wwPDB X-ray Structure Validation Summary Report (i)

Dec 9, 2023 – 09:54 am GMT

PDB ID	:	2JBL
Title	:	PHOTOSYNTHETIC REACTION CENTER FROM BLASTOCHLORIS VIRIDIS
Authors	:	Lancaster, C.R.D.
Deposited on	:	2006-12-08
Resolution	:	2.40 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:

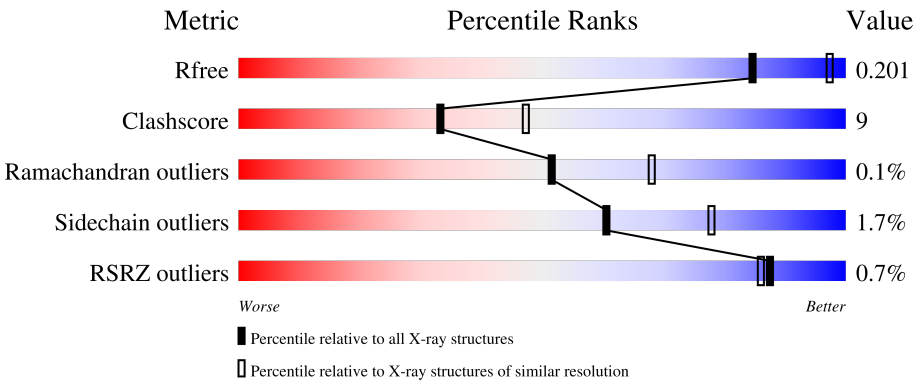
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	356	.% 78% 15% • 7%
2	H	258	83% 17%
3	L	273	87% 13%
4	M	323	.% 82% 17%

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
6	LDA	M	1331	-	-	-	X
8	BCB	L	1274	X	-	-	-
8	BCB	L	1275	X	-	-	-
8	BCB	L	1278	X	-	-	-
8	BCB	M	1324	X	-	-	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 10512 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	2618	1648	471	481	18	51	2	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	258	2018	1292	344	380	2	124	0	0

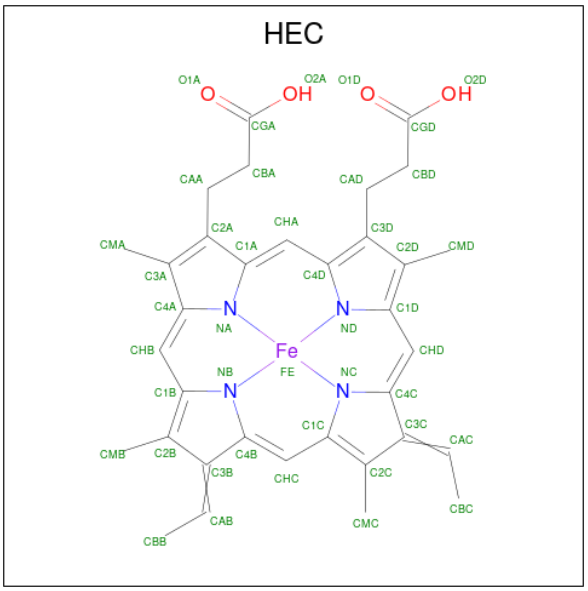
- Molecule 3 is a protein called REACTION CENTER PROTEIN L CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	273	2171	1459	350	355	7	14	0	0

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

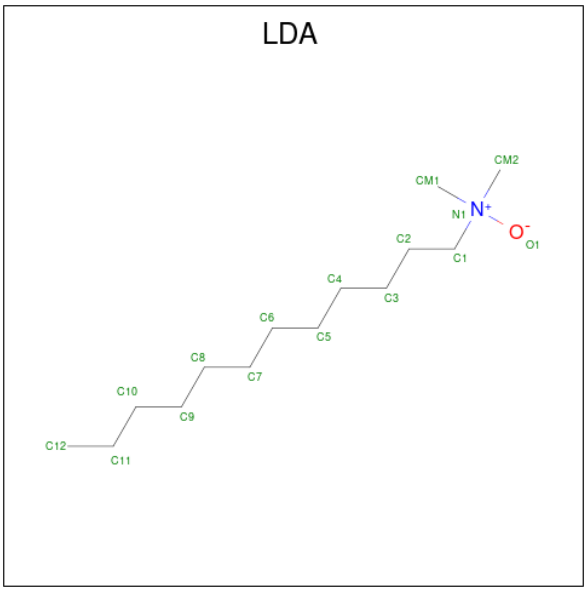
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	M	323	2555	1702	419	423	11	19	0	0

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



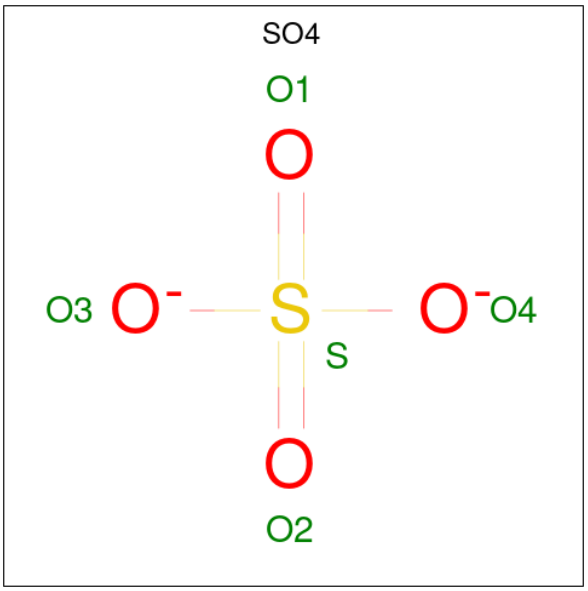
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	C	1	43	34	1	4	4	0	0

- Molecule 6 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	H	1	16	14	1	1	0	0
6	M	1	16	14	1	1	0	0
6	M	1	16	14	1	1	0	0
6	M	1	16	14	1	1	0	0
6	M	1	16	14	1	1	5	0
6	M	1	16	14	1	1	4	0

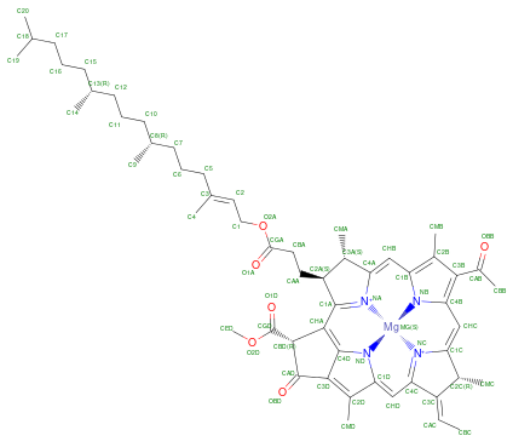
- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 8 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).

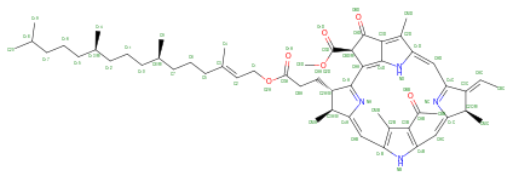
BCB



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

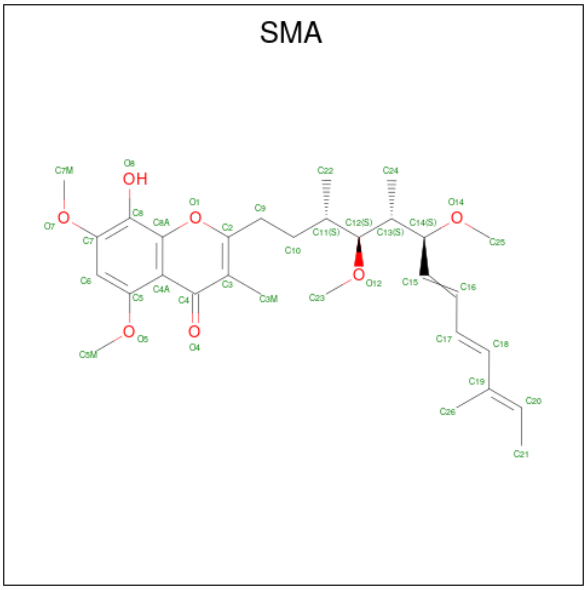
- Molecule 9 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).

BPB



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

- Molecule 10 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).

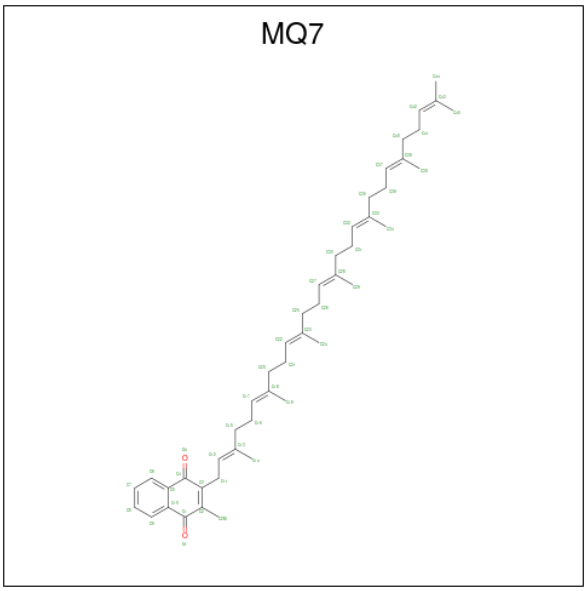


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
10	L	1	37	30	7	0	0

- Molecule 11 is FE (III) ION (three-letter code: FE) (formula: Fe).

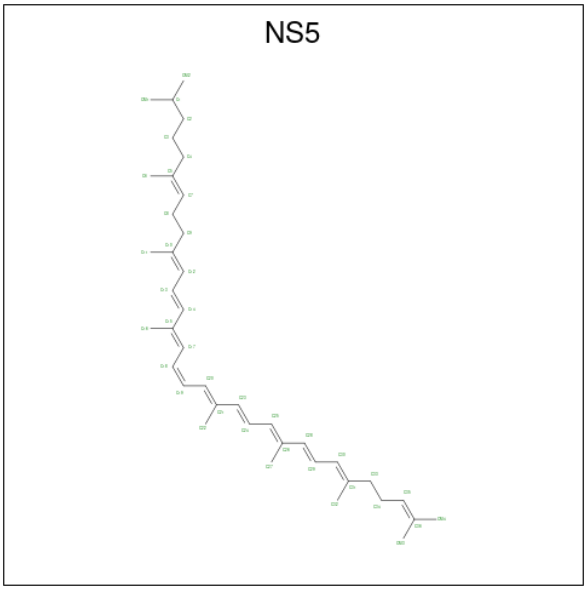
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
11	M	1	1	1	0	0

- Molecule 12 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



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

- Molecule 13 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).



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

- Molecule 14 is water.

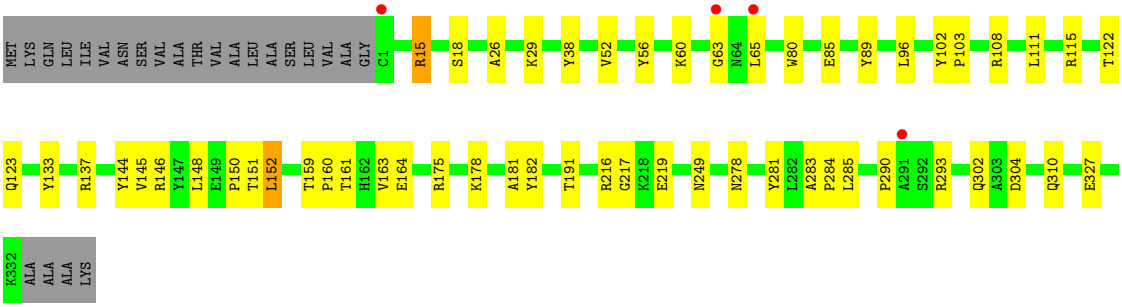
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
14	C	124	124	124	0	0
			Total	O		
14	H	76	76	76	0	0
			Total	O		
14	L	66	66	66	0	0
			Total	O		
14	M	76	76	76	0	0

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:

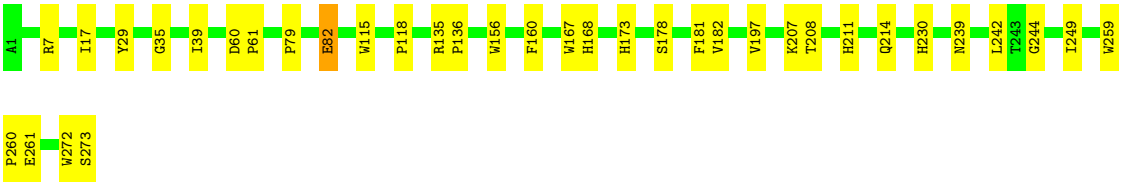


• Molecule 2: REACTION CENTER PROTEIN H CHAIN

Chain H:

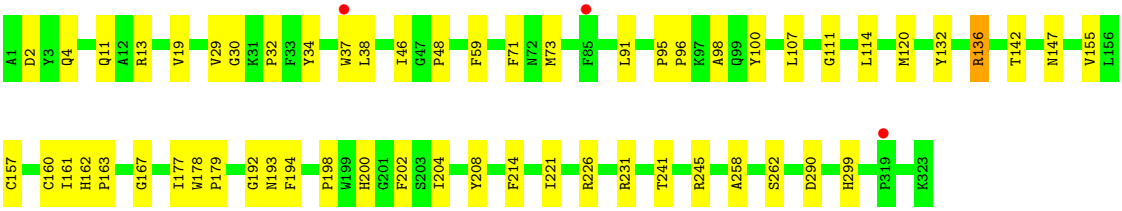
• Molecule 3: REACTION CENTER PROTEIN L CHAIN

Chain L:



• Molecule 4: REACTION CENTER PROTEIN M CHAIN

Chain M:


A1 D2 Y3 Q4 Q11 A12 R13 V19 V29 G30 K31 P32 F33 Y34 W37 L38 I46 G47 P48 F59 F71 N72 M73 F85 L91 P95 P96 K97 A98 Q99 Y100 L107 G111 L114 M120 Y132 R136 T142 N147 V155 L156
C157 C160 I161 H162 P163 G167 I177 W178 P179 G192 N193 F194 P198 W199 H200 G201 F202 S203 I204 Y208 F214 I221 R226 R231 T241 R245 A258 S262 D290 H299 P319 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	223.50Å 223.50Å 113.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.56 – 2.40 47.79 – 2.40	Depositor EDS
% Data completeness (in resolution range)	92.3 (26.56-2.40) 92.4 (47.79-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.206 0.182 , 0.201	Depositor DCC
R_{free} test set	1500 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10512	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.77% 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: BPB, SMA, MQ7, SO4, FE, FME, LDA, HEC, BCB, NS5

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	C	0.32	0/2685	0.60	1/3659 (0.0%)
2	H	0.31	0/2055	0.59	0/2807
3	L	0.39	0/2259	0.58	0/3084
4	M	0.37	0/2659	0.55	0/3637
All	All	0.35	0/9658	0.58	1/13187 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	249	ASN	N-CA-C	-6.31	93.97	111.00

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	2618	0	2587	43	0
2	H	2018	0	2020	31	0
3	L	2171	0	2098	34	0
4	M	2555	0	2452	45	0
5	C	172	0	120	4	0
6	H	16	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	80	0	155	7	0
7	H	5	0	0	0	0
7	M	15	0	0	0	0
8	L	198	0	216	23	0
8	M	66	0	72	10	0
9	L	65	0	74	5	0
9	M	65	0	74	7	0
10	L	37	0	42	2	0
11	M	1	0	0	0	0
12	M	48	0	64	0	0
13	M	40	0	60	3	0
14	C	124	0	0	1	0
14	H	76	0	0	1	0
14	L	66	0	0	1	0
14	M	76	0	0	1	0
All	All	10512	0	10065	170	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 9.

The worst 5 of 170 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)
4:M:32:PRO:HG3	4:M:48:PRO:HD3	1.49	0.95
8:L:1278:BCB:H91	8:L:1278:BCB:H122	1.52	0.87
9:L:1276:BPB:HHC	9:L:1276:BPB:HBBB	1.59	0.84
8:L:1278:BCB:H172	8:L:1278:BCB:H141	1.60	0.82
4:M:136:ARG:HA	4:M:136:ARG:HE	1.45	0.81

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	332/356 (93%)	317 (96%)	15 (4%)	0	100	100
2	H	256/258 (99%)	242 (94%)	14 (6%)	0	100	100
3	L	271/273 (99%)	262 (97%)	9 (3%)	0	100	100
4	M	321/323 (99%)	310 (97%)	10 (3%)	1 (0%)	41	55
All	All	1180/1210 (98%)	1131 (96%)	48 (4%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	M	177	ILE

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	282/297 (95%)	279 (99%)	3 (1%)	73	87
2	H	212/212 (100%)	209 (99%)	3 (1%)	67	82
3	L	218/218 (100%)	215 (99%)	3 (1%)	67	82
4	M	249/249 (100%)	242 (97%)	7 (3%)	43	63
All	All	961/976 (98%)	945 (98%)	16 (2%)	60	78

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	M	214	PHE
4	M	194	PHE
3	L	272	TRP
4	M	136	ARG
3	L	160	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
3	L	211	HIS
3	L	214	GLN
4	M	147	ASN
3	L	239	ASN
2	H	220	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)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FME	H	1	2	8,9,10	0.61	0	7,9,11	3.11	2 (28%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	FME	CA-N-CN	-5.79	113.91	122.82
2	H	1	FME	O1-CN-N	-5.47	110.88	125.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1	FME	CB-CA-N-CN
2	H	1	FME	O1-CN-N-CA

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 24 ligands modelled in this entry, 1 is monoatomic - leaving 23 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	LDA	M	1332	-	12,15,15	2.42	1 (8%)	14,17,17	0.54	0
5	HEC	C	1334	1	32,50,50	1.52	2 (6%)	24,82,82	1.14	1 (4%)
8	BCB	L	1278	4	63,74,74	1.50	9 (14%)	74,115,115	2.01	12 (16%)
5	HEC	C	1333	1	32,50,50	1.53	2 (6%)	24,82,82	0.84	0
6	LDA	M	1330	-	12,15,15	2.36	1 (8%)	14,17,17	0.53	0
13	NS5	M	1328	-	39,39,39	0.67	0	44,46,46	1.10	4 (9%)
5	HEC	C	1335	1	32,50,50	1.50	2 (6%)	24,82,82	0.97	1 (4%)
12	MQ7	M	1327	-	49,49,49	1.48	9 (18%)	60,63,63	1.22	8 (13%)
6	LDA	M	1333	-	12,15,15	2.42	1 (8%)	14,17,17	0.52	0
6	LDA	H	1259	-	12,15,15	2.38	1 (8%)	14,17,17	0.53	0
7	SO4	M	1334	-	4,4,4	0.84	0	6,6,6	0.38	0
7	SO4	M	1335	-	4,4,4	0.61	0	6,6,6	0.07	0
6	LDA	M	1331	-	12,15,15	2.26	1 (8%)	14,17,17	0.46	0
7	SO4	M	1336	-	4,4,4	0.58	0	6,6,6	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	SMA	L	1277	-	38,38,38	1.66	9 (23%)	48,52,52	0.92	2 (4%)
9	BPB	L	1276	-	49,70,70	1.40	6 (12%)	47,101,101	2.15	10 (21%)
5	HEC	C	1336	1	32,50,50	1.45	2 (6%)	24,82,82	0.81	0
6	LDA	M	1329	-	12,15,15	2.22	1 (8%)	14,17,17	0.57	0
8	BCB	L	1275	3	63,74,74	1.44	8 (12%)	74,115,115	1.95	10 (13%)
9	BPB	M	1325	-	49,70,70	1.33	7 (14%)	47,101,101	2.19	8 (17%)
7	SO4	H	1260	-	4,4,4	0.52	0	6,6,6	0.18	0
8	BCB	M	1324	4	63,74,74	1.33	8 (12%)	74,115,115	2.15	16 (21%)
8	BCB	L	1274	3	63,74,74	1.40	8 (12%)	74,115,115	1.98	14 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LDA	M	1332	-	-	0/13/13/13	-
8	BCB	L	1278	4	3/3/21/26	0/37/137/137	-
5	HEC	C	1334	1	-	4/10/54/54	-
5	HEC	C	1333	1	-	4/10/54/54	-
6	LDA	M	1330	-	-	0/13/13/13	-
13	NS5	M	1328	-	-	8/43/43/43	-
5	HEC	C	1335	1	-	2/10/54/54	-
12	MQ7	M	1327	-	-	1/41/61/61	0/2/2/2
6	LDA	M	1333	-	-	0/13/13/13	-
6	LDA	H	1259	-	-	0/13/13/13	-
6	LDA	M	1331	-	-	2/13/13/13	-
10	SMA	L	1277	-	-	7/34/34/34	0/2/2/2
9	BPB	L	1276	-	-	4/37/105/105	0/5/6/6
5	HEC	C	1336	1	-	0/10/54/54	-
6	LDA	M	1329	-	-	0/13/13/13	-
8	BCB	L	1275	3	3/3/21/26	4/37/137/137	-
9	BPB	M	1325	-	-	7/37/105/105	0/5/6/6
8	BCB	M	1324	4	4/4/21/26	7/37/137/137	-
8	BCB	L	1274	3	3/3/21/26	4/37/137/137	-

The worst 5 of 78 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	1332	LDA	O1-N1	-8.37	1.22	1.42
6	M	1333	LDA	O1-N1	-8.36	1.22	1.42
6	H	1259	LDA	O1-N1	-8.24	1.22	1.42
6	M	1330	LDA	O1-N1	-8.15	1.23	1.42
6	M	1331	LDA	O1-N1	-7.79	1.23	1.42

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	M	1325	BPB	O2D-CGD-CBD	9.96	123.61	111.00
8	M	1324	BCB	C4A-NA-C1A	9.55	111.00	106.71
9	L	1276	BPB	O2D-CGD-CBD	9.24	122.71	111.00
8	L	1278	BCB	C4A-NA-C1A	9.00	110.75	106.71
8	L	1274	BCB	C4A-NA-C1A	8.58	110.56	106.71

5 of 13 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	1274	BCB	NC
8	L	1274	BCB	NA
8	L	1274	BCB	ND
8	L	1275	BCB	NC
8	L	1275	BCB	NA

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	M	1324	BCB	CAD-CBD-CGD-O1D
8	M	1324	BCB	CAD-CBD-CGD-O2D
13	M	1328	NS5	C11-C10-C12-C13
13	M	1328	NS5	C10-C12-C13-C14
13	M	1328	NS5	C13-C14-C15-C16

There are no ring outliers.

15 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	1332	LDA	1	0
5	C	1334	HEC	1	0
8	L	1278	BCB	13	0
5	C	1333	HEC	2	0
6	M	1330	LDA	5	0

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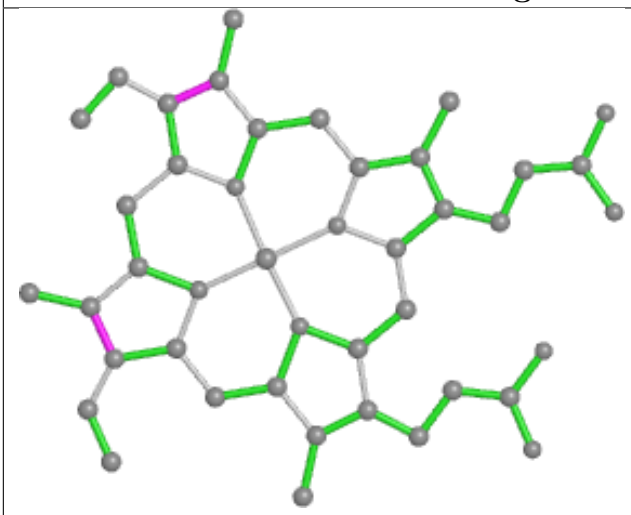
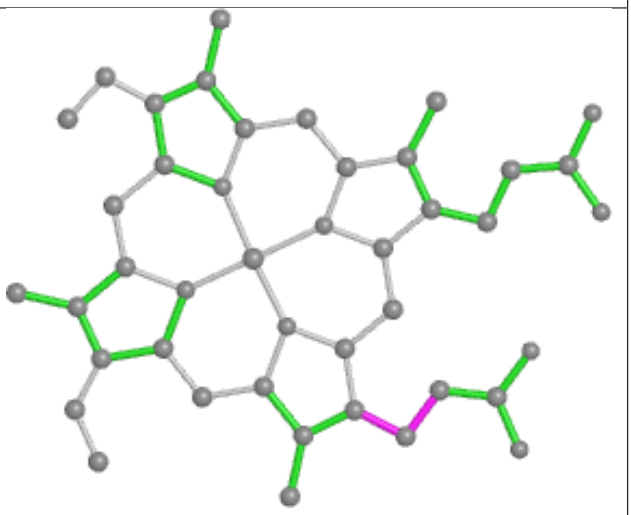
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	M	1328	NS5	3	0
5	C	1335	HEC	1	0
6	H	1259	LDA	1	0
6	M	1331	LDA	1	0
10	L	1277	SMA	2	0
9	L	1276	BPB	5	0
8	L	1275	BCB	5	0
9	M	1325	BPB	7	0
8	M	1324	BCB	10	0
8	L	1274	BCB	6	0

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

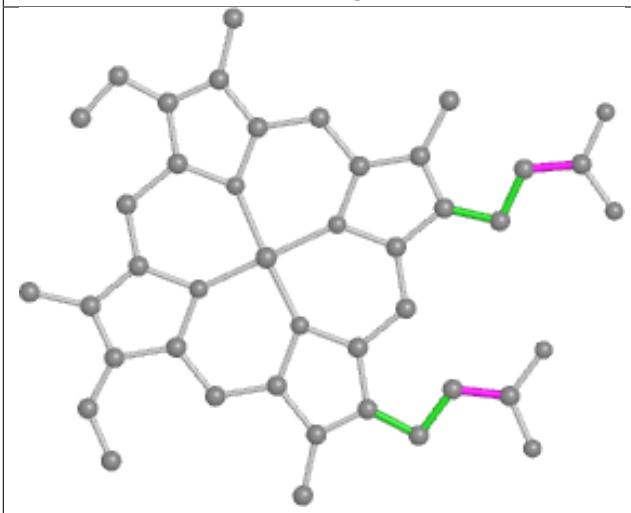
Ligand HEC C 1334



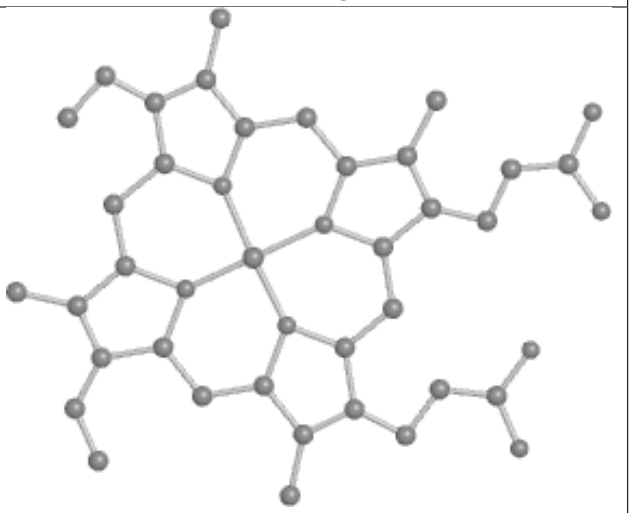
Bond lengths



Bond angles

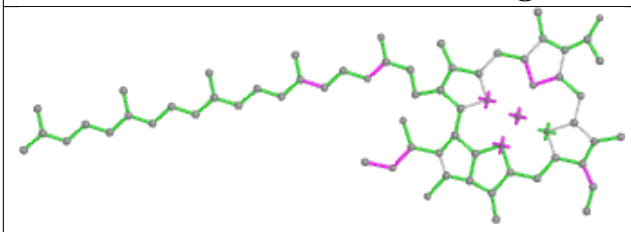


Torsions

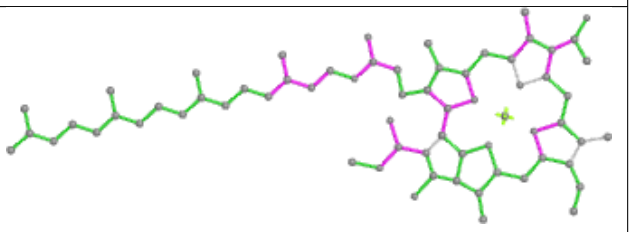


Rings

Ligand BCB L 1278



Bond lengths



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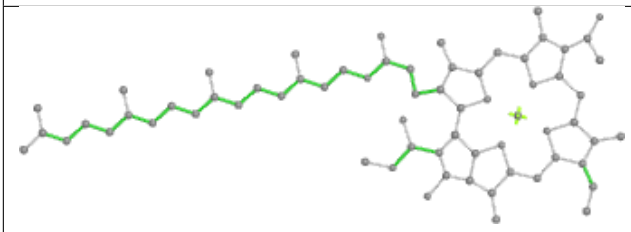
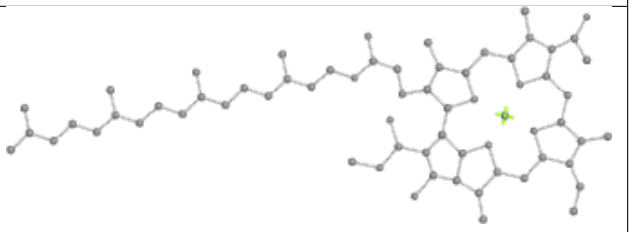
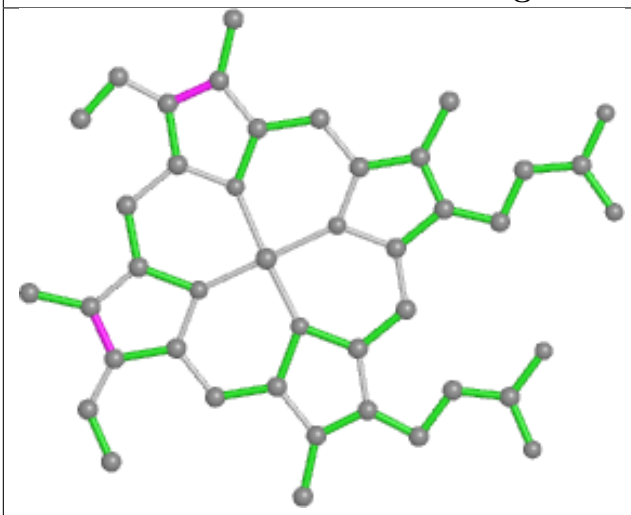


Torsions

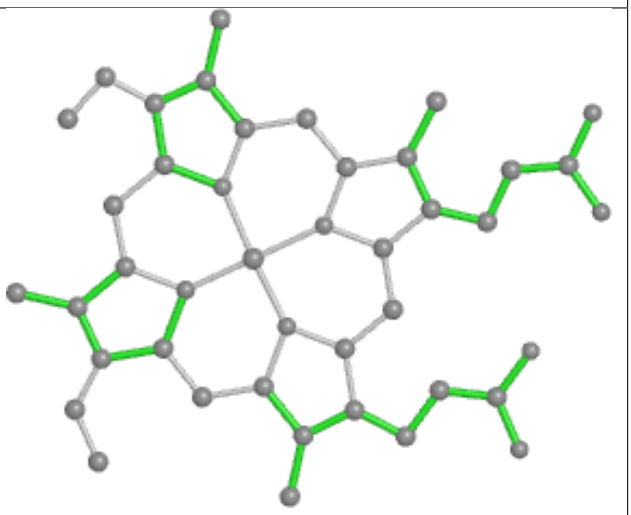


Rings

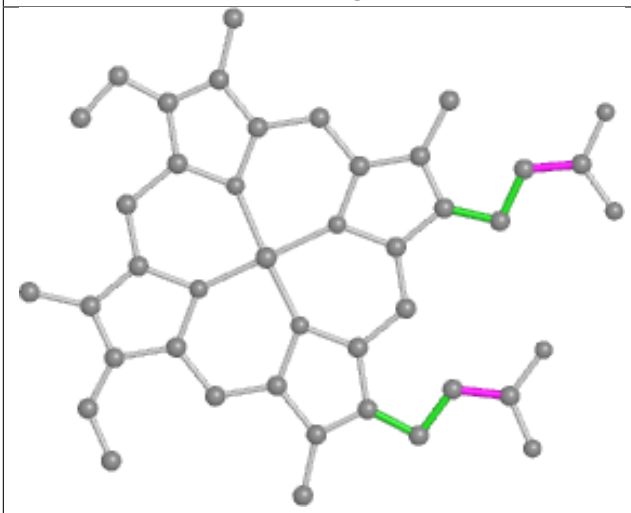
Ligand HEC C 1333



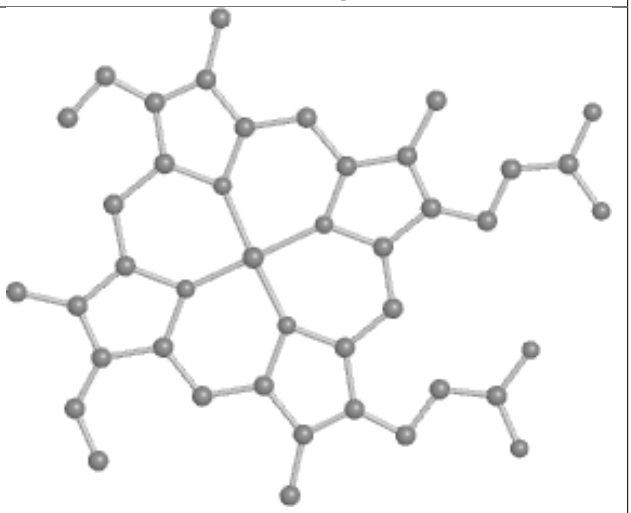
Bond lengths



Bond angles

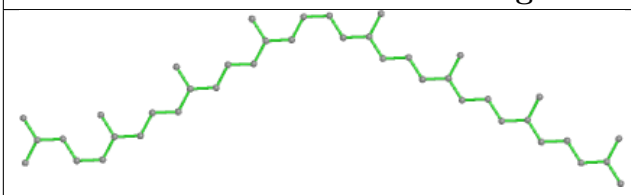


Torsions

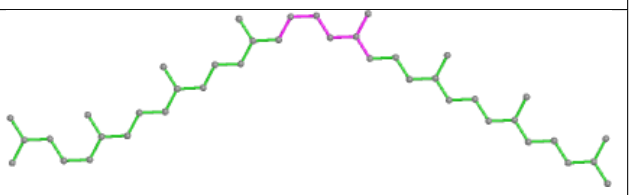


Rings

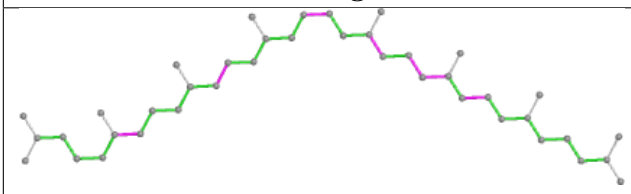
Ligand NS5 M 1328



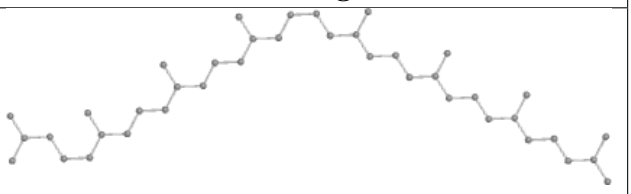
Bond lengths



Bond angles

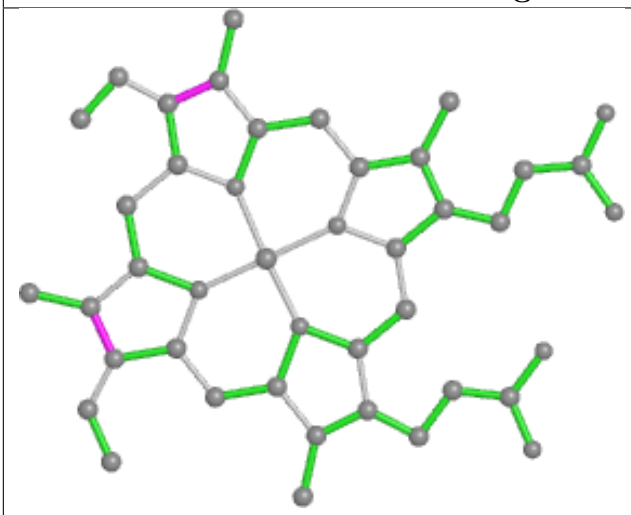


Torsions

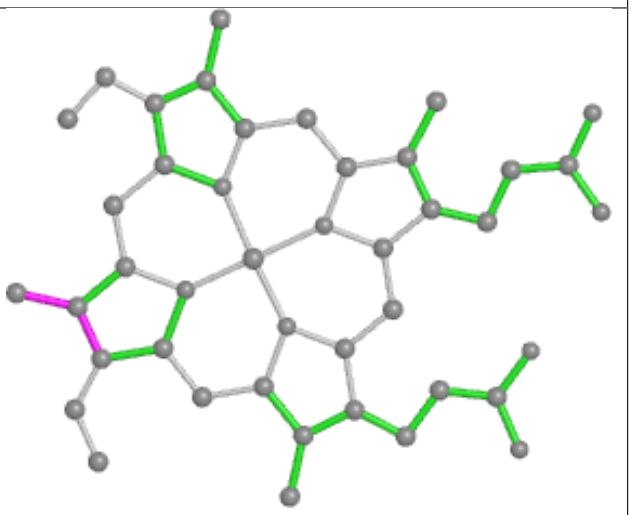


Rings

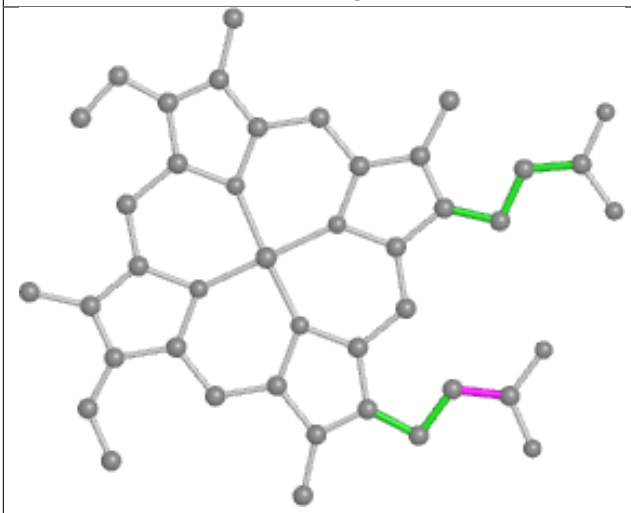
Ligand HEC C 1335



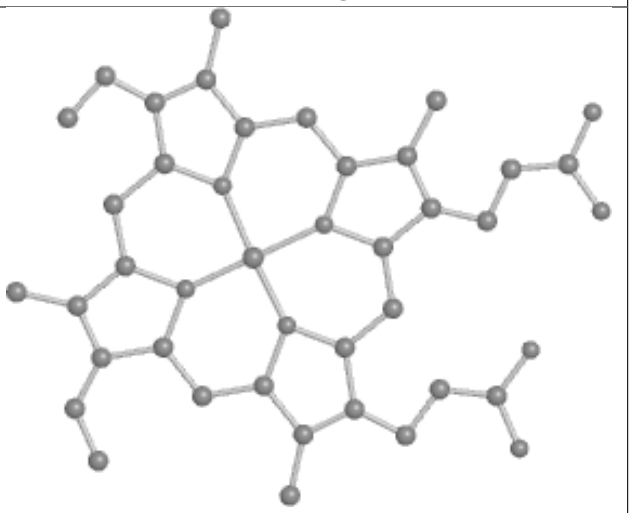
Bond lengths



Bond angles

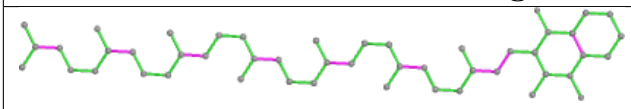


Torsions

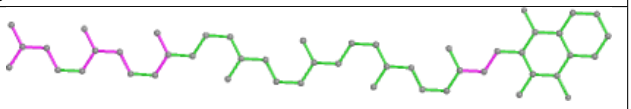


Rings

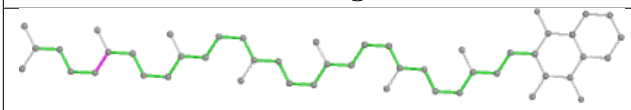
Ligand MQ7 M 1327



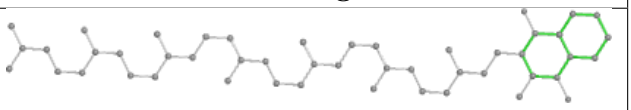
Bond lengths



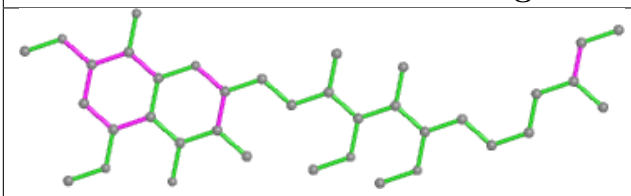
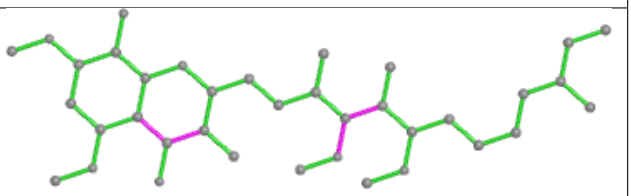
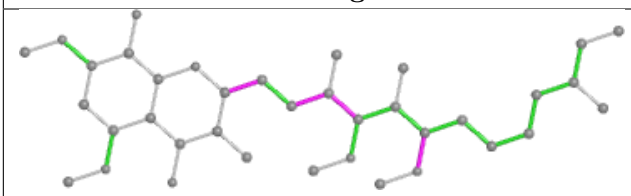
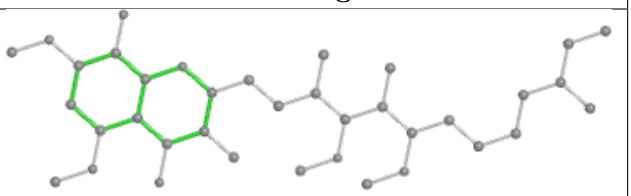
Bond angles

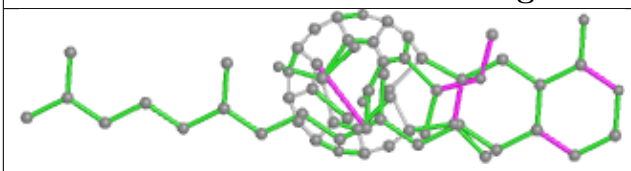
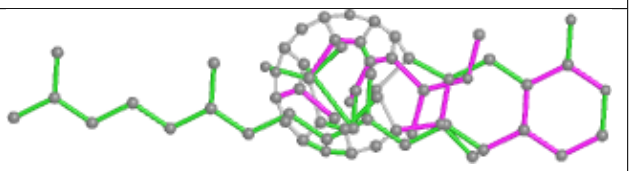
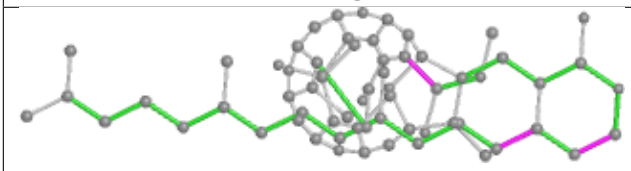
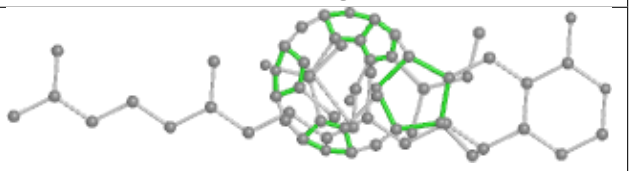


Torsions

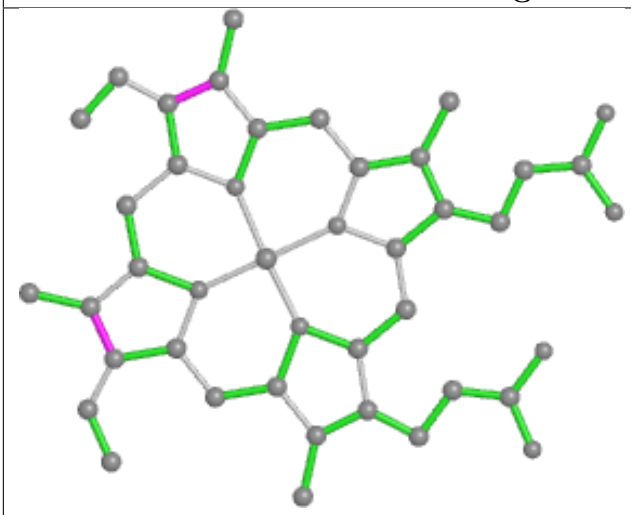


Rings

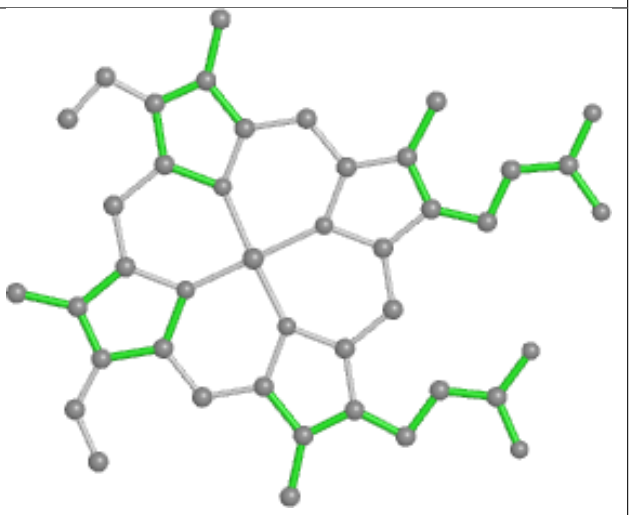
Ligand SMA L 1277	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BPB L 1276	
 Bond lengths	 Bond angles
 Torsions	 Rings

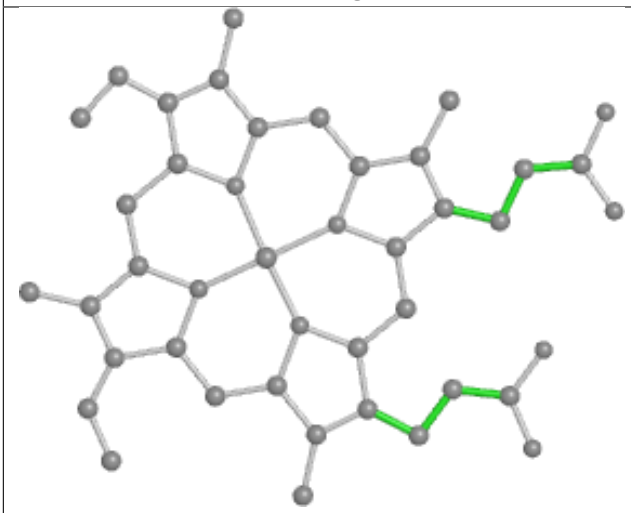
Ligand HEC C 1336



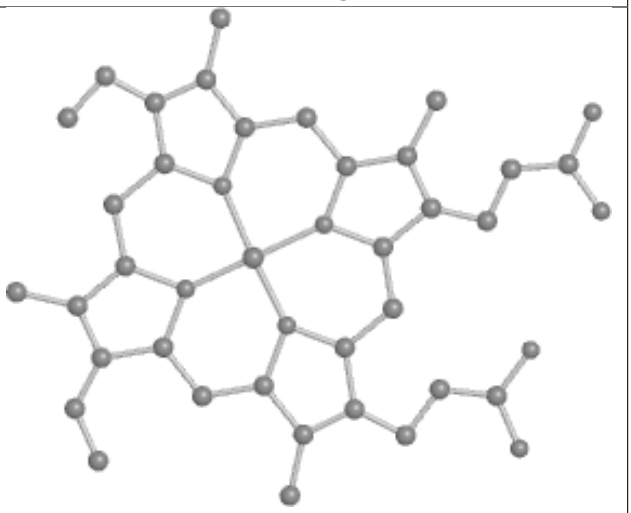
Bond lengths



Bond angles

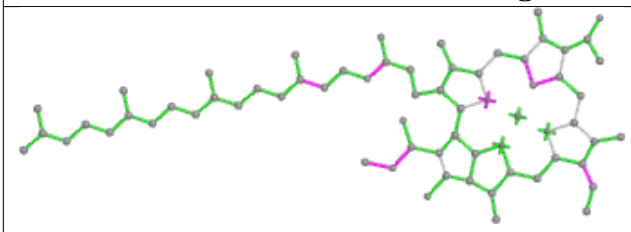


Torsions

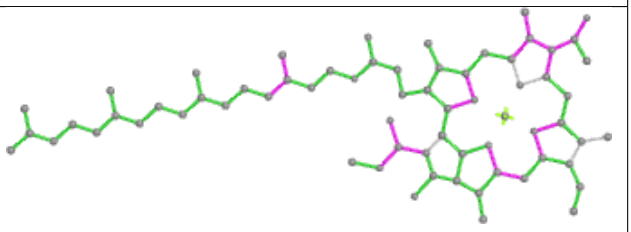


Rings

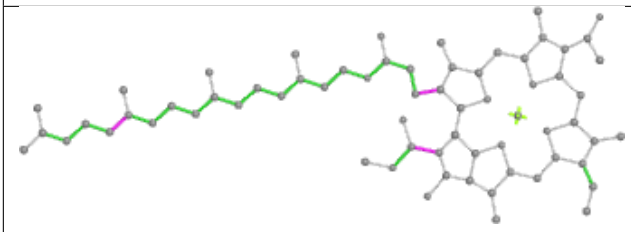
Ligand BCB L 1275



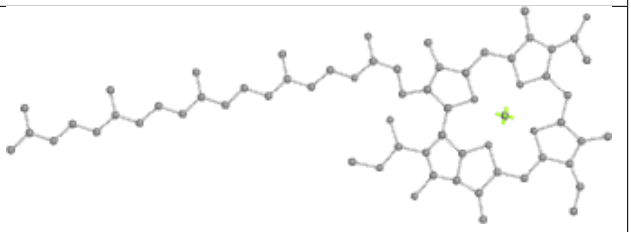
Bond lengths



Bond angles

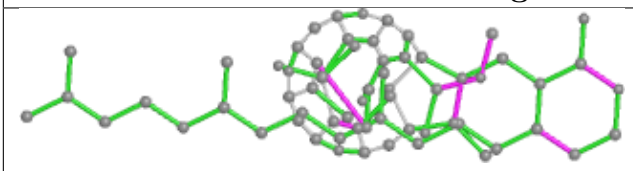


Torsions

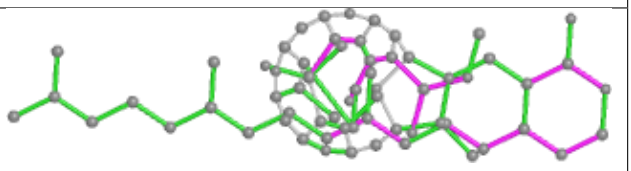


Rings

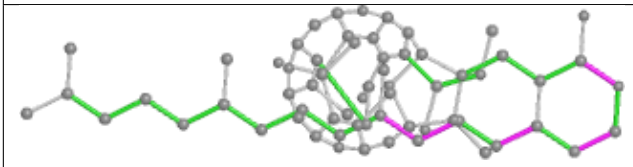
Ligand BPB M 1325



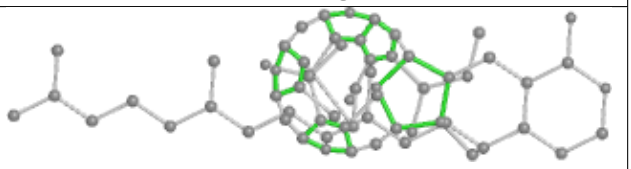
Bond lengths



Bond angles

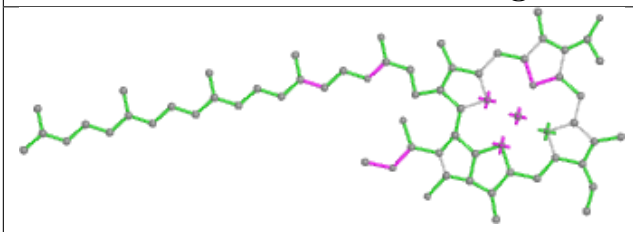


Torsions

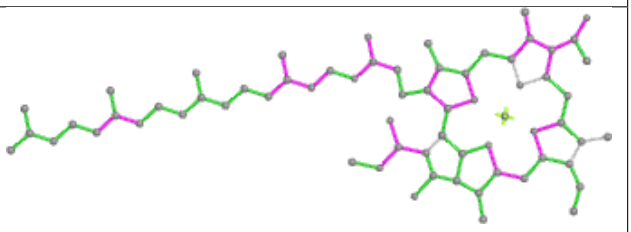


Rings

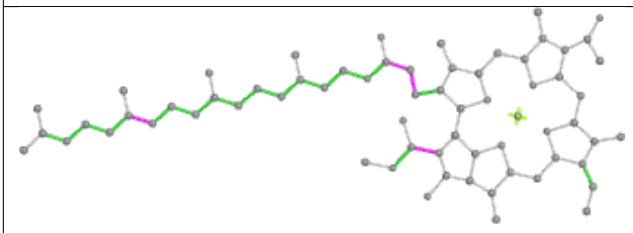
Ligand BCB M 1324



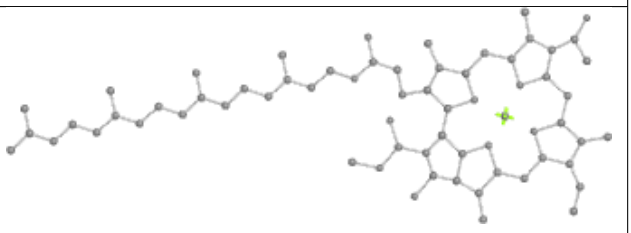
Bond lengths



Bond angles

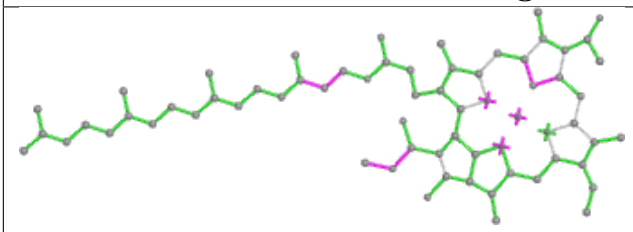


Torsions

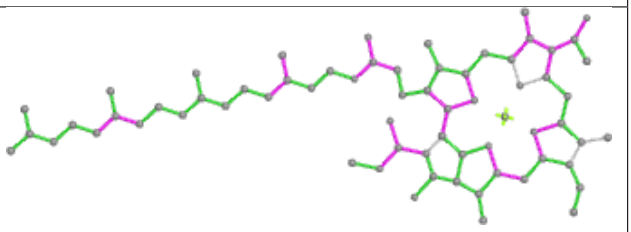


Rings

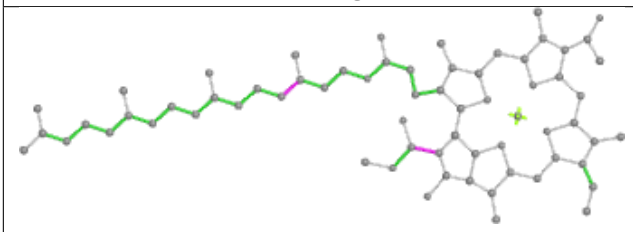
Ligand BCB L 1274



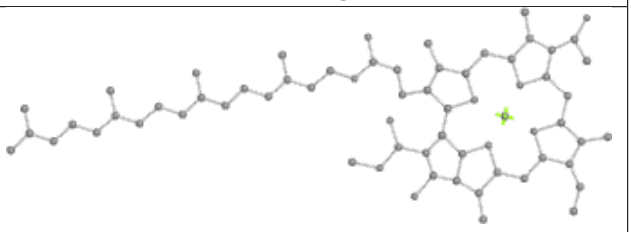
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	332/356 (93%)	-0.52	4 (1%)	79	77	21, 36, 58, 76	19 (5%)
2	H	249/258 (96%)	-0.62	1 (0%)	92	91	24, 41, 66, 81	20 (8%)
3	L	273/273 (100%)	-0.66	0	100	100	21, 30, 51, 62	7 (2%)
4	M	323/323 (100%)	-0.55	3 (0%)	84	82	20, 34, 58, 64	12 (3%)
All	All	1177/1210 (97%)	-0.58	8 (0%)	87	86	20, 35, 59, 81	58 (4%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	M	85	PHE	3.2
1	C	1	CYS	3.1
1	C	65	LEU	2.2
4	M	319	PRO	2.2
1	C	291	ALA	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	FME	H	1	10/11	0.96	0.12	41,44,53,61	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

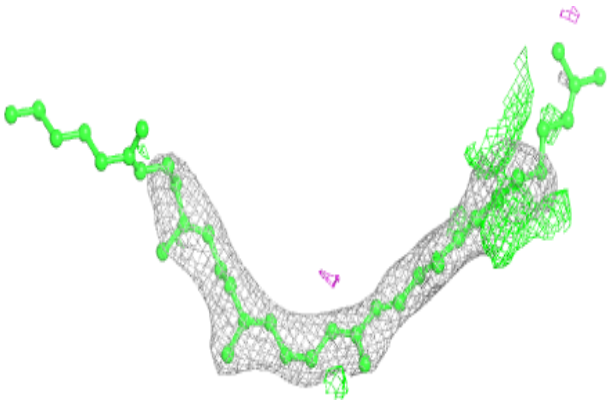
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

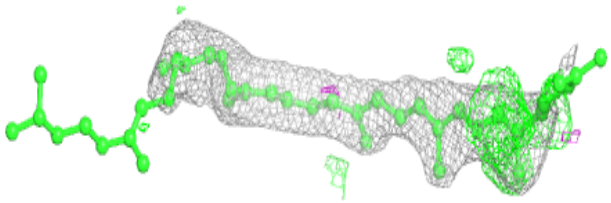
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	LDA	M	1330	16/16	0.60	0.33	52,71,83,83	0
6	LDA	M	1331	16/16	0.71	0.41	83,84,93,93	0
6	LDA	M	1332	16/16	0.72	0.36	86,88,90,90	5
6	LDA	M	1333	16/16	0.81	0.25	86,90,90,90	4
13	NS5	M	1328	40/40	0.92	0.18	50,58,79,80	14
6	LDA	H	1259	16/16	0.93	0.22	52,60,66,67	0
9	BPB	M	1325	65/65	0.94	0.13	25,35,61,62	7
8	BCB	L	1278	66/66	0.95	0.18	20,29,49,50	20
12	MQ7	M	1327	48/48	0.96	0.13	24,27,54,58	0
10	SMA	L	1277	37/37	0.96	0.15	28,36,66,69	0
7	SO4	M	1335	5/5	0.97	0.11	85,86,87,87	0
8	BCB	L	1275	66/66	0.97	0.14	15,22,46,50	0
6	LDA	M	1329	16/16	0.97	0.16	41,44,46,47	0
8	BCB	M	1324	66/66	0.97	0.17	17,24,47,49	0
7	SO4	H	1260	5/5	0.98	0.11	75,76,76,77	0
9	BPB	L	1276	65/65	0.98	0.14	19,27,32,34	0
5	HEC	C	1333	43/43	0.98	0.10	34,39,49,53	0
8	BCB	L	1274	66/66	0.98	0.17	16,21,34,39	0
5	HEC	C	1334	43/43	0.98	0.10	29,35,40,42	0
5	HEC	C	1336	43/43	0.98	0.10	24,29,42,49	0
7	SO4	M	1334	5/5	0.99	0.10	39,41,42,44	0
5	HEC	C	1335	43/43	0.99	0.11	21,25,29,34	0
7	SO4	M	1336	5/5	0.99	0.13	57,57,58,59	0
11	FE	M	1326	1/1	1.00	0.08	25,25,25,25	0

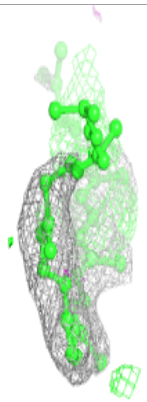
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NS5 M 1328:

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

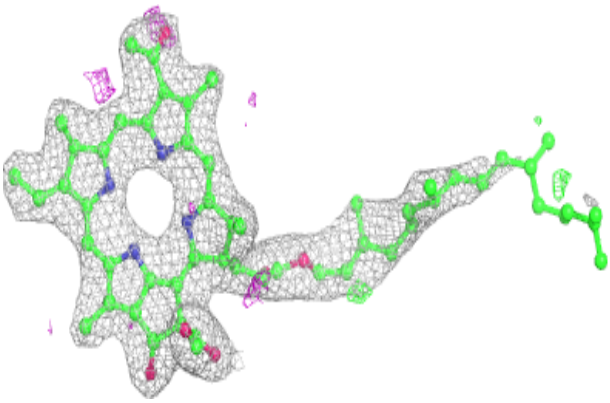


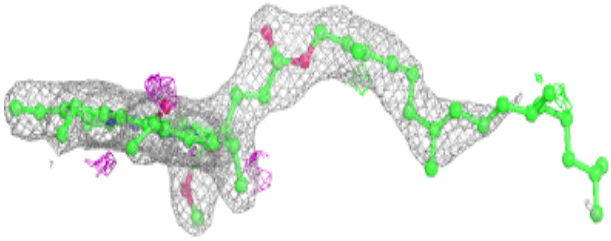


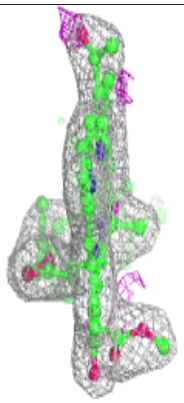


Electron density around BPB M 1325:

$2mF_o$-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 1278:

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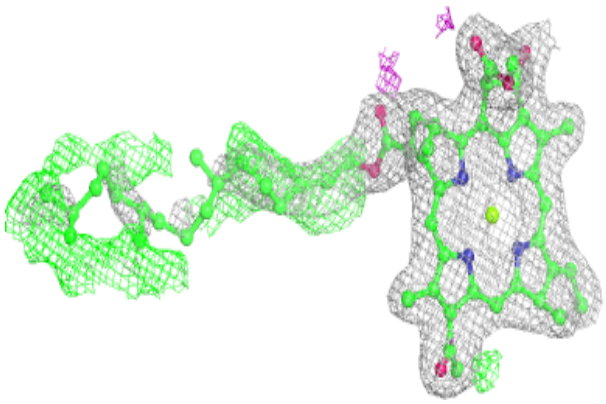
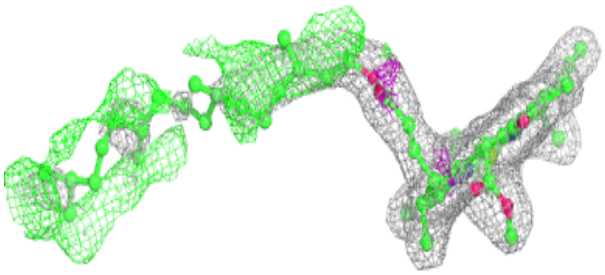
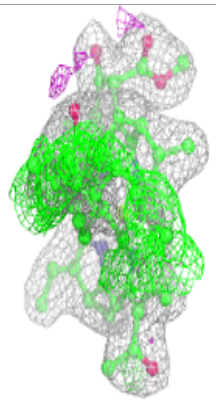
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around MQ7 M 1327:

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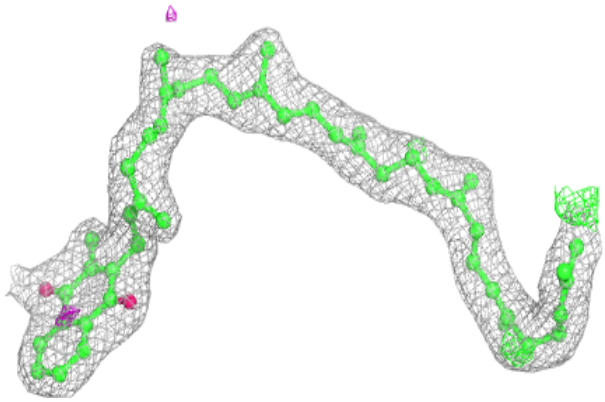
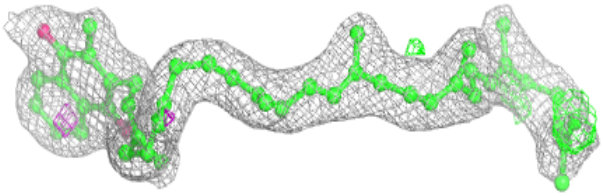
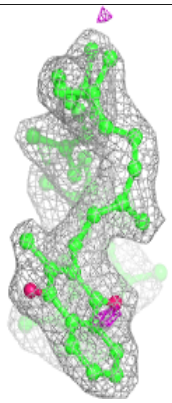
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around SMA L 1277:

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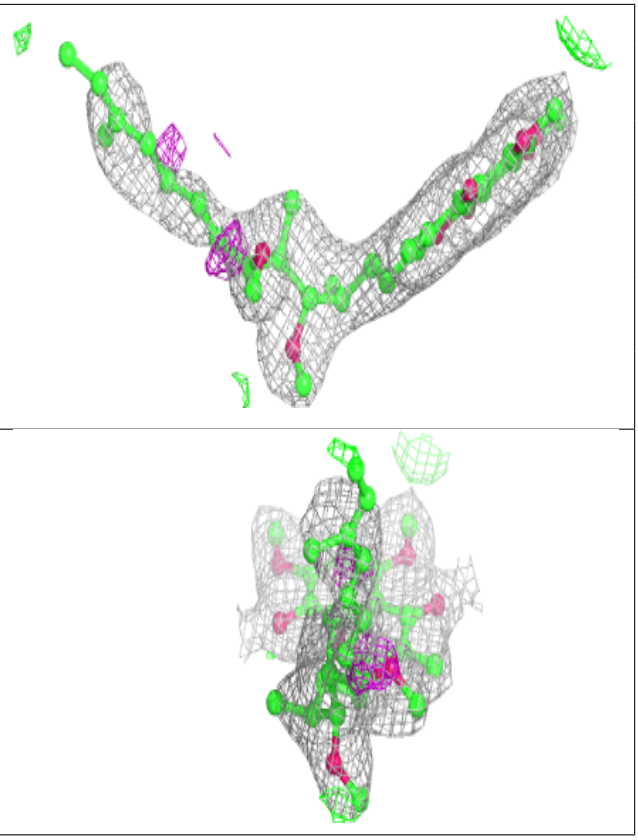
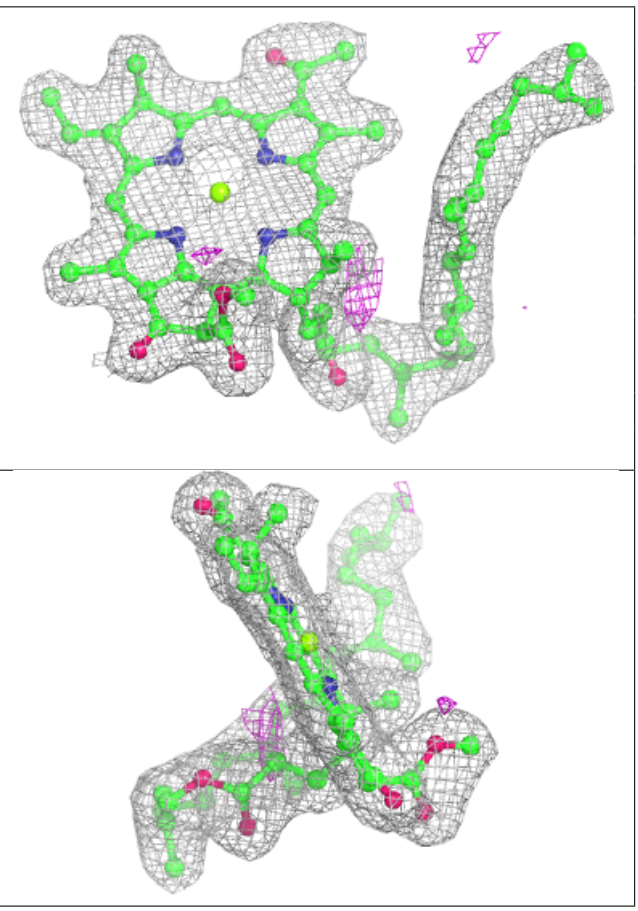
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BCB L 1275:

$2mF_o$-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 1324:

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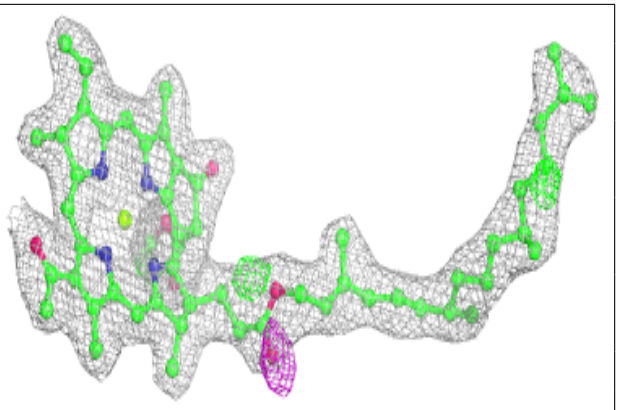
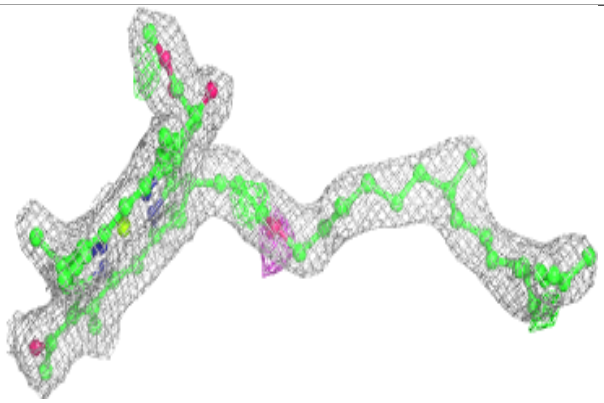
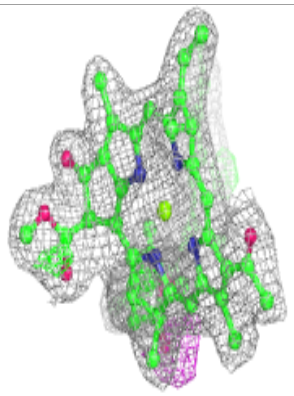
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around BPB L 1276:

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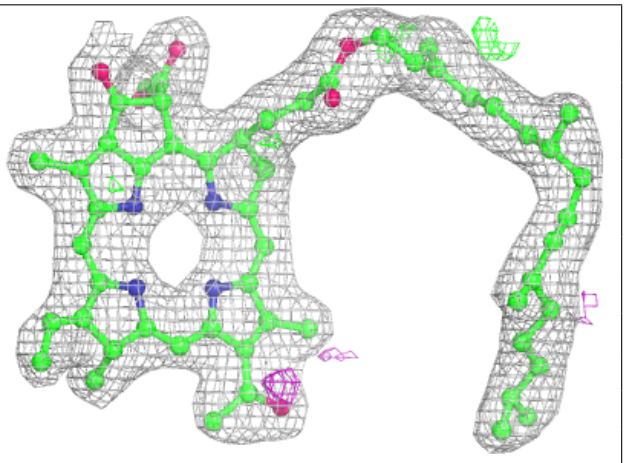
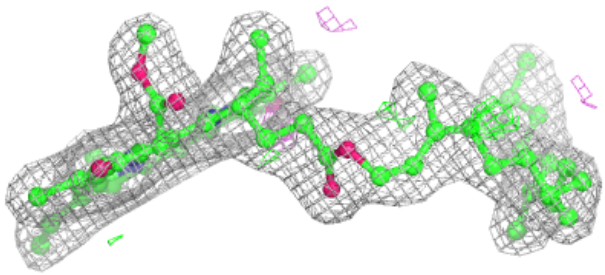
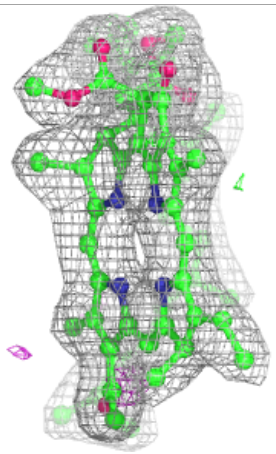
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around HEC C 1333:

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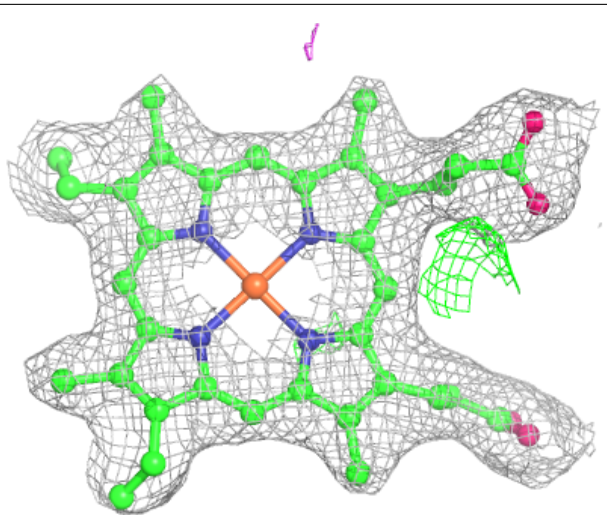
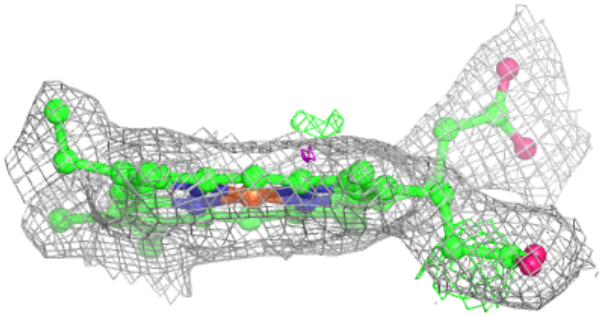
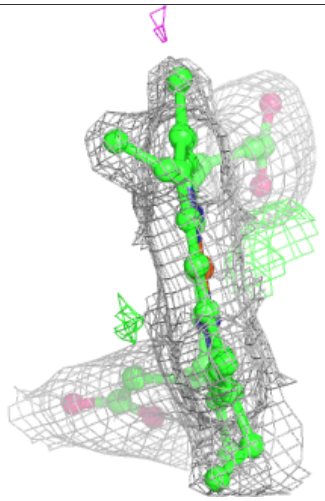
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

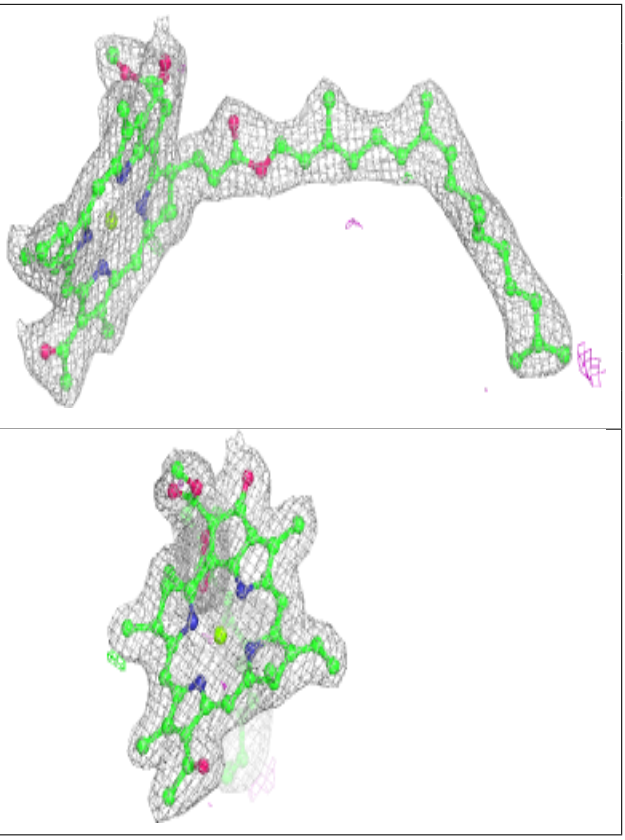






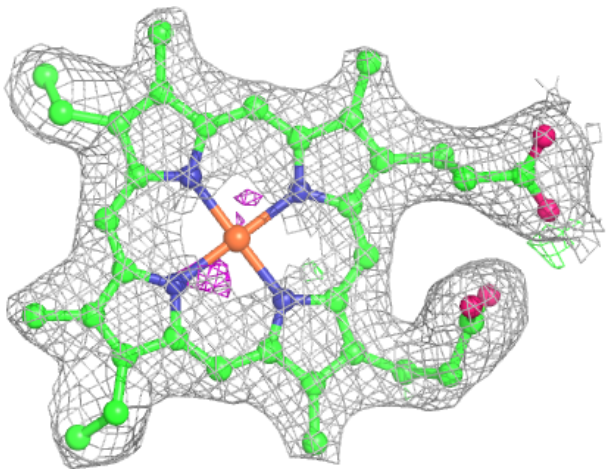
Electron density around BCB L 1274:

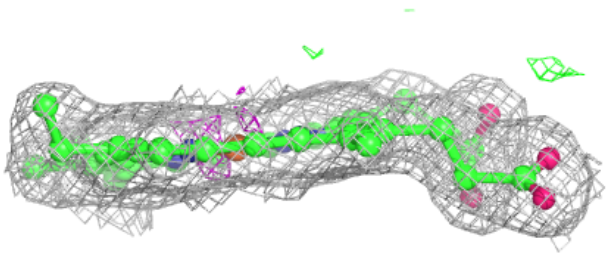
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

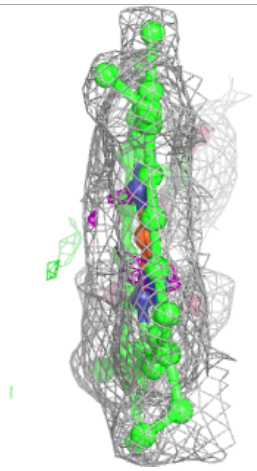


Electron density around HEC C 1334:

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

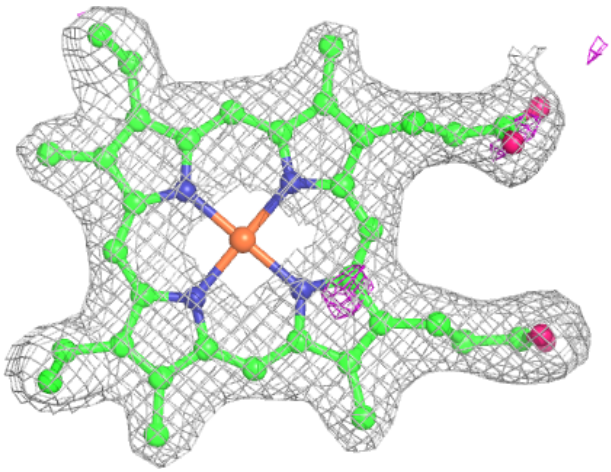


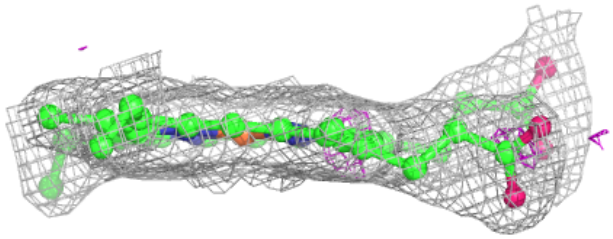


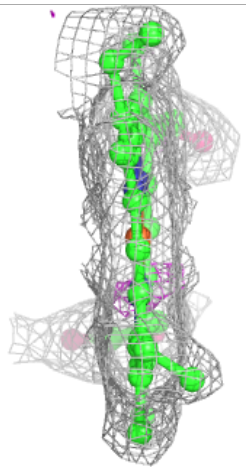


Electron density around HEC C 1336:

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

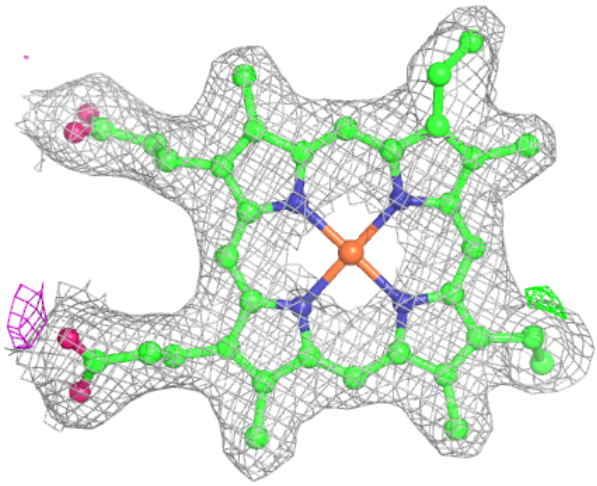


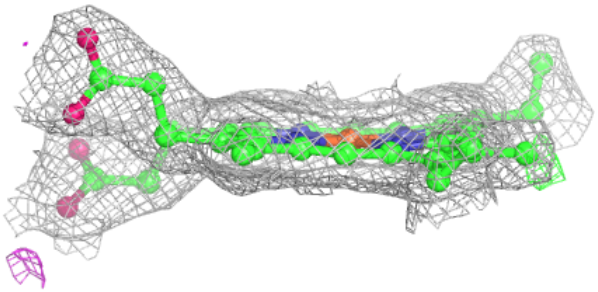


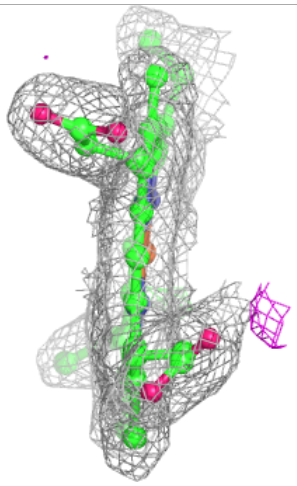


Electron density around HEC C 1335:

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.