wwPDB X-ray Structure Validation Summary Report (i)

Jan 20, 2024 – 02:48 pm 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

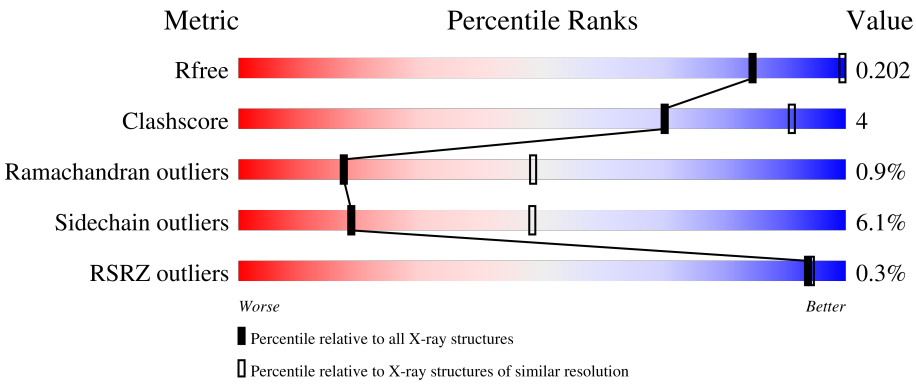
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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)
RSRZ outliers	127900	1115 (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 >=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 <=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	87% 11% ••
2	H	257	% 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
11	BCB	L	301	X	-	-	-
11	BCB	L	302	X	-	-	-
11	BCB	M	402	X	-	-	-
11	BCB	M	403	X	-	-	-
6	DGA	C	405	-	-	-	X
7	SO4	H	305	-	-	-	X
7	SO4	M	407	-	-	X	-

2 Entry composition (i)

There are 16 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
			Total	C	N	O	S			
1	C	332	2602	1640	466	478	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	249	1952	1247	334	370	1	0	0	0

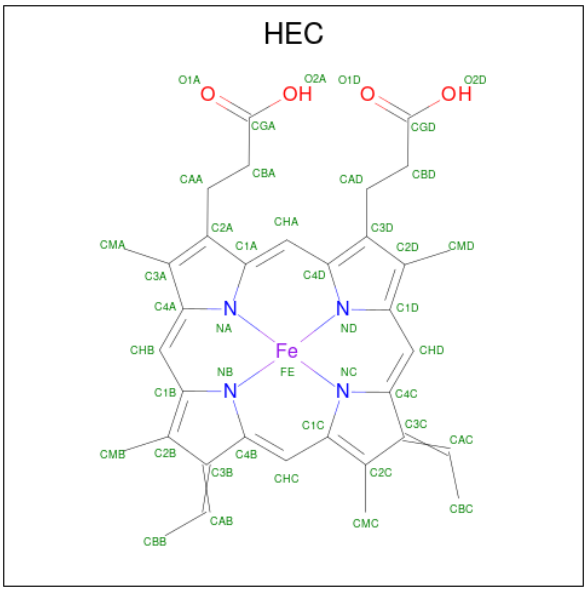
- Molecule 3 is a protein called Reaction center protein L chain.

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

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

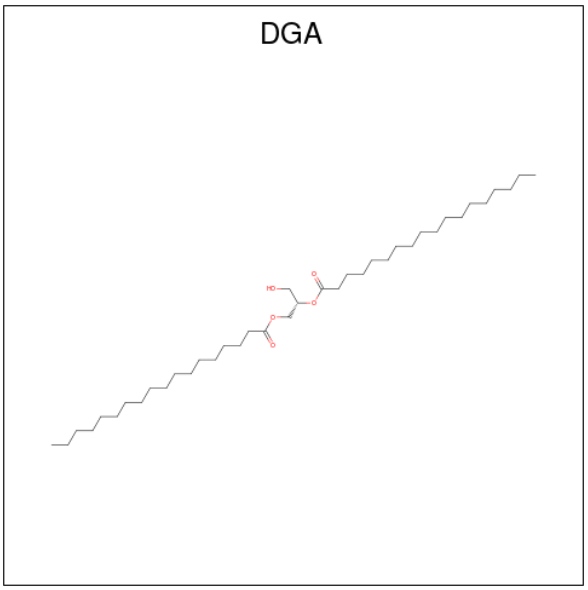
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	323	2555	1702	419	423	11	0	0	0

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



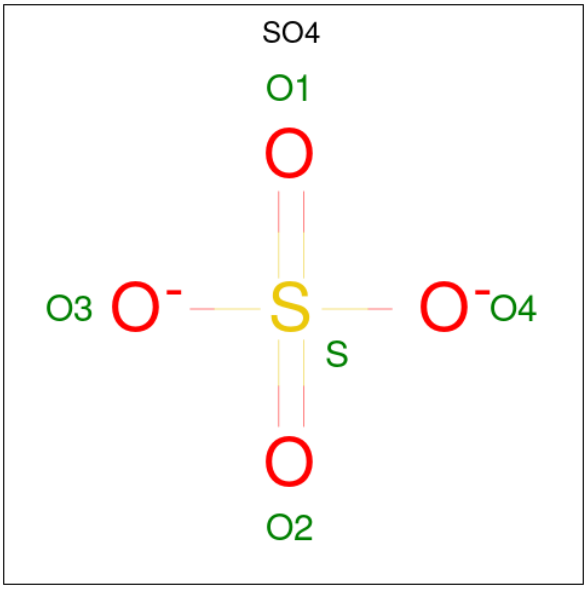
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0

- Molecule 6 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



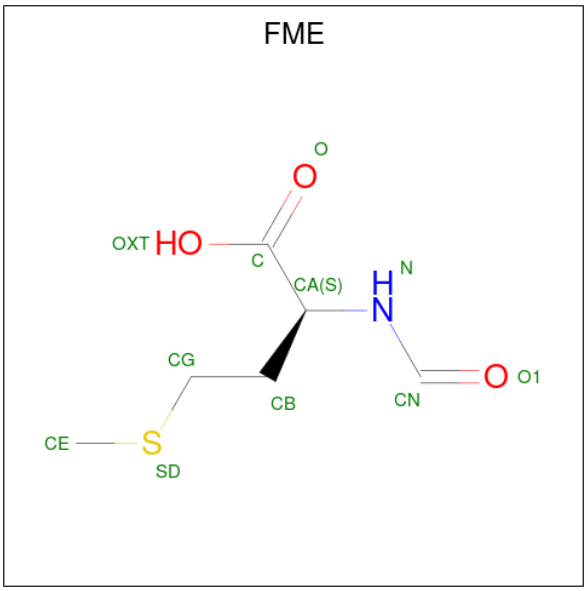
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	C	1	37	33	4	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



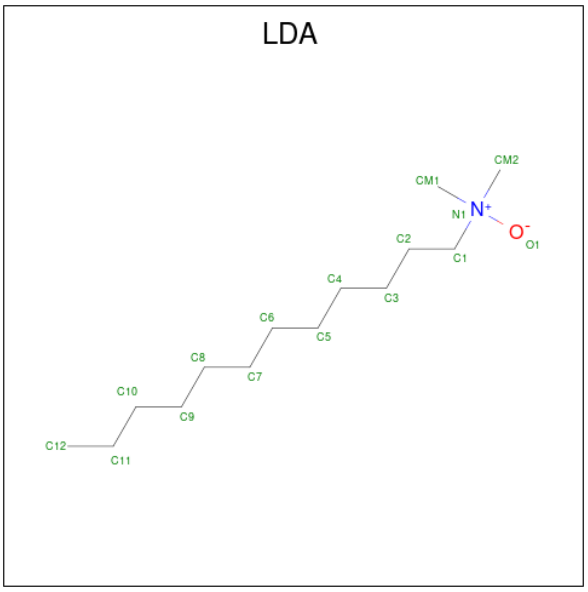
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
7	C	1	5	4	1	0	0
			Total	O	S		
7	H	1	5	4	1	0	0
			Total	O	S		
7	H	1	5	4	1	0	0
			Total	O	S		
7	H	1	5	4	1	0	0
			Total	O	S		
7	M	1	5	4	1	0	0
			Total	O	S		
7	M	1	5	4	1	0	0
			Total	O	S		
7	M	1	5	4	1	0	0
			Total	O	S		
7	M	1	5	4	1	0	0
			Total	O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

- Molecule 8 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
8	H	1	10	6	1	2	1	0	0

- Molecule 9 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



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

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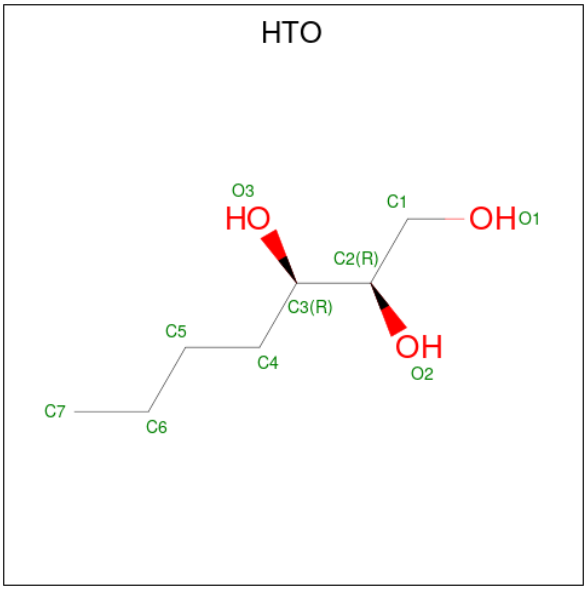
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
9	H	1	16	14	1	1	0	0
			Total	C	N	O		
9	M	1	16	14	1	1	0	0

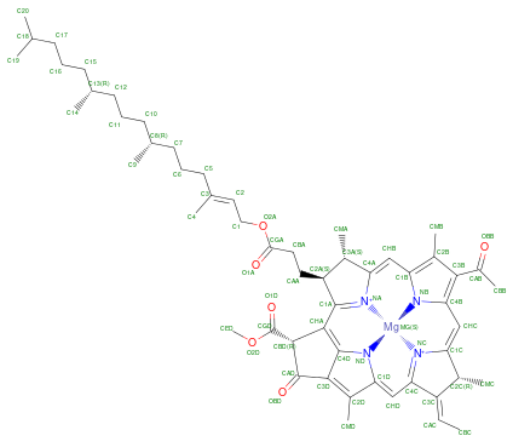
- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



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

- Molecule 11 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).

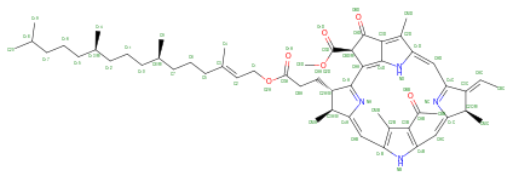
BCB



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

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

BPB

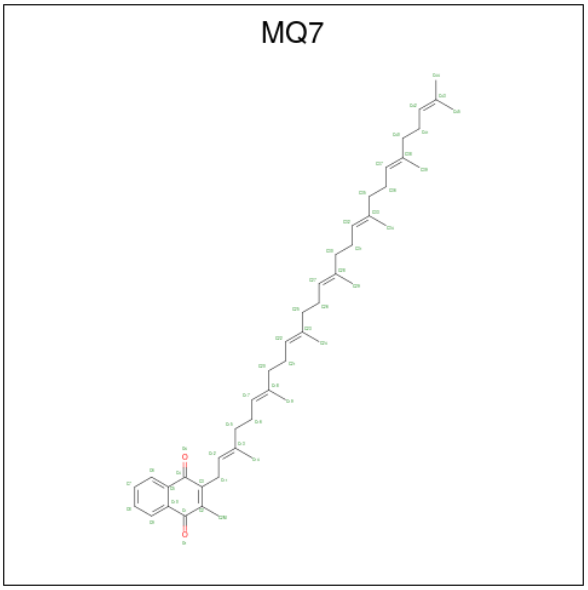


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
12	L	1	65	55	4	6	0	0
12	M	1	65	55	4	6	0	0

- Molecule 13 is FE (II) ION (three-letter code: FE2) (formula: Fe).

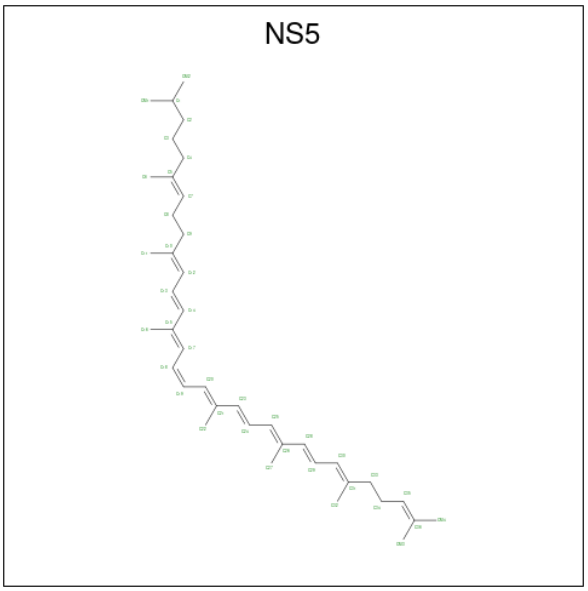
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
13	L	1	1	1	0	0

- Molecule 14 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



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

- Molecule 15 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).



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

- Molecule 16 is water.

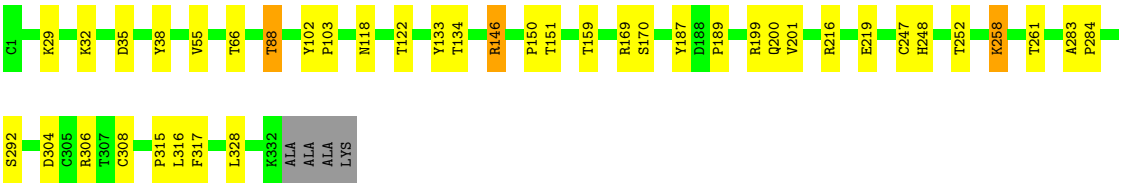
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
16	C	7	7	7	0	0
			Total	O		
16	H	3	3	3	0	0
			Total	O		
16	L	13	13	13	0	0
			Total	O		
16	M	7	7	7	0	0

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.

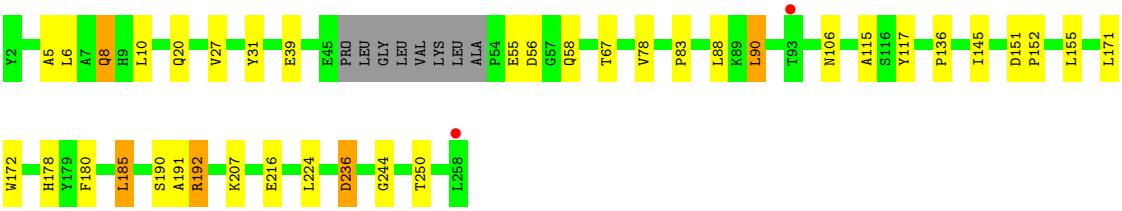
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain C:



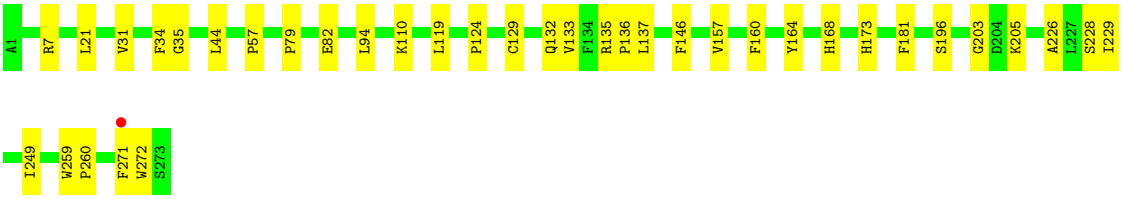
• Molecule 2: Reaction center protein H chain

Chain H:



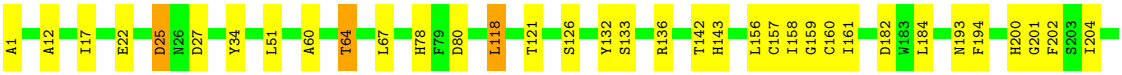
• Molecule 3: Reaction center protein L chain

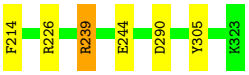
Chain L:



• Molecule 4: Reaction center protein M chain

Chain M:




F214
R226
R239
E244
D290
Y305
K323

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	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^2)	123.8	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 82.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	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^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: FE2, HTO, FME, BPB, LDA, DGA, NS5, MQ7, SO4, HEC, BCB

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(^{o})	Ideal(^{o})
2	H	185	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	1952	0	1939	12	0

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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	10	0	10	0	0
9	H	48	0	93	0	0
9	M	16	0	31	0	0
10	H	10	0	16	0	0
10	L	20	0	32	0	0
11	L	132	0	144	7	0
11	M	132	0	144	4	0
12	L	65	0	74	2	0
12	M	65	0	74	2	0
13	L	1	0	0	0	0
14	M	48	0	64	1	0
15	M	40	0	60	4	0
16	C	7	0	0	0	0
16	H	3	0	0	0	0
16	L	13	0	0	0	0
16	M	7	0	0	0	0
All	All	10157	0	9986	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	14:M:401:MQ7:H401	1.72	0.72
12:L:303:BPB:HBBB	12:L:303:BPB:HMB	1.77	0.67
4:M:159:GLY:HA3	15:M:405: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 (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%)	310 (94%)	18 (6%)	2 (1%)	25	57
2	H	245/257 (95%)	222 (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	1168/1189 (98%)	1081 (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	83	PRO
3	L	203	GLY

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	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	216	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	102	GLN
2	H	106	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 1 is monoatomic - leaving 31 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
14	MQ7	M	401	-	49,49,49	1.48	3 (6%)	60,63,63	1.22	6 (10%)
10	HTO	L	305	-	9,9,9	0.72	0	10,10,10	0.67	0
7	SO4	M	411	-	4,4,4	0.45	0	6,6,6	0.38	0
11	BCB	M	403	-	63,74,74	1.85	14 (22%)	74,115,115	2.79	26 (35%)
5	HEC	C	401	1	32,50,50	1.66	2 (6%)	24,82,82	1.93	5 (20%)
12	BPB	L	303	-	49,70,70	2.12	10 (20%)	47,101,101	1.84	9 (19%)
12	BPB	M	404	-	49,70,70	2.27	10 (20%)	47,101,101	2.18	10 (21%)
7	SO4	M	409	-	4,4,4	0.37	0	6,6,6	0.27	0
7	SO4	H	304	-	4,4,4	0.40	0	6,6,6	0.35	0
8	FME	H	301	2	8,9,10	0.93	0	7,9,11	3.58	4 (57%)
9	LDA	H	306	-	12,15,15	2.13	1 (8%)	14,17,17	0.84	1 (7%)
11	BCB	L	302	-	63,74,74	1.82	13 (20%)	74,115,115	2.61	22 (29%)
7	SO4	C	406	-	4,4,4	0.44	0	6,6,6	0.46	0
5	HEC	C	403	1	32,50,50	1.75	4 (12%)	24,82,82	1.56	4 (16%)
10	HTO	L	304	-	9,9,9	1.23	2 (22%)	10,10,10	1.40	2 (20%)
10	HTO	H	308	-	9,9,9	0.83	0	10,10,10	1.26	2 (20%)
7	SO4	H	303	-	4,4,4	0.49	0	6,6,6	0.50	0
7	SO4	M	406	-	4,4,4	0.36	0	6,6,6	0.58	0
9	LDA	H	307	-	12,15,15	1.94	1 (8%)	14,17,17	0.50	0
5	HEC	C	404	1	32,50,50	1.59	4 (12%)	24,82,82	1.55	5 (20%)
9	LDA	H	302	-	12,15,15	2.09	1 (8%)	14,17,17	0.55	0
11	BCB	L	301	-	63,74,74	1.92	15 (23%)	74,115,115	2.77	28 (37%)
6	DGA	C	405	1	36,36,43	1.46	3 (8%)	38,38,45	1.71	6 (15%)
11	BCB	M	402	-	63,74,74	1.87	15 (23%)	74,115,115	2.61	19 (25%)
9	LDA	M	412	-	12,15,15	2.10	1 (8%)	14,17,17	0.40	0
7	SO4	M	407	-	4,4,4	0.41	0	6,6,6	0.28	0
7	SO4	M	408	-	4,4,4	0.32	0	6,6,6	0.74	0
7	SO4	H	305	-	4,4,4	0.33	0	6,6,6	0.19	0
15	NS5	M	405	-	39,39,39	1.65	4 (10%)	44,46,46	2.39	16 (36%)
7	SO4	M	410	-	4,4,4	0.39	0	6,6,6	0.32	0
5	HEC	C	402	1	32,50,50	1.59	4 (12%)	24,82,82	1.83	7 (29%)

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
14	MQ7	M	401	-	-	2/41/61/61	0/2/2/2
10	HTO	L	305	-	-	3/10/10/10	-
11	BCB	M	403	-	3/3/21/26	11/37/137/137	-
5	HEC	C	401	1	-	4/10/54/54	-
12	BPB	L	303	-	-	10/37/105/105	0/5/6/6
12	BPB	M	404	-	-	16/37/105/105	0/5/6/6
8	FME	H	301	2	-	3/7/9/11	-
9	LDA	H	306	-	-	7/13/13/13	-
11	BCB	L	302	-	3/3/21/26	11/37/137/137	-
5	HEC	C	403	1	-	0/10/54/54	-
10	HTO	L	304	-	-	2/10/10/10	-
10	HTO	H	308	-	-	4/10/10/10	-
9	LDA	H	307	-	-	4/13/13/13	-
5	HEC	C	404	1	-	4/10/54/54	-
9	LDA	H	302	-	-	4/13/13/13	-
11	BCB	L	301	-	3/3/21/26	9/37/137/137	-
6	DGA	C	405	1	-	21/37/37/45	-
9	LDA	M	412	-	-	5/13/13/13	-
15	NS5	M	405	-	-	13/43/43/43	-
11	BCB	M	402	-	3/3/21/26	13/37/137/137	-
5	HEC	C	402	1	-	3/10/54/54	-

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	M	401	MQ7	C3-C2	8.00	1.49	1.35
15	M	405	NS5	C35-C36	7.74	1.54	1.32
12	M	404	BPB	CAC-C3C	7.74	1.53	1.33
12	L	303	BPB	CAC-C3C	7.69	1.53	1.33
9	H	306	LDA	O1-N1	-7.31	1.25	1.42

The worst 5 of 172 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	L	301	BCB	C1C-NC-C4C	-15.11	99.91	106.71
11	M	402	BCB	C1C-NC-C4C	-14.25	100.30	106.71
11	M	403	BCB	C1C-NC-C4C	-13.70	100.55	106.71
11	L	302	BCB	C1C-NC-C4C	-12.94	100.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	301	FME	CA-N-CN	-7.86	110.73	122.82

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	L	301	BCB	ND
11	L	301	BCB	NA
11	L	301	BCB	NC
11	L	302	BCB	ND
11	L	302	BCB	NA

5 of 149 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.

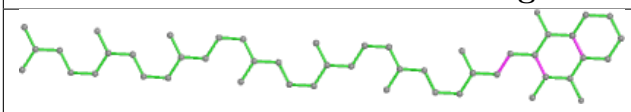
14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	M	401	MQ7	1	0
11	M	403	BCB	1	0
5	C	401	HEC	3	0
12	L	303	BPB	2	0
12	M	404	BPB	2	0
11	L	302	BCB	5	0
7	C	406	SO4	1	0
5	C	403	HEC	1	0
5	C	404	HEC	3	0
11	L	301	BCB	2	0
11	M	402	BCB	3	0
7	M	407	SO4	2	0
15	M	405	NS5	4	0
5	C	402	HEC	2	0

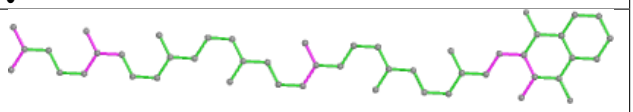
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

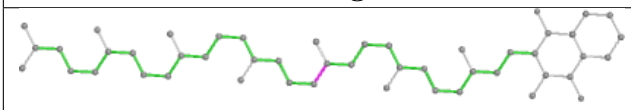
Ligand MQ7 M 401



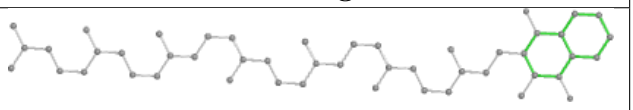
Bond lengths



Bond angles

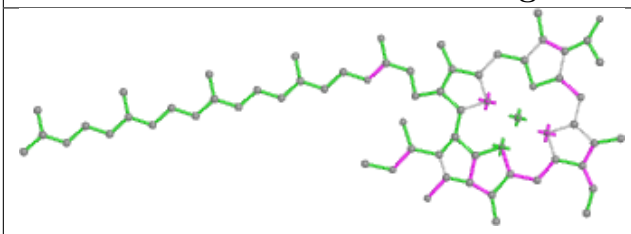


Torsions



Rings

Ligand BCB M 403



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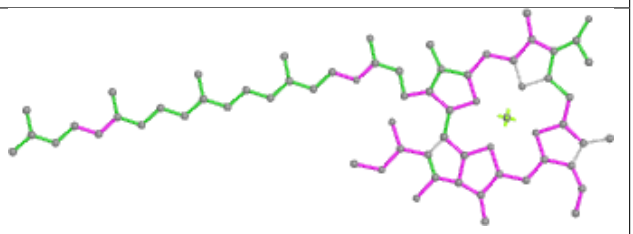

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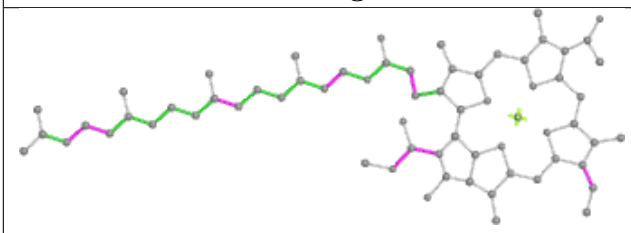

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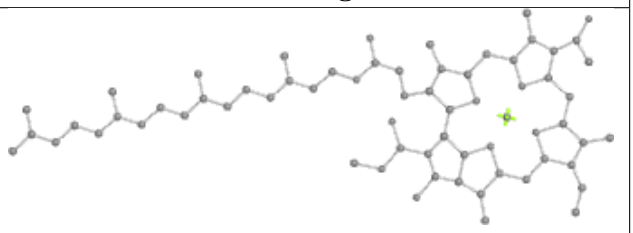
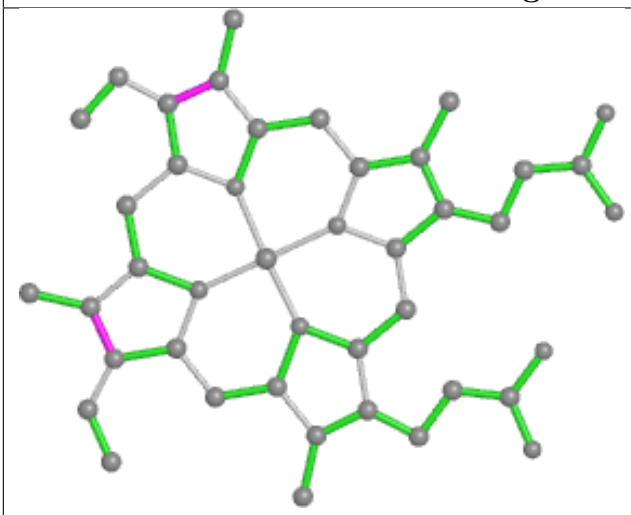


Rings

Ligand HEC C 401



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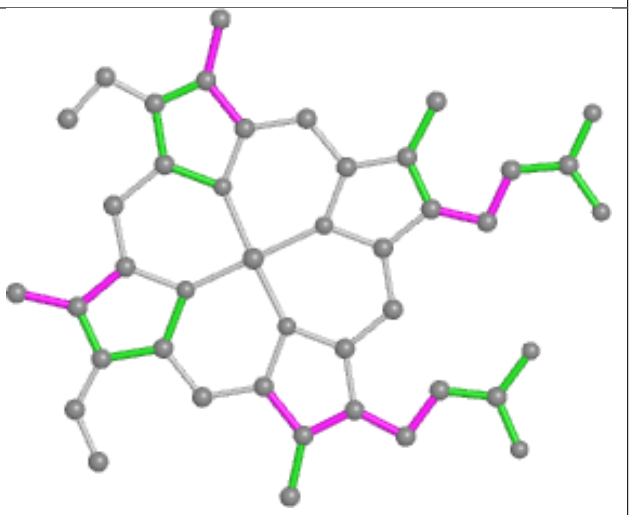
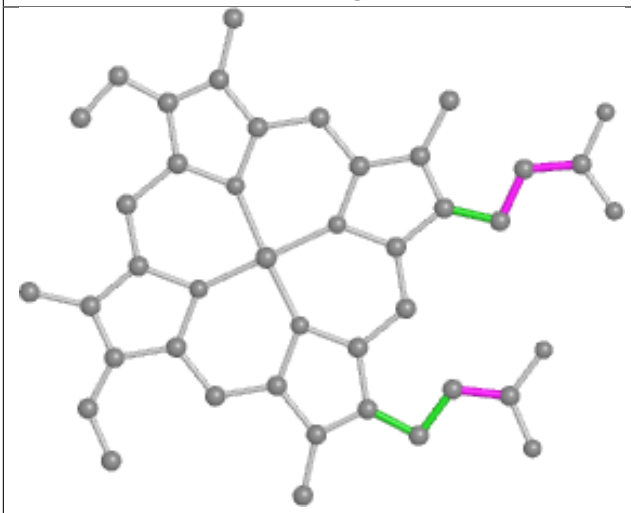


Bond angles



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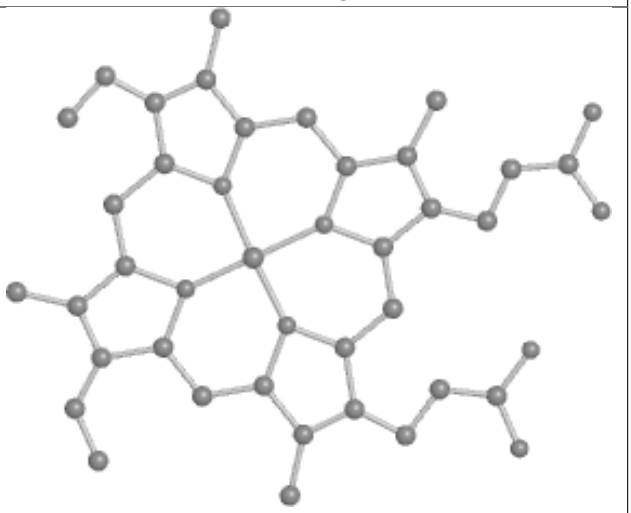
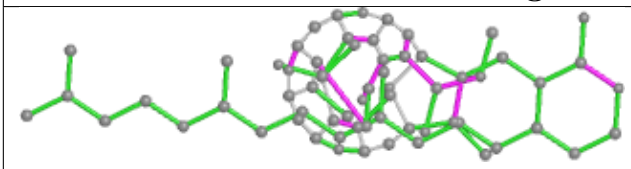


Rings

Ligand BPB L 303



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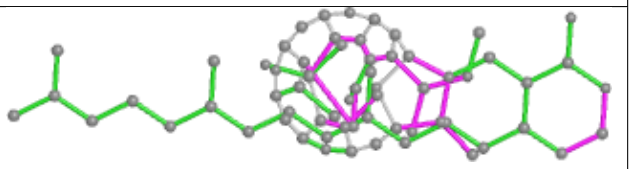

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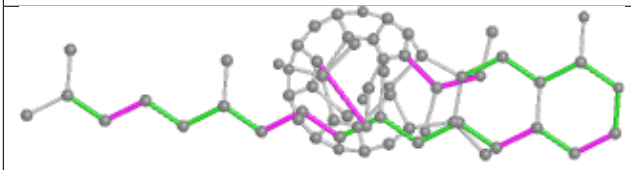
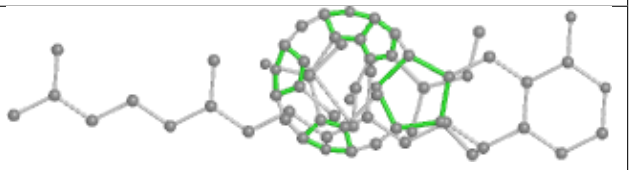
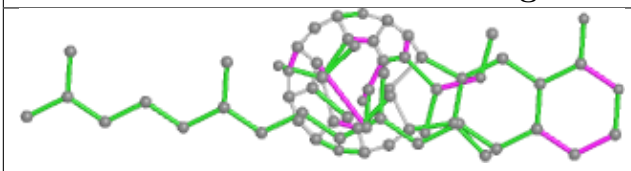
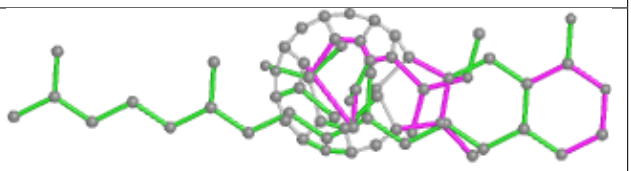
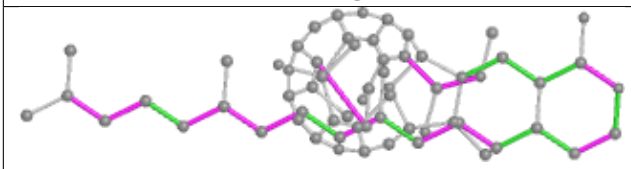
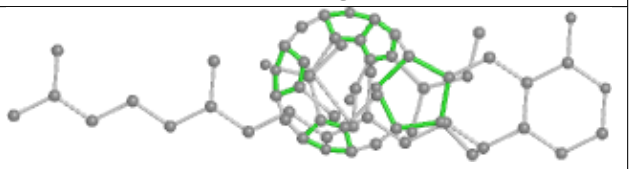


Torsions



Rings

Ligand BPB M 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

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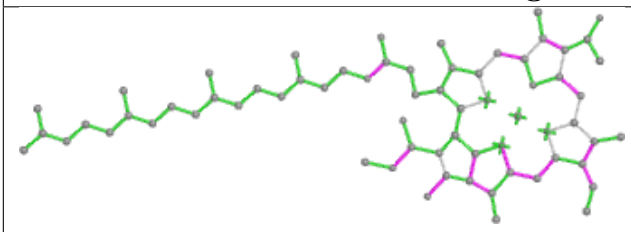
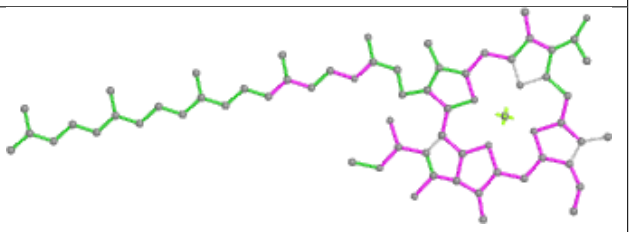
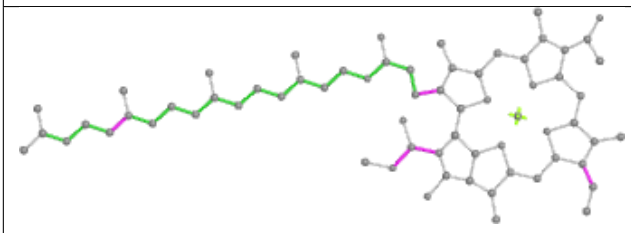
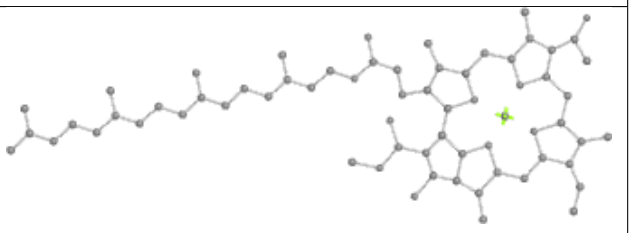
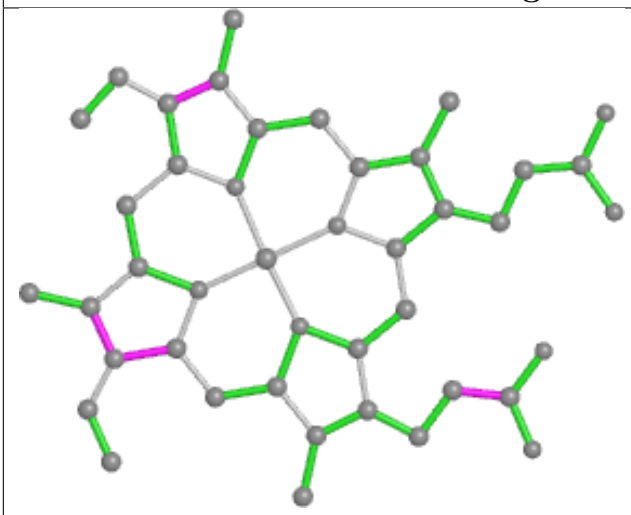
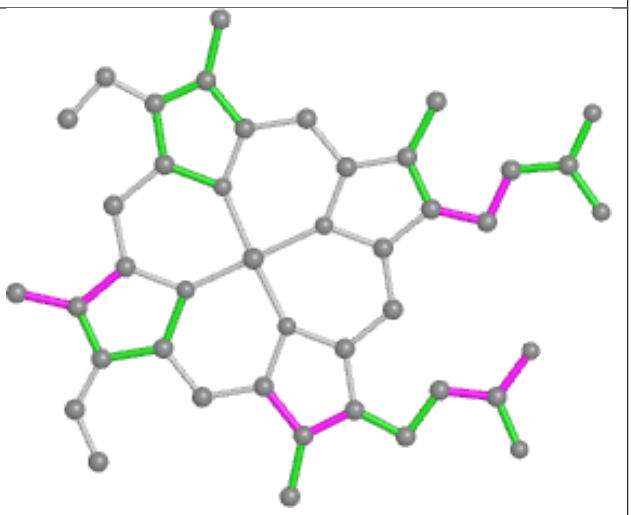
 Bond lengths	 Bond angles
 Torsions	 Rings

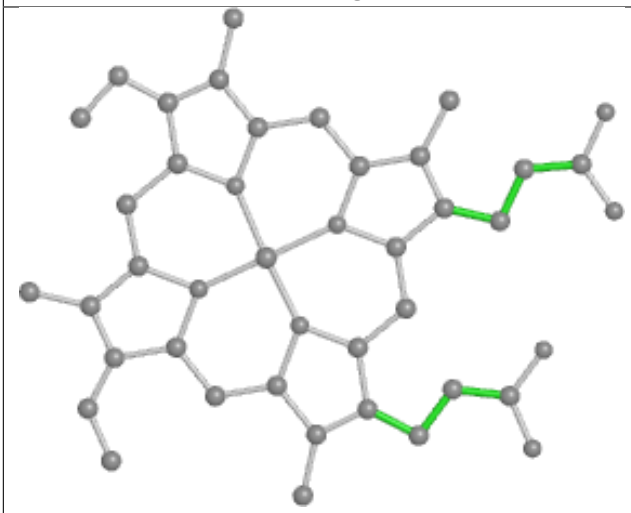
Ligand HEC C 403



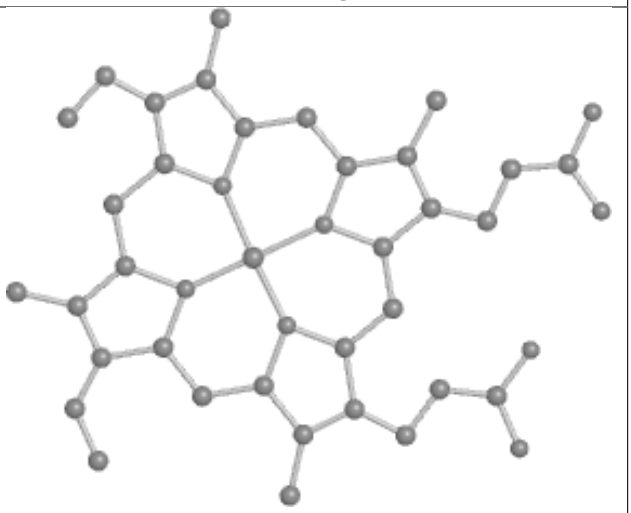
Bond lengths



Bond angles

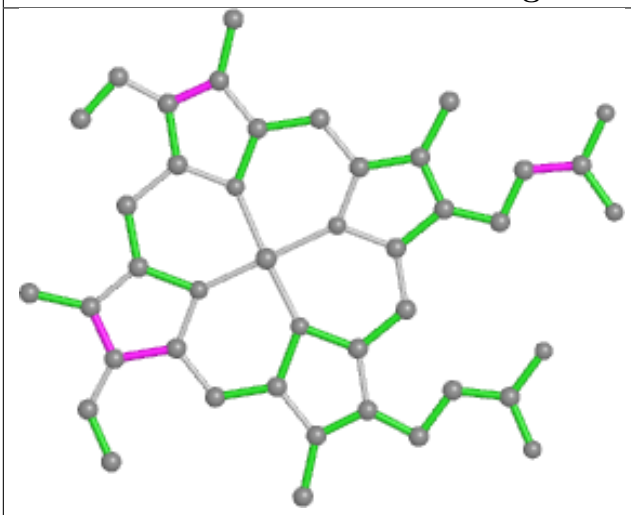


Torsions



Rings

Ligand HEC C 404



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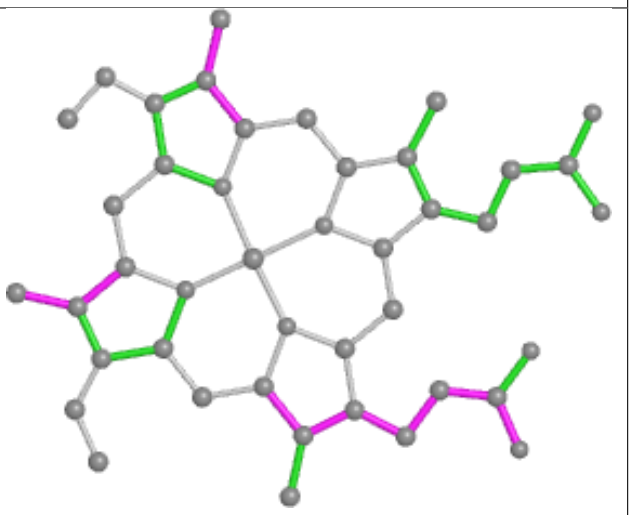
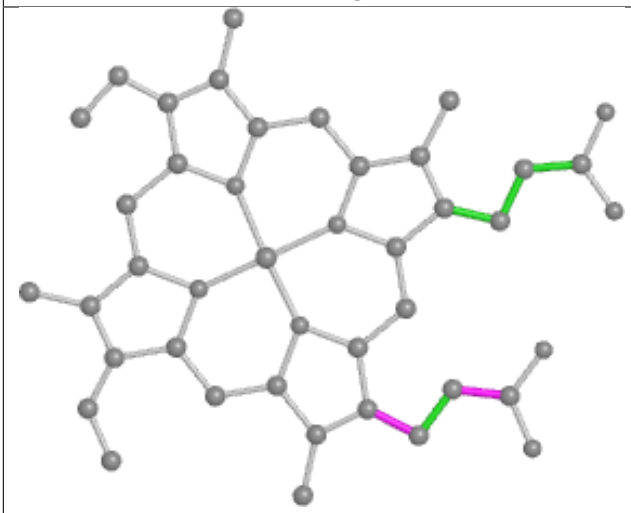
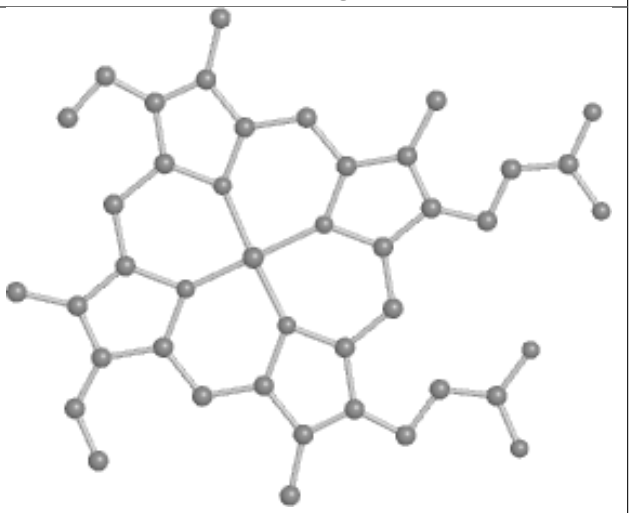


Bond angles

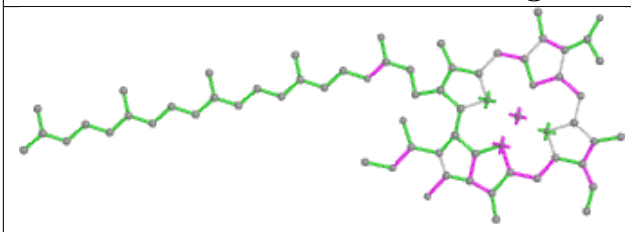


Torsions

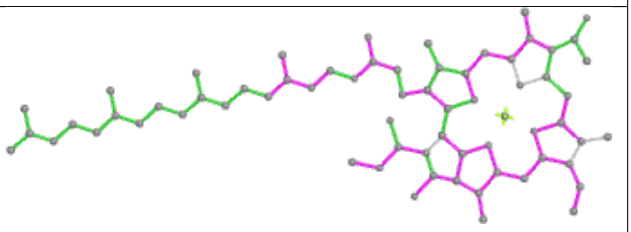


Rings

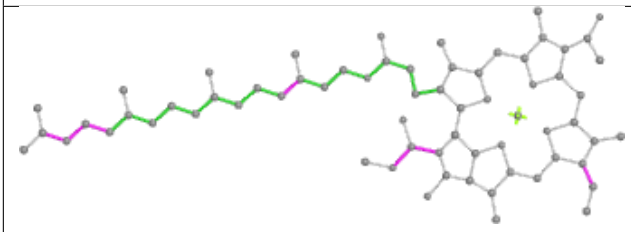
Ligand BCB L 301



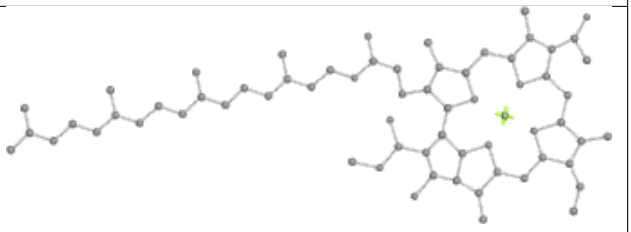
Bond lengths



Bond angles

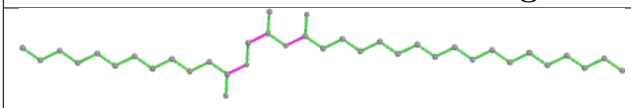


Torsions

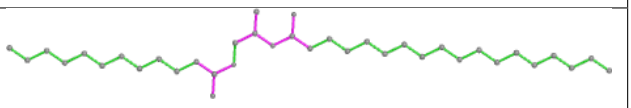


Rings

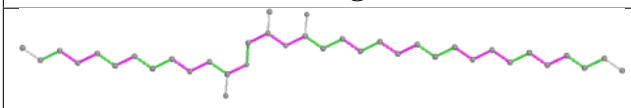
Ligand DGA C 405



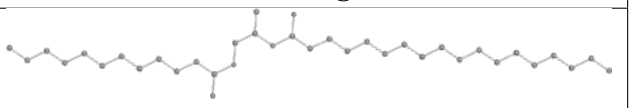
Bond lengths



Bond angles

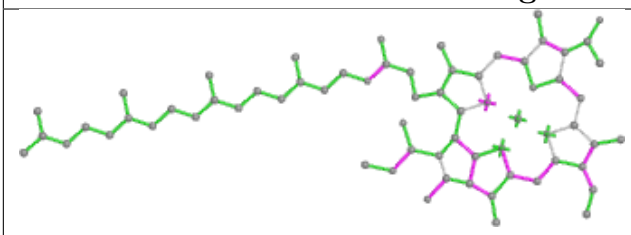


Torsions

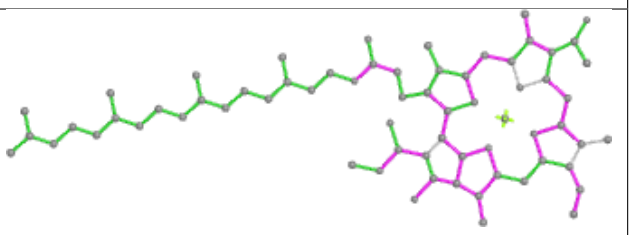


Rings

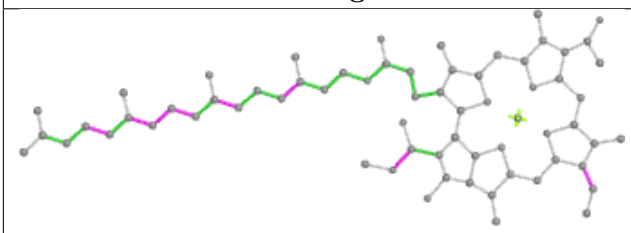
Ligand BCB M 402



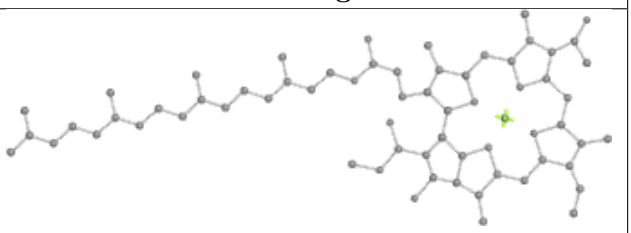
Bond lengths



Bond angles

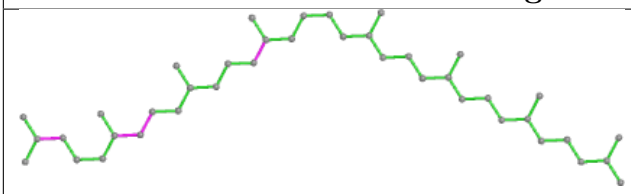


Torsions

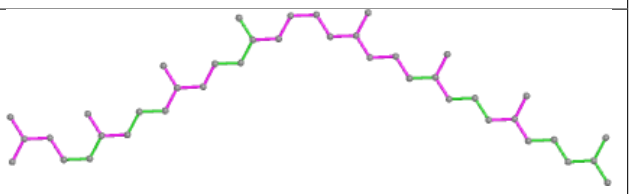


Rings

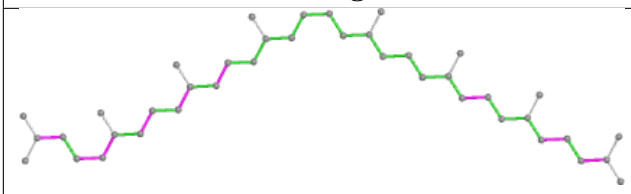
Ligand NS5 M 405



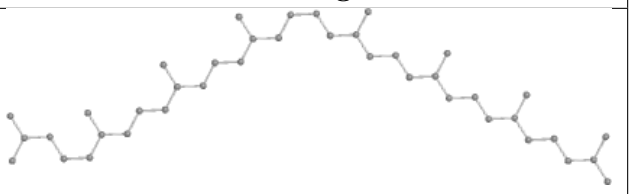
Bond lengths



Bond angles

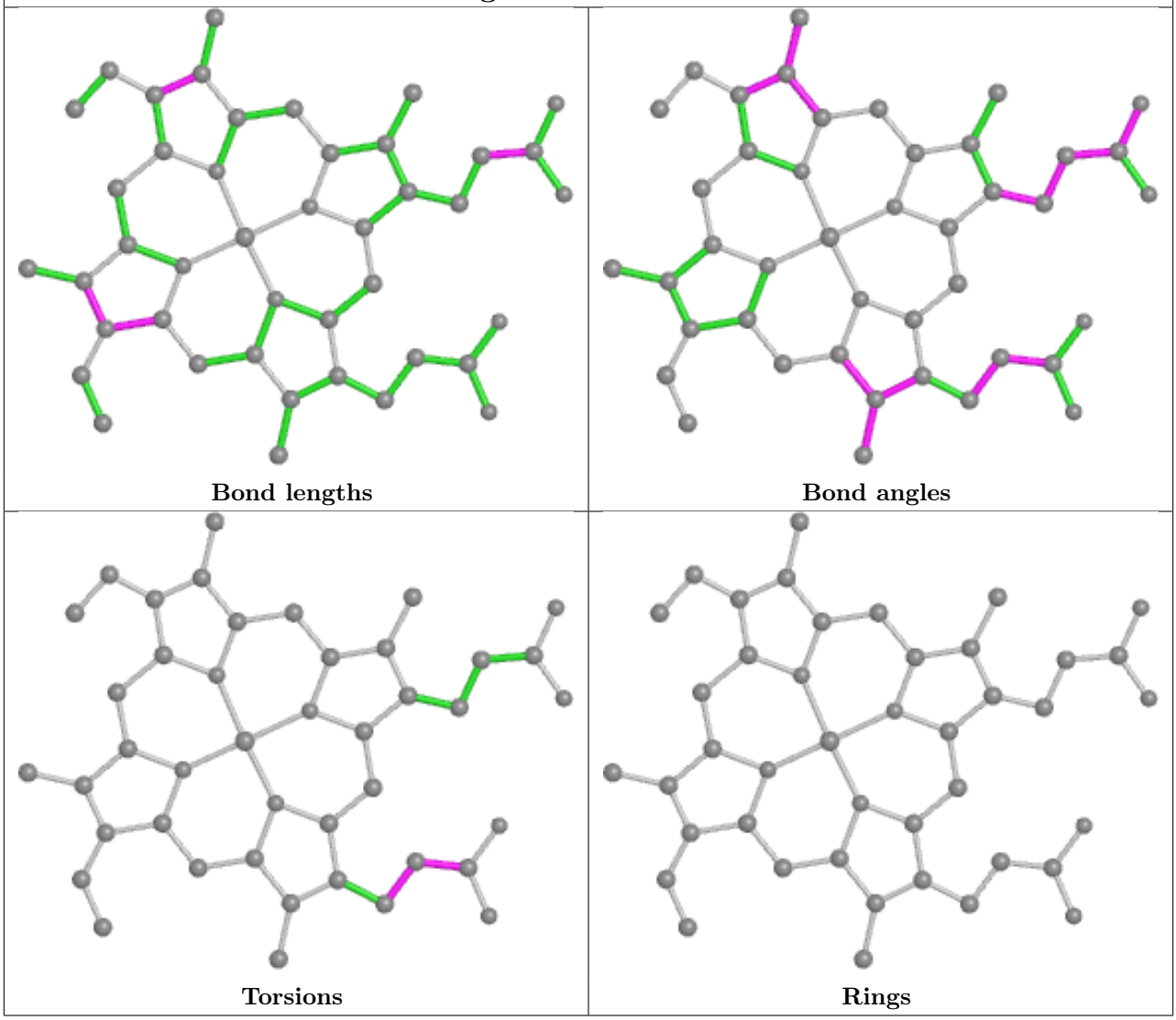


Torsions



Rings

Ligand HEC C 402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	C	332/336 (98%)	-0.41	0 100 100	86, 107, 134, 171	0
2	H	249/257 (96%)	-0.30	2 (0%) 86 86	81, 118, 156, 187	0
3	L	273/273 (100%)	-0.41	1 (0%) 92 93	83, 102, 130, 157	0
4	M	323/323 (100%)	-0.44	0 100 100	82, 104, 129, 165	0
All	All	1177/1189 (98%)	-0.40	3 (0%) 94 94	81, 108, 140, 187	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	258	LEU	2.4
3	L	271	PHE	2.1
2	H	93	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

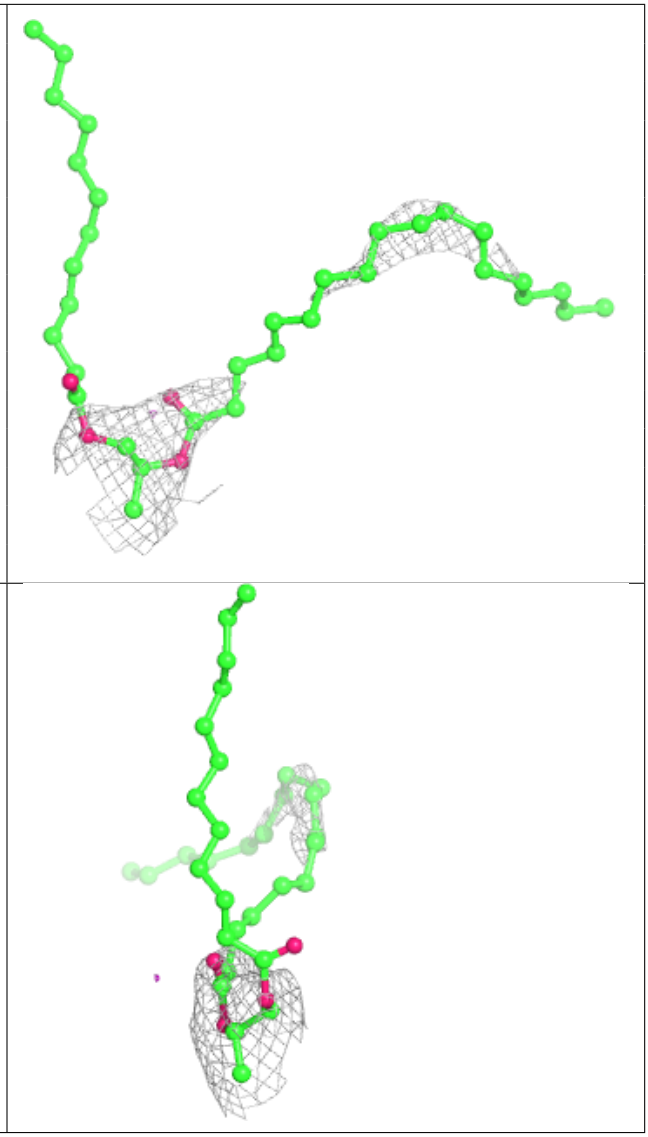
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	SO4	H	305	5/5	0.53	0.58	199,208,215,226	0
7	SO4	M	411	5/5	0.71	0.40	172,177,203,236	0
7	SO4	M	409	5/5	0.76	0.17	177,184,198,201	0
7	SO4	C	406	5/5	0.76	0.23	153,161,204,207	0
6	DGA	C	405	37/44	0.79	0.68	112,148,177,181	0
7	SO4	M	410	5/5	0.82	0.18	169,193,200,213	0
10	HTO	L	304	10/10	0.82	0.76	100,131,162,165	0
9	LDA	H	306	16/16	0.84	0.39	115,138,200,206	0
15	NS5	M	405	40/40	0.86	0.31	96,112,140,141	0
9	LDA	M	412	16/16	0.87	0.69	119,135,175,182	0
10	HTO	H	308	10/10	0.89	0.16	112,132,146,146	0
14	MQ7	M	401	48/48	0.90	0.25	84,100,127,145	0
10	HTO	L	305	10/10	0.90	0.26	108,141,157,183	0
7	SO4	M	407	5/5	0.93	0.29	129,148,154,157	0
12	BPB	M	404	65/65	0.94	0.25	91,107,174,185	0
9	LDA	H	307	16/16	0.94	0.41	117,135,154,155	0
12	BPB	L	303	65/65	0.94	0.26	74,96,106,108	0
8	FME	H	301	10/11	0.95	0.28	114,119,125,134	0
9	LDA	H	302	16/16	0.95	0.20	99,110,120,122	0
7	SO4	M	408	5/5	0.95	0.17	97,104,110,116	0
7	SO4	H	304	5/5	0.95	0.12	114,118,144,147	5
11	BCB	L	302	66/66	0.96	0.21	80,92,107,113	0
11	BCB	M	402	66/66	0.96	0.24	84,97,171,193	0
11	BCB	L	301	66/66	0.98	0.26	76,90,112,120	0
11	BCB	M	403	66/66	0.98	0.21	78,88,128,131	0
7	SO4	H	303	5/5	0.98	0.11	109,124,133,136	0
5	HEC	C	403	43/43	0.99	0.19	72,91,96,99	0
5	HEC	C	404	43/43	0.99	0.17	67,97,120,134	0
5	HEC	C	401	43/43	0.99	0.24	99,109,122,127	0
13	FE2	L	306	1/1	0.99	0.21	97,97,97,97	0
7	SO4	M	406	5/5	0.99	0.12	117,118,138,142	0
5	HEC	C	402	43/43	0.99	0.19	87,107,122,150	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.

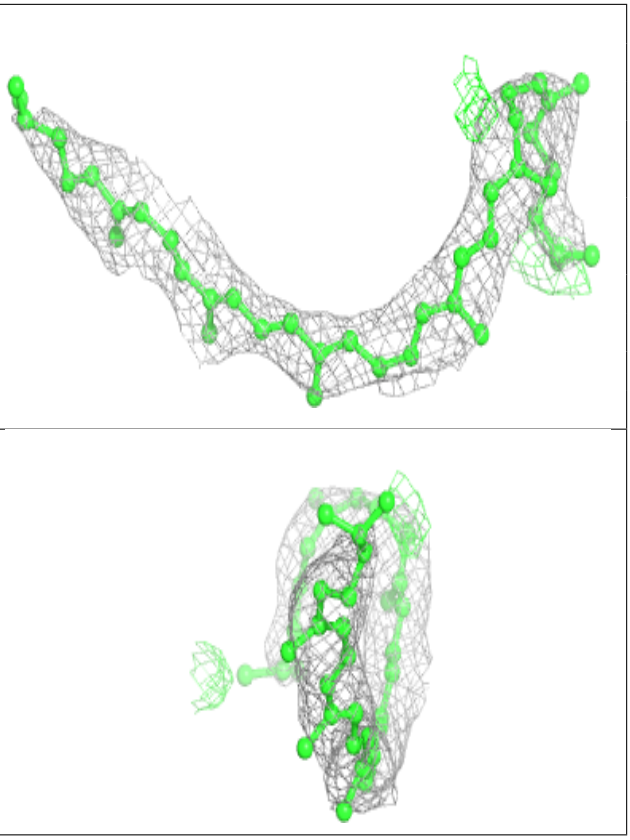
Electron density around DGA C 405:

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



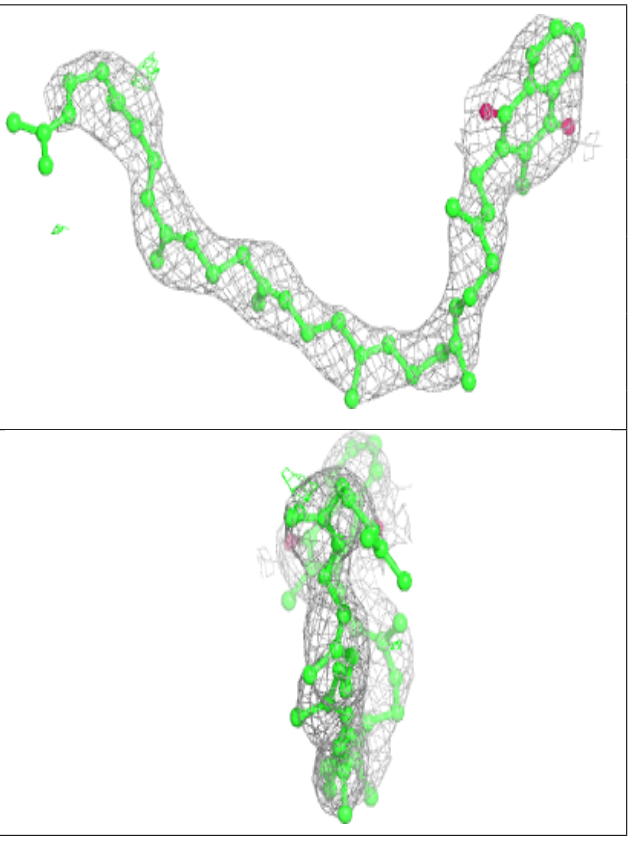
Electron density around NS5 M 405:

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



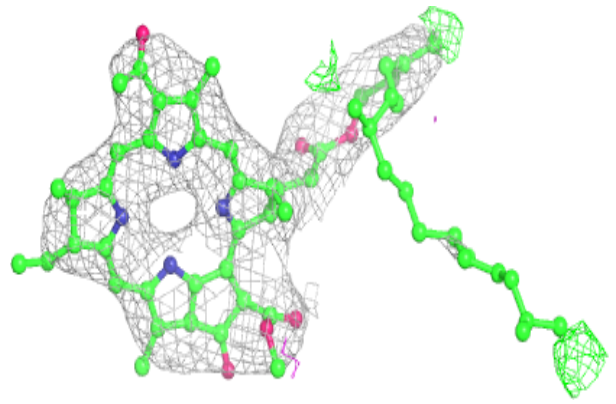
Electron density around MQ7 M 401:

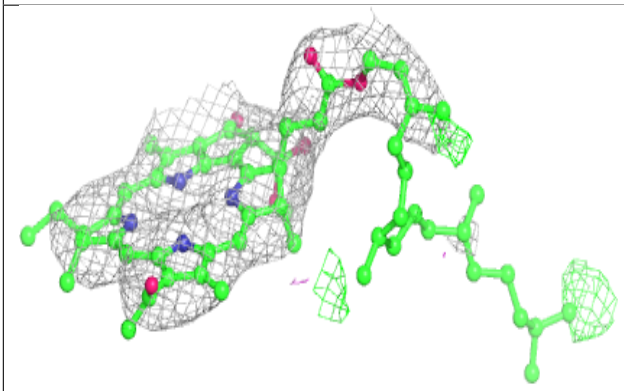
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

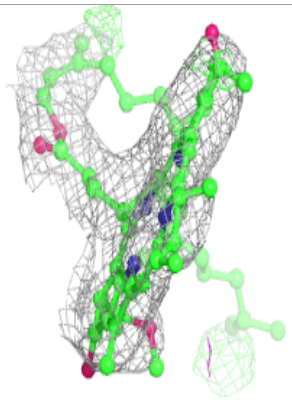


Electron density around BPB M 404:

$2mF_o$-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:

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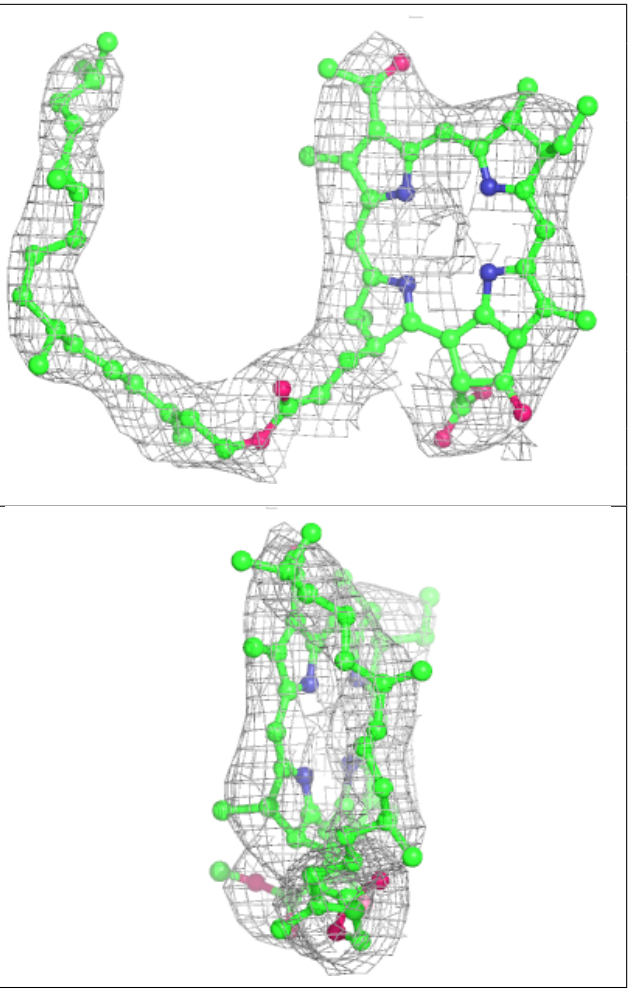
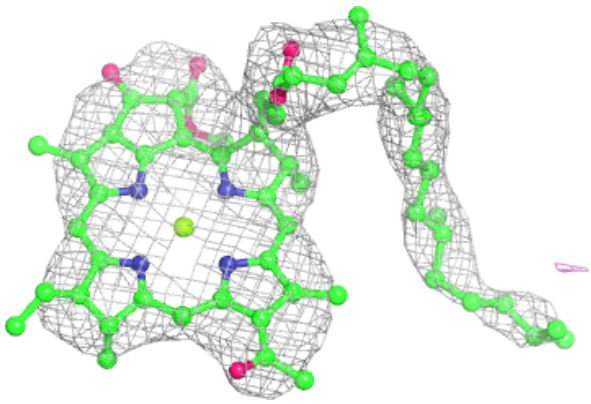
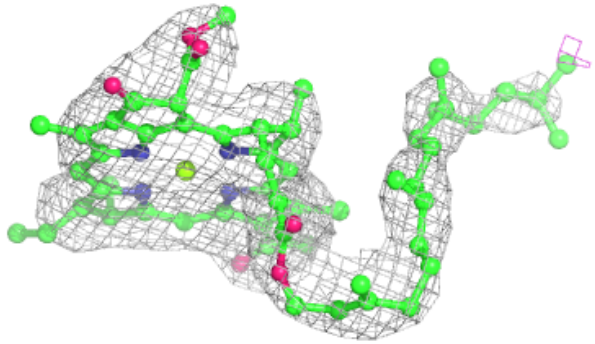
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

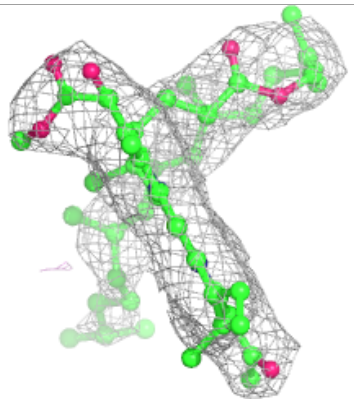


Electron density around BCB L 302:

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

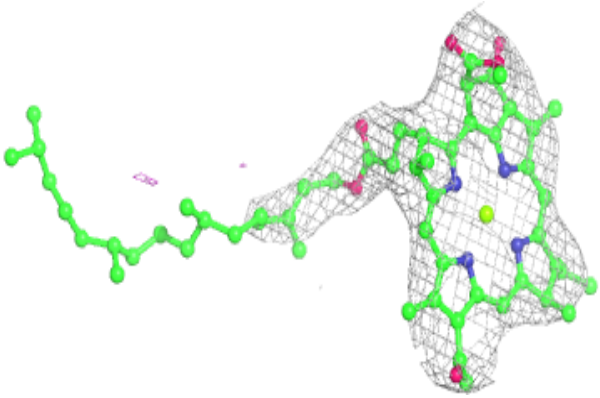


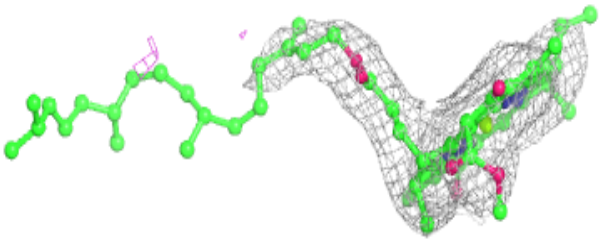


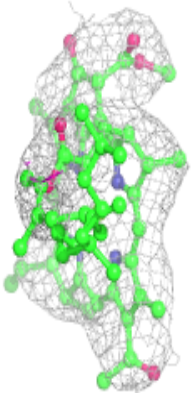


Electron density around BCB M 402:

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

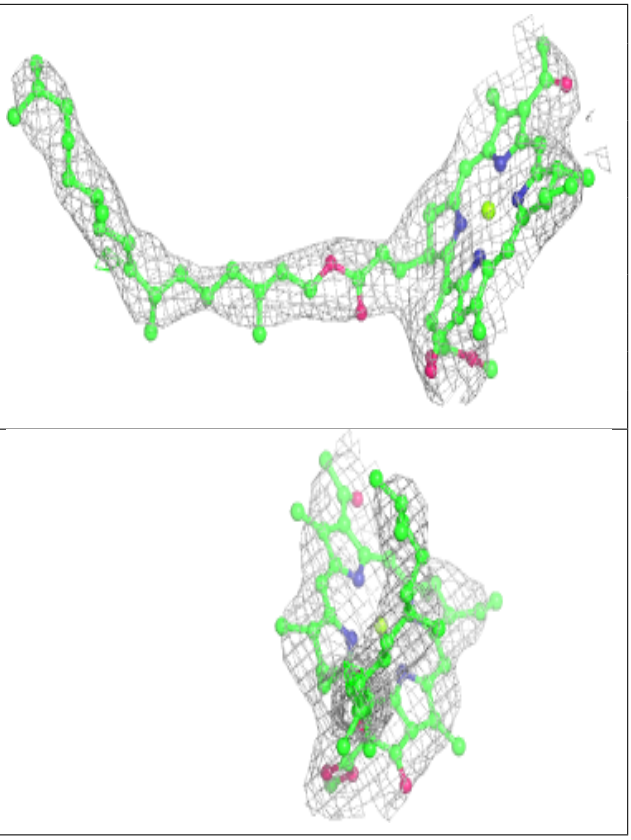


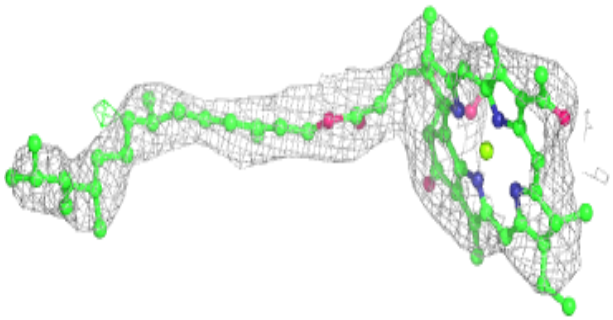




Electron density around BCB L 301:

$2mF_o$-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 403:

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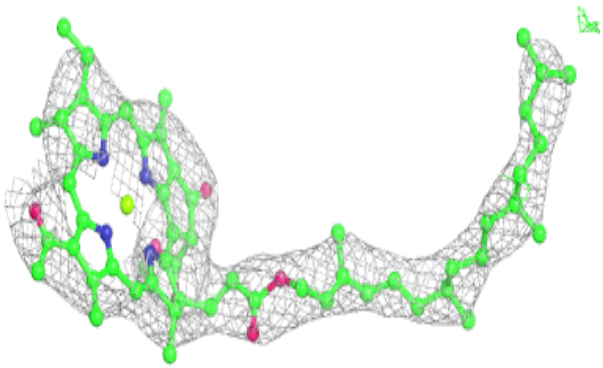
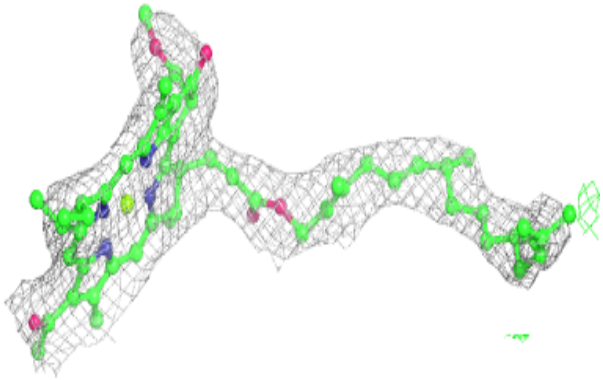
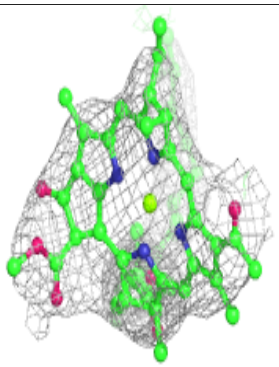
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

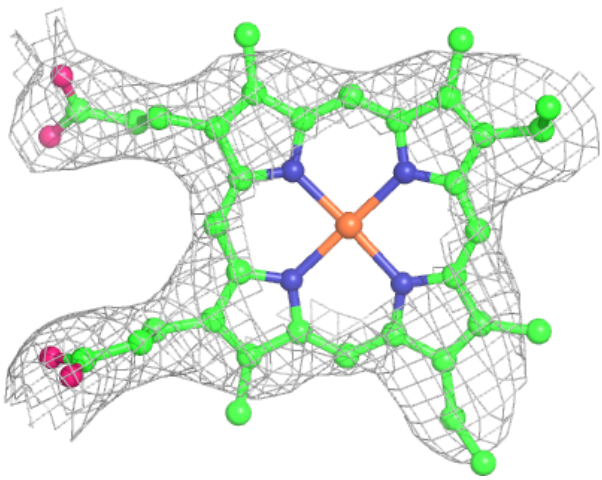


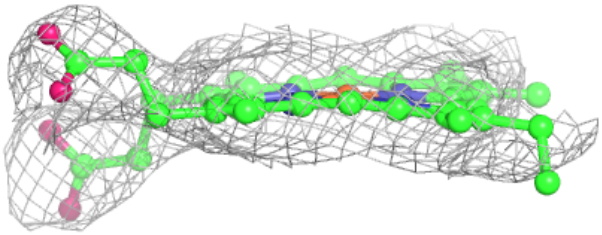


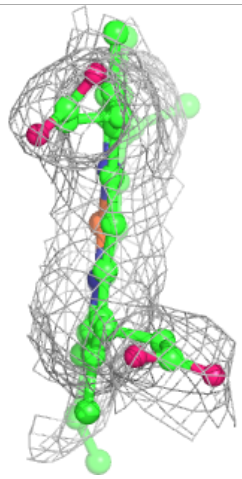


Electron density around HEC C 403:

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

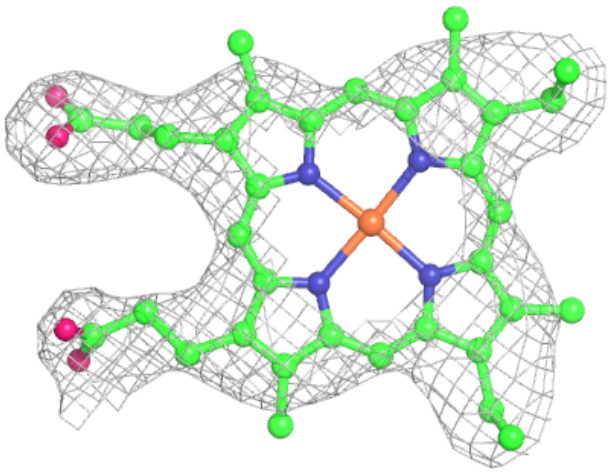


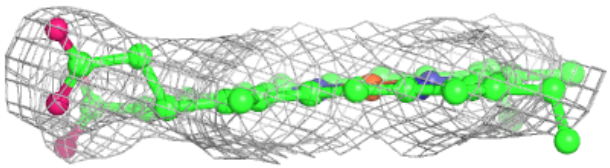


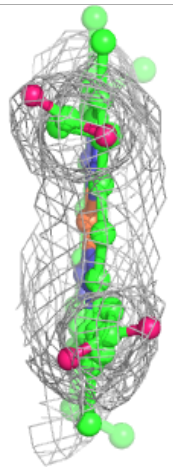


Electron density around HEC C 404:

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

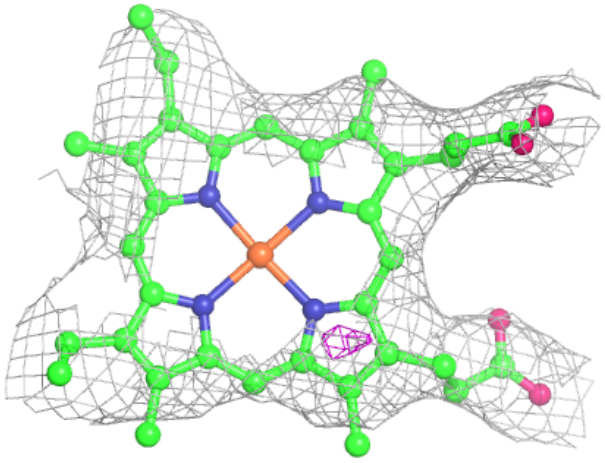


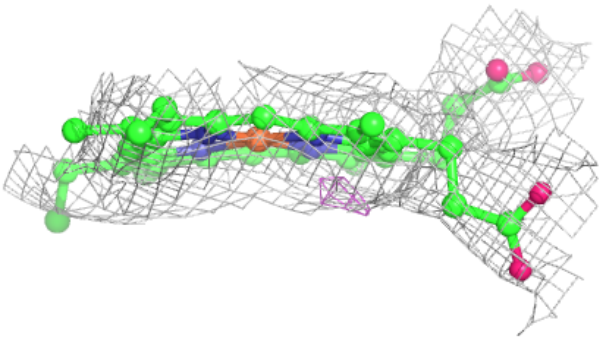


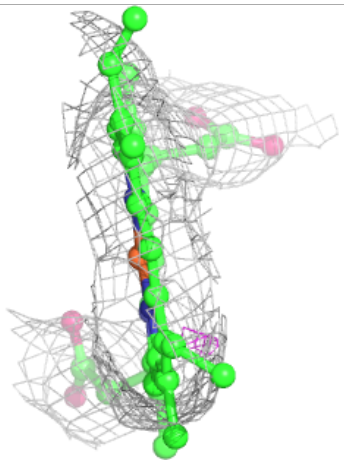


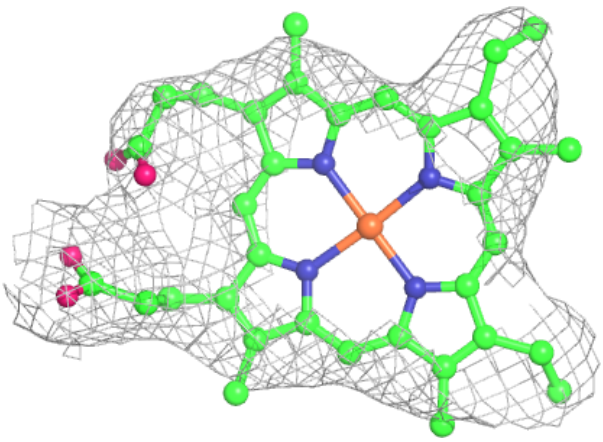
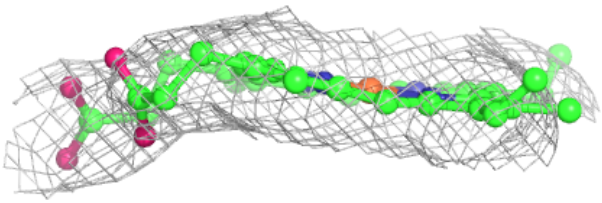
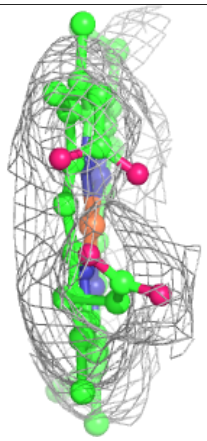
Electron density around HEC C 401:

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)	
	

6.5 Other polymers (i)

There are no such residues in this entry.