wwPDB X-ray Structure Validation Summary Report (i)

Aug 6, 2020 – 09:41 PM BST

PDB ID	:	1EYS
Title	:	CRYSTAL STRUCTURE OF PHOTOSYNTHETIC REACTION CENTER FROM A THERMOPHILIC BACTERIUM, THERMOCHROMATIUM TEPIDUM
Authors	:	Nogi, T.; Fathir, I.; Kobayashi, M.; Nozawa, T.; Miki, K.
Deposited on	:	2000-05-08
Resolution	:	2.20 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 following versions of software and data (see references (1)) were used in the production of this report:

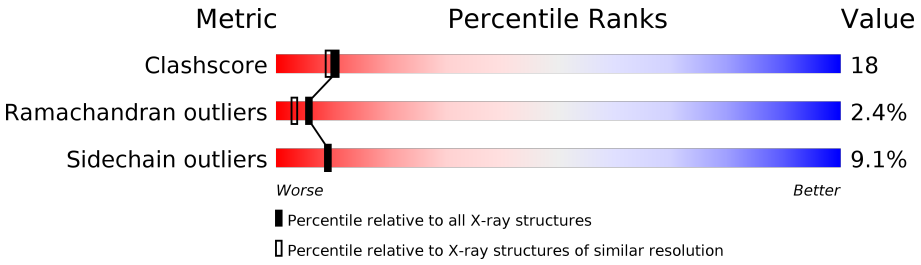
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	382	53% 24% • 19%
2	L	280	66% 31% •
3	M	324	60% 33% 5% • •
4	H	259	55% 29% 7% • 8%

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
8	BPH	L	606	X	-	-	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 10044 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	310	Total	C	N	O	S	0	0	0
			2402	1514	421	451	16			

- Molecule 2 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	280	Total	C	N	O	S	0	0	0
			2233	1501	361	361	10			

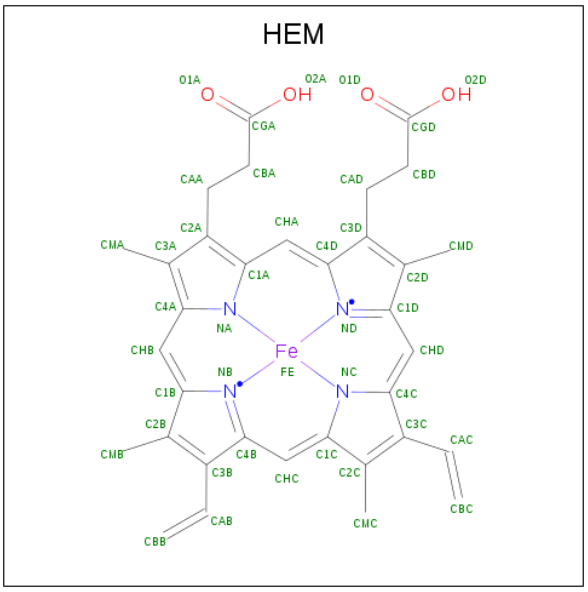
- Molecule 3 is a protein called PHOTOSYNTHETIC REACTION CENTER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	318	Total	C	N	O	S	0	0	0
			2537	1705	413	409	10			

- Molecule 4 is a protein called PHOTOSYNTHETIC REACTION CENTER.

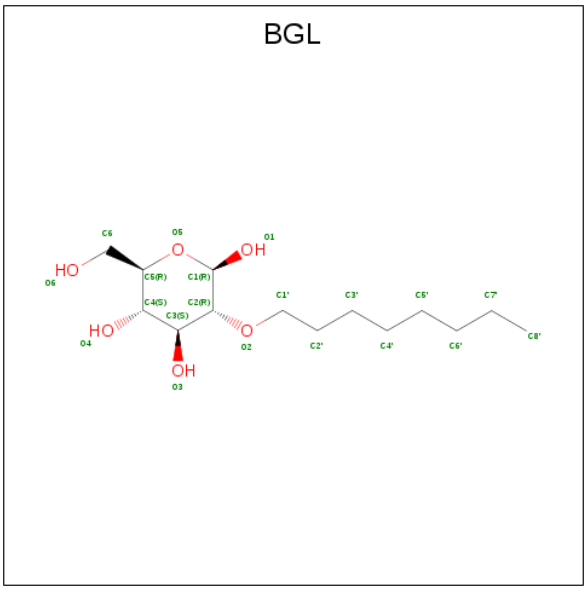
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	238	Total	C	N	O	S	0	0	0
			1837	1187	309	336	5			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



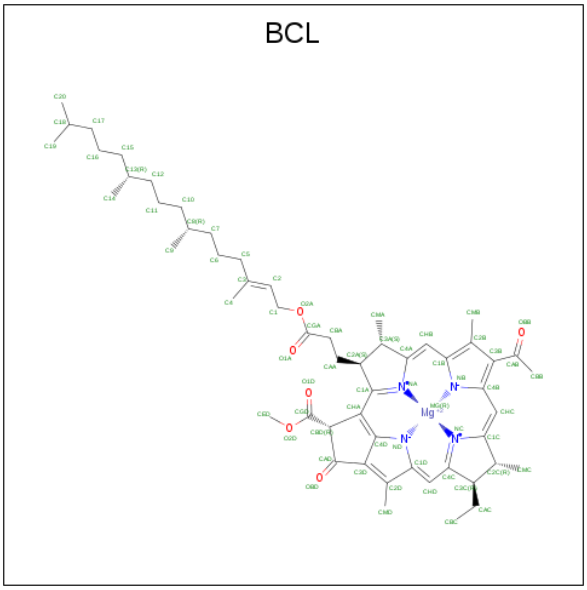
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is 2-O-octyl-beta-D-glucopyranose (three-letter code: BGL) (formula: $C_{14}H_{28}O_6$).



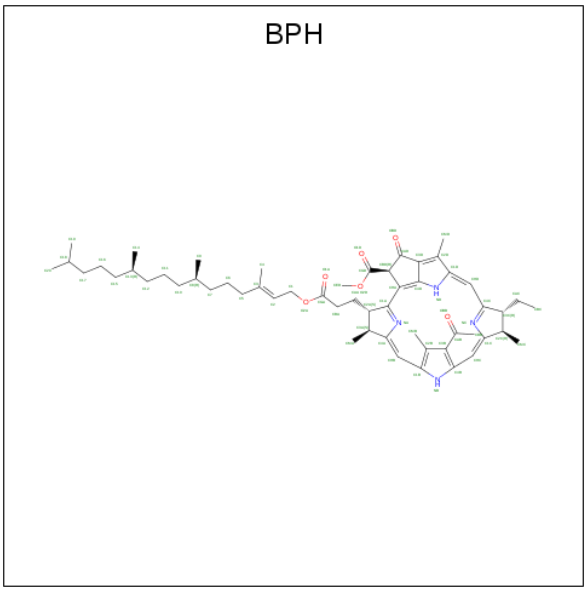
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	1	Total C O 20 14 6	0	0
6	L	1	Total C O 20 14 6	0	0
6	L	1	Total C O 20 14 6	0	0
6	M	1	Total C O 20 14 6	0	0
6	M	1	Total C O 20 14 6	0	0
6	M	1	Total C O 20 14 6	0	0

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$).



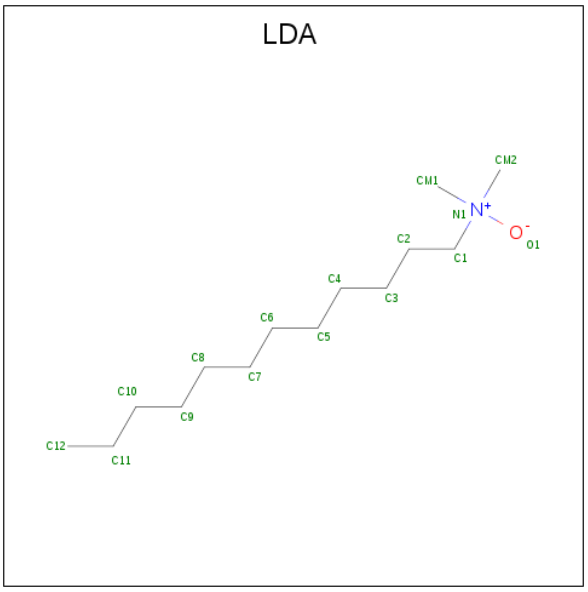
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	L	1	Total C Mg N O 66 55 1 4 6	0	0
7	L	1	Total C Mg N O 66 55 1 4 6	0	0
7	M	1	Total C Mg N O 66 55 1 4 6	0	0
7	M	1	Total C Mg N O 66 55 1 4 6	0	0

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



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

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

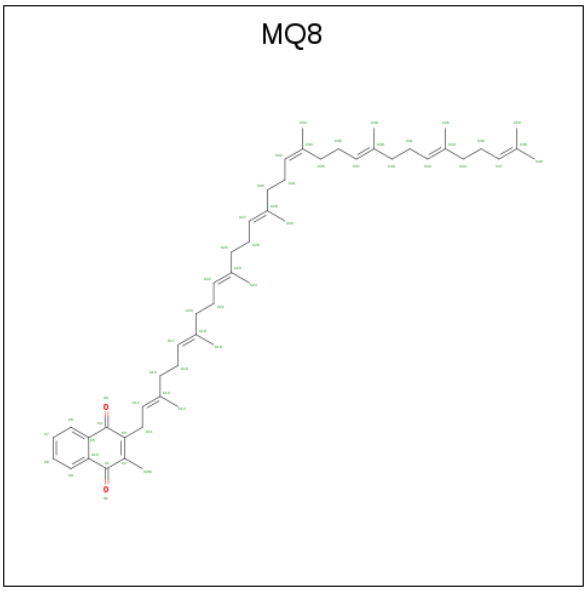


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	L	1	Total	C	N	O	0	0
			16	14	1	1		

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

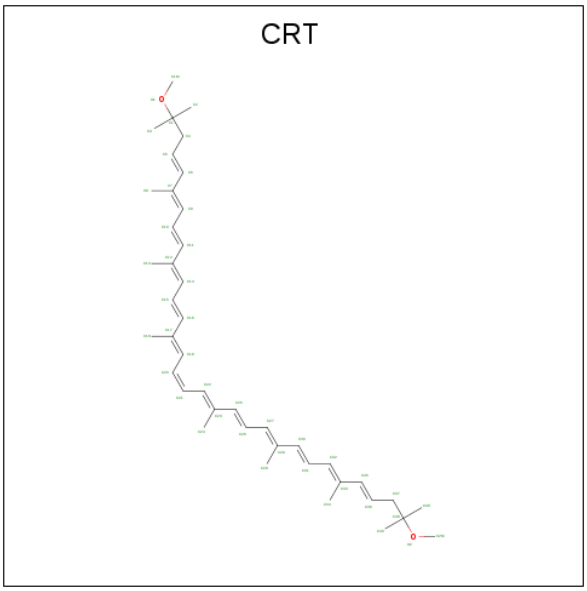
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	M	1	Total Fe 1 1	0	0

- Molecule 11 is MENAQUINONE 8 (three-letter code: MQ8) (formula: $C_{51}H_{72}O_2$).



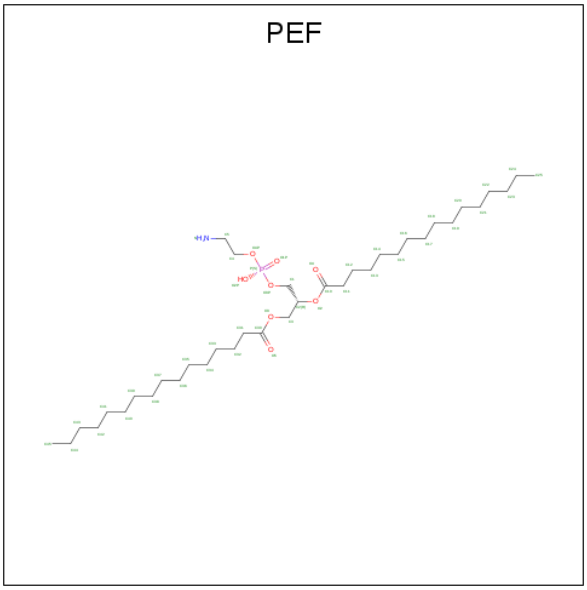
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	M	1	Total C O 53 51 2	0	0

- Molecule 12 is SPIRILLOXANTHIN (three-letter code: CRT) (formula: $C_{42}H_{60}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	M	1	Total C O 44 42 2	0	0

- Molecule 13 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	H	1	Total C N O P 47 37 1 8 1	0	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	94	Total O 94 94	0	0
14	L	37	Total O 37 37	0	0
14	M	35	Total O 35 35	0	0
14	H	22	Total O 22 22	0	0

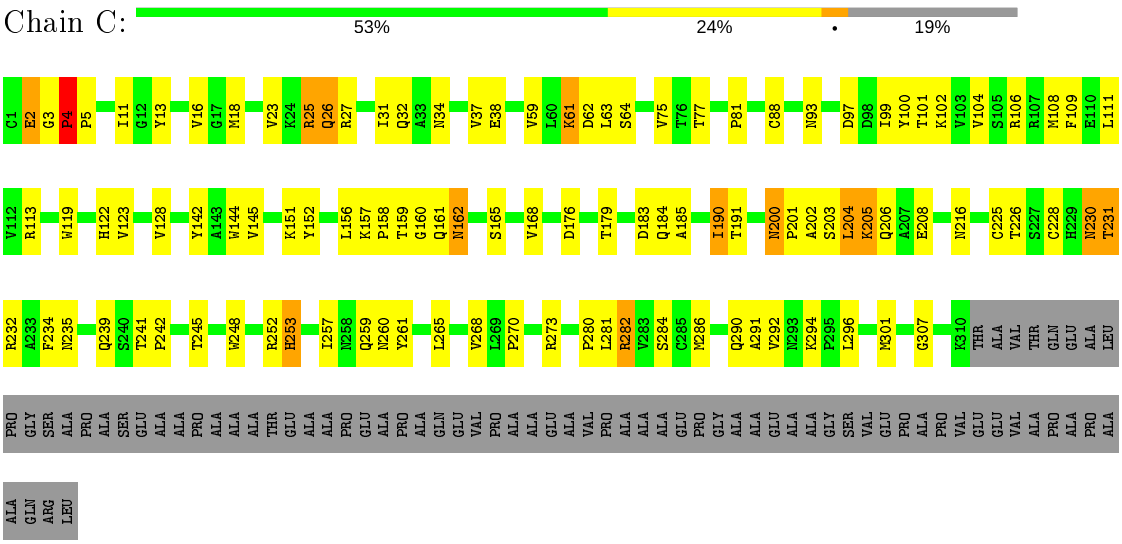
3 Residue-property plots (i)

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.

Note EDS was not executed.

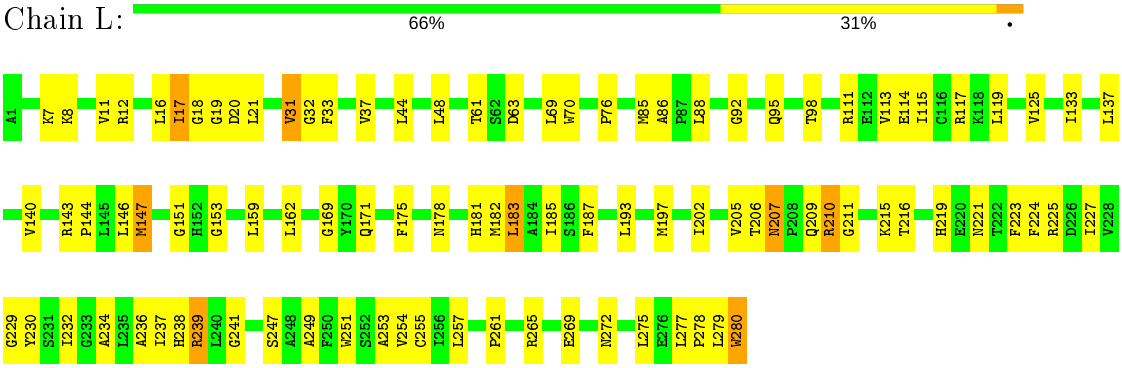
- Molecule 1: PHOTOSYNTHETIC REACTION CENTER

Chain C:



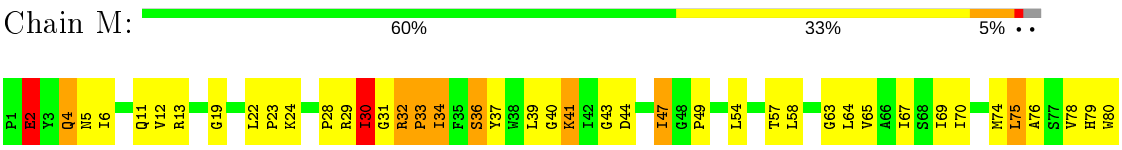
- Molecule 2: PHOTOSYNTHETIC REACTION CENTER

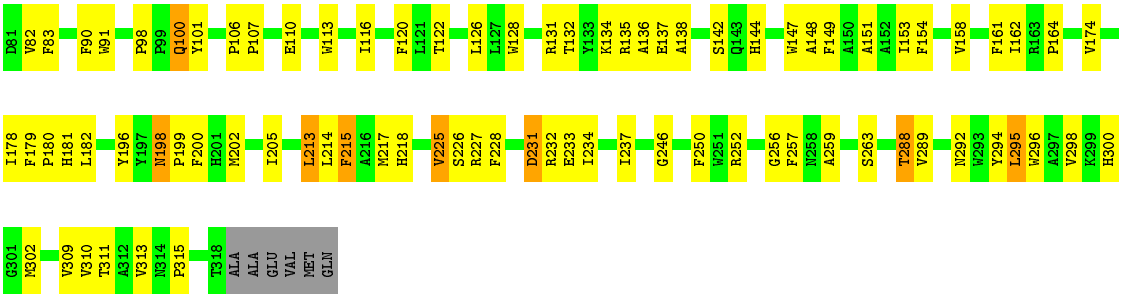
Chain L:



- Molecule 3: PHOTOSYNTHETIC REACTION CENTER

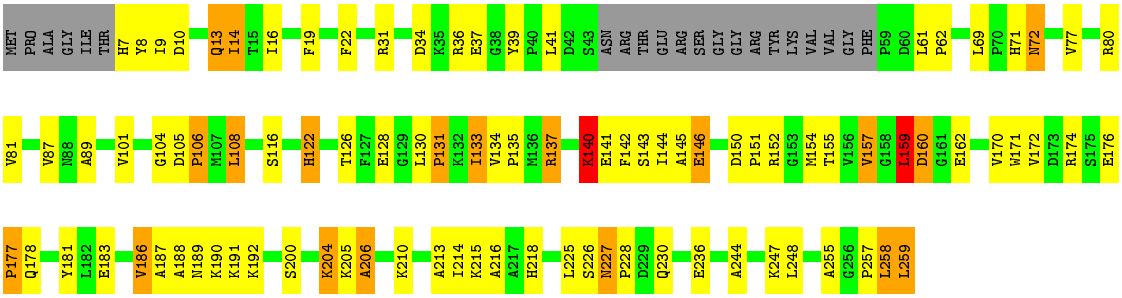
Chain M:





- Molecule 4: PHOTOSYNTHETIC REACTION CENTER

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	133.30Å 196.60Å 84.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.231 , 0.287	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10044	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, LDA, CRT, BPH, BGL, FE, MQ8, HEM, PEF

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	0.53	1/2471 (0.0%)	0.72	2/3374 (0.1%)
2	L	0.50	0/2320	0.65	0/3170
3	M	0.49	0/2637	0.67	1/3610 (0.0%)
4	H	0.47	0/1890	0.76	1/2576 (0.0%)
All	All	0.50	1/9318 (0.0%)	0.69	4/12730 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	225	CYS	CB-SG	-5.56	1.72	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	159	LEU	CA-CB-CG	7.48	132.51	115.30
1	C	230	ASN	N-CA-C	-6.83	92.55	111.00
3	M	47	ILE	N-CA-C	-5.57	95.95	111.00
1	C	3	GLY	N-CA-C	5.11	125.88	113.10

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	C	2402	0	2323	74	0
2	L	2233	0	2195	85	0
3	M	2537	0	2511	123	0
4	H	1837	0	1831	82	0
5	C	172	0	120	5	0
6	L	60	0	84	10	0
6	M	60	0	84	1	0
7	L	132	0	148	14	0
7	M	132	0	148	16	0
8	L	65	0	75	6	0
8	M	65	0	75	4	0
9	L	16	0	31	2	0
10	M	1	0	0	0	0
11	M	53	0	72	1	0
12	M	44	0	60	2	0
13	H	47	0	73	7	0
14	C	94	0	0	0	0
14	H	22	0	0	1	0
14	L	37	0	0	0	0
14	M	35	0	0	1	0
All	All	10044	0	9830	364	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 18.

The worst 5 of 364 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)
3:M:69:ILE:HD13	3:M:116:ILE:HG23	1.36	1.06
4:H:7:HIS:HB3	4:H:9:ILE:HG12	1.40	1.00
4:H:151:PRO:HA	4:H:154:MET:SD	2.07	0.94
3:M:33:PRO:HG3	3:M:49:PRO:HD3	1.52	0.92
2:L:86:ALA:H	2:L:95:GLN:HE22	1.06	0.90

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	308/382 (81%)	268 (87%)	31 (10%)	9 (3%)	4 2
2	L	278/280 (99%)	249 (90%)	27 (10%)	2 (1%)	22 22
3	M	316/324 (98%)	279 (88%)	31 (10%)	6 (2%)	8 5
4	H	234/259 (90%)	191 (82%)	33 (14%)	10 (4%)	2 1
All	All	1136/1245 (91%)	987 (87%)	122 (11%)	27 (2%)	6 3

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	GLU
1	C	4	PRO
4	H	140	LYS
4	H	142	PHE
4	H	146	GLU

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	259/300 (86%)	239 (92%)	20 (8%)	13 13
2	L	228/228 (100%)	212 (93%)	16 (7%)	15 16
3	M	254/258 (98%)	234 (92%)	20 (8%)	12 12
4	H	195/211 (92%)	166 (85%)	29 (15%)	3 2
All	All	936/997 (94%)	851 (91%)	85 (9%)	9 9

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	24	LYS
3	M	181	HIS
4	H	186	VAL
3	M	30	ILE
3	M	41	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	174	HIS
2	L	207	ASN
4	H	13	GLN
1	C	290	GLN
2	L	95	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	$\#\|Z\|>2$
8	BPH	L	606	-	64,70,70	1.57	8 (12%)	76,101,101	2.03	25 (32%)
7	BCL	L	604	2	58,74,74	2.17	10 (17%)	69,115,115	2.41	26 (37%)
6	BGL	M	705	-	20,20,20	1.28	2 (10%)	24,25,25	2.04	6 (25%)
9	LDA	L	707	-	12,15,15	2.14	1 (8%)	14,17,17	0.64	0
6	BGL	M	702	-	20,20,20	1.07	1 (5%)	24,25,25	2.42	8 (33%)
5	HEM	C	609	1	27,50,50	2.20	10 (37%)	17,82,82	0.95	0
12	CRT	M	613	-	41,43,43	2.75	14 (34%)	50,54,54	1.44	4 (8%)
11	MQ8	M	608	-	54,54,54	2.41	16 (29%)	66,69,69	2.90	21 (31%)
6	BGL	L	704	-	20,20,20	1.23	2 (10%)	24,25,25	2.42	8 (33%)
5	HEM	C	612	1	27,50,50	1.91	6 (22%)	17,82,82	0.88	0
6	BGL	L	703	-	20,20,20	0.92	1 (5%)	24,25,25	2.04	7 (29%)
6	BGL	M	706	-	20,20,20	0.97	1 (5%)	24,25,25	2.07	6 (25%)
5	HEM	C	611	1	27,50,50	2.08	9 (33%)	17,82,82	1.16	0
5	HEM	C	610	1	27,50,50	2.00	7 (25%)	17,82,82	1.18	1 (5%)
7	BCL	L	602	2	58,74,74	2.07	8 (13%)	69,115,115	2.23	21 (30%)
6	BGL	L	701	-	20,20,20	1.25	2 (10%)	24,25,25	1.96	7 (29%)
8	BPH	M	605	-	64,70,70	1.67	8 (12%)	76,101,101	2.01	18 (23%)
7	BCL	M	603	3	58,74,74	2.03	6 (10%)	69,115,115	2.28	23 (33%)
7	BCL	M	601	3	58,74,74	2.23	10 (17%)	69,115,115	2.47	25 (36%)
13	PEF	H	708	-	46,46,46	2.17	7 (15%)	49,51,51	1.38	6 (12%)

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
8	BPH	L	606	-	1/1/18/22	21/54/105/105	0/5/6/6
7	BCL	L	604	2	-	8/37/137/137	-
6	BGL	M	705	-	-	4/11/31/31	0/1/1/1
9	LDA	L	707	-	-	4/13/13/13	-
6	BGL	M	702	-	-	8/11/31/31	0/1/1/1
5	HEM	C	609	1	-	0/6/54/54	-
12	CRT	M	613	-	-	5/51/51/51	-
11	MQ8	M	608	-	-	12/47/67/67	0/2/2/2
6	BGL	L	704	-	-	5/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	C	612	1	-	0/6/54/54	-
6	BGL	L	703	-	-	6/11/31/31	0/1/1/1
6	BGL	M	706	-	-	5/11/31/31	0/1/1/1
5	HEM	C	611	1	-	0/6/54/54	-
5	HEM	C	610	1	-	1/6/54/54	-
7	BCL	L	602	2	-	10/37/137/137	-
6	BGL	L	701	-	-	7/11/31/31	0/1/1/1
8	BPH	M	605	-	-	14/54/105/105	0/5/6/6
7	BCL	M	603	3	-	10/37/137/137	-
7	BCL	M	601	3	-	23/37/137/137	-
13	PEF	H	708	-	-	35/50/50/50	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	601	BCL	C3C-C4C	-12.13	1.36	1.51
7	L	604	BCL	C3C-C4C	-12.06	1.36	1.51
7	M	603	BCL	C3C-C4C	-10.55	1.38	1.51
7	L	602	BCL	C3C-C4C	-10.39	1.38	1.51
8	M	605	BPH	C3C-C4C	-8.84	1.38	1.50

The worst 5 of 212 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	L	604	BCL	C4A-NA-C1A	8.95	110.73	106.71
7	M	601	BCL	C4A-NA-C1A	8.67	110.61	106.71
11	M	608	MQ8	C34-C33-C35	8.53	129.63	115.27
7	L	602	BCL	C4A-NA-C1A	8.45	110.50	106.71
11	M	608	MQ8	C11-C3-C4	-8.11	109.82	118.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	L	606	BPH	C8

5 of 178 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	604	BCL	C2C-C3C-CAC-CBC
7	L	604	BCL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
6	M	705	BGL	C2'-C1'-O2-C2
8	L	606	BPH	C4C-C3C-CAC-CBC
8	L	606	BPH	C2C-C3C-CAC-CBC

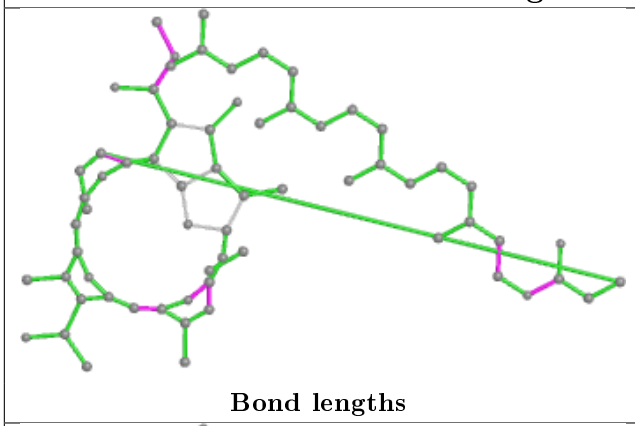
There are no ring outliers.

17 monomers are involved in 65 short contacts:

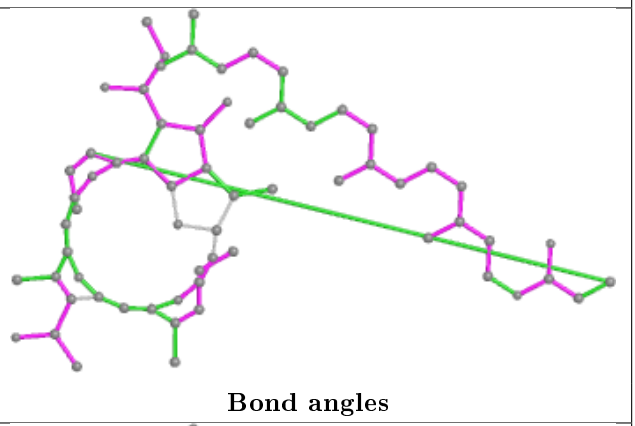
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	L	606	BPH	6	0
7	L	604	BCL	10	0
9	L	707	LDA	2	0
6	M	702	BGL	1	0
5	C	609	HEM	1	0
12	M	613	CRT	2	0
11	M	608	MQ8	1	0
6	L	704	BGL	3	0
5	C	612	HEM	2	0
6	L	703	BGL	4	0
5	C	610	HEM	2	0
7	L	602	BCL	7	0
6	L	701	BGL	3	0
8	M	605	BPH	4	0
7	M	603	BCL	6	0
7	M	601	BCL	10	0
13	H	708	PEF	7	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.

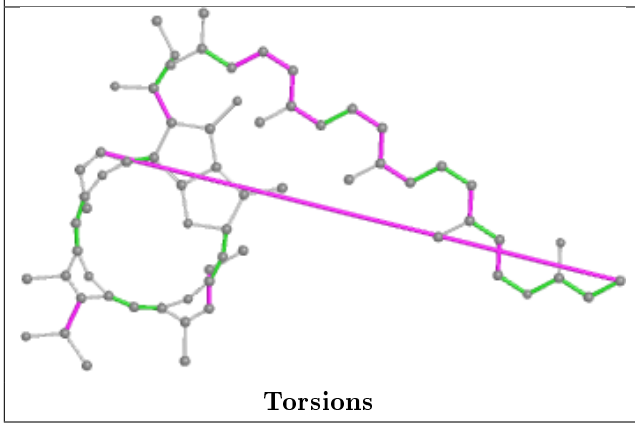
Ligand BPH L 606



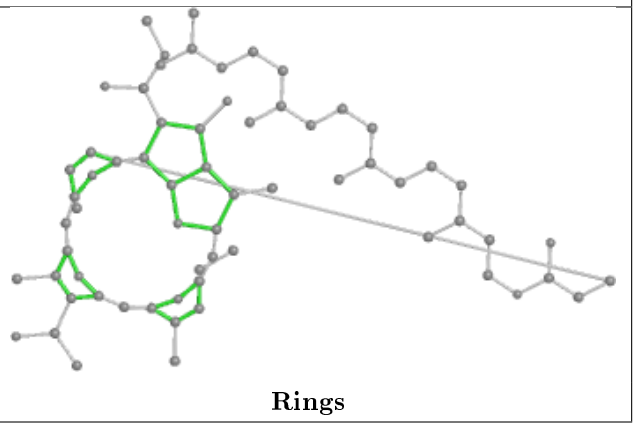
Bond lengths



Bond angles

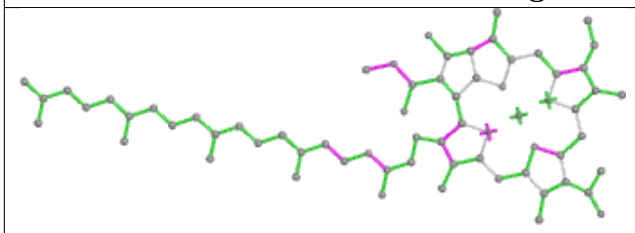


Torsions

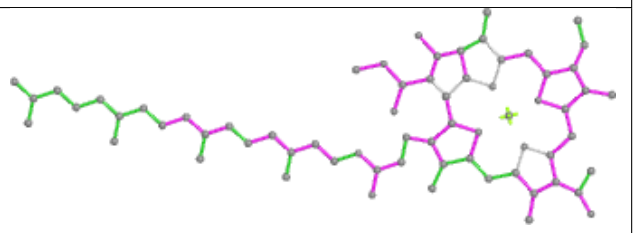


Rings

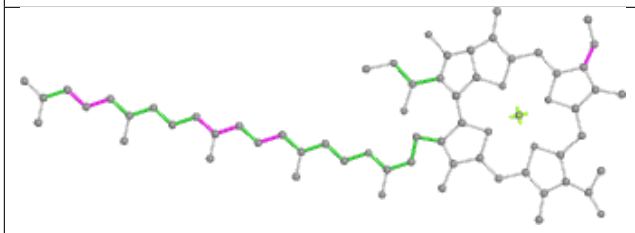
Ligand BCL L 604



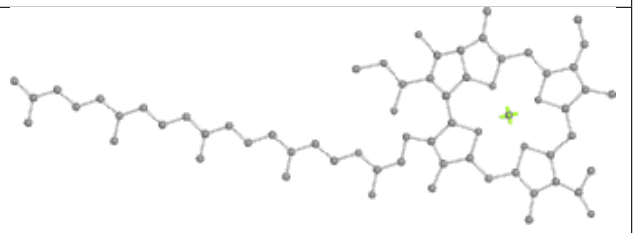
Bond lengths



Bond angles

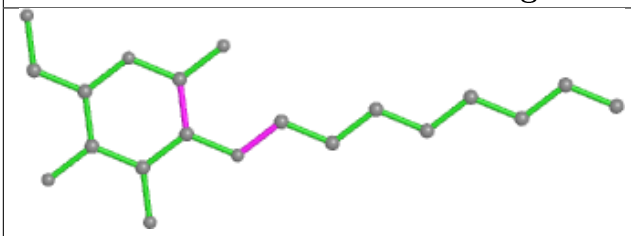


Torsions

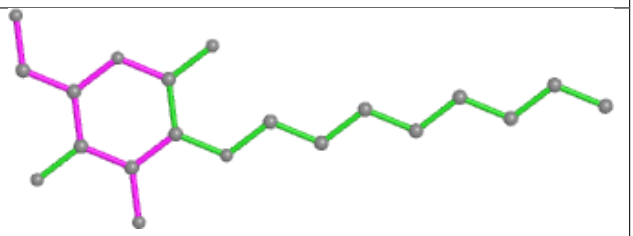


Rings

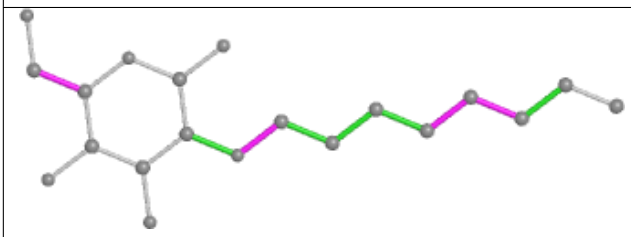
Ligand BGL M 705



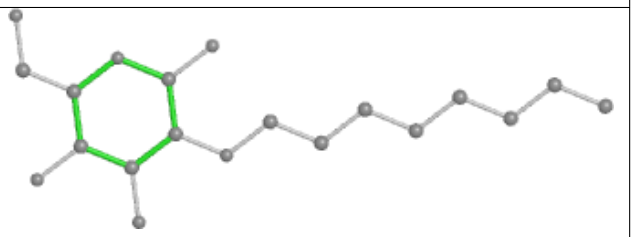
Bond lengths



Bond angles

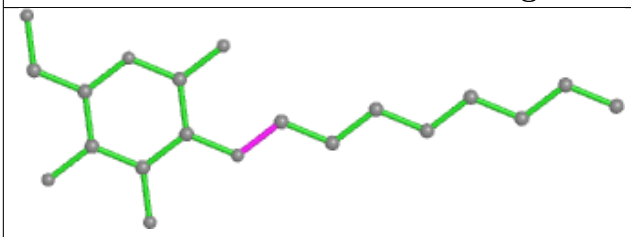


Torsions

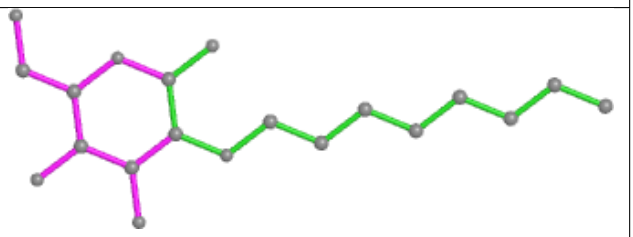


Rings

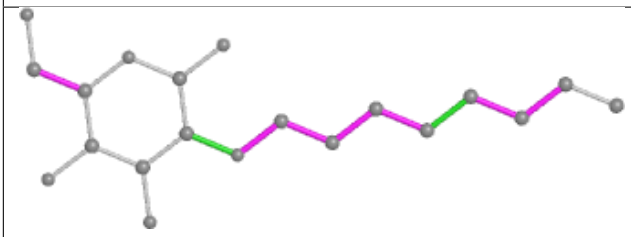
Ligand BGL M 702



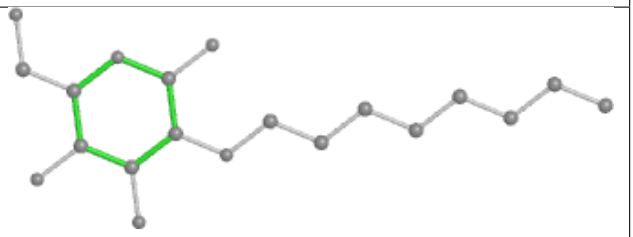
Bond lengths



Bond angles

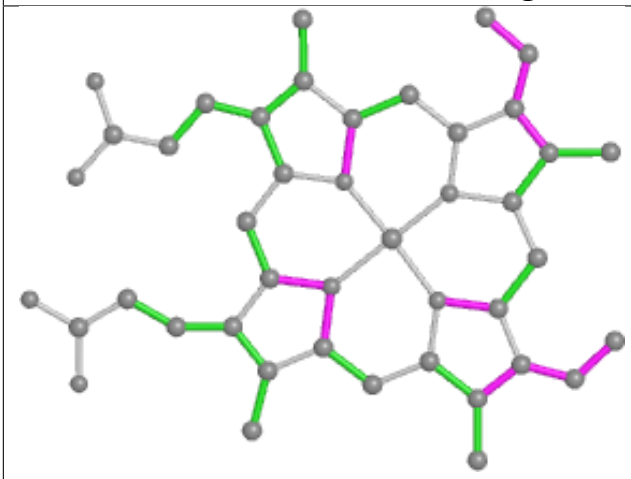


Torsions

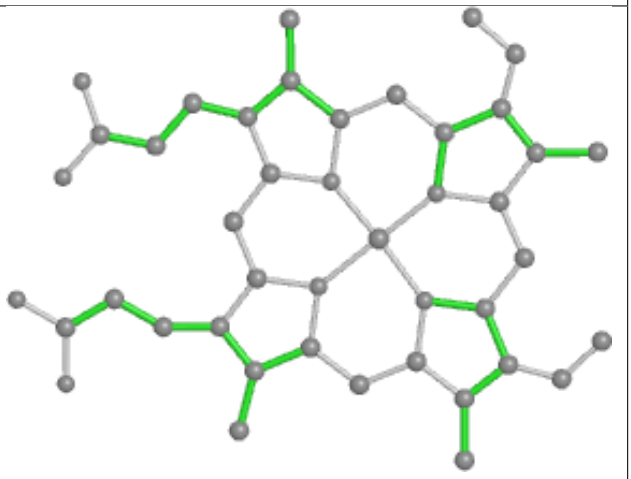


Rings

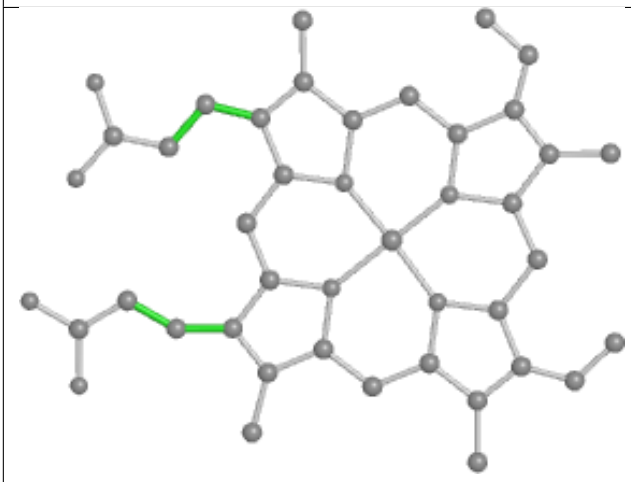
Ligand HEM C 609



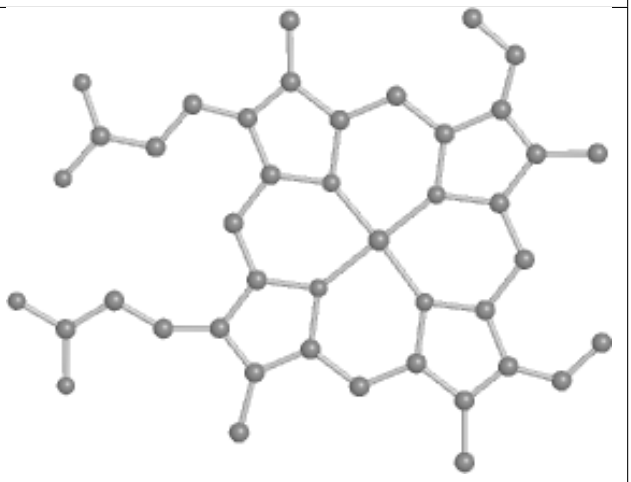
Bond lengths



Bond angles

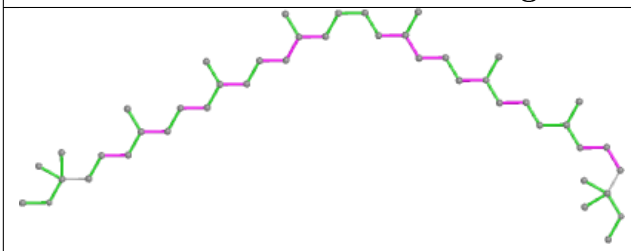


Torsions

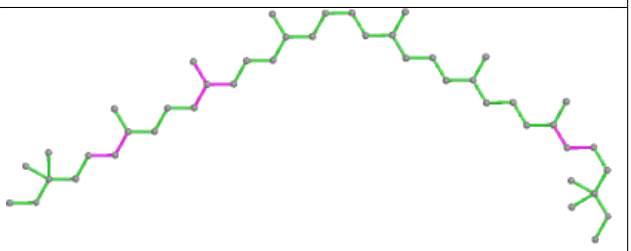


Rings

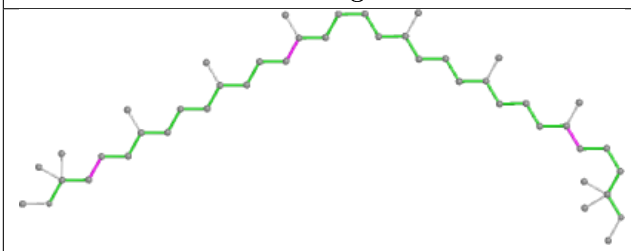
Ligand CRT M 613



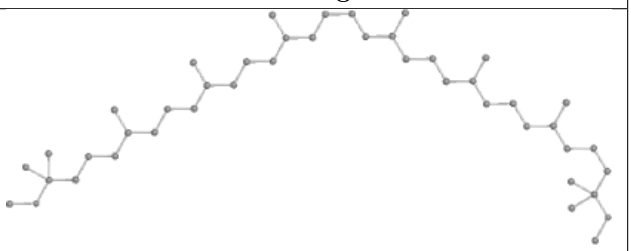
Bond lengths



Bond angles

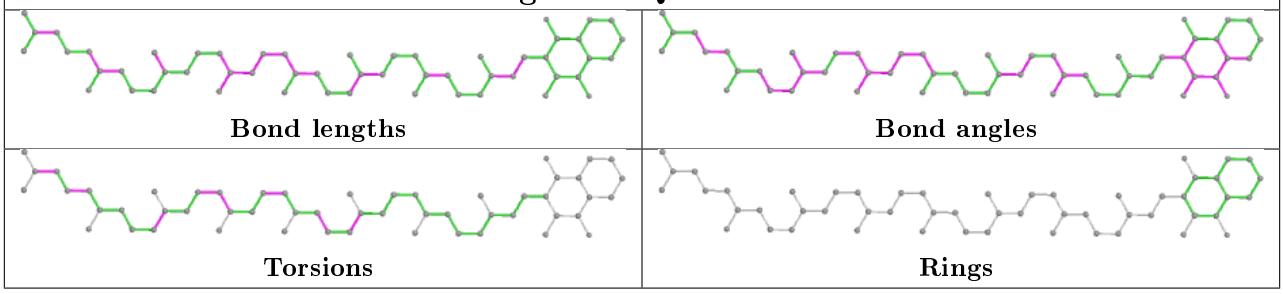


Torsions

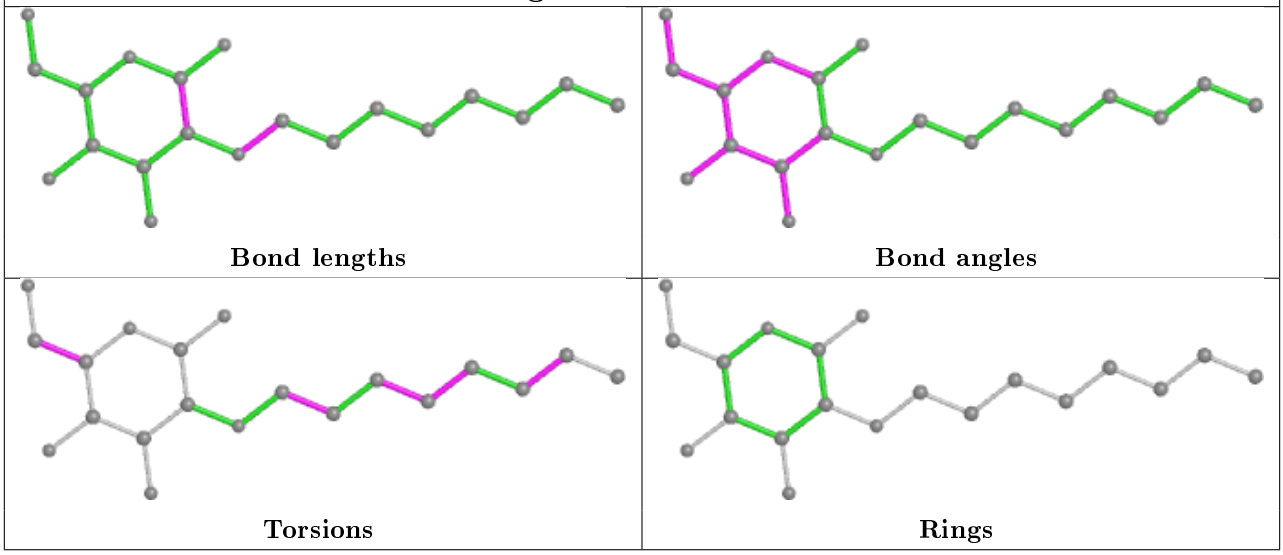


Rings

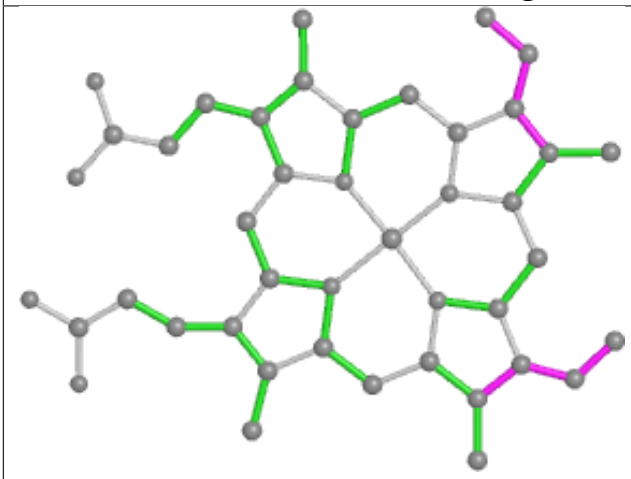
Ligand MQ8 M 608



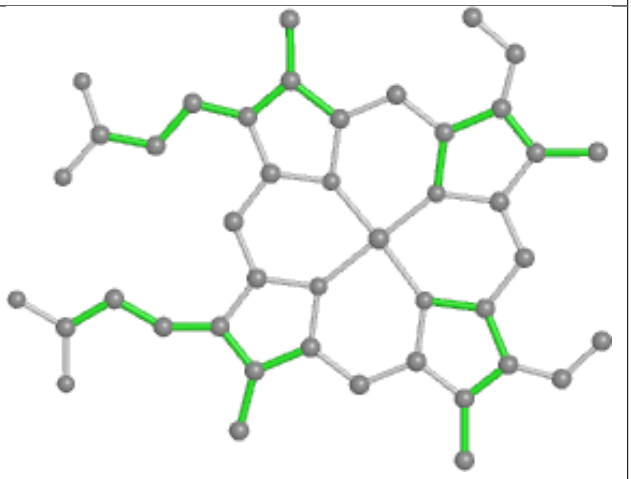
Ligand BGL L 704



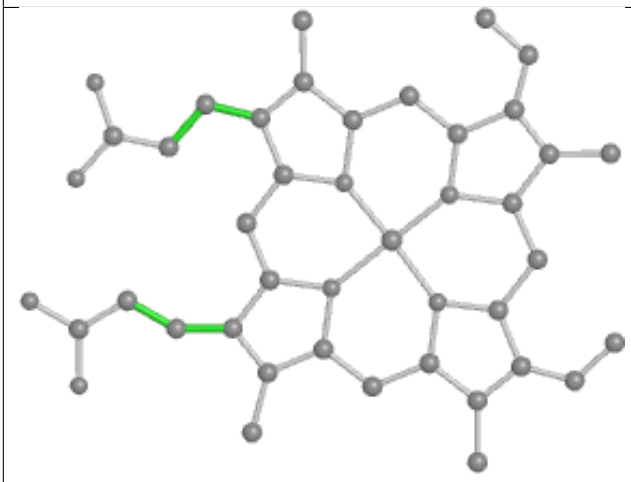
Ligand HEM C 612



Bond lengths



Bond angles



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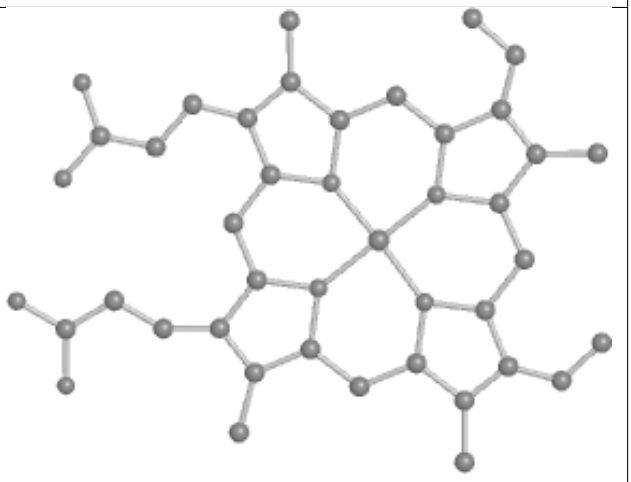
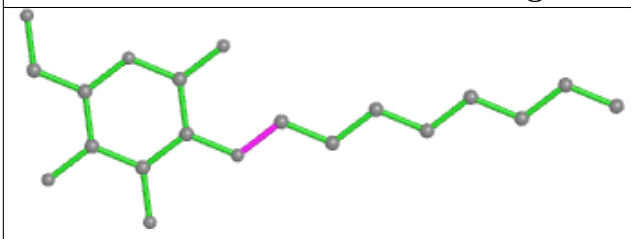
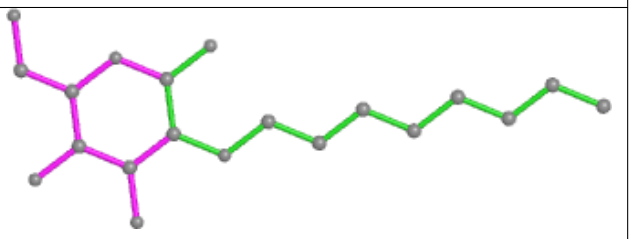


Rings

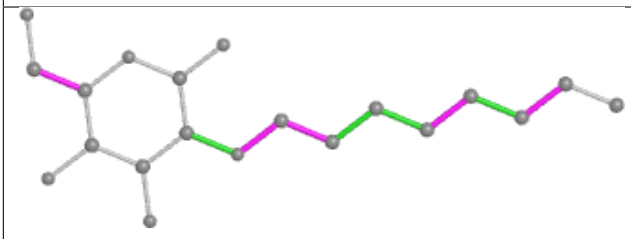
Ligand BGL L 703



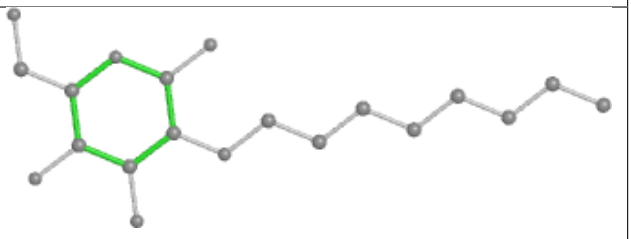
Bond lengths



Bond angles

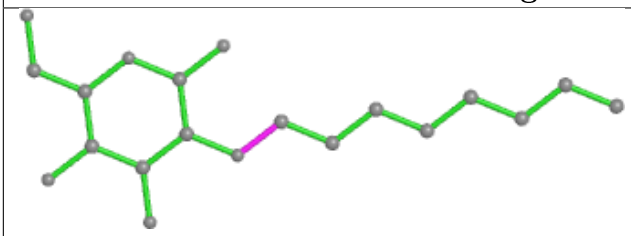


Torsions

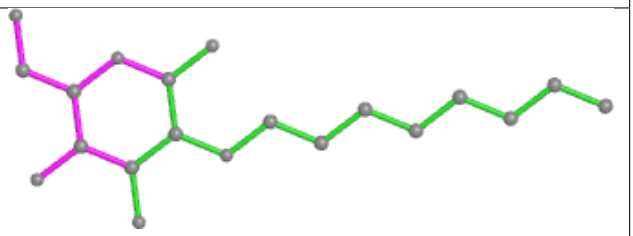


Rings

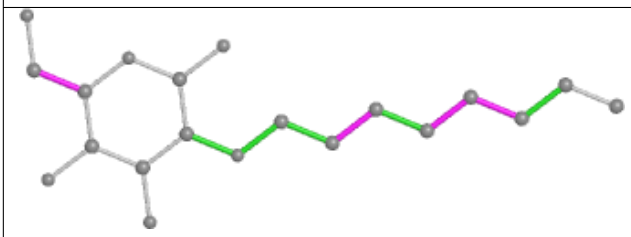
Ligand BGL M 706



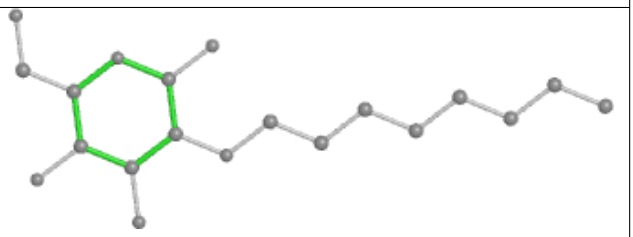
Bond lengths



Bond angles

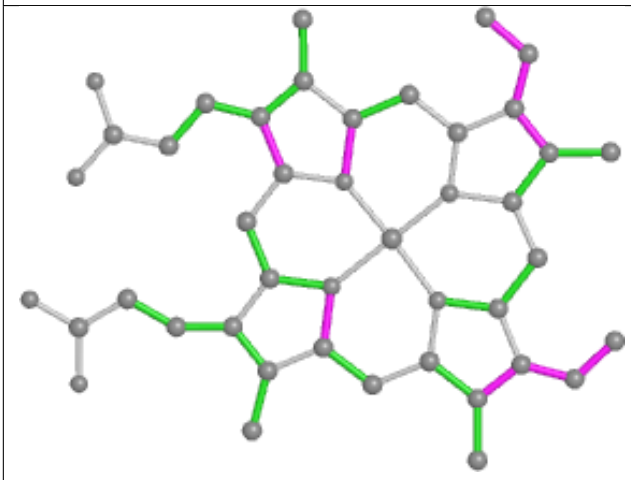


Torsions

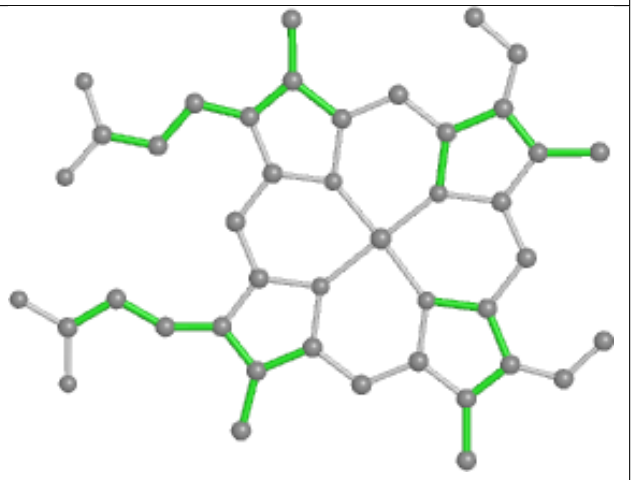


Rings

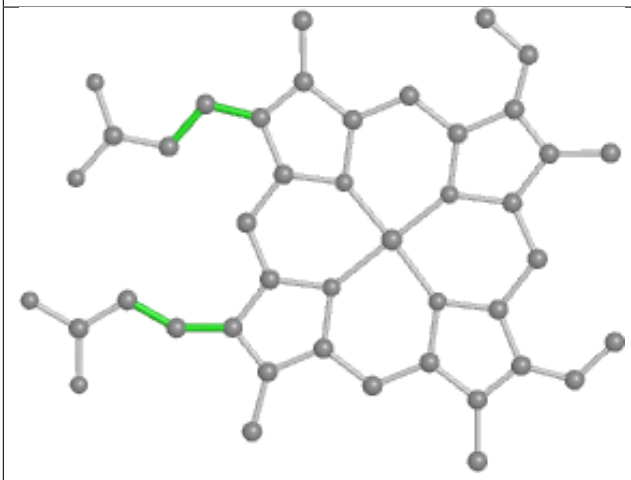
Ligand HEM C 611



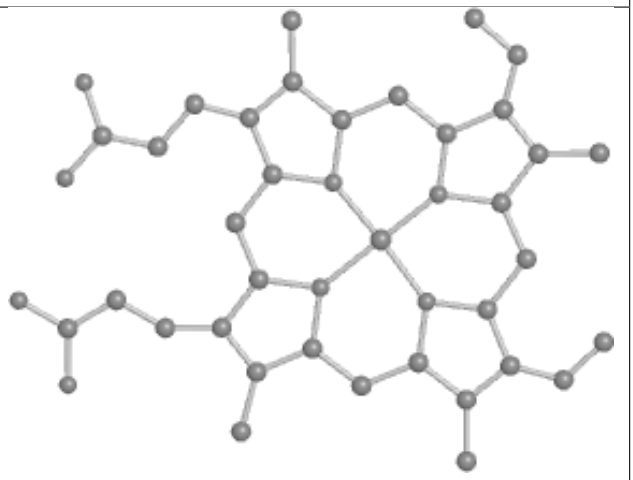
Bond lengths



Bond angles

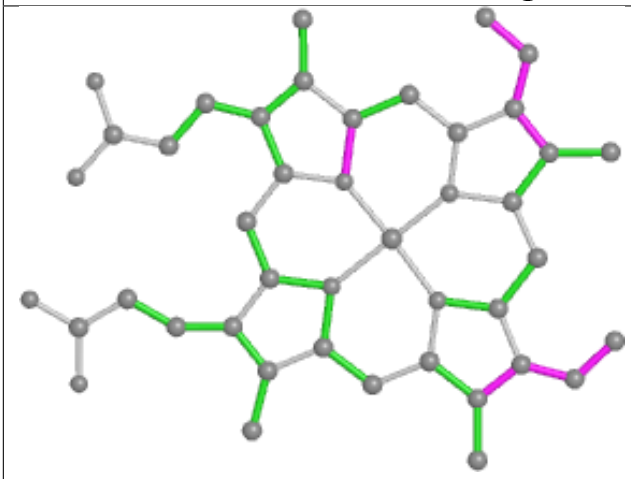


Torsions

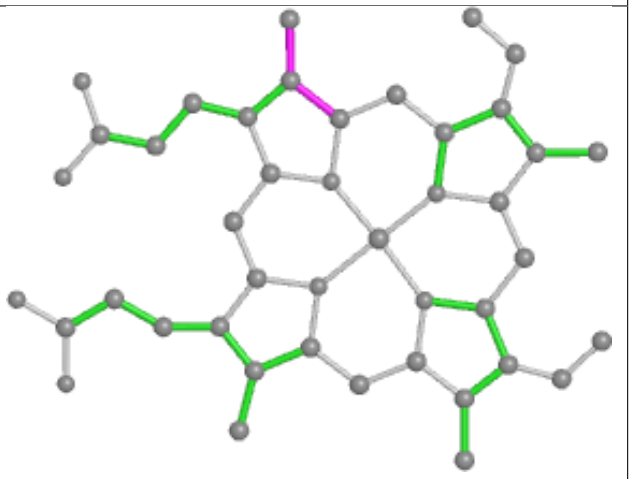


Rings

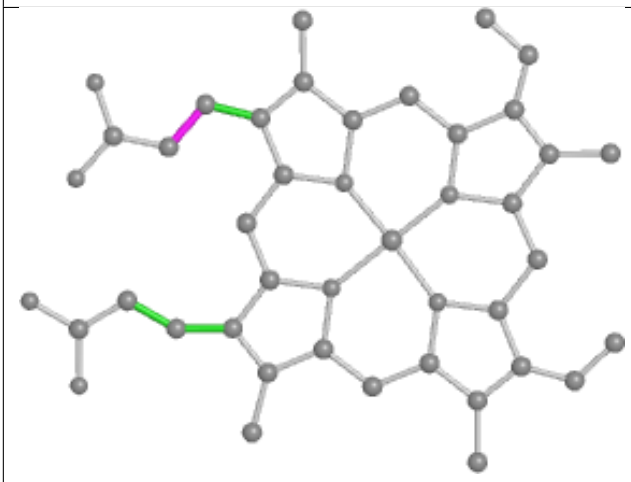
Ligand HEM C 610



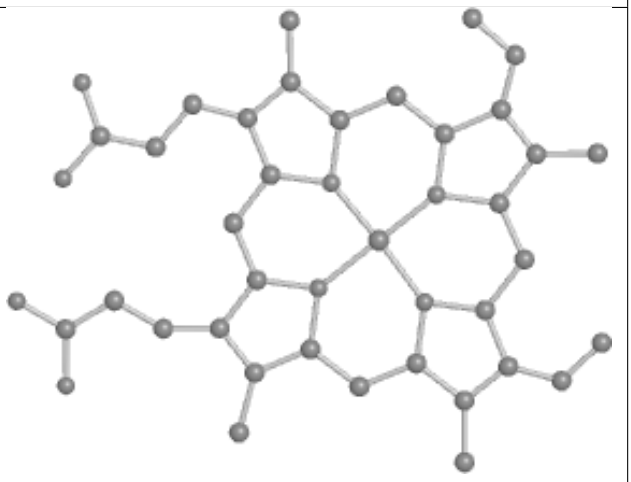
Bond lengths



Bond angles

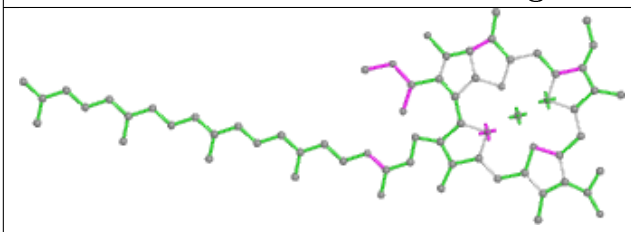


Torsions

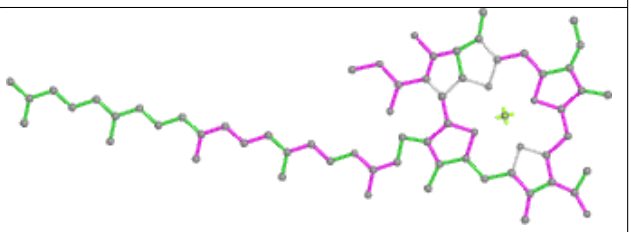


Rings

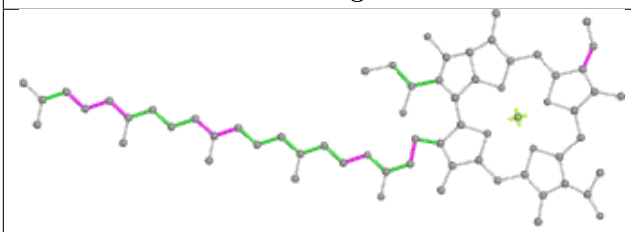
Ligand BCL L 602



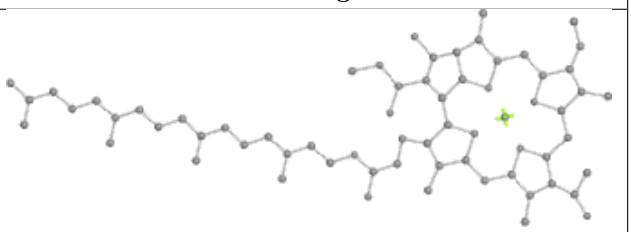
Bond lengths



Bond angles

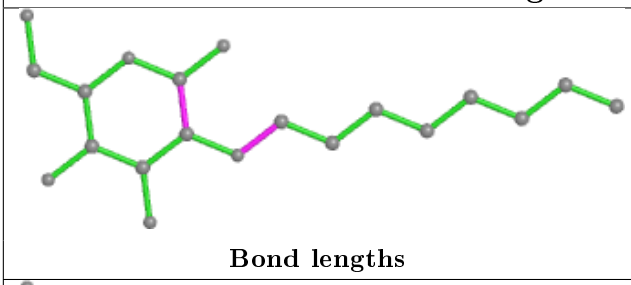


Torsions

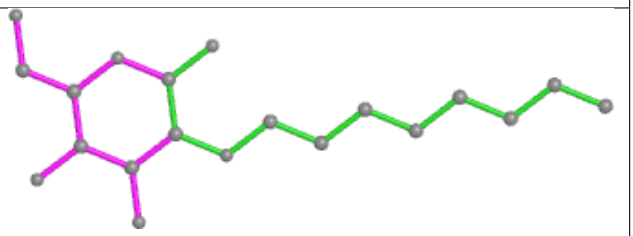


Rings

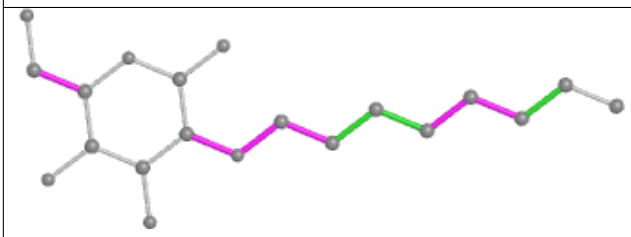
Ligand BGL L 701



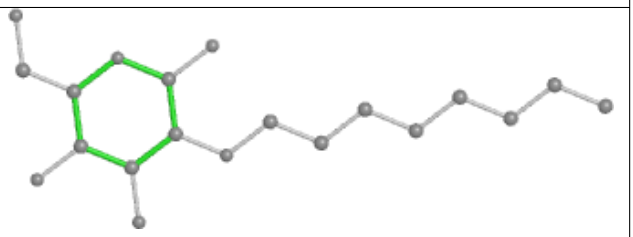
Bond lengths



Bond angles

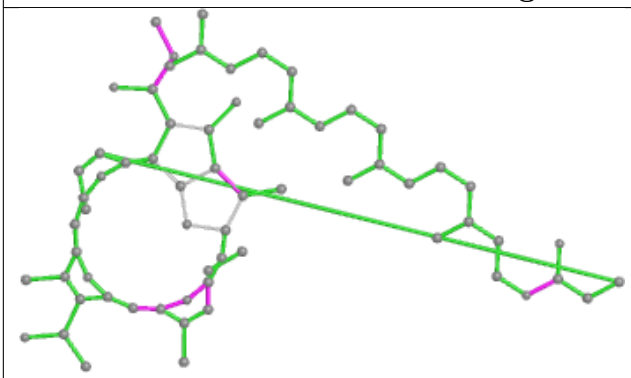


Torsions

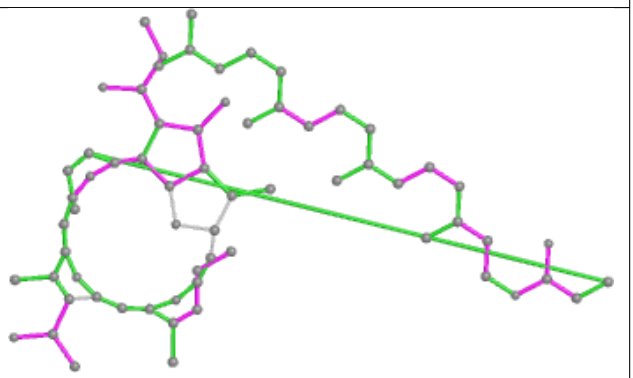


Rings

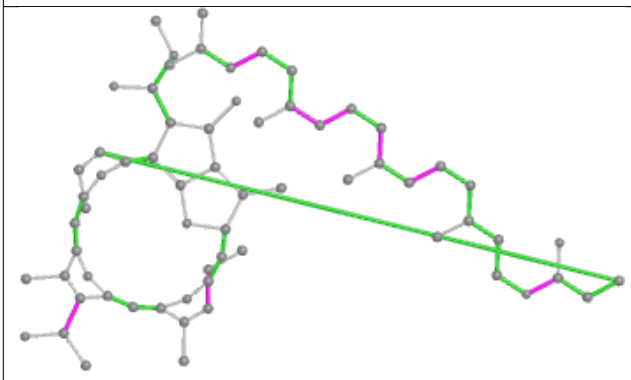
Ligand BPH M 605



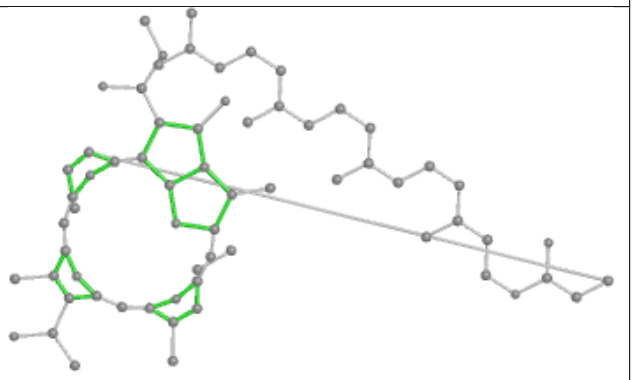
Bond lengths



Bond angles

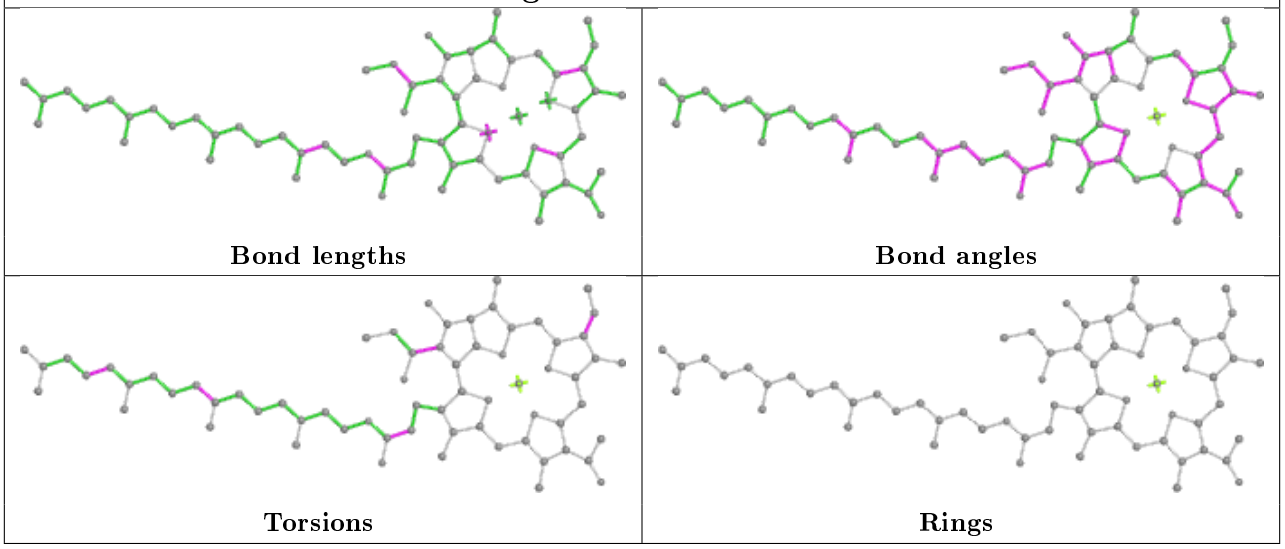


Torsions

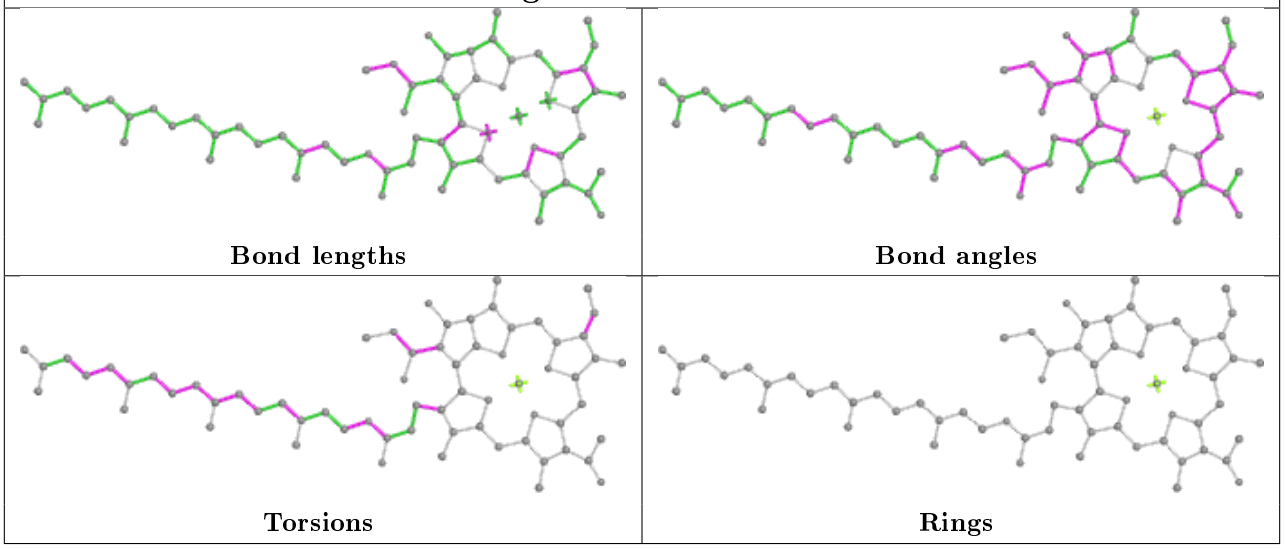


Rings

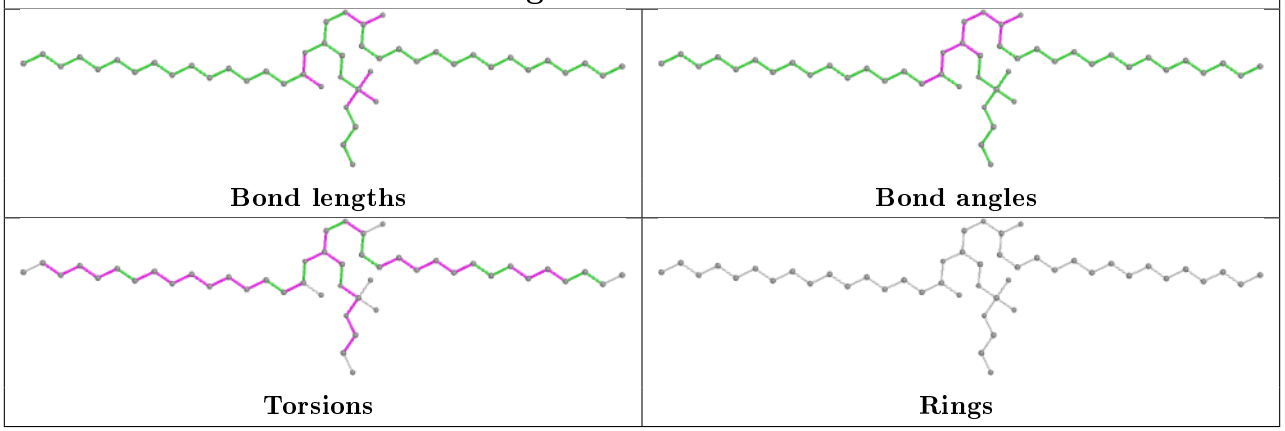
Ligand BCL M 603



Ligand BCL M 601



Ligand PEF H 708



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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.