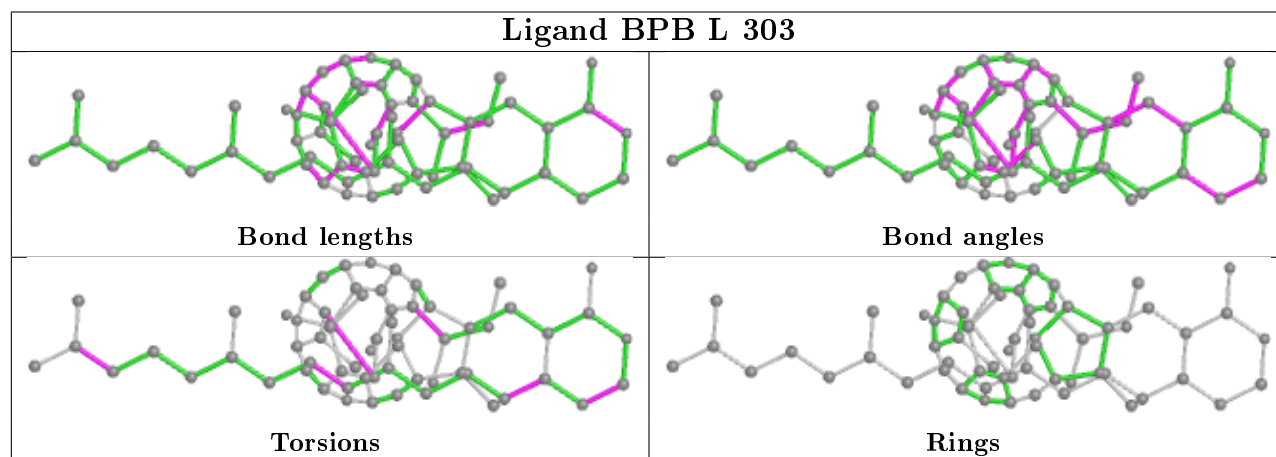
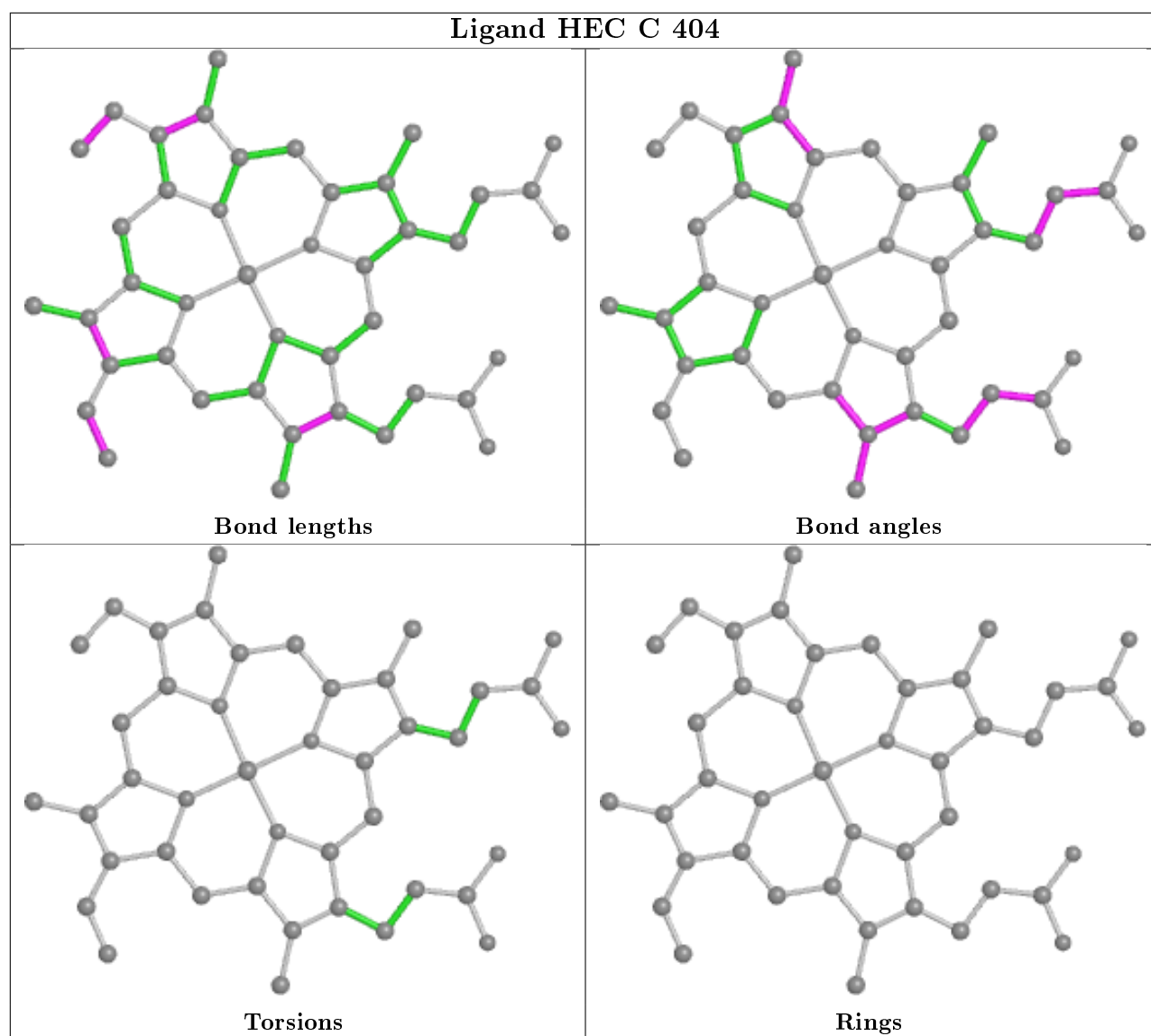


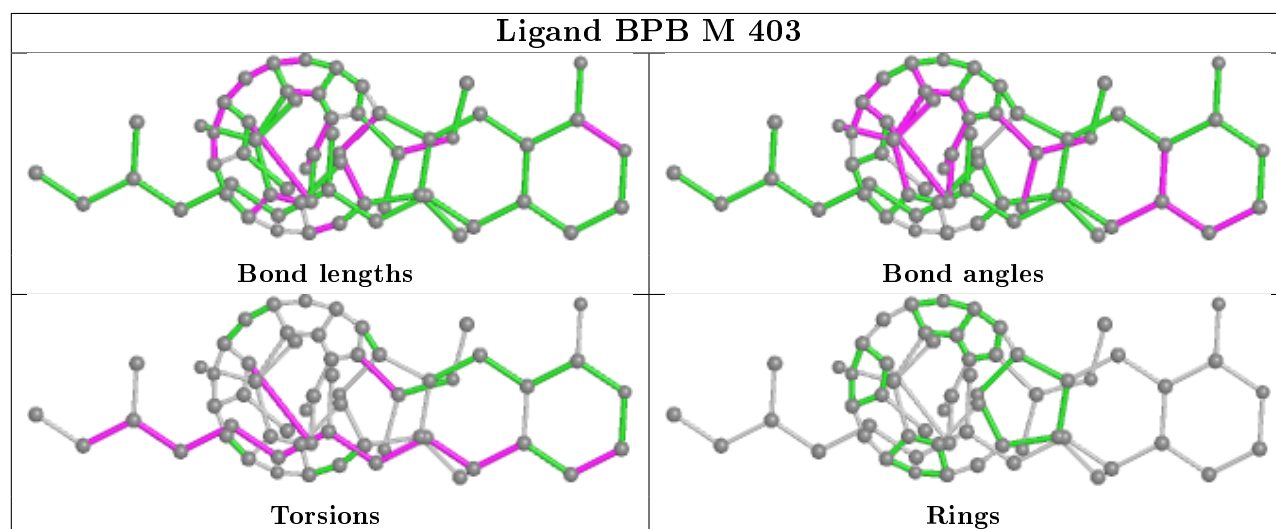
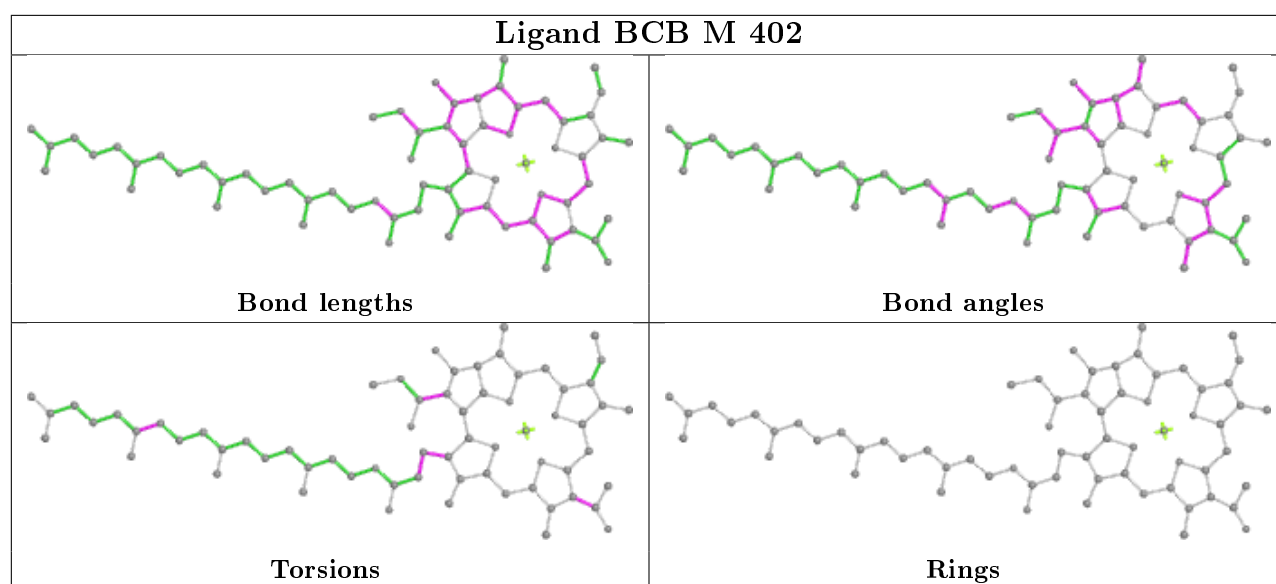
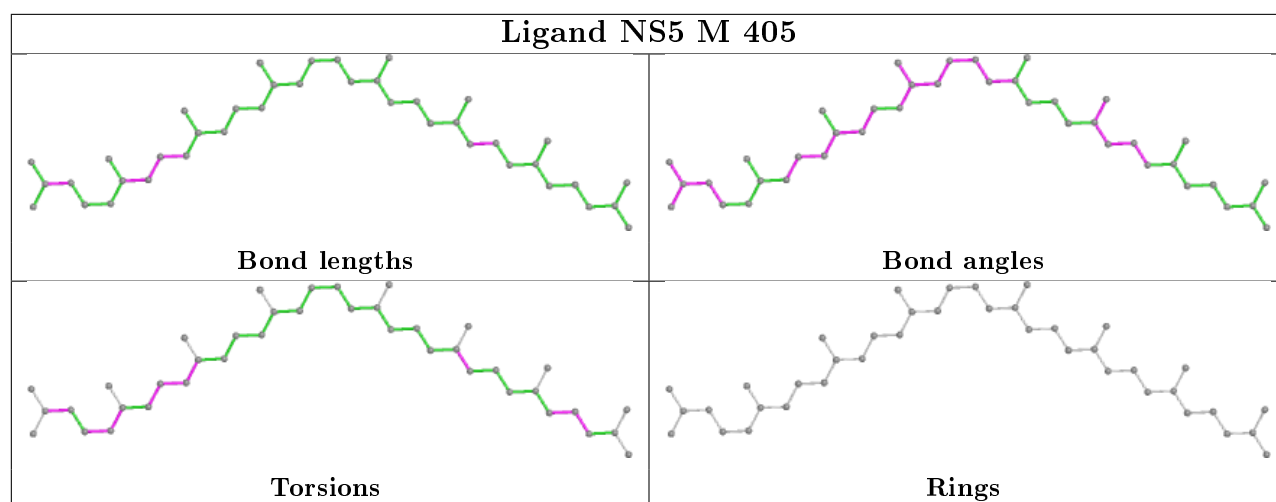












## 5.7 Other polymers [i](#)

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%)	0.37	13 (3%) 39 49	27, 32, 38, 53	0
2	H	242/258 (93%)	0.62	29 (11%) 4 7	26, 31, 43, 58	0
3	L	273/274 (99%)	0.75	31 (11%) 5 8	28, 32, 41, 54	0
4	M	323/324 (99%)	0.49	20 (6%) 20 29	27, 31, 40, 43	0
All	All	1170/1192 (98%)	0.54	93 (7%) 12 19	26, 32, 41, 58	0

The worst 5 of 93 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	85	THR	7.2
2	H	8	GLN	5.8
2	H	7	ALA	5.8
2	H	9	HIS	5.4
3	L	21	LEU	5.1

### 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	0.69	0.32	31,36,49,51	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

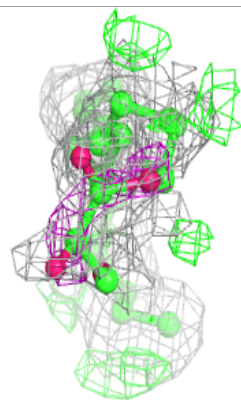
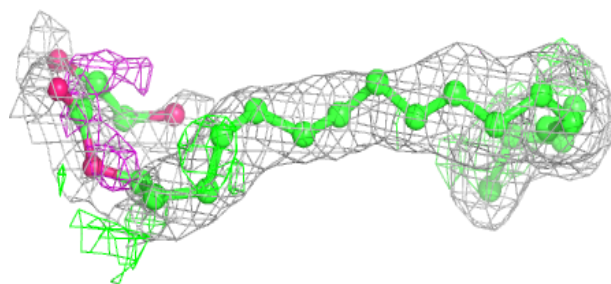
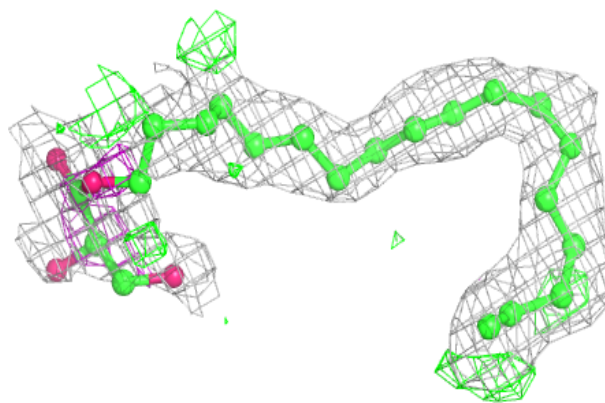
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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
9	MPG	L	304	25/25	0.49	0.27	47,56,76,76	0
6	DGA	C	405	37/44	0.52	0.34	54,66,76,76	0
9	MPG	L	305	25/25	0.78	0.28	34,43,48,49	25
12	NS5	M	405	40/40	0.78	0.25	38,50,65,66	0
9	MPG	M	406	17/25	0.80	0.16	53,56,57,57	0
13	PO4	M	407	5/5	0.81	0.27	50,52,60,61	0
13	PO4	M	408	5/5	0.91	0.33	42,45,49,54	0
11	MQ7	M	404	48/48	0.93	0.11	26,30,44,46	0
8	BPB	M	403	61/65	0.93	0.12	19,25,56,58	0
7	BCB	M	401	65/66	0.95	0.11	20,23,65,67	0
8	BPB	L	303	65/65	0.95	0.09	22,29,34,36	0
7	BCB	L	302	66/66	0.95	0.10	22,25,49,52	0
7	BCB	L	301	66/66	0.96	0.10	19,25,35,38	0
7	BCB	M	402	66/66	0.96	0.09	19,22,35,36	0
5	HEC	C	402	43/43	0.97	0.10	23,26,32,35	0
5	HEC	C	401	43/43	0.97	0.12	26,30,32,33	0
5	HEC	C	404	43/43	0.97	0.09	20,24,35,43	0
5	HEC	C	403	43/43	0.98	0.08	19,23,25,27	0
10	FE2	L	306	1/1	1.00	0.03	26,26,26,26	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 MPG L 304:**

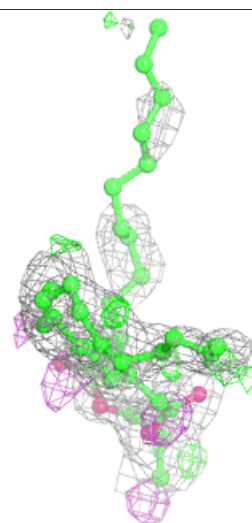
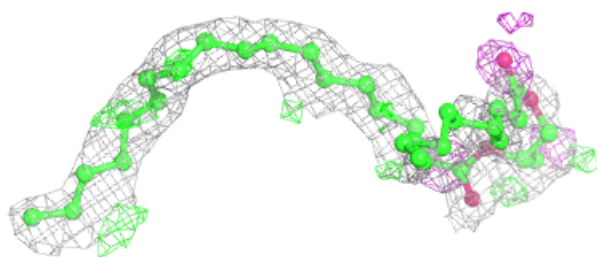
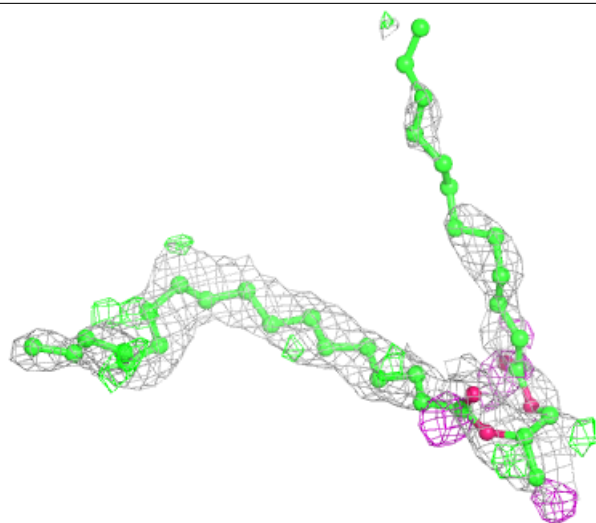
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





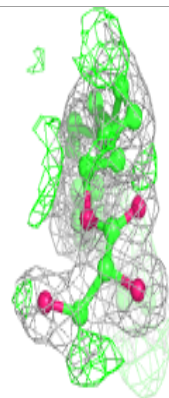
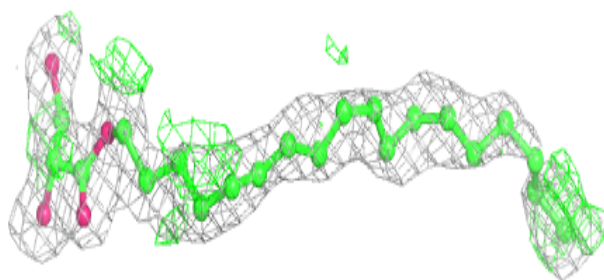
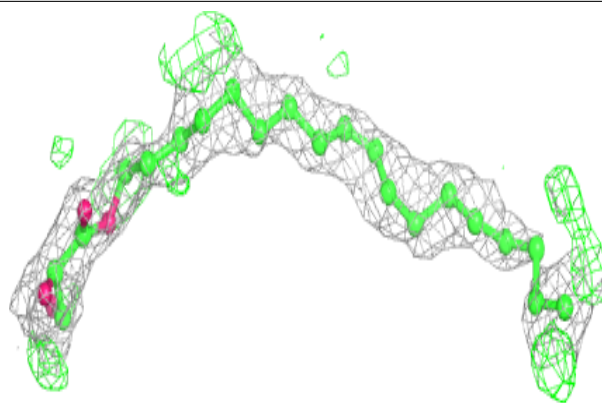
**Electron density around DGA C 405:**

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

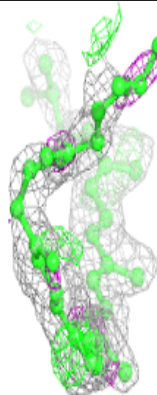
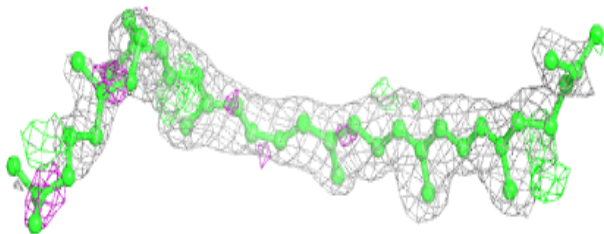
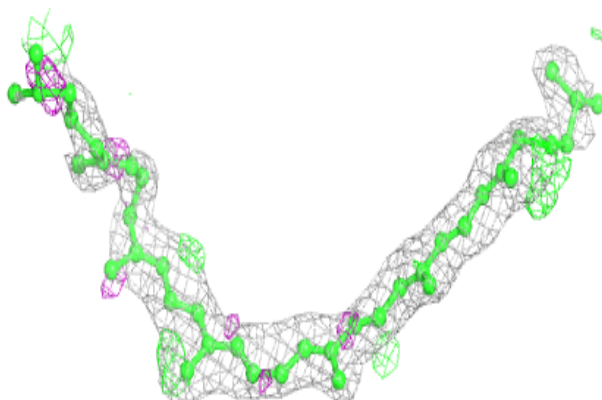


**Electron density around MPG L 305:**

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

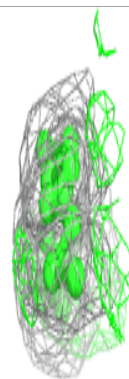
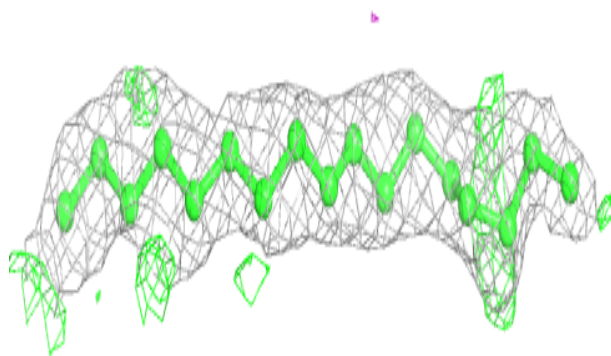
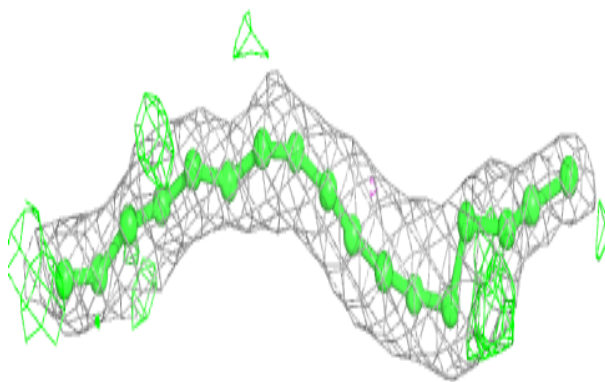
**Electron density around NS5 M 405:**

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

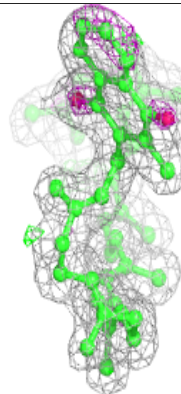
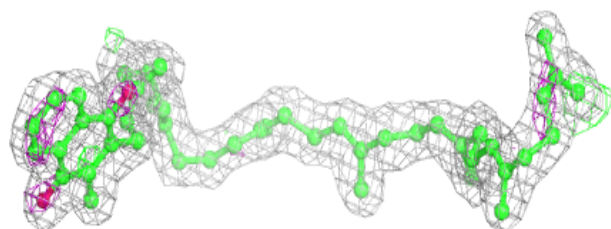
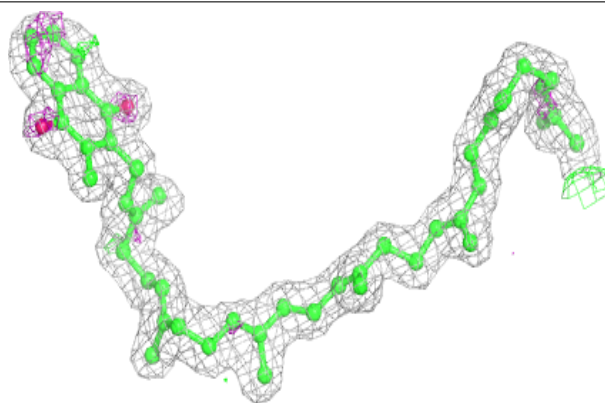


**Electron density around MPG M 406:**

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

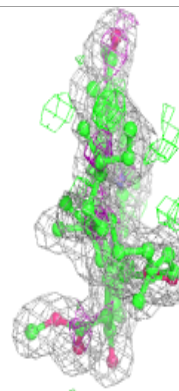
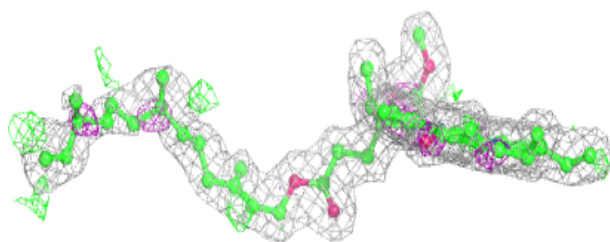
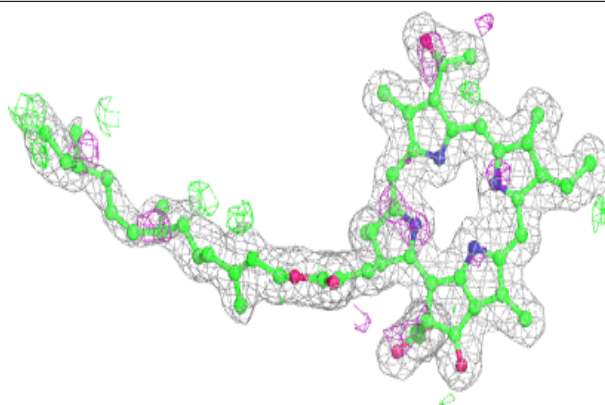
**Electron density around MQ7 M 404:**

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

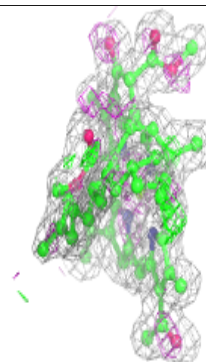
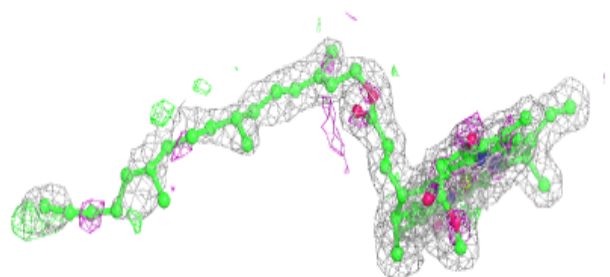
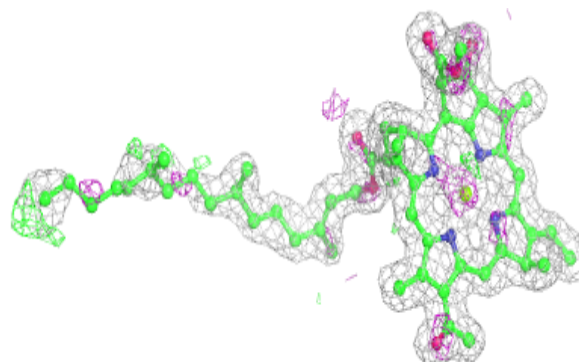


**Electron density around BPB M 403:**

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

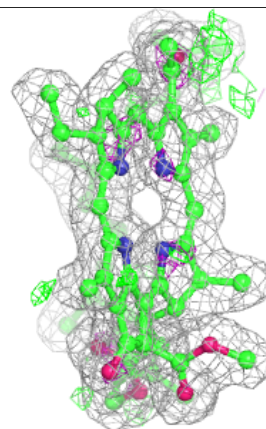
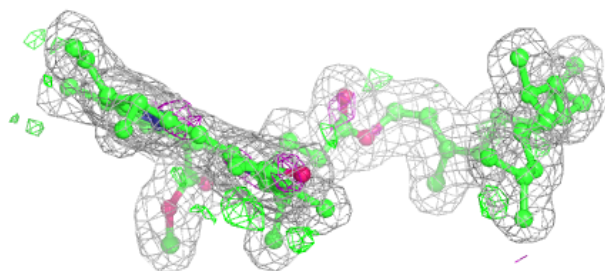
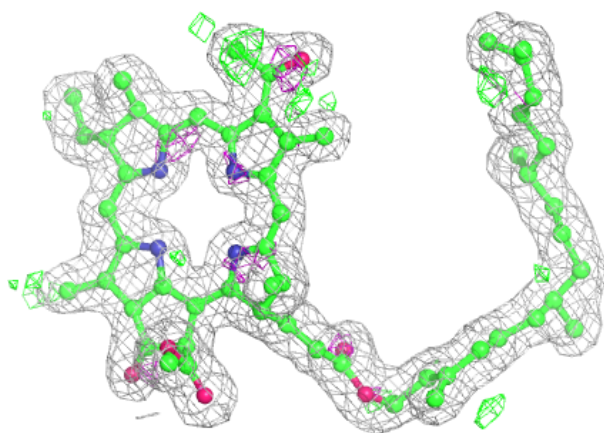
**Electron density around BCB M 401:**

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



**Electron density around BPB L 303:**

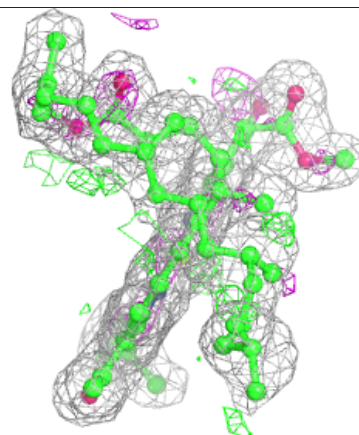
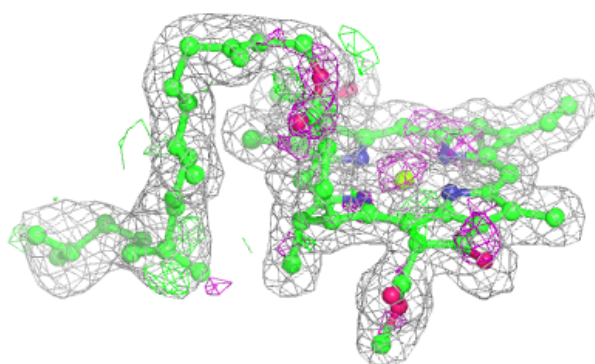
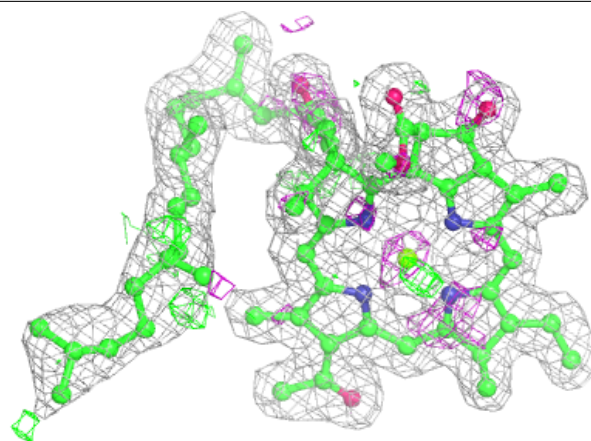
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



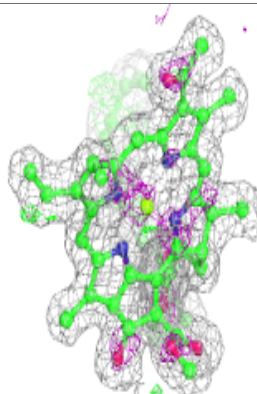
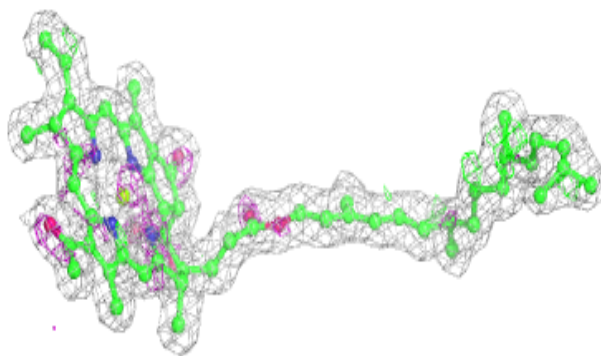
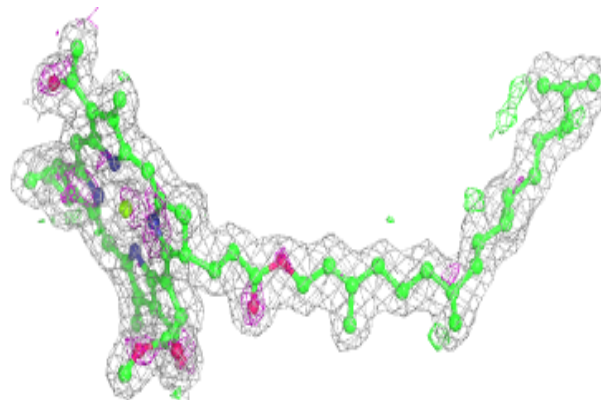


**Electron density around BCB L 302:**

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

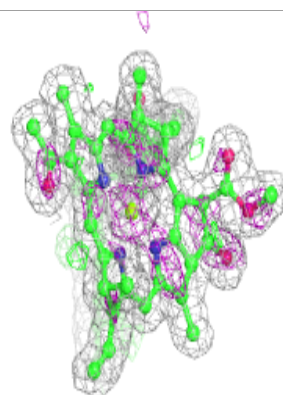
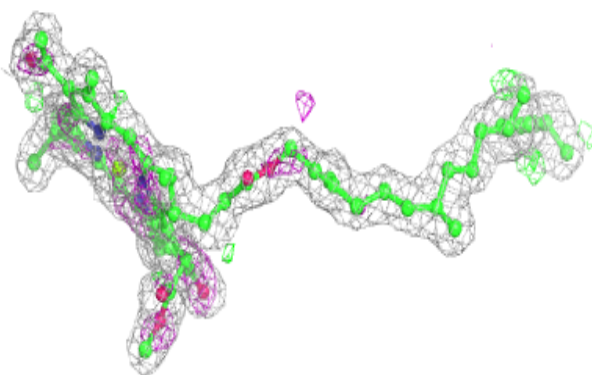
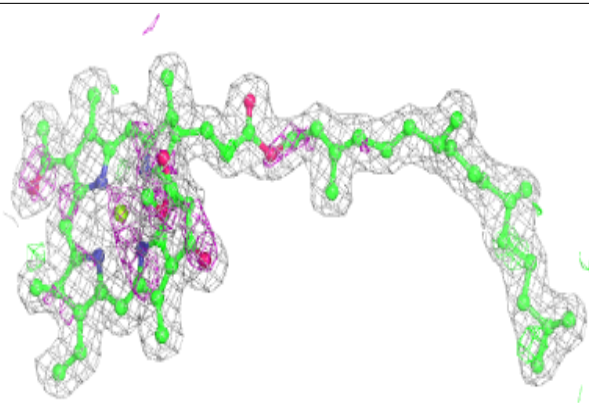
**Electron density around BCB L 301:**

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



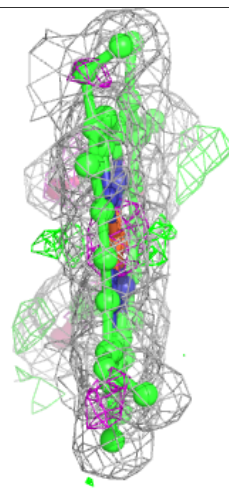
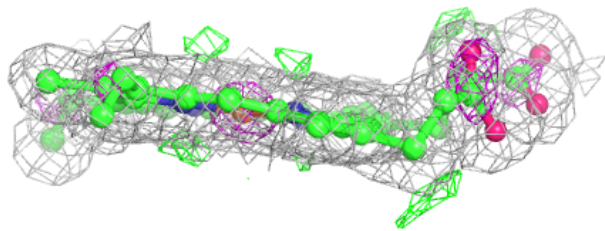
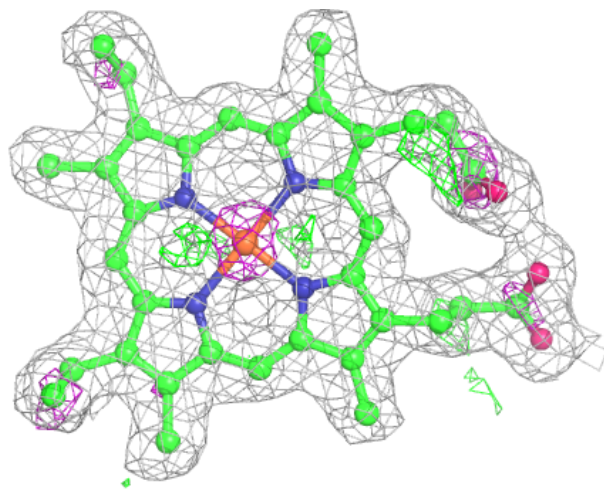
**Electron density around BCB M 402:**

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



**Electron density around HEC C 402:**

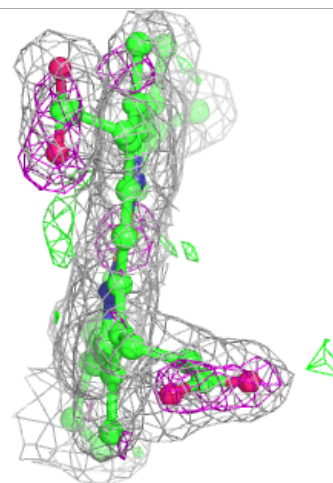
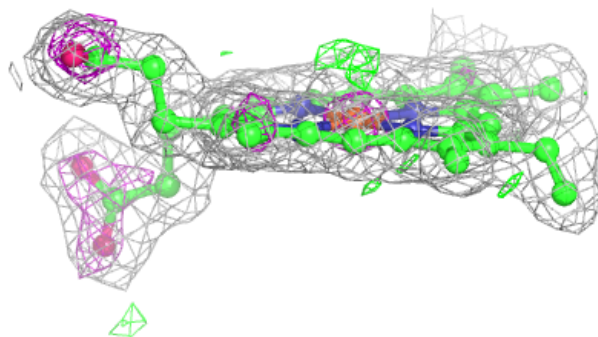
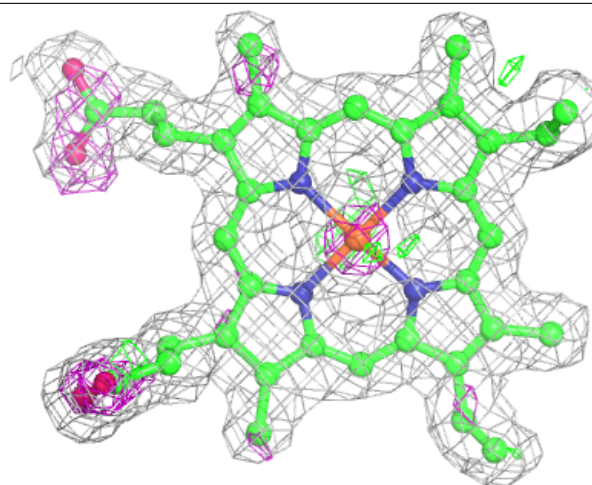
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





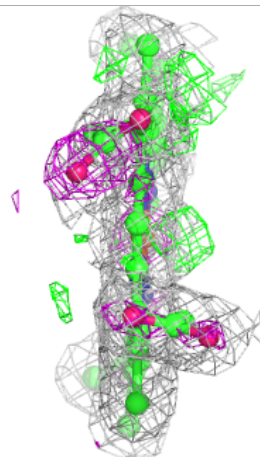
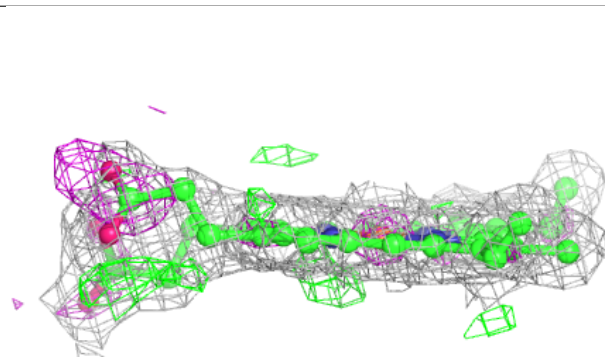
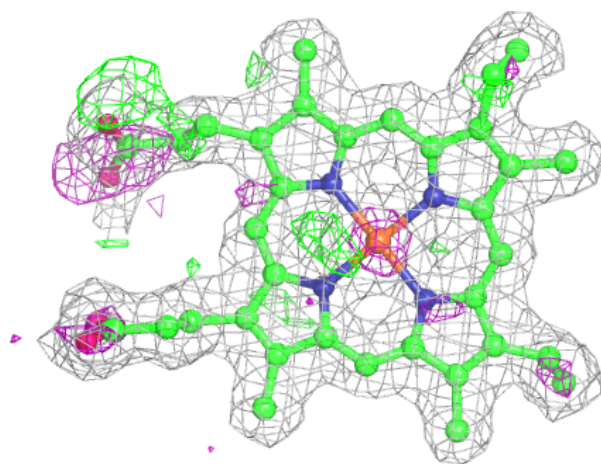
**Electron density around HEC C 401:**

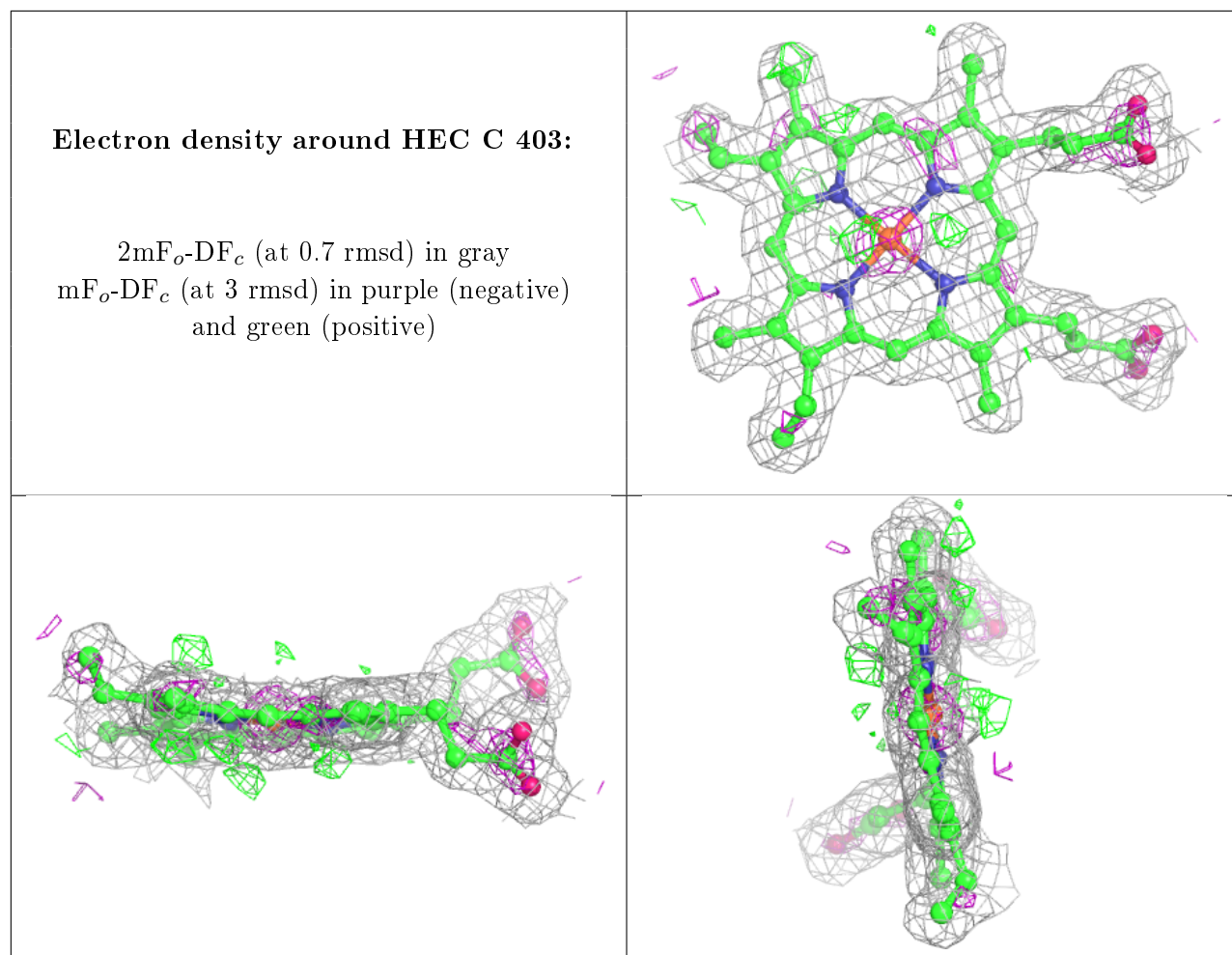
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEC C 404:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.