



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 30, 2022 – 12:40 am GMT

PDB ID : 5O64  
Title : From macrocrystals to microcrystals: a strategy for membrane protein serial crystallography  
Authors : Dods, R.; Baath, P.; Branden, G.; Neutze, R.  
Deposited on : 2017-06-05  
Resolution : 3.30 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

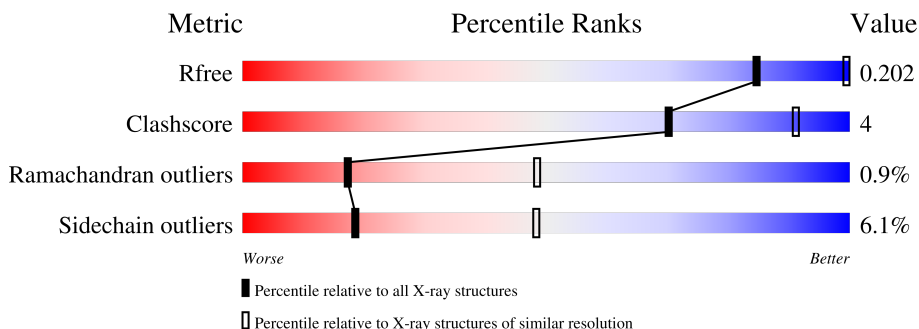
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 of 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	C	336	87% 11% ..
2	H	258	82% 13% . .
3	L	273	86% 14%
4	M	323	87% 11% .

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	SO4	M	408	-	-	X	-

## 2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 10157 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
			2602	1640	466	478	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	250	Total	C	N	O	S	0	0	0
			1962	1253	335	372	2			

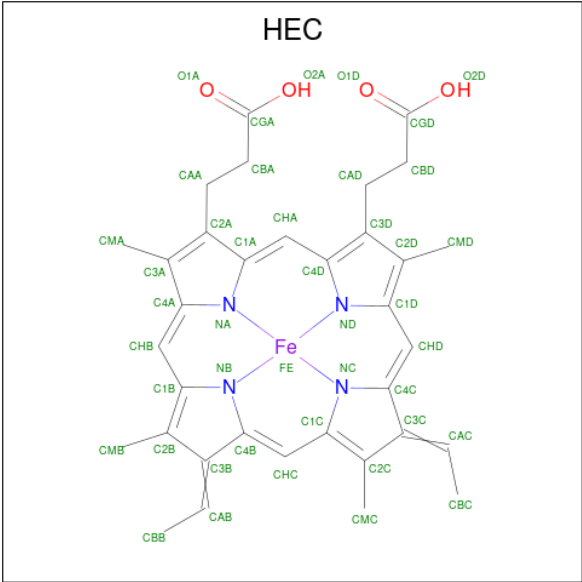
- Molecule 3 is a protein called Reaction center protein L chain.

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

- Molecule 4 is a protein called Reaction center protein M chain.

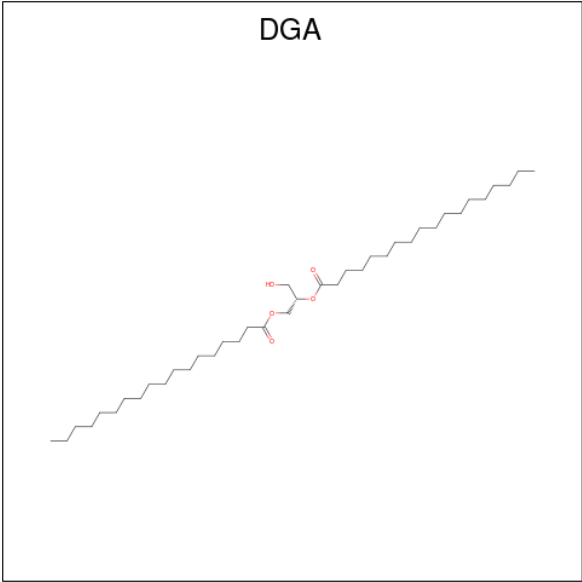
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	323	Total	C	N	O	S	0	0	0
			2555	1702	419	423	11			

- Molecule 5 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



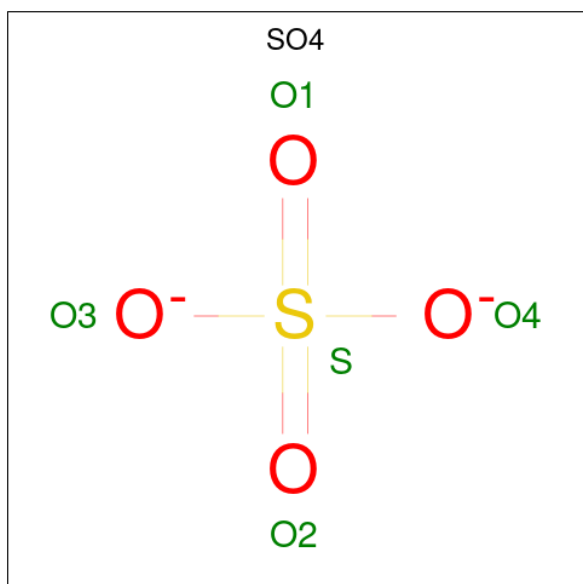
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
5	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C<sub>39</sub>H<sub>76</sub>O<sub>5</sub>).



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

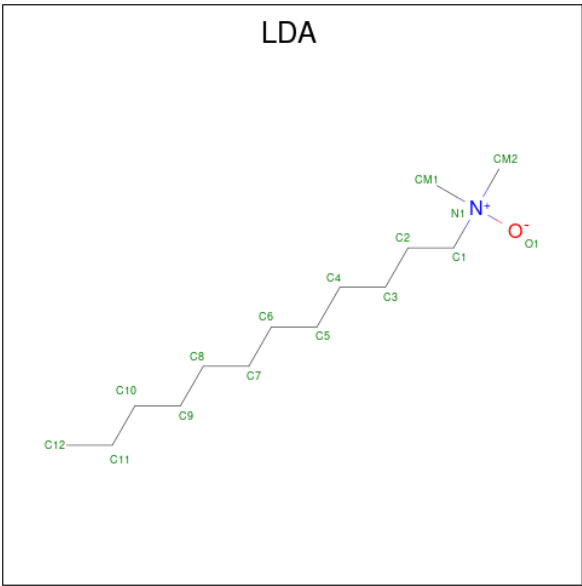
- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

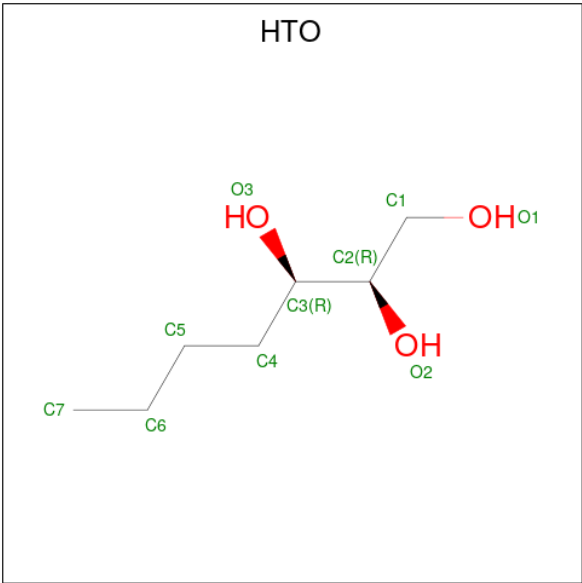
- Molecule 8 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C<sub>14</sub>H<sub>31</sub>NO).



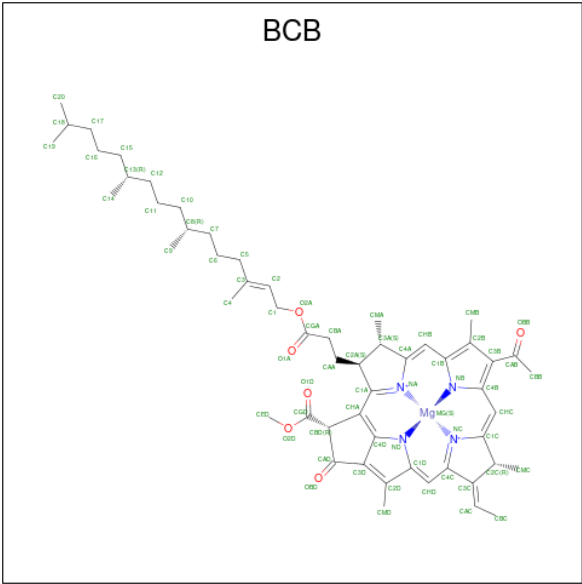
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	H	1	Total	C	N	O	0	0
			16	14	1	1		
8	M	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 9 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
9	H	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		
9	L	1	Total	C	O	0	0
			10	7	3		

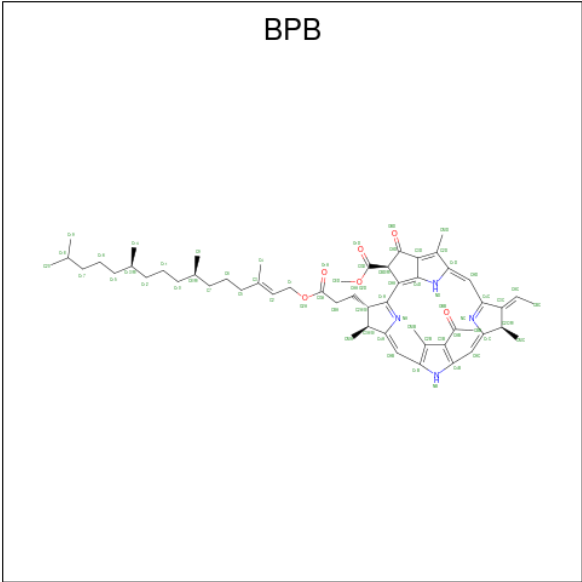
- Molecule 10 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>6</sub>).



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

- Molecule 11 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>6</sub>).



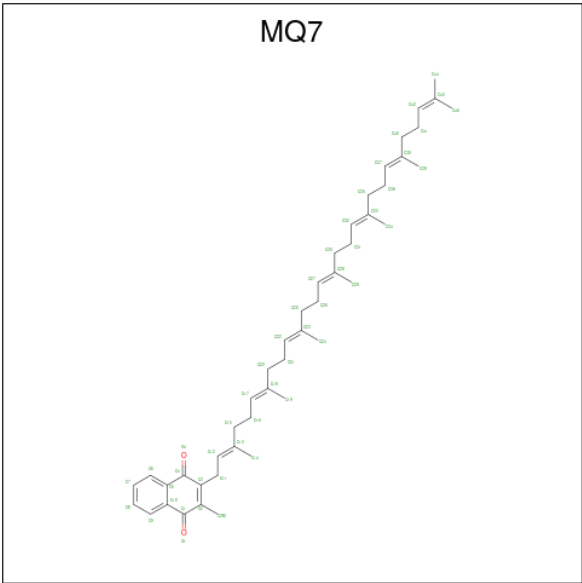


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	L	1	Total	C	N	O	0	0
			65	55	4	6		
11	M	1	Total	C	N	O	0	0
			65	55	4	6		

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

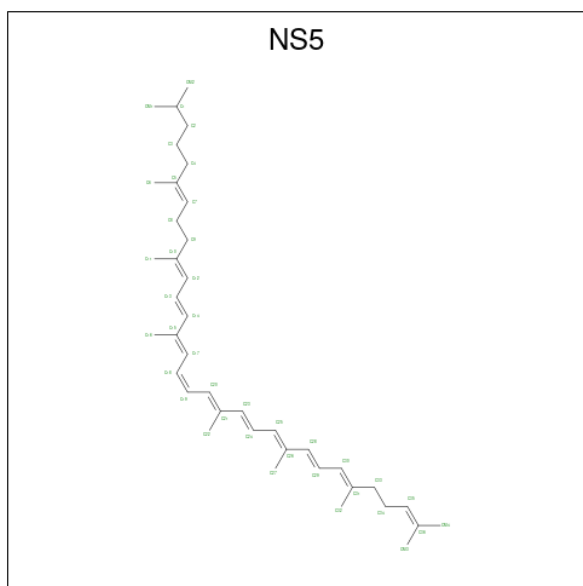
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	M	1	Total	Fe	0	0
			1	1		

- Molecule 13 is MENAQUINONE-7 (three-letter code: MQ7) (formula: C<sub>46</sub>H<sub>64</sub>O<sub>2</sub>).



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

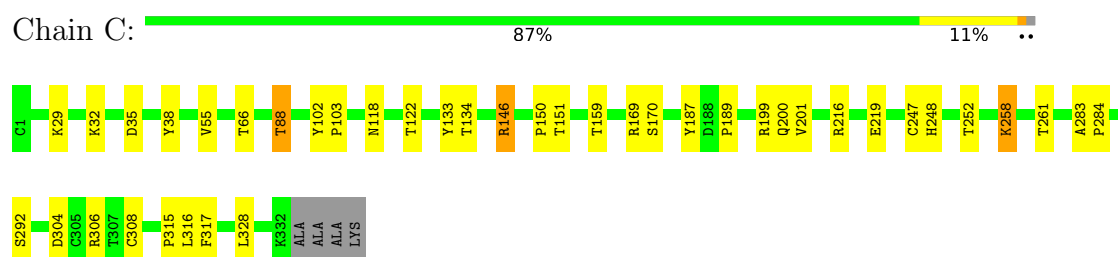
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	7	Total	O	0	0
			7	7		
15	H	3	Total	O	0	0
			3	3		
15	L	13	Total	O	0	0
			13	13		
15	M	7	Total	O	0	0
			7	7		

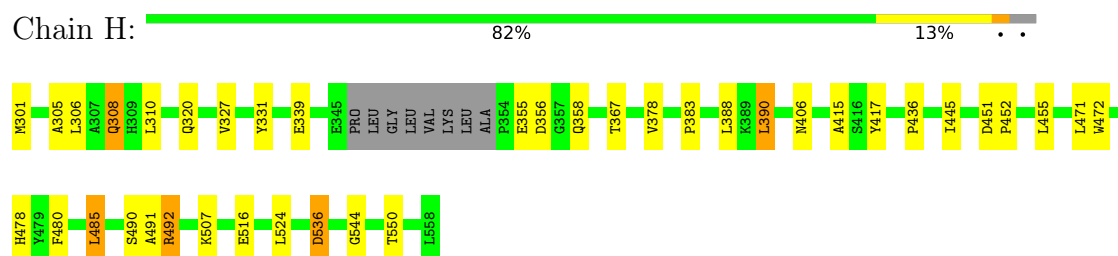
### 3 Residue-property plots

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. 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. 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.

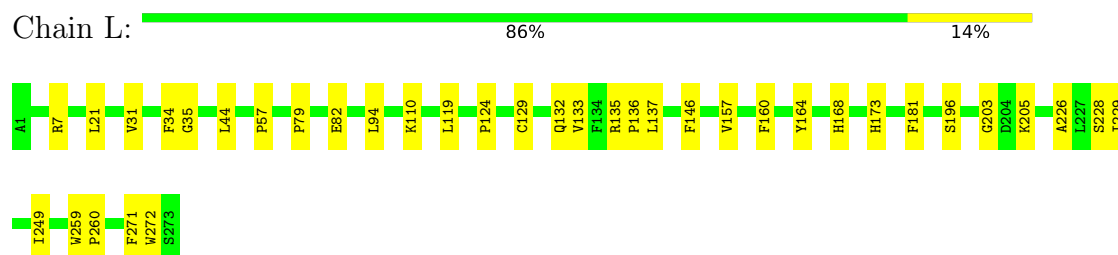
- Molecule 1: Photosynthetic reaction center cytochrome c subunit



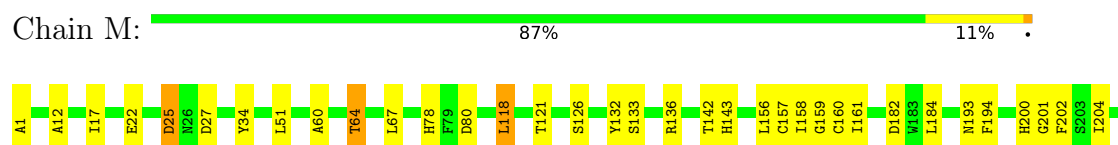
- Molecule 2: Reaction center protein H chain



- 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, $\alpha$ , $\beta$ , $\gamma$	226.60Å 226.60Å 113.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.39 – 3.30 46.39 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.39-3.30) 100.0 (46.39-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.154 , 0.196 0.167 , 0.202	Depositor DCC
$R_{free}$ test set	2294 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	123.8	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10157	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: FME, NS5, LDA, HEC, SO4, BCB, DGA, FE2, HTO, BPB, MQ7

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	0.56	0/2669	0.83	2/3637 (0.1%)
2	H	0.59	0/1997	0.83	1/2725 (0.0%)
3	L	0.59	0/2267	0.77	0/3095
4	M	0.57	0/2659	0.77	3/3637 (0.1%)
All	All	0.58	0/9592	0.80	6/13094 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	485	LEU	CA-CB-CG	5.68	128.36	115.30
4	M	80	ASP	CB-CG-OD1	5.56	123.31	118.30
1	C	146	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	C	306	ARG	NE-CZ-NH2	-5.36	117.62	120.30
4	M	239	ARG	NE-CZ-NH1	5.10	122.85	120.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2602	0	2578	14	0
2	H	1962	0	1950	12	0

*Continued on next page...*

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	2172	0	2097	17	0
4	M	2555	0	2452	21	0
5	C	172	0	120	7	0
6	C	37	0	58	0	0
7	C	5	0	0	1	0
7	H	15	0	0	0	0
7	M	30	0	0	2	0
8	H	48	0	93	0	0
8	M	16	0	31	0	0
9	H	10	0	16	0	0
9	L	20	0	32	0	0
10	L	132	0	144	7	0
10	M	132	0	144	4	0
11	L	65	0	74	2	0
11	M	65	0	74	2	0
12	M	1	0	0	0	0
13	M	48	0	64	1	0
14	M	40	0	60	4	0
15	C	7	0	0	0	0
15	H	3	0	0	0	0
15	L	13	0	0	0	0
15	M	7	0	0	0	0
All	All	10157	0	9987	73	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 4.

The worst 5 of 73 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)
5:C:401:HEC:HMB1	5:C:401:HEC:HBB3	1.69	0.75
3:L:31:VAL:HG22	13:M:402:MQ7:H401	1.72	0.72
11:L:303:BPB:HBBB	11:L:303:BPB:HMB	1.77	0.67
4:M:159:GLY:HA3	14:M:406:NS5:H272	1.80	0.63
3:L:132:GLN:HE22	3:L:146:PHE:H	1.47	0.61

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%)	310 (94%)	18 (6%)	2 (1%)	25	57
2	H	246/258 (95%)	223 (91%)	20 (8%)	3 (1%)	13	42
3	L	272/273 (100%)	248 (91%)	21 (8%)	3 (1%)	14	45
4	M	321/323 (99%)	301 (94%)	18 (6%)	2 (1%)	25	57
All	All	1169/1190 (98%)	1082 (93%)	77 (7%)	10 (1%)	17	48

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	55	VAL
3	L	57	PRO
3	L	271	PHE
2	H	383	PRO
3	L	203	GLY

### 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	281/282 (100%)	267 (95%)	14 (5%)	24	55
2	H	206/212 (97%)	188 (91%)	18 (9%)	10	34
3	L	219/218 (100%)	209 (95%)	10 (5%)	27	58
4	M	249/249 (100%)	233 (94%)	16 (6%)	17	46
All	All	955/961 (99%)	897 (94%)	58 (6%)	18	48



5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	516	GLU
4	M	214	PHE
3	L	110	LYS
4	M	194	PHE
4	M	118	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	158	ASN
3	L	239	ASN
4	M	143	HIS
2	H	402	GLN
2	H	406	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	301	2	8,9,10	0.93	0	7,9,11	3.58	4 (57%)

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	301	2	-	3/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	FME	CA-N-CN	-7.86	110.73	122.82
2	H	301	FME	CE-SD-CG	4.05	114.32	100.40
2	H	301	FME	O-C-CA	-2.28	118.81	124.78
2	H	301	FME	O1-CN-N	-2.11	119.71	125.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	301	FME	O1-CN-N-CA
2	H	301	FME	O-C-CA-CB
2	H	301	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 1 is monoatomic - leaving 30 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	404	1	32,50,50	1.59	4 (12%)	24,82,82	1.55	5 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SO4	M	411	-	4,4,4	0.39	0	6,6,6	0.32	0
7	SO4	H	602	-	4,4,4	0.49	0	6,6,6	0.50	0
10	BCB	L	302	-	54,74,74	2.36	16 (29%)	52,115,115	2.62	14 (26%)
9	HTO	L	304	-	9,9,9	1.23	2 (22%)	10,10,10	1.40	2 (20%)
8	LDA	H	601	-	12,15,15	2.09	1 (8%)	14,17,17	0.55	0
8	LDA	H	605	-	12,15,15	2.13	1 (8%)	14,17,17	0.84	1 (7%)
10	BCB	M	404	-	54,74,74	2.40	13 (24%)	52,115,115	2.48	13 (25%)
6	DGA	C	405	1	36,36,43	1.46	3 (8%)	38,38,45	1.71	6 (15%)
7	SO4	M	410	-	4,4,4	0.37	0	6,6,6	0.27	0
7	SO4	H	603	-	4,4,4	0.40	0	6,6,6	0.35	0
5	HEC	C	401	1	32,50,50	1.66	2 (6%)	24,82,82	1.93	5 (20%)
9	HTO	H	607	-	9,9,9	0.83	0	10,10,10	1.26	2 (20%)
5	HEC	C	402	1	32,50,50	1.59	4 (12%)	24,82,82	1.83	7 (29%)
14	NS5	M	406	-	39,39,39	1.65	4 (10%)	44,46,46	2.39	16 (36%)
7	SO4	M	408	-	4,4,4	0.41	0	6,6,6	0.28	0
7	SO4	H	604	-	4,4,4	0.33	0	6,6,6	0.19	0
11	BPB	M	405	-	49,70,70	2.27	10 (20%)	47,101,101	2.18	10 (21%)
11	BPB	L	303	-	49,70,70	2.12	10 (20%)	47,101,101	1.84	9 (19%)
10	BCB	M	403	-	54,74,74	2.41	15 (27%)	52,115,115	2.49	12 (23%)
10	BCB	L	301	-	54,74,74	2.36	14 (25%)	52,115,115	2.30	15 (28%)
7	SO4	C	406	-	4,4,4	0.44	0	6,6,6	0.46	0
8	LDA	H	606	-	12,15,15	1.94	1 (8%)	14,17,17	0.50	0
7	SO4	M	409	-	4,4,4	0.32	0	6,6,6	0.74	0
7	SO4	M	407	-	4,4,4	0.36	0	6,6,6	0.58	0
9	HTO	L	305	-	9,9,9	0.72	0	10,10,10	0.67	0
8	LDA	M	413	-	12,15,15	2.10	1 (8%)	14,17,17	0.40	0
13	MQ7	M	402	-	49,49,49	1.48	3 (6%)	60,63,63	1.22	6 (10%)
5	HEC	C	403	1	32,50,50	1.75	4 (12%)	24,82,82	1.56	4 (16%)
7	SO4	M	412	-	4,4,4	0.45	0	6,6,6	0.38	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
5	HEC	C	404	1	-	4/10/54/54	-
10	BCB	L	302	-	-	8/37/177/177	-

*Continued on next page...*

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HTO	L	304	-	-	2/10/10/10	-
8	LDA	H	601	-	-	4/13/13/13	-
8	LDA	H	605	-	-	7/13/13/13	-
10	BCB	M	404	-	-	9/37/177/177	-
6	DGA	C	405	1	-	21/37/37/45	-
5	HEC	C	401	1	-	4/10/54/54	-
9	HTO	H	607	-	-	4/10/10/10	-
5	HEC	C	402	1	-	3/10/54/54	-
14	NS5	M	406	-	-	13/43/43/43	-
11	BPB	M	405	-	-	16/37/105/105	0/5/6/6
11	BPB	L	303	-	-	10/37/105/105	0/5/6/6
10	BCB	M	403	-	-	13/37/177/177	-
10	BCB	L	301	-	-	9/37/177/177	-
8	LDA	H	606	-	-	4/13/13/13	-
9	HTO	L	305	-	-	3/10/10/10	-
8	LDA	M	413	-	-	5/13/13/13	-
13	MQ7	M	402	-	-	2/41/61/61	0/2/2/2
5	HEC	C	403	1	-	0/10/54/54	-

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	404	BCB	C1A-CHA	8.63	1.49	1.39
13	M	402	MQ7	C3-C2	8.00	1.49	1.35
10	L	301	BCB	C1A-CHA	7.98	1.48	1.39
14	M	406	NS5	C35-C36	7.74	1.54	1.32
11	M	405	BPB	CAC-C3C	7.74	1.53	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	403	BCB	C4D-C3D-CAD	-10.81	100.39	116.53
10	M	404	BCB	C4D-C3D-CAD	-10.57	100.74	116.53
10	L	302	BCB	C4D-C3D-CAD	-10.21	101.29	116.53
10	L	301	BCB	C4D-C3D-CAD	-9.52	102.32	116.53
10	L	302	BCB	O2D-CGD-CBD	8.09	121.24	111.00

There are no chirality outliers.

5 of 141 torsion outliers are listed below:

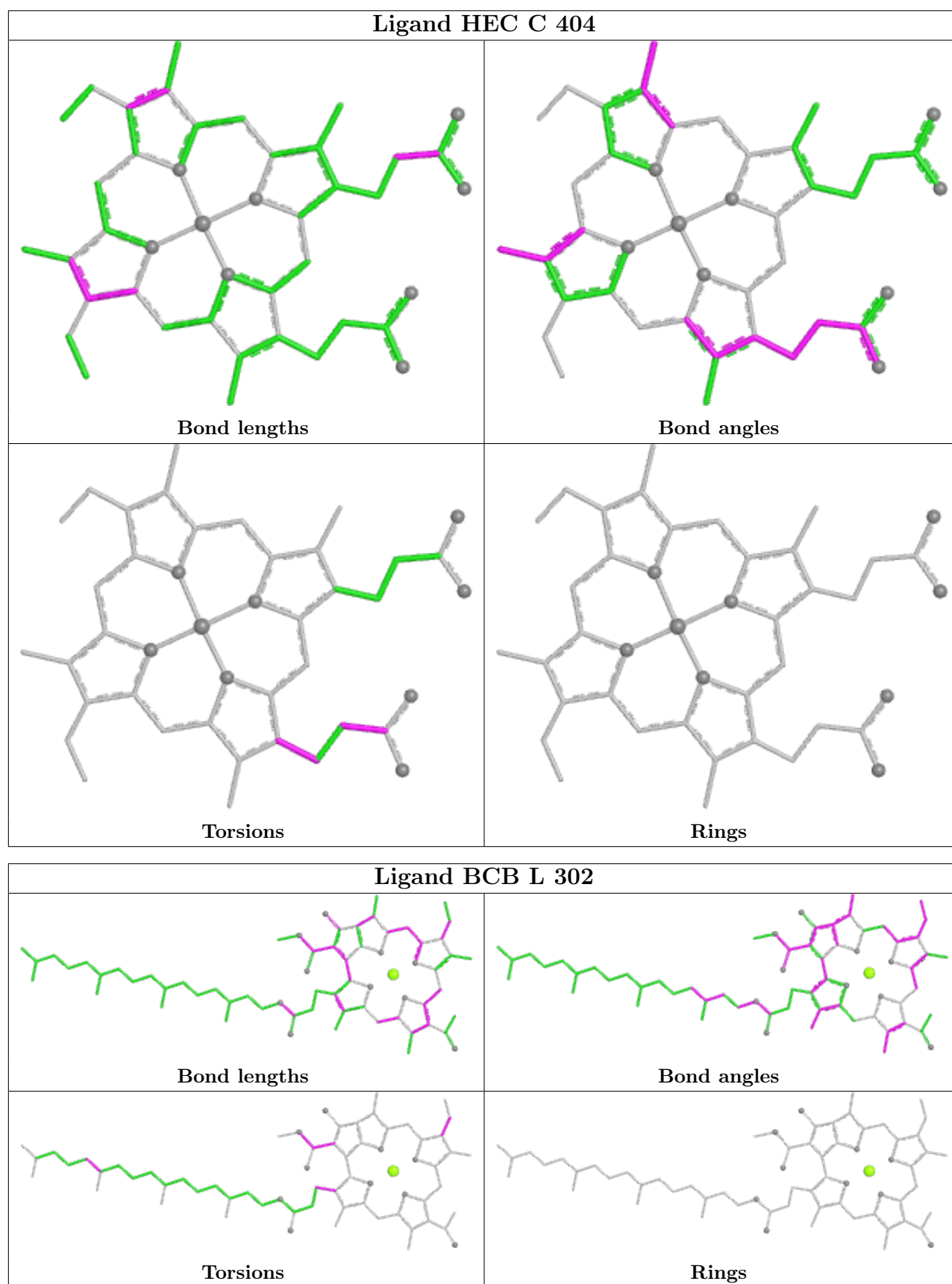
Mol	Chain	Res	Type	Atoms
5	C	401	HEC	C2A-CAA-CBA-CGA
5	C	404	HEC	C2D-C3D-CAD-CBD
5	C	404	HEC	C4D-C3D-CAD-CBD
6	C	405	DGA	OG1-CG1-CG2-OG2
6	C	405	DGA	OG1-CG1-CG2-CG3

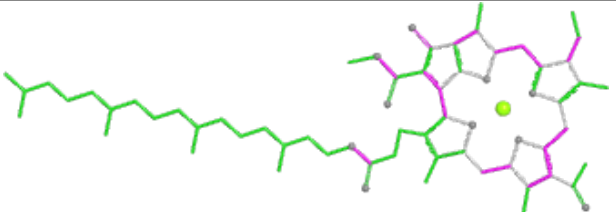
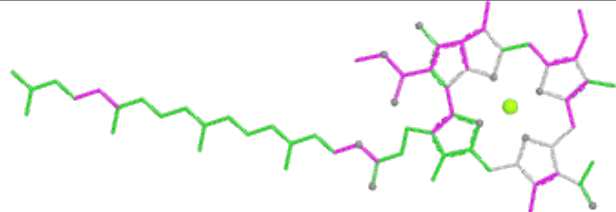
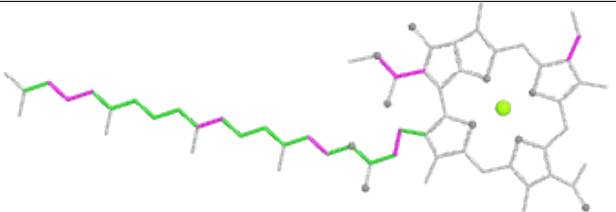
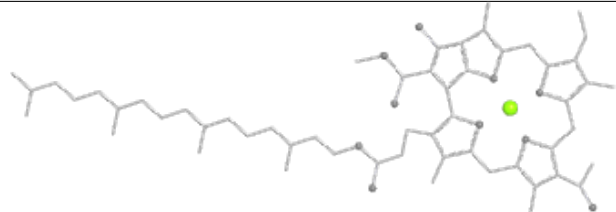
There are no ring outliers.

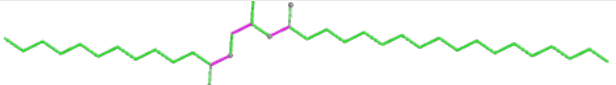
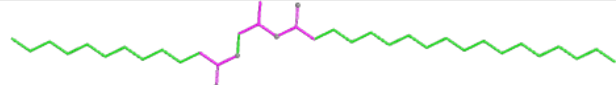
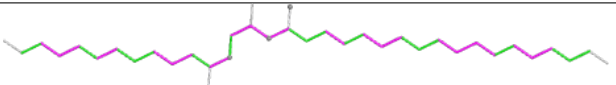
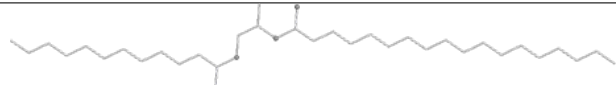
14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	404	HEC	3	0
10	L	302	BCB	5	0
10	M	404	BCB	1	0
5	C	401	HEC	3	0
5	C	402	HEC	2	0
14	M	406	NS5	4	0
7	M	408	SO4	2	0
11	M	405	BPB	2	0
11	L	303	BPB	2	0
10	M	403	BCB	3	0
10	L	301	BCB	2	0
7	C	406	SO4	1	0
13	M	402	MQ7	1	0
5	C	403	HEC	1	0

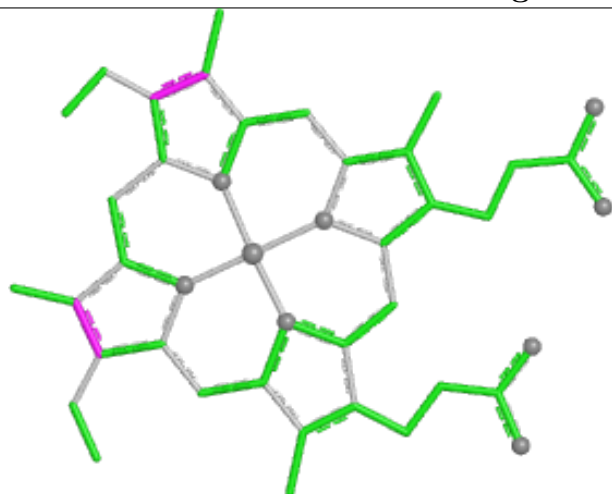
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



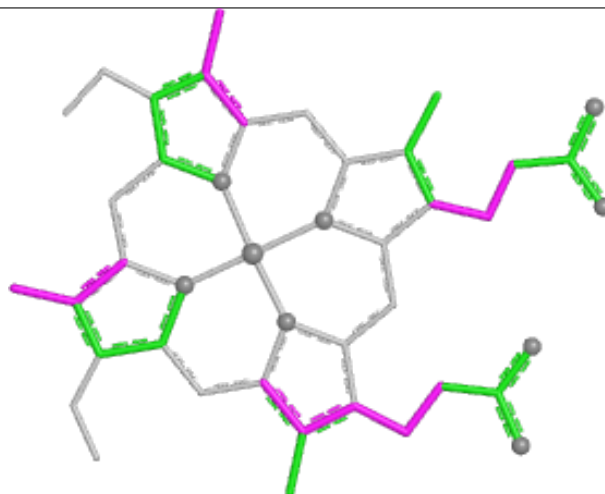
Ligand BCB M 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGA C 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

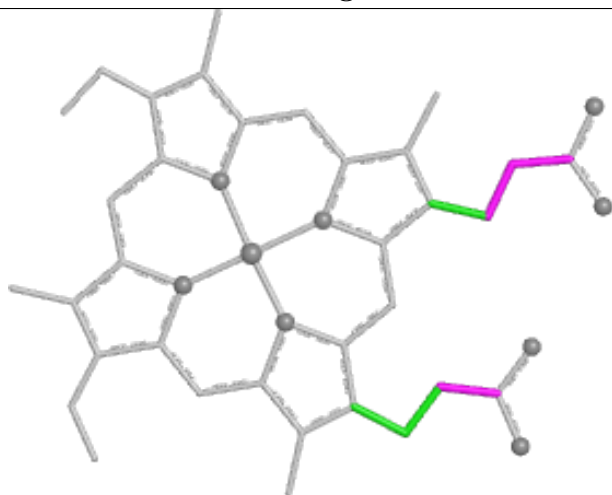
## Ligand HEC C 401



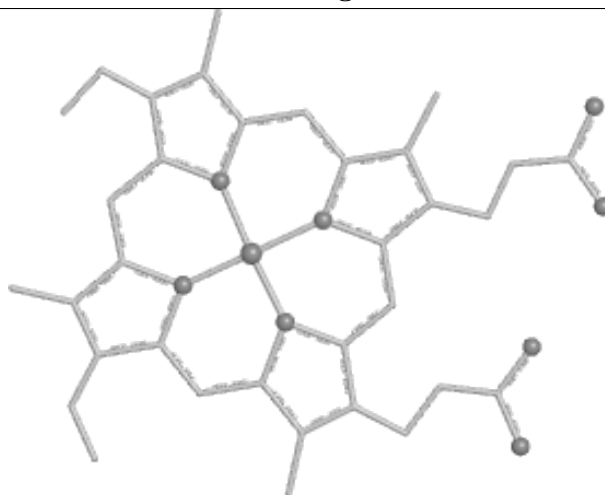
Bond lengths



Bond angles

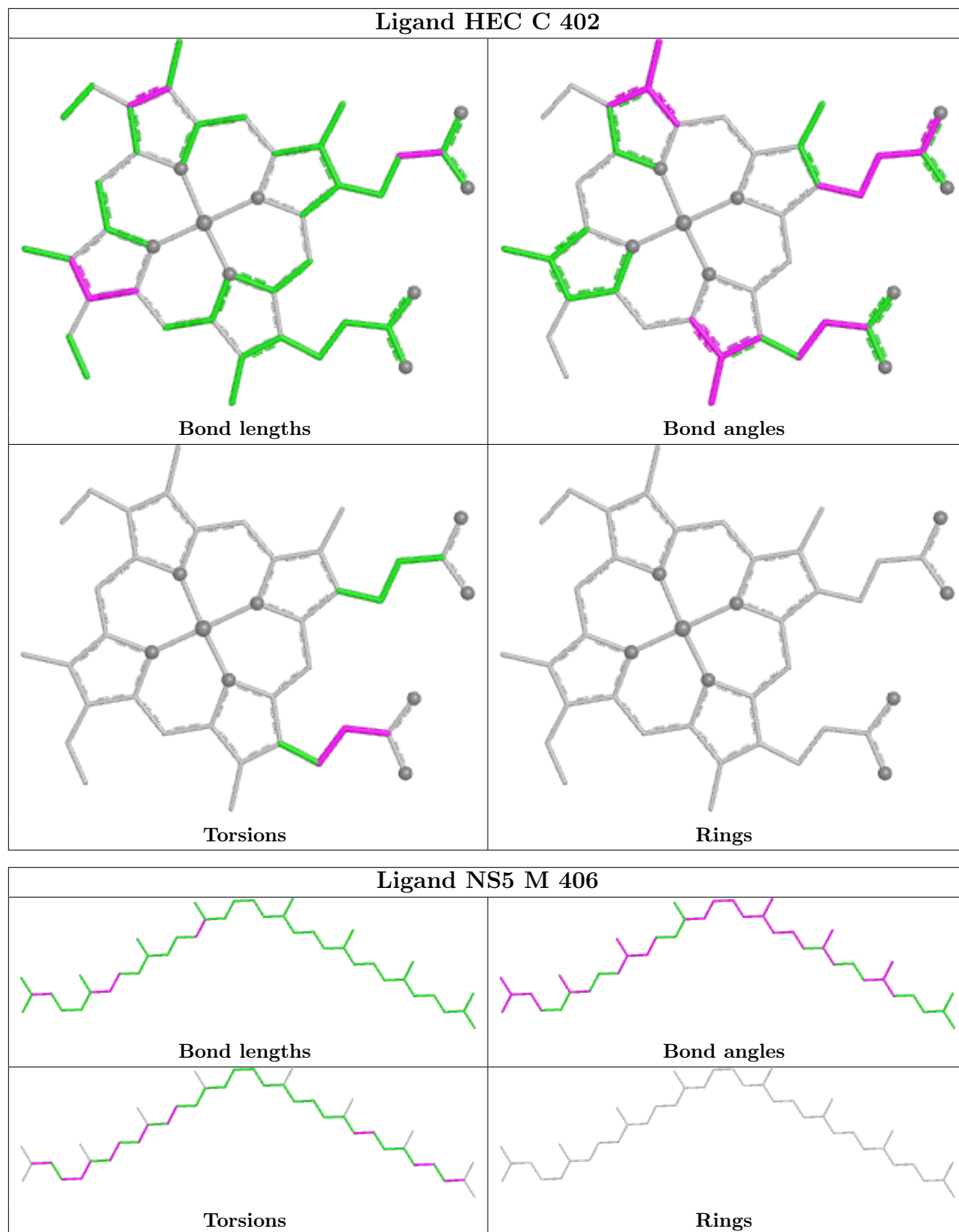


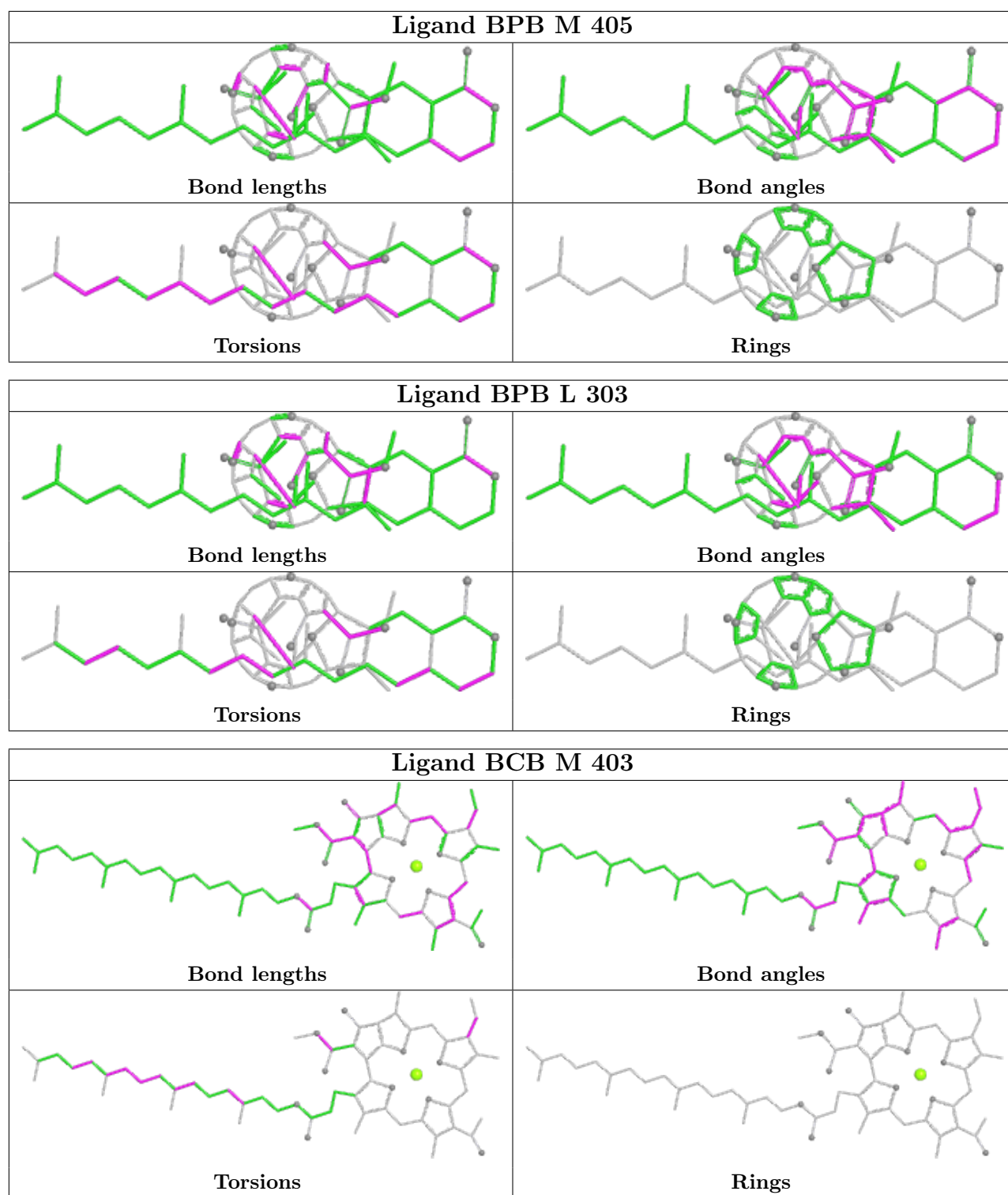
Torsions

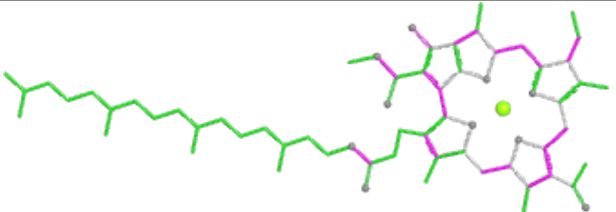
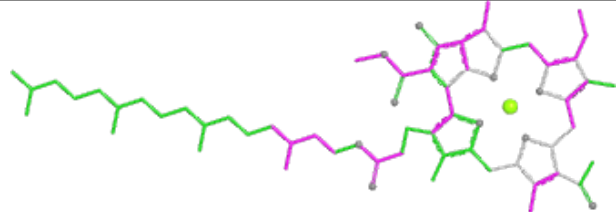
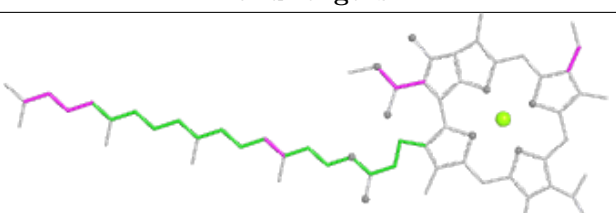
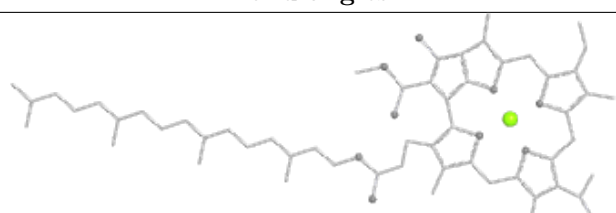


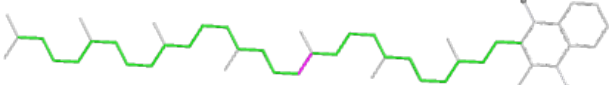
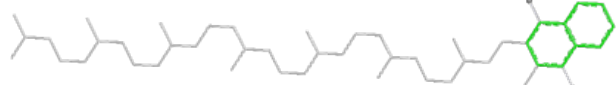


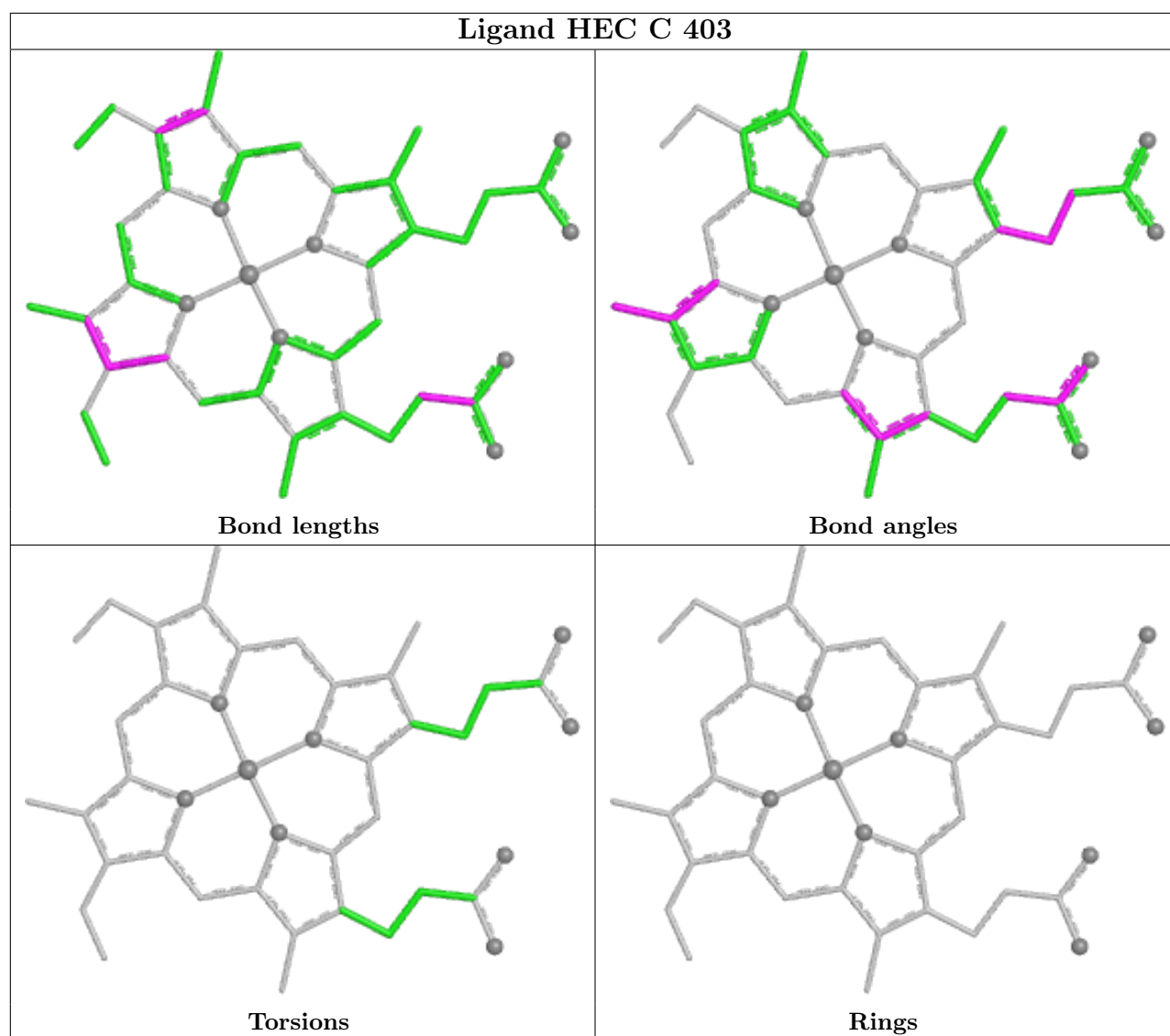
Rings







Ligand BCB L 301	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand MQ7 M 402	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



## 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

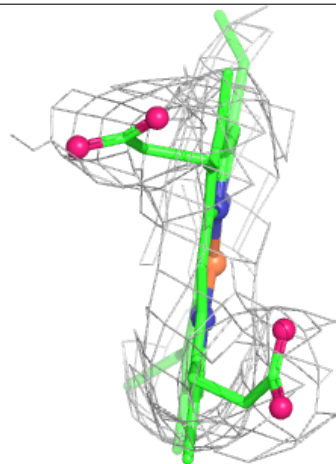
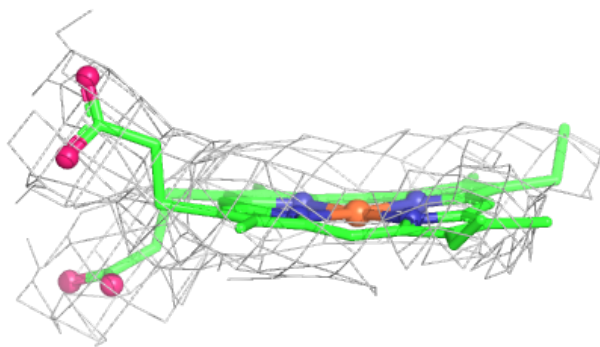
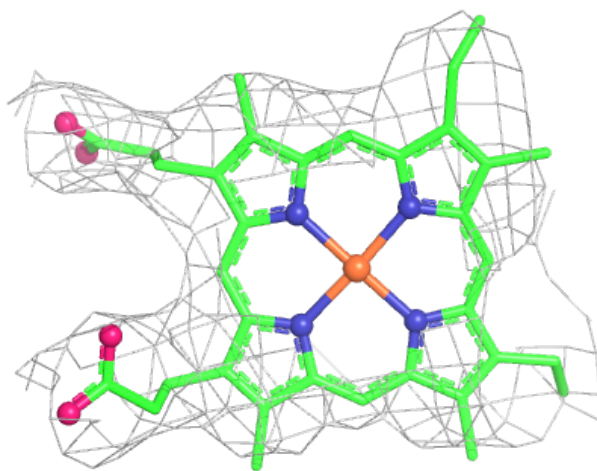
### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

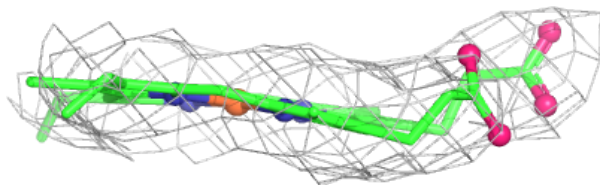
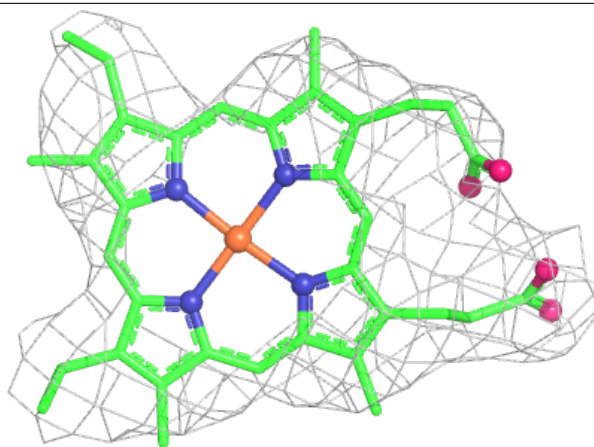
**Electron density around HEC C 401:**

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



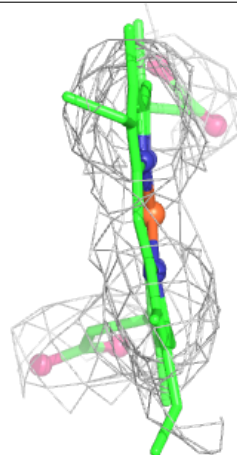
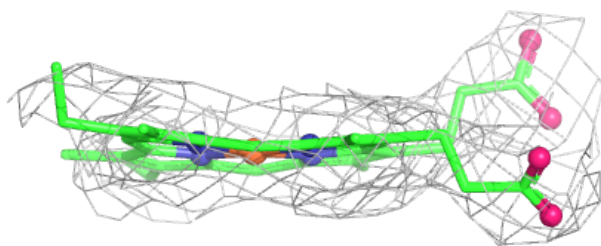
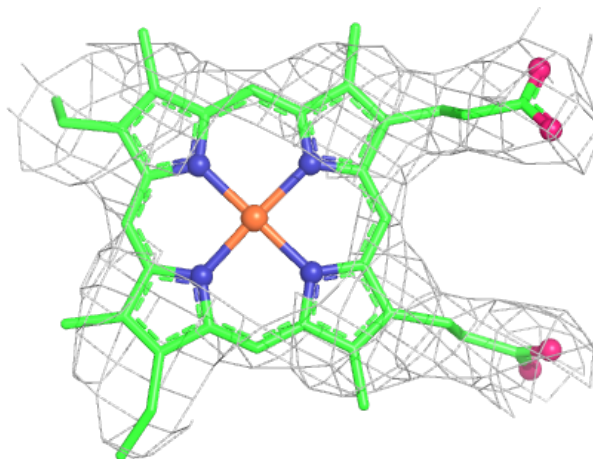
**Electron density around HEC C 402:**

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



**Electron density around HEC C 403:**

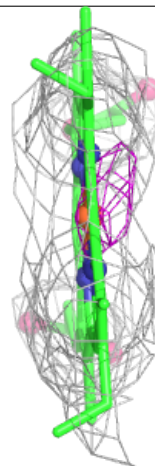
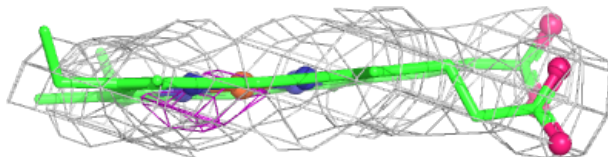
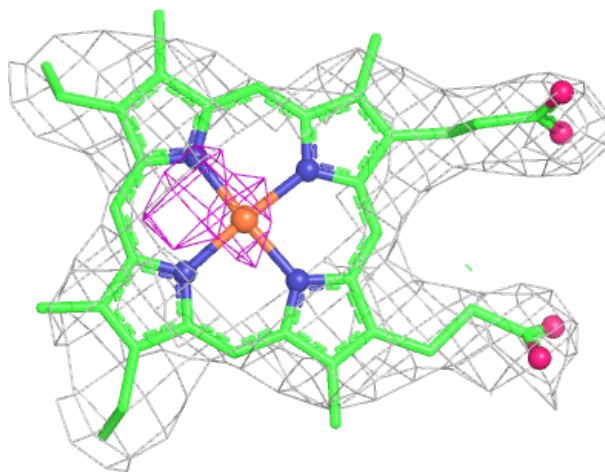
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





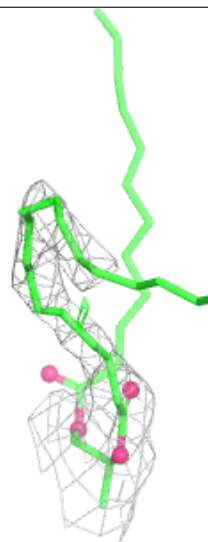
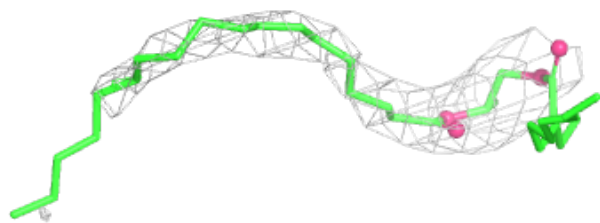
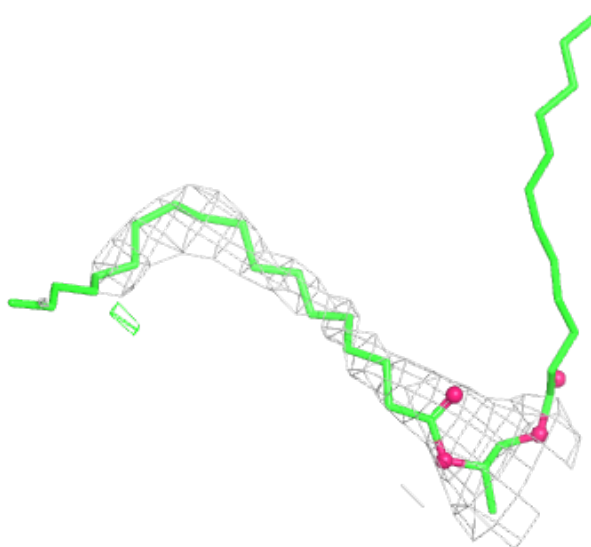
**Electron density around HEC C 404:**

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



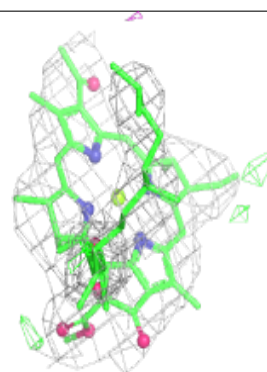
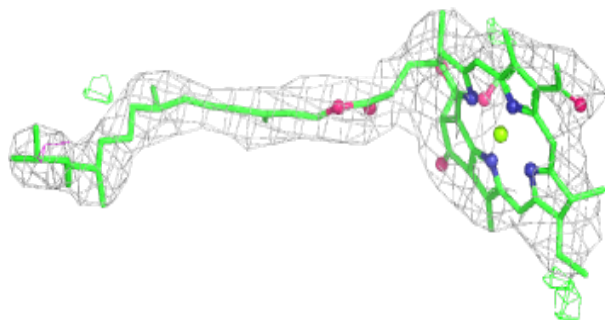
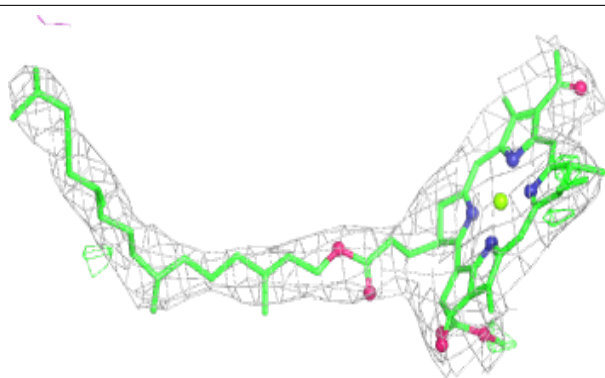
**Electron density around DGA C 405:**

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

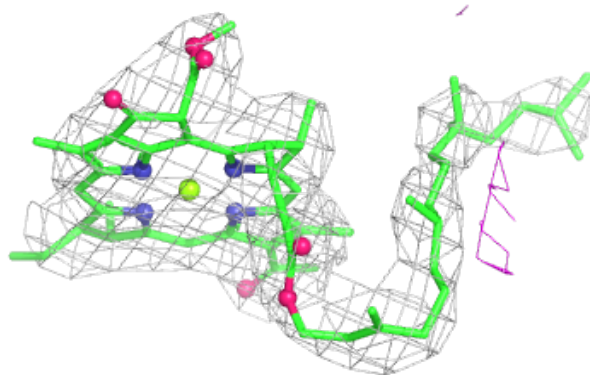
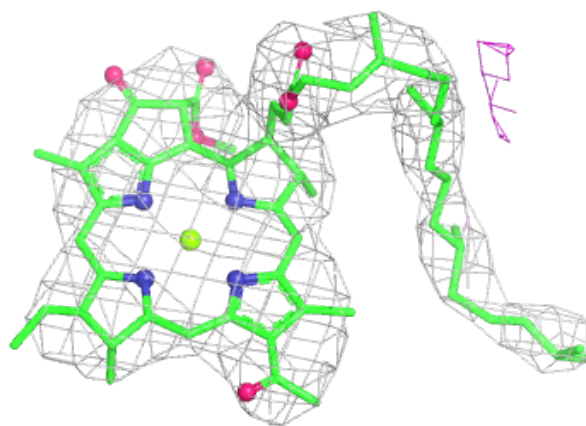


**Electron density around BCB L 301:**

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

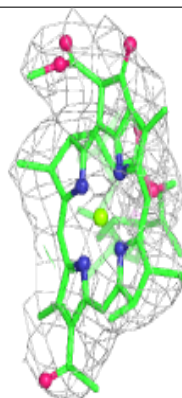
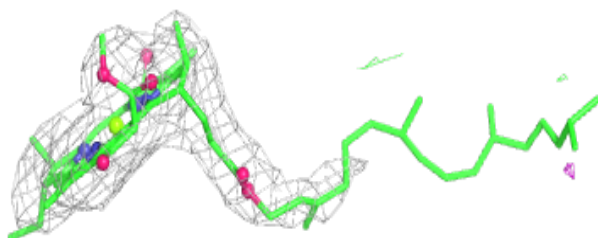
**Electron density around BCB L 302:**

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

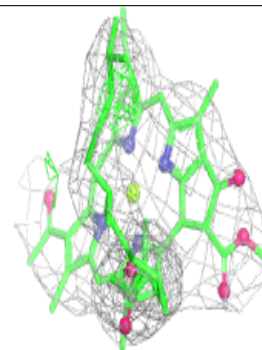
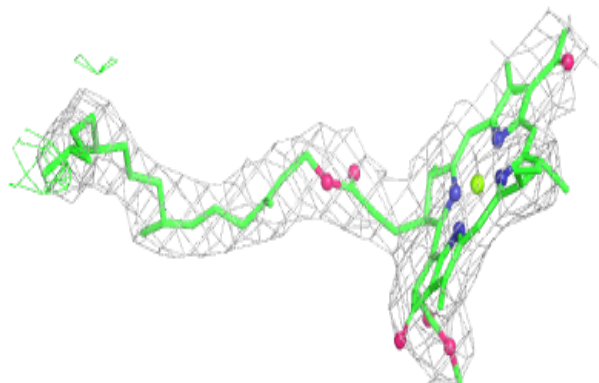
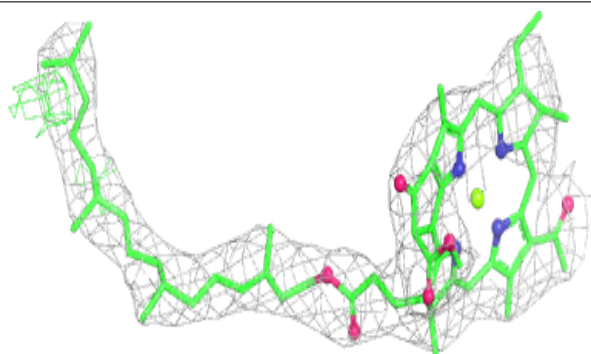


**Electron density around BCB M 403:**

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

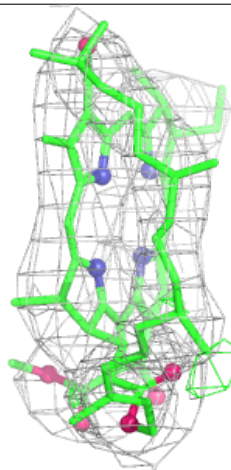
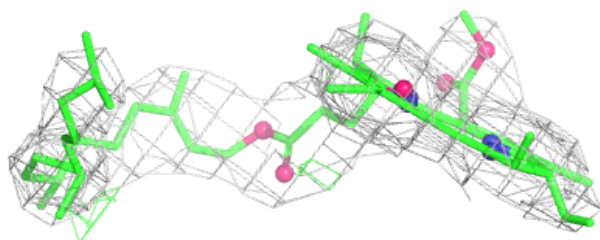
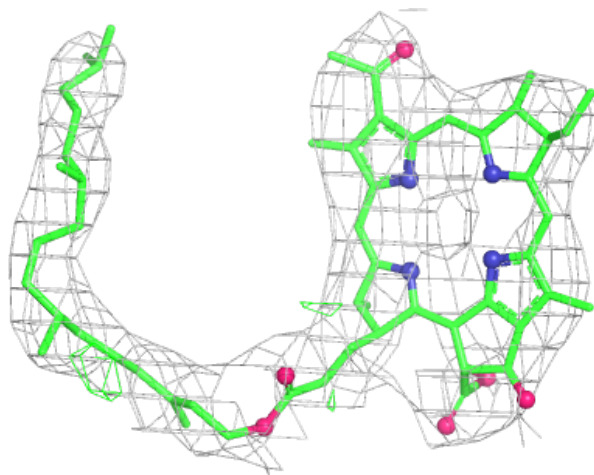
**Electron density around BCB M 404:**

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



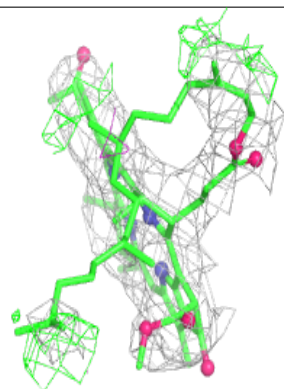
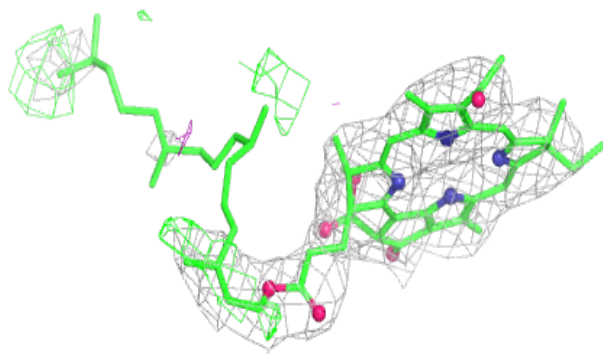
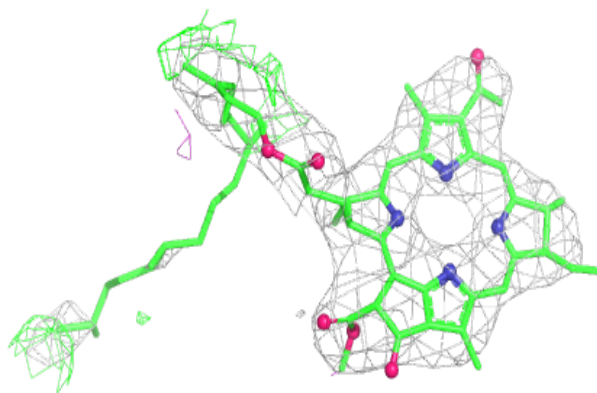
**Electron density around BPB L 303:**

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

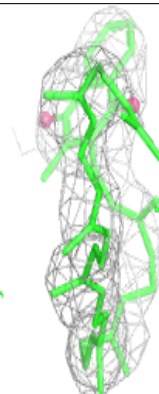
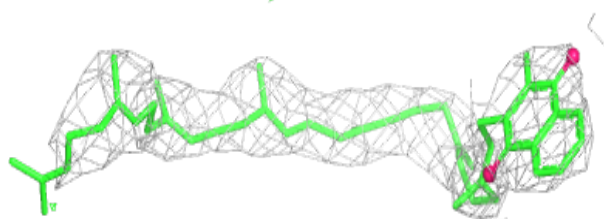
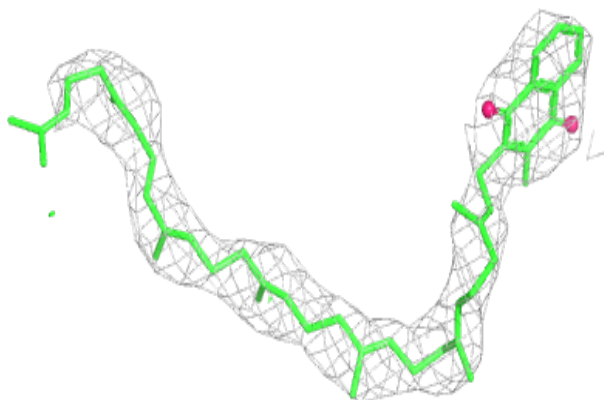


**Electron density around BPB M 405:**

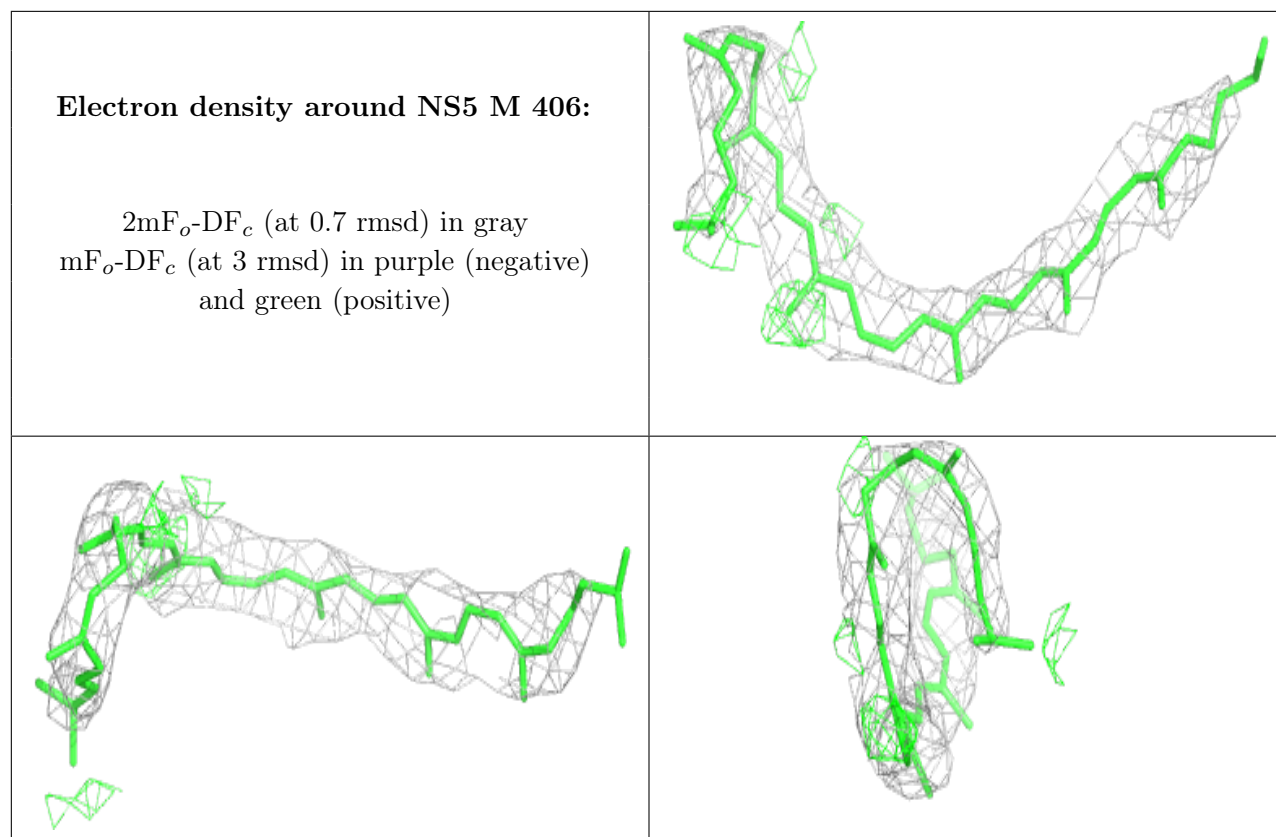
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around MQ7 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)







## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.