wwPDB EM Validation Summary Report

May 26, 2024 – 07:31 AM EDT

PDB ID	:	7SA3
EMDB ID	:	EMD-24943
Title	:	Structure of a monomeric photosystem II core complex from a cyanobacterium acclimated to far-red light
Authors	:	Gisriel, C.J.; Bryant, D.A.; Brudvig, G.W.
Deposited on	:	2021-09-22
Resolution	:	2.25 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

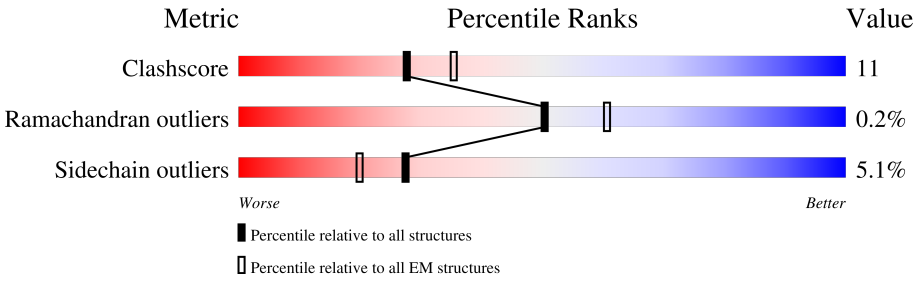
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.25 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	5% 63% 20% • 16%
2	B	509	• 74% 13% • 12%
3	C	482	8% 69% 17% • 13%
4	D	352	6% 71% 22% • 5%
5	E	80	11% 41% 10% 49%
6	F	44	11% 43% 25% 32%
7	I	38	5% 61% 11% 29%
8	K	45	31% 69% 9% • 18%

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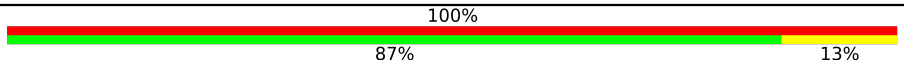
Mol	Chain	Length	Quality of chain
9	N	23	

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
12	CLA	A	403	X	-	-	-
12	CLA	A	405	X	-	-	-
12	CLA	A	407	X	-	-	-
12	CLA	B	601	X	-	-	-
12	CLA	B	602	X	-	-	-
12	CLA	B	604	X	-	-	-
12	CLA	B	605	X	-	-	-
12	CLA	B	607	X	-	-	-
12	CLA	B	608	X	-	-	-
12	CLA	B	609	X	-	-	-
12	CLA	B	610	X	-	-	-
12	CLA	B	611	X	-	-	-
12	CLA	B	613	X	-	-	-
12	CLA	B	614	X	-	-	-
12	CLA	C	501	X	-	-	-
12	CLA	C	502	X	-	-	-
12	CLA	C	503	X	-	-	-
12	CLA	C	504	X	-	-	-
12	CLA	C	505	X	-	-	-
12	CLA	C	506	X	-	-	-
12	CLA	C	508	X	-	-	-
12	CLA	C	509	X	-	-	-
12	CLA	C	510	X	-	-	-
12	CLA	C	511	X	-	-	-
12	CLA	C	512	X	-	-	-
12	CLA	C	513	X	-	-	-
12	CLA	D	403	X	-	-	-
12	CLA	D	404	X	-	-	-
13	CL7	A	404	X	-	-	-

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 15960 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Photosystem q(B) protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	303	2382	1572	392	403	15	0	0

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	conflict	UNP B4WKH9
A	2	THR	-	conflict	UNP B4WKH9
A	3	THR	-	conflict	UNP B4WKH9
A	4	ILE	-	conflict	UNP B4WKH9
A	5	SER	-	conflict	UNP B4WKH9
A	6	THR	-	conflict	UNP B4WKH9
A	7	ARG	-	conflict	UNP B4WKH9
A	8	PRO	-	conflict	UNP B4WKH9
A	9	THR	-	conflict	UNP B4WKH9
A	10	SER	-	conflict	UNP B4WKH9
A	11	ARG	-	conflict	UNP B4WKH9
A	12	PHE	-	conflict	UNP B4WKH9
A	13	PRO	-	conflict	UNP B4WKH9
A	14	THR	-	conflict	UNP B4WKH9
A	15	TRP	-	conflict	UNP B4WKH9
A	16	ASP	-	conflict	UNP B4WKH9
A	17	ARG	-	conflict	UNP B4WKH9
A	18	PHE	-	conflict	UNP B4WKH9
A	19	CYS	-	conflict	UNP B4WKH9
A	20	ASN	-	conflict	UNP B4WKH9
A	21	TRP	-	conflict	UNP B4WKH9
A	22	VAL	-	conflict	UNP B4WKH9
A	23	THR	-	conflict	UNP B4WKH9
A	24	SER	-	conflict	UNP B4WKH9
A	25	THR	-	conflict	UNP B4WKH9
A	26	GLU	-	conflict	UNP B4WKH9
A	27	ASN	-	conflict	UNP B4WKH9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	28	ARG	-	conflict	UNP B4WKH9
A	29	LEU	-	conflict	UNP B4WKH9
A	30	TYR	-	conflict	UNP B4WKH9
A	31	ILE	-	conflict	UNP B4WKH9
A	32	GLY	-	conflict	UNP B4WKH9
A	33	TRP	-	conflict	UNP B4WKH9
A	34	PHE	-	conflict	UNP B4WKH9
A	35	GLY	-	conflict	UNP B4WKH9
A	36	VAL	-	conflict	UNP B4WKH9
A	37	LEU	-	conflict	UNP B4WKH9

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	450	Total	C	N	O	S	0	0
			3528	2316	593	607	12		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	420	Total	C	N	O	S	0	0
			3272	2154	553	554	11		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	336	Total	C	N	O	S	0	0
			2671	1770	435	452	14		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	41	Total	C	N	O	0	0
			330	225	49	56		

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			243	165	41	36	1		

- Molecule 7 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	27	Total	C	N	O	S	0	0
			213	150	28	34	1		

- Molecule 8 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	37	Total	C	N	O	0	0
			294	206	45	43		

- Molecule 9 is a protein called Unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	N	23	Total	C	N	O	0	0
			115	69	23	23		

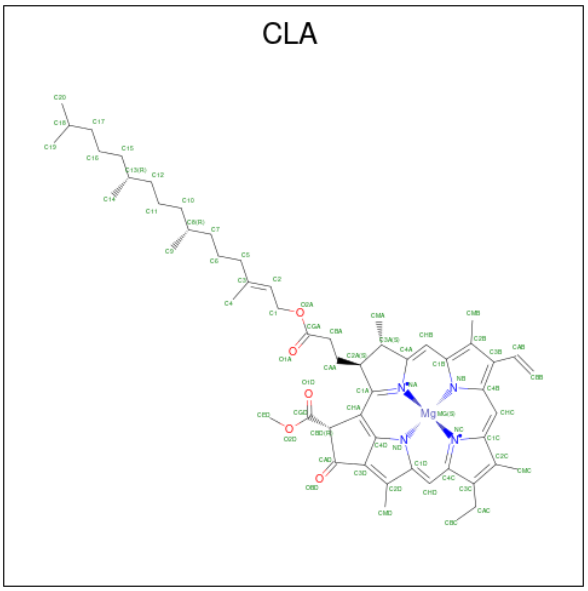
- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Ca	0
			1	1	

- Molecule 11 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
11	A	1	Total	Cl	0
			1	1	

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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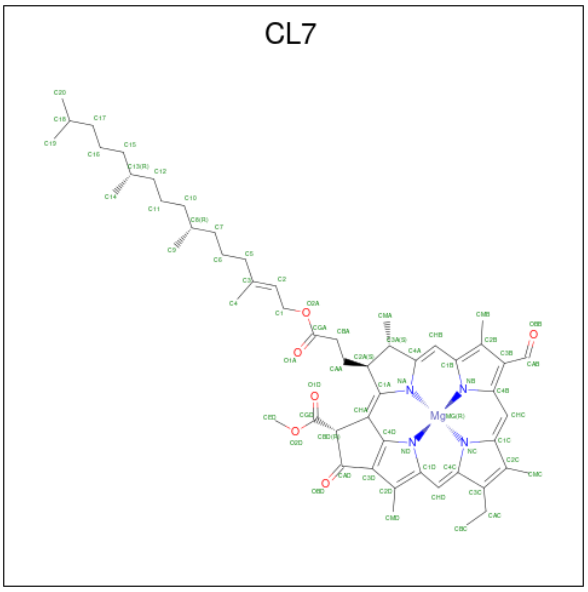
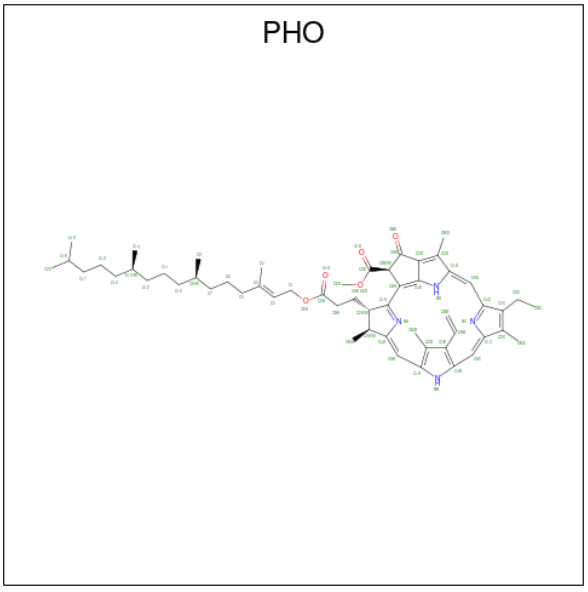
Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	D	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	D	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 13 is CHLOROPHYLL D (three-letter code: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



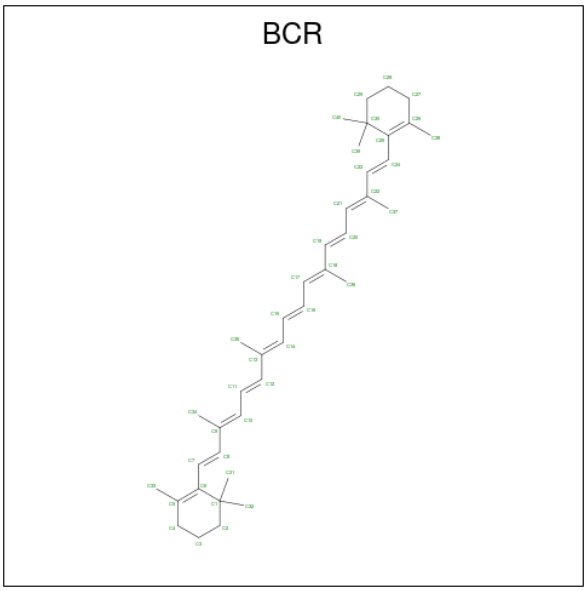
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	54	1	4	6	

- Molecule 14 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



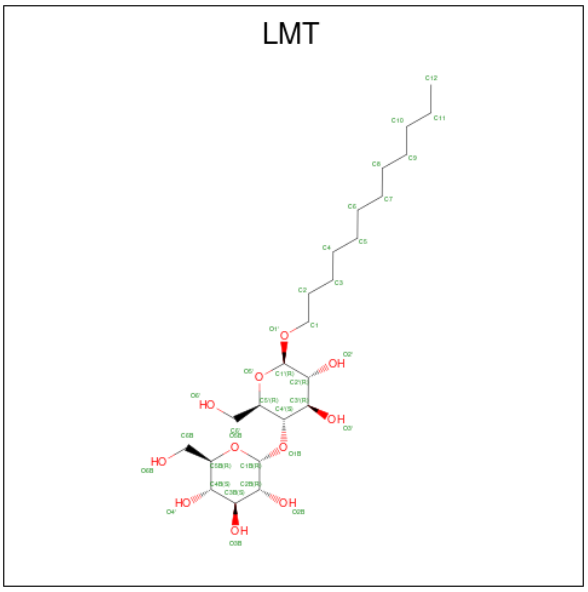
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	N	O	0
			64	55	4	5	
14	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



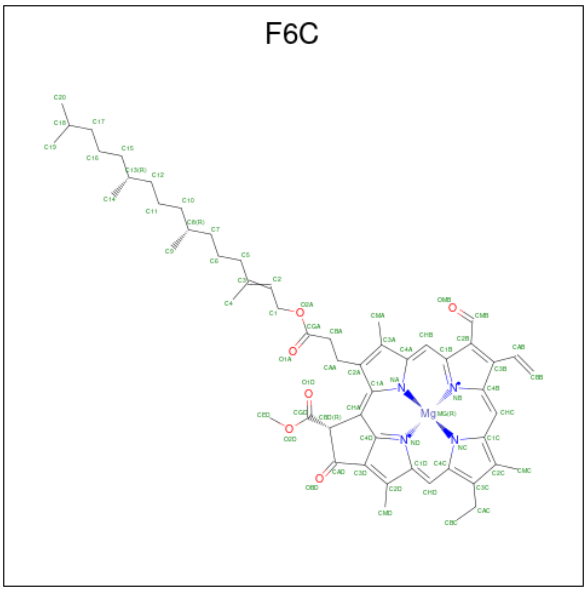
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	C	1	Total C 40 40	0
15	C	1	Total C 40 40	0
15	D	1	Total C 26 26	0

- Molecule 16 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



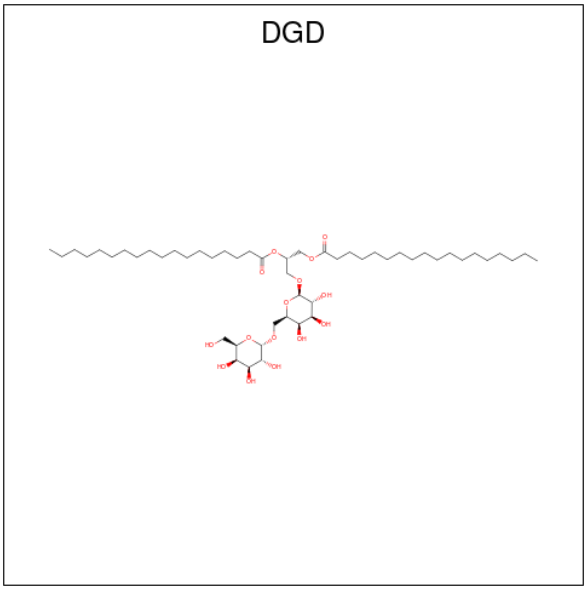
Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total C O 35 24 11	0
16	A	1	Total C O 31 20 11	0
16	B	1	Total C O 35 24 11	0
16	B	1	Total C O 30 19 11	0
16	C	1	Total C O 34 23 11	0
16	D	1	Total C O 20 15 5	0

- Molecule 17 is Chlorophyll F (three-letter code: F6C) (formula: $C_{55}H_{68}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



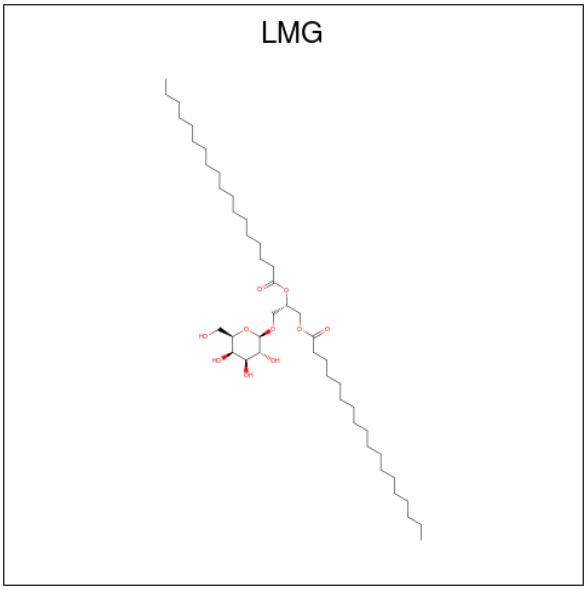
Mol	Chain	Residues	Atoms					AltConf
17	B	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	B	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
17	B	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
17	C	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 18 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total 47	C 38	O 9	0
18	C	1	Total 47	C 32	O 15	0

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).

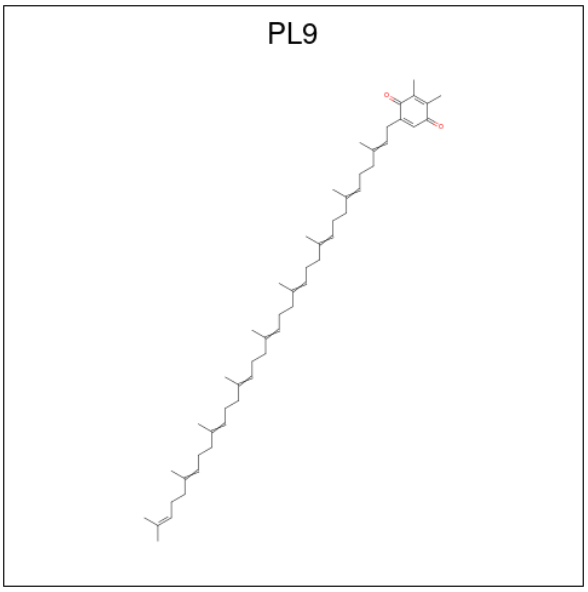


Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total 40	C 30	O 10	0
19	D	1	Total 33	C 23	O 10	0

- Molecule 20 is FE (II) ION (three-letter code: FE2) (formula: Fe).

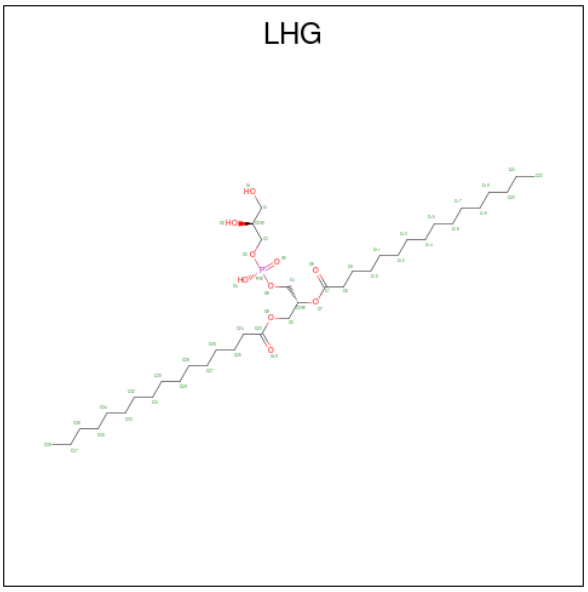
Mol	Chain	Residues	Atoms		AltConf
20	D	1	Total 1	Fe 1	0

- Molecule 21 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula: $C_{53}H_{80}O_2$).



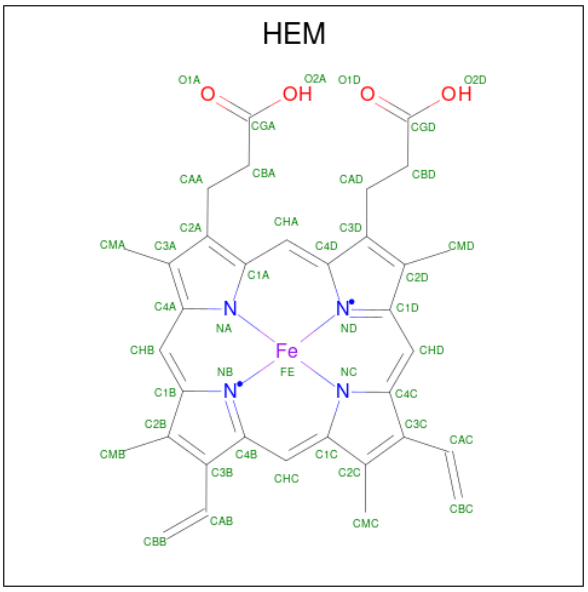
Mol	Chain	Residues	Atoms			AltConf
21	D	1	Total	C	O	0
			45	43	2	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
22	D	1	Total	C	O	P	0
			46	35	10	1	

- Molecule 23 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					AltConf
23	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 24 is water.

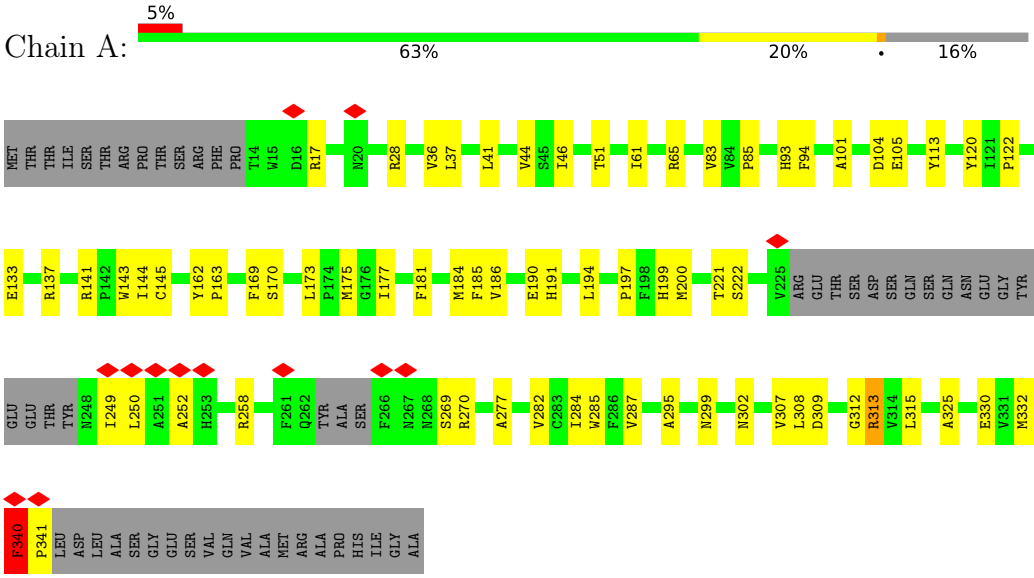
Mol	Chain	Residues	Atoms		AltConf
24	A	61	Total	O	0
			61	61	
24	B	59	Total	O	0
			59	59	
24	C	44	Total	O	0
			44	44	
24	D	65	Total	O	0
			65	65	
24	I	1	Total	O	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

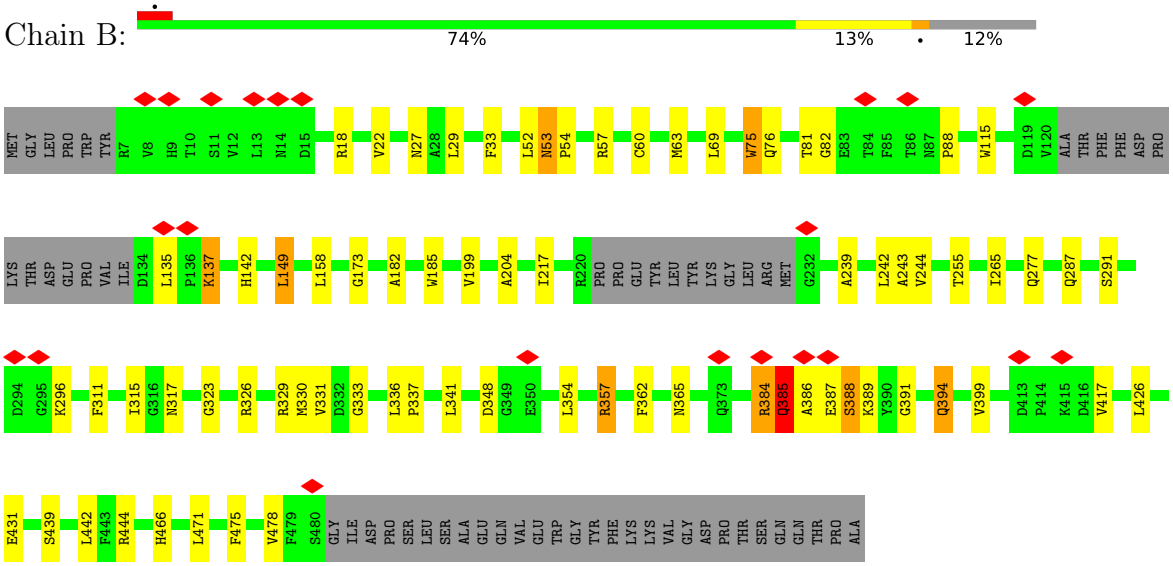
• Molecule 1: Photosystem q(B) protein

Chain A:



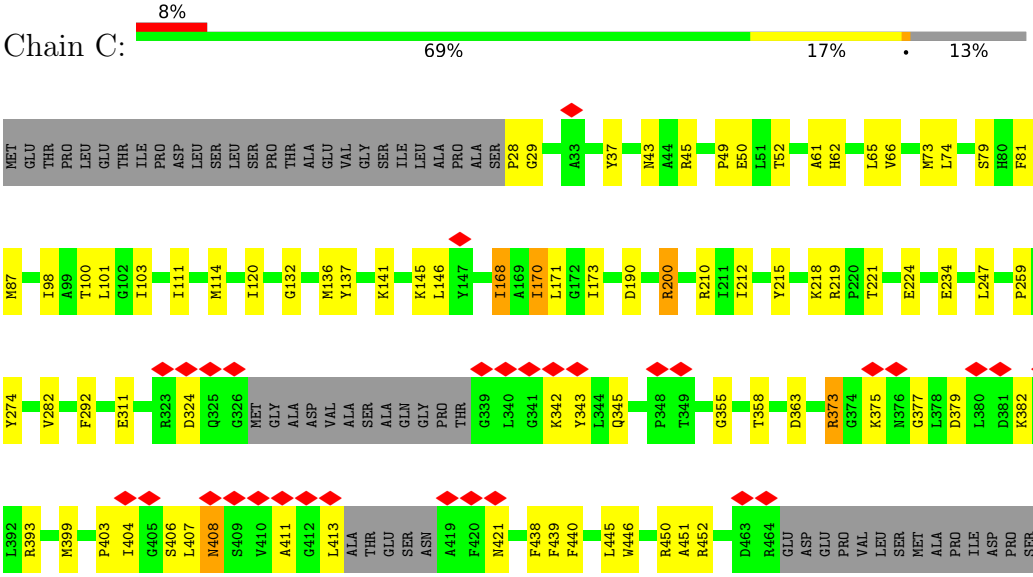
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



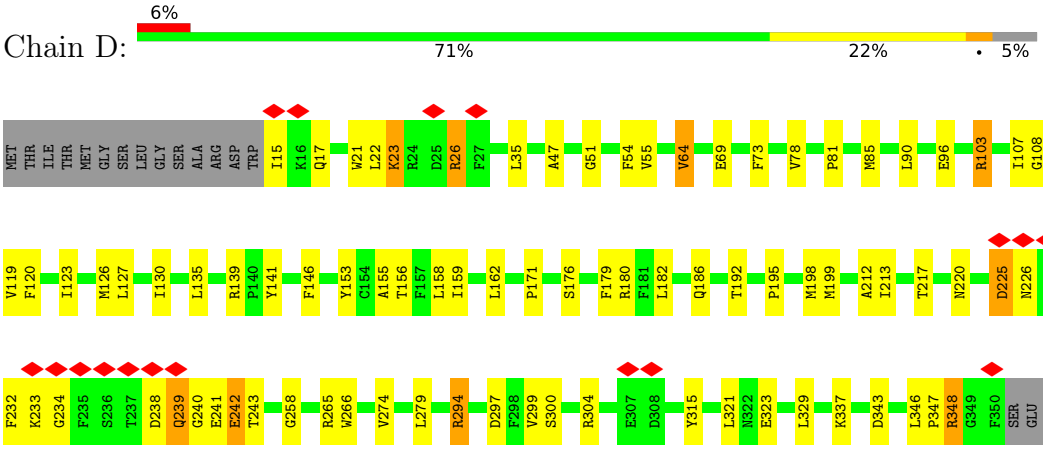
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



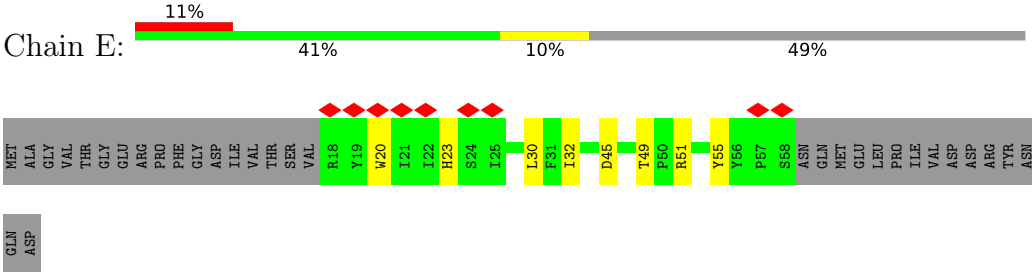
• Molecule 4: Photosystem II D2 protein

Chain D:



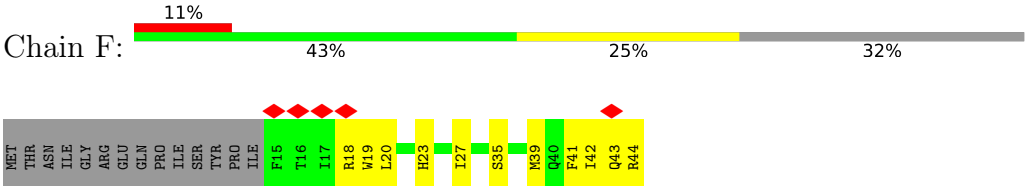
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



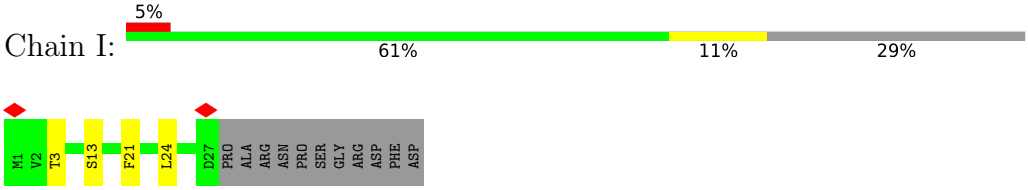
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



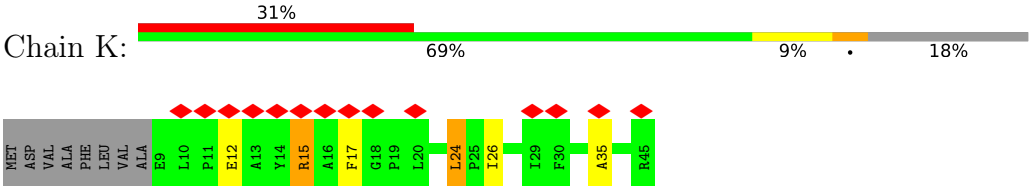
• Molecule 7: Photosystem II reaction center protein I

Chain I:



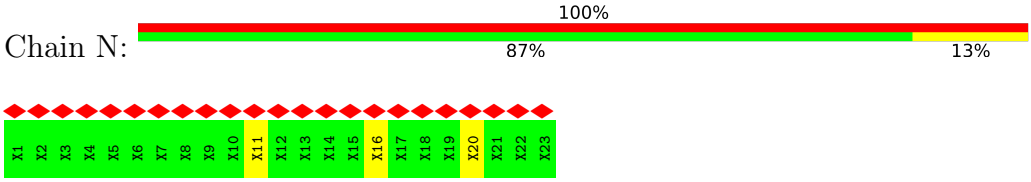
• Molecule 8: Photosystem II reaction center protein K

Chain K:



• Molecule 9: Unknown

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	315307	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.129	Depositor
Minimum map value	-0.059	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	316.8, 316.8, 316.8	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PL9, LHG, LMG, CL7, LMT, HEM, PHO, F6C, CL, CA, CLA, DGD, BCR, FE2

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	A	0.42	0/2462	0.53	0/3362
2	B	0.40	0/3651	0.51	0/4966
3	C	0.37	0/3384	0.51	0/4608
4	D	0.43	0/2760	0.54	0/3751
5	E	0.38	0/345	0.49	0/476
6	F	0.29	0/250	0.73	0/337
7	I	0.31	0/218	0.50	0/294
8	K	0.32	0/305	0.65	0/417
All	All	0.40	0/13375	0.53	0/18211

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	6
8	K	0	1
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	335	ARG	Peptide
1	A	340	PHE	Peptide

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Mol	Chain	Res	Type	Group
2	B	135	LEU	Peptide
2	B	384	ARG	Peptide
2	B	385	GLN	Peptide

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	A	2382	0	2311	73	0
2	B	3528	0	3377	44	0
3	C	3272	0	3190	66	0
4	D	2671	0	2592	83	0
5	E	330	0	310	6	0
6	F	243	0	252	6	0
7	I	213	0	226	3	0
8	K	294	0	301	4	0
9	N	115	0	25	2	0
10	A	1	0	0	0	0
11	A	1	0	0	0	0
12	A	175	0	170	14	0
12	B	610	0	562	37	0
12	C	695	0	688	47	0
12	D	105	0	92	5	0
13	A	65	0	70	4	0
14	A	64	0	74	5	0
14	D	64	0	74	3	0
15	A	40	0	49	5	0
15	B	40	0	49	2	0
15	C	80	0	98	6	0
15	D	26	0	29	1	0
16	A	66	0	78	3	0
16	B	65	0	78	1	0
16	C	34	0	40	2	0
16	D	20	0	24	0	0
17	B	168	0	0	9	0
17	C	61	0	0	1	0
18	B	47	0	66	1	0
18	C	47	0	52	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	40	0	50	1	0
19	D	33	0	36	2	0
20	D	1	0	0	0	0
21	D	45	0	61	4	0
22	D	46	0	65	8	0
23	F	43	0	30	4	0
24	A	61	0	0	6	0
24	B	59	0	0	1	0
24	C	44	0	0	6	0
24	D	65	0	0	2	0
24	I	1	0	0	0	0
All	All	15960	0	15119	331	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 11.

The worst 5 of 331 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)
1:A:330:GLU:OE1	3:C:408:ASN:ND2	1.64	1.30
1:A:190:GLU:O	3:C:407:LEU:HG	1.30	1.29
24:A:556:HOH:O	3:C:407:LEU:HD23	1.55	1.05
1:A:335:ARG:NH2	24:A:501:HOH:O	1.89	1.03
2:B:388:SER:OG	2:B:394:GLN:NE2	2.01	0.93

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 PDB entries followed by that with respect to all EM entries.

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	A	297/361 (82%)	290 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	444/509 (87%)	427 (96%)	16 (4%)	1 (0%)	47 55
3	C	414/482 (86%)	391 (94%)	22 (5%)	1 (0%)	47 55
4	D	334/352 (95%)	324 (97%)	8 (2%)	2 (1%)	25 25
5	E	39/80 (49%)	37 (95%)	2 (5%)	0	100 100
6	F	28/44 (64%)	25 (89%)	3 (11%)	0	100 100
7	I	25/38 (66%)	25 (100%)	0	0	100 100
8	K	35/45 (78%)	33 (94%)	2 (6%)	0	100 100
All	All	1616/1911 (85%)	1552 (96%)	60 (4%)	4 (0%)	50 55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	384	ARG
3	C	86	PRO
4	D	242	GLU
4	D	232	PHE

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 PDB entries followed by that with respect to all EM entries.

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	A	249/299 (83%)	239 (96%)	10 (4%)	31 37
2	B	358/410 (87%)	344 (96%)	14 (4%)	32 38
3	C	321/372 (86%)	300 (94%)	21 (6%)	17 16
4	D	273/290 (94%)	259 (95%)	14 (5%)	24 25
5	E	33/69 (48%)	31 (94%)	2 (6%)	18 18
6	F	24/37 (65%)	21 (88%)	3 (12%)	4 3
7	I	24/33 (73%)	23 (96%)	1 (4%)	30 34
8	K	29/37 (78%)	27 (93%)	2 (7%)	15 14
All	All	1311/1547 (85%)	1244 (95%)	67 (5%)	27 25

5 of 67 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	300	SER
5	E	20	TRP
8	K	15	ARG
3	C	73	MET
2	B	394	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	314	GLN
3	C	408	ASN
3	C	391	GLN
3	C	421	ASN
2	B	365	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 3 are monoatomic - leaving 53 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	$\#\|Z\|>2$
12	CLA	A	405	24	50,58,73	2.53	19 (38%)	58,95,113	2.93	25 (43%)
16	LMT	A	410	-	32,32,36	1.32	5 (15%)	43,43,47	1.24	5 (11%)
12	CLA	C	509	-	65,73,73	2.26	20 (30%)	76,113,113	2.56	25 (32%)
12	CLA	D	404	-	45,53,73	2.53	19 (42%)	52,89,113	2.98	21 (40%)
15	BCR	C	514	-	41,41,41	2.89	6 (14%)	56,56,56	6.39	19 (33%)
16	LMT	C	516	-	35,35,36	1.20	6 (17%)	46,46,47	0.95	0
12	CLA	B	605	-	55,63,73	2.45	19 (34%)	64,101,113	2.78	26 (40%)
17	F6C	B	606	24	64,69,74	2.85	26 (40%)	64,108,114	3.68	29 (45%)
19	LMG	B	617	-	40,40,55	1.15	4 (10%)	48,48,63	1.25	4 (8%)
15	BCR	A	408	-	41,41,41	2.95	6 (14%)	56,56,56	6.44	24 (42%)
16	LMT	D	409	-	20,20,36	1.41	4 (20%)	23,24,47	1.70	4 (17%)
12	CLA	B	613	-	65,73,73	2.21	18 (27%)	76,113,113	2.62	25 (32%)
12	CLA	D	403	-	60,68,73	2.27	18 (30%)	70,107,113	2.93	22 (31%)
12	CLA	B	611	-	65,73,73	2.20	18 (27%)	76,113,113	2.59	21 (27%)
15	BCR	B	615	-	41,41,41	2.99	6 (14%)	56,56,56	6.36	23 (41%)
15	BCR	C	517	-	41,41,41	2.84	6 (14%)	56,56,56	6.42	21 (37%)
15	BCR	D	405	-	26,26,41	3.31	5 (19%)	34,34,56	7.81	15 (44%)
17	F6C	B	603	-	54,59,74	3.12	26 (48%)	52,96,114	3.65	29 (55%)
16	LMT	B	619	-	31,31,36	1.40	7 (22%)	42,42,47	1.25	4 (9%)
12	CLA	C	501	-	65,73,73	2.19	19 (29%)	76,113,113	2.62	25 (32%)
16	LMT	A	409	-	36,36,36	1.20	6 (16%)	47,47,47	1.13	3 (6%)
12	CLA	A	403	-	65,73,73	2.18	18 (27%)	76,113,113	2.65	25 (32%)
12	CLA	B	614	-	50,58,73	2.49	21 (42%)	58,95,113	2.97	24 (41%)
12	CLA	C	506	-	55,63,73	2.45	20 (36%)	64,101,113	2.71	24 (37%)
12	CLA	C	512	-	45,53,73	2.55	18 (40%)	52,89,113	2.98	20 (38%)
12	CLA	B	609	-	45,53,73	2.57	19 (42%)	52,89,113	3.03	21 (40%)
18	DGD	C	515	-	48,48,67	1.16	5 (10%)	62,62,81	1.36	4 (6%)
12	CLA	C	511	3	45,53,73	2.54	18 (40%)	52,89,113	2.98	20 (38%)
23	HEM	F	101	5,6	41,50,50	1.45	4 (9%)	45,82,82	1.40	6 (13%)
13	CL7	A	404	24	66,73,73	2.72	22 (33%)	65,113,113	2.42	18 (27%)
17	F6C	C	507	24	64,69,74	2.86	26 (40%)	64,108,114	3.34	27 (42%)
12	CLA	B	601	-	55,63,73	2.41	19 (34%)	64,101,113	2.76	22 (34%)
12	CLA	B	602	-	55,63,73	2.41	18 (32%)	64,101,113	2.78	27 (42%)
17	F6C	B	612	-	59,64,74	2.97	26 (44%)	58,102,114	3.53	27 (46%)
18	DGD	B	616	-	47,47,67	0.96	3 (6%)	55,55,81	1.40	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	B	607	-	65,73,73	2.26	20 (30%)	76,113,113	2.53	27 (35%)
19	LMG	D	408	-	33,33,55	1.15	2 (6%)	41,41,63	1.09	1 (2%)
21	PL9	D	406	-	45,45,55	1.56	5 (11%)	56,57,69	1.54	11 (19%)
12	CLA	A	407	-	60,68,73	2.31	18 (30%)	70,107,113	2.64	22 (31%)
12	CLA	C	504	24	50,58,73	2.51	19 (38%)	58,95,113	2.94	23 (39%)
16	LMT	B	618	-	36,36,36	1.16	4 (11%)	47,47,47	1.10	3 (6%)
22	LHG	D	407	-	45,45,48	0.92	2 (4%)	48,51,54	1.11	5 (10%)
12	CLA	C	502	-	65,73,73	2.21	19 (29%)	76,113,113	2.63	25 (32%)
12	CLA	C	503	-	65,73,73	2.18	18 (27%)	76,113,113	2.57	24 (31%)
12	CLA	C	505	-	65,73,73	2.23	18 (27%)	76,113,113	2.49	23 (30%)
12	CLA	B	604	-	55,63,73	2.44	20 (36%)	64,101,113	2.76	24 (37%)
12	CLA	B	610	-	55,63,73	2.42	19 (34%)	64,101,113	2.80	25 (39%)
12	CLA	C	510	-	65,73,73	2.22	20 (30%)	76,113,113	2.69	28 (36%)
12	CLA	C	513	-	45,53,73	2.59	18 (40%)	52,89,113	2.87	19 (36%)
14	PHO	A	406	-	51,69,69	1.00	4 (7%)	47,99,99	1.22	5 (10%)
12	CLA	B	608	-	45,53,73	2.57	20 (44%)	52,89,113	2.98	20 (38%)
14	PHO	D	402	-	51,69,69	1.00	4 (7%)	47,99,99	1.39	8 (17%)
12	CLA	C	508	-	65,73,73	2.24	20 (30%)	76,113,113	2.60	23 (30%)

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
12	CLA	A	405	24	1/1/12/20	7/19/97/115	-
16	LMT	A	410	-	-	7/17/57/61	0/2/2/2
12	CLA	C	509	-	1/1/15/20	12/37/115/115	-
12	CLA	D	404	-	1/1/11/20	4/13/91/115	-
15	BCR	C	514	-	-	5/29/63/63	0/2/2/2
16	LMT	C	516	-	-	11/20/60/61	0/2/2/2
12	CLA	B	605	-	1/1/13/20	10/25/103/115	-
17	F6C	B	606	24	-	19/35/91/97	-
19	LMG	B	617	-	-	9/35/55/70	0/1/1/1
15	BCR	A	408	-	-	10/29/63/63	0/2/2/2
16	LMT	D	409	-	-	9/12/28/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	613	-	1/1/15/20	16/37/115/115	-
12	CLA	D	403	-	1/1/14/20	6/31/109/115	-
12	CLA	B	611	-	1/1/15/20	16/37/115/115	-
15	BCR	B	615	-	-	9/29/63/63	0/2/2/2
15	BCR	C	517	-	-	11/29/63/63	0/2/2/2
15	BCR	D	405	-	-	8/20/37/63	0/1/1/2
17	F6C	B	603	-	-	8/23/79/97	-
16	LMT	B	619	-	-	6/16/56/61	0/2/2/2
12	CLA	C	501	-	1/1/15/20	10/37/115/115	-
16	LMT	A	409	-	-	7/21/61/61	0/2/2/2
12	CLA	A	403	-	1/1/15/20	8/37/115/115	-
12	CLA	B	614	-	1/1/12/20	2/19/97/115	-
12	CLA	C	506	-	1/1/13/20	10/25/103/115	-
12	CLA	C	512	-	1/1/11/20	9/13/91/115	-
12	CLA	B	609	-	1/1/11/20	7/13/91/115	-
18	DGD	C	515	-	-	13/36/76/95	0/2/2/2
12	CLA	C	511	3	1/1/11/20	5/13/91/115	-
23	HEM	F	101	5,6	-	3/12/54/54	-
13	CL7	A	404	24	2/2/15/20	24/37/115/115	-
17	F6C	C	507	24	-	17/35/91/97	-
12	CLA	B	601	-	1/1/13/20	8/25/103/115	-
12	CLA	B	602	-	1/1/13/20	11/25/103/115	-
17	F6C	B	612	-	-	12/29/85/97	-
18	DGD	B	616	-	-	19/41/61/95	0/1/1/2
12	CLA	B	607	-	1/1/15/20	16/37/115/115	-
19	LMG	D	408	-	-	4/28/48/70	0/1/1/1
21	PL9	D	406	-	-	14/41/61/73	0/1/1/1
12	CLA	A	407	-	1/1/14/20	12/31/109/115	-
12	CLA	C	504	24	1/1/12/20	7/19/97/115	-
16	LMT	B	618	-	-	11/21/61/61	0/2/2/2
22	LHG	D	407	-	-	21/50/50/53	-
12	CLA	C	502	-	1/1/15/20	19/37/115/115	-
12	CLA	C	503	-	1/1/15/20	11/37/115/115	-
12	CLA	C	505	-	1/1/15/20	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	604	-	1/1/13/20	14/25/103/115	-
12	CLA	B	610	-	1/1/13/20	11/25/103/115	-
12	CLA	C	510	-	1/1/15/20	21/37/115/115	-
12	CLA	C	513	-	1/1/11/20	6/13/91/115	-
14	PHO	A	406	-	-	10/37/103/103	0/5/6/6
12	CLA	B	608	-	1/1/11/20	11/13/91/115	-
14	PHO	D	402	-	-	6/37/103/103	0/5/6/6
12	CLA	C	508	-	1/1/15/20	19/37/115/115	-

The worst 5 of 750 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	B	603	F6C	MG-NA	9.33	2.24	2.05
17	C	507	F6C	MG-NA	9.24	2.24	2.05
17	B	612	F6C	MG-NA	9.08	2.23	2.05
17	B	606	F6C	MG-NA	8.91	2.23	2.05
17	B	606	F6C	C1A-CHA	8.84	1.51	1.35

The worst 5 of 957 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	405	BCR	C20-C19-C18	22.01	149.85	126.59
15	C	517	BCR	C20-C21-C22	20.90	157.14	127.31
15	B	615	BCR	C15-C16-C17	20.83	166.15	123.47
15	A	408	BCR	C15-C16-C17	20.68	165.83	123.47
15	C	517	BCR	C15-C16-C17	20.65	165.77	123.47

5 of 30 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	403	CLA	ND
12	A	405	CLA	ND
12	A	407	CLA	ND
12	B	601	CLA	ND
12	B	602	CLA	ND

5 of 582 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	403	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
12	B	604	CLA	C2A-CAA-CBA-CGA
12	B	607	CLA	C2-C1-O2A-CGA
12	B	607	CLA	CBD-CGD-O2D-CED
12	B	608	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

48 monomers are involved in 154 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	405	CLA	2	0
16	A	410	LMT	1	0
12	C	509	CLA	7	0
12	D	404	CLA	3	0
15	C	514	BCR	2	0
16	C	516	LMT	2	0
12	B	605	CLA	2	0
19	B	617	LMG	1	0
15	A	408	BCR	5	0
12	B	613	CLA	3	0
12	D	403	CLA	2	0
12	B	611	CLA	7	0
15	B	615	BCR	2	0
15	C	517	BCR	4	0
15	D	405	BCR	1	0
17	B	603	F6C	5	0
16	B	619	LMT	1	0
12	C	501	CLA	4	0
16	A	409	LMT	2	0
12	A	403	CLA	7	0
12	B	614	CLA	1	0
12	C	506	CLA	3	0
12	C	512	CLA	1	0
12	B	609	CLA	1	0
18	C	515	DGD	2	0
12	C	511	CLA	2	0
23	F	101	HEM	4	0
13	A	404	CL7	4	0
17	C	507	F6C	1	0
12	B	601	CLA	1	0
12	B	602	CLA	5	0
17	B	612	F6C	4	0
18	B	616	DGD	1	0

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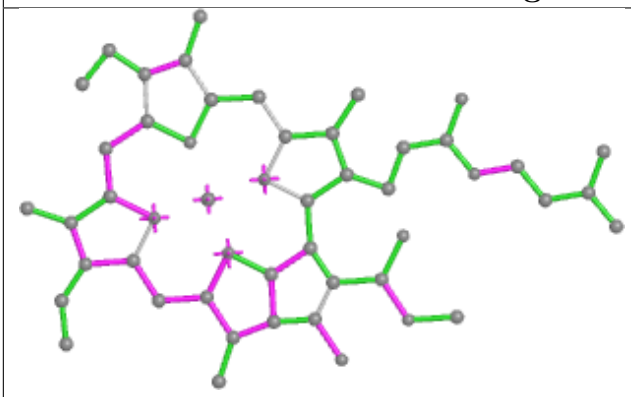
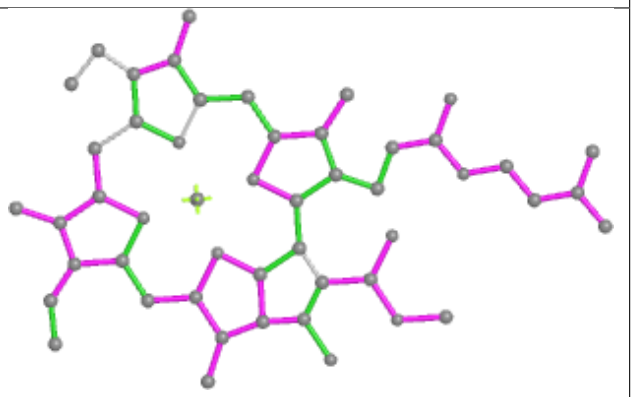
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	607	CLA	5	0
19	D	408	LMG	2	0
21	D	406	PL9	4	0
12	A	407	CLA	5	0
12	C	504	CLA	1	0
22	D	407	LHG	8	0
12	C	502	CLA	5	0
12	C	503	CLA	9	0
12	C	505	CLA	5	0
12	B	604	CLA	11	0
12	B	610	CLA	5	0
12	C	510	CLA	6	0
14	A	406	PHO	5	0
14	D	402	PHO	3	0
12	C	508	CLA	9	0

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.

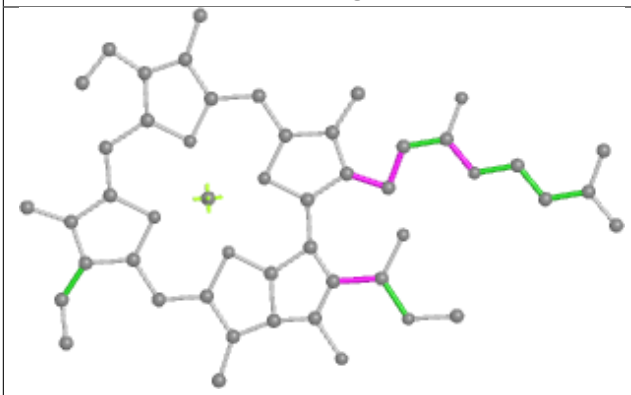
Ligand CLA A 405



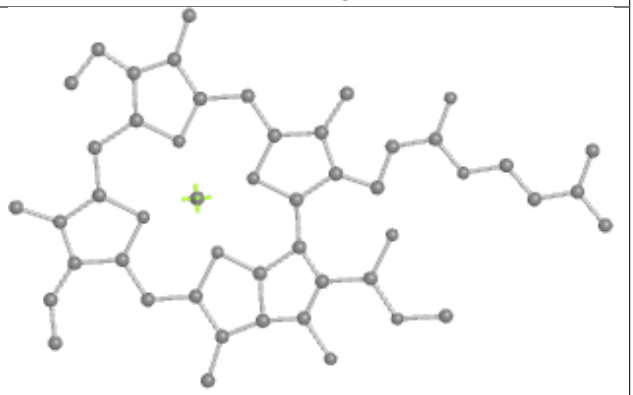
Bond lengths



Bond angles

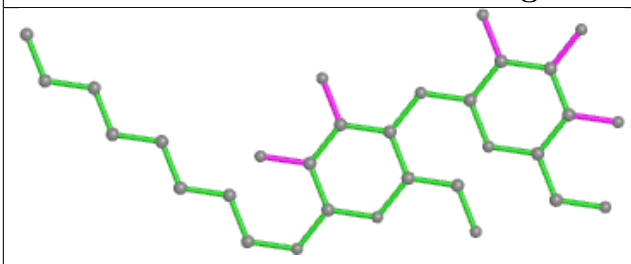


Torsions

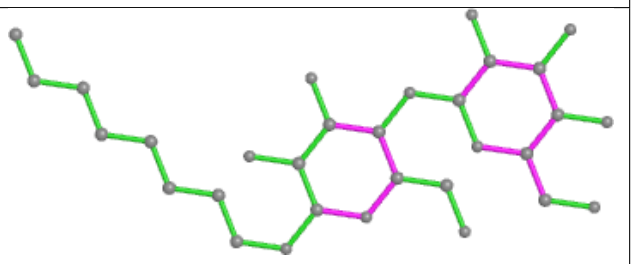


Rings

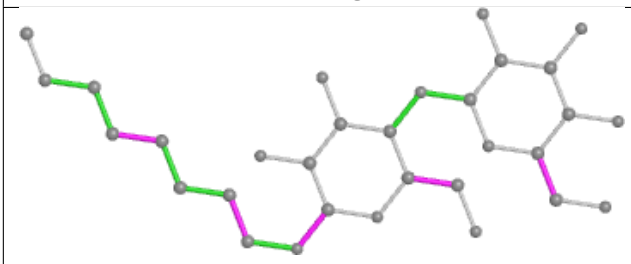
Ligand LMT A 410



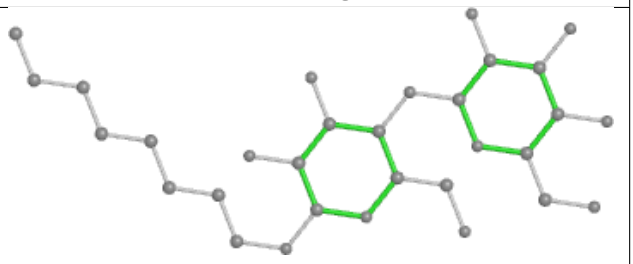
Bond lengths



Bond angles

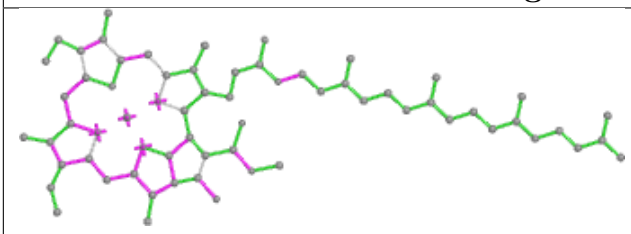


Torsions



Rings

Ligand CLA C 509



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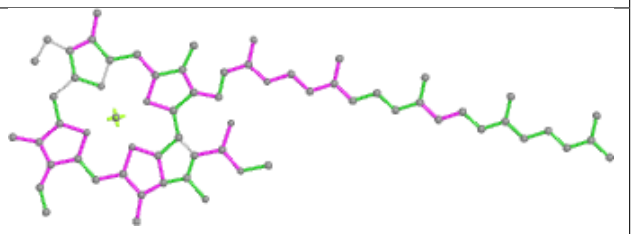
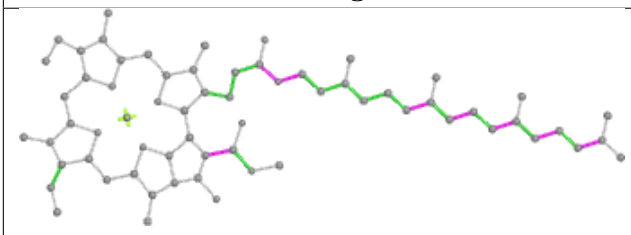
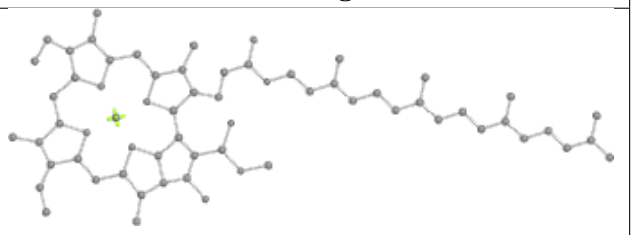


Bond angles

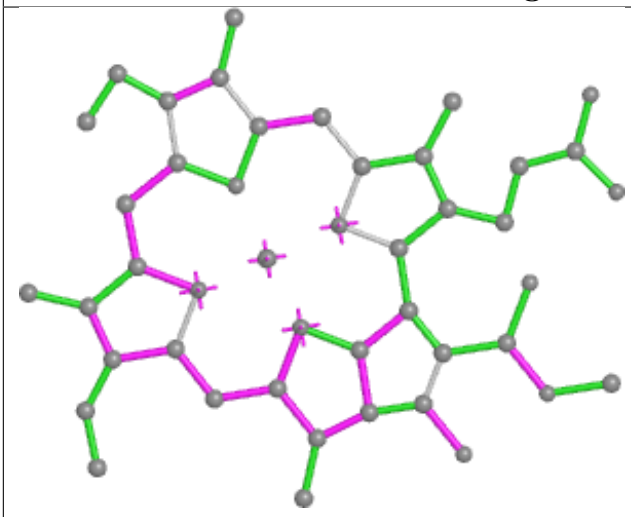


Torsions



Rings

Ligand CLA D 404



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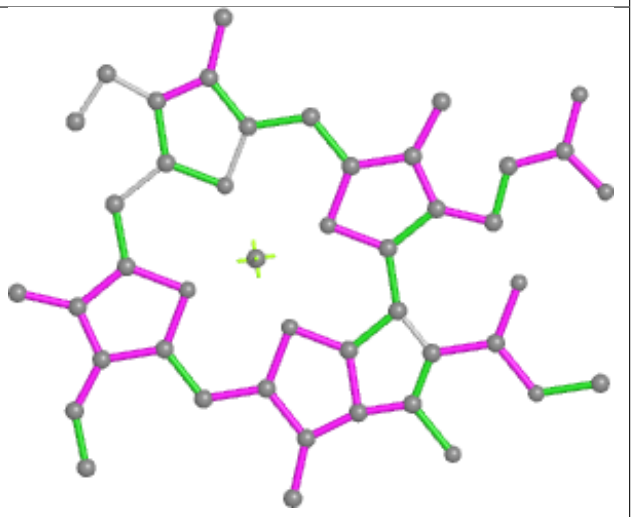
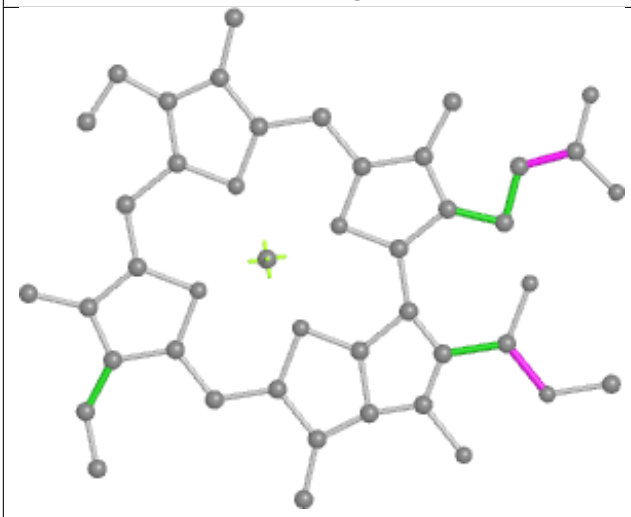


Bond angles



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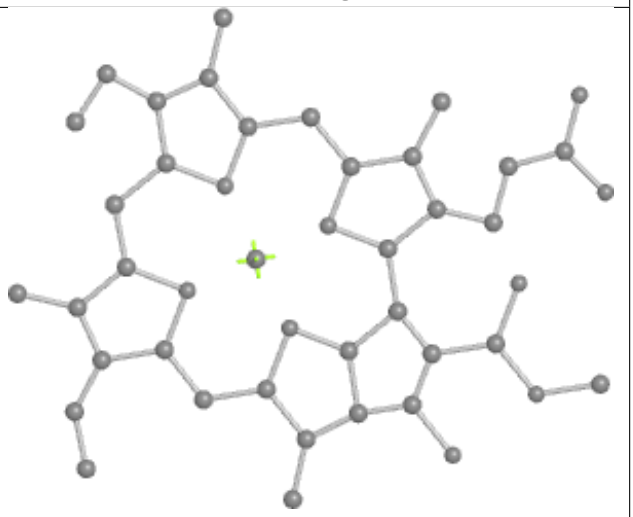
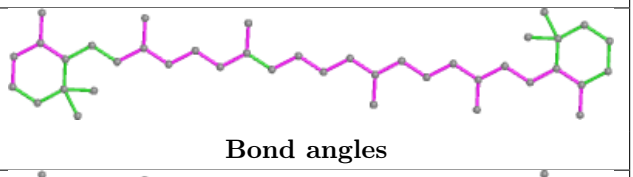


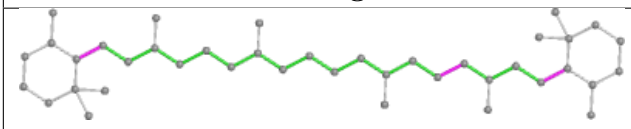
Rings

Ligand BCR C 514

Bond lengths



Bond angles



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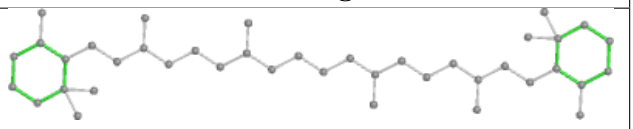
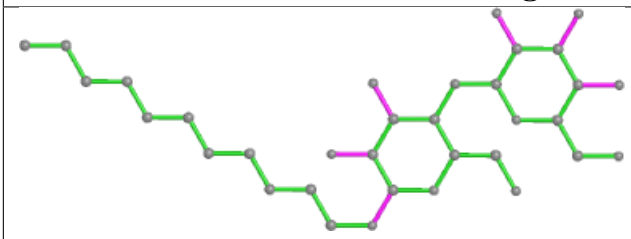


Rings

Ligand LMT C 516



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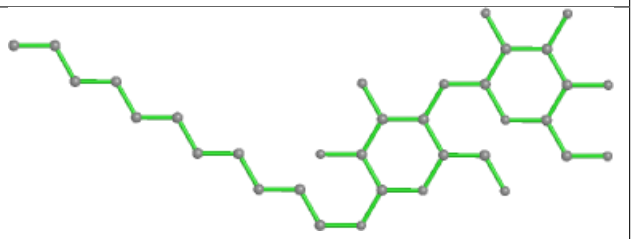

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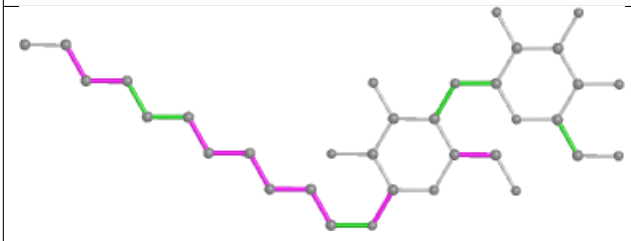

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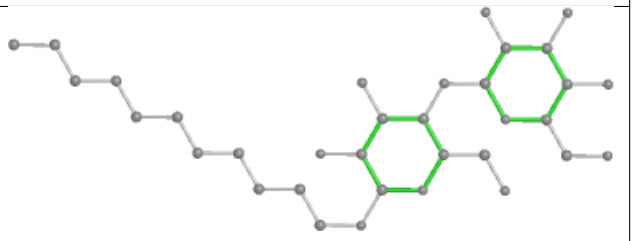
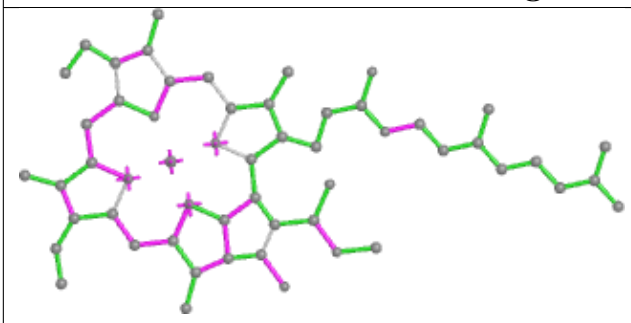


Rings

Ligand CLA B 605



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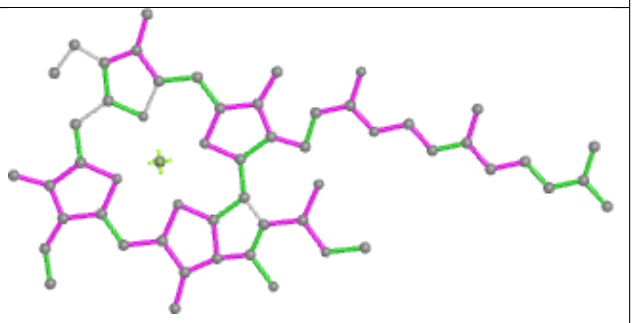

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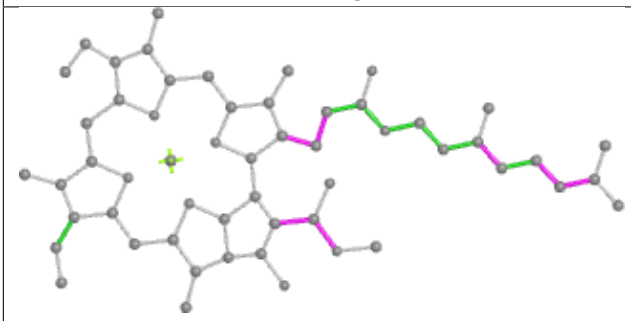

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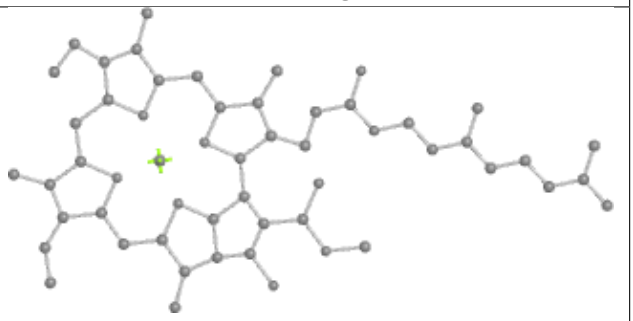
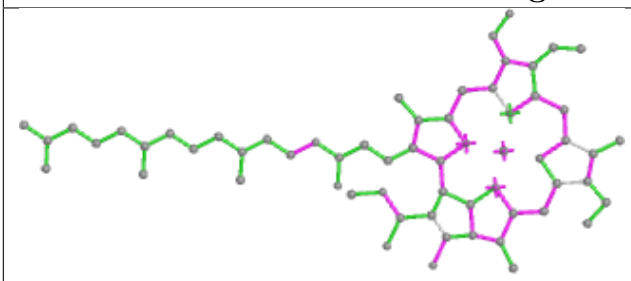


Rings

Ligand F6C B 606



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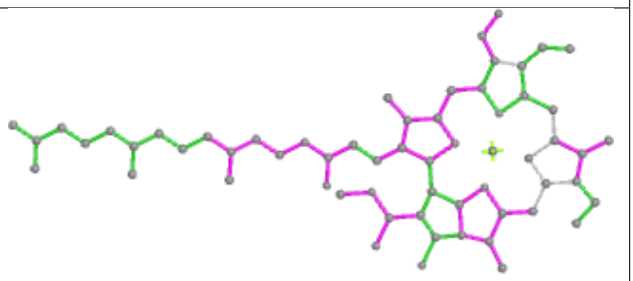

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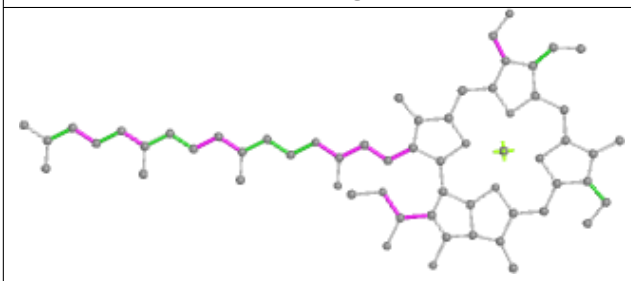
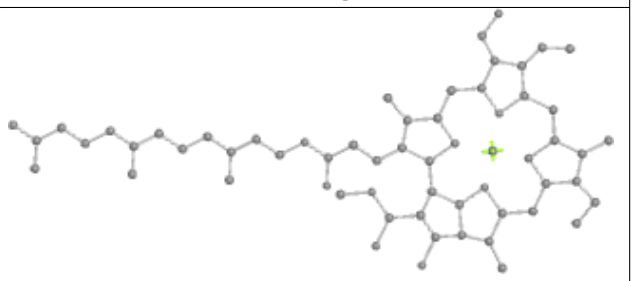
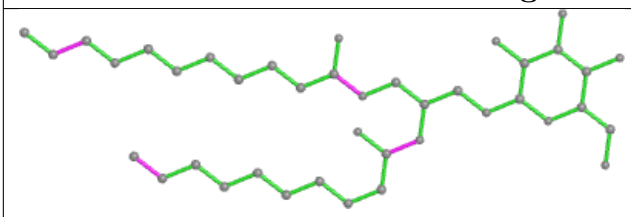


Torsions



Rings

Ligand LMG B 617



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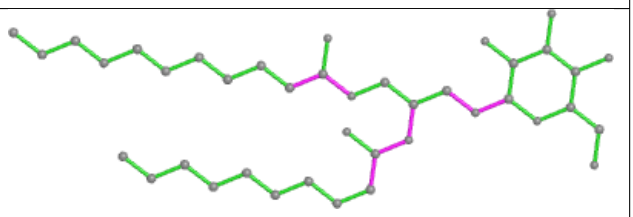
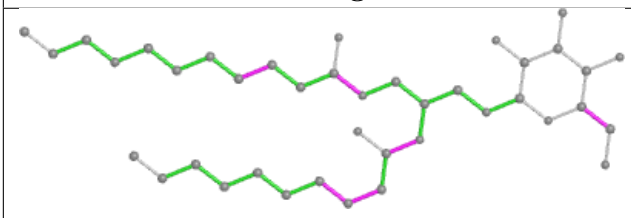
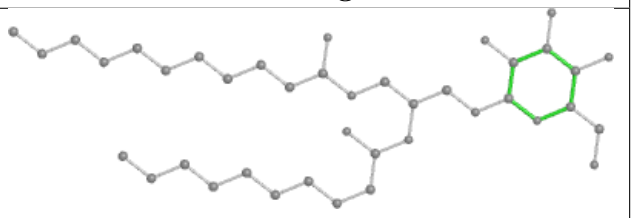


Bond angles

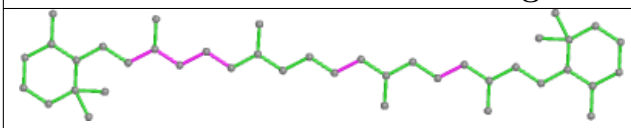


Torsions

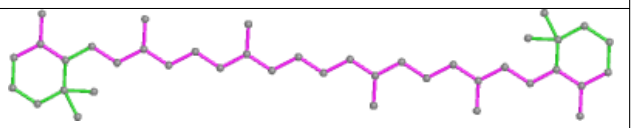


Rings

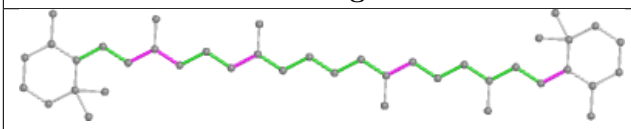
Ligand BCR A 408



Bond lengths



Bond angles



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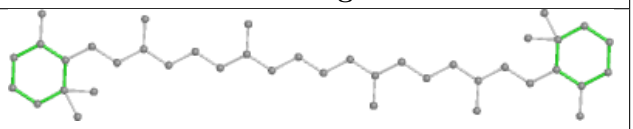
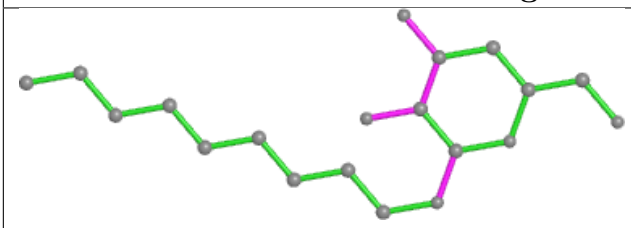
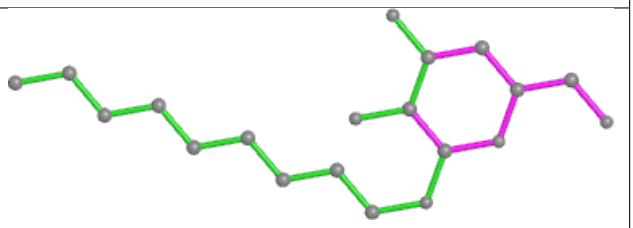


Rings

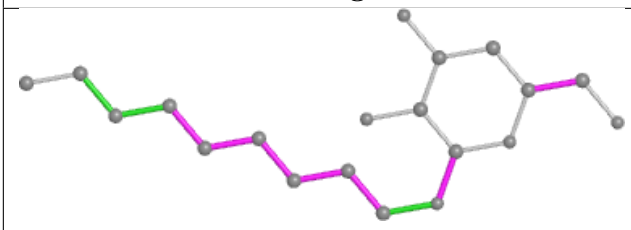
Ligand LMT D 409



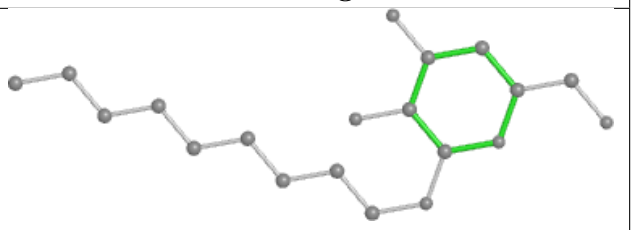
Bond lengths



Bond angles

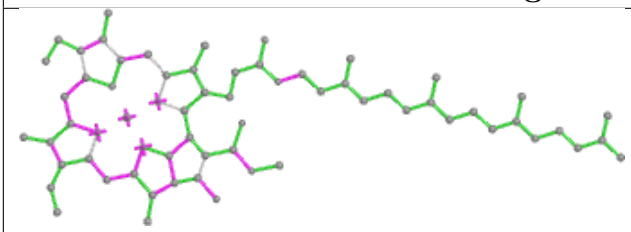


Torsions

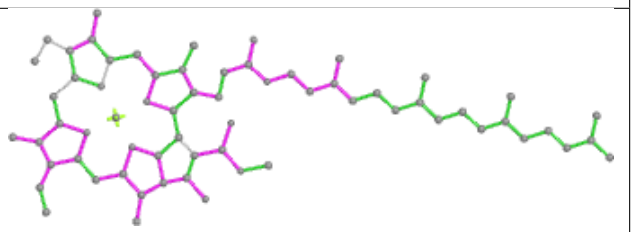


Rings

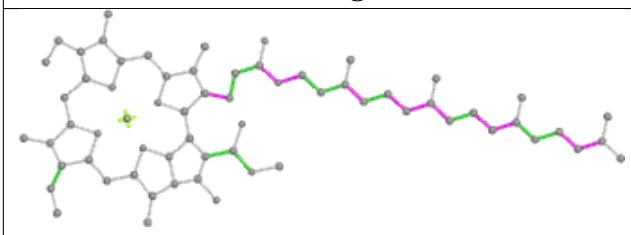
Ligand CLA B 613



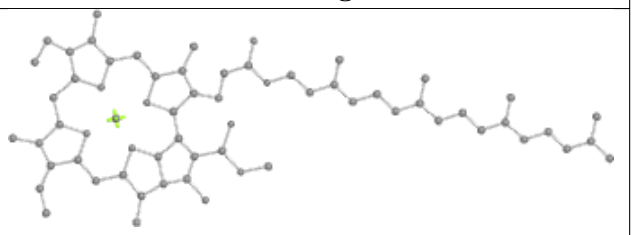
Bond lengths



Bond angles

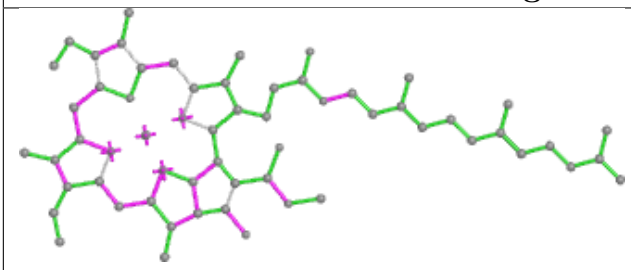


Torsions

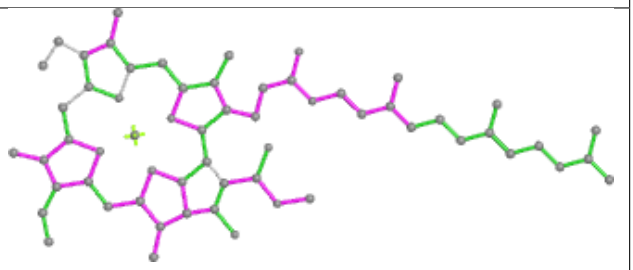


Rings

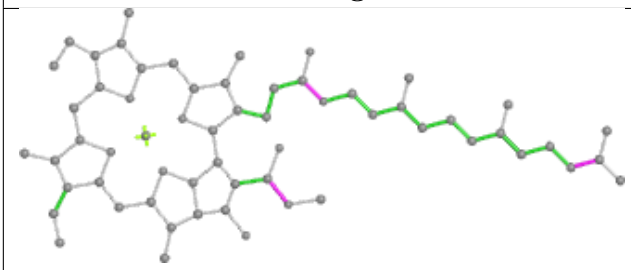
Ligand CLA D 403



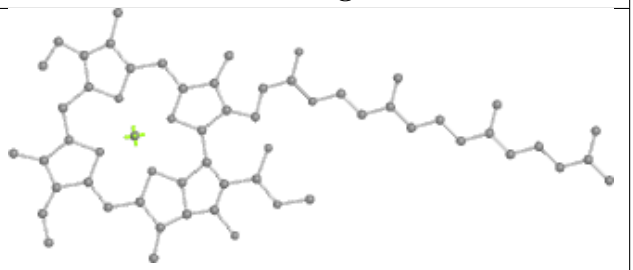
Bond lengths



Bond angles

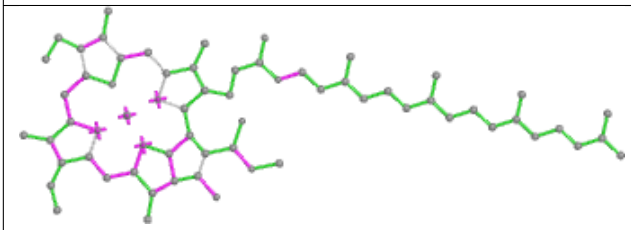


Torsions

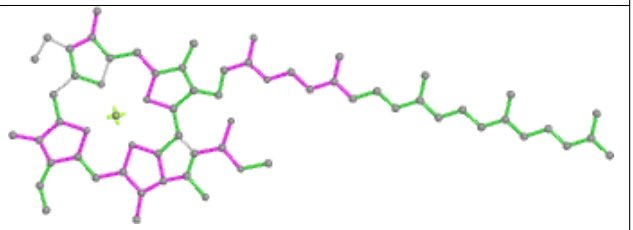


Rings

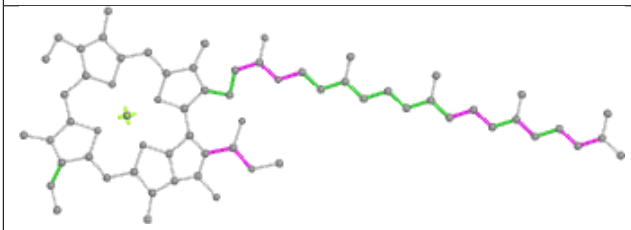
Ligand CLA B 611



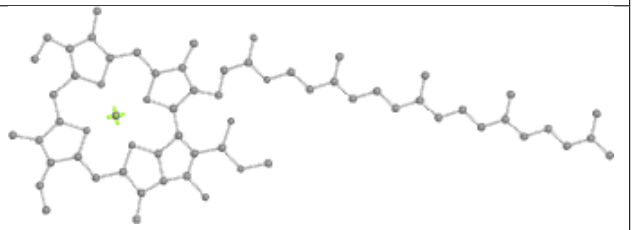
Bond lengths



Bond angles

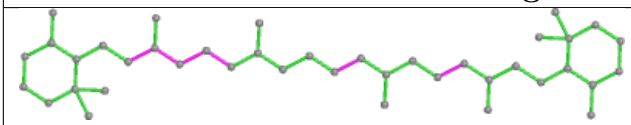


Torsions

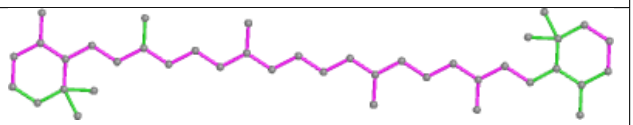


Rings

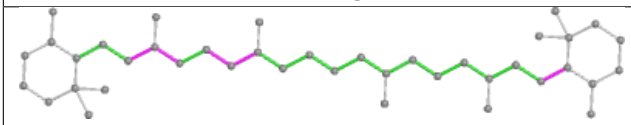
Ligand BCR B 615



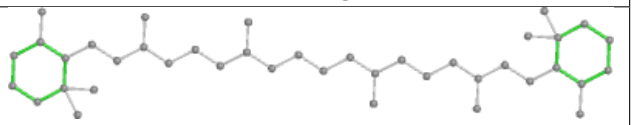
Bond lengths



Bond angles



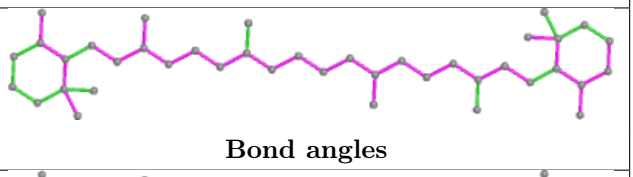
Torsions



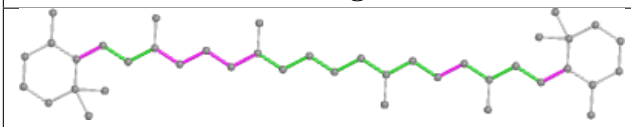
Rings

Ligand BCR C 517

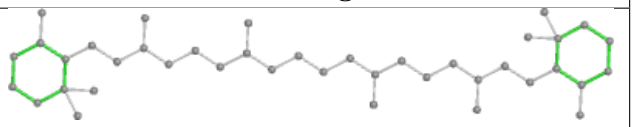
Bond lengths



Bond angles

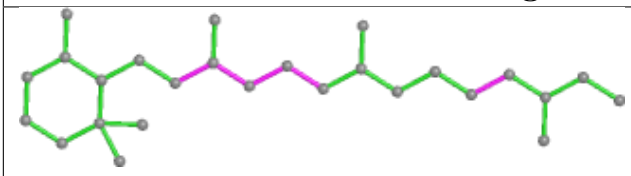


Torsions

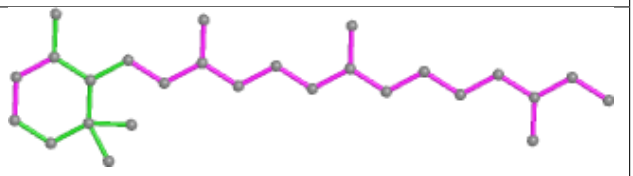


Rings

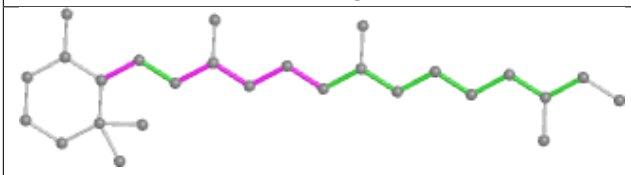
Ligand BCR D 405



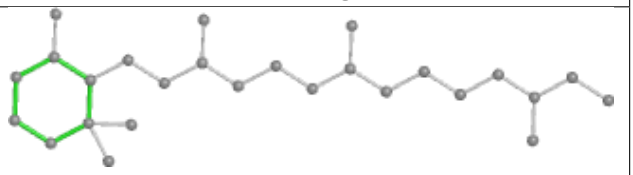
Bond lengths



Bond angles

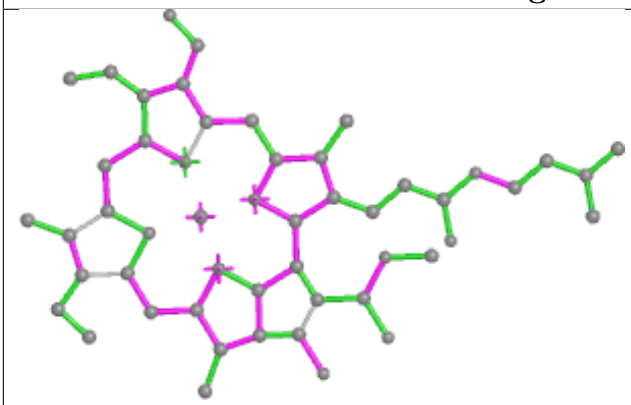


Torsions

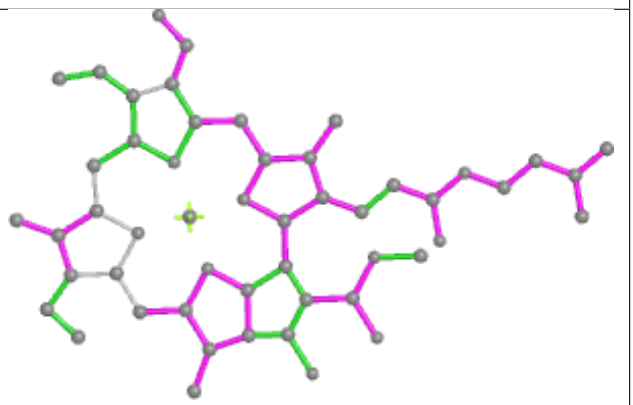


Rings

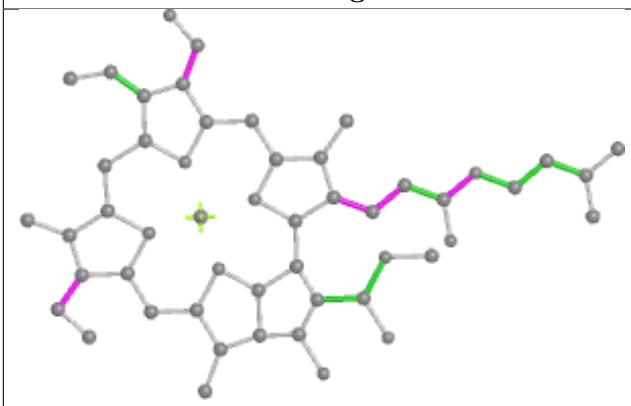
Ligand F6C B 603



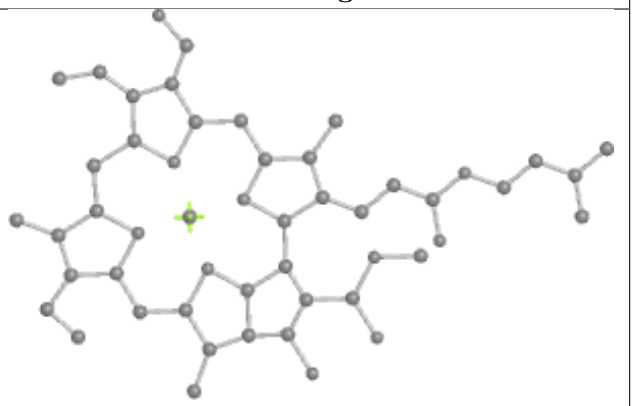
Bond lengths



Bond angles

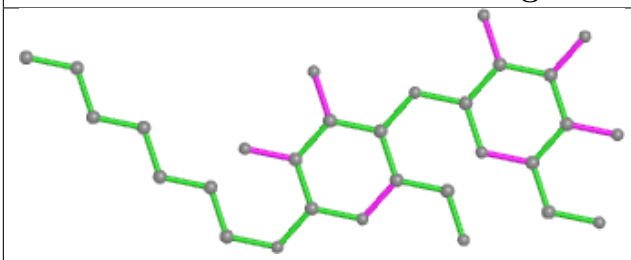


Torsions

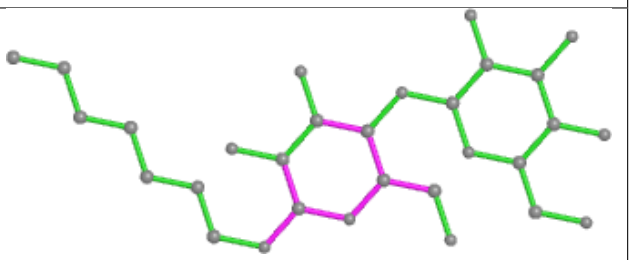


Rings

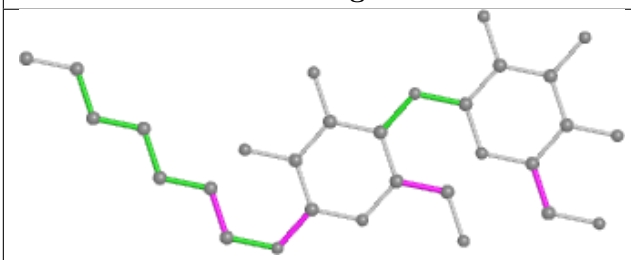
Ligand LMT B 619



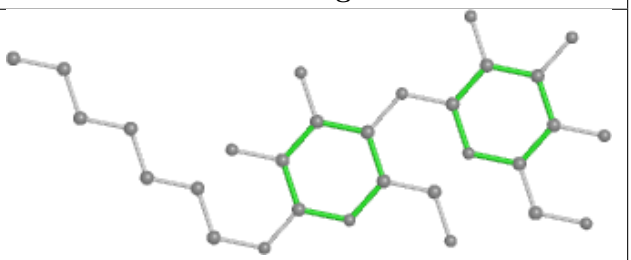
Bond lengths



Bond angles

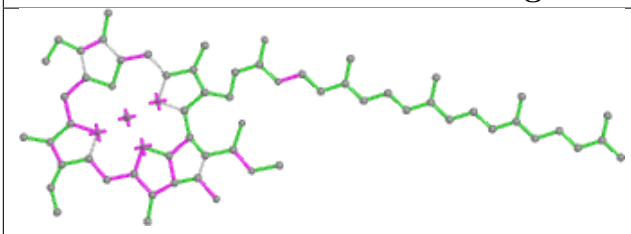


Torsions



Rings

Ligand CLA C 501



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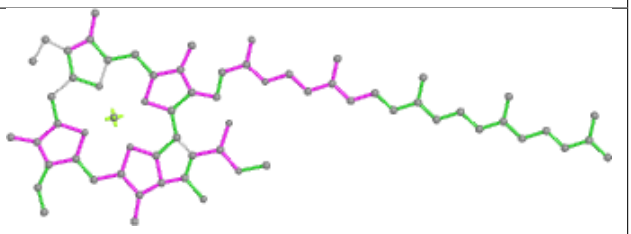
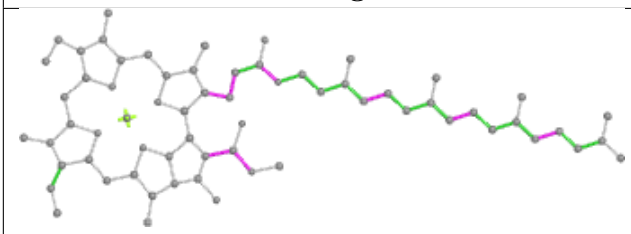
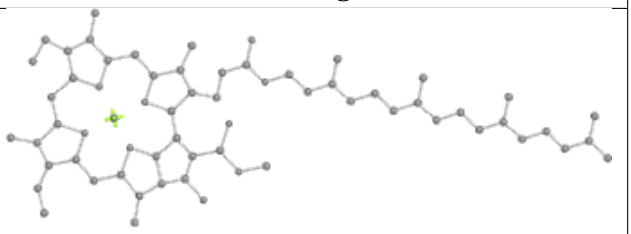


Bond angles

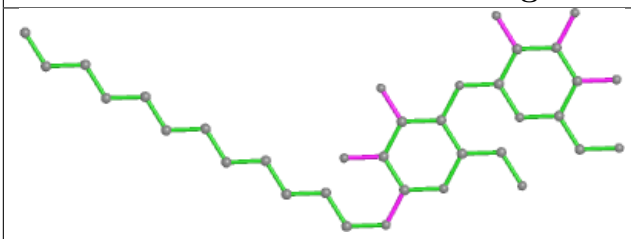


Torsions



Rings

Ligand LMT A 409



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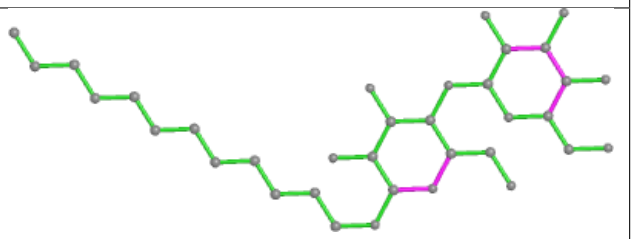
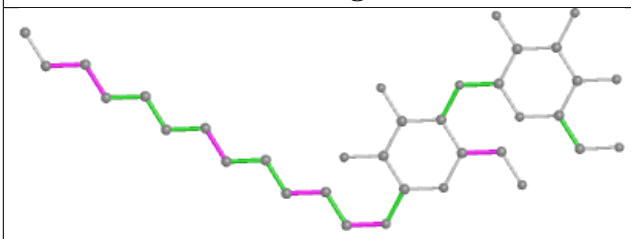
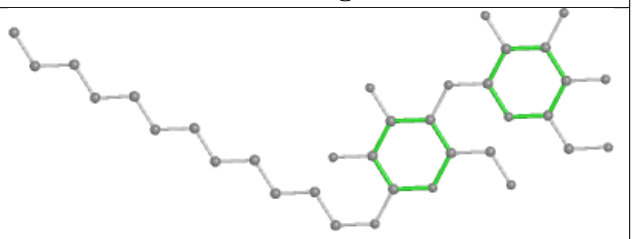


Bond angles

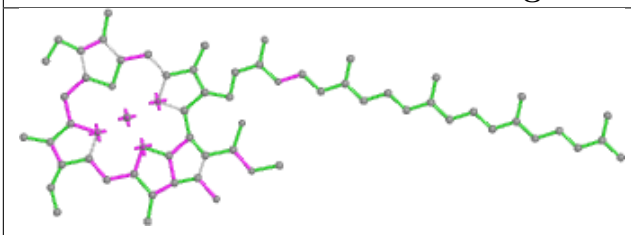


Torsions



Rings

Ligand CLA A 403



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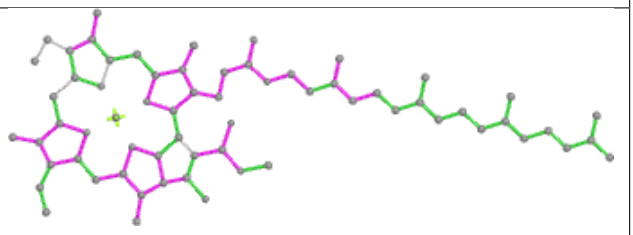
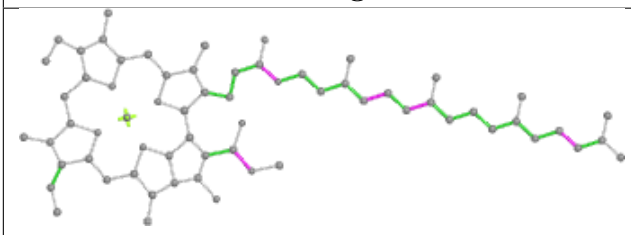
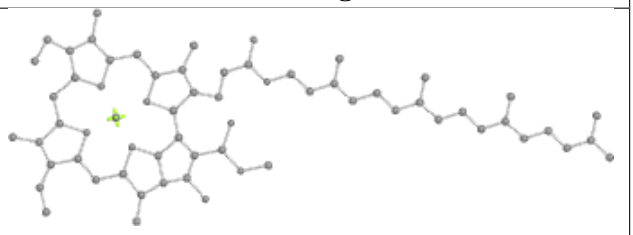


Bond angles

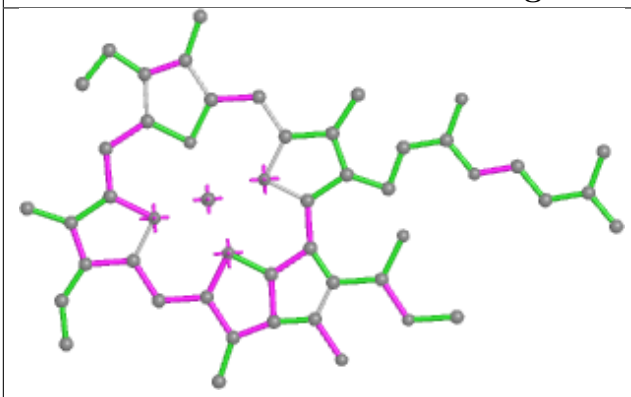


Torsions

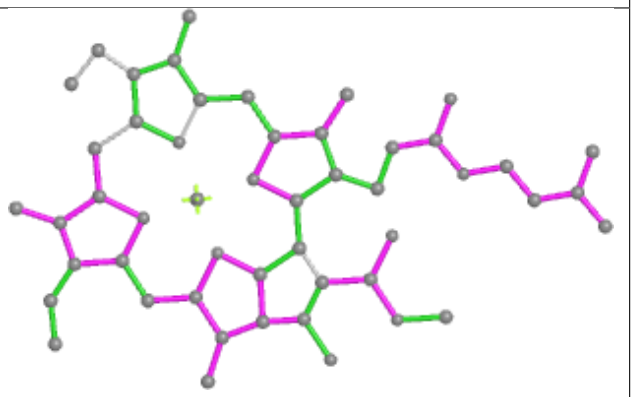


Rings

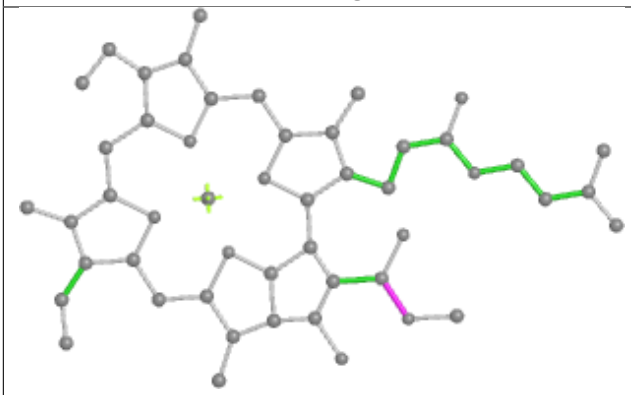
Ligand CLA B 614



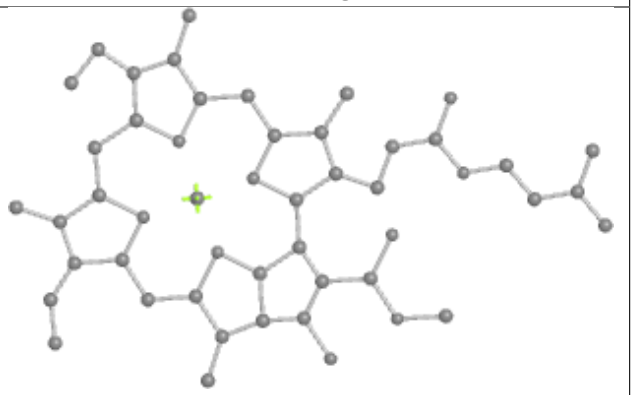
Bond lengths



Bond angles

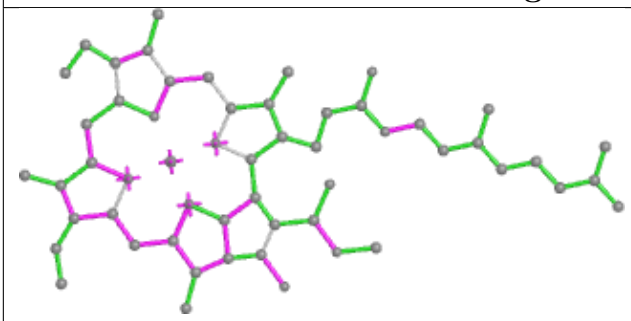


Torsions

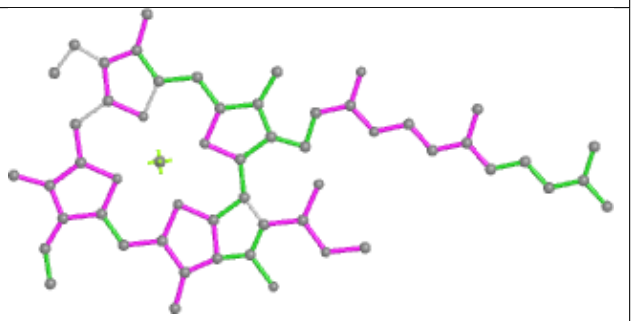


Rings

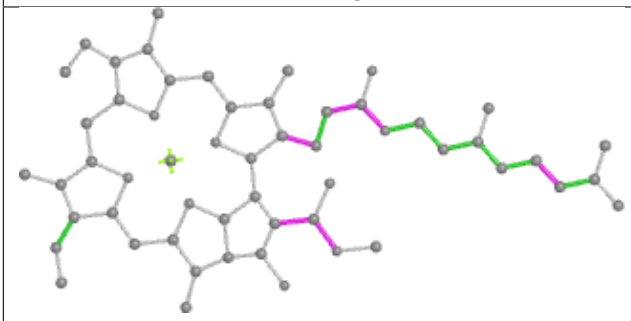
Ligand CLA C 506



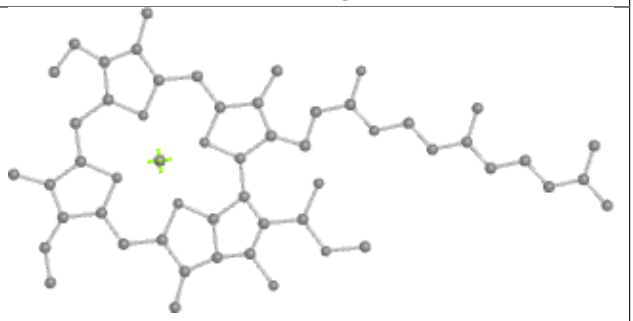
Bond lengths



Bond angles

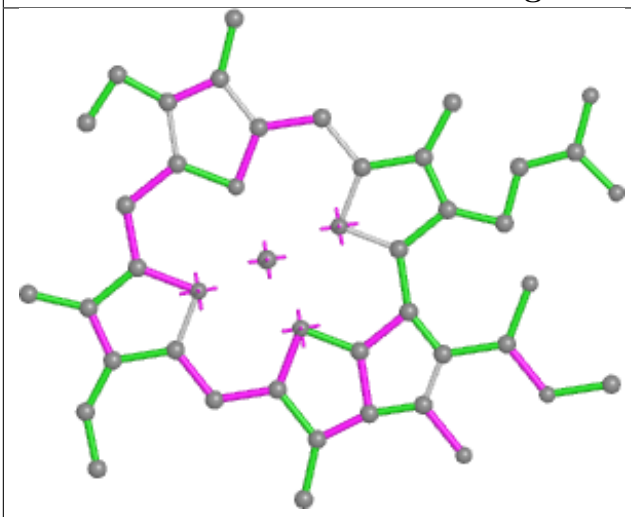


Torsions

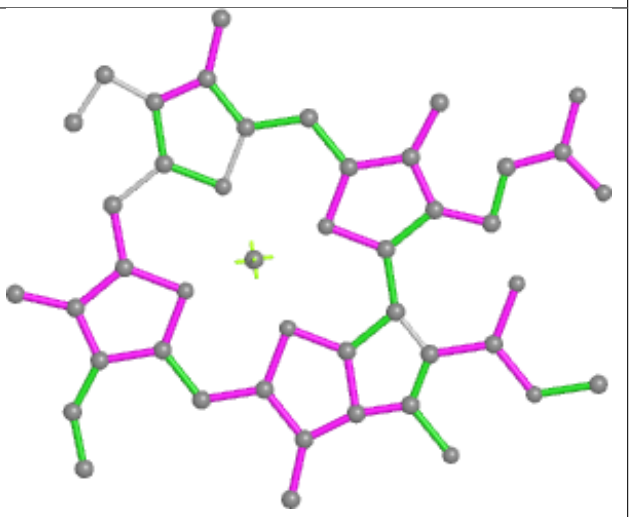


Rings

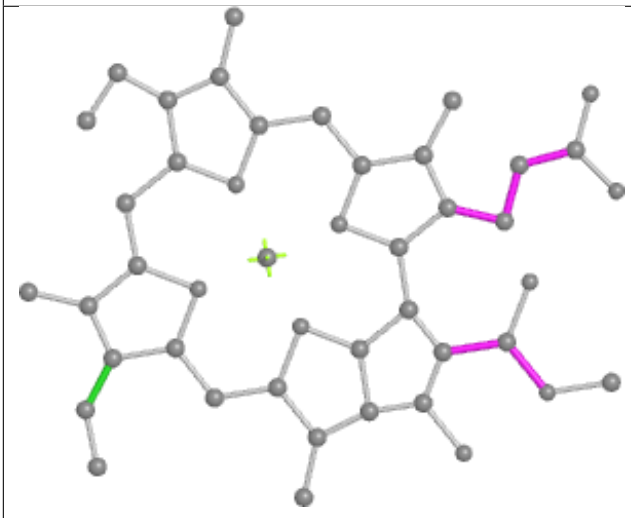
Ligand CLA C 512



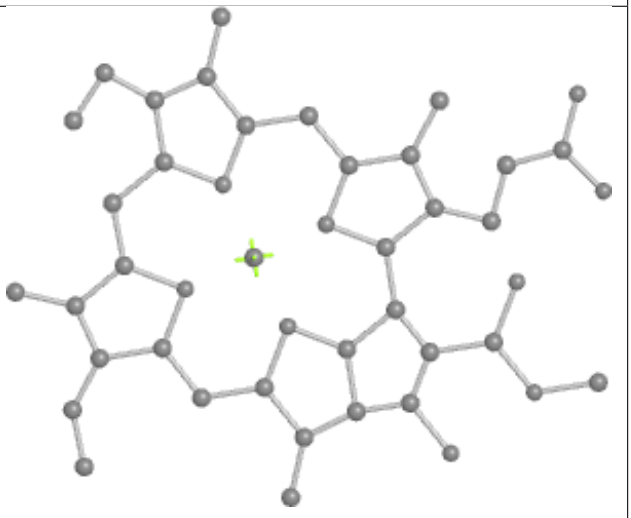
Bond lengths



Bond angles

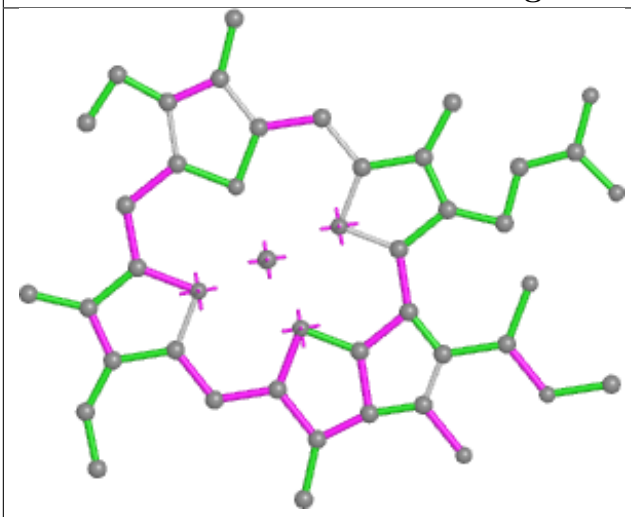


Torsions

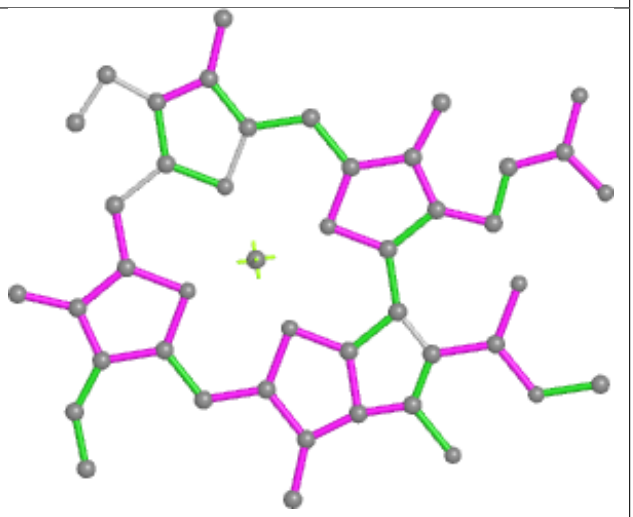


Rings

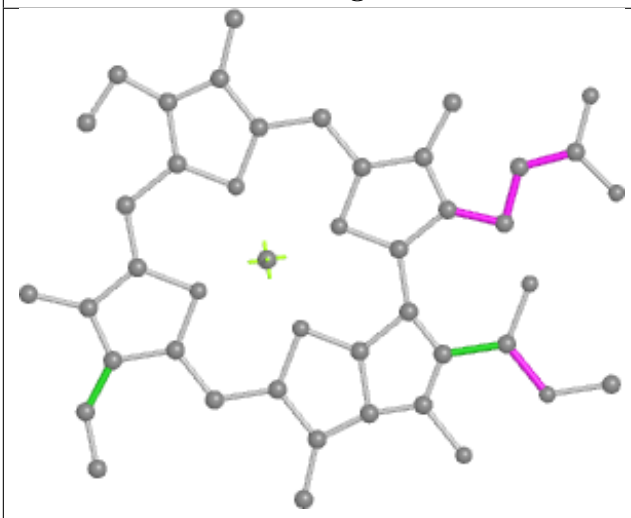
Ligand CLA B 609



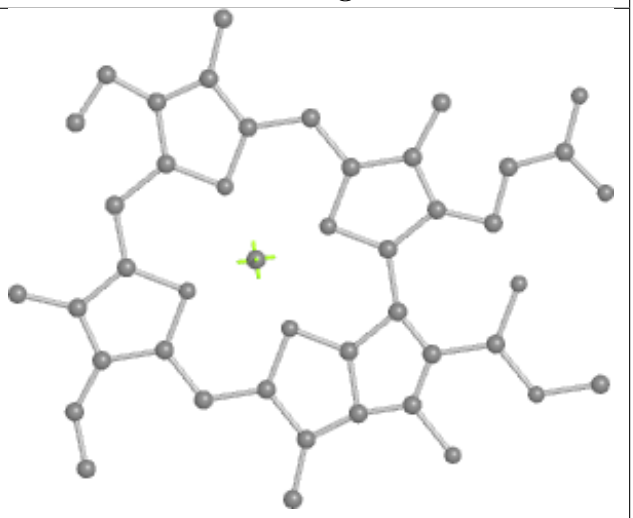
Bond lengths



Bond angles

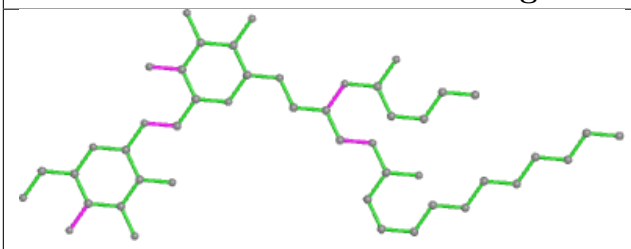


Torsions



Rings

Ligand DGD C 515



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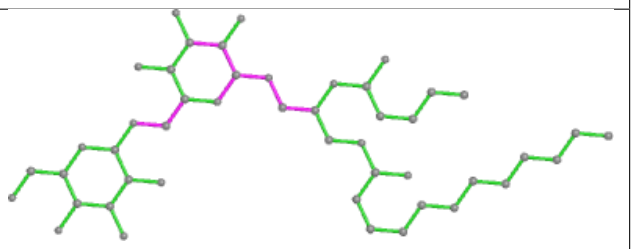
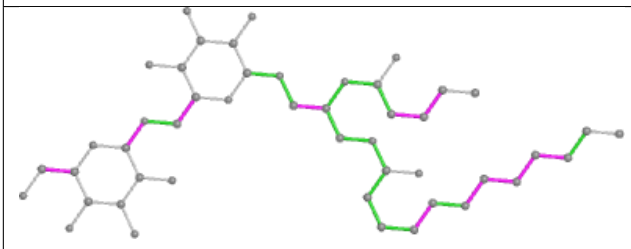
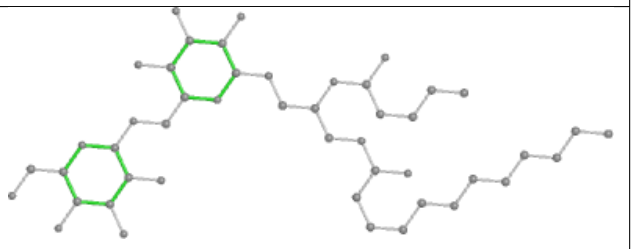


Bond angles

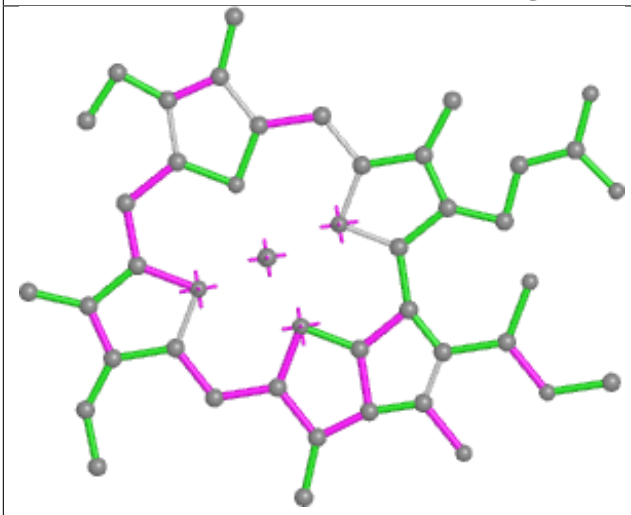


Torsions



Rings

Ligand CLA C 511



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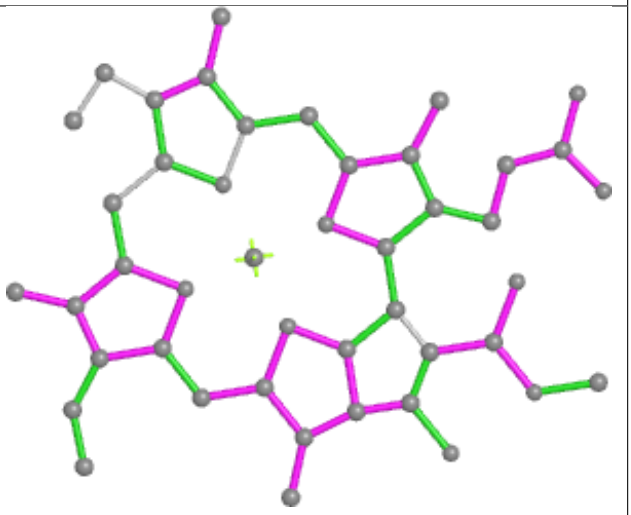
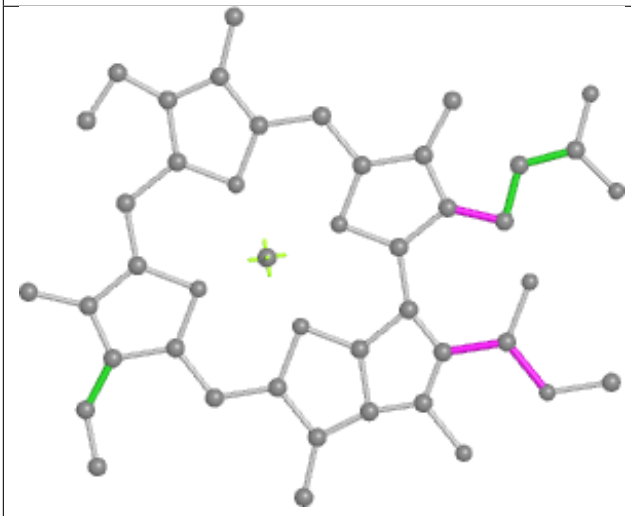
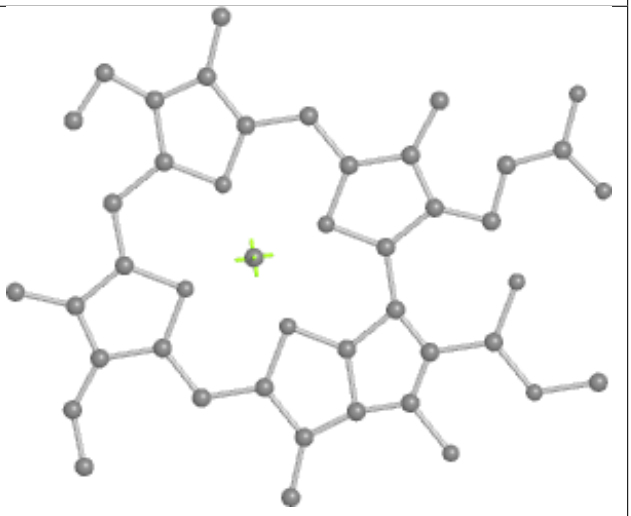


Bond angles

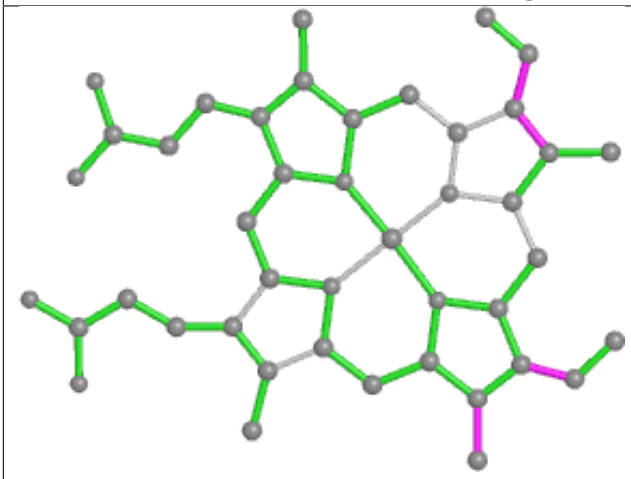


Torsions



Rings

Ligand HEM F 101



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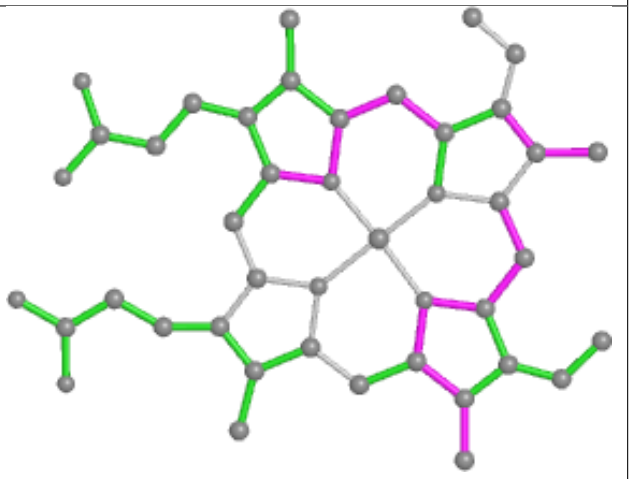
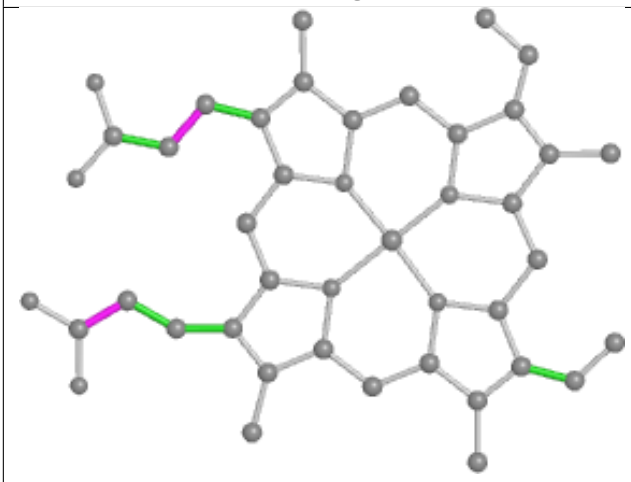
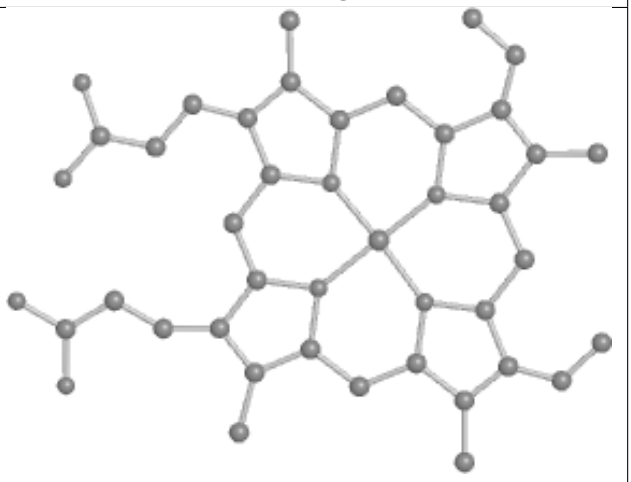


Bond angles

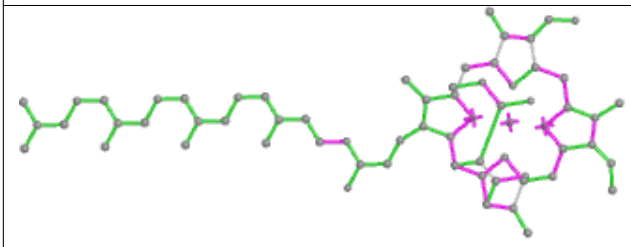


Torsions



Rings

Ligand CL7 A 404



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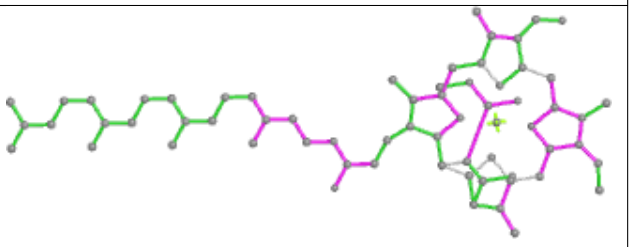
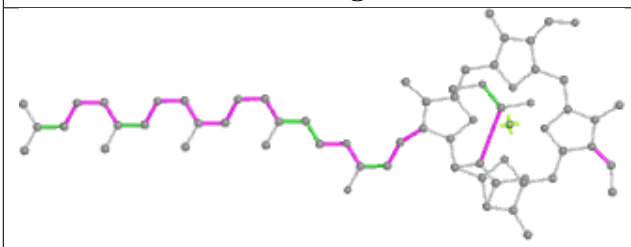
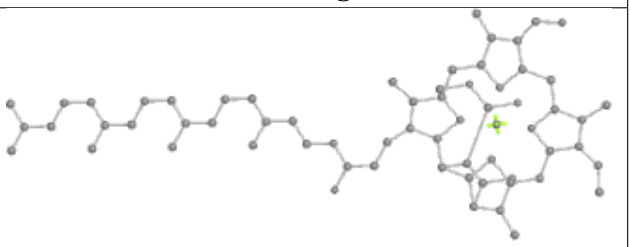


Bond angles

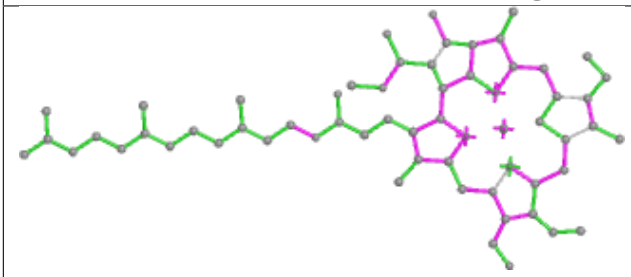


Torsions



Rings

Ligand F6C C 507



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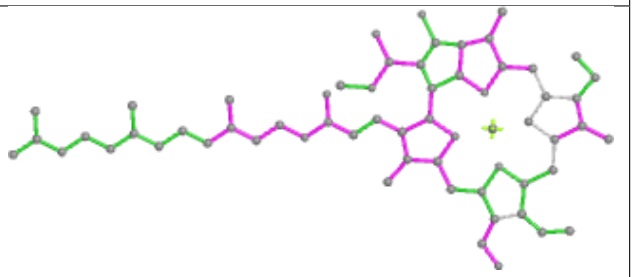
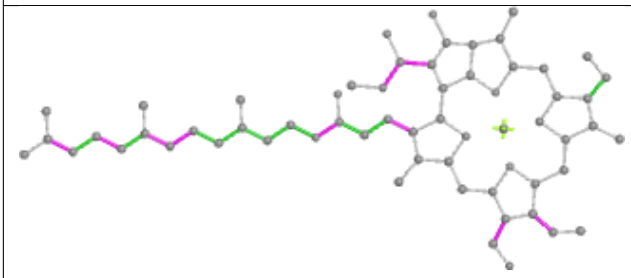


Bond angles



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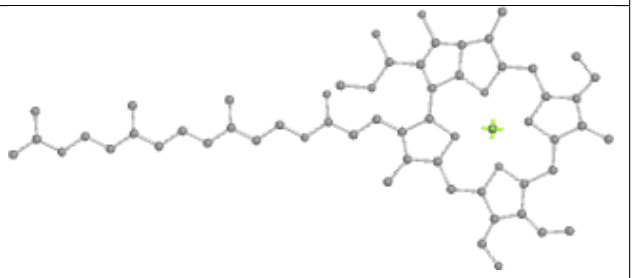
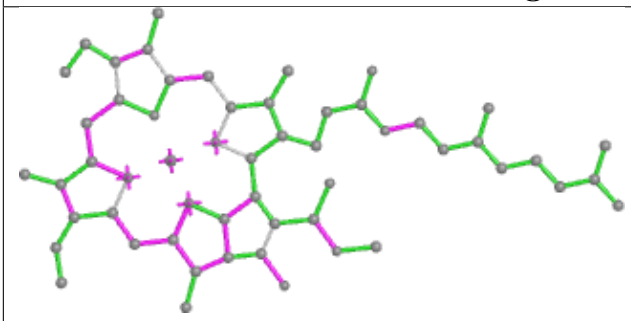


Rings

Ligand CLA B 601



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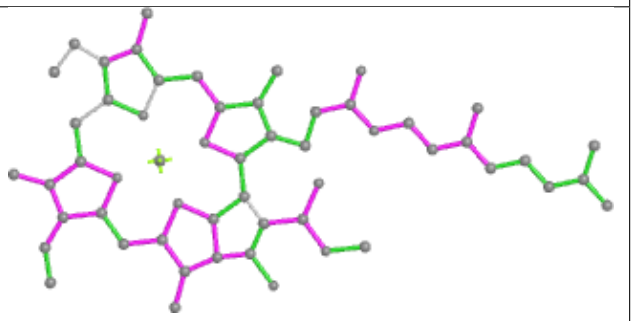
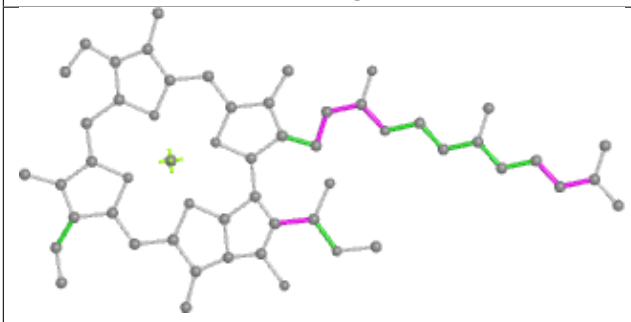
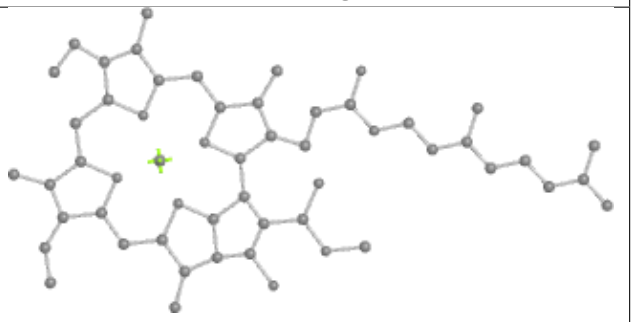


Bond angles

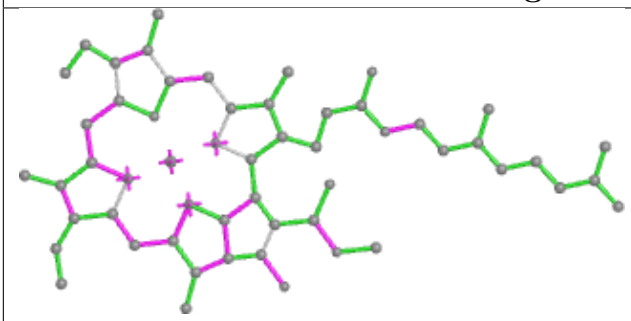


Torsions



Rings

Ligand CLA B 602



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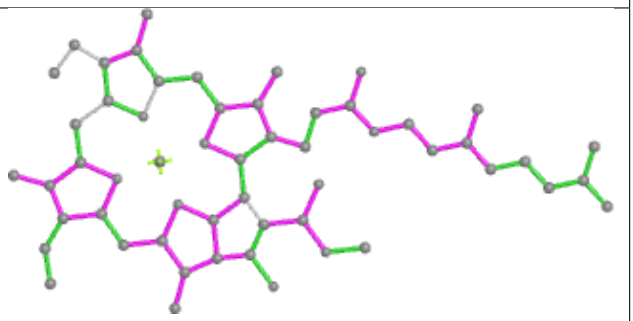
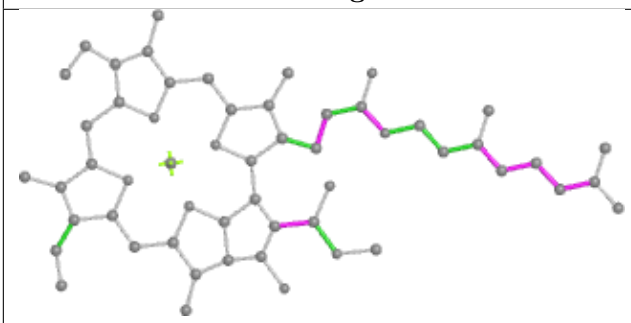


Bond angles



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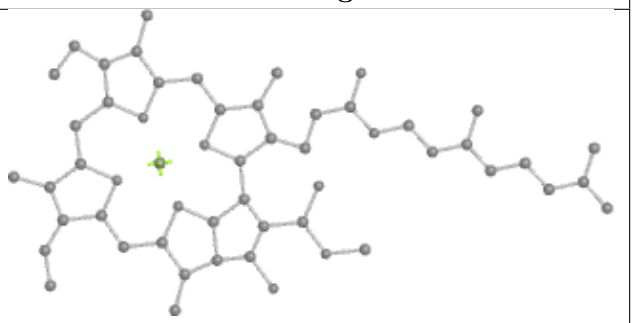
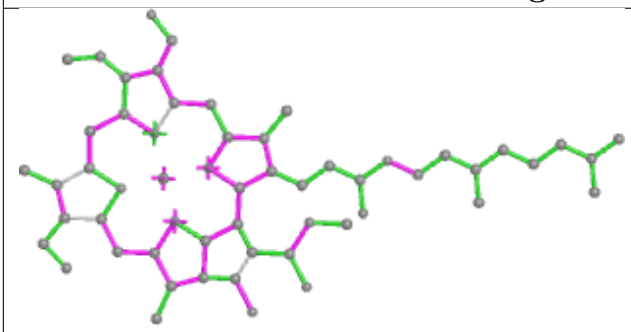


Rings

Ligand F6C B 612



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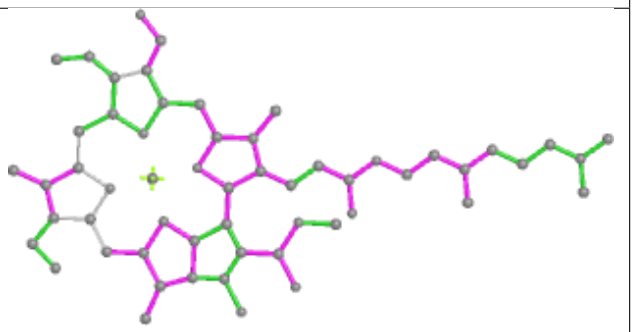
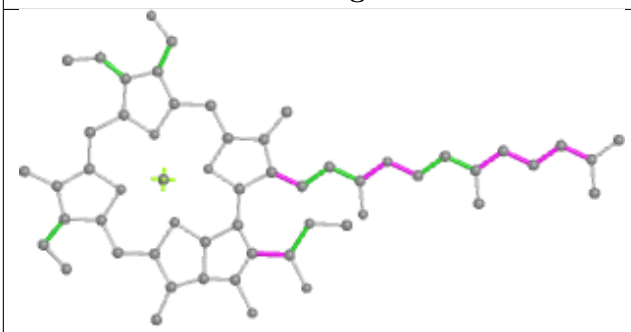
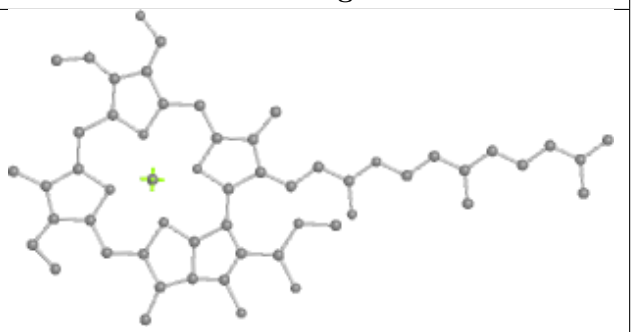


Bond angles

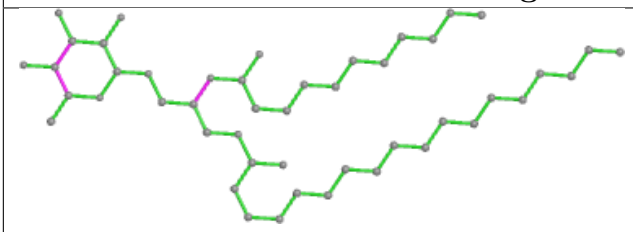


Torsions



Rings

Ligand DGD B 616



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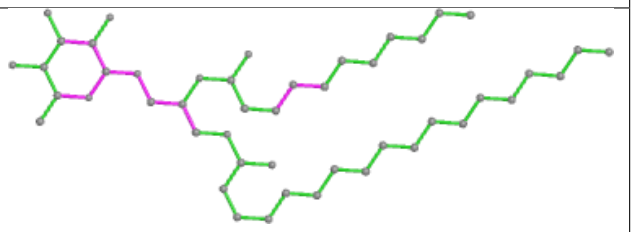
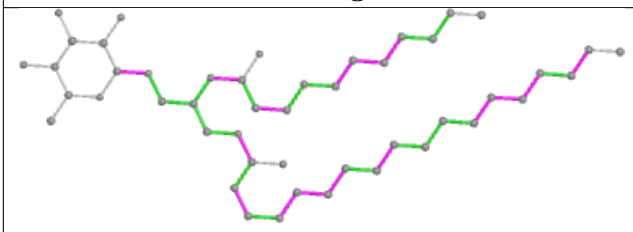
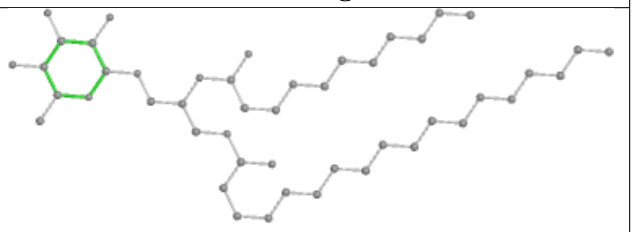


Bond angles

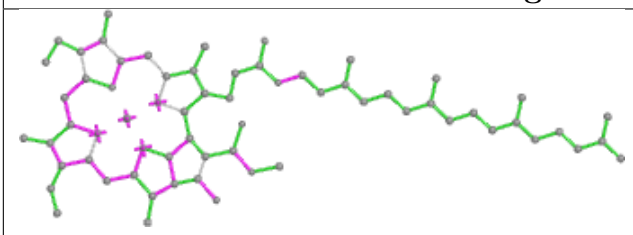


Torsions



Rings

Ligand CLA B 607



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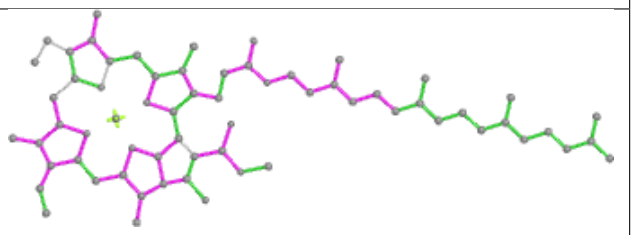
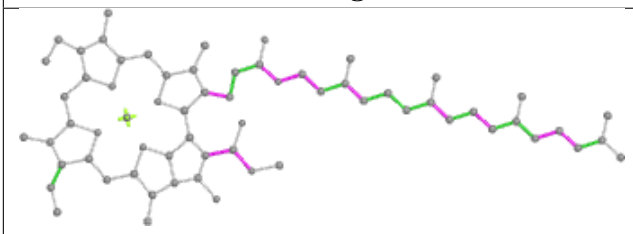


Bond angles



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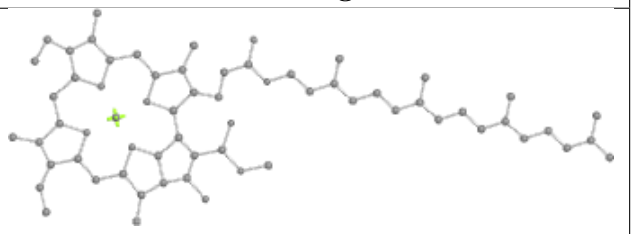
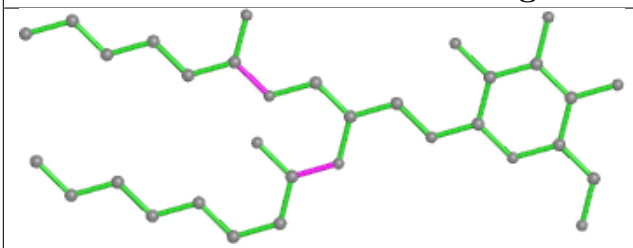


Rings

Ligand LMG D 408



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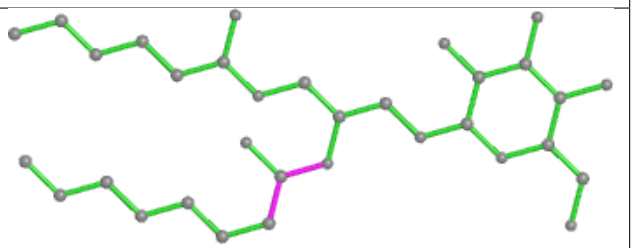
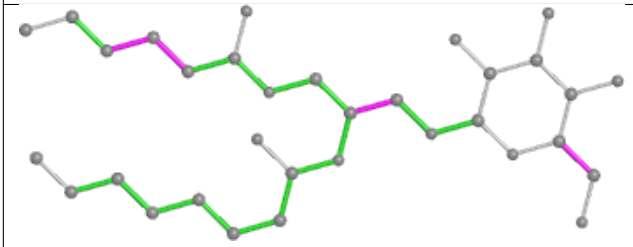
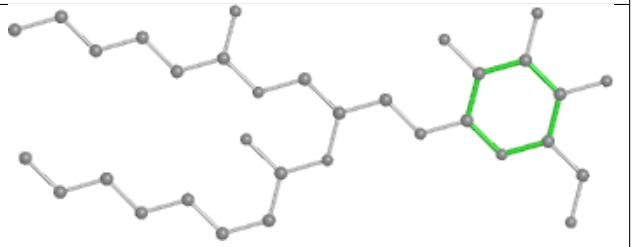


Bond angles

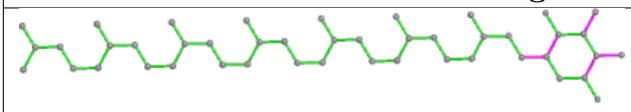


Torsions



Rings

Ligand PL9 D 406



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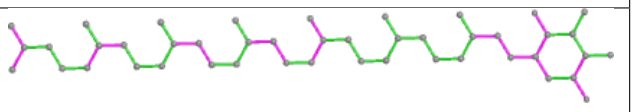
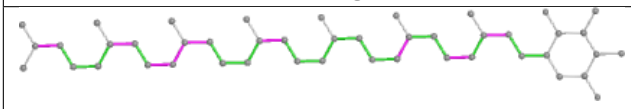
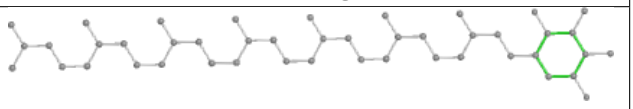


Bond angles

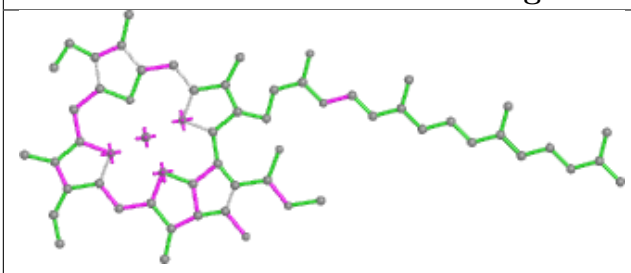


Torsions

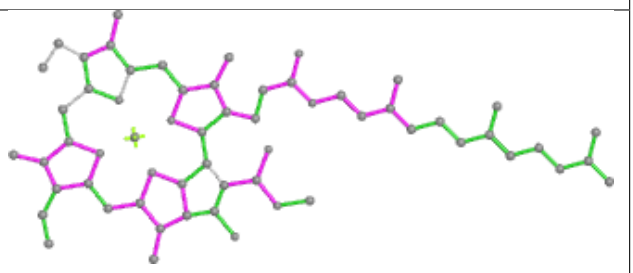


Rings

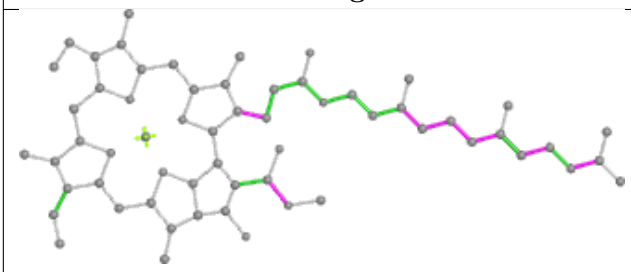
Ligand CLA A 407



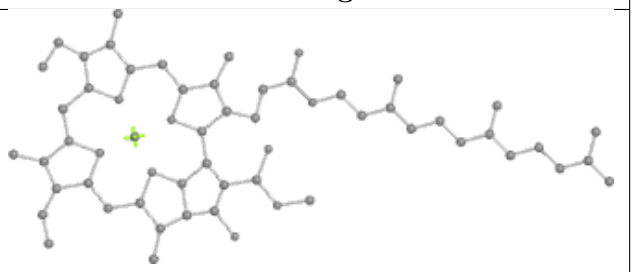
Bond lengths



Bond angles

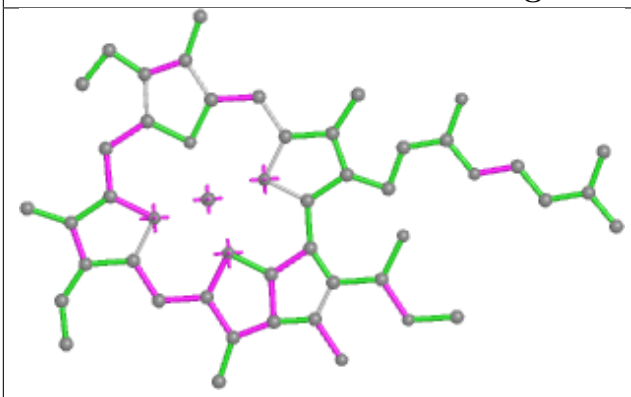


Torsions

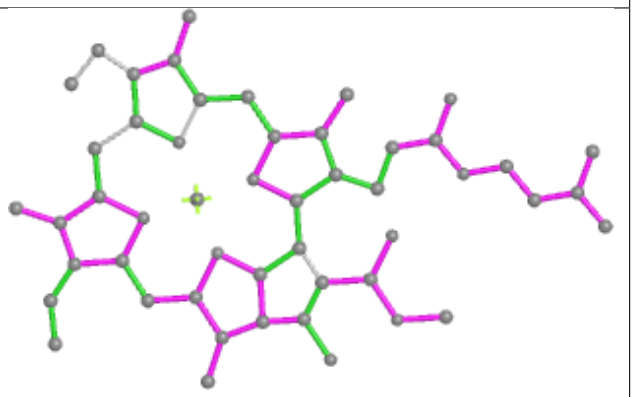


Rings

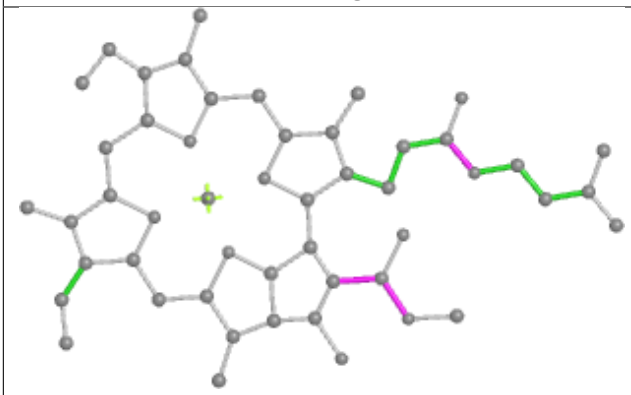
Ligand CLA C 504



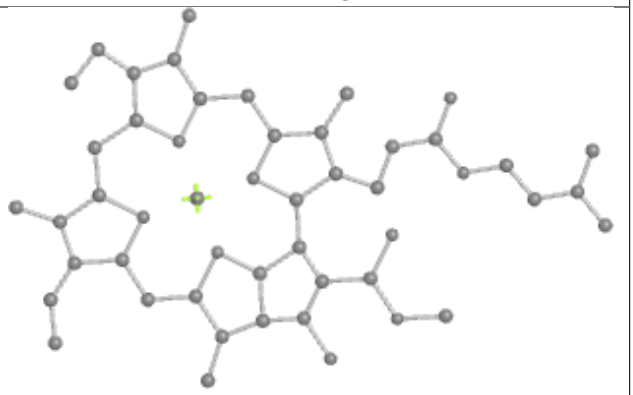
Bond lengths



Bond angles

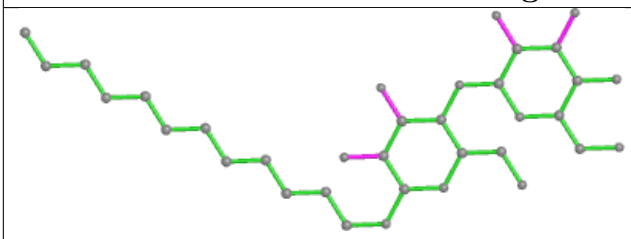


Torsions

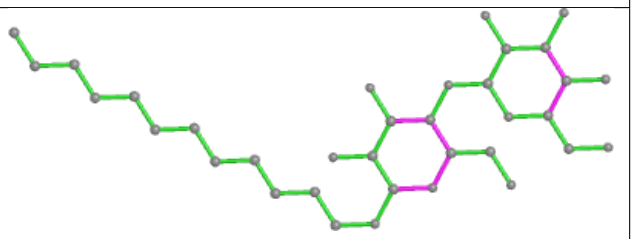


Rings

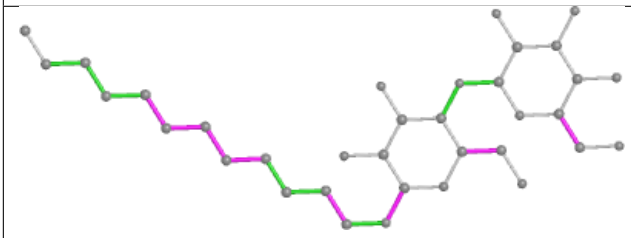
Ligand LMT B 618



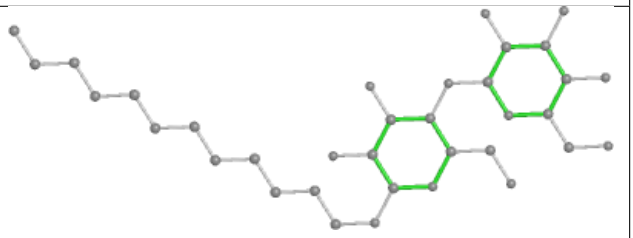
Bond lengths



Bond angles

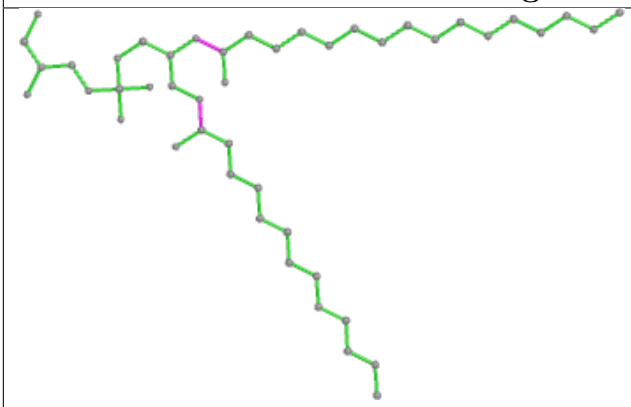


Torsions



Rings

Ligand LHG D 407



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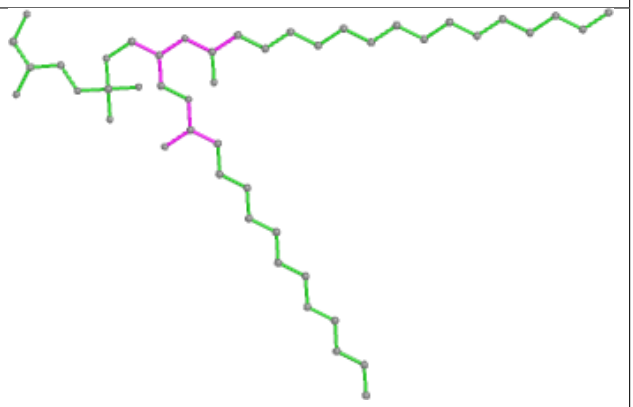
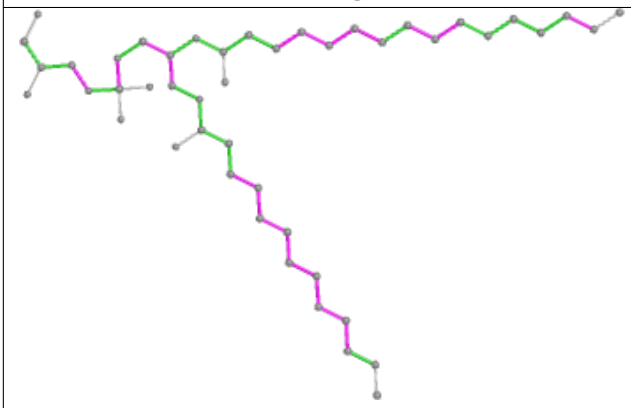


Bond angles



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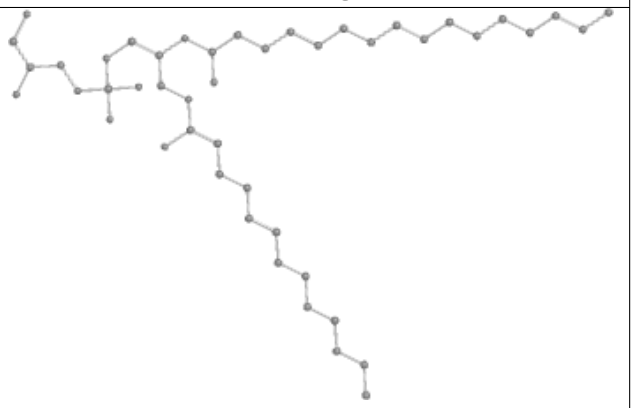
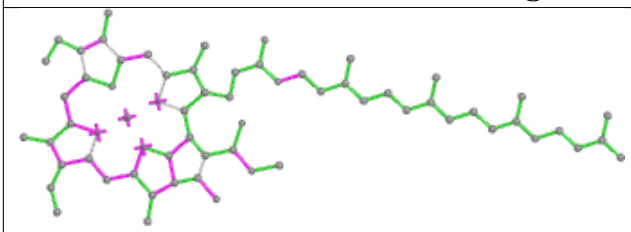


Rings

Ligand CLA C 502



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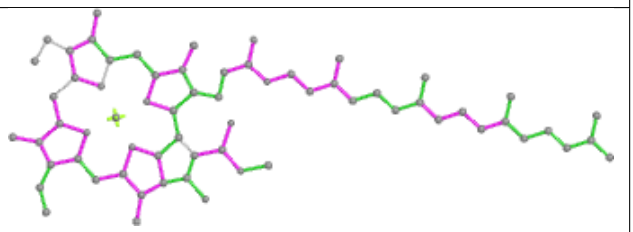
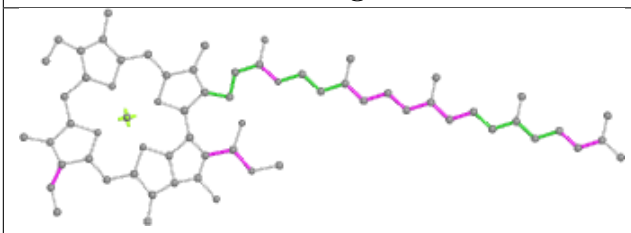
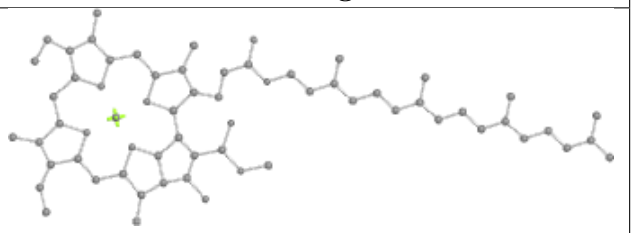


Bond angles

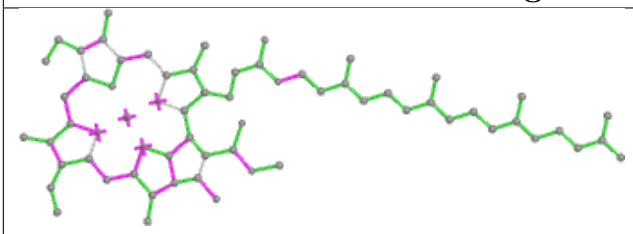


Torsions

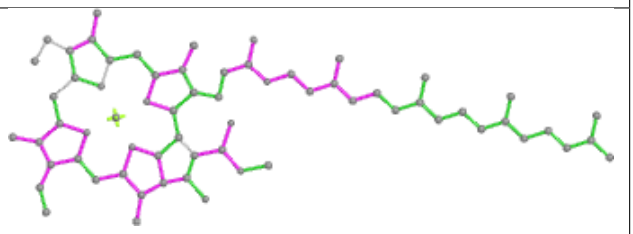


Rings

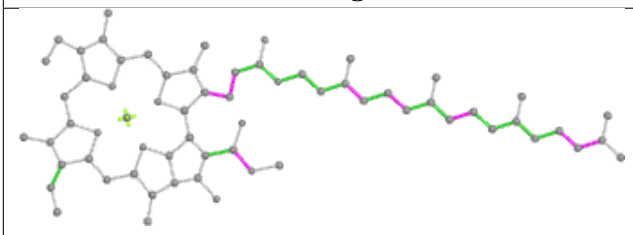
Ligand CLA C 503



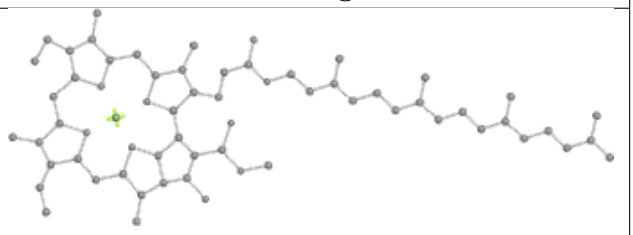
Bond lengths



Bond angles

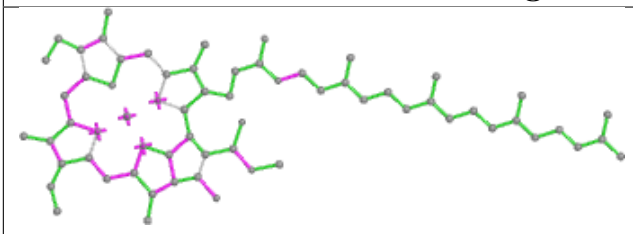


Torsions

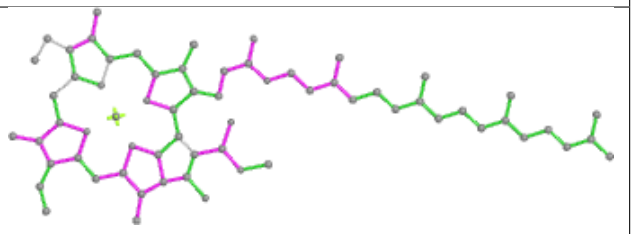


Rings

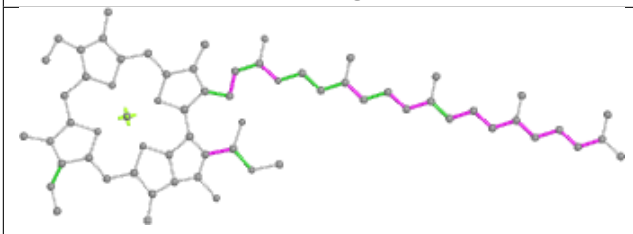
Ligand CLA C 505



Bond lengths



Bond angles



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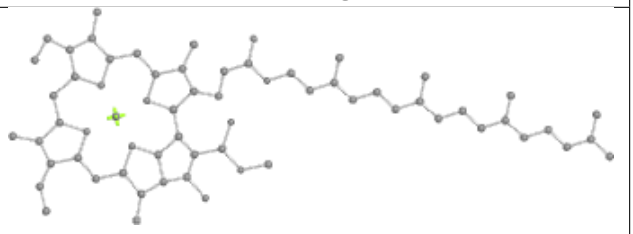
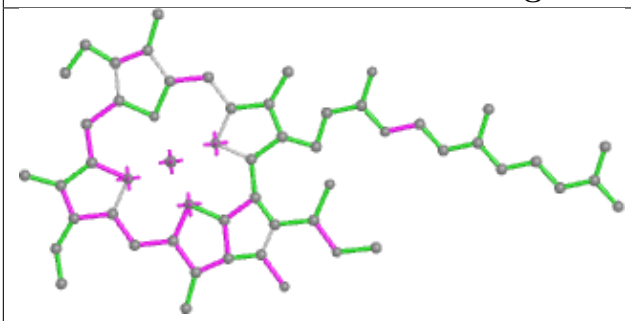


Rings

Ligand CLA B 604



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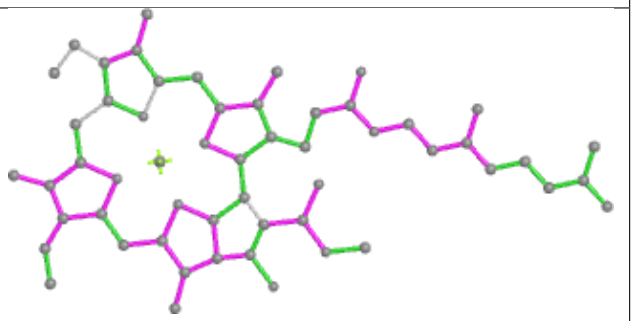
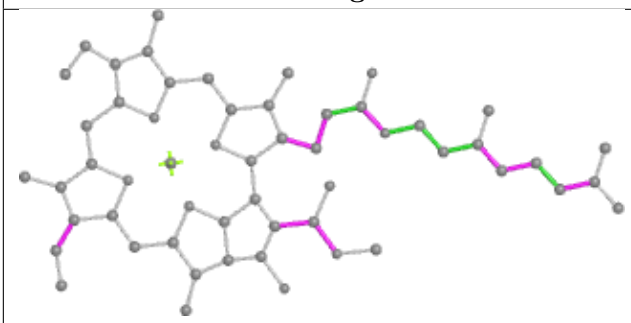
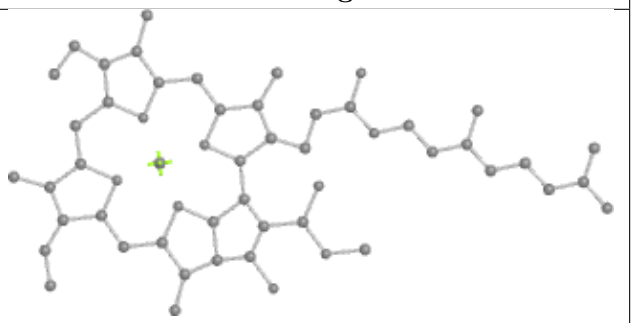


Bond angles

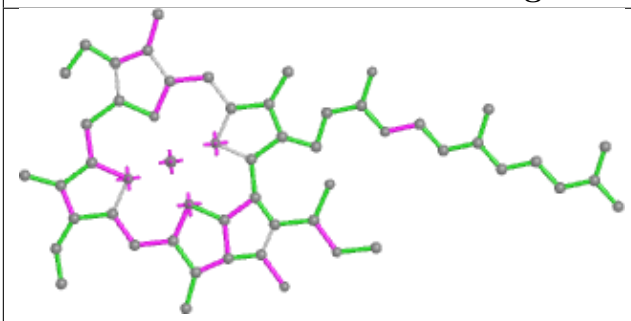


Torsions

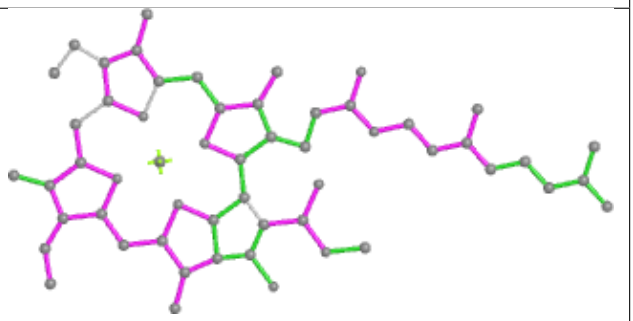


Rings

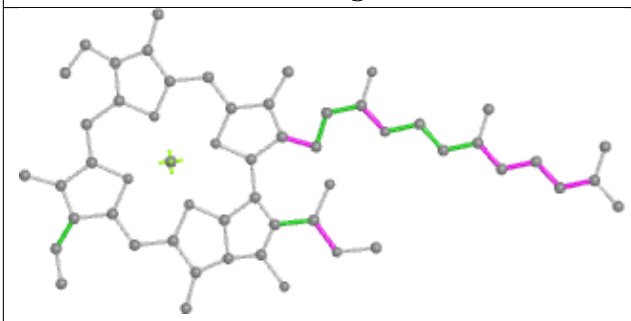
Ligand CLA B 610



Bond lengths



Bond angles



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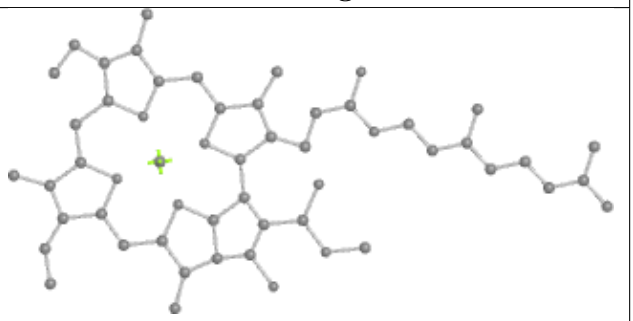
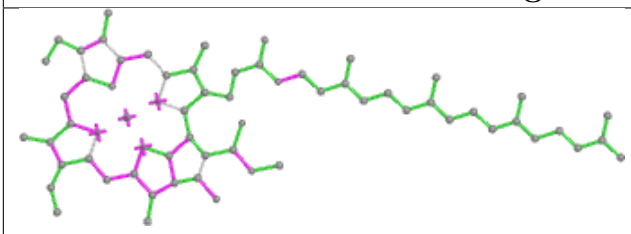


Rings

Ligand CLA C 510



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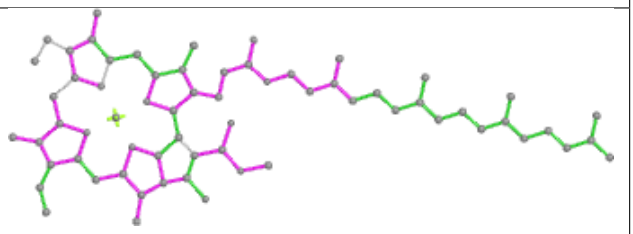
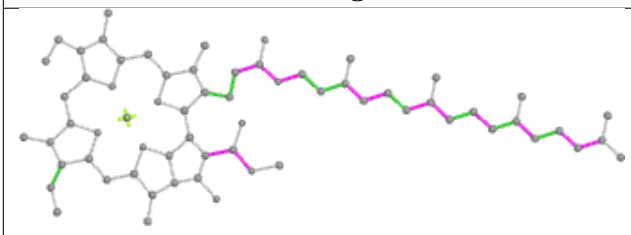


Bond angles



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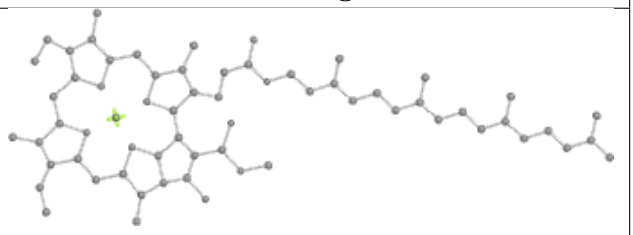
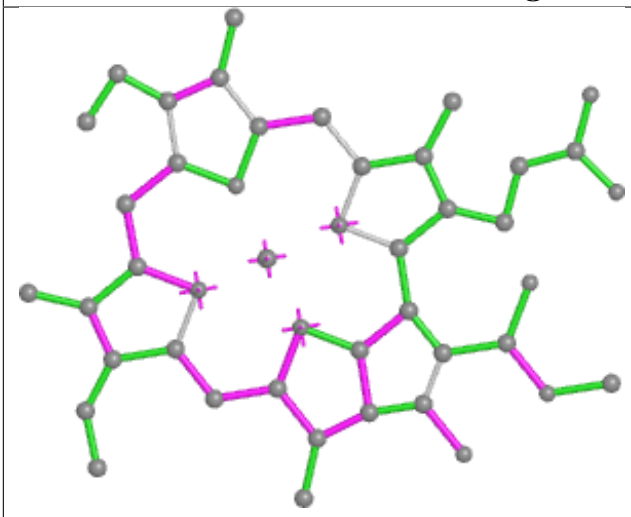
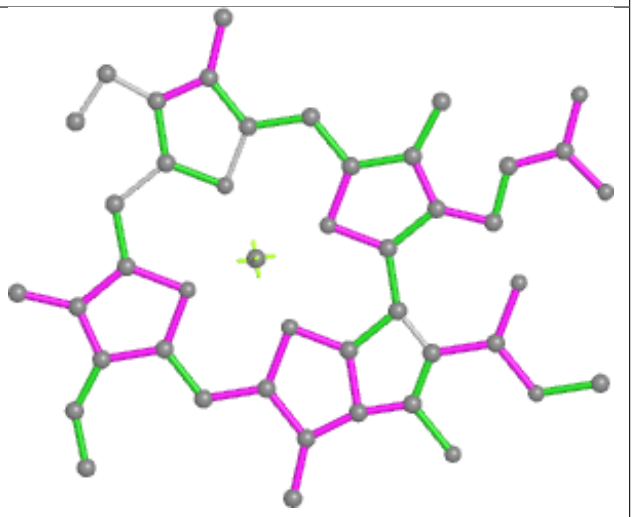


Rings

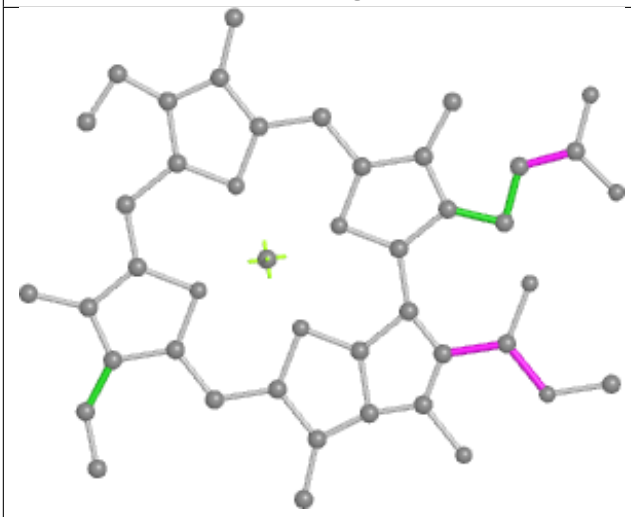
Ligand CLA C 513



Bond lengths



Bond angles



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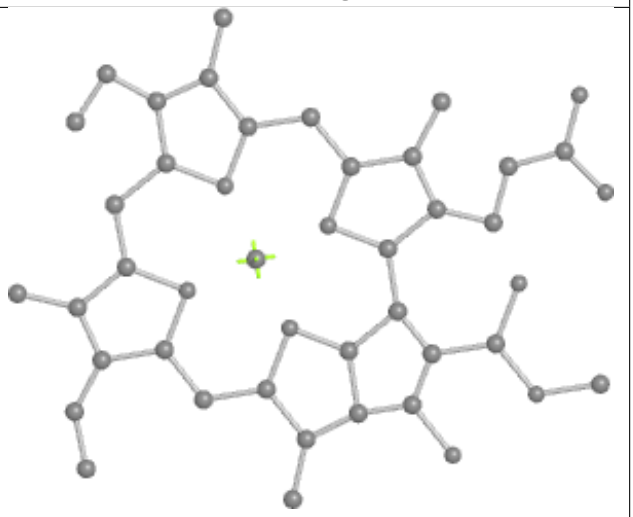
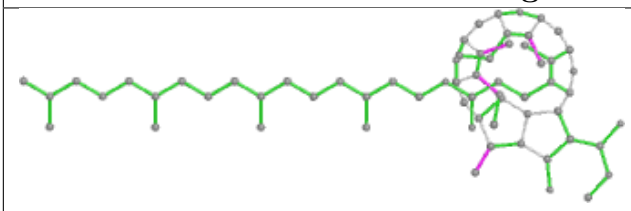
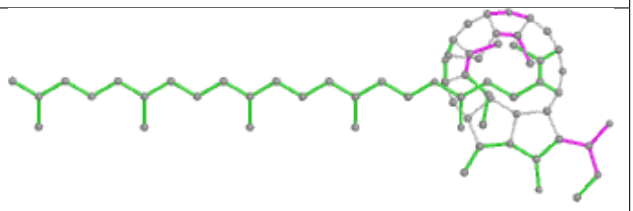


Rings

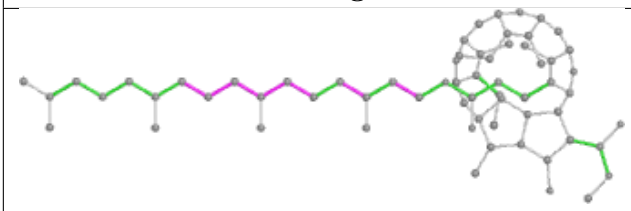
Ligand PHO A 406



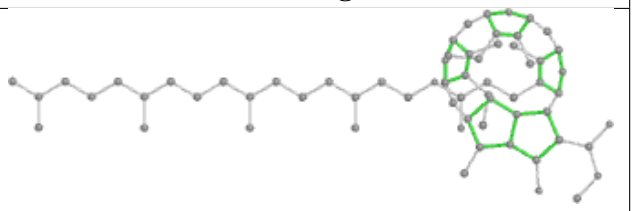
Bond lengths



Bond angles

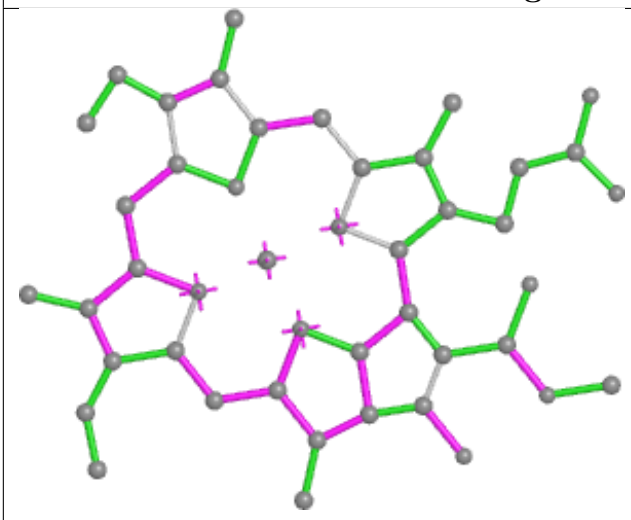


Torsions

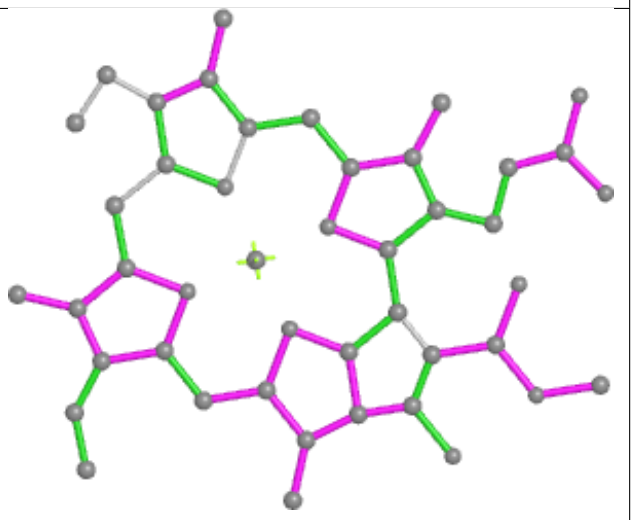


Rings

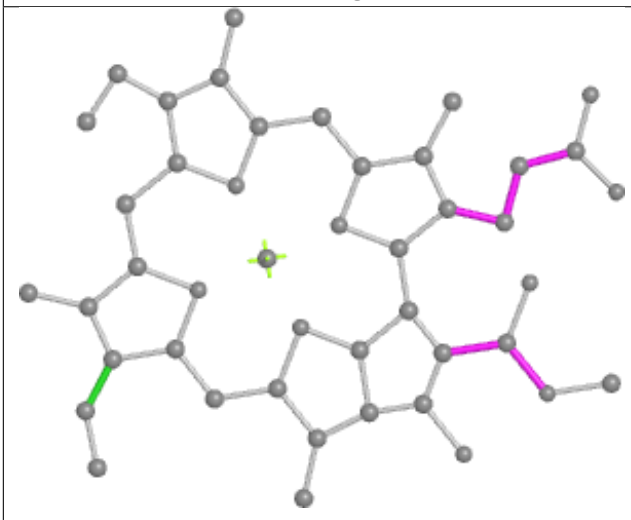
Ligand CLA B 608



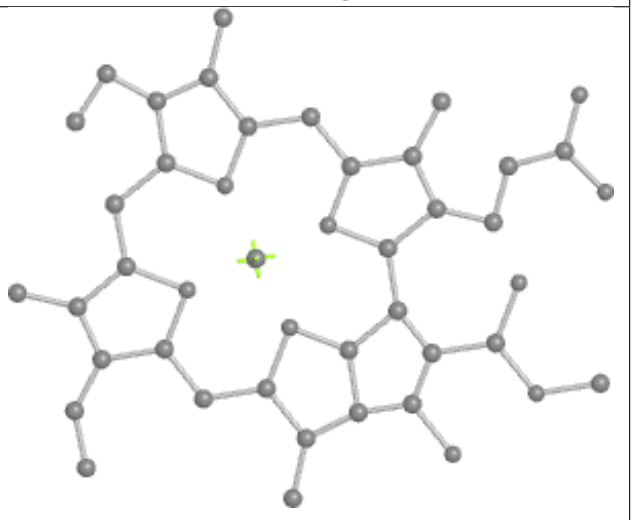
Bond lengths



Bond angles

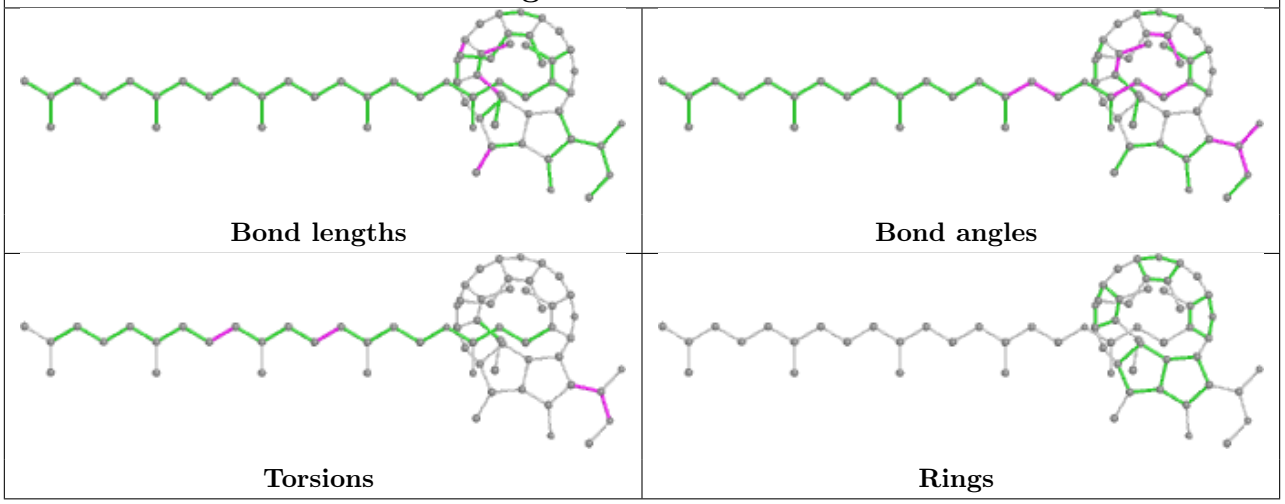


Torsions

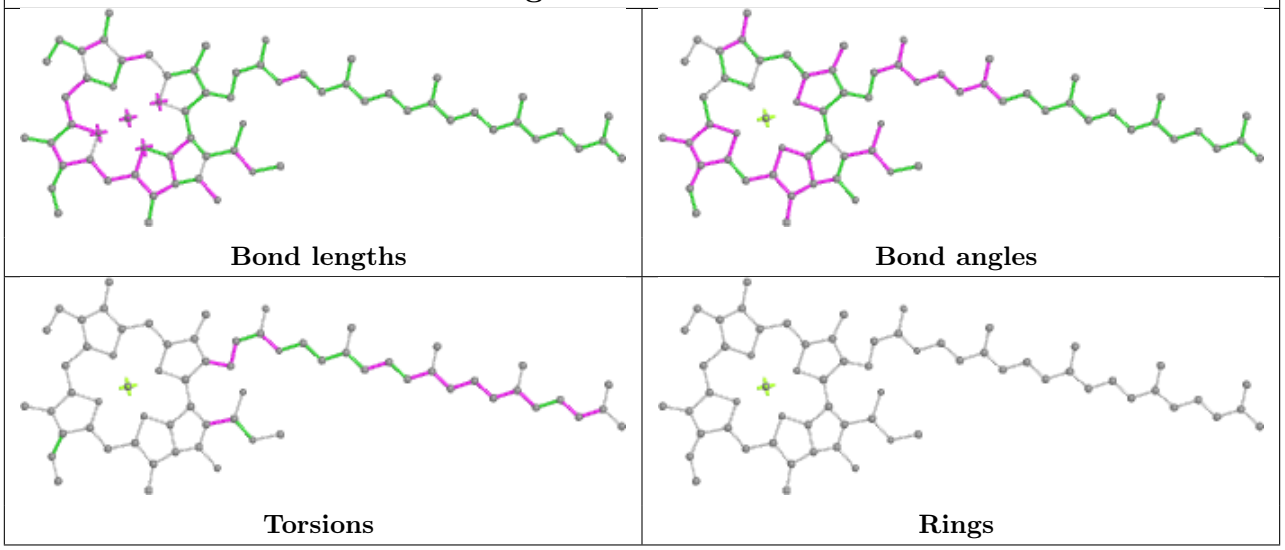


Rings

Ligand PHO D 402



Ligand CLA C 508



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.

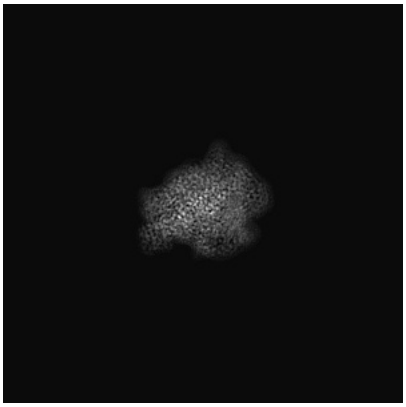
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24943. These allow visual inspection of the internal detail of the map and identification of artifacts.

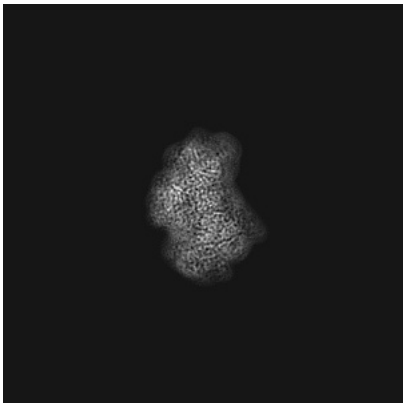
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

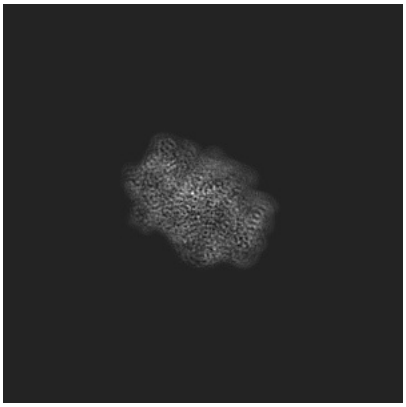
6.1.1 Primary map



X



Y

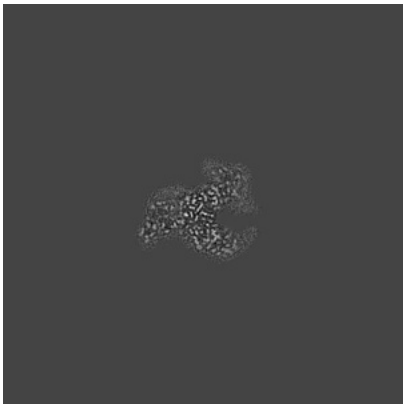


Z

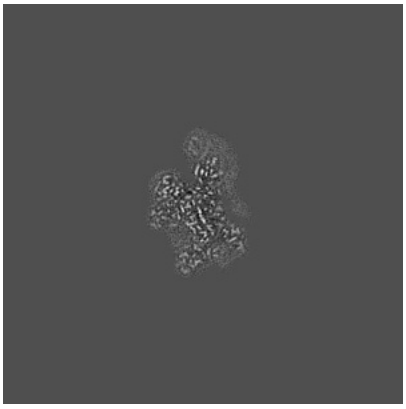
The images above show the map projected in three orthogonal directions.

6.2 Central slices

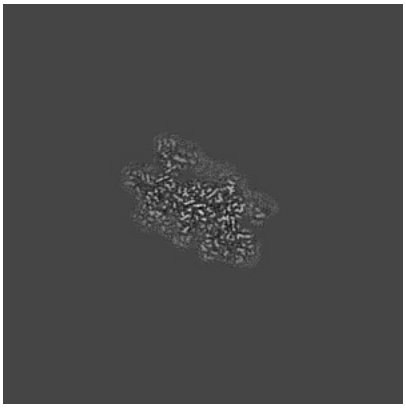
6.2.1 Primary map



X Index: 192



Y Index: 192

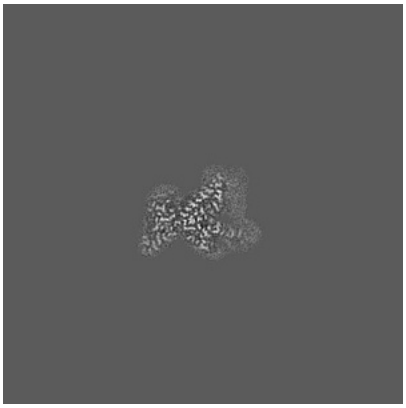


Z Index: 192

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 202

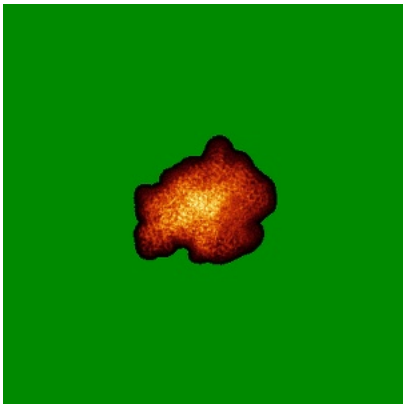
Y Index: 190

Z Index: 187

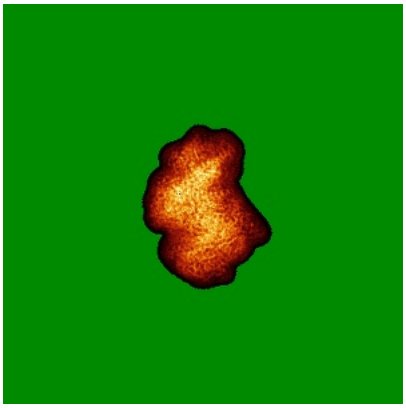
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

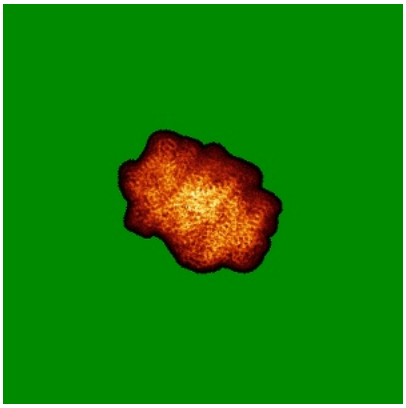
6.4.1 Primary map



X



Y

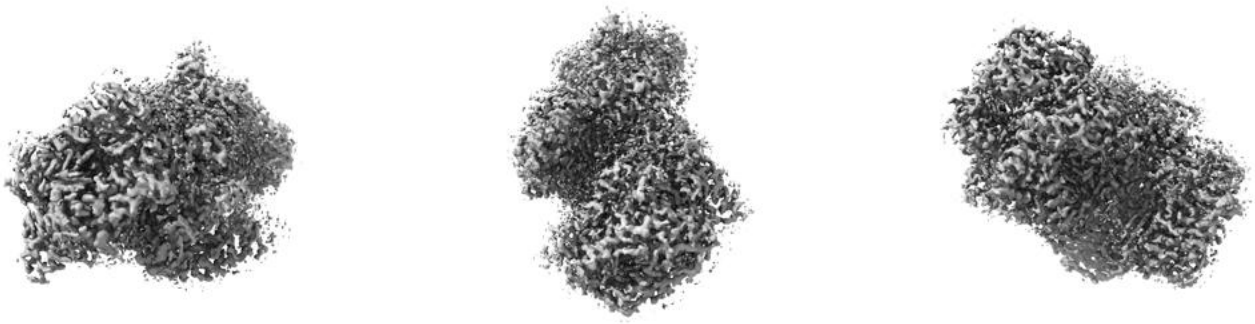


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

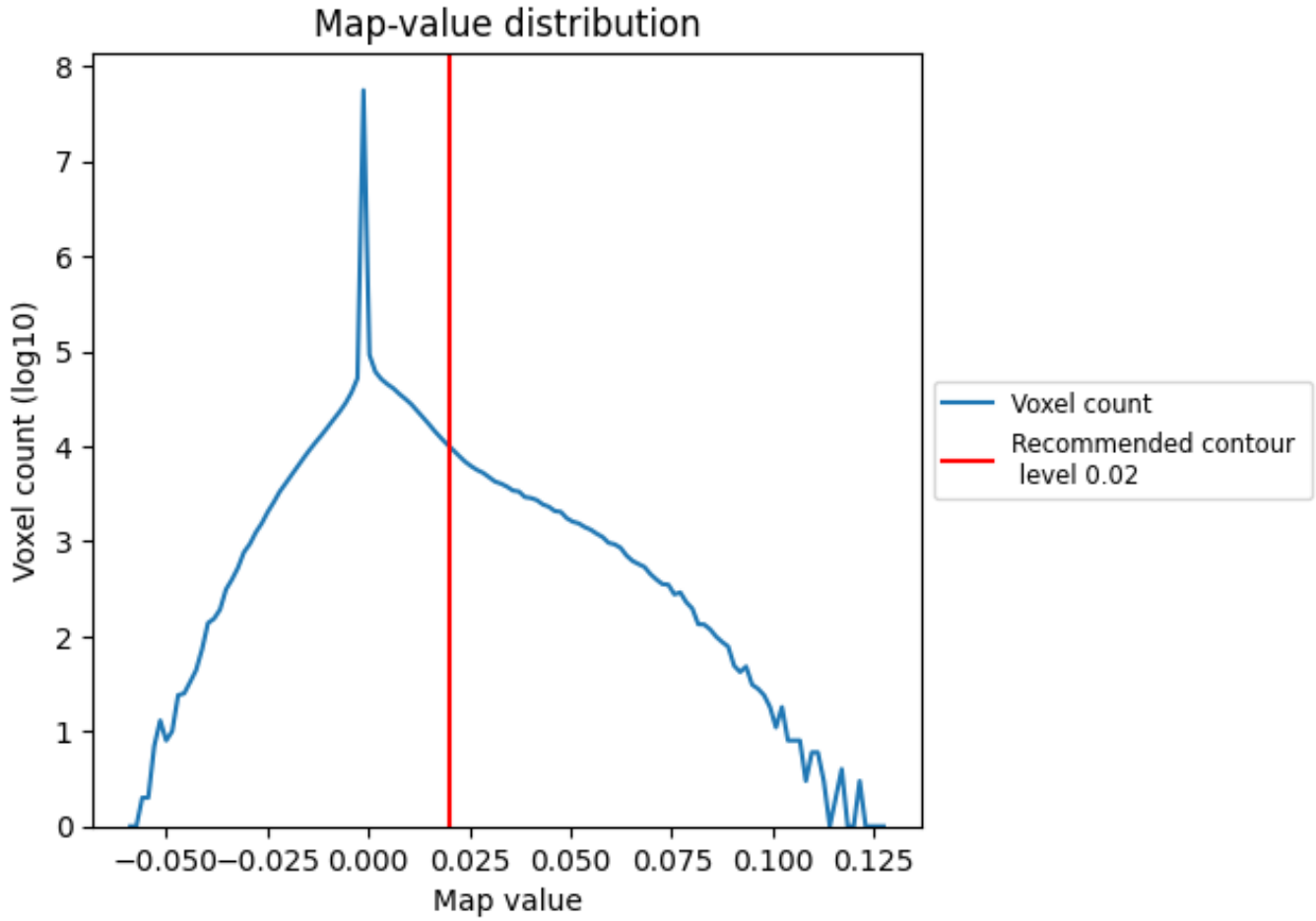
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

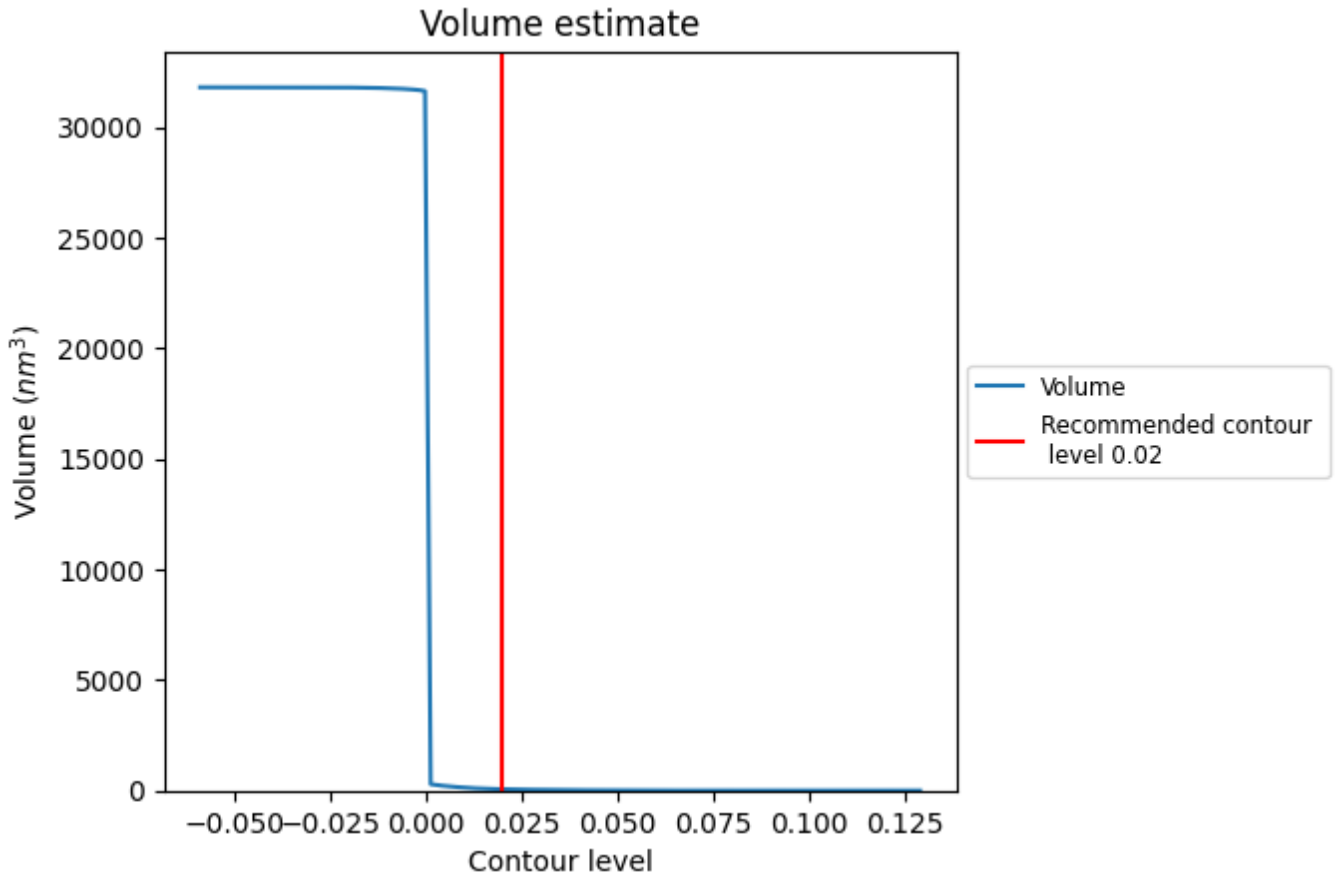
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

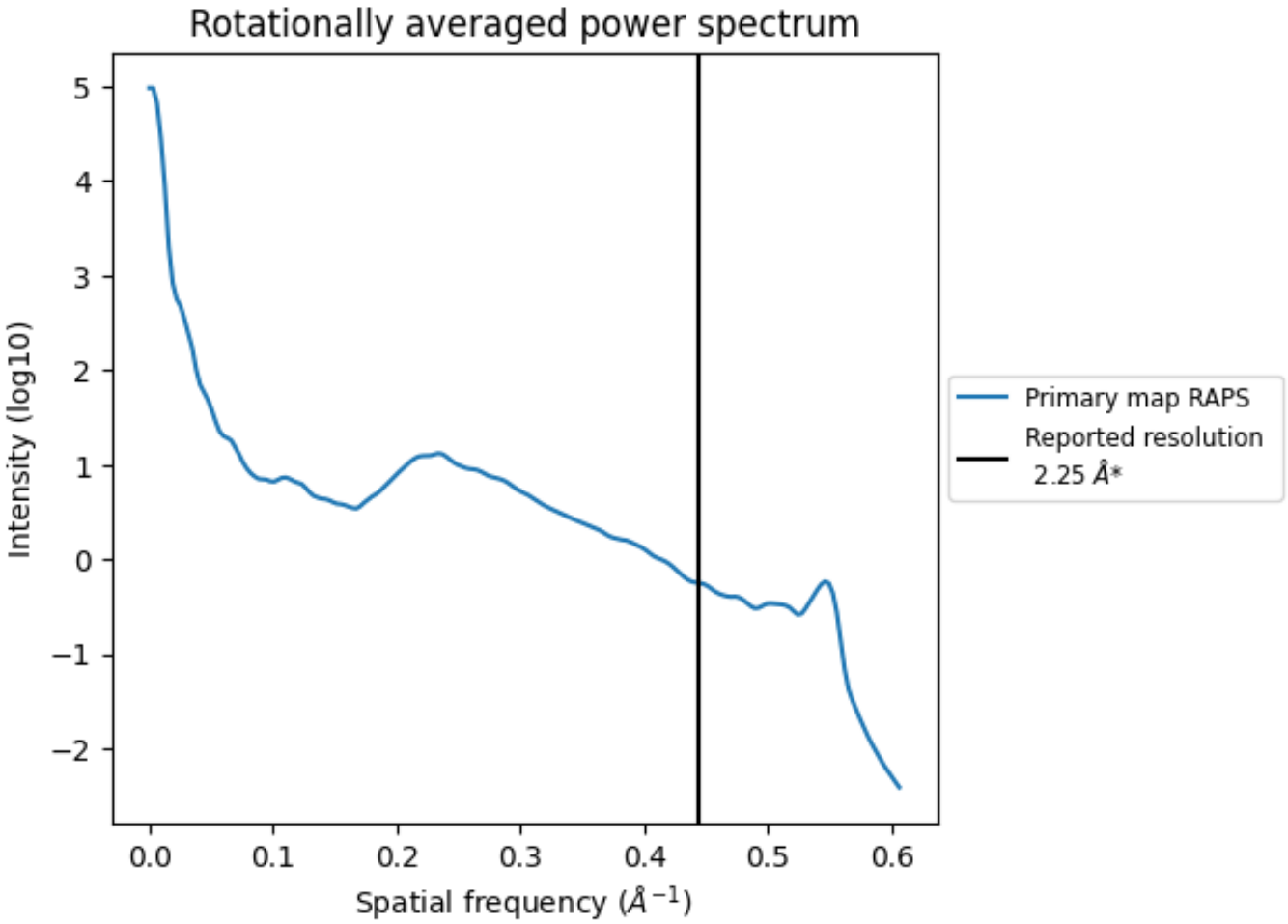
7.2 Volume estimate (i)



The volume at the recommended contour level is 60 nm^3; this corresponds to an approximate mass of 54 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

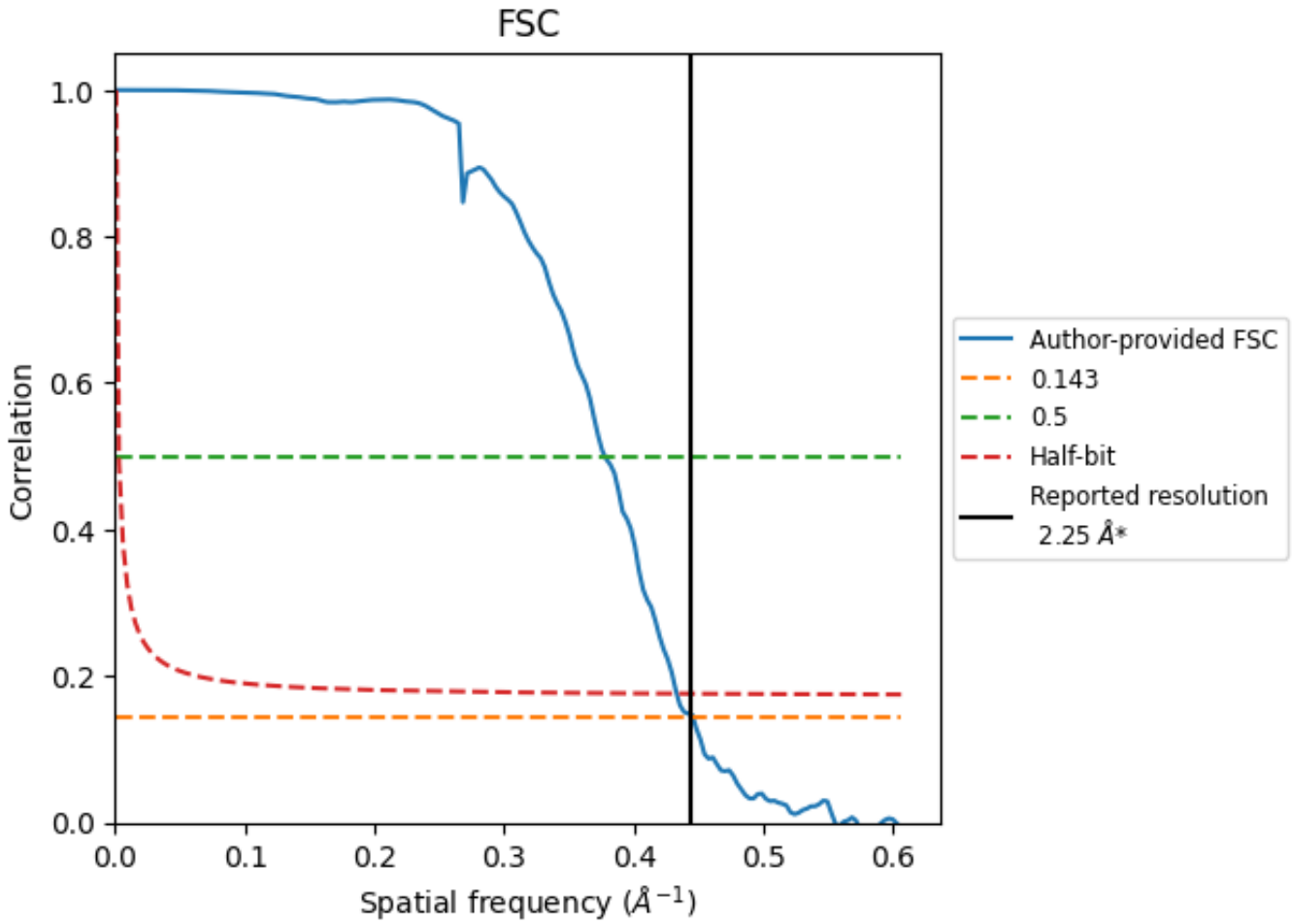


*Reported resolution corresponds to spatial frequency of 0.444 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.444 Å^{-1}

8.2 Resolution estimates (i)

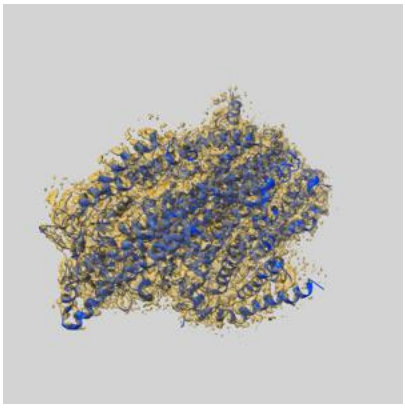
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.25	-	-
Author-provided FSC curve	2.24	2.65	2.31
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

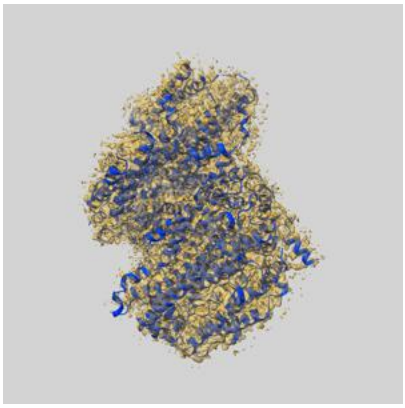
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24943 and PDB model 7SA3. Per-residue inclusion information can be found in section 3 on page 16.

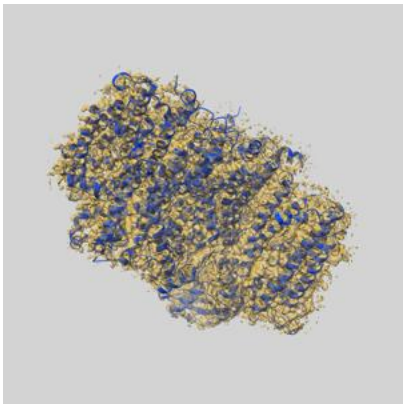
9.1 Map-model overlay



X



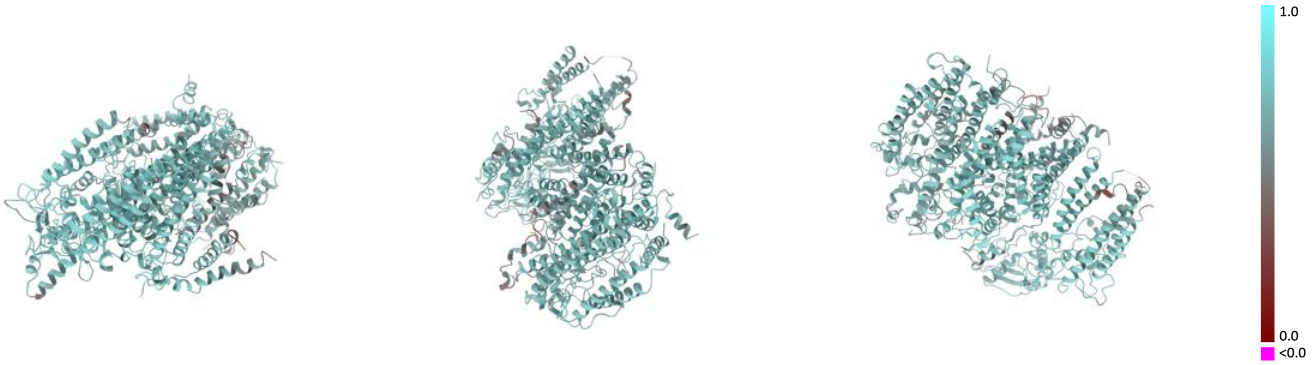
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

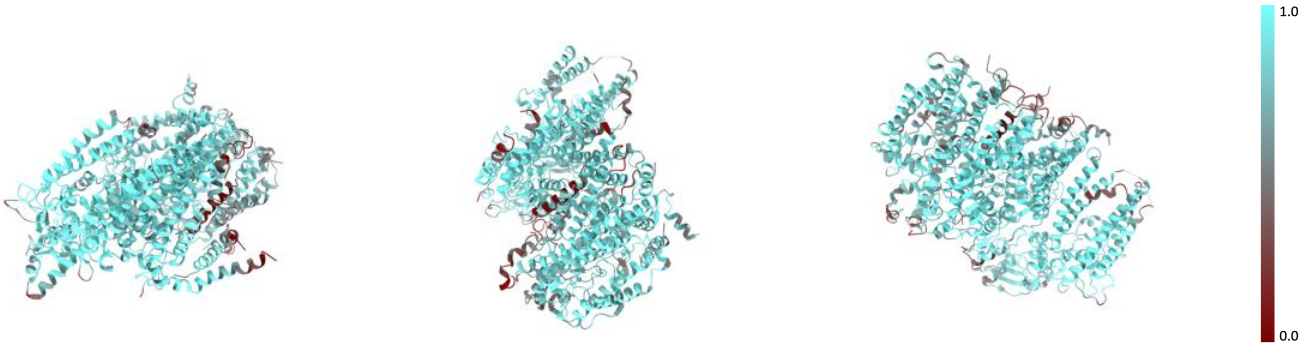
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

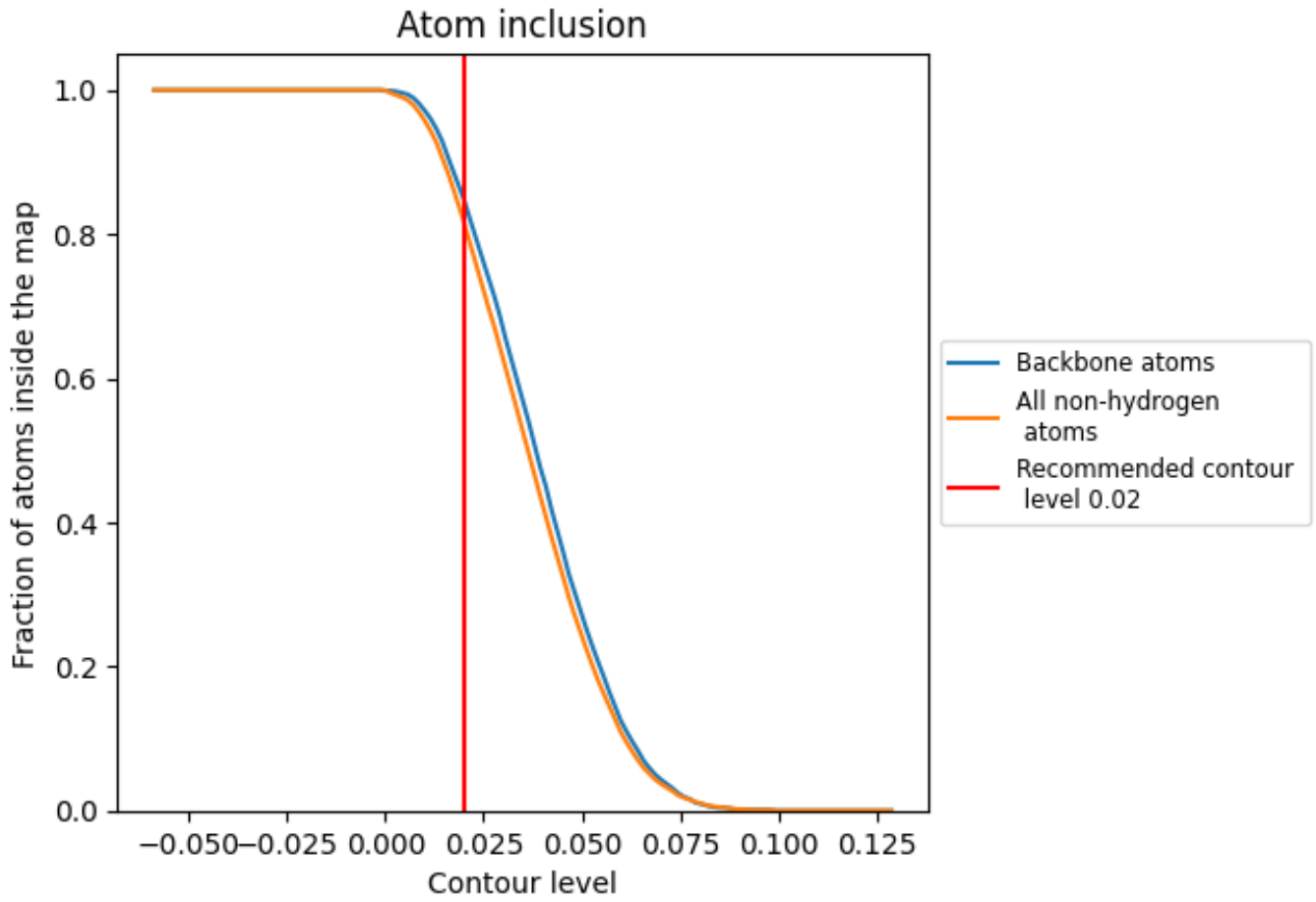
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8170	0.6800
A	0.8630	0.7030
B	0.8470	0.6850
C	0.7830	0.6650
D	0.8710	0.7060
E	0.7170	0.6340
F	0.6390	0.5940
I	0.7500	0.6480
K	0.4760	0.5710
N	0.1300	0.4730