wwPDB X-ray Structure Validation Summary Report (i)

Jan 20, 2024 – 04:53 pm GMT

PDB ID	:	7Q7P
Title	:	LIPIDIC CUBIC PHASE SERIAL FEMTOSECOND CRYSTALLOGRAPHY STRUCTURE OF A PHOTOSYNTHETIC REACTION CENTRE
Authors	:	Baath, P.; Banacore, A.; Neutze, R.
Deposited on	:	2021-11-09
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:

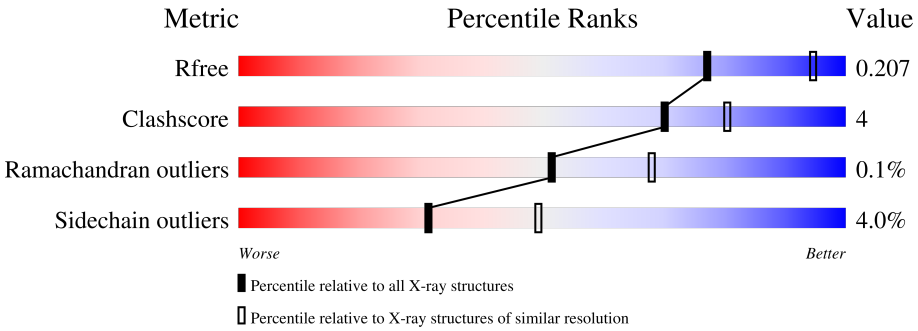
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

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%

Mol	Chain	Length	Quality of chain
1	CCC	356	86% 7% 7%
2	HHH	258	83% 12% • •
3	LLL	273	93% 6% •
4	MMM	323	94% 6% •

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
10	BCB	LLL	301	X	-	-	-
10	BCB	LLL	302	X	-	-	-
10	BCB	MMM	403	X	-	-	-
10	BCB	MMM	404	X	-	-	-
11	BPB	LLL	303	X	-	-	-
11	BPB	MMM	405	X	-	-	-
6	DGA	CCC	405	X	-	-	-

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 10442 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	CCC	332	2618	1649	471	480	18	0	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	HHH	247	1941	1242	332	365	2	0	0	0

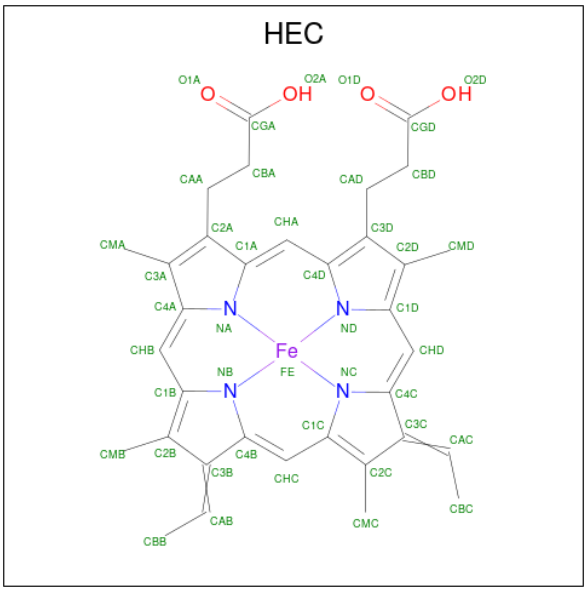
- Molecule 3 is a protein called Reaction center protein L chain.

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

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

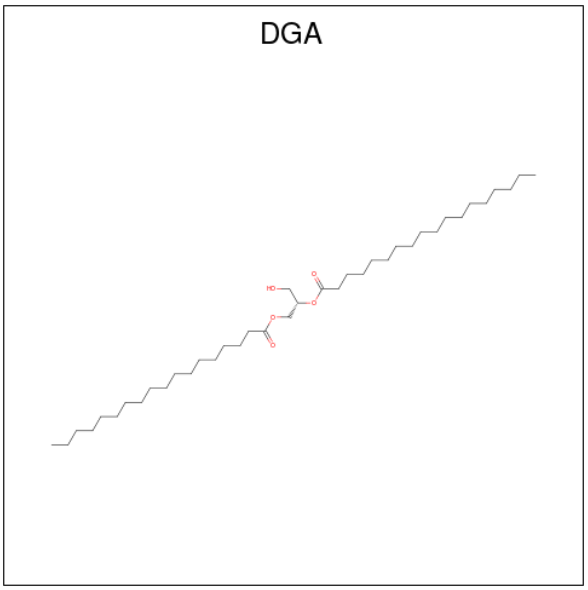
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	MMM	323	2555	1702	419	423	11	0	0	0

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



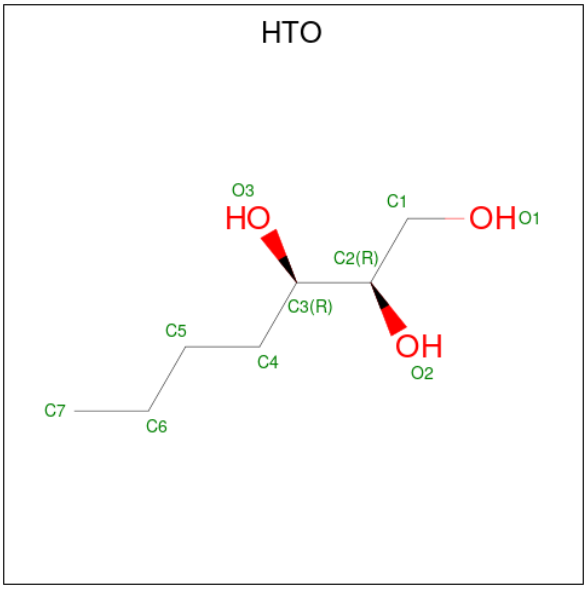
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	CCC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	CCC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	CCC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	CCC	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



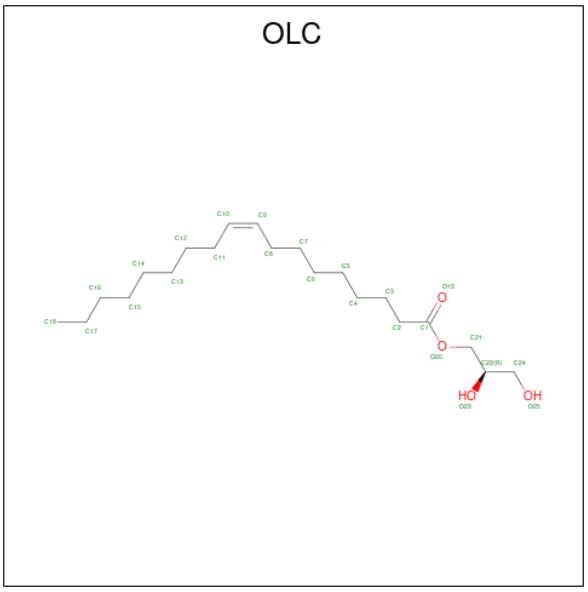
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	CCC	1	Total C O 44 39 5	41	0

- Molecule 7 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



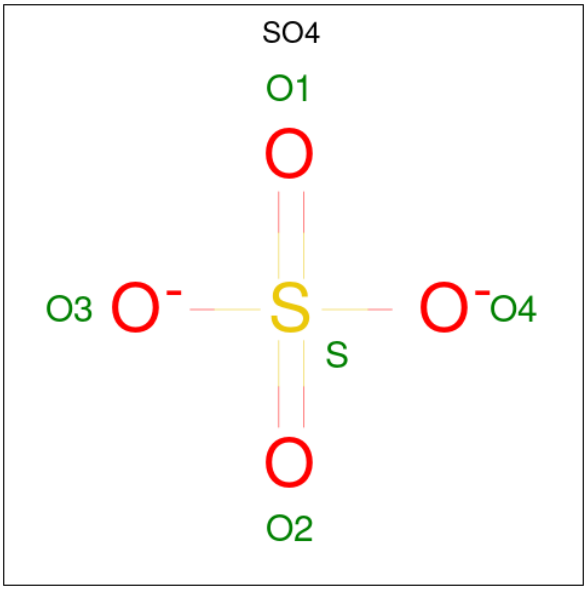
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	HHH	1	Total C O 10 7 3	0	0
7	LLL	1	Total C O 10 7 3	0	0
7	LLL	1	Total C O 10 7 3	0	0
7	LLL	1	Total C O 10 7 3	0	0
7	LLL	1	Total C O 10 7 3	0	0
7	LLL	1	Total C O 10 7 3	0	0
7	MMM	1	Total C O 10 7 3	0	0
7	MMM	1	Total C O 10 7 3	0	0
7	MMM	1	Total C O 10 7 3	0	0

- Molecule 8 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	HHH	1	Total C O 25 21 4	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	HHH	1	Total O S 5 4 1	0	0
9	LLL	1	Total O S 5 4 1	0	0
9	MMM	1	Total O S 5 4 1	0	0

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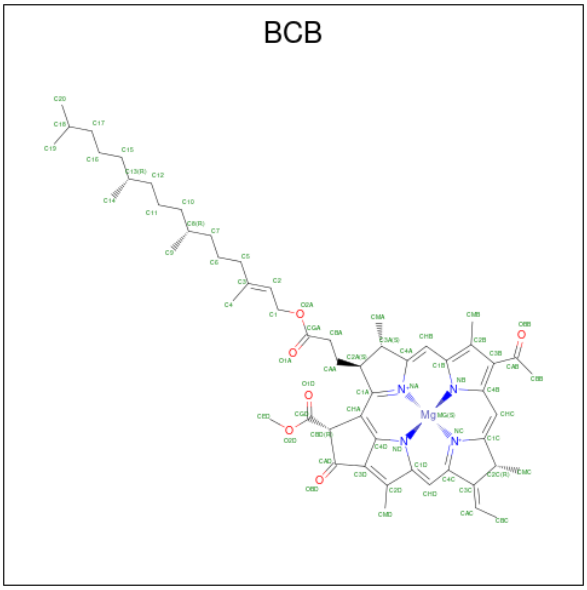
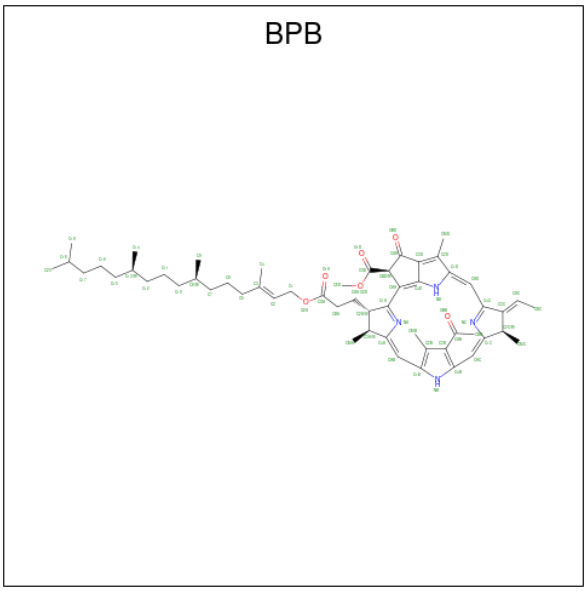
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	MMM	1	Total O S 5 4 1	0	0
9	MMM	1	Total O S 5 4 1	0	0
9	MMM	1	Total O S 5 4 1	0	0

- Molecule 10 is BACTERIOCHLOROPHYLL B (three-letter code: BCB) (formula: $C_{55}H_{72}MgN_4O_6$).



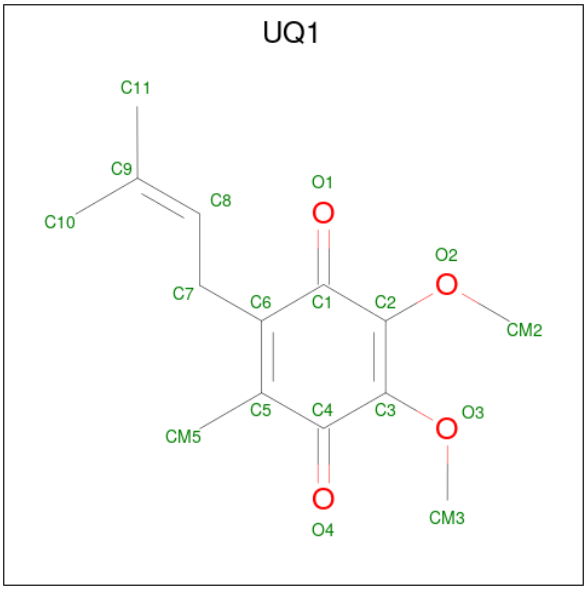
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	LLL	1	Total C Mg N O 66 55 1 4 6	0	0
10	LLL	1	Total C Mg N O 66 55 1 4 6	0	0
10	MMM	1	Total C Mg N O 66 55 1 4 6	0	0
10	MMM	1	Total C Mg N O 66 55 1 4 6	0	0

- Molecule 11 is BACTERIOPHEOPHYTIN B (three-letter code: BPB) (formula: $C_{55}H_{74}N_4O_6$).



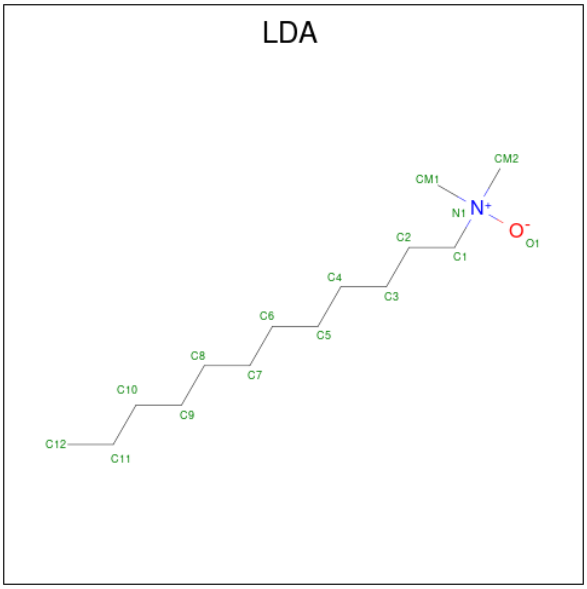
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	LLL	1	Total	C	N	O	0	0
			65	55	4	6		
11	MMM	1	Total	C	N	O	0	0
			65	55	4	6		

- Molecule 12 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	LLL	1	Total	C	O		0	0
			18	14	4			
12	LLL	1	Total	C	O		0	0
			18	14	4			

- Molecule 13 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

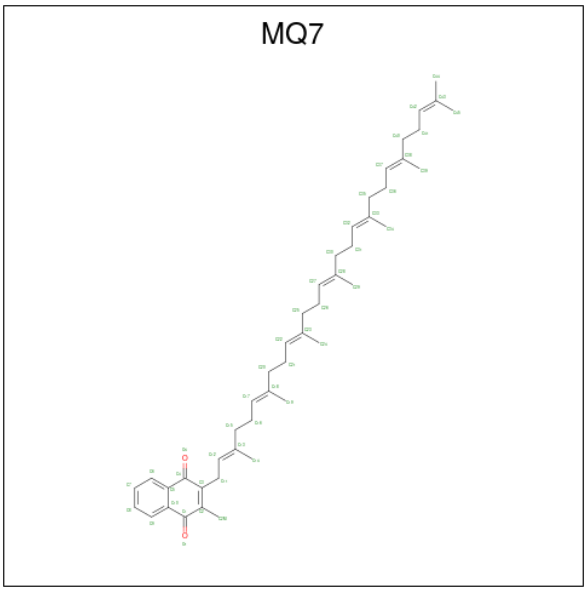


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	LLL	1	Total C N O 16 14 1 1	0	0
13	MMM	1	Total C N O 16 14 1 1	0	0

- Molecule 14 is FE (II) ION (three-letter code: FE2) (formula: Fe).

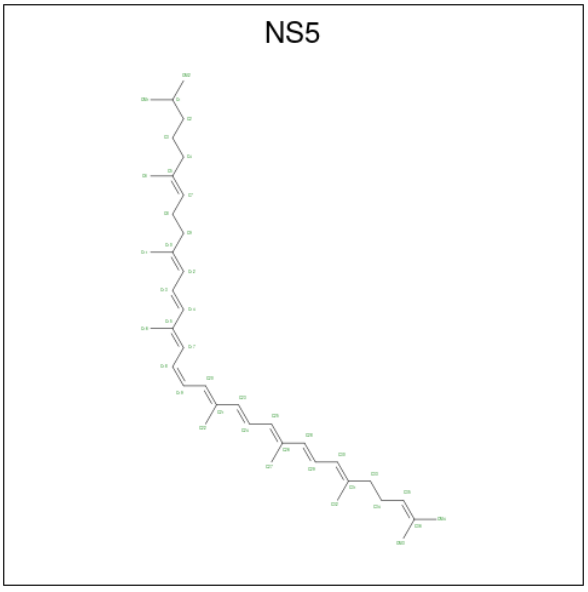
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	MMM	1	Total Fe 1 1	0	0

- Molecule 15 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	MMM	1	Total C O 48 46 2	0	0

- Molecule 16 is 15-cis-1,2-dihydroneurosporene (three-letter code: NS5) (formula: $C_{40}H_{60}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	MMM	1	Total C 40 40	0	0

- Molecule 17 is water.

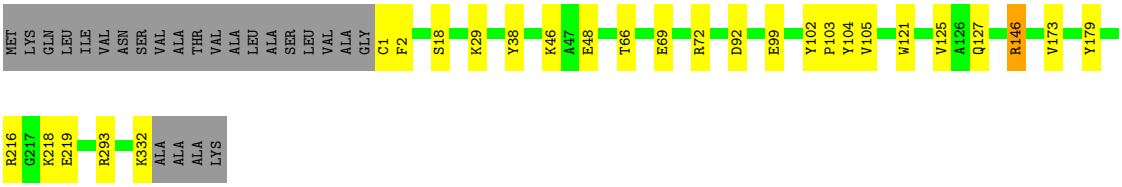
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	CCC	95	Total O 95 95	0	0
17	HHH	43	Total O 43 43	0	0
17	LLL	42	Total O 42 42	0	0
17	MMM	64	Total O 64 64	0	0

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

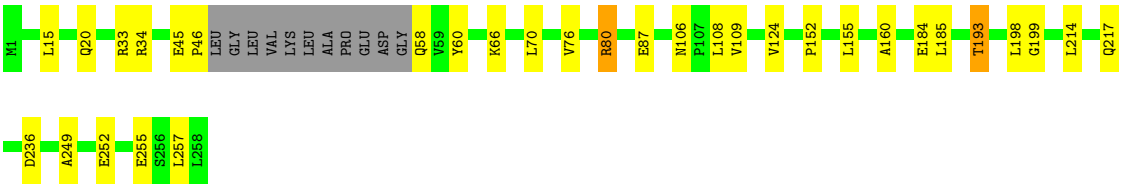
• Molecule 1: Photosynthetic reaction center cytochrome c subunit

Chain CCC:



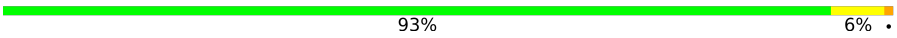
• Molecule 2: Reaction center protein H chain

Chain HHH:



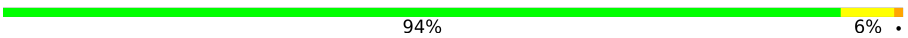
• Molecule 3: Reaction center protein L chain

Chain LLL:



• Molecule 4: Reaction center protein M chain

Chain MMM:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	84.90Å 125.30Å 182.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.92 – 2.40 73.82 – 0.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.92-2.40) 4.0 (73.82-0.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.165 , 0.204 0.175 , 0.207	Depositor DCC
R_{free} test set	10006 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 91.5	EDS
L-test for twinning[1]	$< \|L\| >$ = (Not available), $< L^2 >$ = (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	10442	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

[1]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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BPB, UQ1, NS5, BCB, FE2, LDA, FME, OLC, HTO, DGA, MQ7, HEC, SO4

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	CCC	0.68	0/2688	0.80	0/3662
2	HHH	0.66	0/1976	0.81	0/2698
3	LLL	0.66	0/2267	0.75	0/3095
4	MMM	0.64	0/2659	0.76	0/3637
All	All	0.66	0/9590	0.78	0/13092

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CCC	2618	0	2596	11	0
2	HHH	1941	0	1936	16	0
3	LLL	2172	0	2097	15	0
4	MMM	2555	0	2452	11	0
5	CCC	172	0	120	5	0
6	CCC	44	0	69	0	0
7	HHH	10	0	16	0	0
7	LLL	50	0	80	0	0
7	MMM	30	0	48	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	HHH	25	0	40	3	0
9	HHH	5	0	0	0	0
9	LLL	5	0	0	0	0
9	MMM	20	0	0	1	0
10	LLL	132	0	144	9	0
10	MMM	132	0	144	2	0
11	LLL	65	0	74	2	0
11	MMM	65	0	74	6	0
12	LLL	36	0	36	2	0
13	LLL	16	0	31	0	0
13	MMM	16	0	31	0	0
14	MMM	1	0	0	0	0
15	MMM	48	0	64	2	0
16	MMM	40	0	60	5	0
17	CCC	95	0	0	0	0
17	HHH	43	0	0	1	0
17	LLL	42	0	0	0	0
17	MMM	64	0	0	2	0
All	All	10442	0	10112	72	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 72 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)
11:MMM:405:BPB:HHC	11:MMM:405:BPB:HBBB	1.62	0.80
4:MMM:159:GLY:HA3	16:MMM:406:NS5:H272	1.68	0.76
3:LLL:181:PHE:HB3	11:MMM:405:BPB:HBBA	1.69	0.74
11:LLL:303:BPB:HBBB	11:LLL:303:BPB:HMB	1.69	0.74
3:LLL:132:GLN:HE22	3:LLL:146:PHE:H	1.32	0.73

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CCC	332/356 (93%)	317 (96%)	15 (4%)	0	100	100
2	HHH	243/258 (94%)	233 (96%)	10 (4%)	0	100	100
3	LLL	272/273 (100%)	265 (97%)	7 (3%)	0	100	100
4	MMM	321/323 (99%)	313 (98%)	7 (2%)	1 (0%)	41	55
All	All	1168/1210 (96%)	1128 (97%)	39 (3%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	MMM	193	ASN

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	CCC	283/297 (95%)	269 (95%)	14 (5%)	25	40
2	HHH	204/212 (96%)	191 (94%)	13 (6%)	17	28
3	LLL	219/218 (100%)	214 (98%)	5 (2%)	50	70
4	MMM	249/249 (100%)	242 (97%)	7 (3%)	43	63
All	All	955/976 (98%)	916 (96%)	39 (4%)	31	48

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	LLL	20	ASP
4	MMM	194	PHE
3	LLL	21	LEU
4	MMM	51	LEU
4	MMM	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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	HHH	1	2	8,9,10	0.45	0	7,9,11	0.89	0

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 1 is monoatomic - leaving 33 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	HTO	MMM	408	-	9,9,9	0.72	0	10,10,10	0.99	1 (10%)
11	BPB	LLL	303	-	49,70,70	1.94	10 (20%)	47,101,101	1.81	7 (14%)
5	HEC	CCC	403	1	32,50,50	1.59	5 (15%)	24,82,82	1.57	7 (29%)
10	BCB	MMM	403	-	63,74,74	1.72	14 (22%)	74,115,115	2.86	27 (36%)
9	SO4	HHH	403	-	4,4,4	0.37	0	6,6,6	0.13	0
12	UQ1	LLL	309	-	18,18,18	2.32	3 (16%)	22,25,25	1.64	4 (18%)
13	LDA	LLL	311	-	12,15,15	0.29	0	14,17,17	0.34	0
7	HTO	LLL	312	-	9,9,9	0.94	0	10,10,10	1.49	2 (20%)
15	MQ7	MMM	402	-	49,49,49	1.36	3 (6%)	60,63,63	1.07	3 (5%)
5	HEC	CCC	404	1	32,50,50	1.50	4 (12%)	24,82,82	2.21	9 (37%)
7	HTO	LLL	305	-	9,9,9	0.73	0	10,10,10	1.20	1 (10%)
6	DGA	CCC	405	-	43,43,43	4.46	4 (9%)	45,45,45	4.51	8 (17%)
9	SO4	MMM	414	-	4,4,4	0.37	0	6,6,6	0.07	0
7	HTO	MMM	409	-	9,9,9	0.88	0	10,10,10	1.01	1 (10%)
9	SO4	MMM	412	-	4,4,4	0.34	0	6,6,6	0.13	0
10	BCB	LLL	301	-	63,74,74	1.75	14 (22%)	74,115,115	3.00	25 (33%)
16	NS5	MMM	406	-	39,39,39	0.95	0	44,46,46	1.68	10 (22%)
10	BCB	LLL	302	-	63,74,74	1.72	13 (20%)	74,115,115	2.93	18 (24%)
7	HTO	LLL	306	-	9,9,9	0.69	0	10,10,10	0.95	0
5	HEC	CCC	402	1	32,50,50	1.62	4 (12%)	24,82,82	2.25	7 (29%)
7	HTO	MMM	407	-	9,9,9	0.97	0	10,10,10	1.29	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	SO4	LLL	308	-	4,4,4	0.37	0	6,6,6	0.04	0
8	OLC	HHH	402	-	24,24,24	1.19	1 (4%)	25,25,25	1.37	3 (12%)
5	HEC	CCC	401	1	32,50,50	1.80	5 (15%)	24,82,82	1.82	3 (12%)
7	HTO	LLL	307	-	9,9,9	0.98	0	10,10,10	1.01	2 (20%)
9	SO4	MMM	411	-	4,4,4	0.33	0	6,6,6	0.07	0
10	BCB	MMM	404	-	63,74,74	1.73	13 (20%)	74,115,115	3.02	25 (33%)
11	BPB	MMM	405	-	49,70,70	1.99	9 (18%)	47,101,101	2.54	15 (31%)
12	UQ1	LLL	310	-	18,18,18	2.57	3 (16%)	22,25,25	1.46	6 (27%)
7	HTO	HHH	401	-	9,9,9	0.94	0	10,10,10	0.70	0
9	SO4	MMM	413	-	4,4,4	0.36	0	6,6,6	0.07	0
13	LDA	MMM	410	-	12,15,15	0.28	0	14,17,17	0.34	0
7	HTO	LLL	304	-	9,9,9	0.81	0	10,10,10	0.76	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	BPB	LLL	303	-	1/1/18/23	9/37/105/105	0/5/6/6
7	HTO	MMM	408	-	-	4/10/10/10	-
10	BCB	MMM	403	-	3/3/21/26	9/37/137/137	-
5	HEC	CCC	403	1	-	0/10/54/54	-
12	UQ1	LLL	309	-	-	0/9/33/33	0/1/1/1
13	LDA	LLL	311	-	-	5/13/13/13	-
7	HTO	LLL	312	-	-	3/10/10/10	-
15	MQ7	MMM	402	-	-	2/41/61/61	0/2/2/2
5	HEC	CCC	404	1	-	3/10/54/54	-
7	HTO	LLL	305	-	-	6/10/10/10	-
6	DGA	CCC	405	-	1/1/3/3	28/45/45/45	-
7	HTO	MMM	409	-	-	5/10/10/10	-
10	BCB	LLL	301	-	3/3/21/26	8/37/137/137	-
16	NS5	MMM	406	-	-	6/43/43/43	-
10	BCB	LLL	302	-	3/3/21/26	7/37/137/137	-
7	HTO	LLL	306	-	-	6/10/10/10	-
5	HEC	CCC	402	1	-	4/10/54/54	-
7	HTO	MMM	407	-	-	6/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	OLC	HHH	402	-	-	8/24/24/24	-
5	HEC	CCC	401	1	-	4/10/54/54	-
7	HTO	LLL	307	-	-	6/10/10/10	-
10	BCB	MMM	404	-	3/3/21/26	11/37/137/137	-
11	BPB	MMM	405	-	1/1/18/23	11/37/105/105	0/5/6/6
12	UQ1	LLL	310	-	-	3/9/33/33	0/1/1/1
7	HTO	HHH	401	-	-	5/10/10/10	-
13	LDA	MMM	410	-	-	11/13/13/13	-
7	HTO	LLL	304	-	-	4/10/10/10	-

The worst 5 of 105 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	CCC	405	DGA	OG1-CG1	-20.66	0.98	1.45
6	CCC	405	DGA	CG1-CG2	-13.44	1.09	1.50
6	CCC	405	DGA	OG2-CG2	-12.10	1.16	1.46
6	CCC	405	DGA	CB2-CB1	-9.70	1.22	1.50
12	LLL	310	UQ1	C6-C5	8.95	1.51	1.35

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	LLL	302	BCB	C1C-NC-C4C	-18.18	98.53	106.71
10	LLL	301	BCB	C1C-NC-C4C	-17.82	98.70	106.71
10	MMM	404	BCB	C1C-NC-C4C	-15.67	99.66	106.71
10	MMM	403	BCB	C1C-NC-C4C	-15.45	99.76	106.71
6	CCC	405	DGA	OG2-CG2-CG3	-14.69	55.66	108.36

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	CCC	405	DGA	CG2
10	LLL	301	BCB	ND
10	LLL	301	BCB	NA
10	LLL	301	BCB	NC
10	LLL	302	BCB	ND

5 of 174 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	CCC	405	DGA	CB2-CB1-OG2-CG2
6	CCC	405	DGA	CG1-CG2-CG3-OXT
7	HHH	401	HTO	C1-C2-C3-O3
7	HHH	401	HTO	C1-C2-C3-C4
7	HHH	401	HTO	O2-C2-C3-O3

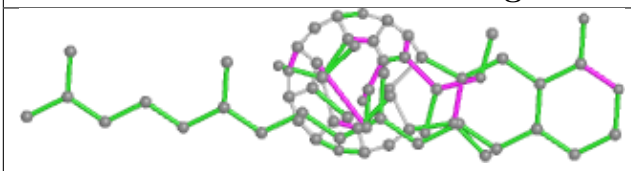
There are no ring outliers.

14 monomers are involved in 35 short contacts:

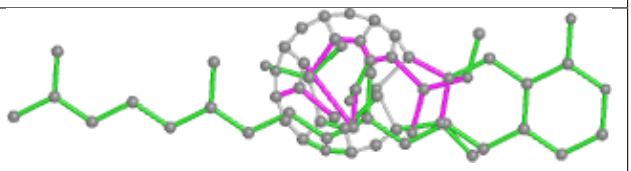
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	LLL	303	BPB	2	0
5	CCC	403	HEC	2	0
10	MMM	403	BCB	1	0
12	LLL	309	UQ1	2	0
15	MMM	402	MQ7	2	0
10	LLL	301	BCB	7	0
16	MMM	406	NS5	5	0
10	LLL	302	BCB	2	0
5	CCC	402	HEC	1	0
8	HHH	402	OLC	3	0
5	CCC	401	HEC	2	0
9	MMM	411	SO4	1	0
10	MMM	404	BCB	1	0
11	MMM	405	BPB	6	0

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

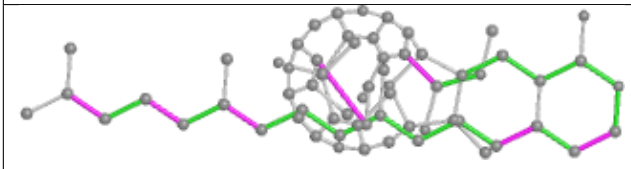
Ligand BPB LLL 303



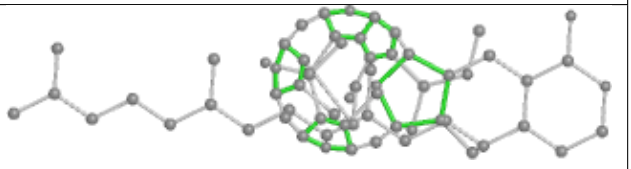
Bond lengths



Bond angles

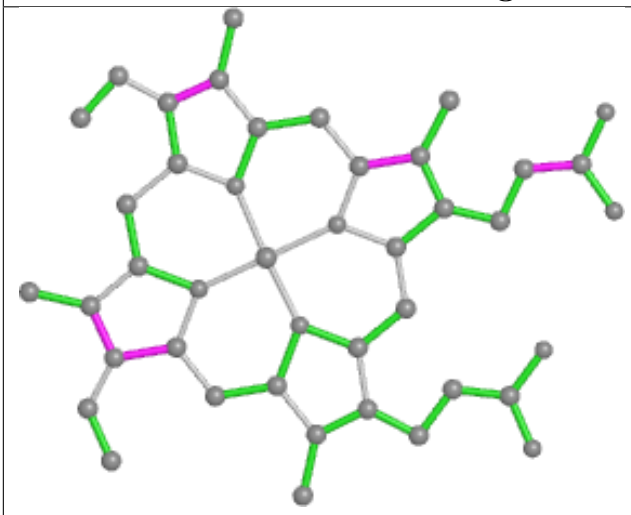


Torsions

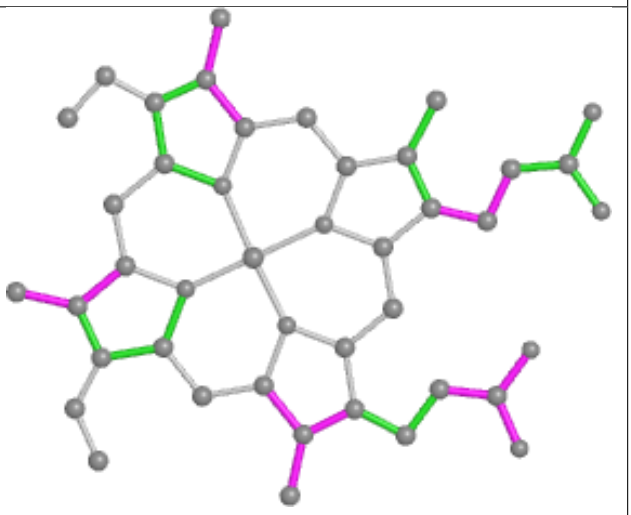


Rings

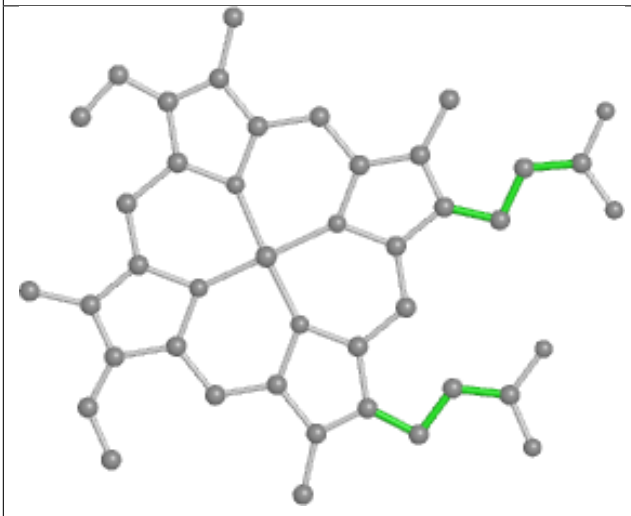
Ligand HEC CCC 403



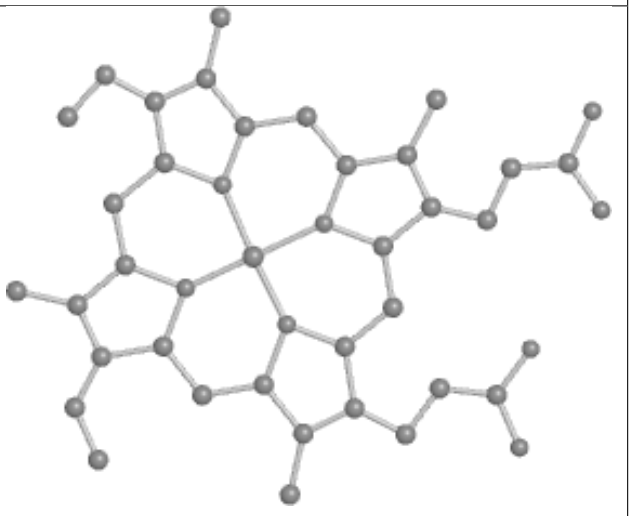
Bond lengths



Bond angles

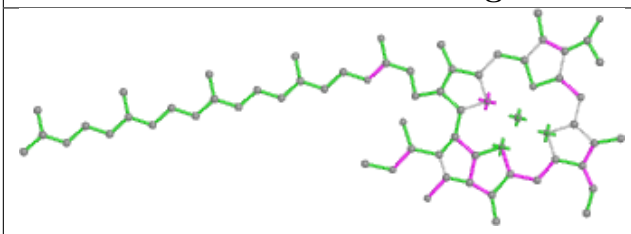


Torsions

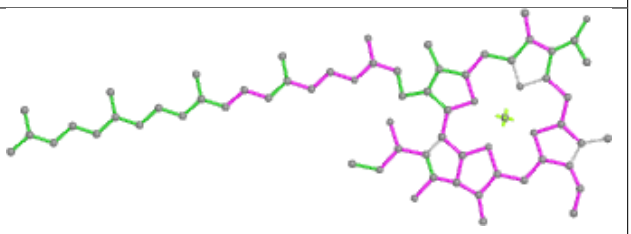


Rings

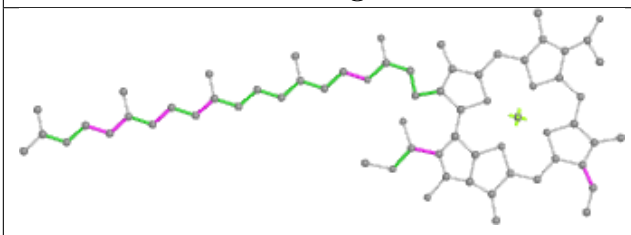
Ligand BCB MMM 403



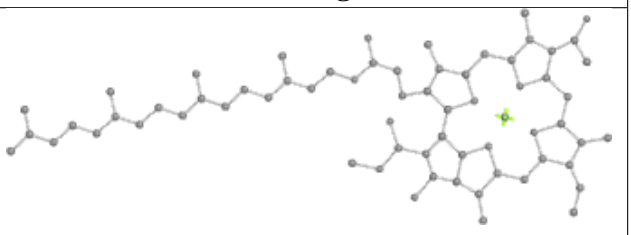
Bond lengths



Bond angles

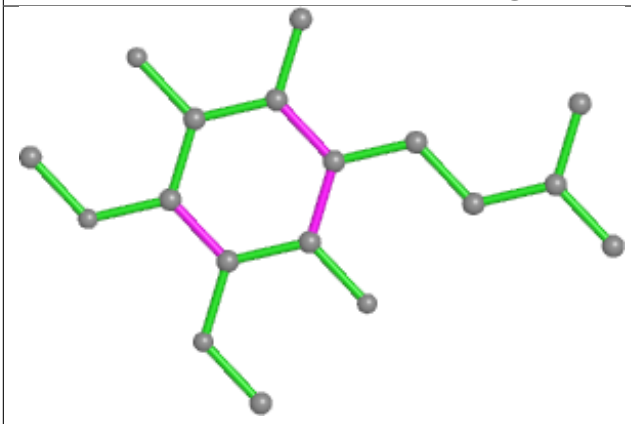


Torsions

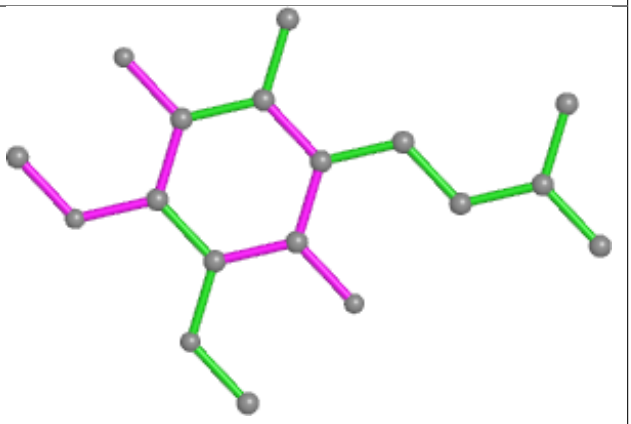


Rings

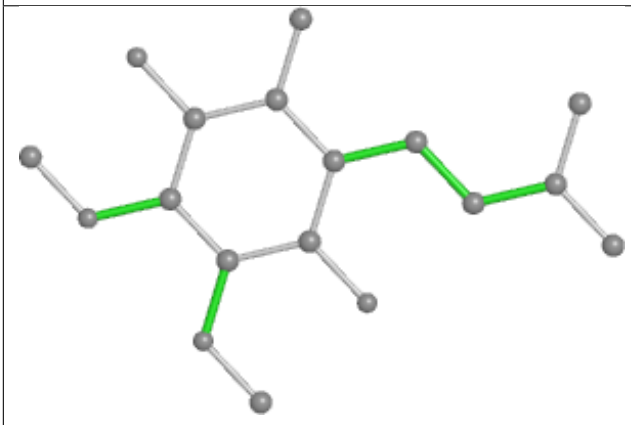
Ligand UQ1 LLL 309



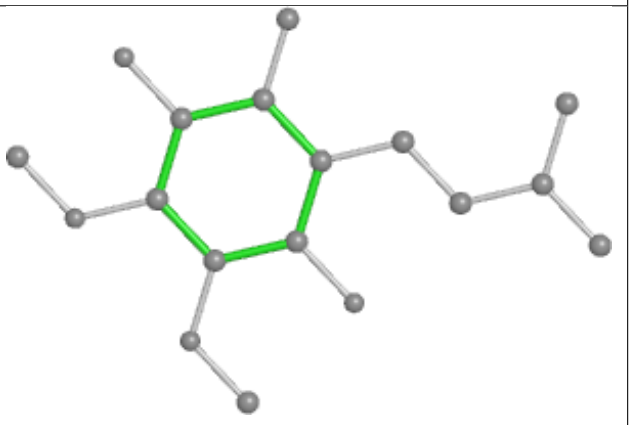
Bond lengths



Bond angles

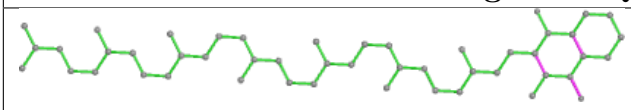


Torsions

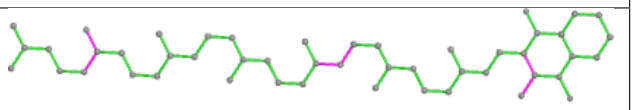


Rings

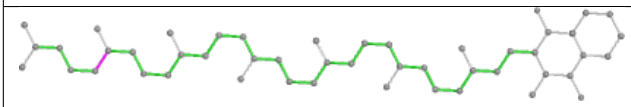
Ligand MQ7 MMM 402



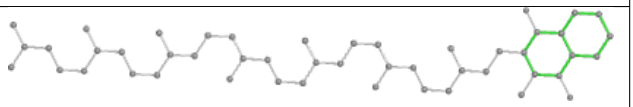
Bond lengths



Bond angles

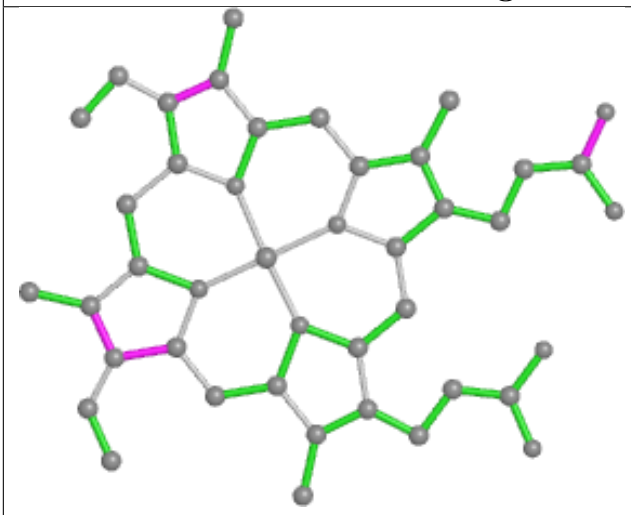


Torsions

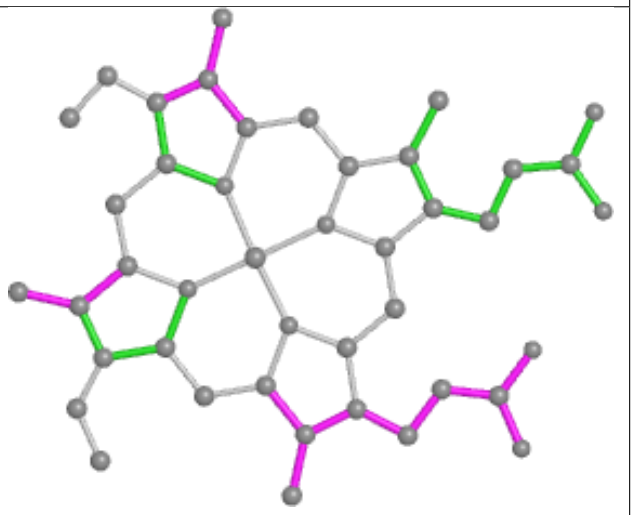


Rings

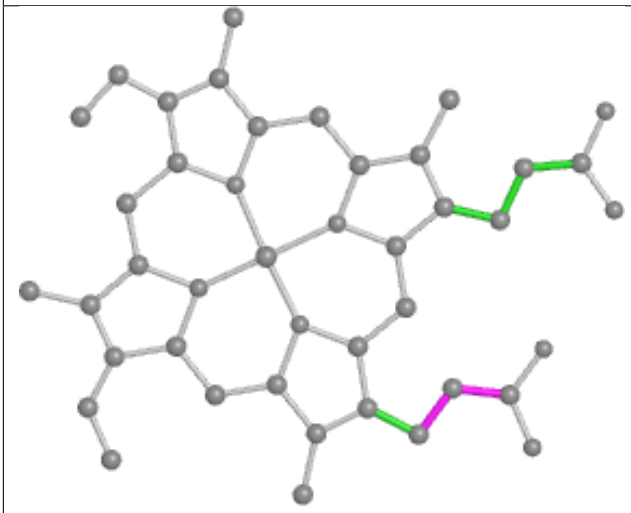
Ligand HEC CCC 404



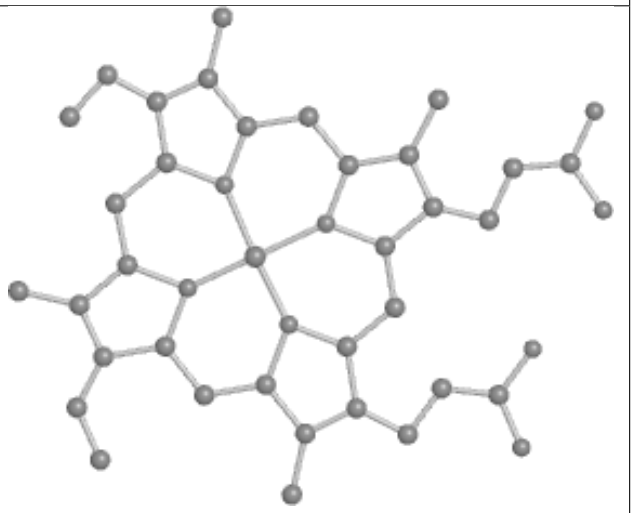
Bond lengths



Bond angles

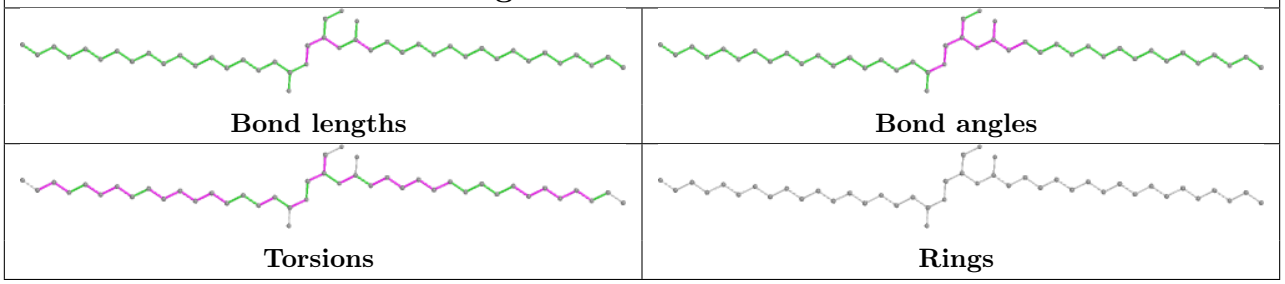


Torsions

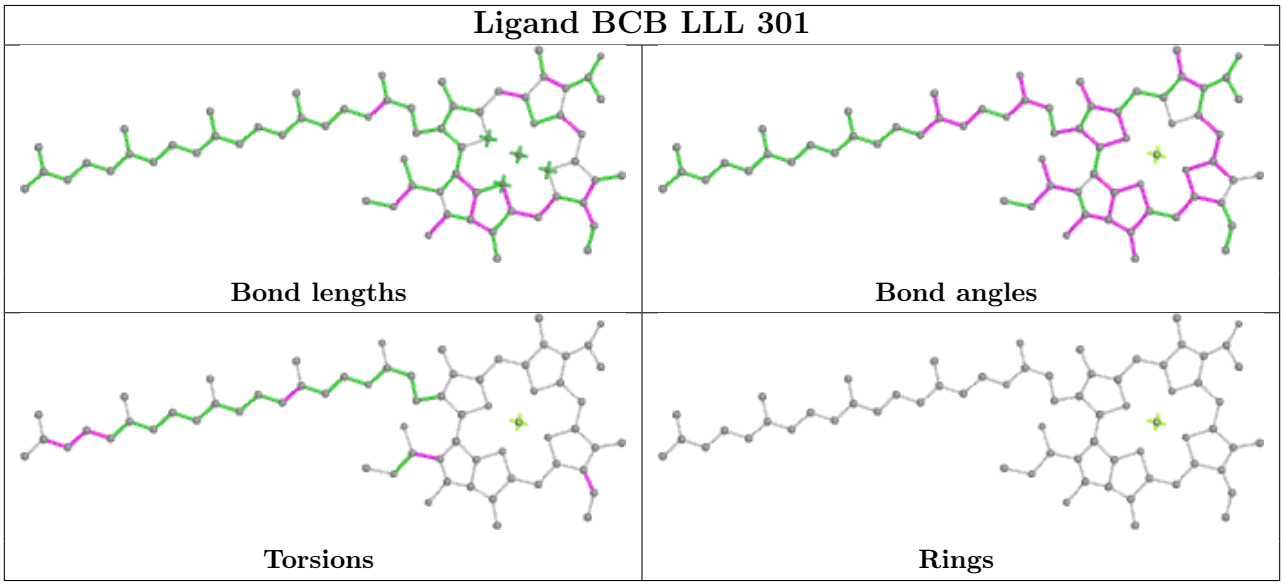


Rings

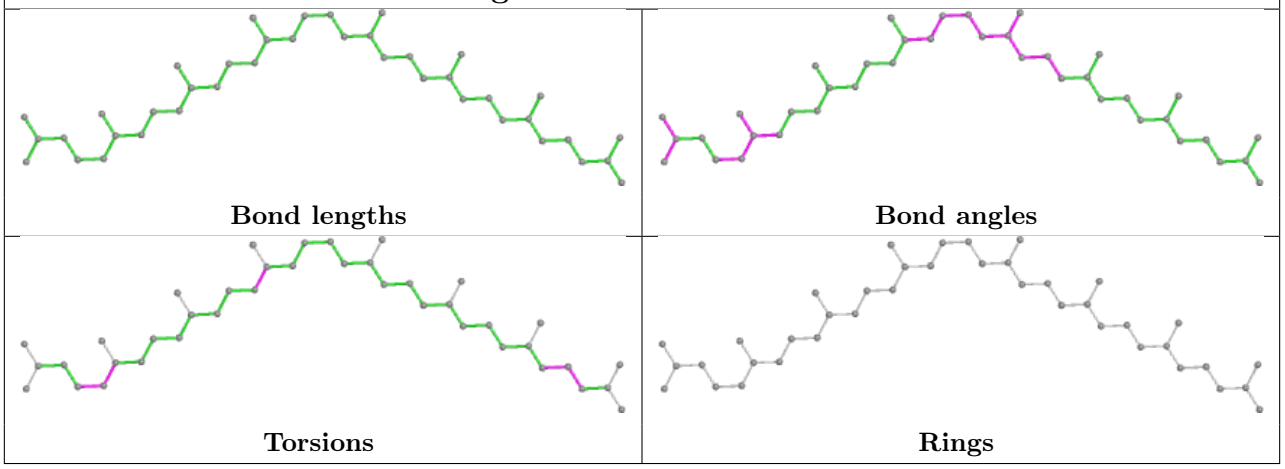
Ligand DGA CCC 405



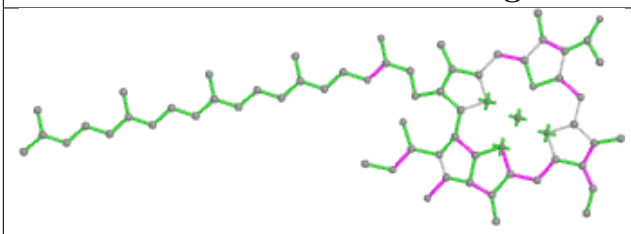
Ligand BCB LLL 301



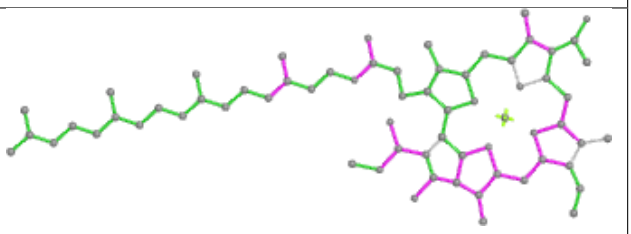
Ligand NS5 MMM 406



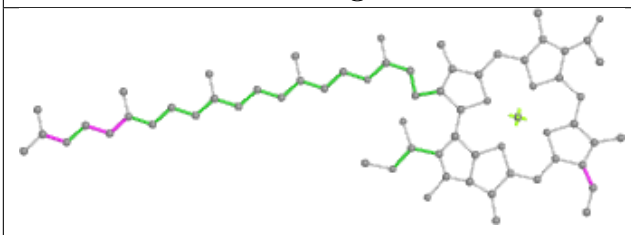
Ligand BCB LLL 302



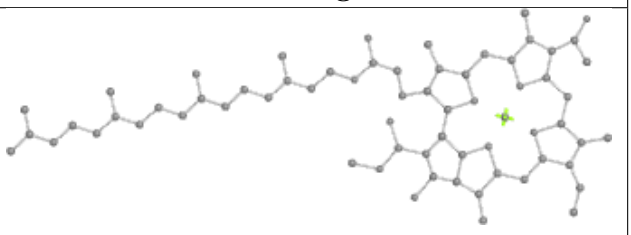
Bond lengths



Bond angles

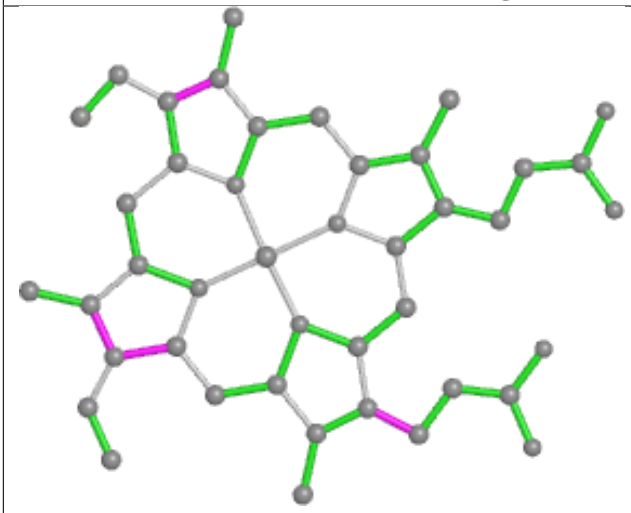


Torsions

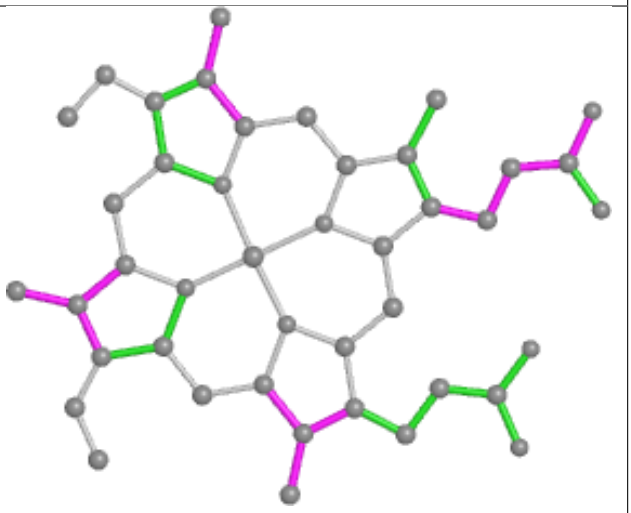


Rings

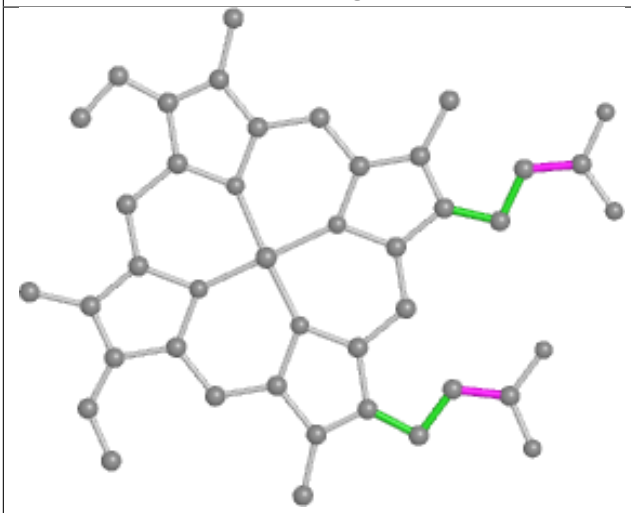
Ligand HEC CCC 402



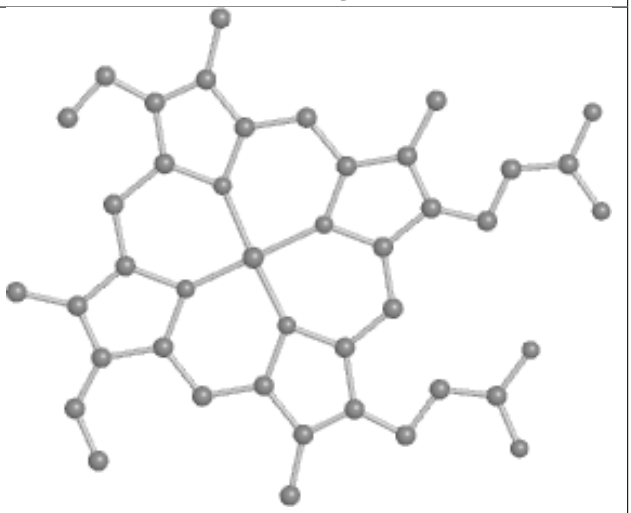
Bond lengths



Bond angles

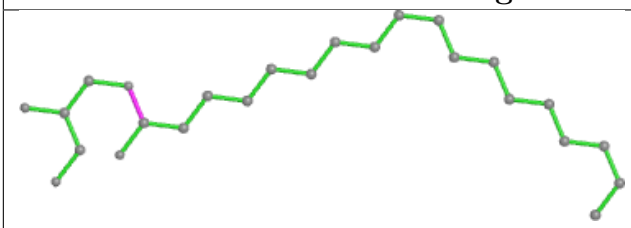


Torsions

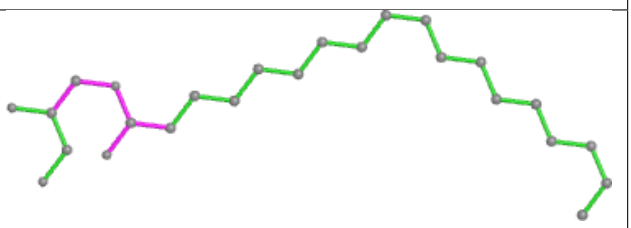


Rings

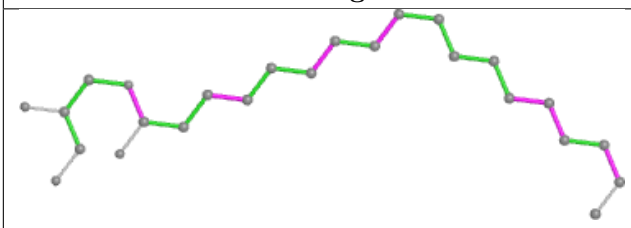
Ligand OLC HHH 402



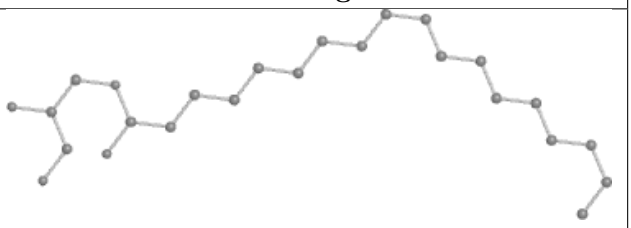
Bond lengths



Bond angles

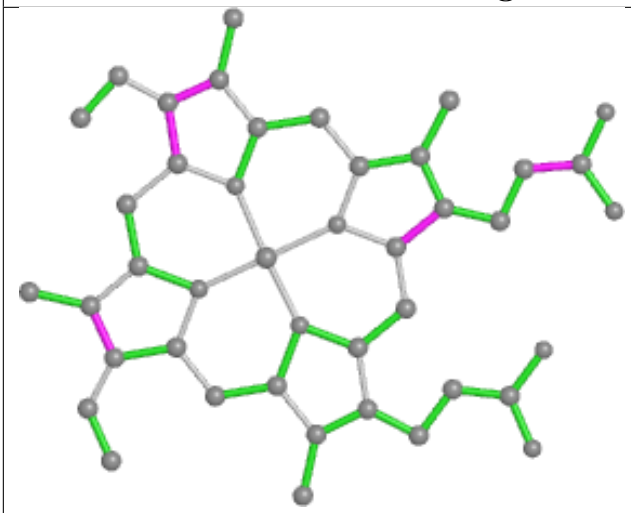


Torsions

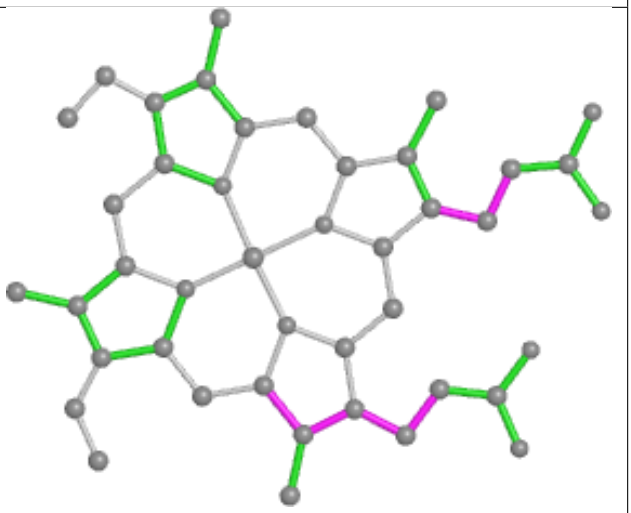


Rings

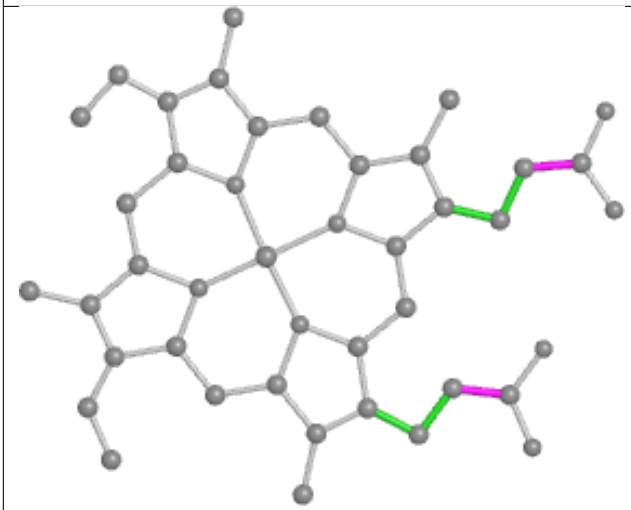
Ligand HEC CCC 401



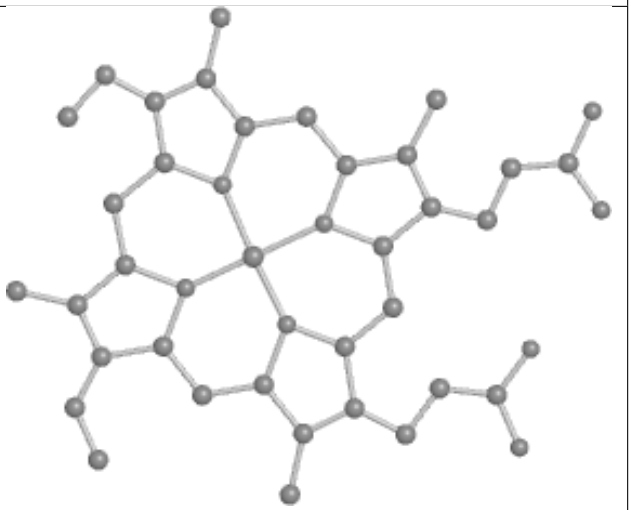
Bond lengths



Bond angles

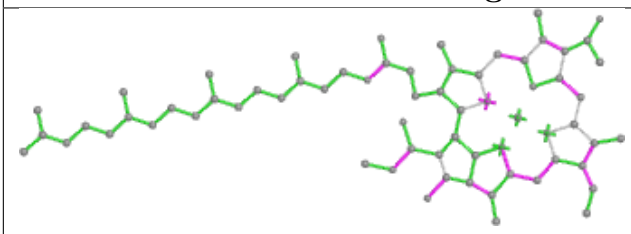


Torsions

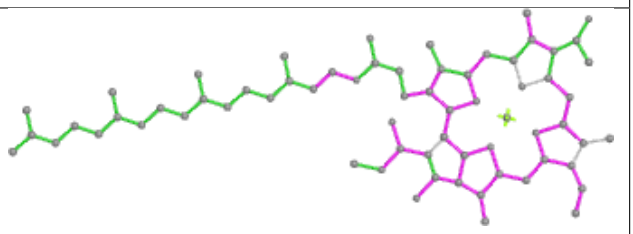


Rings

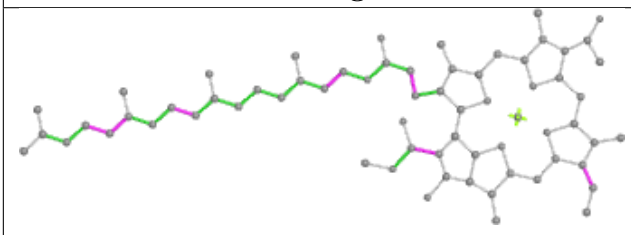
Ligand BCB MMM 404



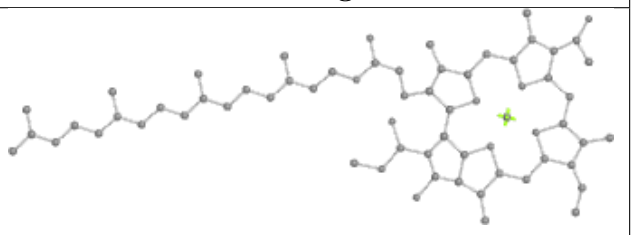
Bond lengths



Bond angles

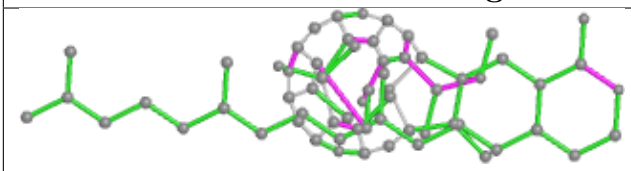


Torsions

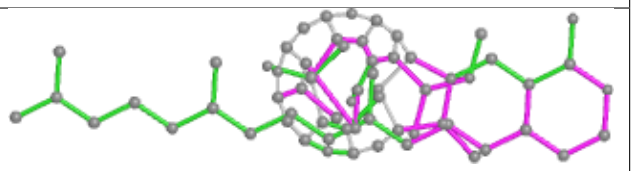


Rings

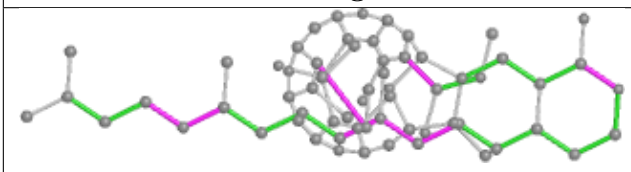
Ligand BPB MMM 405



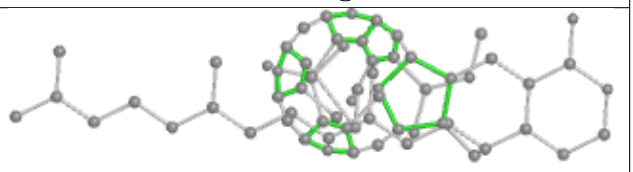
Bond lengths



Bond angles

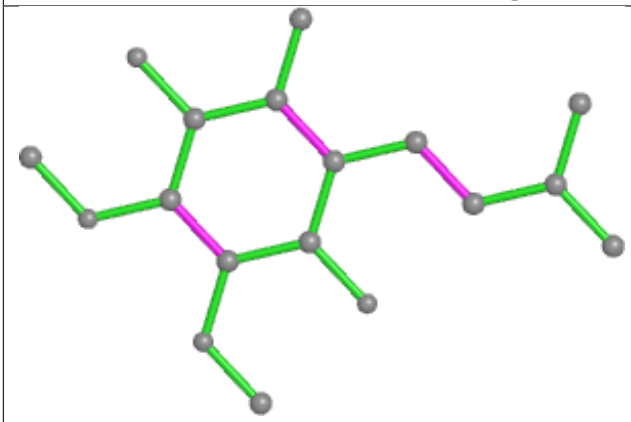


Torsions

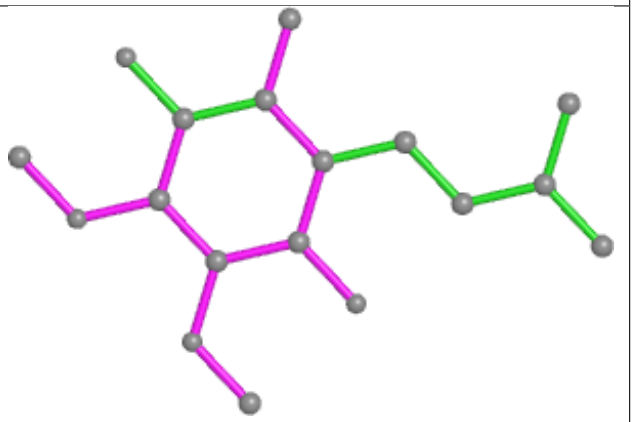


Rings

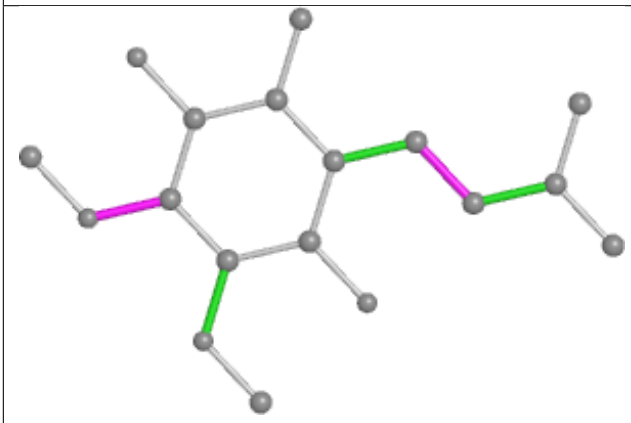
Ligand UQ1 LLL 310



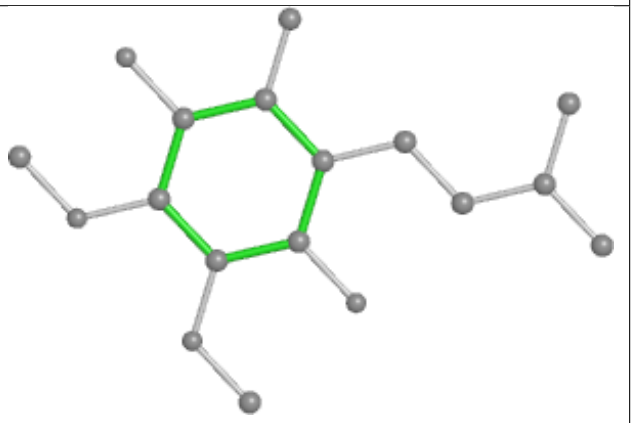
Bond lengths



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

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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