wwPDB EM Validation Summary Report

May 6, 2025 – 12:17 PM JST

PDB ID	:	9IIU / pdb_00009iiu
EMDB ID	:	EMD-60605
Title	:	Cryo-EM structure of an TEF30-associated intermediate PSII core complex from Chlamydomonas reinhardtii
Authors	:	Wang, Y.; Wang, C.; Li, A.; Liu, Z.
Deposited on	:	2024-06-21
Resolution	:	2.98 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:

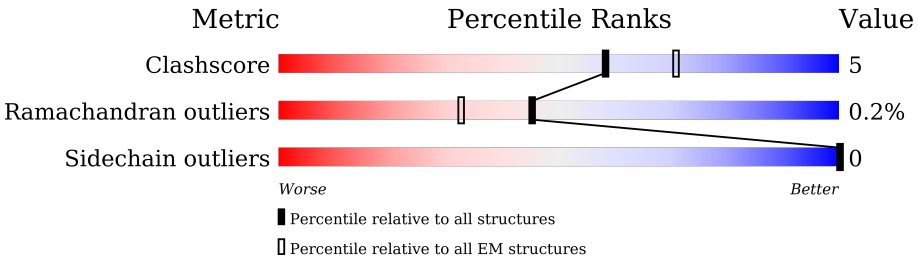
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.98 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	326	82% 10% 8%
2	B	480	91% 9%
3	C	450	85% 12%
4	D	349	83% 13%
5	E	75	92% 8%
6	F	31	6% 90% 10%
7	G	258	24% 91% 9%
8	H	70	90% 9%

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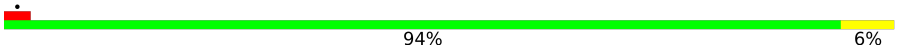
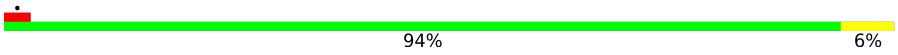
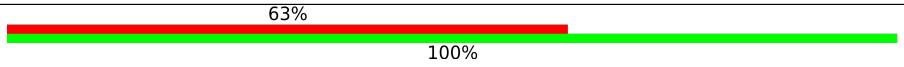
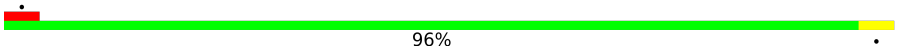
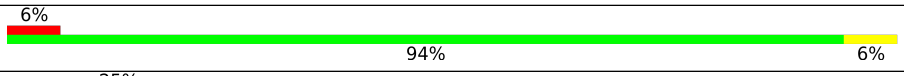
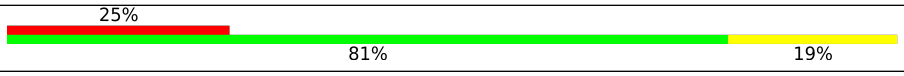
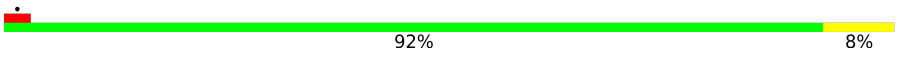
Mol	Chain	Length	Quality of chain
9	I	34	
10	J	32	
11	K	37	
12	L	35	
13	M	27	
14	T	24	
15	V	32	
16	X	32	
17	Z	61	

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
19	CLA	A	402	X	-	-	-
19	CLA	A	403	X	-	-	-
19	CLA	B	501	X	-	-	-
19	CLA	B	502	X	-	-	-
19	CLA	B	503	X	-	-	-
19	CLA	B	504	X	-	-	-
19	CLA	B	505	X	-	-	-
19	CLA	B	506	X	-	-	-
19	CLA	B	507	X	-	-	-
19	CLA	B	508	X	-	-	-
19	CLA	B	509	X	-	-	-
19	CLA	B	510	X	-	-	-
19	CLA	B	511	X	-	-	-
19	CLA	B	512	X	-	-	-
19	CLA	B	513	X	-	-	-
19	CLA	B	514	X	-	-	-
19	CLA	B	515	X	-	-	-
19	CLA	B	516	X	-	-	-
19	CLA	C	501	X	-	-	-
19	CLA	C	502	X	-	-	-
19	CLA	C	503	X	-	-	-
19	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	C	505	X	-	-	-
19	CLA	C	506	X	-	-	-
19	CLA	C	507	X	-	-	-
19	CLA	C	508	X	-	-	-
19	CLA	C	509	X	-	-	-
19	CLA	C	510	X	-	-	-
19	CLA	C	511	X	-	-	-
19	CLA	C	512	X	-	-	-
19	CLA	C	513	X	-	-	-
19	CLA	D	401	X	-	-	-
19	CLA	D	405	X	-	-	-

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 21452 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 II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	301	2355	1547	389	404	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	480	3755	2462	630	651	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	438	3431	2249	571	594	17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	335	2671	1767	437	455	12	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	75	610	399	101	110	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	31	251	171	42	37	1	0	0

- Molecule 7 is a protein called PDZ domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	258	Total	C	N	O	S	0	0
			1806	1116	334	349	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	69	Total	C	N	O	S	0	0
			532	356	79	95	2		

- Molecule 9 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	34	Total	C	N	O	S	0	0
			275	189	41	43	2		

- Molecule 10 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	32	Total	C	N	O	0	0
			232	160	33	39		

- Molecule 11 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	209	43	45		

- Molecule 12 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	35	Total	C	N	O	0	0
			290	196	45	49		

- Molecule 13 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	27	Total	C	N	O	0	0
			210	146	29	35		

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	24	Total	C	N	O	S	0	0
			198	140	27	30	1		

- Molecule 15 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	V	32	Total	C	N	O	0	0
			224	147	37	40		

- Molecule 16 is a protein called Chloroplast photosystem II subunit X.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	X	32	Total	C	N	O	0	0
			214	140	35	39		

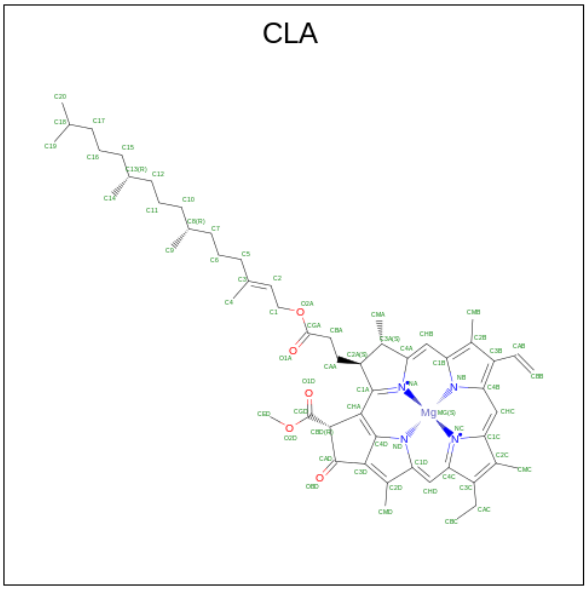
- Molecule 17 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

- Molecule 18 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	Fe	0
			1	1	

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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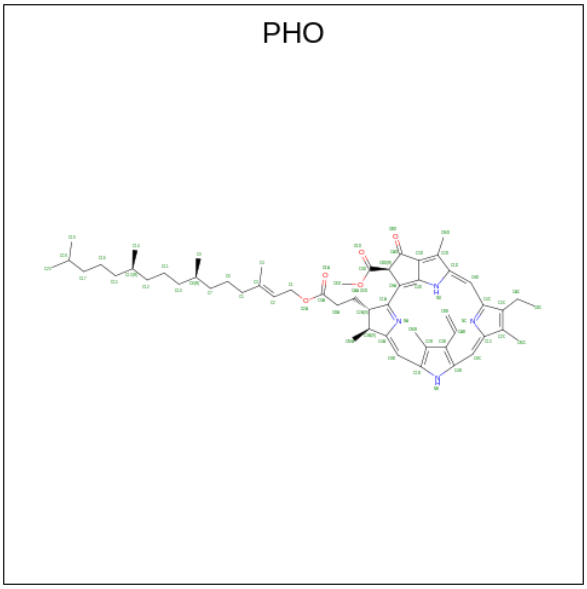
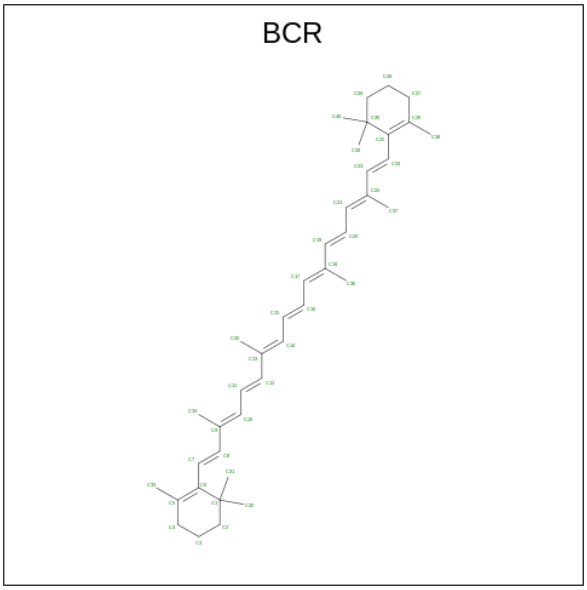
Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 45 35 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	B	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	C	1	Total C Mg N O 65 55 1 4 5	0
19	D	1	Total C Mg N O 65 55 1 4 5	0
19	D	1	Total C Mg N O 65 55 1 4 5	0
19	D	1	Total C Mg N O 65 55 1 4 5	0

- Molecule 20 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



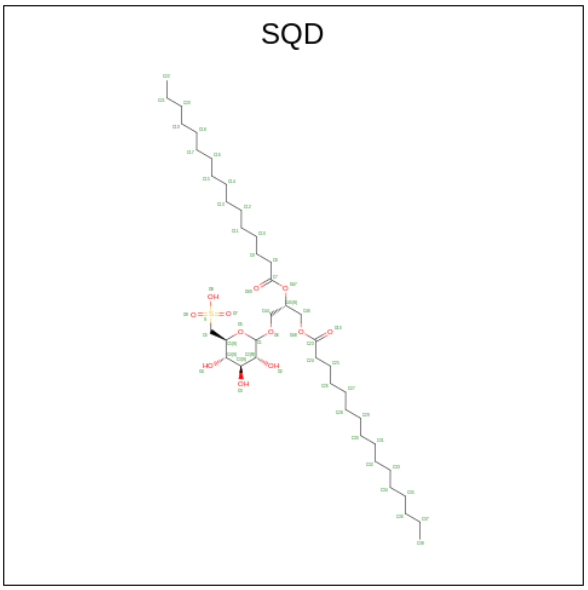
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	N	O	0
			64	55	4	5	
20	D	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



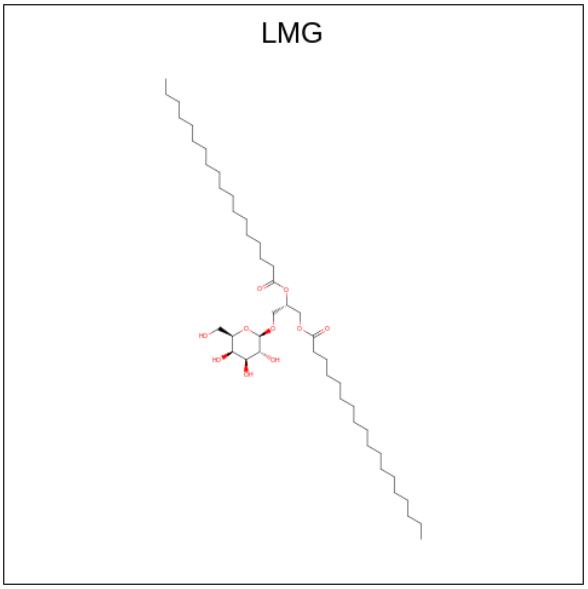
Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	C	1	Total C 40 40	0
21	D	1	Total C 40 40	0
21	H	1	Total C 40 40	0
21	K	1	Total C 40 40	0

- Molecule 22 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



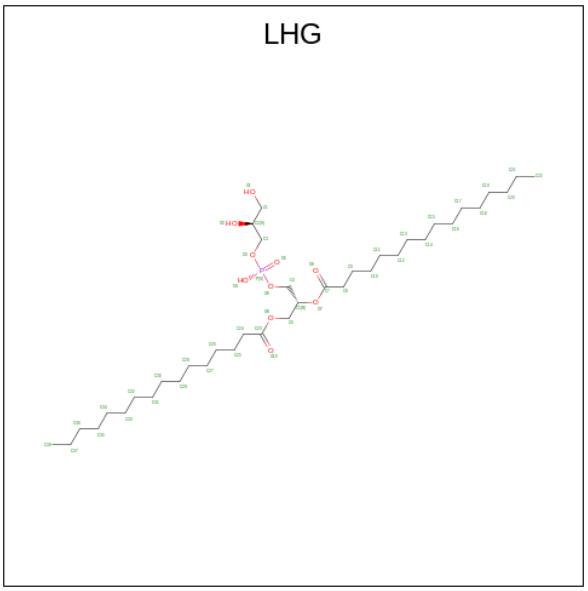
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total C O S 51 38 12 1	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



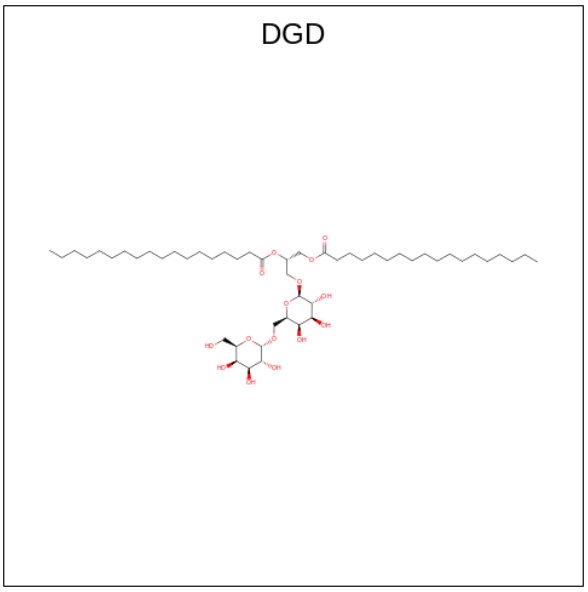
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C O 46 36 10	0
23	B	1	Total C O 42 32 10	0
23	B	1	Total C O 48 38 10	0
23	C	1	Total C O 51 41 10	0
23	D	1	Total C O 46 36 10	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



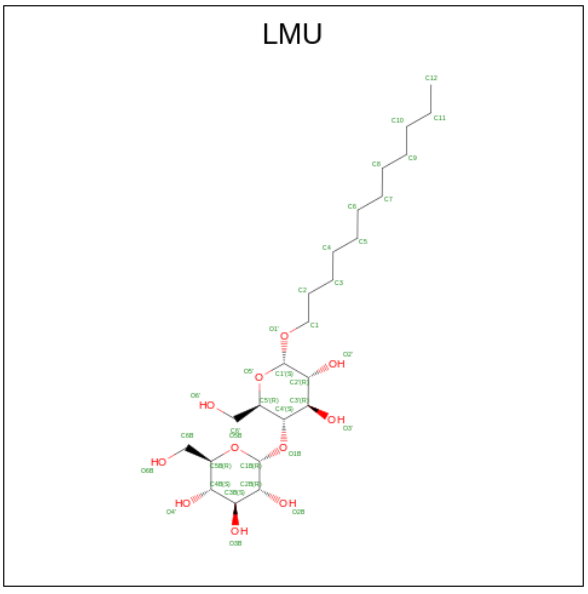
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			43	32	10	1	
24	B	1	Total	C	O	P	0
			44	33	10	1	
24	D	1	Total	C	O	P	0
			49	38	10	1	
24	D	1	Total	C	O	P	0
			49	38	10	1	
24	D	1	Total	C	O	P	0
			49	38	10	1	
24	L	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



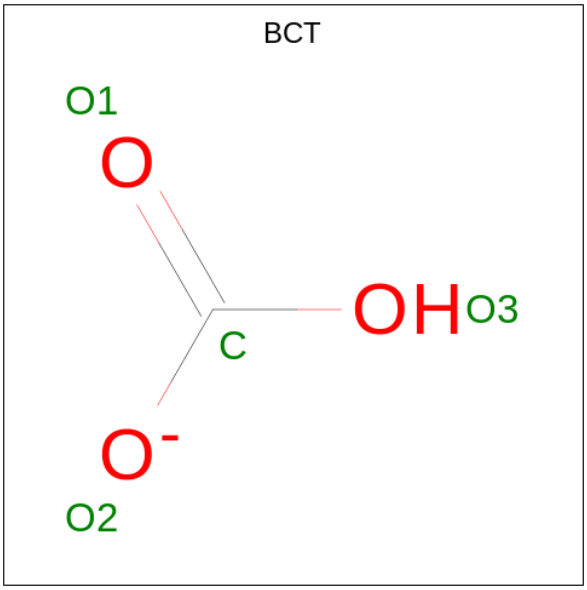
Mol	Chain	Residues	Atoms			AltConf
25	C	1	Total 53	C 38	O 15	0
25	C	1	Total 62	C 47	O 15	0
25	J	1	Total 59	C 44	O 15	0

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



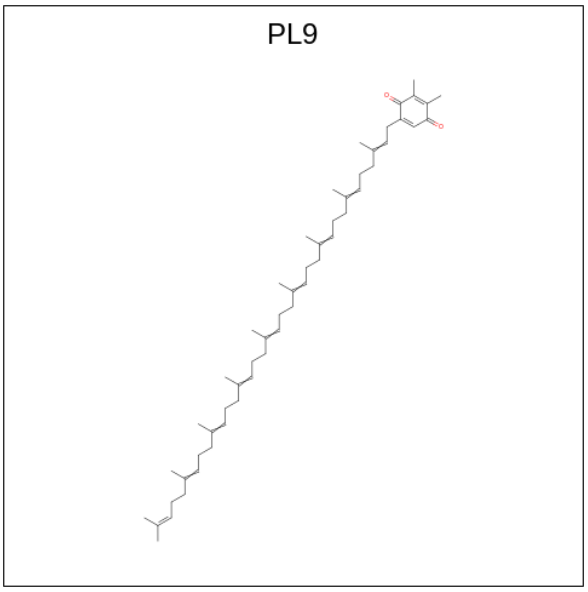
Mol	Chain	Residues	Atoms			AltConf
26	C	1	Total	C	O	0
			35	24	11	

- Molecule 27 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



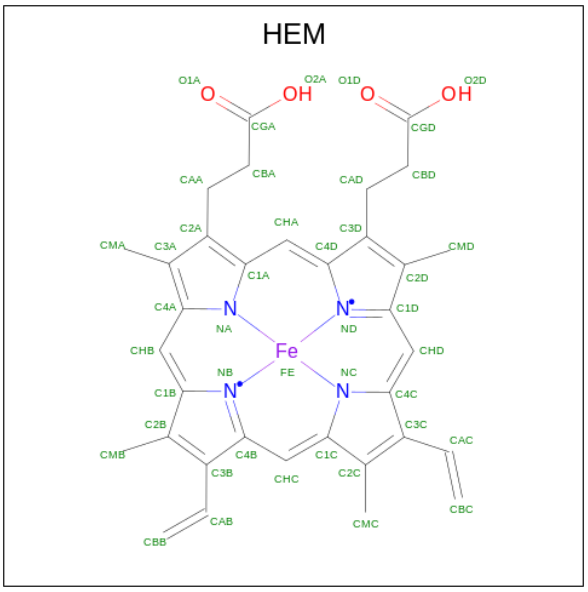
Mol	Chain	Residues	Atoms			AltConf
27	D	1	Total	C	O	0
			4	1	3	

- Molecule 28 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 (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
28	D	1	Total	C	O	0
			55	53	2	

- Molecule 29 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



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

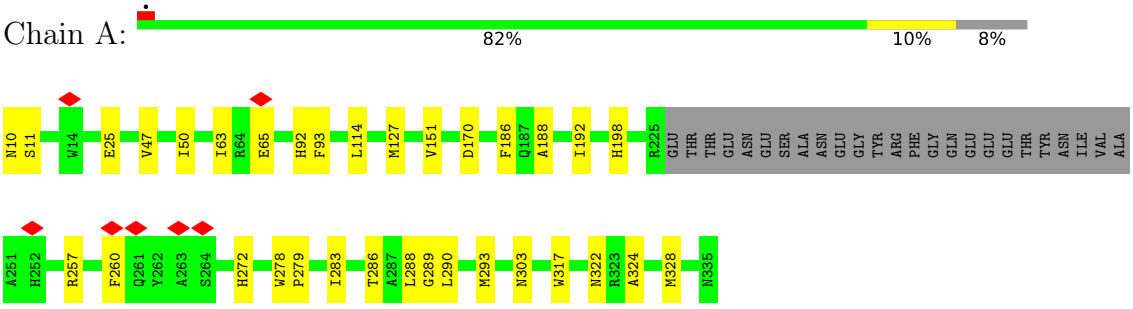
- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	A	2	Total	O	0
			2	2	

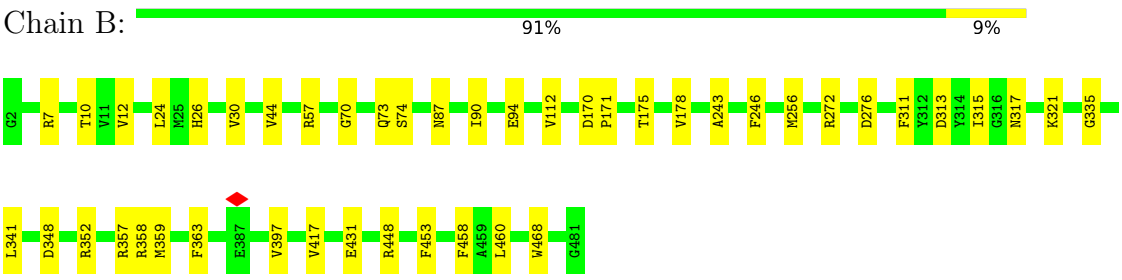
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

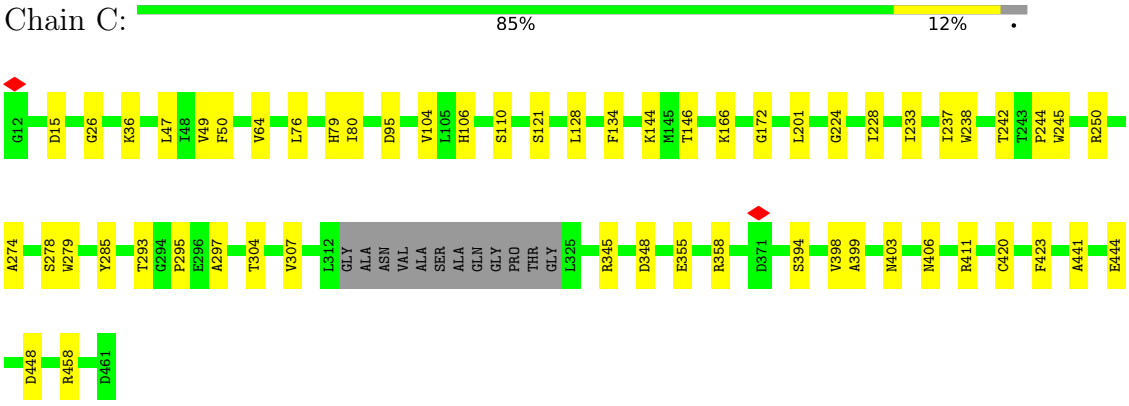
• Molecule 1: Photosystem II protein D1



• Molecule 2: Photosystem II CP47 reaction center protein

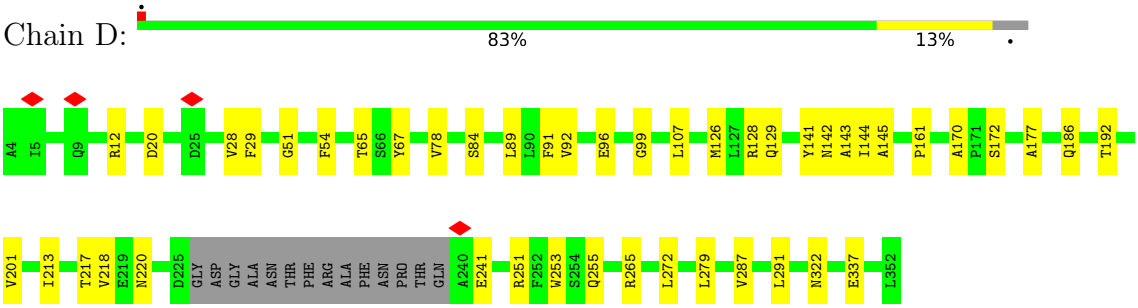


• Molecule 3: Photosystem II CP43 reaction center protein



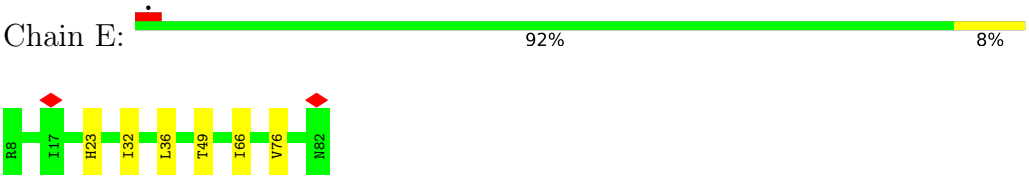
• Molecule 4: Photosystem II D2 protein

Chain D:



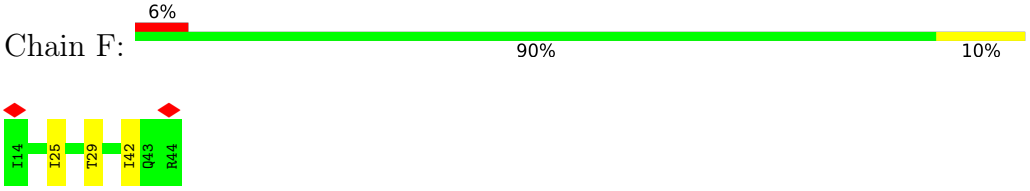
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



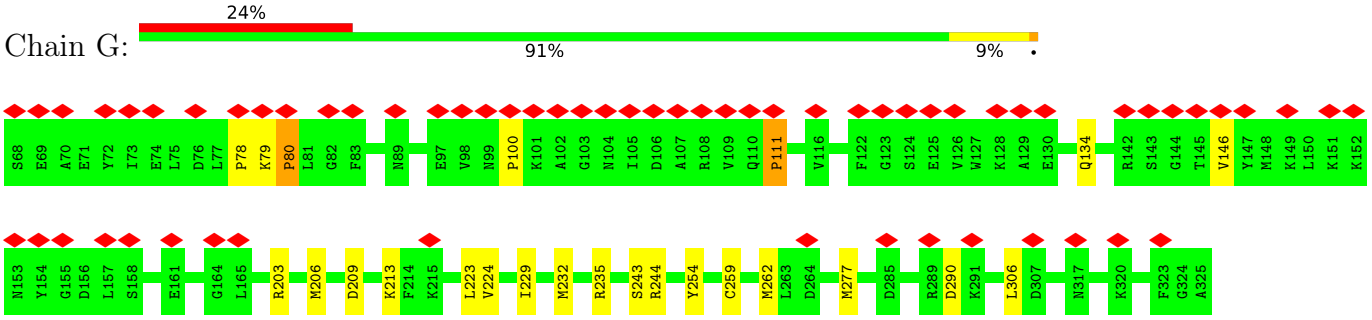
• Molecule 6: Cytochrome b559 subunit beta

Chain F:



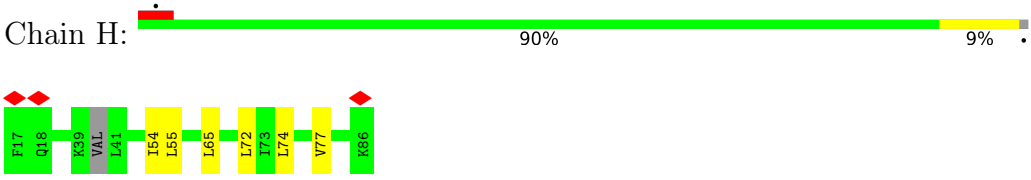
• Molecule 7: PDZ domain-containing protein

Chain G:



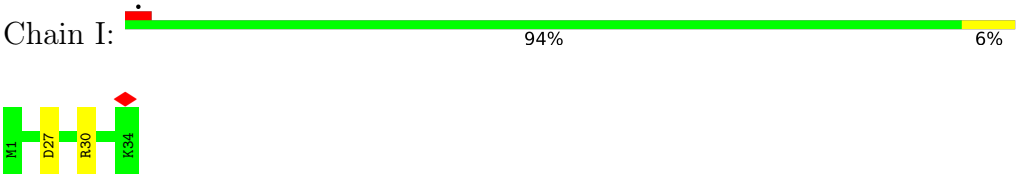
• Molecule 8: Photosystem II reaction center protein H

Chain H:



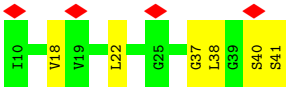
• Molecule 9: Photosystem II reaction center protein I

Chain I:



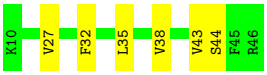
• Molecule 10: Photosystem II reaction center protein J

Chain J:



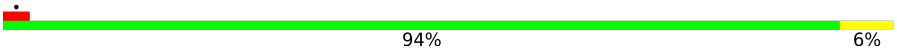
• Molecule 11: Photosystem II reaction center protein K

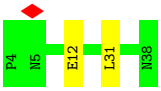
Chain K:



• Molecule 12: Photosystem II reaction center protein L

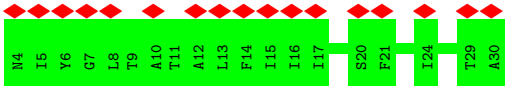
Chain L:





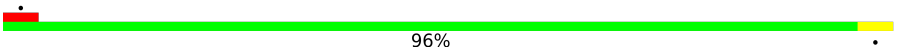
• Molecule 13: Photosystem II reaction center protein M

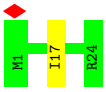
Chain M:



• Molecule 14: Photosystem II reaction center protein T

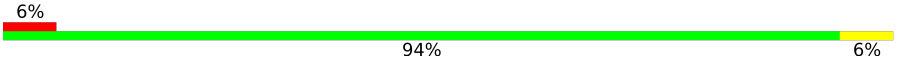
Chain T:

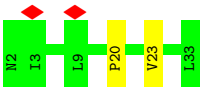




• Molecule 15: Photosystem II reaction center protein Psb30

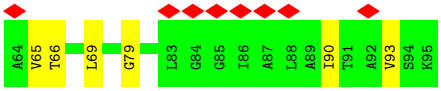
Chain V:





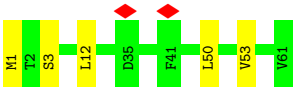
• Molecule 16: Chloroplast photosystem II subunit X

Chain X:



• Molecule 17: Photosystem II reaction center protein Z

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45968	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.397	Depositor
Minimum map value	-0.883	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.174	Depositor
Map size (Å)	280.0, 280.0, 280.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, LHG, LMG, HEM, BCT, BCR, FE2, LMU, PHO, CLA, PL9, DGD

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	0.16	0/2430	0.31	0/3312
2	B	0.13	0/3883	0.26	0/5286
3	C	0.13	0/3550	0.27	0/4834
4	D	0.14	0/2762	0.27	0/3766
5	E	0.11	0/628	0.27	0/857
6	F	0.12	0/258	0.27	0/349
7	G	0.16	0/1830	0.43	4/2476 (0.2%)
8	H	0.11	0/543	0.27	0/740
9	I	0.16	0/283	0.24	0/383
10	J	0.10	0/238	0.23	0/326
11	K	0.16	0/309	0.37	0/425
12	L	0.11	0/298	0.22	0/405
13	M	0.10	0/214	0.28	0/293
14	T	0.15	0/203	0.25	0/273
15	V	0.10	0/224	0.25	0/307
16	X	0.11	0/215	0.27	0/292
17	Z	0.15	0/469	0.29	0/644
All	All	0.14	0/18337	0.29	4/24968 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	78	PRO	N-CA-CB	7.86	110.28	103.36
7	G	80	PRO	N-CA-CB	7.31	110.92	103.25
7	G	100	PRO	N-CA-CB	7.13	109.97	103.20
7	G	111	PRO	N-CA-CB	6.93	110.53	103.25

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2355	0	2291	30	0
2	B	3755	0	3642	30	0
3	C	3431	0	3308	45	0
4	D	2671	0	2567	40	0
5	E	610	0	599	5	0
6	F	251	0	263	2	0
7	G	1806	0	1549	13	0
8	H	532	0	556	6	0
9	I	275	0	287	2	0
10	J	232	0	242	5	0
11	K	297	0	308	5	0
12	L	290	0	298	2	0
13	M	210	0	231	0	0
14	T	198	0	209	2	0
15	V	224	0	256	1	0
16	X	214	0	240	4	0
17	Z	458	0	490	4	0
18	A	1	0	0	0	0
19	A	174	0	170	2	0
19	B	1020	0	1113	9	0
19	C	845	0	936	5	0
19	D	195	0	216	7	0
20	A	64	0	74	1	0
20	D	64	0	74	3	0
21	A	40	0	56	3	0
21	B	120	0	168	3	0
21	C	120	0	168	12	0
21	D	40	0	56	2	0
21	H	40	0	56	3	0
21	K	40	0	56	1	0
22	A	51	0	69	0	0
23	A	46	0	62	0	0
23	B	90	0	120	1	0
23	C	51	0	72	0	0
23	D	46	0	62	2	0
24	A	43	0	56	1	0
24	B	44	0	61	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	D	147	0	222	2	0
24	L	49	0	74	2	0
25	C	115	0	146	0	0
25	J	59	0	76	0	0
26	C	35	0	46	1	0
27	D	4	0	0	0	0
28	D	55	0	80	1	0
29	F	43	0	30	5	0
30	A	2	0	0	0	0
All	All	21452	0	21655	195	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 5.

The worst 5 of 195 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)
2:B:272:ARG:NH1	2:B:276:ASP:OD2	2.10	0.85
1:A:286:THR:OG1	19:A:402:CLA:O1D	2.01	0.77
3:C:285:TYR:O	3:C:411:ARG:NH2	2.20	0.74
3:C:104:VAL:HG11	21:C:514:BCR:H333	1.69	0.74
4:D:217:THR:HG21	4:D:253:TRP:HE1	1.54	0.72

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	297/326 (91%)	289 (97%)	8 (3%)	0	100	100
2	B	478/480 (100%)	466 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	434/450 (96%)	418 (96%)	16 (4%)	0	100	100
4	D	331/349 (95%)	324 (98%)	7 (2%)	0	100	100
5	E	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
6	F	29/31 (94%)	29 (100%)	0	0	100	100
7	G	256/258 (99%)	236 (92%)	16 (6%)	4 (2%)	8	32
8	H	65/70 (93%)	64 (98%)	1 (2%)	0	100	100
9	I	32/34 (94%)	32 (100%)	0	0	100	100
10	J	30/32 (94%)	30 (100%)	0	0	100	100
11	K	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
12	L	33/35 (94%)	33 (100%)	0	0	100	100
13	M	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
14	T	22/24 (92%)	22 (100%)	0	0	100	100
15	V	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
16	X	30/32 (94%)	30 (100%)	0	0	100	100
17	Z	59/61 (97%)	59 (100%)	0	0	100	100
All	All	2259/2353 (96%)	2189 (97%)	66 (3%)	4 (0%)	45	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	79	LYS
7	G	80	PRO
7	G	111	PRO
7	G	146	VAL

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	245/266 (92%)	245 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	382/382 (100%)	382 (100%)	0	100	100
3	C	346/352 (98%)	346 (100%)	0	100	100
4	D	268/278 (96%)	268 (100%)	0	100	100
5	E	66/66 (100%)	66 (100%)	0	100	100
6	F	25/25 (100%)	25 (100%)	0	100	100
7	G	141/211 (67%)	141 (100%)	0	100	100
8	H	59/60 (98%)	59 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
10	J	24/24 (100%)	24 (100%)	0	100	100
11	K	31/31 (100%)	31 (100%)	0	100	100
12	L	33/33 (100%)	33 (100%)	0	100	100
13	M	23/23 (100%)	23 (100%)	0	100	100
14	T	21/21 (100%)	21 (100%)	0	100	100
15	V	26/26 (100%)	26 (100%)	0	100	100
16	X	22/22 (100%)	22 (100%)	0	100	100
17	Z	51/51 (100%)	51 (100%)	0	100	100
All	All	1794/1902 (94%)	1794 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	ASN
4	D	142	ASN
7	G	134	GLN
7	G	220	GLN
12	L	38	ASN

5.3.3 RNA

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 67 ligands modelled in this entry, 1 is monoatomic - leaving 66 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	$\#\|Z\| > 2$
19	CLA	A	402	-	65,73,73	1.51	7 (10%)	76,113,113	1.25	8 (10%)
19	CLA	B	502	-	65,73,73	1.51	5 (7%)	76,113,113	1.22	8 (10%)
23	LMG	A	408	-	46,46,55	0.99	2 (4%)	54,54,63	1.00	3 (5%)
19	CLA	B	503	-	65,73,73	1.53	7 (10%)	76,113,113	1.31	8 (10%)
19	CLA	B	515	-	65,73,73	1.50	6 (9%)	76,113,113	1.20	7 (9%)
19	CLA	C	501	-	65,73,73	1.50	6 (9%)	76,113,113	1.27	10 (13%)
19	CLA	B	507	-	65,73,73	1.52	6 (9%)	76,113,113	1.20	8 (10%)
21	BCR	C	514	-	41,41,41	0.74	0	56,56,56	2.26	22 (39%)
19	CLA	A	405	-	60,68,73	1.56	8 (13%)	70,107,113	1.25	9 (12%)
23	LMG	D	409	-	46,46,55	1.01	2 (4%)	54,54,63	1.04	3 (5%)
24	LHG	A	409	-	42,42,48	1.01	2 (4%)	45,48,54	1.02	2 (4%)
19	CLA	C	512	-	65,73,73	1.52	7 (10%)	76,113,113	1.31	9 (11%)
21	BCR	B	518	-	41,41,41	0.77	0	56,56,56	2.06	19 (33%)
21	BCR	B	517	-	41,41,41	0.78	0	56,56,56	2.08	20 (35%)
23	LMG	B	520	-	42,42,55	1.01	2 (4%)	50,50,63	1.00	2 (4%)
20	PHO	D	402	-	51,69,69	1.02	5 (9%)	47,99,99	1.12	4 (8%)
19	CLA	B	510	-	65,73,73	1.48	6 (9%)	76,113,113	1.23	7 (9%)
23	LMG	C	519	-	51,51,55	0.93	2 (3%)	59,59,63	0.93	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	CLA	B	508	-	65,73,73	1.50	7 (10%)	76,113,113	1.23	8 (10%)
19	CLA	B	509	-	65,73,73	1.54	7 (10%)	76,113,113	1.26	9 (11%)
19	CLA	B	516	-	65,73,73	1.52	5 (7%)	76,113,113	1.18	7 (9%)
19	CLA	D	405	-	65,73,73	1.53	5 (7%)	76,113,113	1.25	8 (10%)
21	BCR	H	101	-	41,41,41	0.71	0	56,56,56	2.11	21 (37%)
19	CLA	C	507	-	65,73,73	1.50	6 (9%)	76,113,113	1.24	7 (9%)
25	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	1.02	3 (3%)
21	BCR	B	519	-	41,41,41	0.78	0	56,56,56	1.92	18 (32%)
21	BCR	K	101	-	41,41,41	0.77	1 (2%)	56,56,56	2.21	20 (35%)
21	BCR	D	406	-	41,41,41	0.70	0	56,56,56	2.19	23 (41%)
21	BCR	A	406	-	41,41,41	0.70	0	56,56,56	2.03	18 (32%)
19	CLA	C	509	-	65,73,73	1.47	6 (9%)	76,113,113	1.26	7 (9%)
19	CLA	B	513	-	65,73,73	1.48	6 (9%)	76,113,113	1.24	8 (10%)
19	CLA	C	508	-	65,73,73	1.49	7 (10%)	76,113,113	1.29	8 (10%)
24	LHG	L	101	-	48,48,48	0.93	2 (4%)	51,54,54	0.95	3 (5%)
28	PL9	D	407	-	55,55,55	1.09	4 (7%)	68,69,69	1.58	12 (17%)
19	CLA	D	401	-	65,73,73	1.49	6 (9%)	76,113,113	1.30	8 (10%)
27	BCT	D	403	18	2,3,3	1.25	0	2,3,3	4.17	2 (100%)
19	CLA	C	504	-	65,73,73	1.52	8 (12%)	76,113,113	1.16	8 (10%)
25	DGD	C	517	-	54,54,67	0.95	2 (3%)	68,68,81	1.03	3 (4%)
24	LHG	D	408	-	48,48,48	0.94	2 (4%)	51,54,54	0.91	2 (3%)
19	CLA	C	505	-	65,73,73	1.50	6 (9%)	76,113,113	1.16	7 (9%)
19	CLA	B	504	-	65,73,73	1.52	7 (10%)	76,113,113	1.26	6 (7%)
19	CLA	A	403	-	49,57,73	1.74	7 (14%)	55,93,113	1.39	8 (14%)
19	CLA	C	510	-	65,73,73	1.52	6 (9%)	76,113,113	1.25	8 (10%)
19	CLA	C	511	3	65,73,73	1.55	6 (9%)	76,113,113	1.20	9 (11%)
21	BCR	C	516	-	41,41,41	0.70	0	56,56,56	1.88	17 (30%)
22	SQD	A	407	-	50,51,54	1.22	4 (8%)	59,62,65	1.16	8 (13%)
19	CLA	B	506	-	65,73,73	1.52	6 (9%)	76,113,113	1.22	7 (9%)
23	LMG	B	522	-	48,48,55	0.96	2 (4%)	56,56,63	0.94	2 (3%)
19	CLA	D	404	-	65,73,73	1.50	7 (10%)	76,113,113	1.21	8 (10%)
29	HEM	F	101	6,5	41,50,50	1.49	5 (12%)	45,82,82	1.32	6 (13%)
19	CLA	B	512	-	65,73,73	1.48	6 (9%)	76,113,113	1.30	8 (10%)
24	LHG	D	410	-	48,48,48	0.95	2 (4%)	51,54,54	0.95	2 (3%)
26	LMU	C	520	-	36,36,36	1.17	2 (5%)	47,47,47	0.87	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	LHG	B	521	-	43,43,48	1.00	2 (4%)	46,49,54	1.08	3 (6%)
20	PHO	A	404	-	51,69,69	1.03	4 (7%)	47,99,99	1.15	6 (12%)
19	CLA	B	514	-	45,53,73	1.80	6 (13%)	52,89,113	1.35	7 (13%)
19	CLA	C	503	-	65,73,73	1.52	6 (9%)	76,113,113	1.20	9 (11%)
24	LHG	D	411	-	48,48,48	0.94	2 (4%)	51,54,54	0.97	3 (5%)
19	CLA	C	513	-	65,73,73	1.51	5 (7%)	76,113,113	1.21	8 (10%)
19	CLA	B	501	-	65,73,73	1.53	7 (10%)	76,113,113	1.22	7 (9%)
21	BCR	C	515	-	41,41,41	0.77	1 (2%)	56,56,56	1.99	16 (28%)
25	DGD	J	101	-	60,60,67	0.92	2 (3%)	74,74,81	0.96	3 (4%)
19	CLA	B	511	-	65,73,73	1.51	8 (12%)	76,113,113	1.24	9 (11%)
19	CLA	C	502	-	65,73,73	1.52	8 (12%)	76,113,113	1.29	8 (10%)
19	CLA	B	505	-	65,73,73	1.50	5 (7%)	76,113,113	1.17	6 (7%)
19	CLA	C	506	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	9 (11%)

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
19	CLA	A	402	-	1/1/15/20	11/37/115/115	-
19	CLA	B	502	-	1/1/15/20	11/37/115/115	-
23	LMG	A	408	-	-	11/41/61/70	0/1/1/1
19	CLA	B	503	-	1/1/15/20	8/37/115/115	-
19	CLA	B	515	-	1/1/15/20	12/37/115/115	-
19	CLA	C	501	-	1/1/15/20	12/37/115/115	-
19	CLA	B	507	-	1/1/15/20	15/37/115/115	-
21	BCR	C	514	-	-	5/29/63/63	0/2/2/2
19	CLA	A	405	-	-	10/31/109/115	-
23	LMG	D	409	-	-	6/41/61/70	0/1/1/1
24	LHG	A	409	-	-	7/47/47/53	-
19	CLA	C	512	-	1/1/15/20	14/37/115/115	-
21	BCR	B	518	-	-	4/29/63/63	0/2/2/2
21	BCR	B	517	-	-	6/29/63/63	0/2/2/2
23	LMG	B	520	-	-	9/37/57/70	0/1/1/1
20	PHO	D	402	-	-	13/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	510	-	1/1/15/20	16/37/115/115	-
23	LMG	C	519	-	-	5/46/66/70	0/1/1/1
19	CLA	B	508	-	1/1/15/20	12/37/115/115	-
19	CLA	B	509	-	1/1/15/20	16/37/115/115	-
19	CLA	B	516	-	1/1/15/20	13/37/115/115	-
19	CLA	D	405	-	1/1/15/20	17/37/115/115	-
21	BCR	H	101	-	-	6/29/63/63	0/2/2/2
19	CLA	C	507	-	1/1/15/20	13/37/115/115	-
25	DGD	C	518	-	-	11/51/91/95	0/2/2/2
21	BCR	B	519	-	-	4/29/63/63	0/2/2/2
21	BCR	K	101	-	-	6/29/63/63	0/2/2/2
21	BCR	D	406	-	-	0/29/63/63	0/2/2/2
21	BCR	A	406	-	-	5/29/63/63	0/2/2/2
19	CLA	C	509	-	1/1/15/20	14/37/115/115	-
19	CLA	B	513	-	1/1/15/20	18/37/115/115	-
19	CLA	C	508	-	1/1/15/20	9/37/115/115	-
24	LHG	L	101	-	-	15/53/53/53	-
28	PL9	D	407	-	-	10/53/73/73	0/1/1/1
19	CLA	D	401	-	1/1/15/20	13/37/115/115	-
19	CLA	C	504	-	1/1/15/20	7/37/115/115	-
25	DGD	C	517	-	-	9/42/82/95	0/2/2/2
24	LHG	D	408	-	-	6/53/53/53	-
19	CLA	C	505	-	1/1/15/20	9/37/115/115	-
19	CLA	B	504	-	1/1/15/20	17/37/115/115	-
19	CLA	A	403	-	1/1/11/20	12/18/96/115	-
19	CLA	C	510	-	1/1/15/20	14/37/115/115	-
19	CLA	C	511	3	1/1/15/20	24/37/115/115	-
21	BCR	C	516	-	-	3/29/63/63	0/2/2/2
22	SQD	A	407	-	-	12/46/66/69	0/1/1/1
19	CLA	B	506	-	1/1/15/20	8/37/115/115	-
23	LMG	B	522	-	-	8/43/63/70	0/1/1/1
19	CLA	D	404	-	-	14/37/115/115	-
29	HEM	F	101	6,5	-	0/12/54/54	-
19	CLA	B	512	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	D	410	-	-	10/53/53/53	-
26	LMU	C	520	-	-	12/21/61/61	0/2/2/2
24	LHG	B	521	-	-	12/48/48/53	-
20	PHO	A	404	-	-	13/37/103/103	0/5/6/6
19	CLA	B	514	-	1/1/11/20	4/13/91/115	-
19	CLA	C	503	-	1/1/15/20	17/37/115/115	-
24	LHG	D	411	-	-	19/53/53/53	-
19	CLA	C	513	-	1/1/15/20	14/37/115/115	-
19	CLA	B	501	-	1/1/15/20	14/37/115/115	-
21	BCR	C	515	-	-	4/29/63/63	0/2/2/2
25	DGD	J	101	-	-	6/48/88/95	0/2/2/2
19	CLA	B	511	-	1/1/15/20	11/37/115/115	-
19	CLA	C	502	-	1/1/15/20	19/37/115/115	-
19	CLA	B	505	-	1/1/15/20	17/37/115/115	-
19	CLA	C	506	-	1/1/15/20	17/37/115/115	-

The worst 5 of 277 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	405	CLA	C4B-NB	7.85	1.42	1.35
19	B	509	CLA	C4B-NB	7.77	1.42	1.35
19	B	516	CLA	C4B-NB	7.75	1.42	1.35
19	B	507	CLA	C4B-NB	7.75	1.42	1.35
19	C	511	CLA	C4B-NB	7.73	1.42	1.35

The worst 5 of 545 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	D	406	BCR	C28-C27-C26	-6.00	103.36	114.08
21	C	514	BCR	C3-C4-C5	-5.89	103.56	114.08
19	B	513	CLA	C4A-NA-C1A	5.86	109.34	106.71
28	D	407	PL9	C7-C3-C4	5.80	121.59	116.88
21	A	406	BCR	C28-C27-C26	-5.80	103.72	114.08

5 of 33 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	402	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A	403	CLA	ND
19	B	501	CLA	ND
19	B	502	CLA	ND
19	B	503	CLA	ND

5 of 703 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	402	CLA	O2A-C1-C2-C3
19	A	405	CLA	C1A-C2A-CAA-CBA
19	A	405	CLA	C3A-C2A-CAA-CBA
19	B	501	CLA	C1A-C2A-CAA-CBA
19	B	501	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

33 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	402	CLA	1	0
19	B	502	CLA	4	0
21	C	514	BCR	4	0
19	A	405	CLA	1	0
23	D	409	LMG	2	0
24	A	409	LHG	1	0
21	B	518	BCR	1	0
20	D	402	PHO	3	0
19	B	510	CLA	1	0
19	B	516	CLA	1	0
19	D	405	CLA	2	0
21	H	101	BCR	3	0
21	B	519	BCR	2	0
21	K	101	BCR	1	0
21	D	406	BCR	2	0
21	A	406	BCR	3	0
19	B	513	CLA	2	0
24	L	101	LHG	2	0
28	D	407	PL9	1	0
24	D	408	LHG	2	0
19	B	504	CLA	2	0
19	C	511	CLA	1	0
21	C	516	BCR	2	0
23	B	522	LMG	1	0

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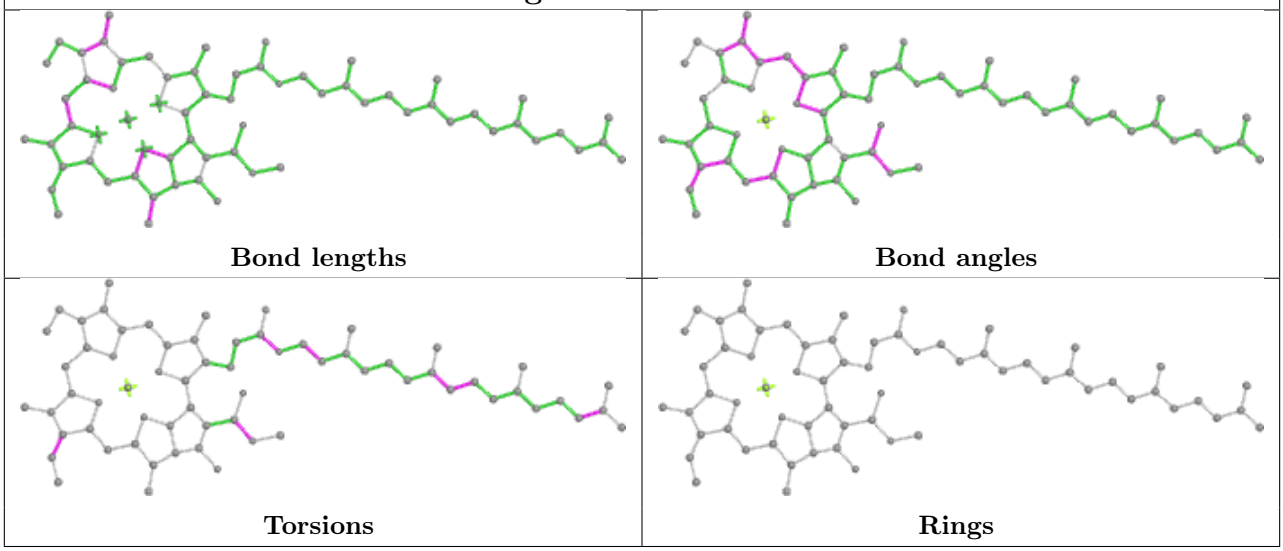
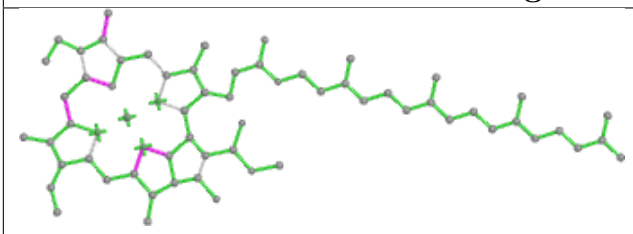
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	D	404	CLA	5	0
29	F	101	HEM	5	0
26	C	520	LMU	1	0
24	B	521	LHG	3	0
20	A	404	PHO	1	0
21	C	515	BCR	6	0
19	C	502	CLA	3	0
19	B	505	CLA	1	0
19	C	506	CLA	1	0

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.

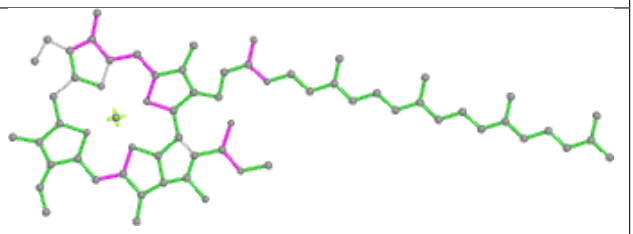
Ligand CLA A 402



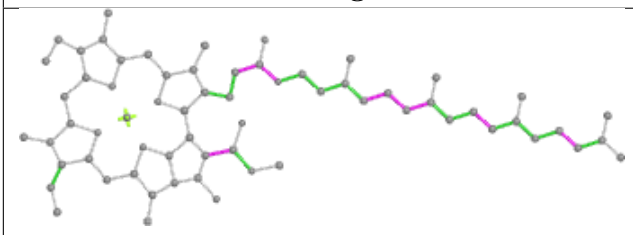
Ligand CLA B 502



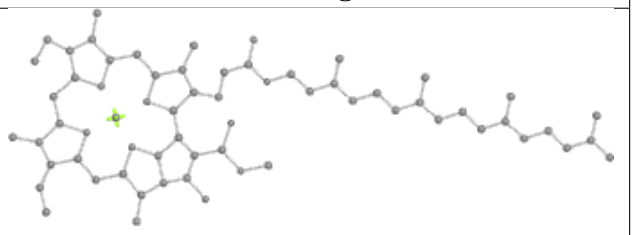
Bond lengths



Bond angles

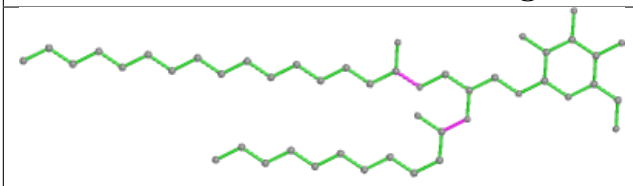


Torsions

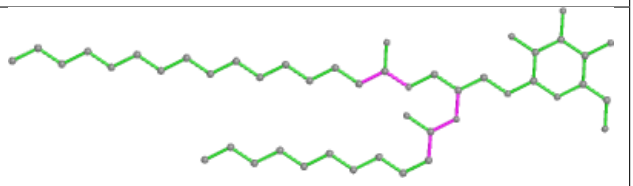


Rings

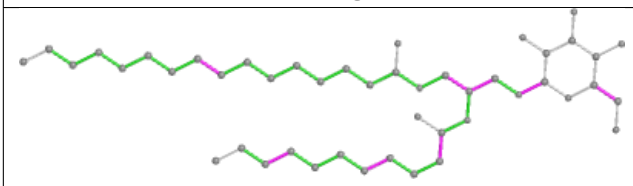
Ligand LMG A 408



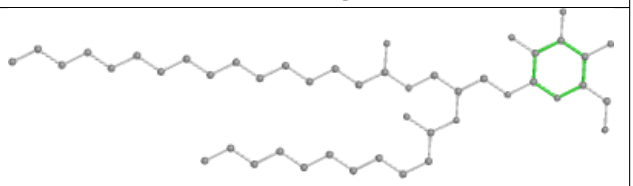
Bond lengths



Bond angles

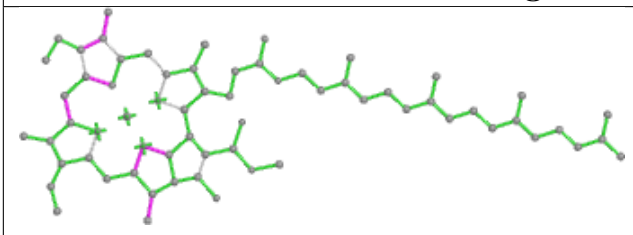


Torsions

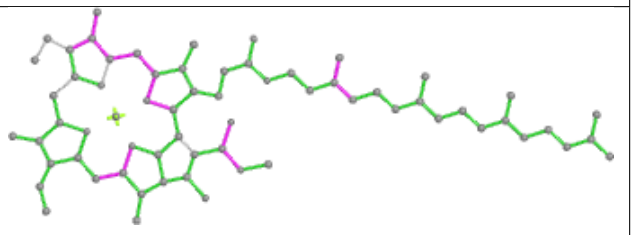


Rings

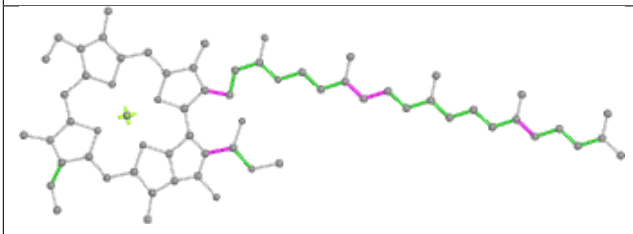
Ligand CLA B 503



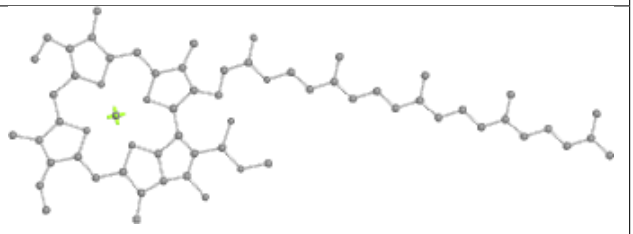
Bond lengths



Bond angles

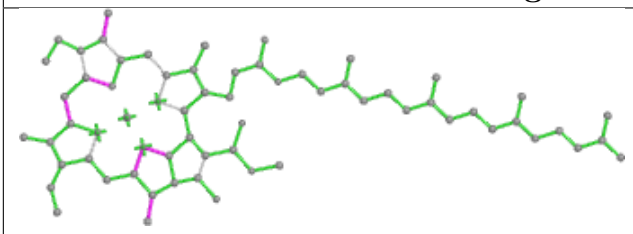


Torsions

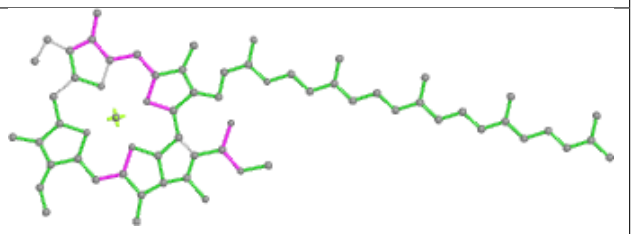


Rings

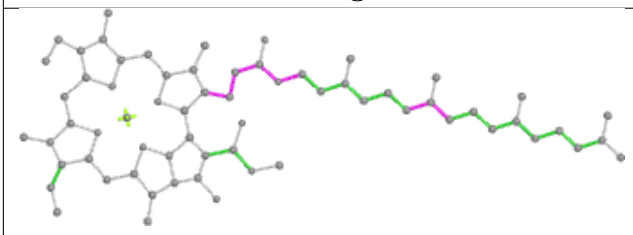
Ligand CLA B 515



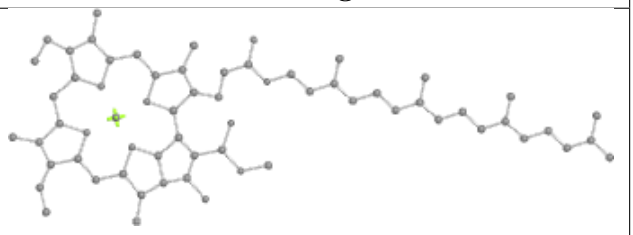
Bond lengths



Bond angles

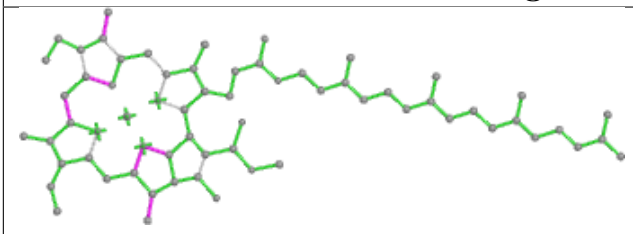


Torsions

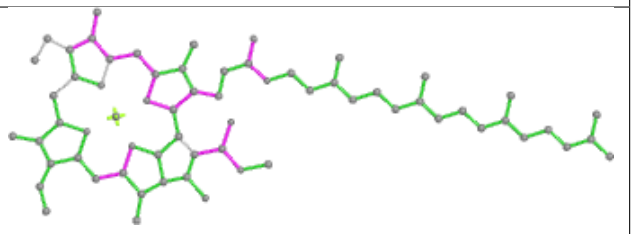


Rings

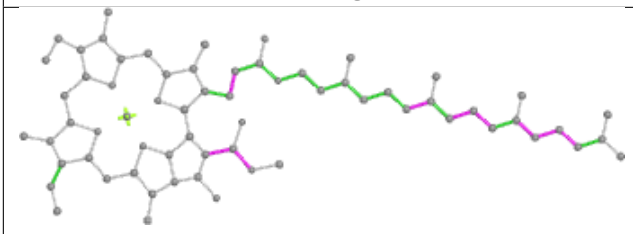
Ligand CLA C 501



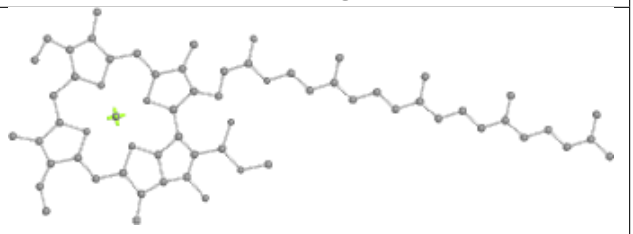
Bond lengths



Bond angles

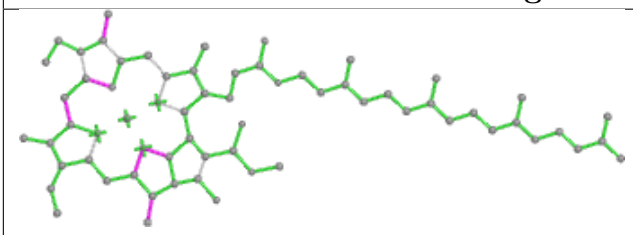


Torsions

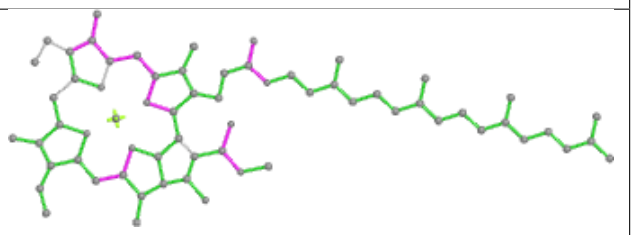


Rings

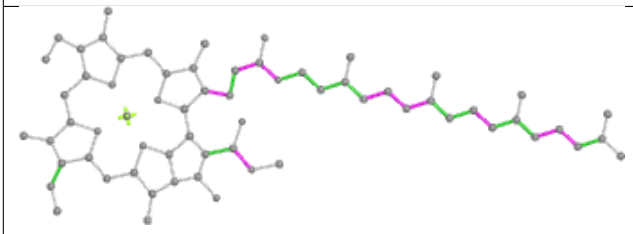
Ligand CLA B 507



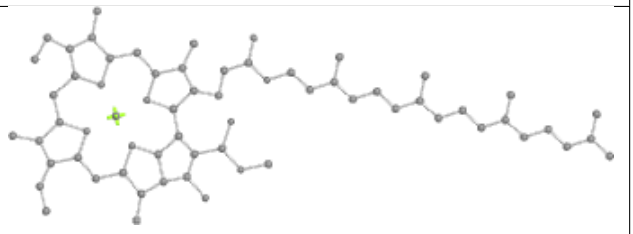
Bond lengths



Bond angles

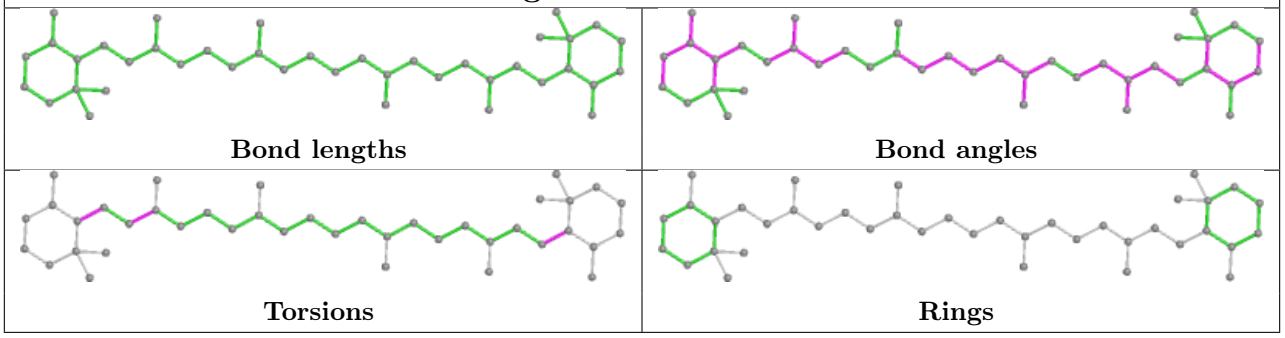


Torsions

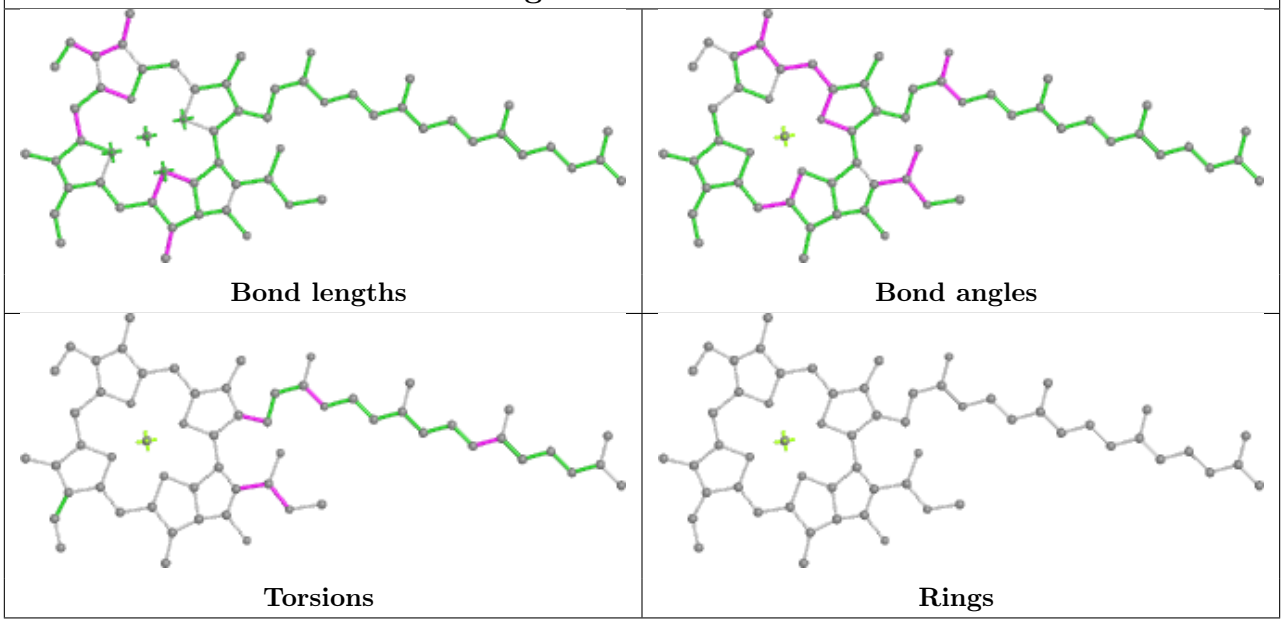


Rings

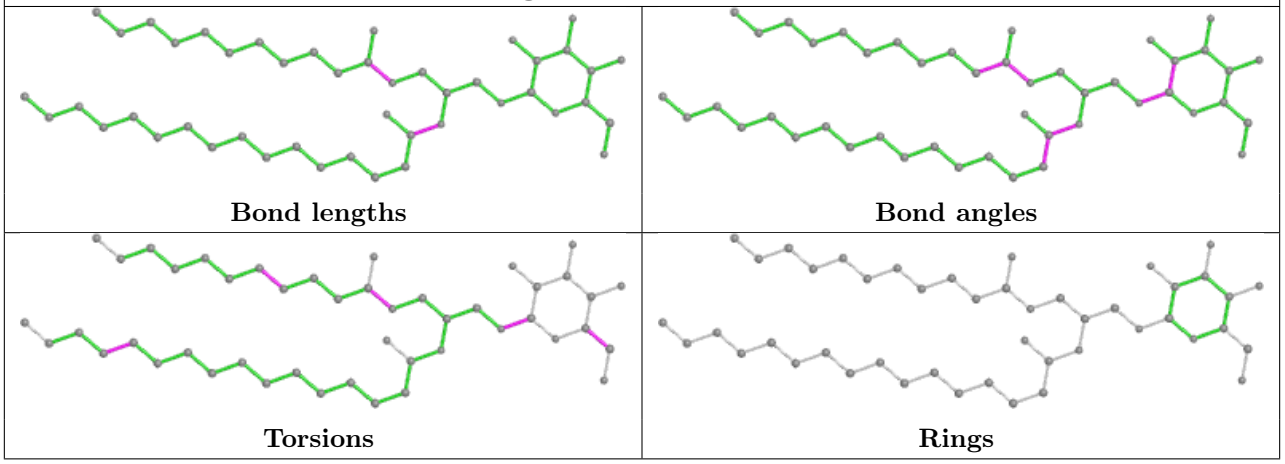
Ligand BCR C 514



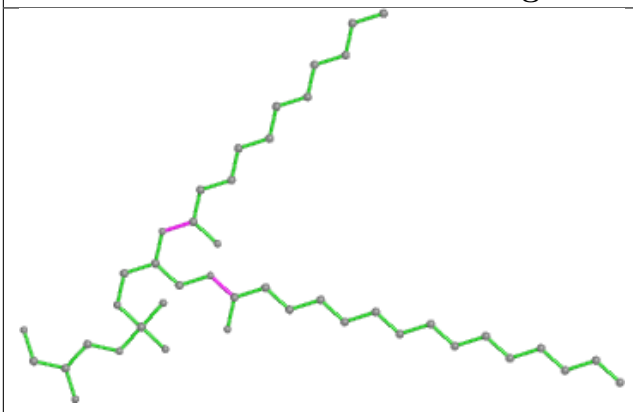
Ligand CLA A 405



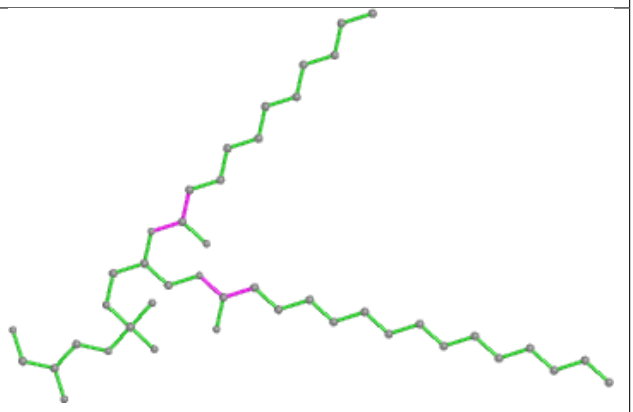
Ligand LMG D 409



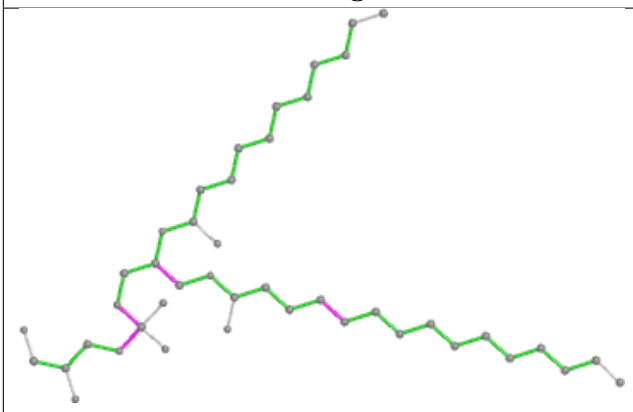
Ligand LHG A 409



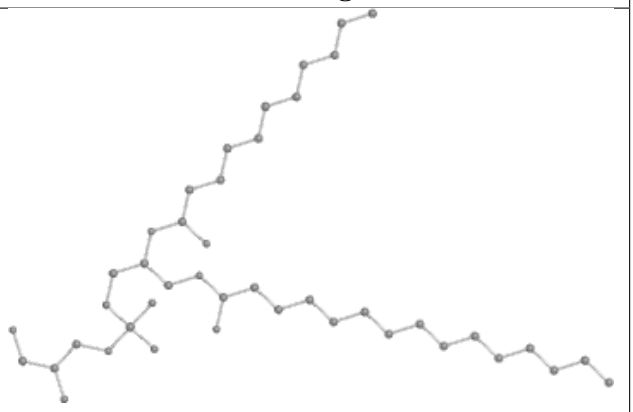
Bond lengths



Bond angles

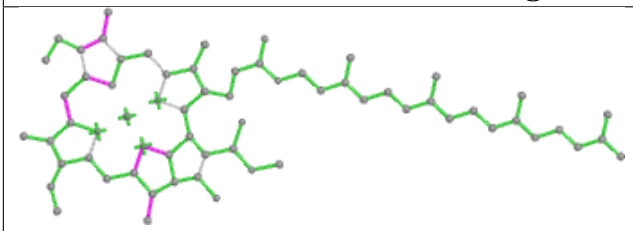


Torsions

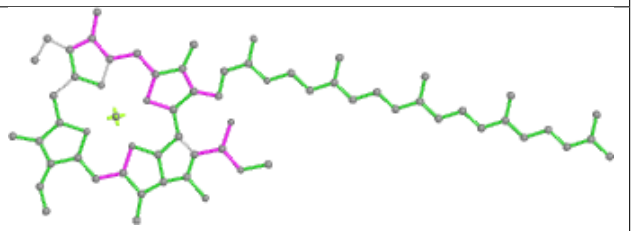


Rings

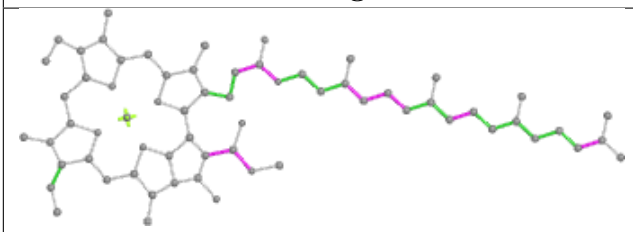
Ligand CLA C 512



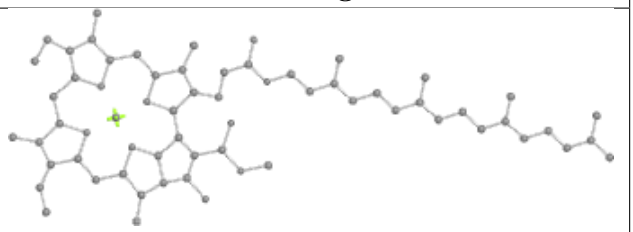
Bond lengths



Bond angles

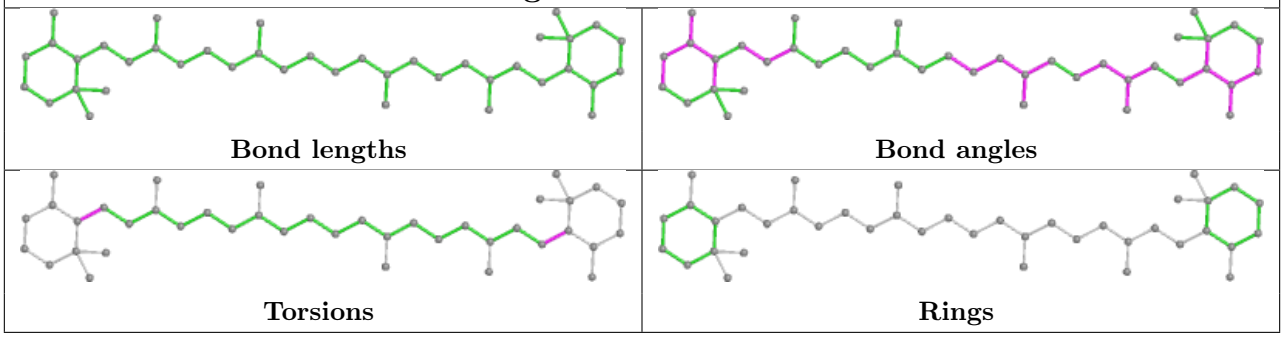


Torsions

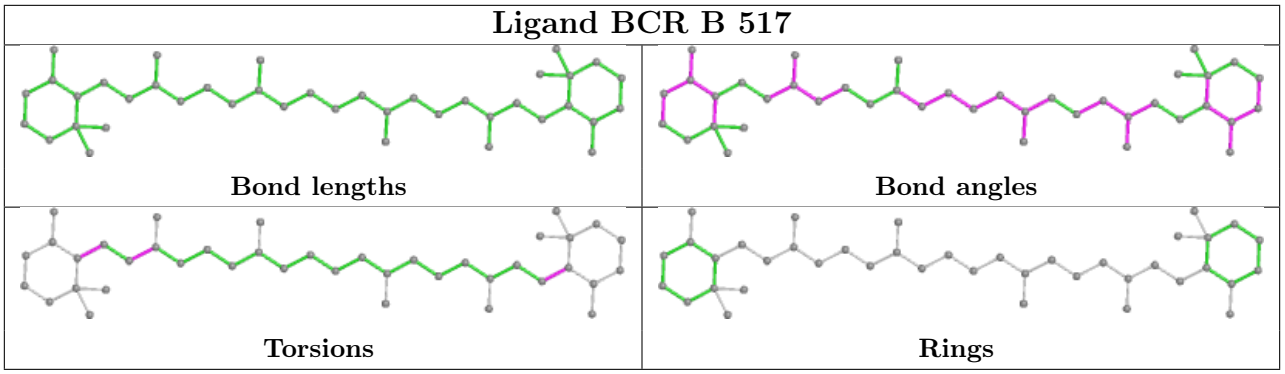


Rings

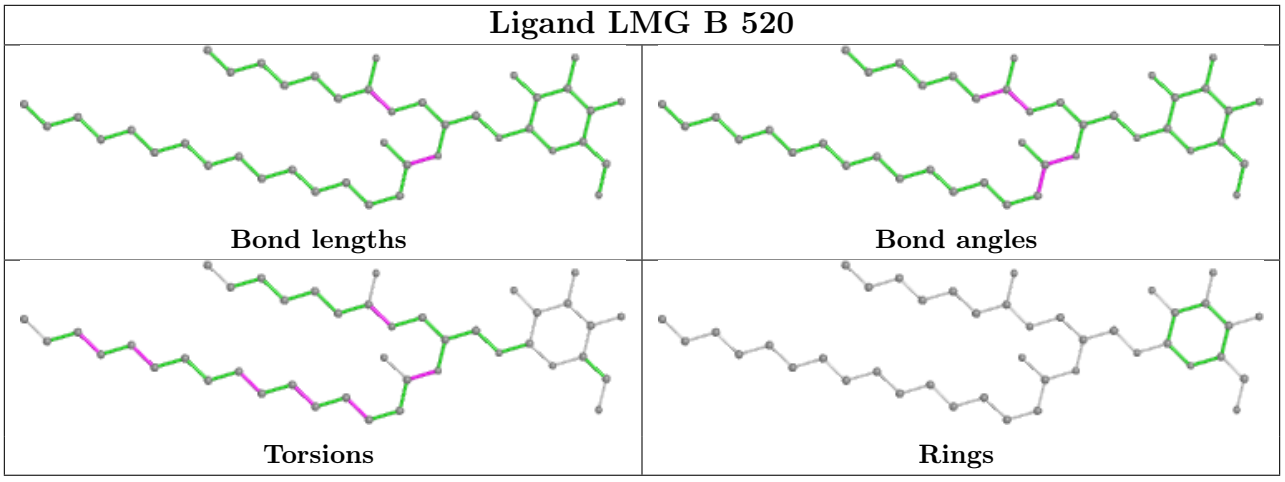
Ligand BCR B 518



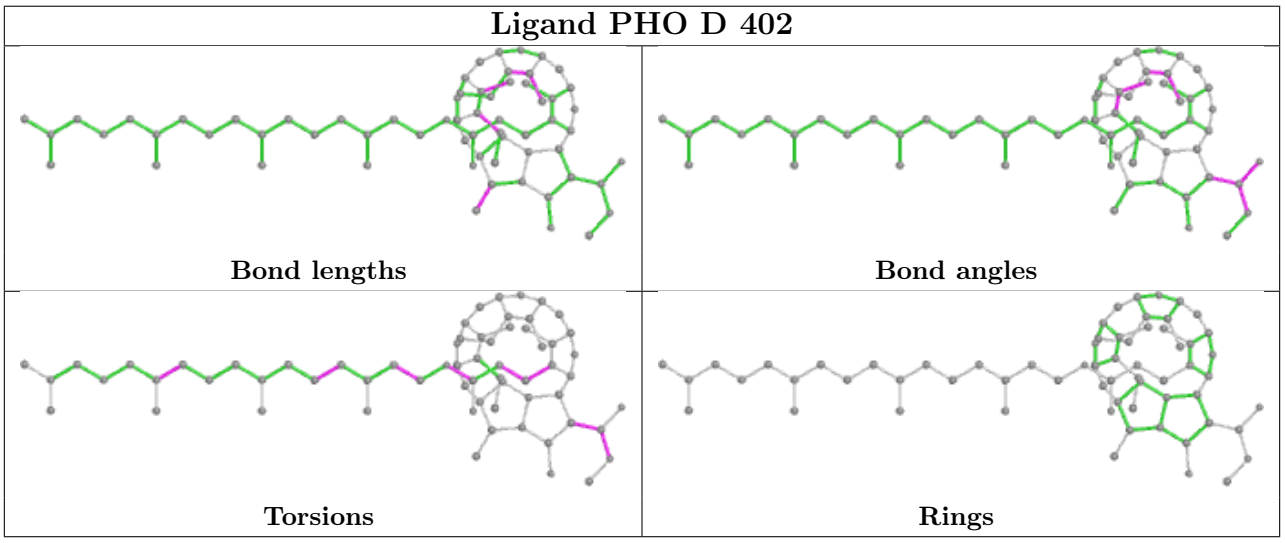
Ligand BCR B 517



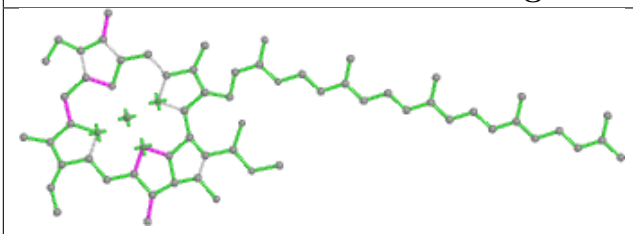
Ligand LMG B 520



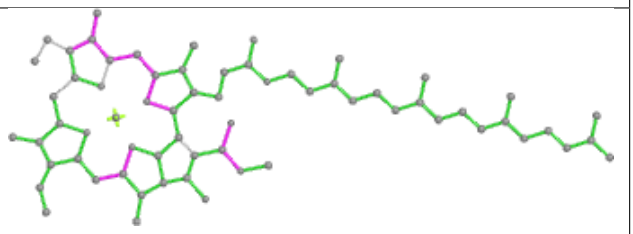
Ligand PHO D 402



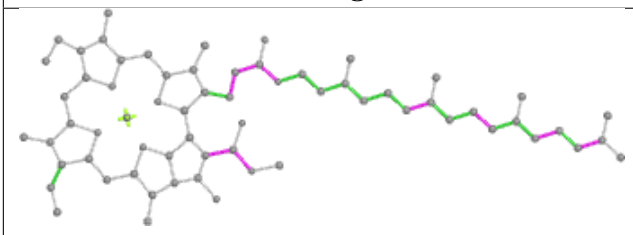
Ligand CLA B 510



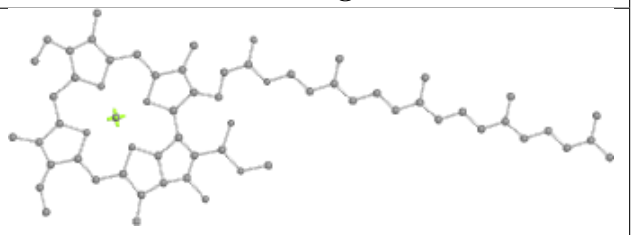
Bond lengths



Bond angles

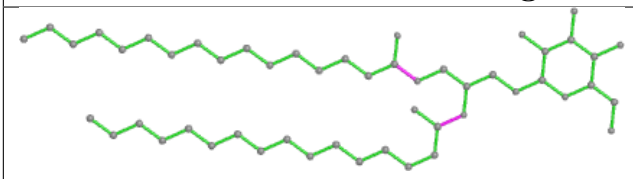


Torsions

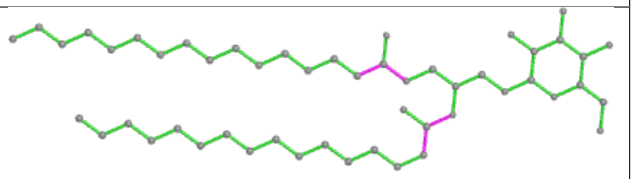


Rings

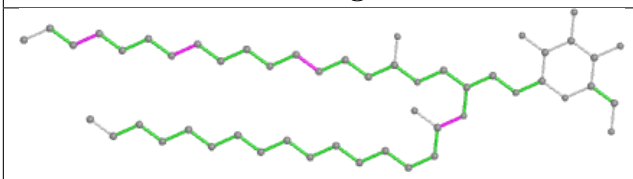
Ligand LMG C 519



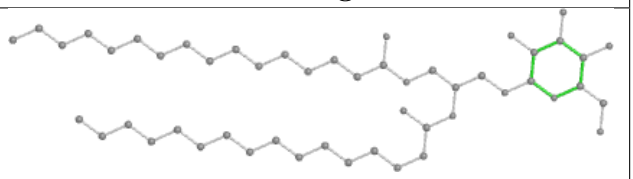
Bond lengths



Bond angles

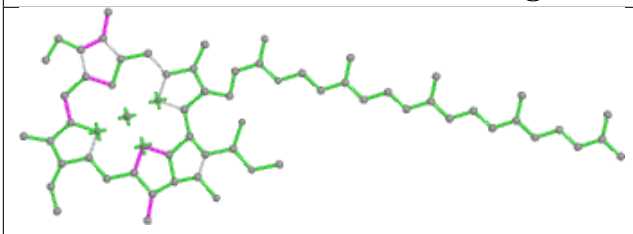


Torsions

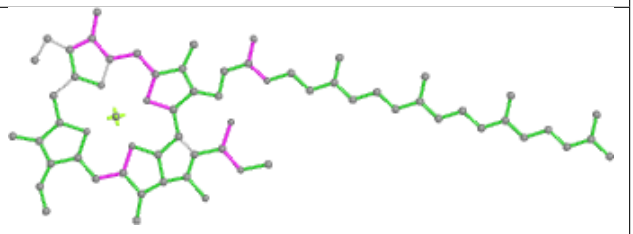


Rings

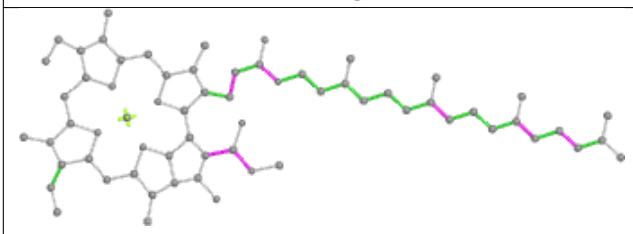
Ligand CLA B 508



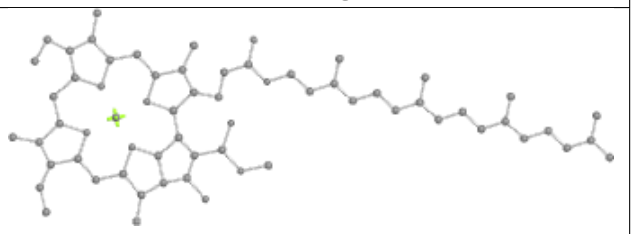
Bond lengths



Bond angles

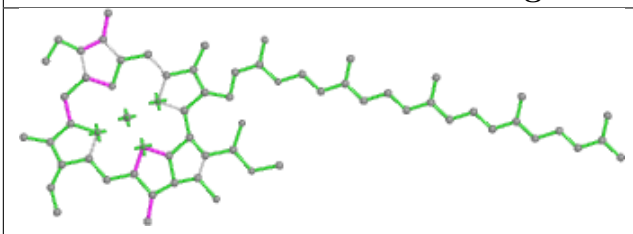


Torsions

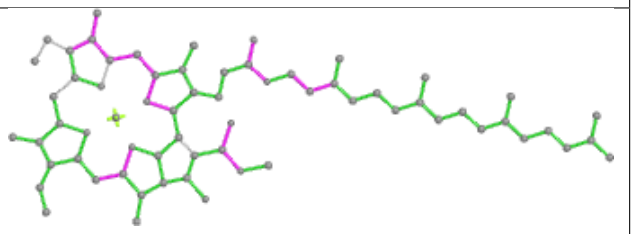


Rings

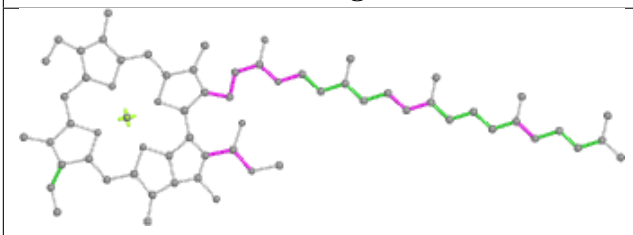
Ligand CLA B 509



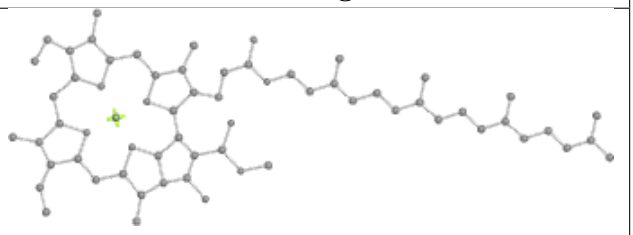
Bond lengths



Bond angles

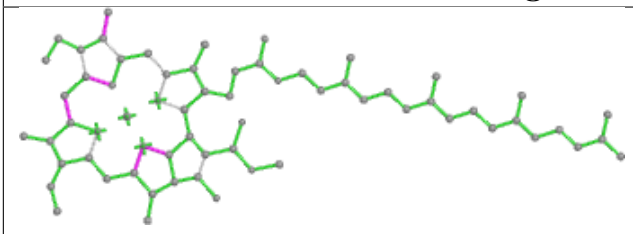


Torsions

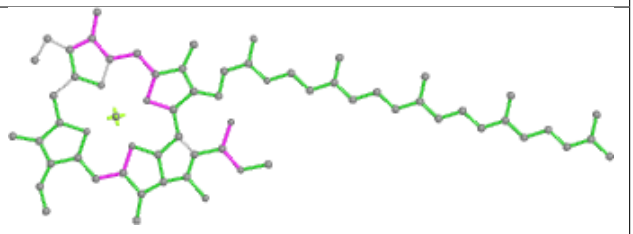


Rings

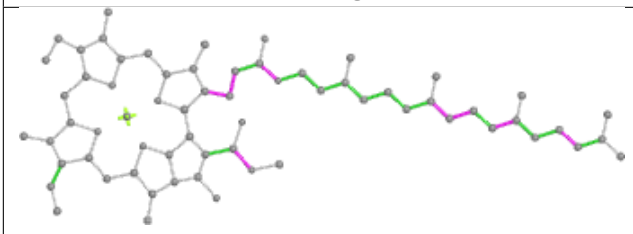
Ligand CLA B 516



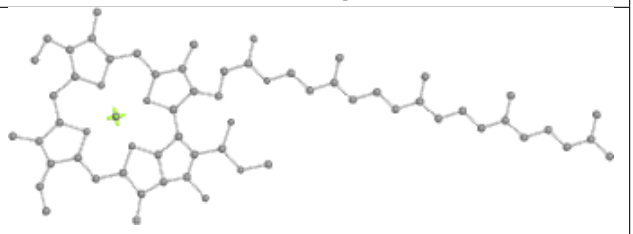
Bond lengths



Bond angles

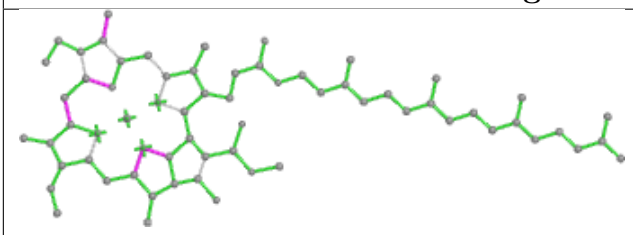


Torsions

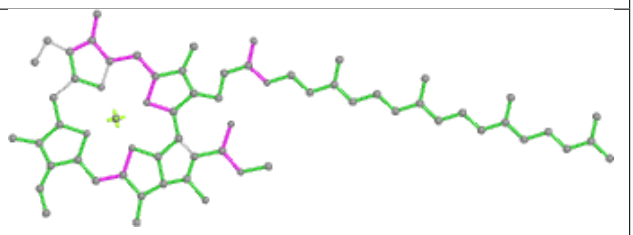


Rings

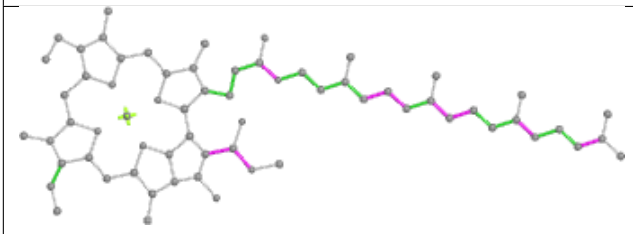
Ligand CLA D 405



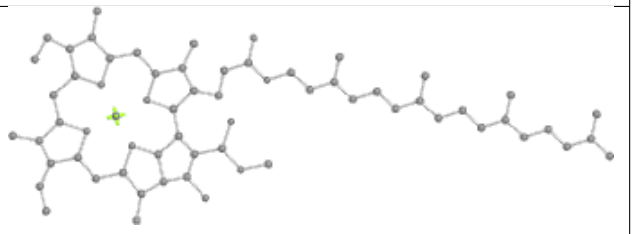
Bond lengths



Bond angles

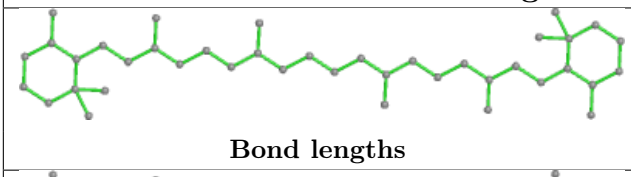


Torsions

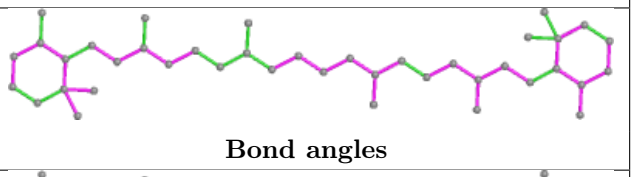


Rings

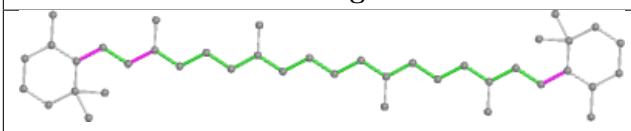
Ligand BCR H 101



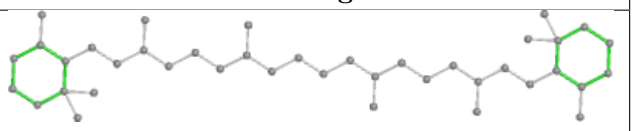
Bond lengths



Bond angles

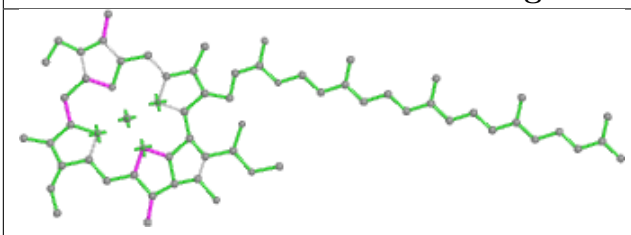


Torsions

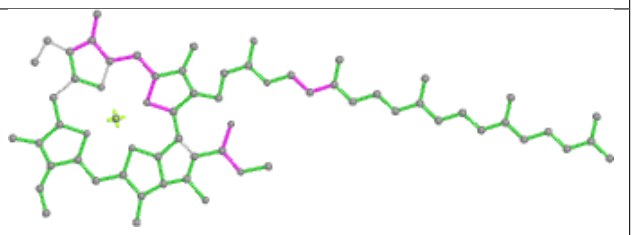


Rings

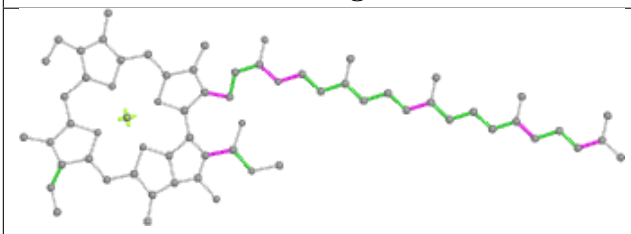
Ligand CLA C 507



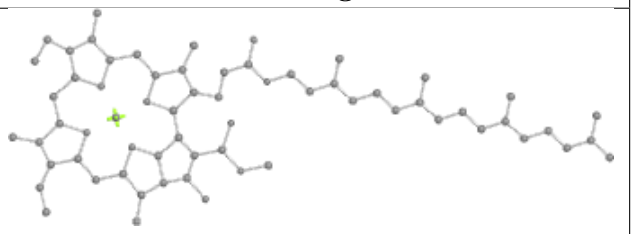
Bond lengths



Bond angles

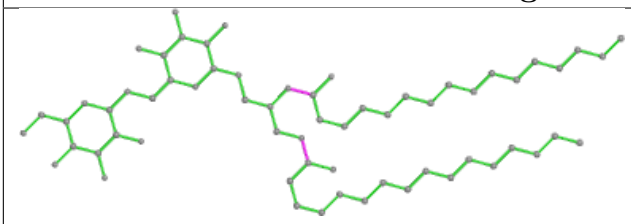


Torsions

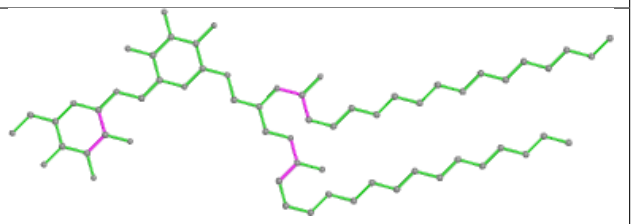


Rings

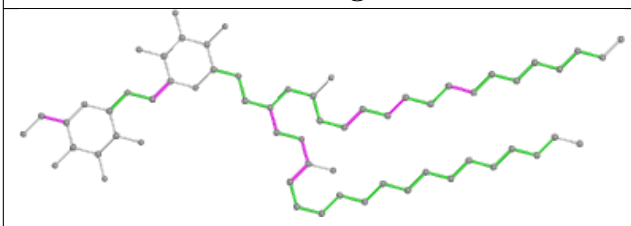
Ligand DGD C 518



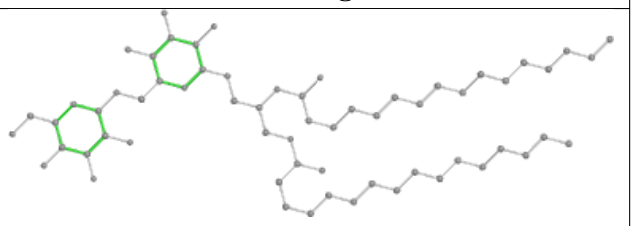
Bond lengths



Bond angles

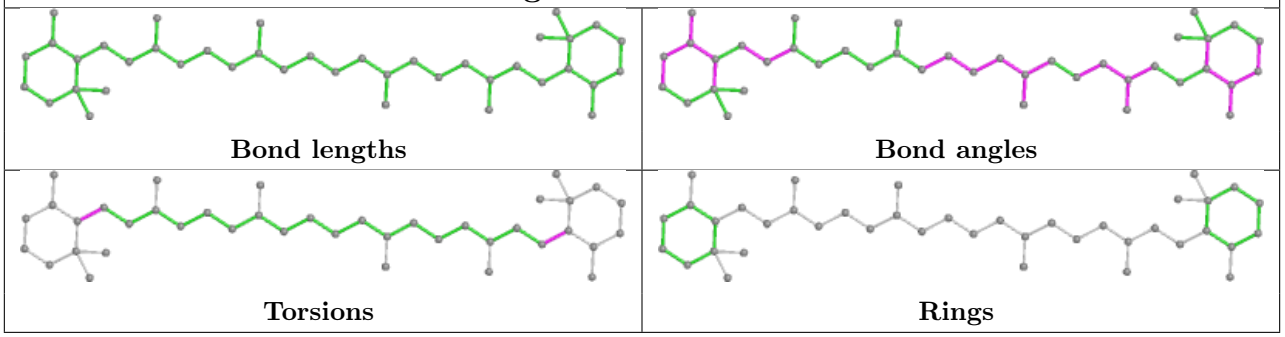


Torsions

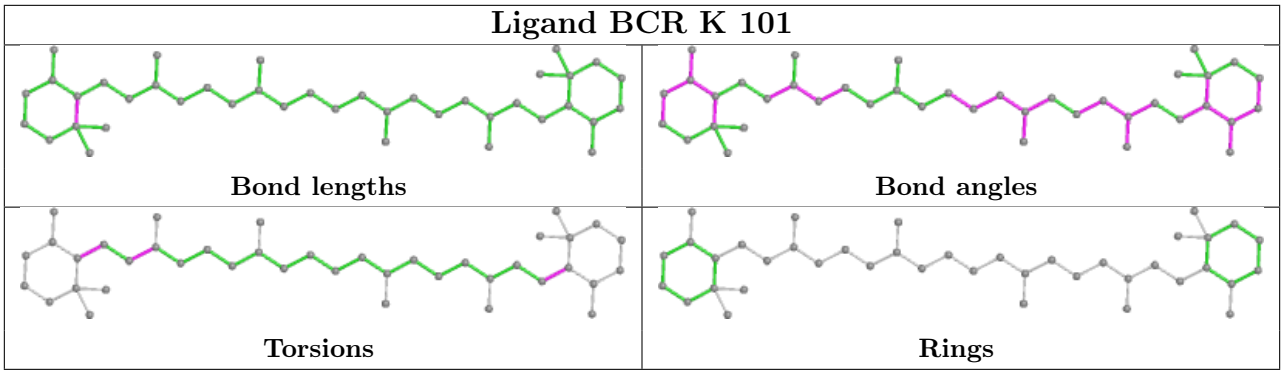


Rings

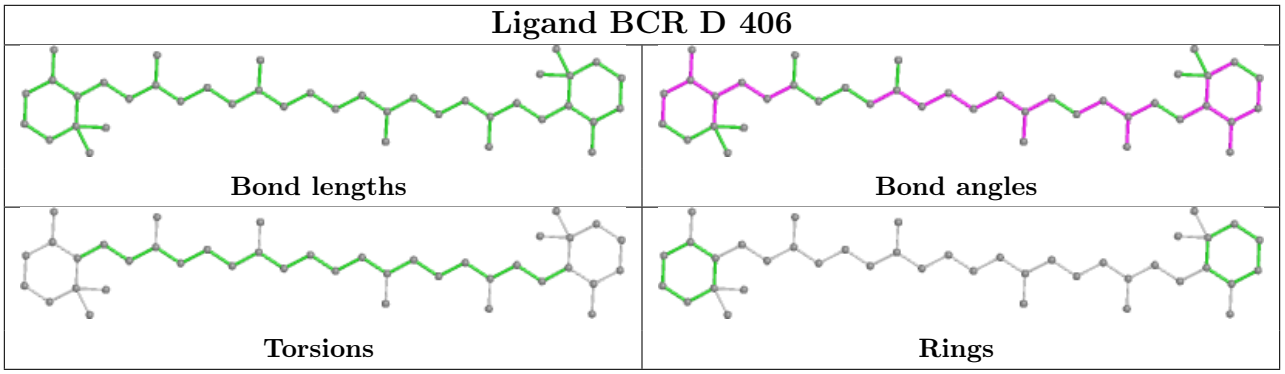
Ligand BCR B 519



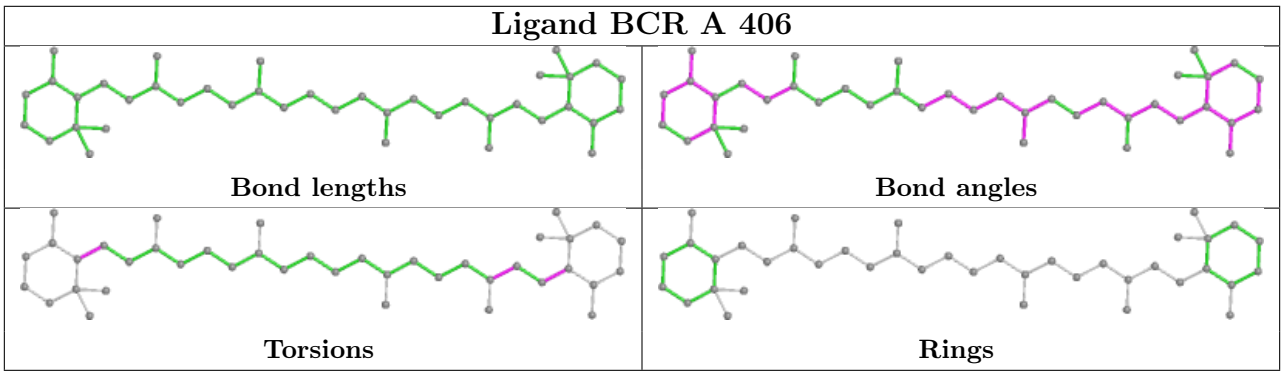
Ligand BCR K 101



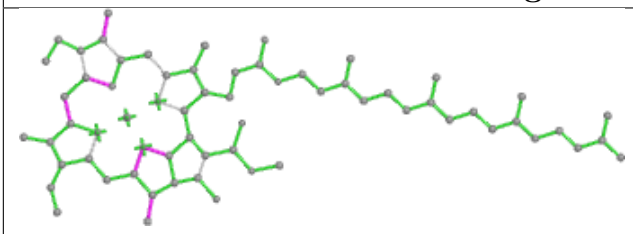
Ligand BCR D 406



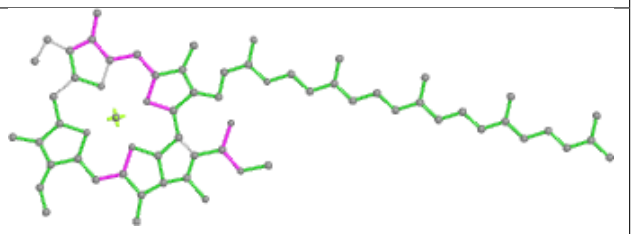
Ligand BCR A 406



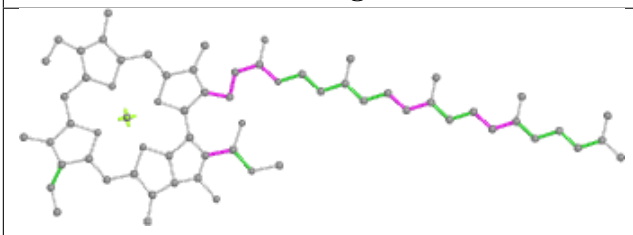
Ligand CLA C 509



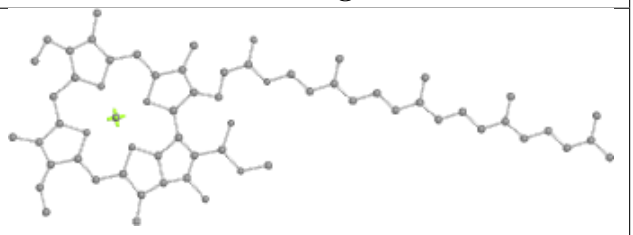
Bond lengths



Bond angles

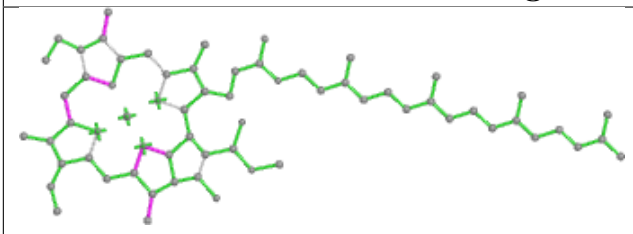


Torsions

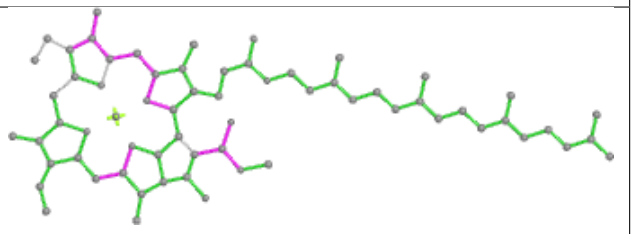


Rings

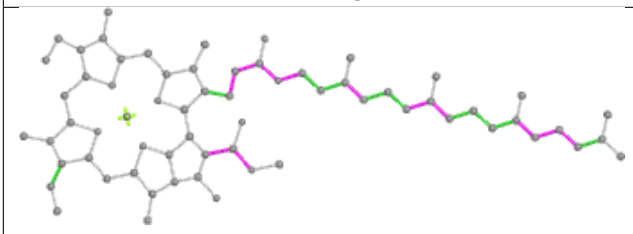
Ligand CLA B 513



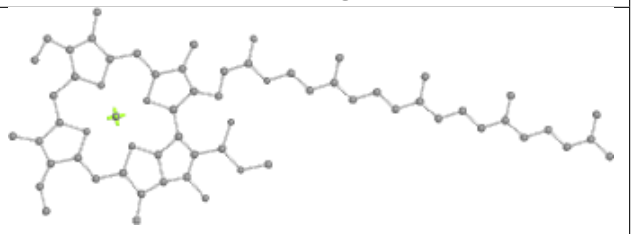
Bond lengths



Bond angles

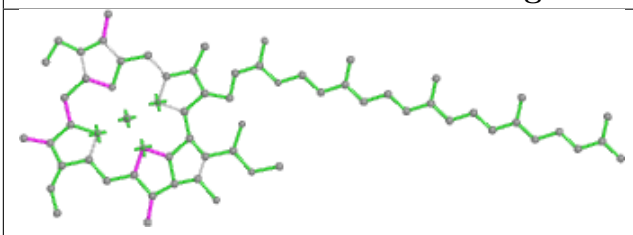


Torsions

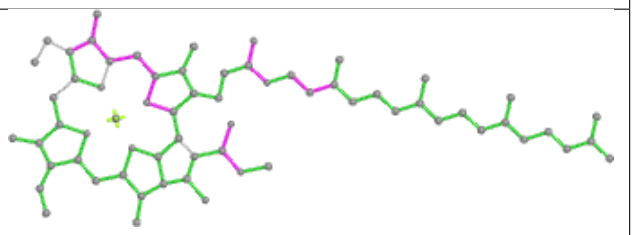


Rings

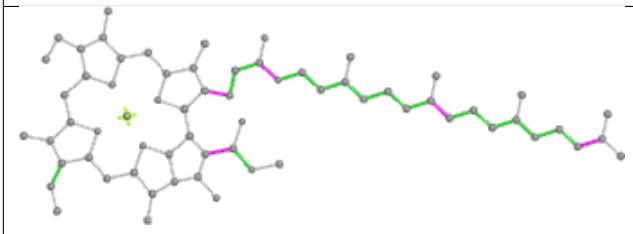
Ligand CLA C 508



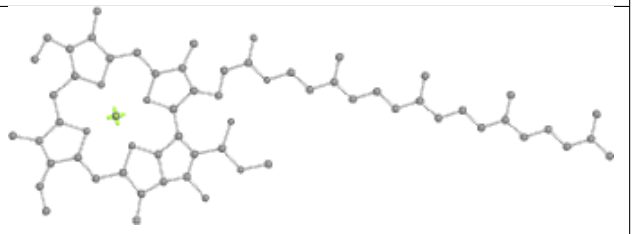
Bond lengths



Bond angles

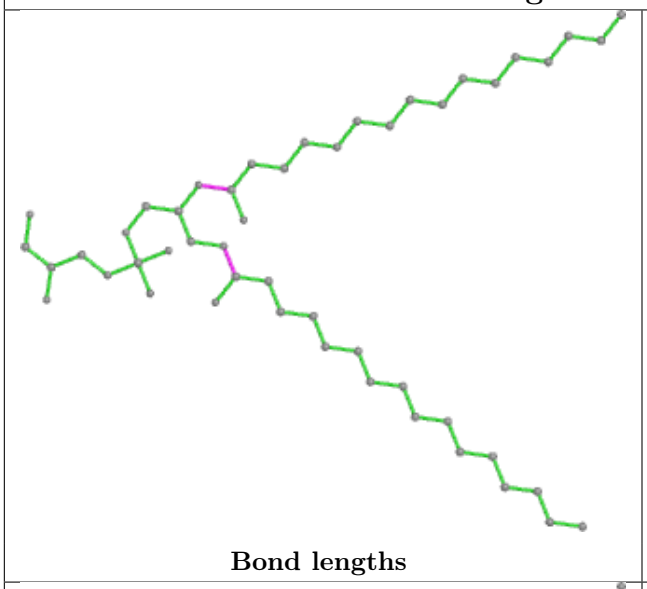


Torsions

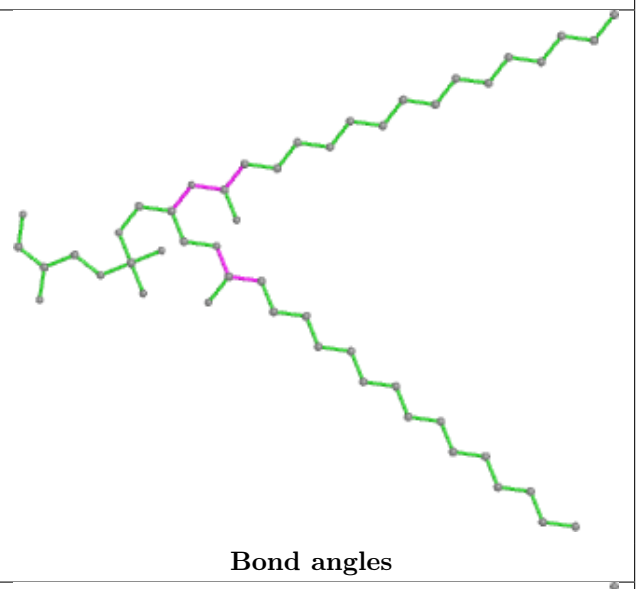


Rings

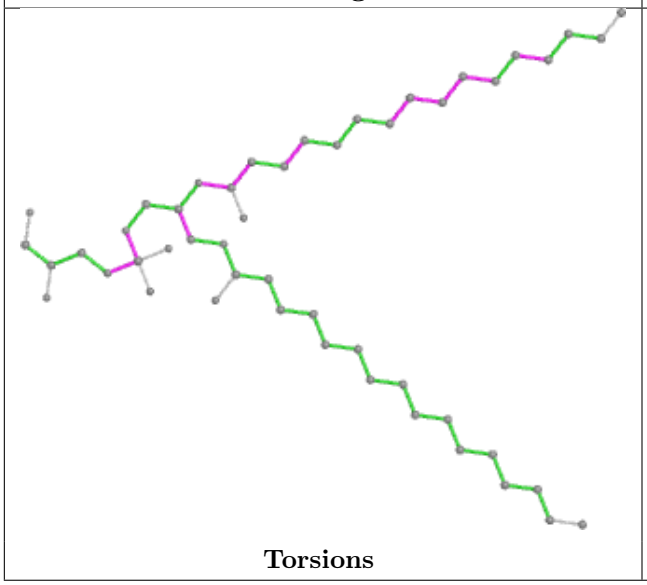
Ligand LHG L 101



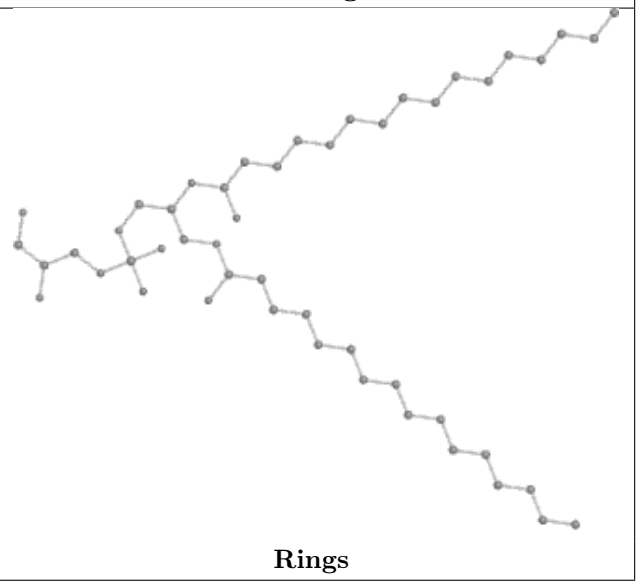
Bond lengths



Bond angles

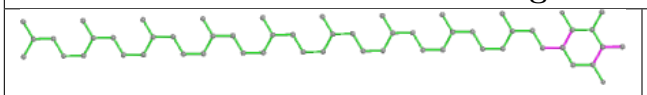


Torsions

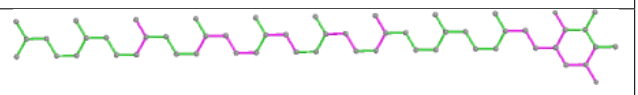


Rings

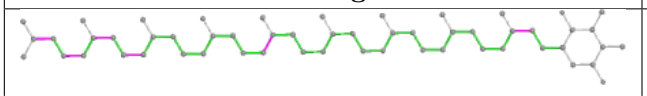
Ligand PL9 D 407



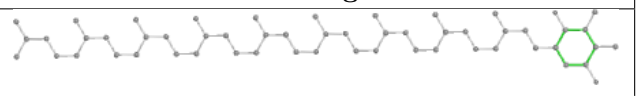
Bond lengths



Bond angles

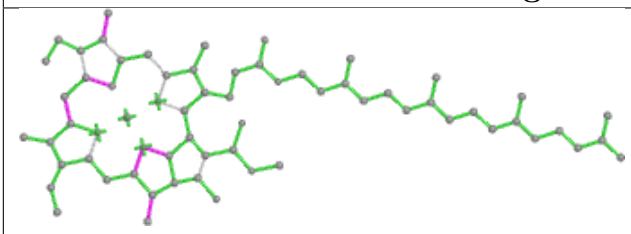


Torsions

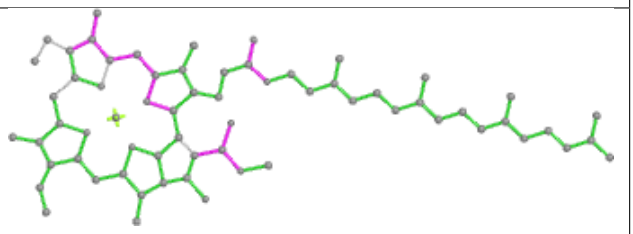


Rings

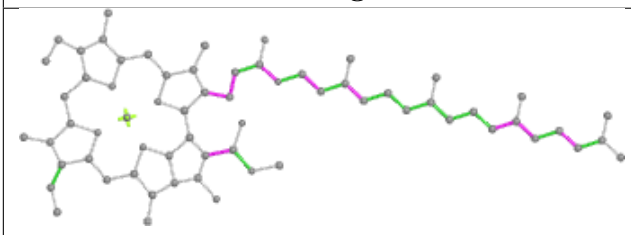
Ligand CLA D 401



Bond lengths



Bond angles



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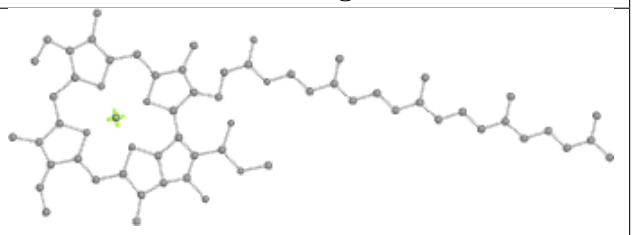
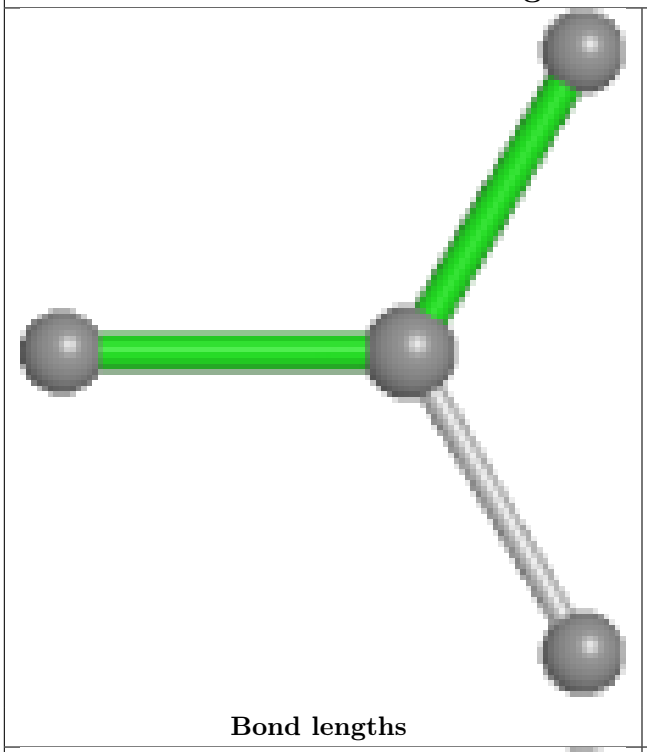
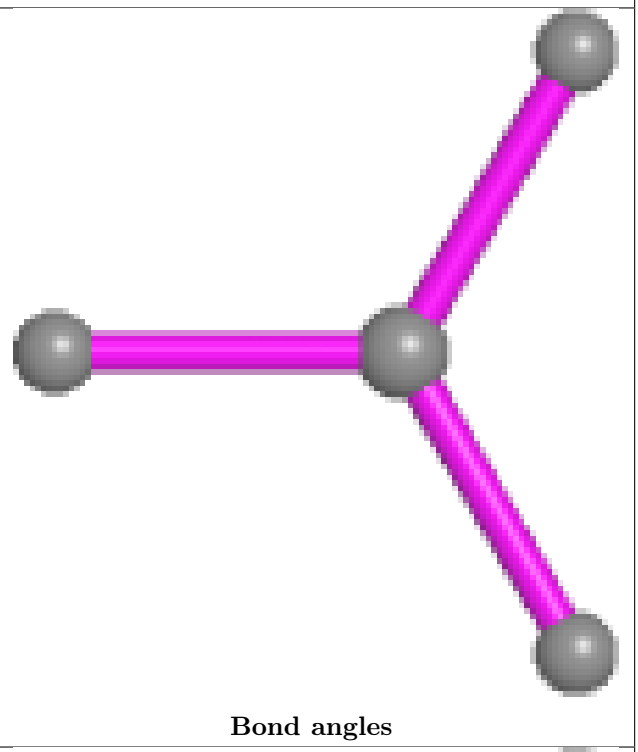


Rings

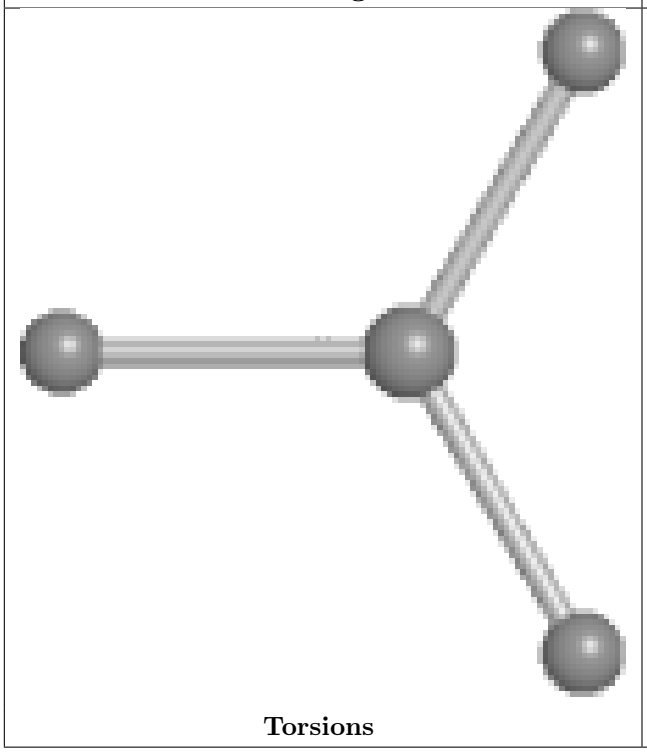
Ligand BCT D 403



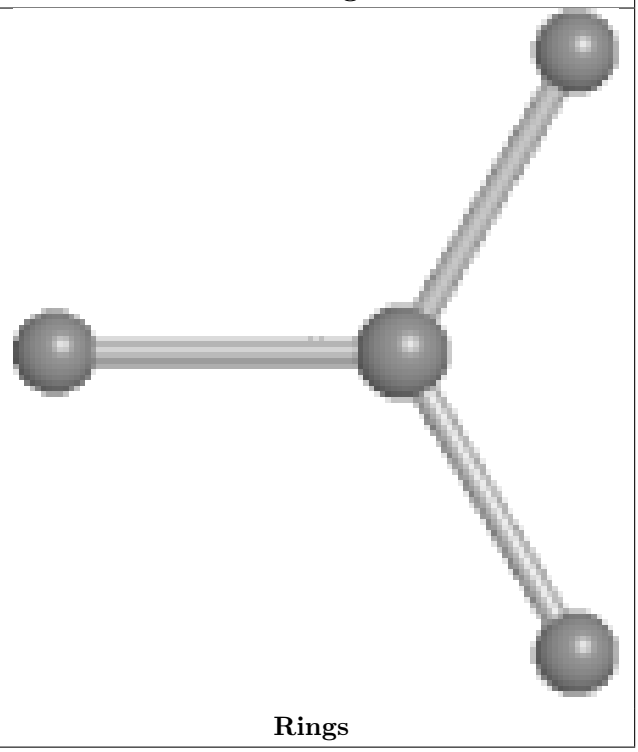
Bond lengths



Bond angles

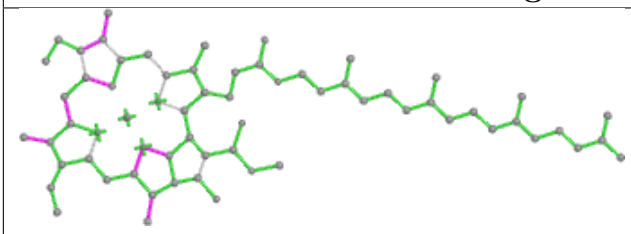


Torsions

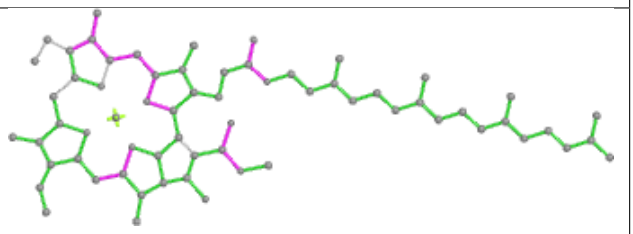


Rings

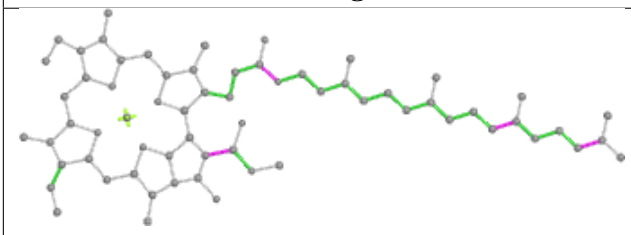
Ligand CLA C 504



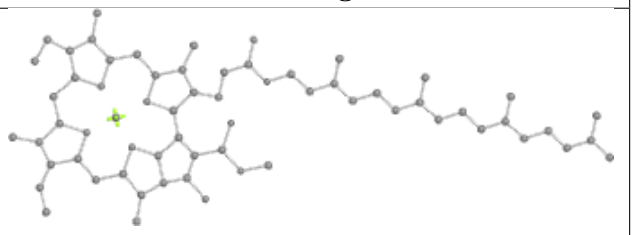
Bond lengths



Bond angles

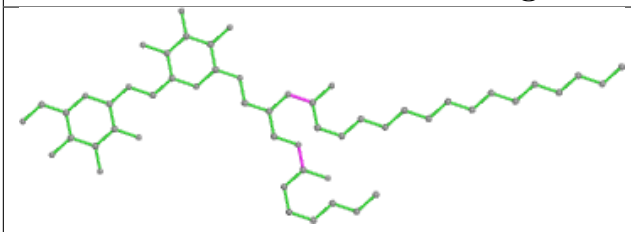


Torsions

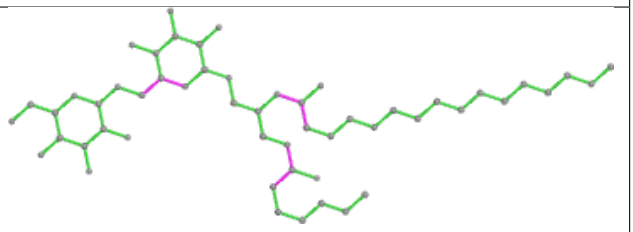


Rings

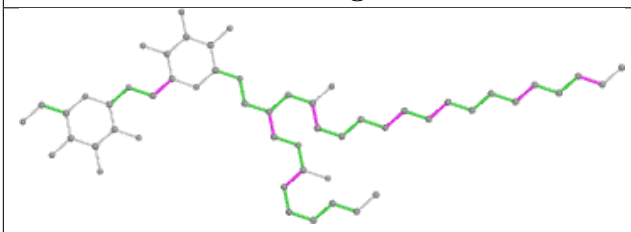
Ligand DGD C 517



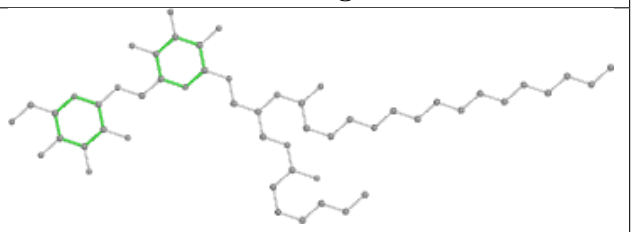
Bond lengths



Bond angles

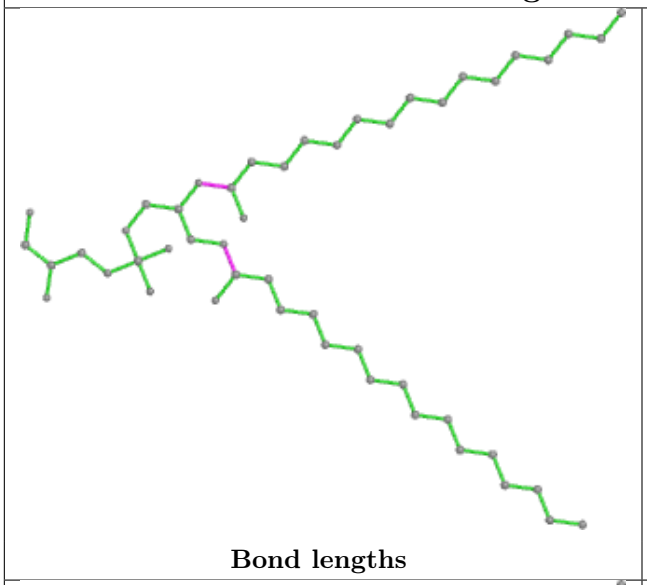


Torsions

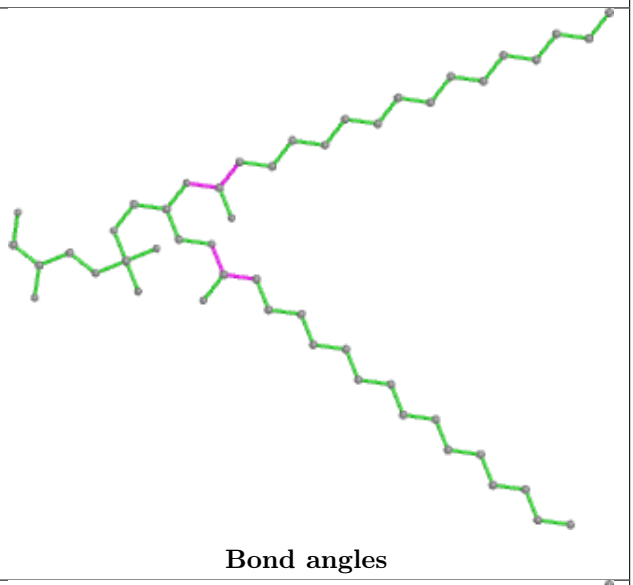


Rings

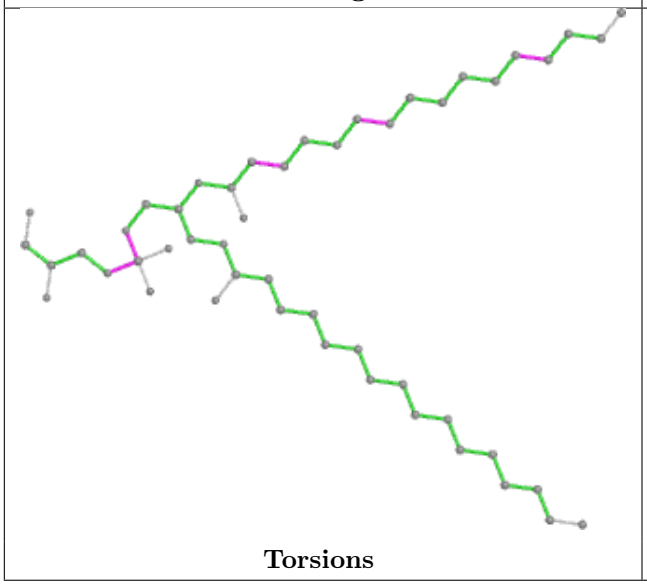
Ligand LHG D 408



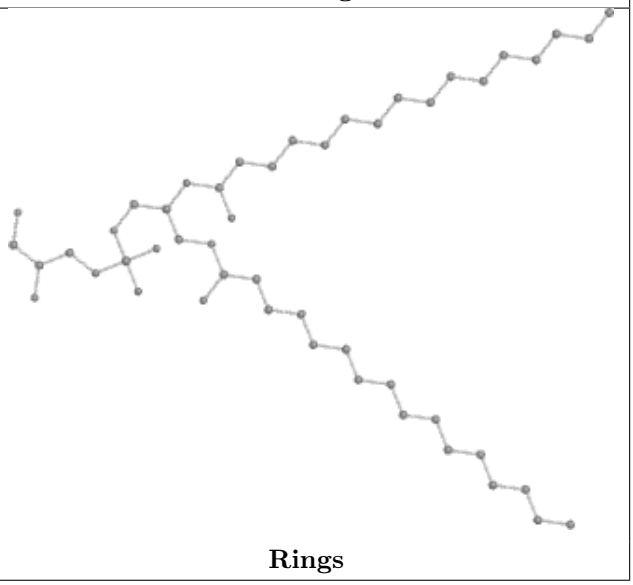
Bond lengths



Bond angles

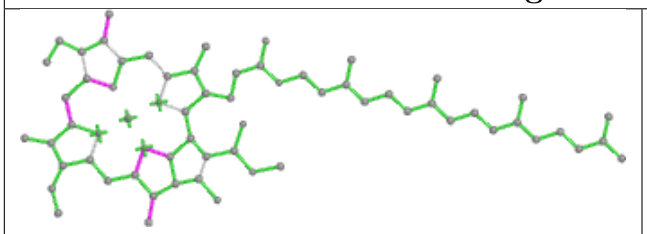


Torsions

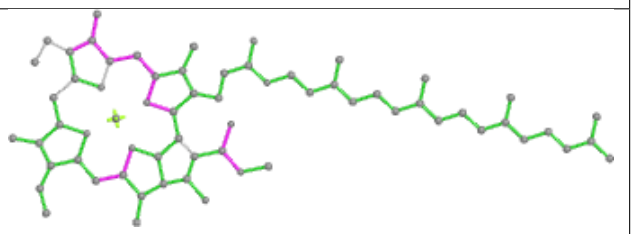


Rings

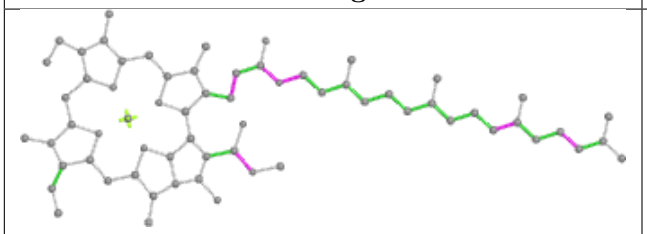
Ligand CLA C 505



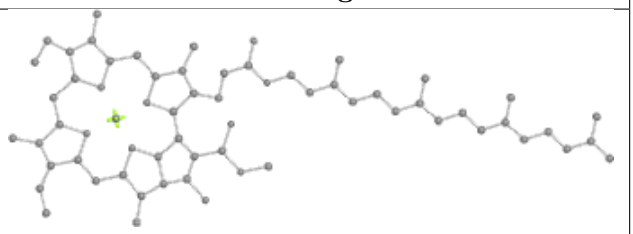
Bond lengths



Bond angles

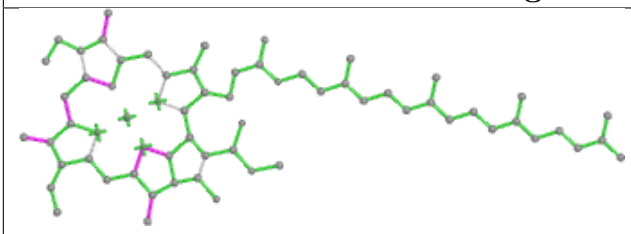


Torsions

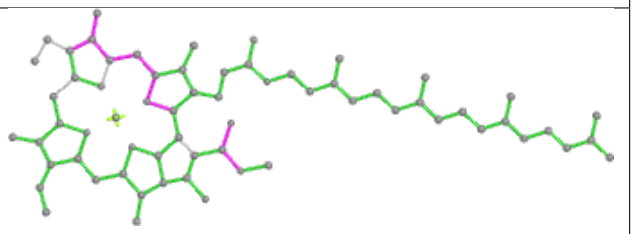


Rings

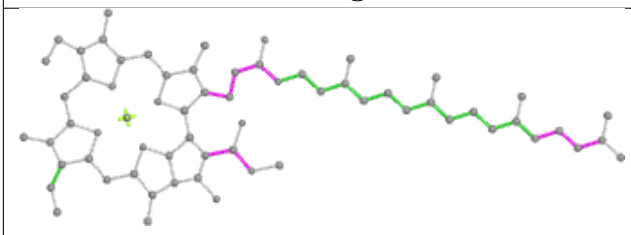
Ligand CLA B 504



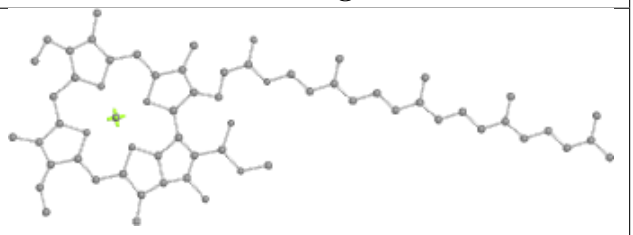
Bond lengths



Bond angles

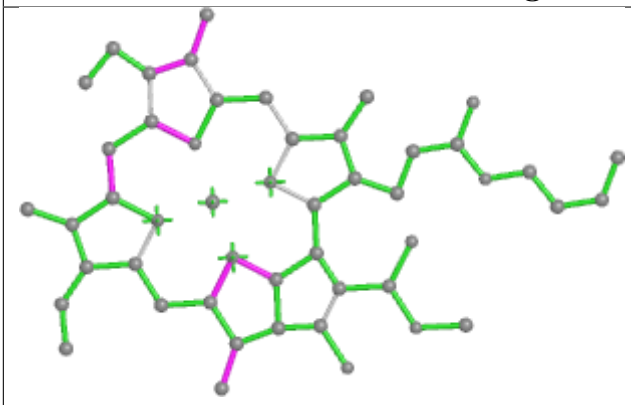


Torsions

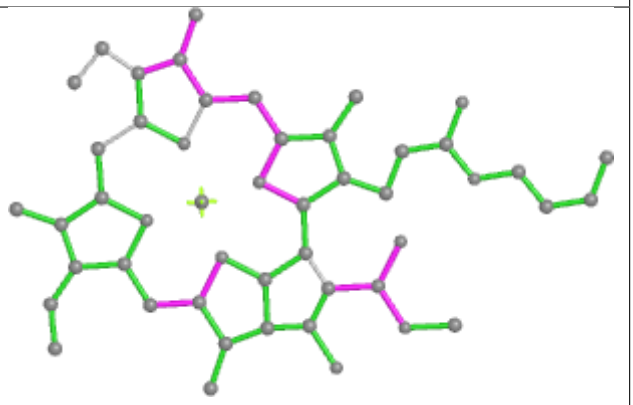


Rings

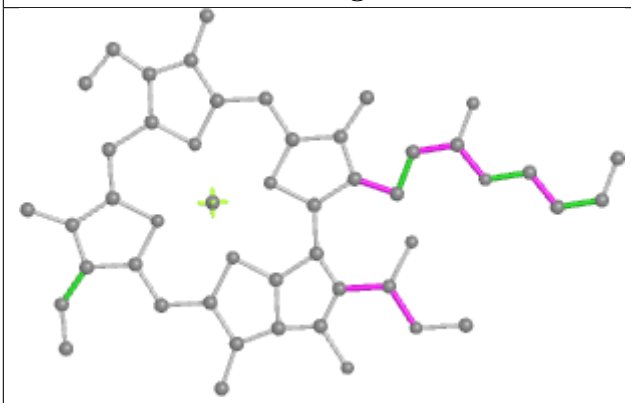
Ligand CLA A 403



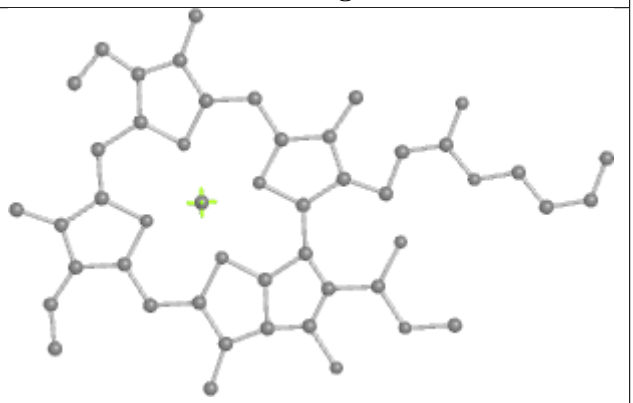
Bond lengths



Bond angles

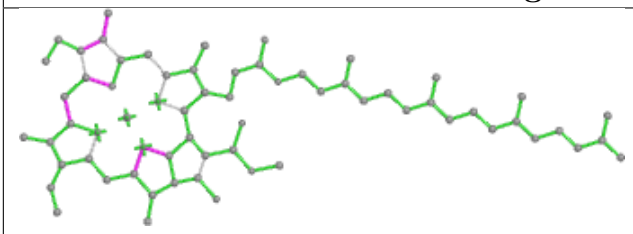


Torsions

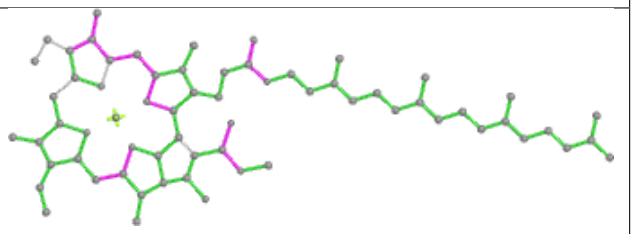


Rings

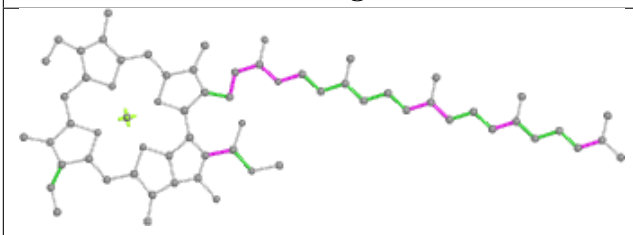
Ligand CLA C 510



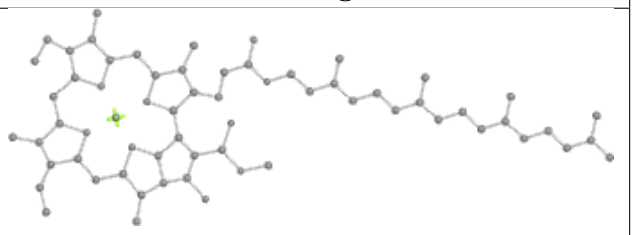
Bond lengths



Bond angles

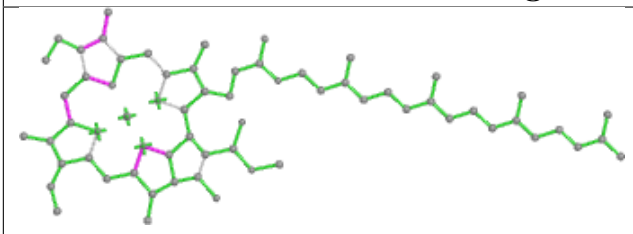


Torsions

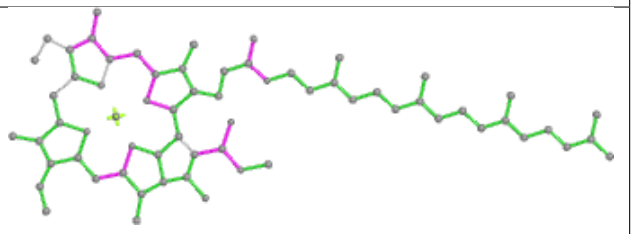


Rings

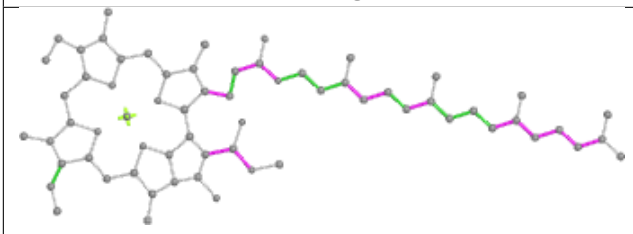
Ligand CLA C 511



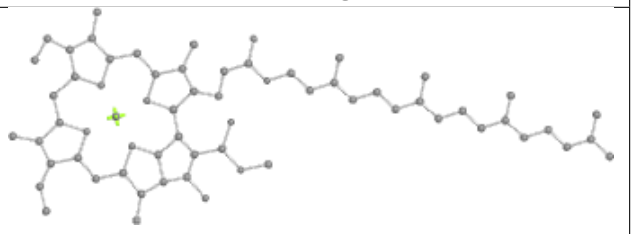
Bond lengths



Bond angles

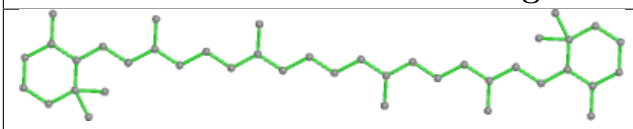


Torsions

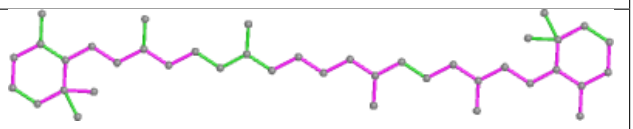


Rings

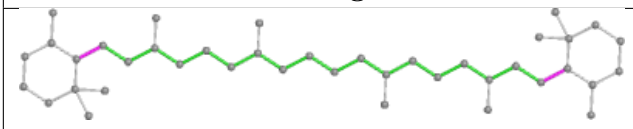
Ligand BCR C 516



Bond lengths



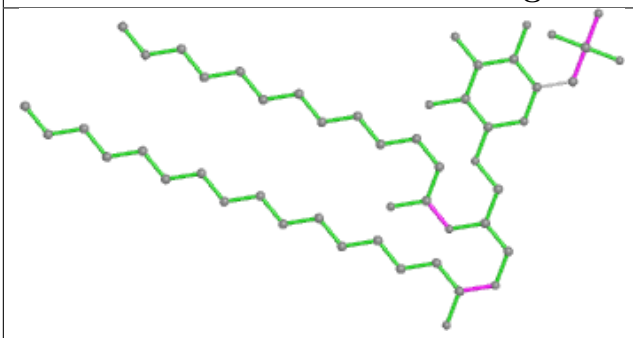
Bond angles



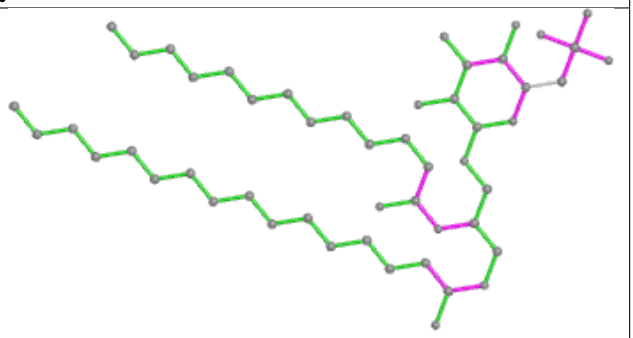
Torsions

Rings

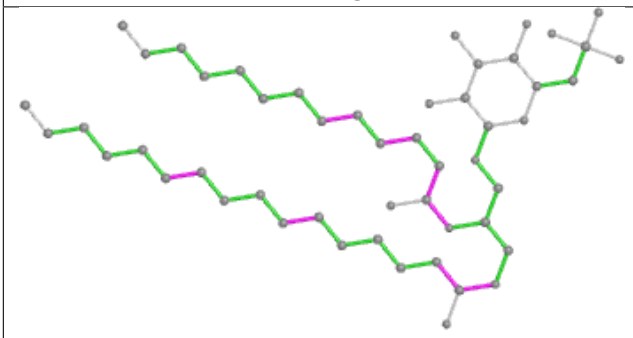
Ligand SQD A 407



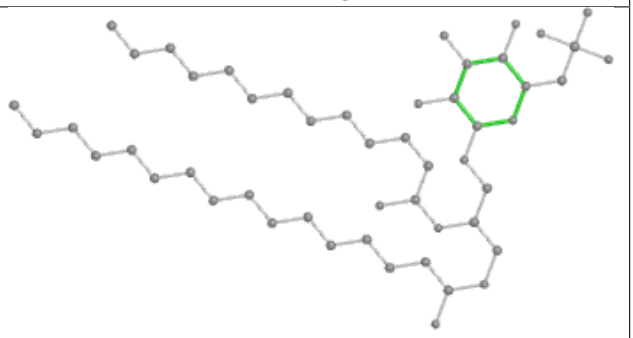
Bond lengths



Bond angles

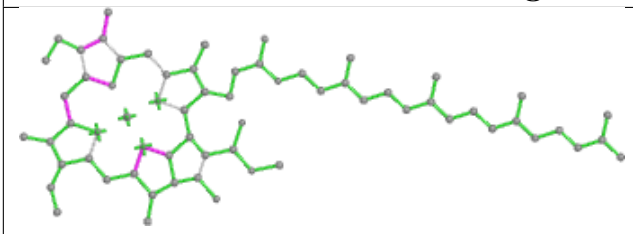


Torsions

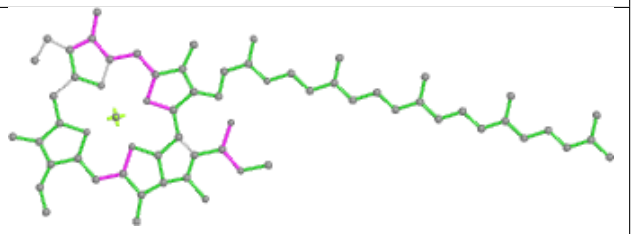


Rings

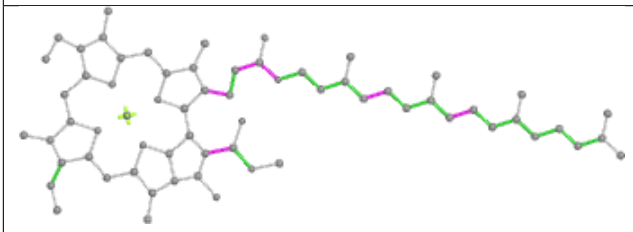
Ligand CLA B 506



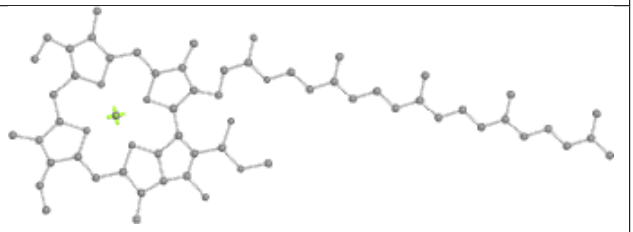
Bond lengths



Bond angles

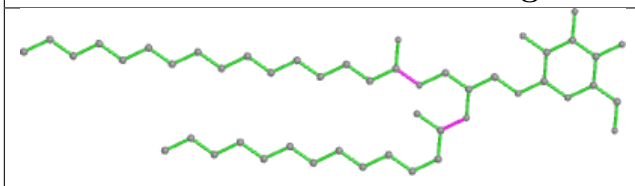


Torsions

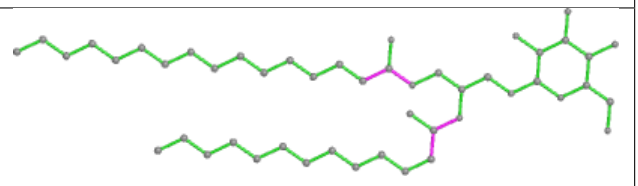


Rings

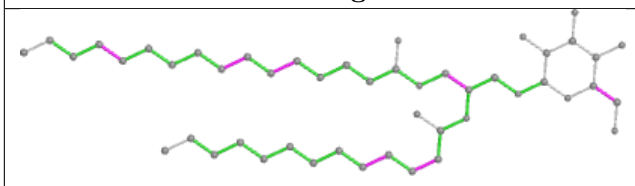
Ligand LMG B 522



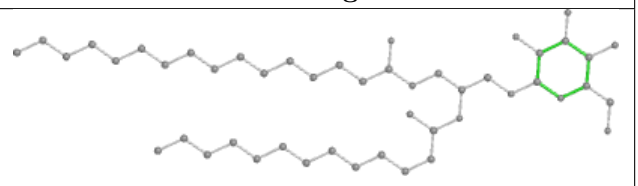
Bond lengths



Bond angles

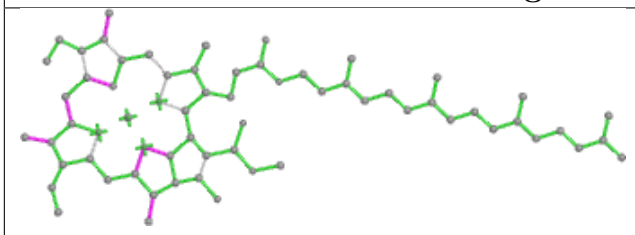


Torsions

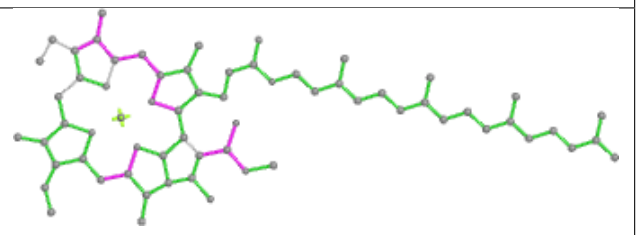


Rings

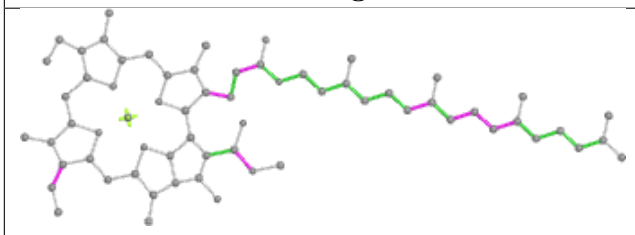
Ligand CLA D 404



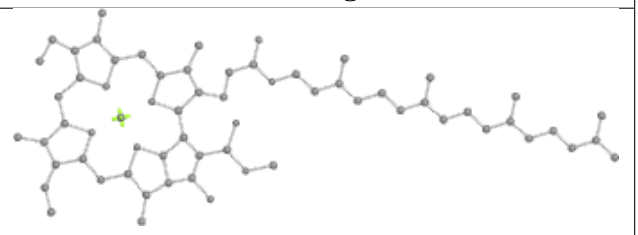
Bond lengths



Bond angles

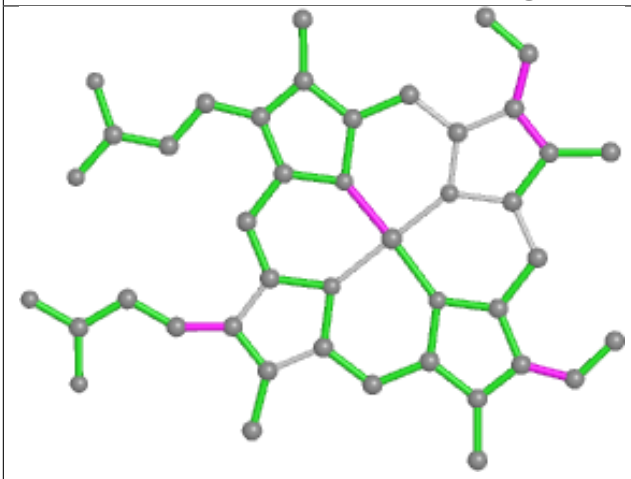


Torsions

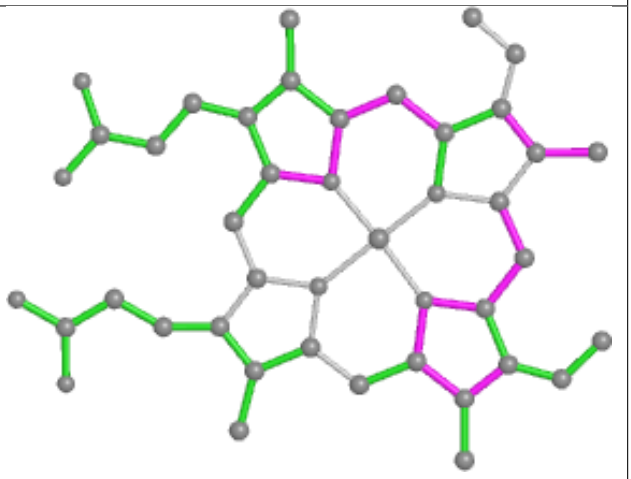


Rings

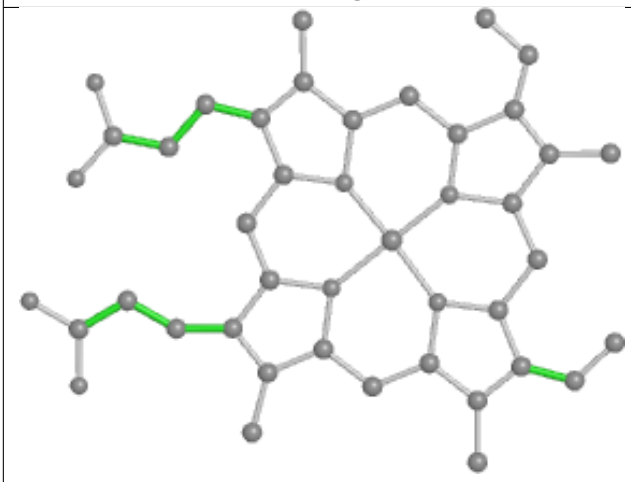
Ligand HEM F 101



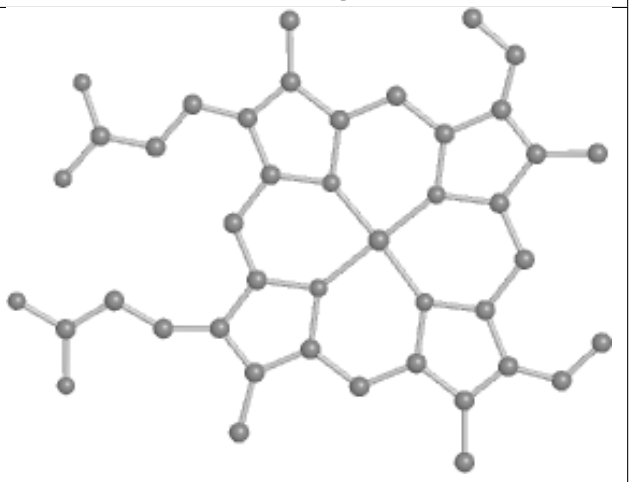
Bond lengths



Bond angles

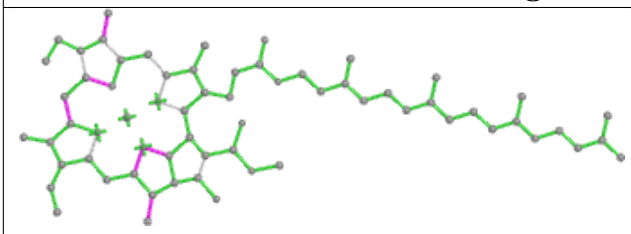


Torsions

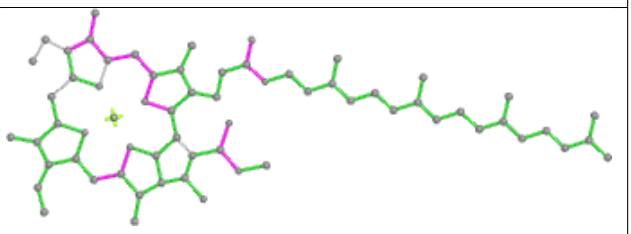


Rings

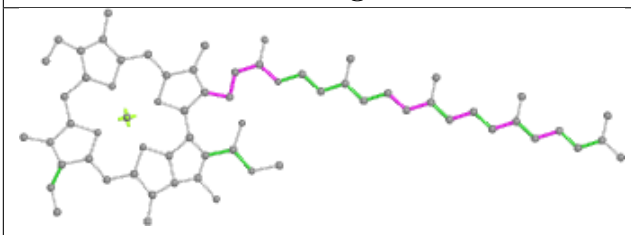
Ligand CLA B 512



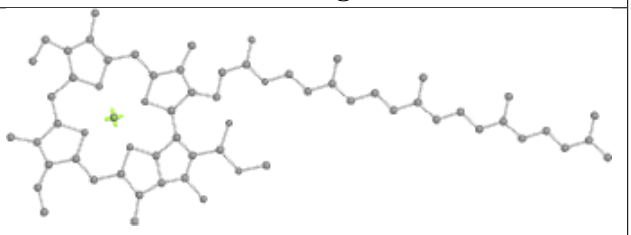
Bond lengths



Bond angles

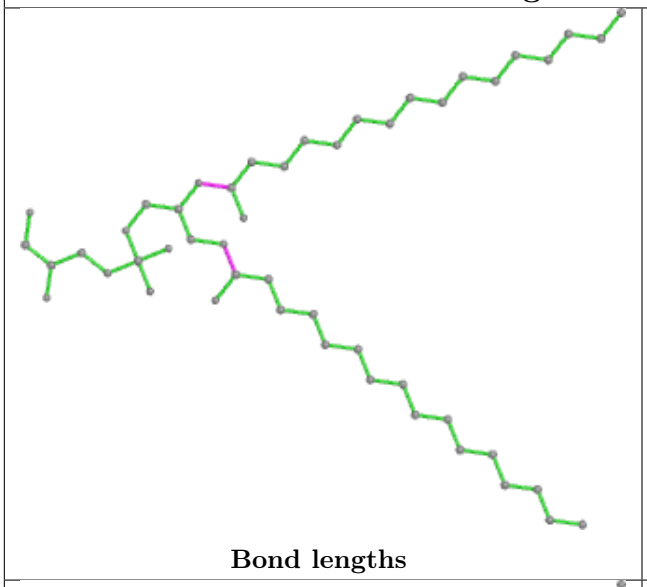


Torsions

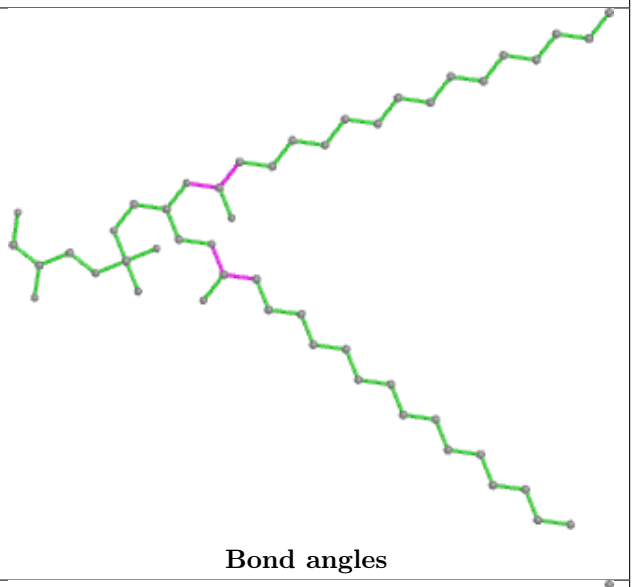


Rings

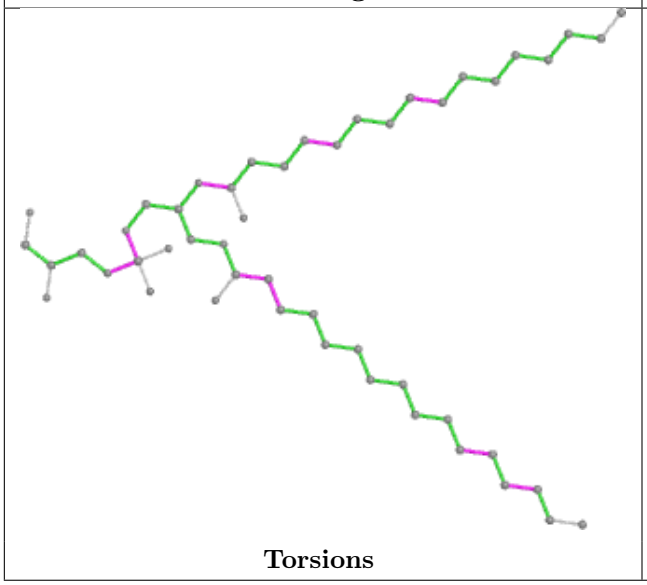
Ligand LHG D 410



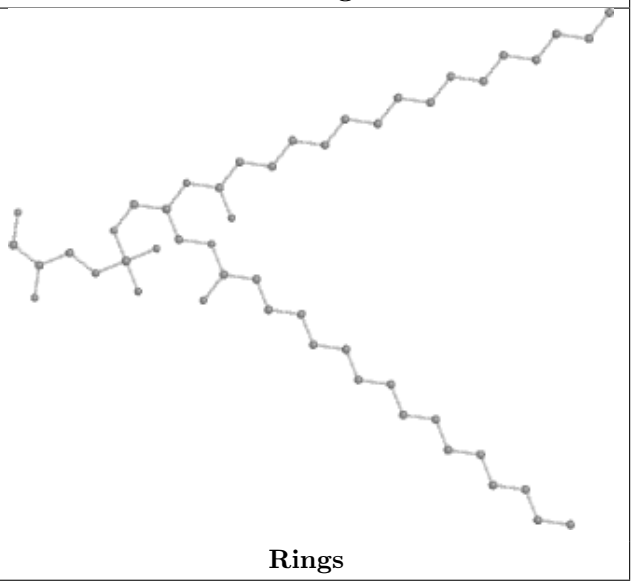
Bond lengths



Bond angles

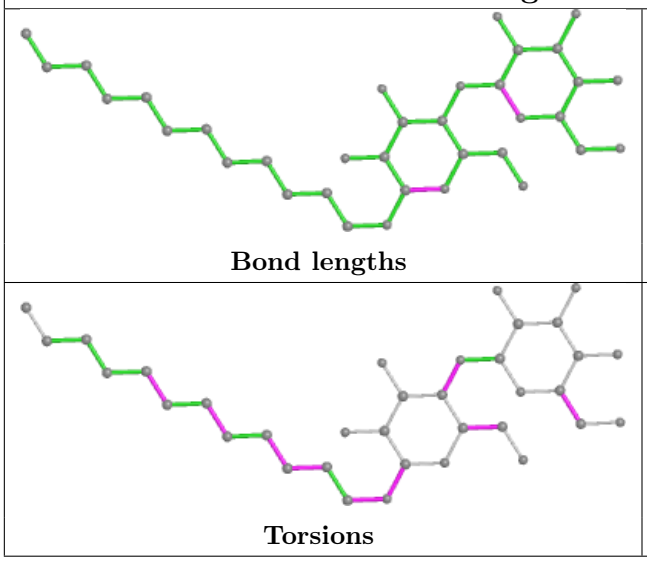


Torsions

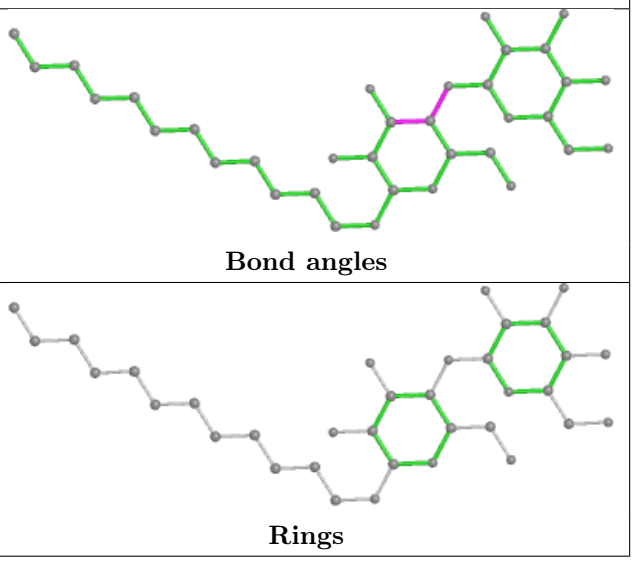


Rings

Ligand LMU C 520



Bond lengths

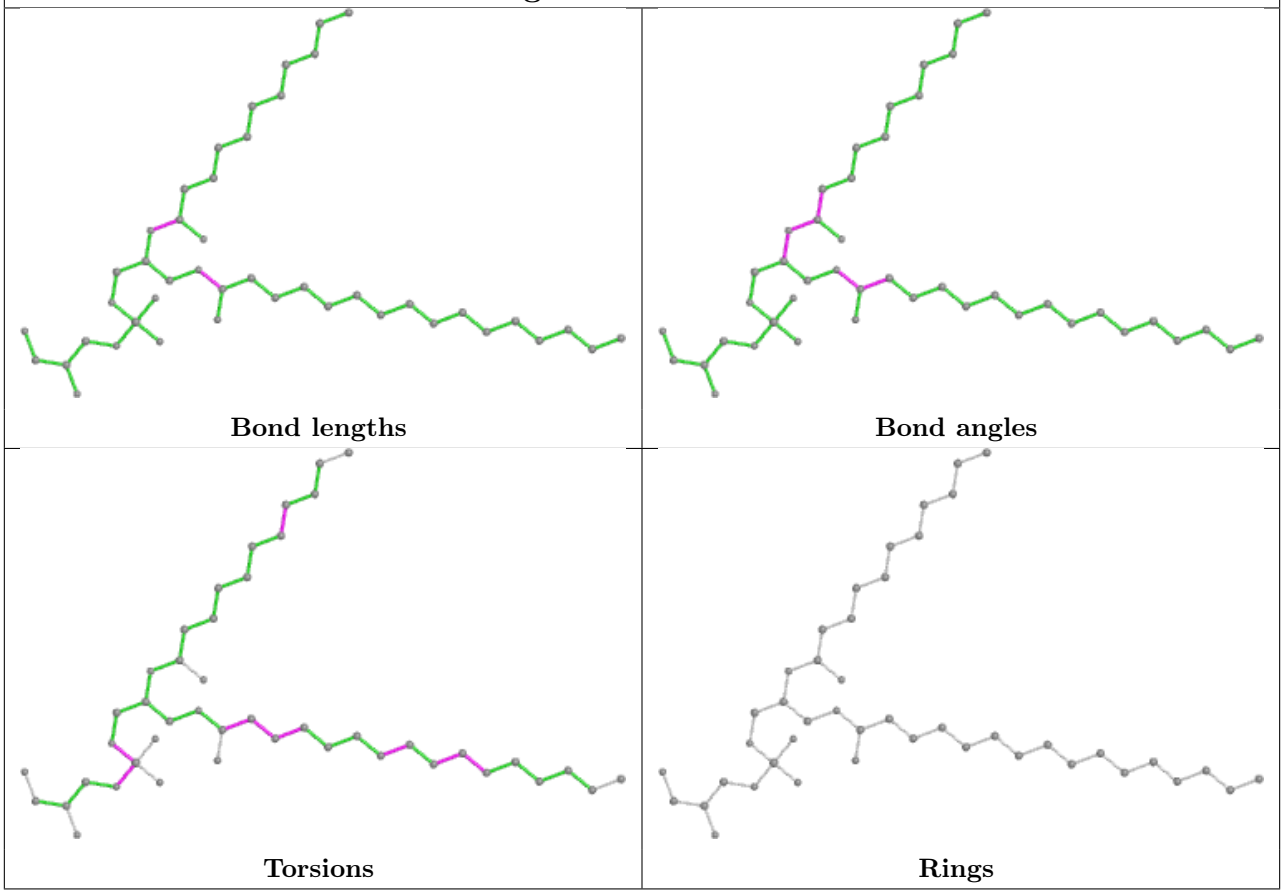


Bond angles

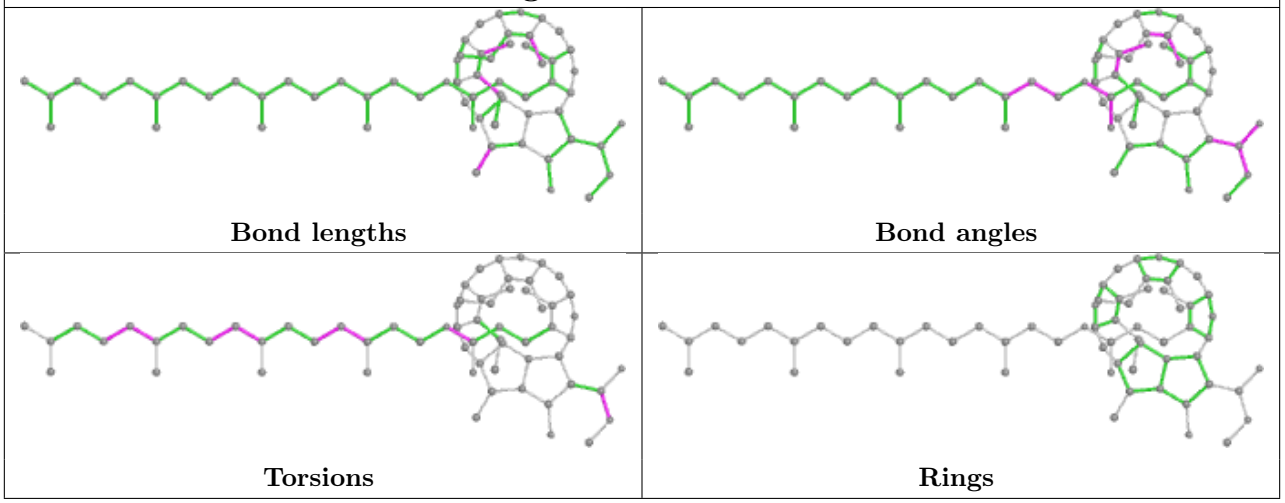
Torsions

Rings

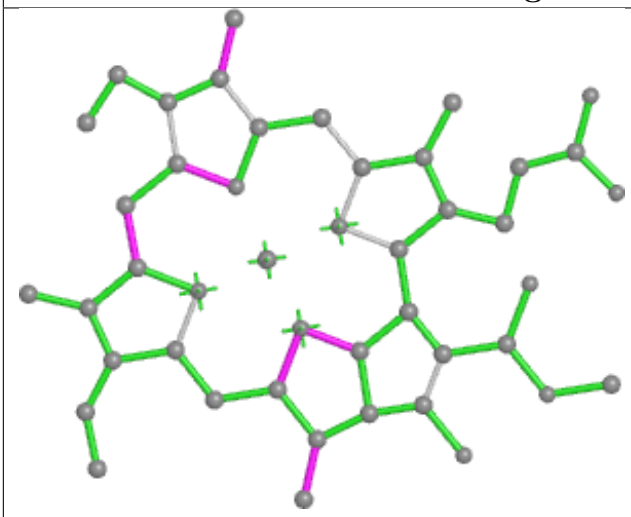
Ligand LHG B 521



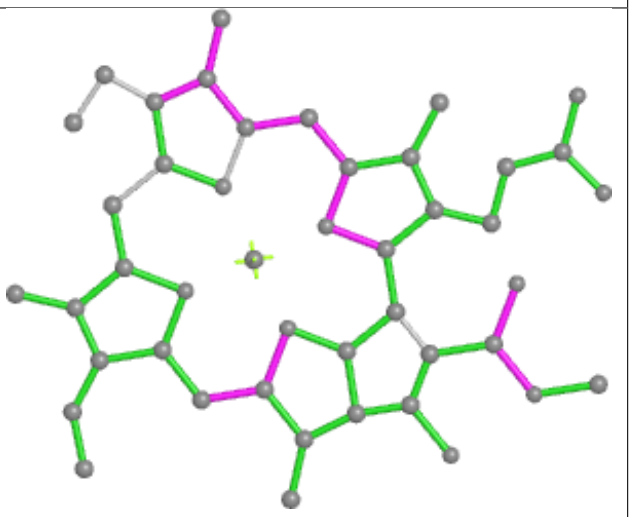
Ligand PHO A 404



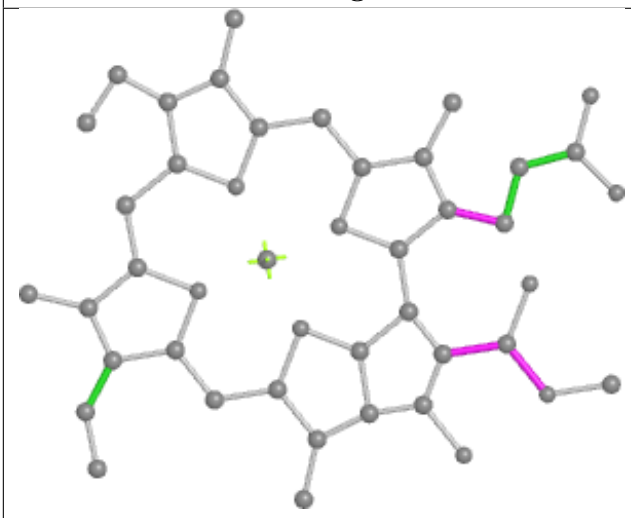
Ligand CLA B 514



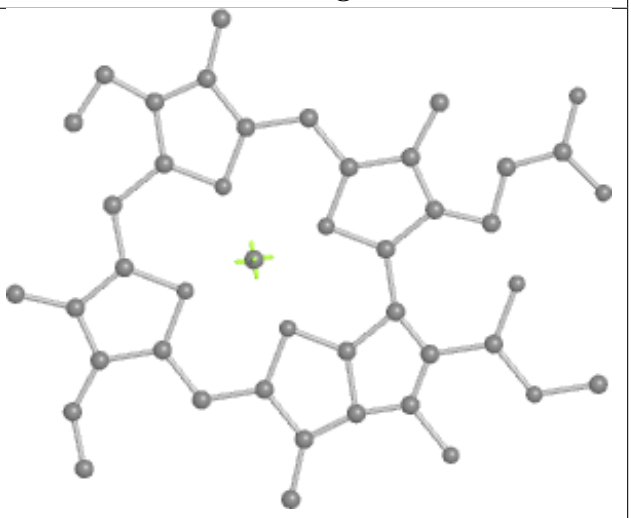
Bond lengths



Bond angles

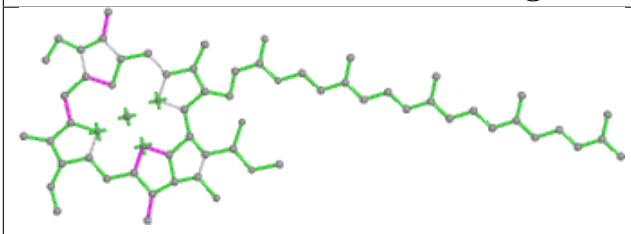


Torsions

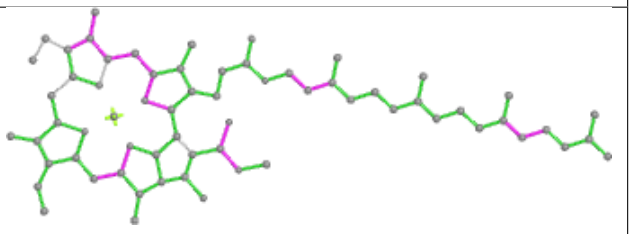


Rings

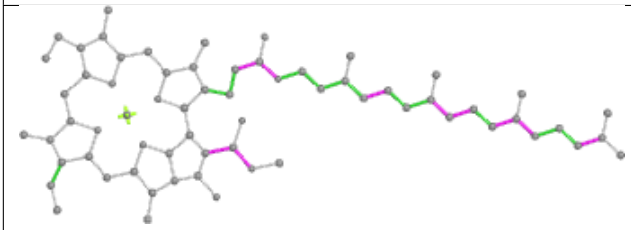
Ligand CLA C 503



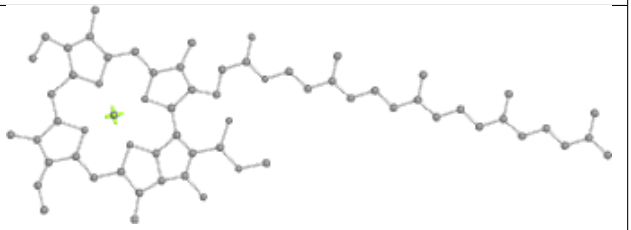
Bond lengths



Bond angles

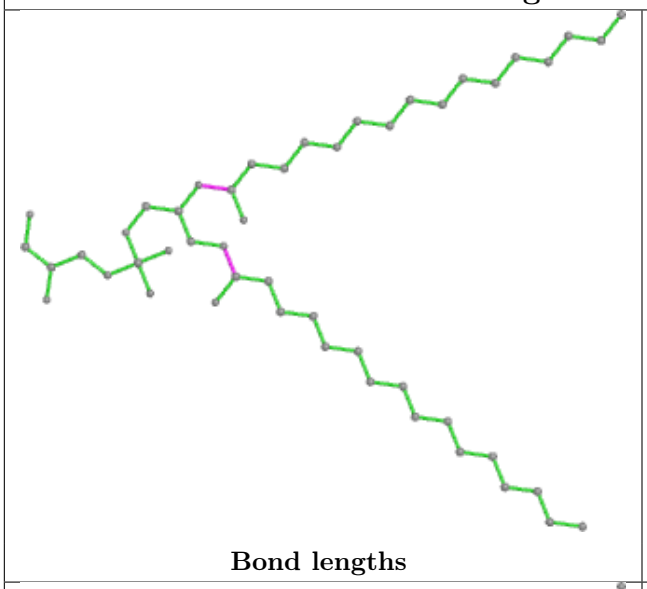


Torsions

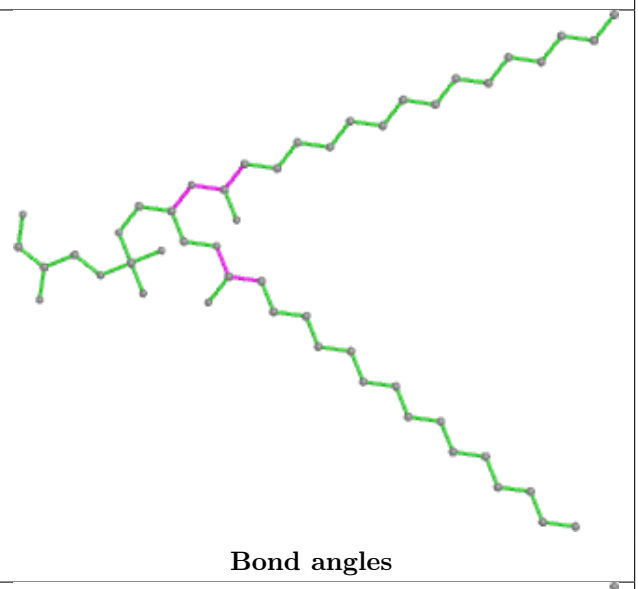


Rings

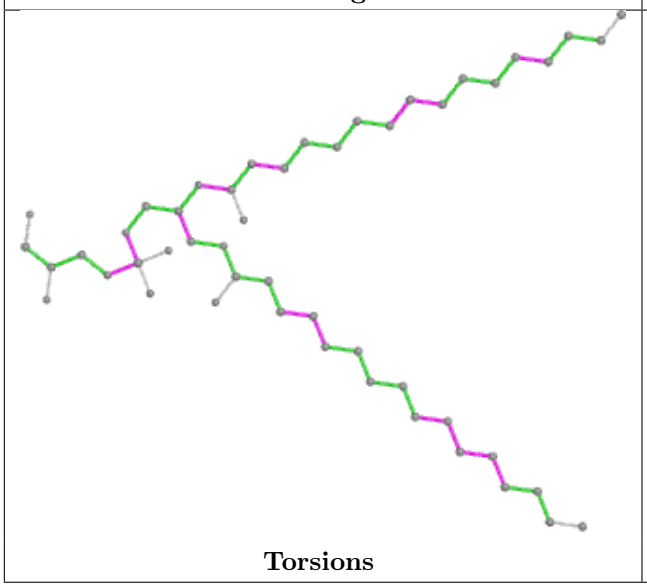
Ligand LHG D 411



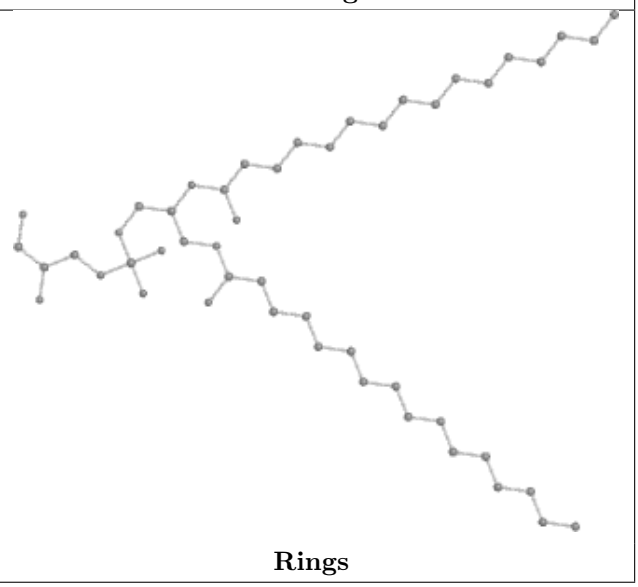
Bond lengths



Bond angles

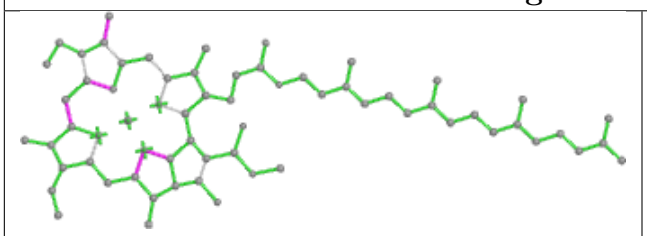


Torsions

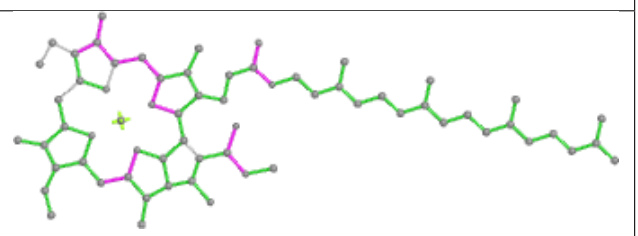


Rings

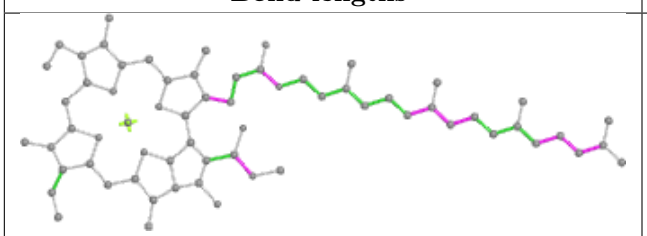
Ligand CLA C 513



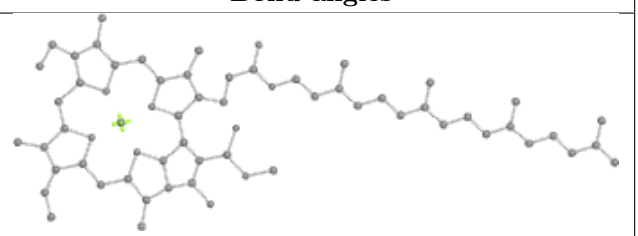
Bond lengths



Bond angles

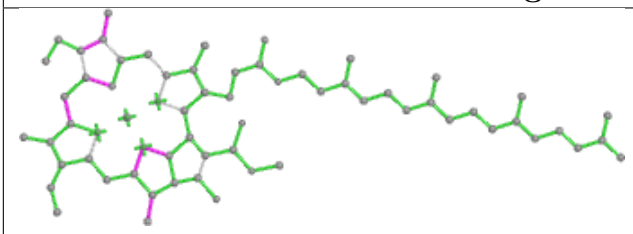


Torsions

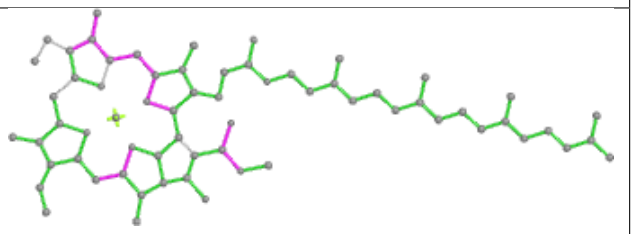


Rings

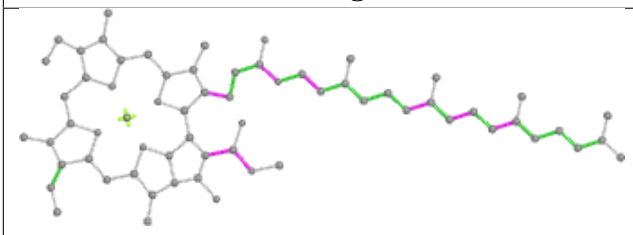
Ligand CLA B 501



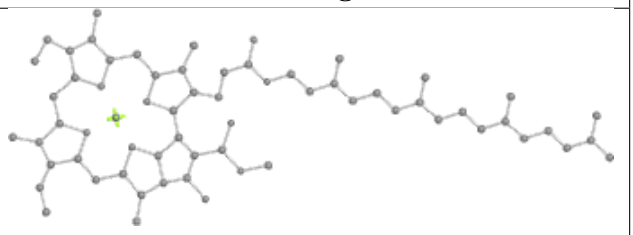
Bond lengths



Bond angles

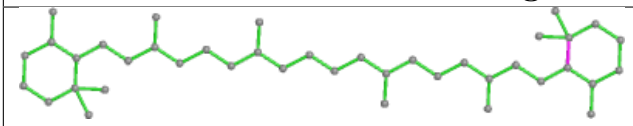


Torsions

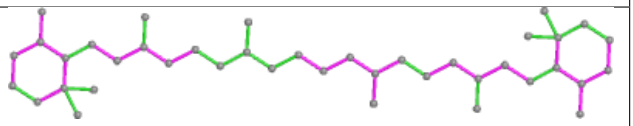


Rings

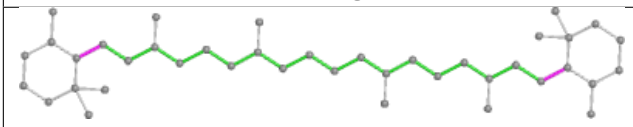
Ligand BCR C 515



Bond lengths



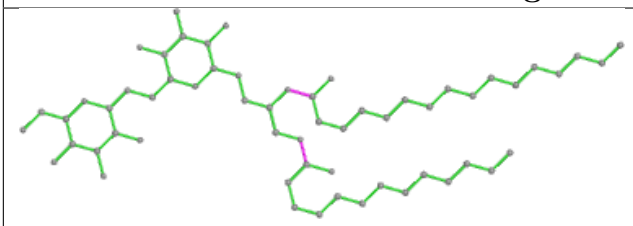
Bond angles



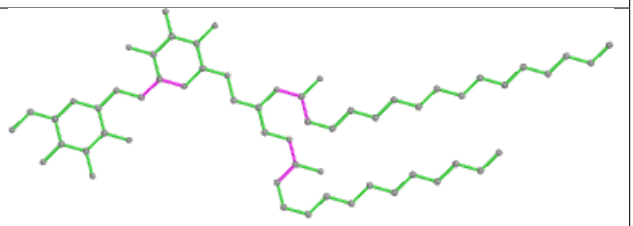
Torsions

Rings

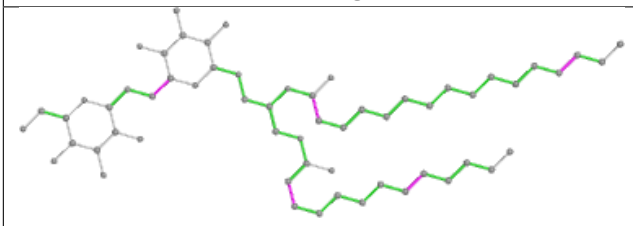
Ligand DGD J 101



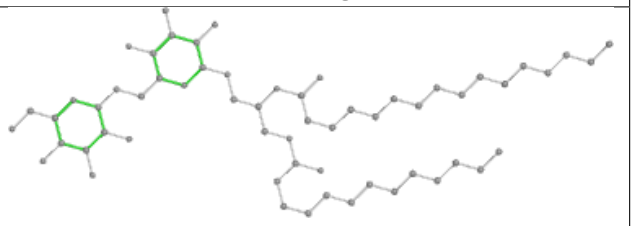
Bond lengths



Bond angles

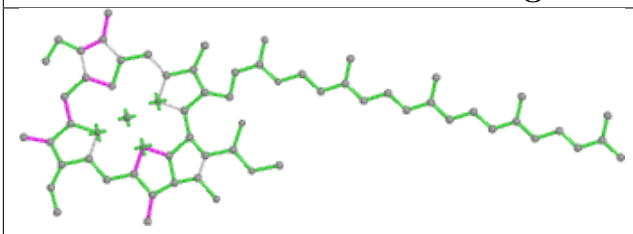


Torsions

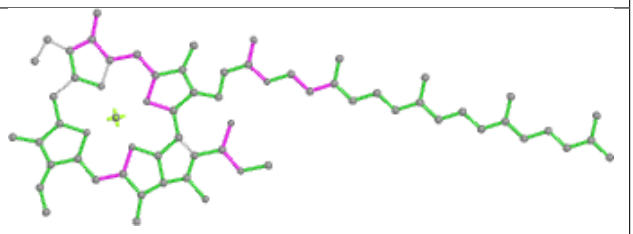


Rings

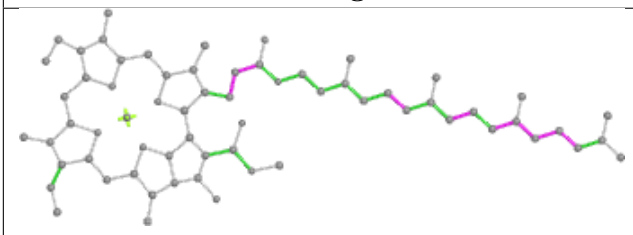
Ligand CLA B 511



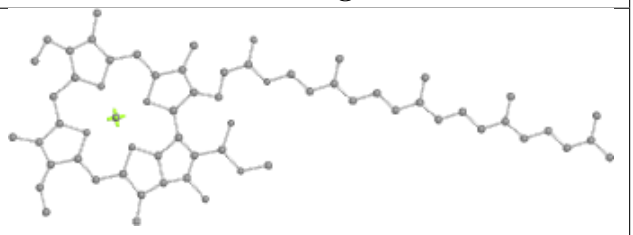
Bond lengths



Bond angles

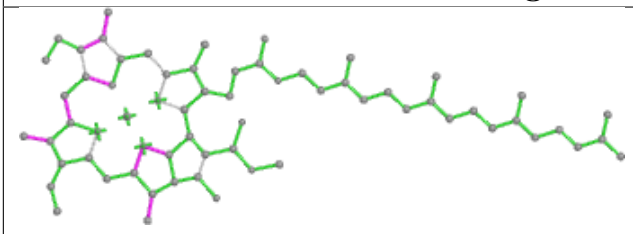


Torsions

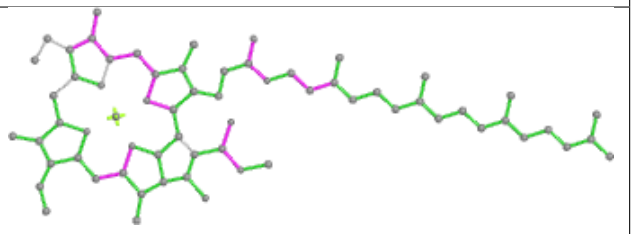


Rings

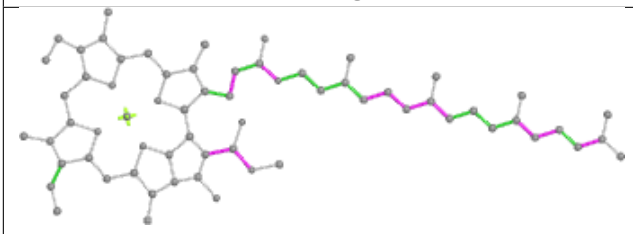
Ligand CLA C 502



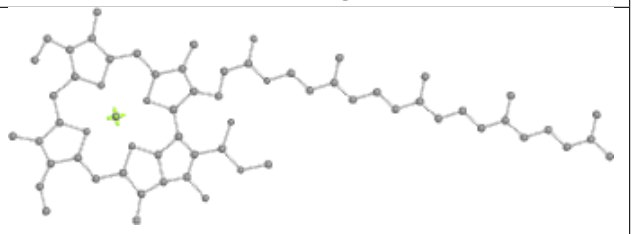
Bond lengths



Bond angles

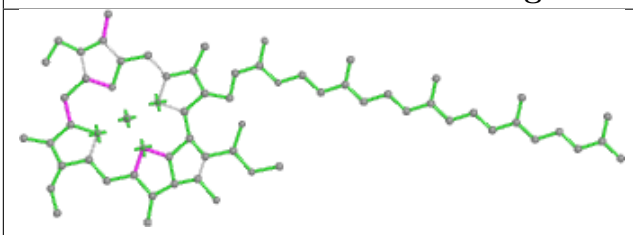


Torsions

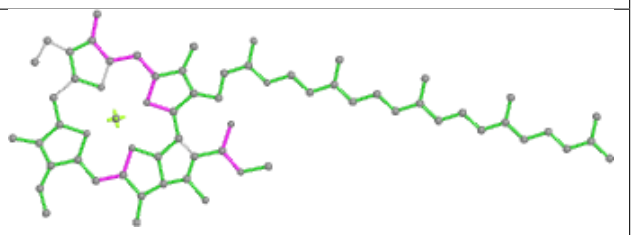


Rings

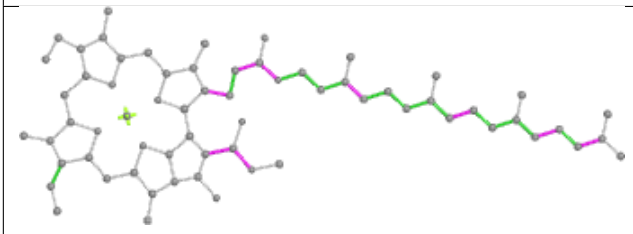
Ligand CLA B 505



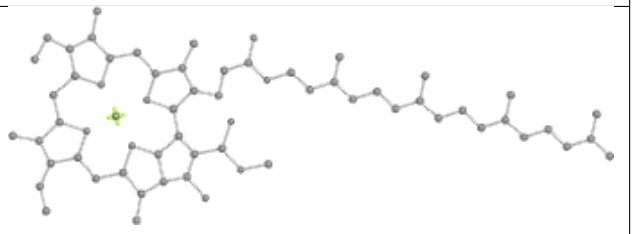
Bond lengths



Bond angles

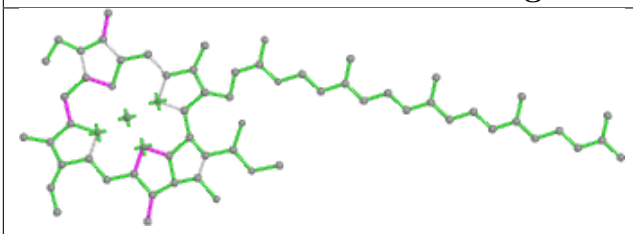


Torsions

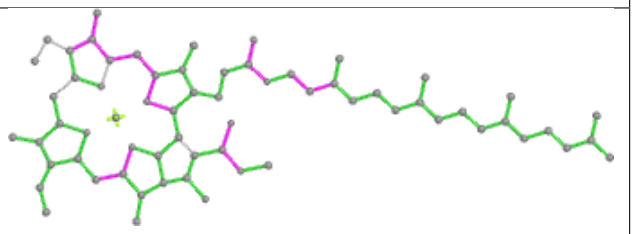


Rings

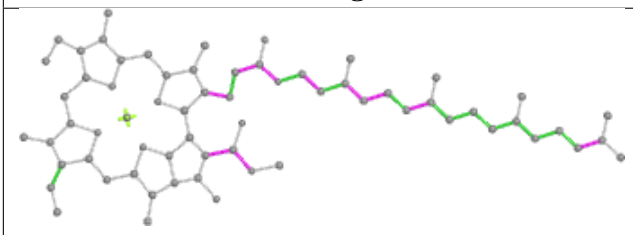
Ligand CLA C 506



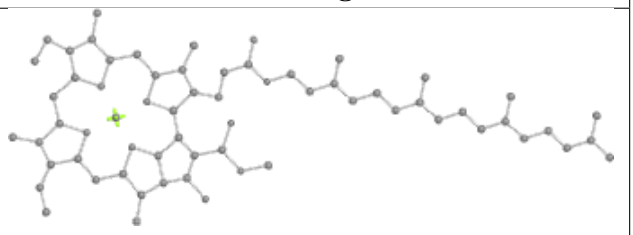
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

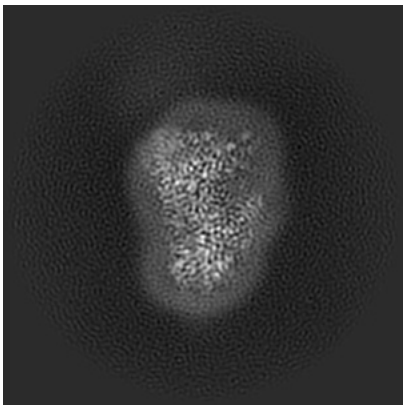
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-60605. These allow visual inspection of the internal detail of the map and identification of artifacts.

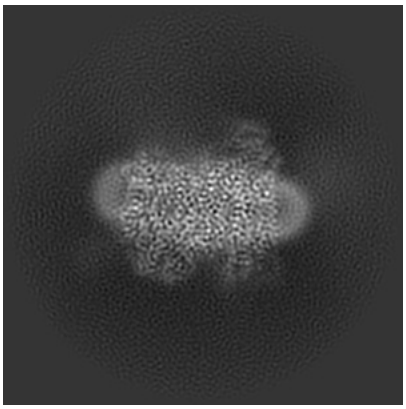
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

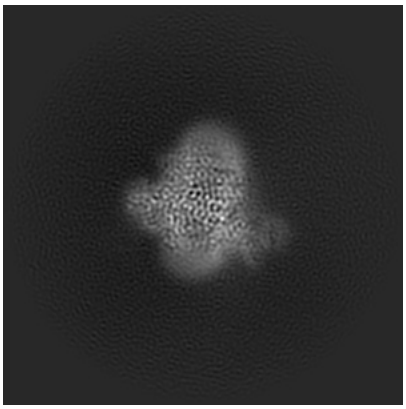
6.1.1 Primary map



X

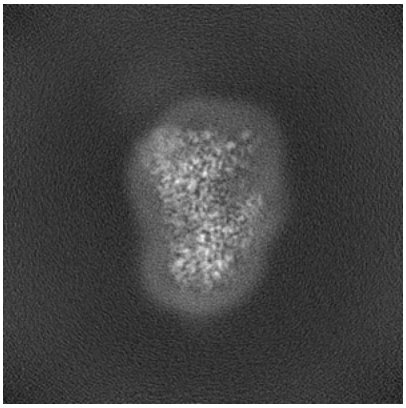


Y

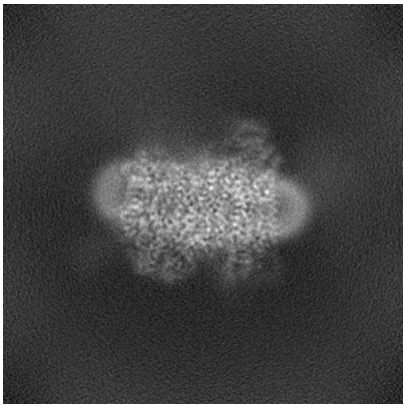


Z

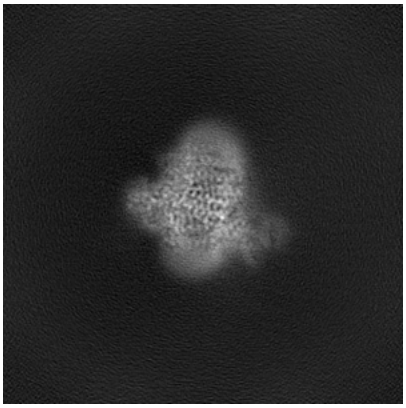
6.1.2 Raw map



X



Y

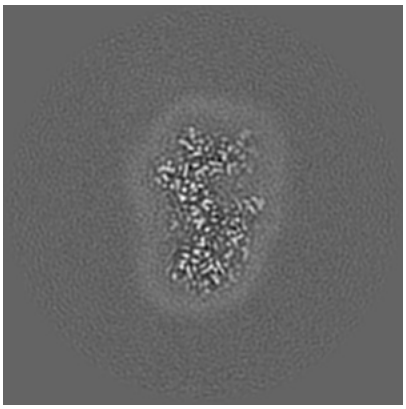


Z

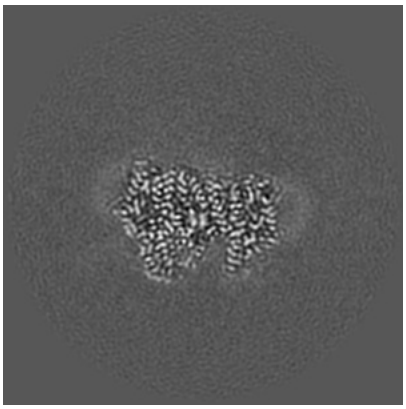
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

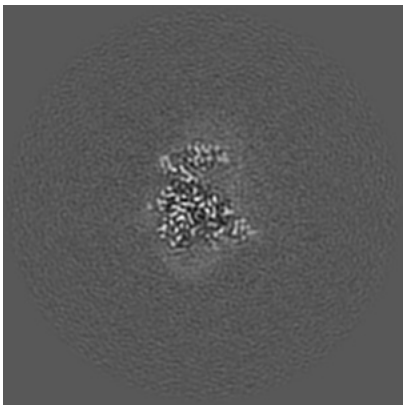
6.2.1 Primary map



X Index: 140

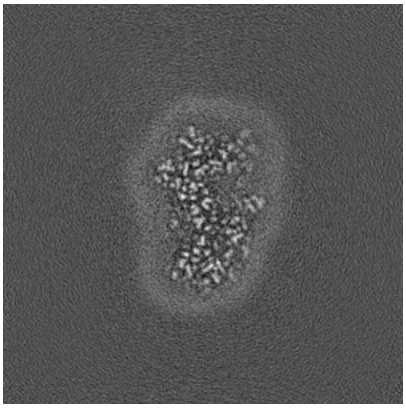


Y Index: 140

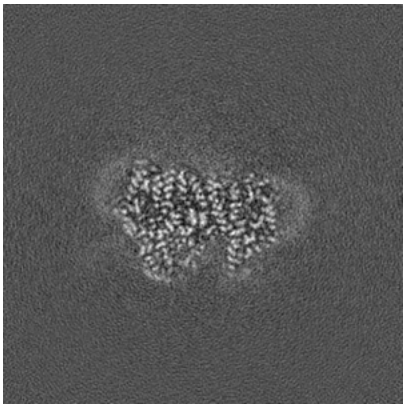


Z Index: 140

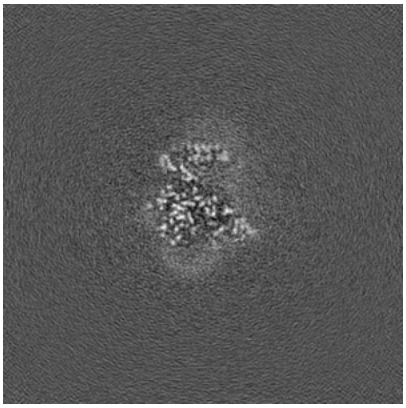
6.2.2 Raw map



X Index: 140



Y Index: 140

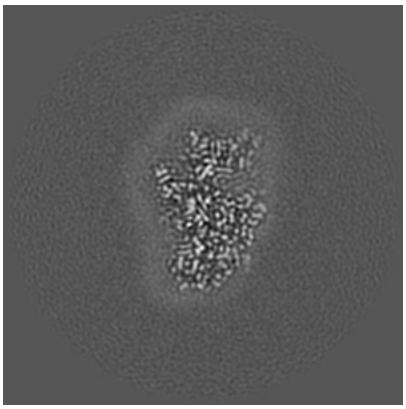


Z Index: 140

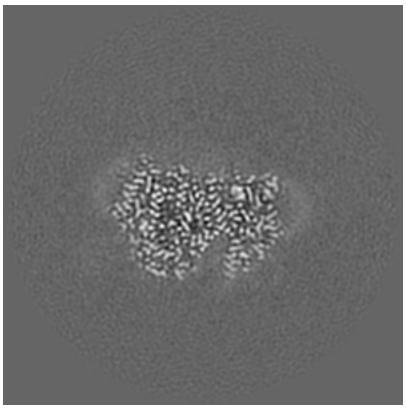
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

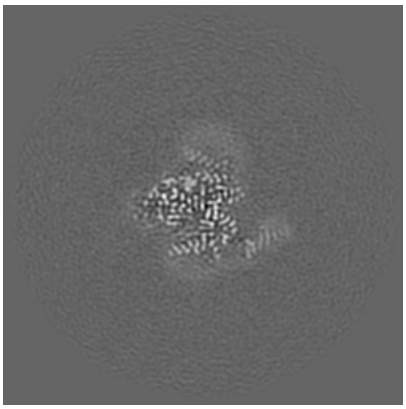
6.3.1 Primary map



X Index: 130

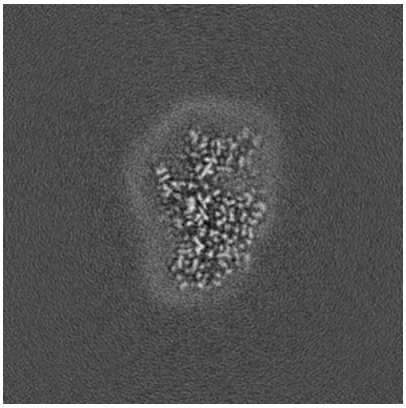


Y Index: 142

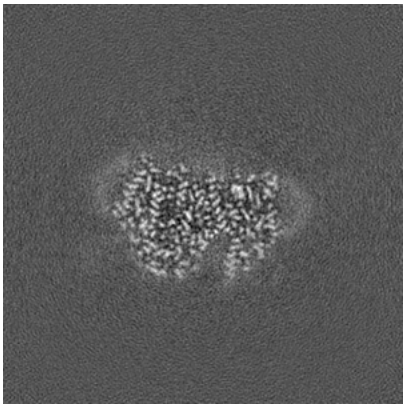


Z Index: 164

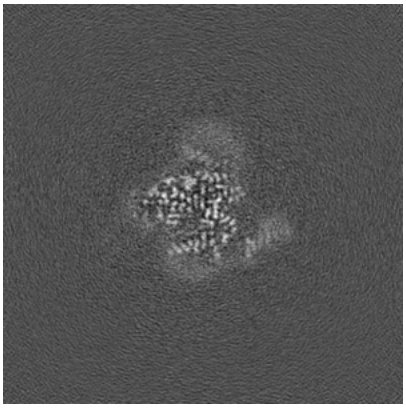
6.3.2 Raw map



X Index: 130



Y Index: 142

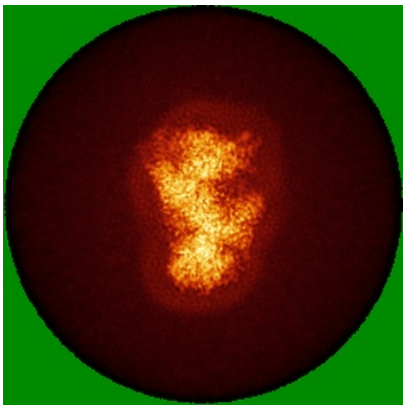


Z Index: 164

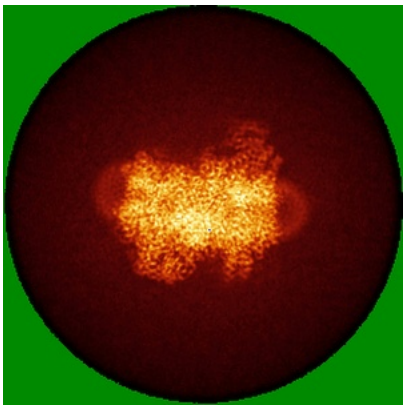
The images above show the largest variance slices of the map in three orthogonal directions.

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

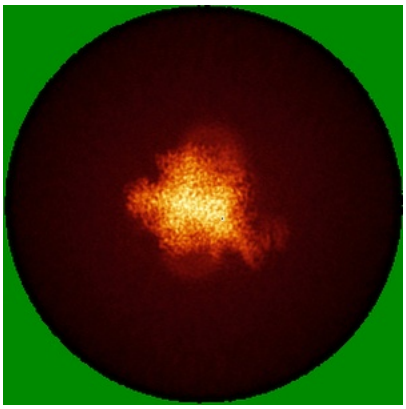
6.4.1 Primary map



X

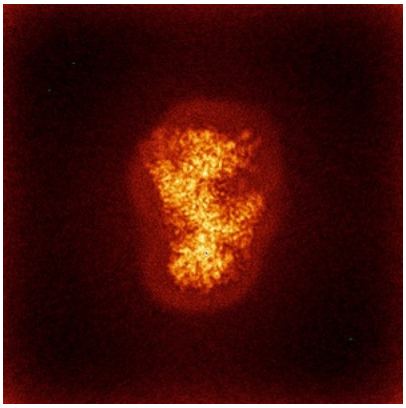


Y

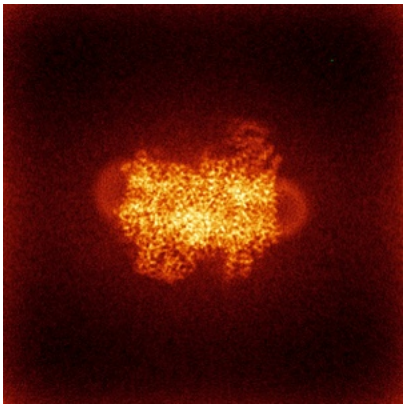


Z

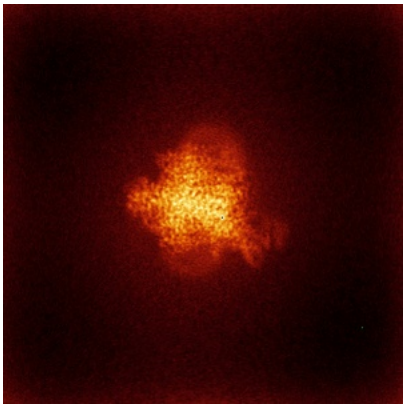
6.4.2 Raw map



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.

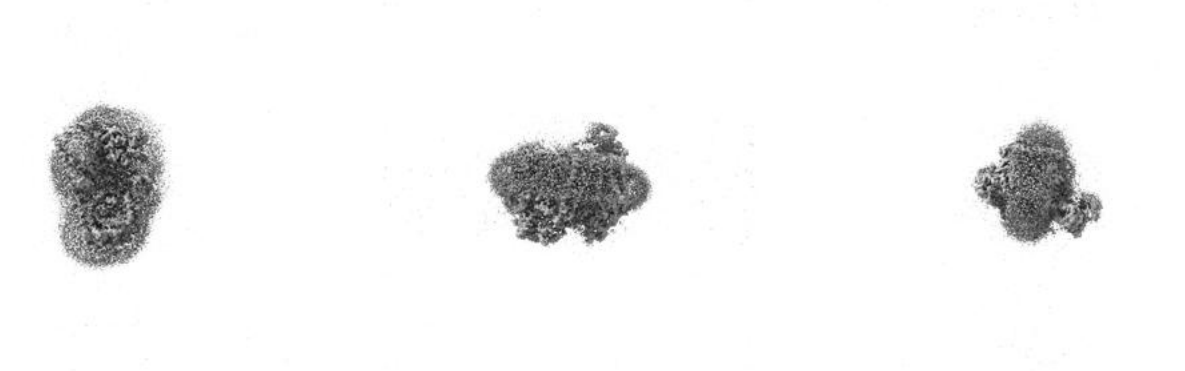
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.174. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

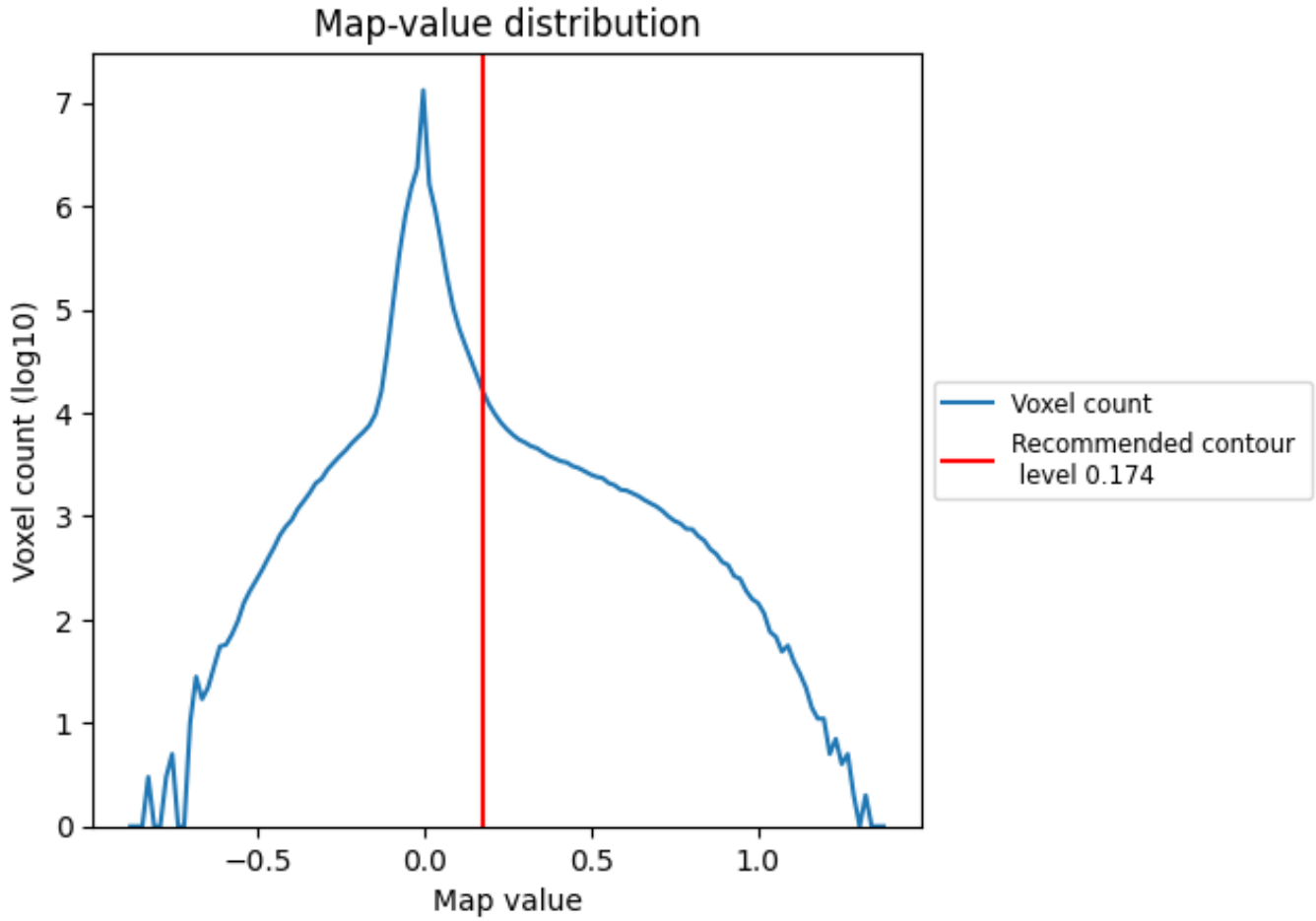
6.6 Mask visualisation (i)

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

7 Map analysis

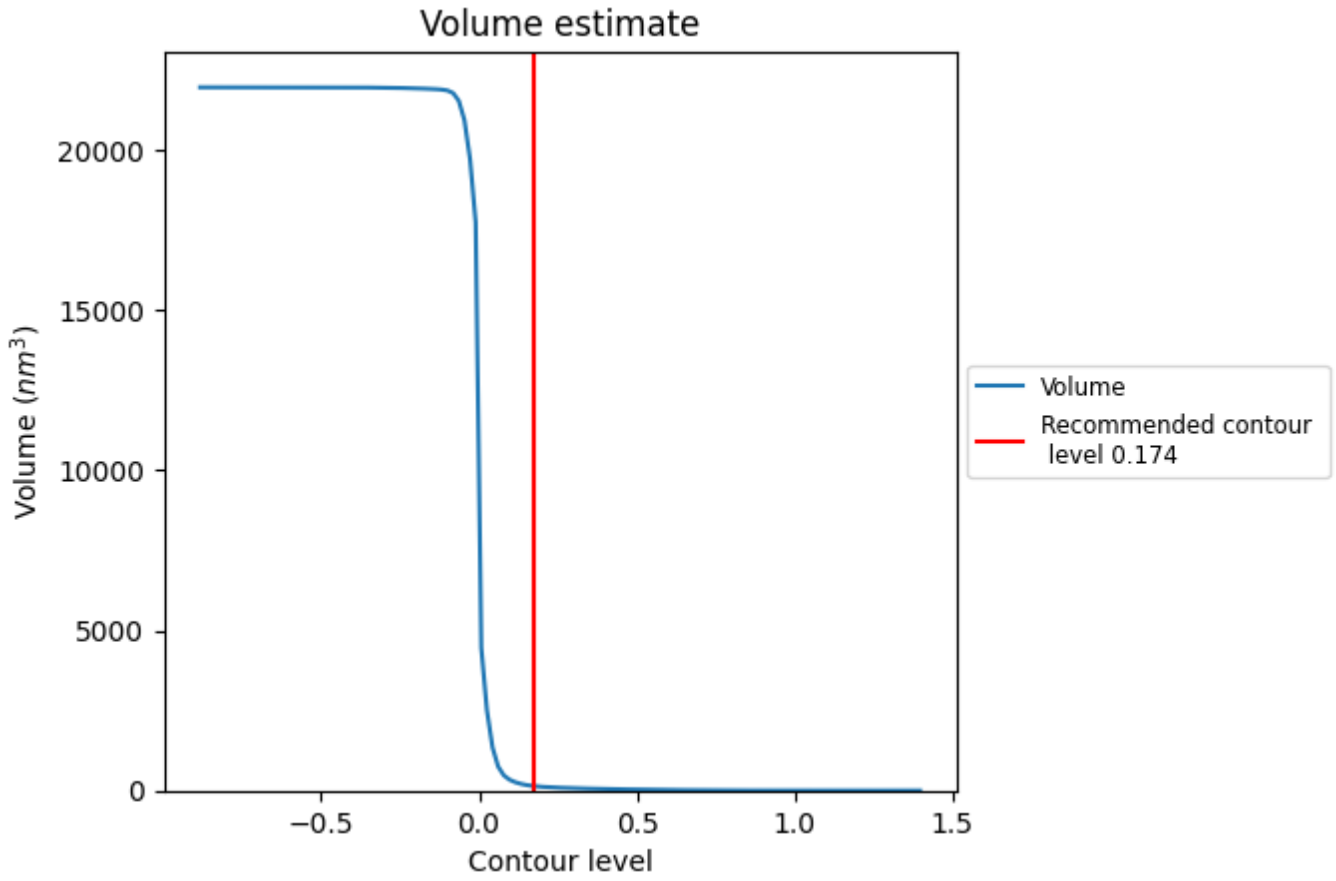
This section contains the results of statistical analysis of the map.

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.

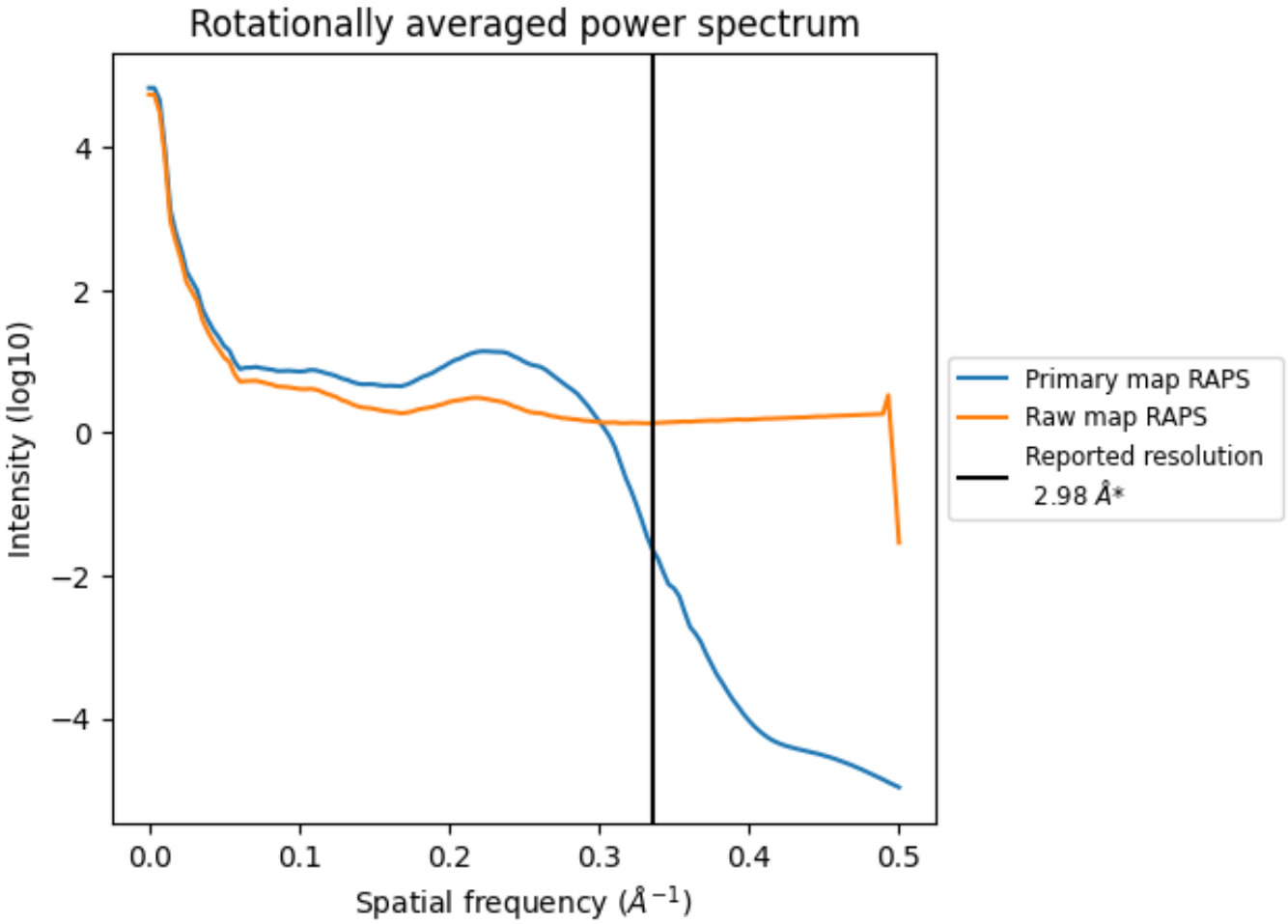
7.2 Volume estimate (i)



The volume at the recommended contour level is 140 nm^3; this corresponds to an approximate mass of 127 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)

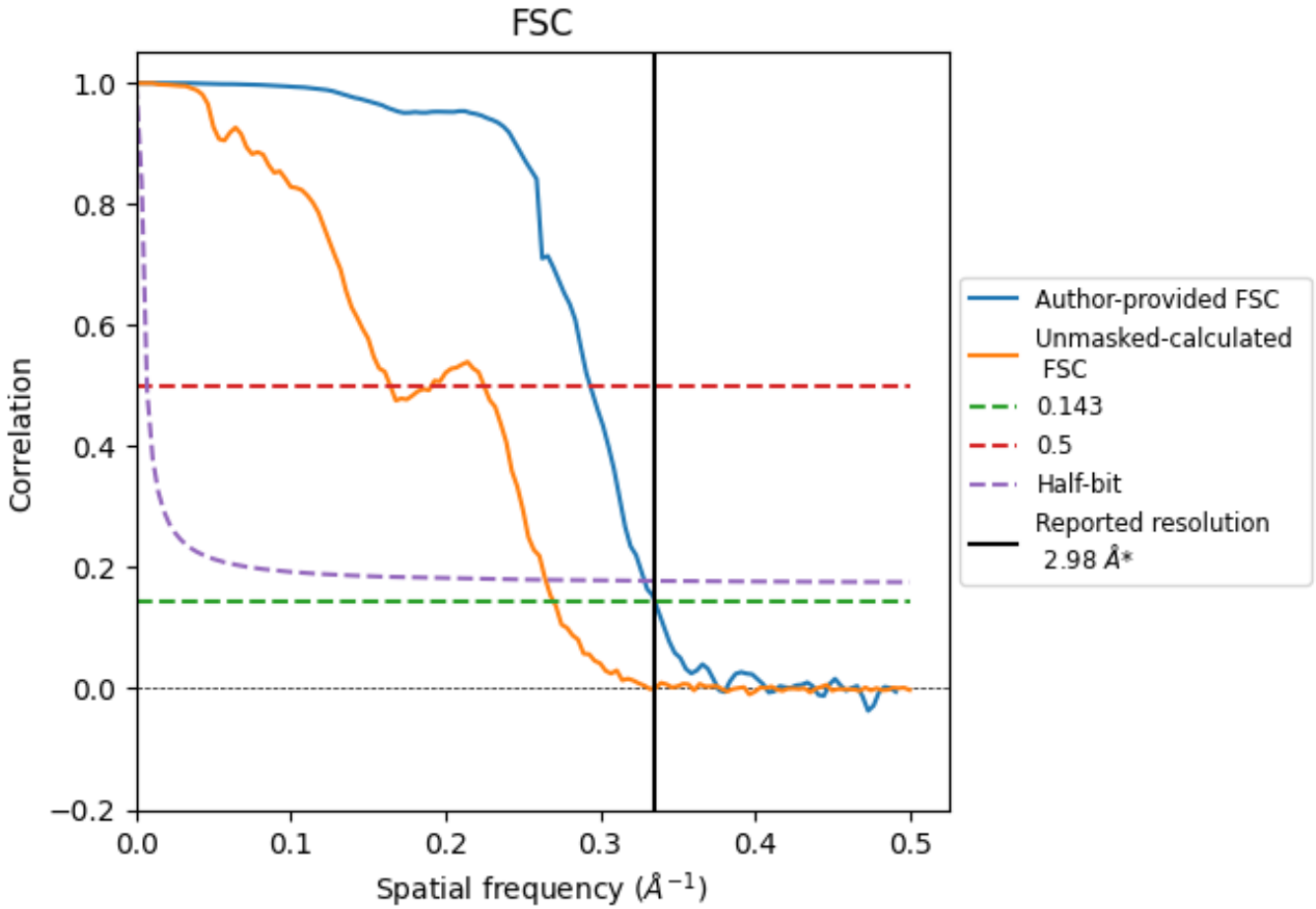


*Reported resolution corresponds to spatial frequency of 0.336 Å^{-1}

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 0.336 Å^{-1}

8.2 Resolution estimates (i)

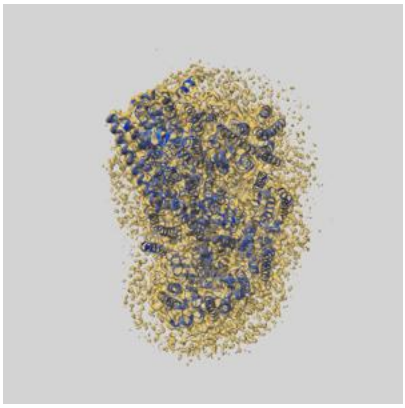
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.41	3.04
Unmasked-calculated*	3.70	6.09	3.78

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.70 differs from the reported value 2.98 by more than 10 %

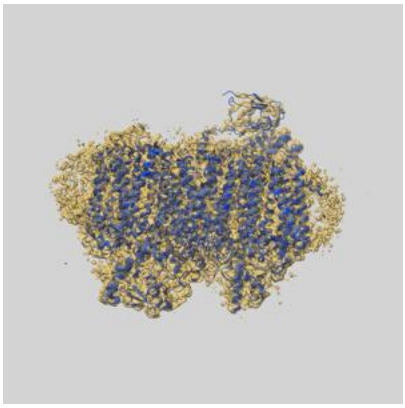
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-60605 and PDB model 9IIU. Per-residue inclusion information can be found in section 3 on page 18.

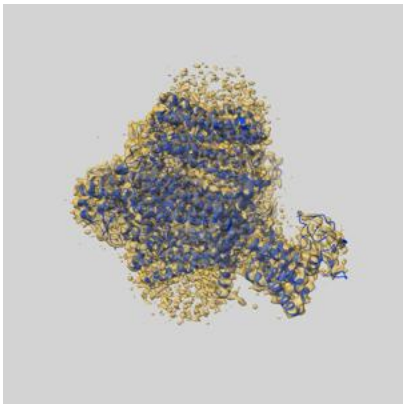
9.1 Map-model overlay



X



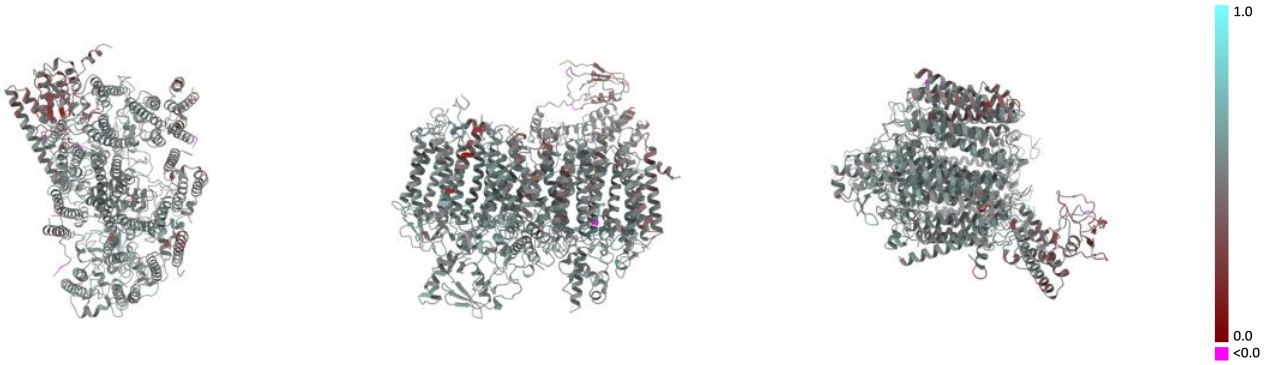
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.174 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.

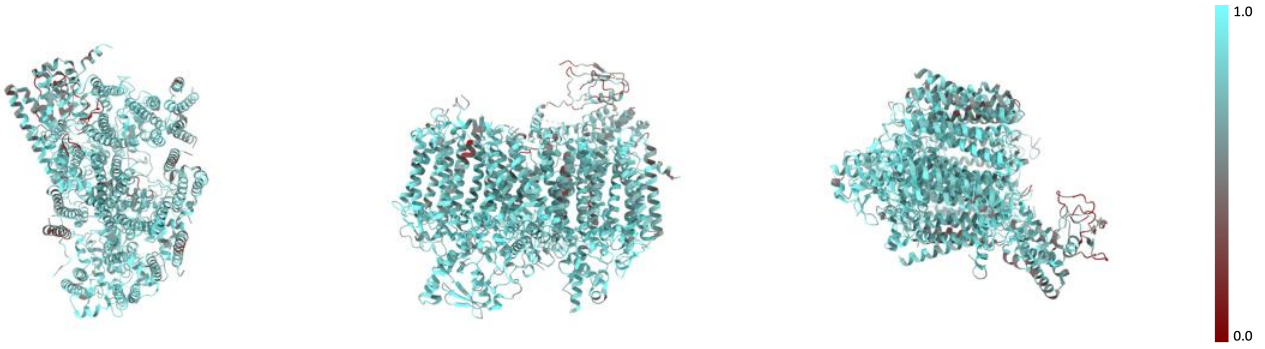
9.2 Q-score mapped to coordinate model (i)



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.

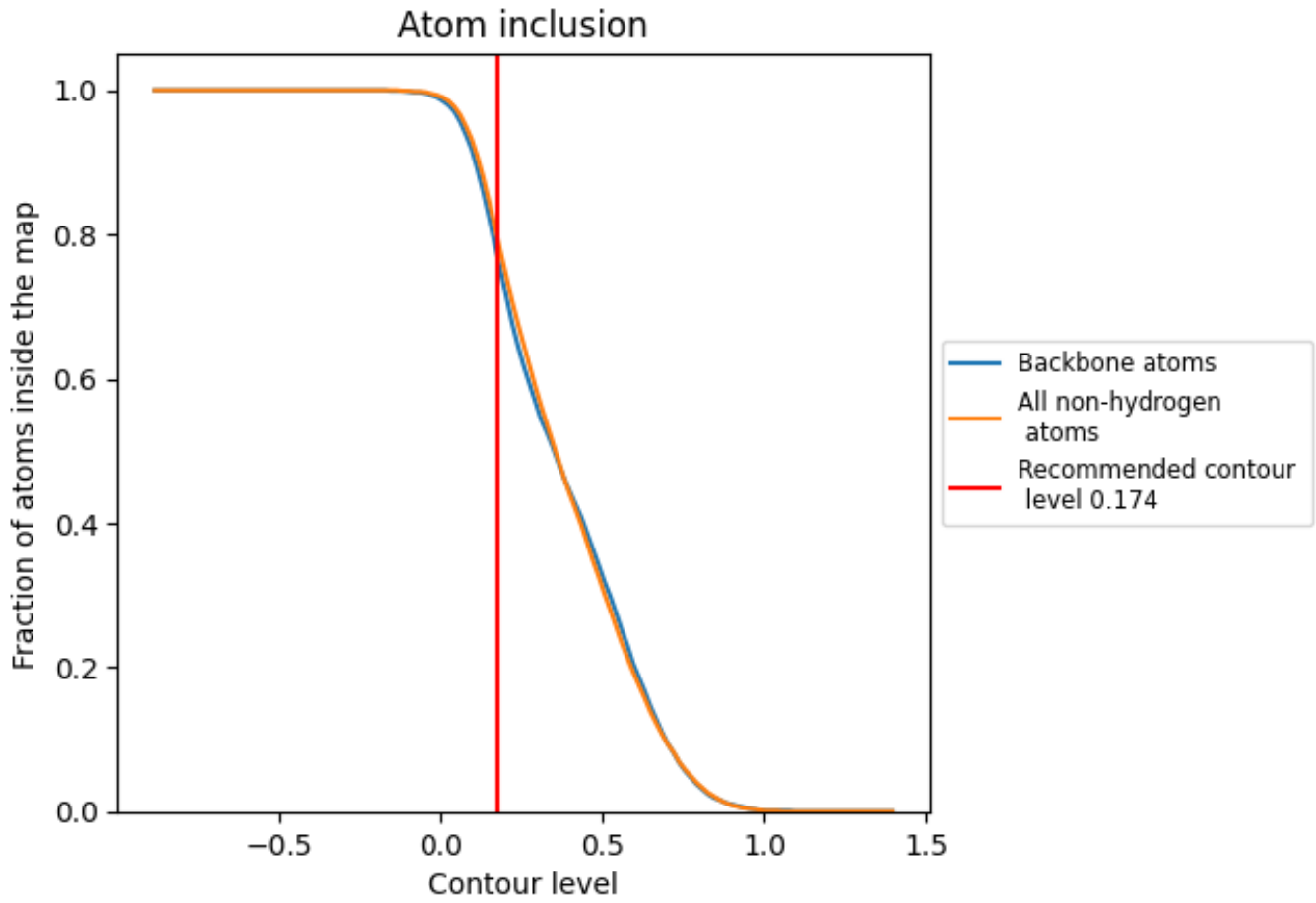
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.174).

9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.174) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8000	0.5230
A	0.8410	0.5330
B	0.8480	0.5460
C	0.8420	0.5380
D	0.8560	0.5520
E	0.7710	0.4940
F	0.7820	0.4970
G	0.6600	0.4410
H	0.7690	0.5110
I	0.7940	0.5280
J	0.6770	0.4810
K	0.8050	0.5050
L	0.7430	0.5030
M	0.3560	0.4110
T	0.6260	0.4700
V	0.6260	0.4280
X	0.6400	0.4260
Z	0.6890	0.4500