wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 07:25 AM JST

PDB ID	:	7DXA / pdb_00007dxa
EMDB ID	:	EMD-30902
Title	:	PSII intermediate Psb28-RC47
Authors	:	Sui, S.F.; Shen, J.R.; Han, G.Y.; Xiao, Y.N.; Huang, G.Q.
Deposited on	:	2021-01-18
Resolution	:	3.14 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 (i) symbol.

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

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

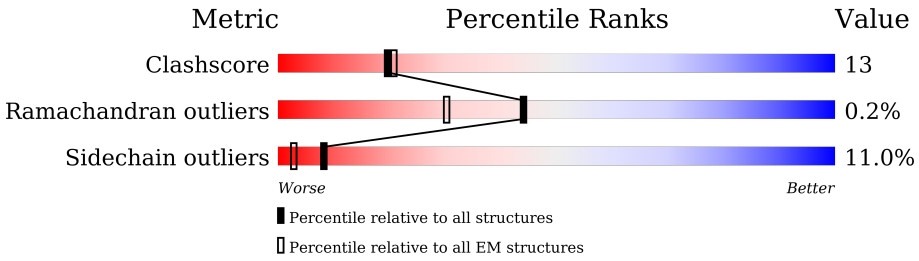
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

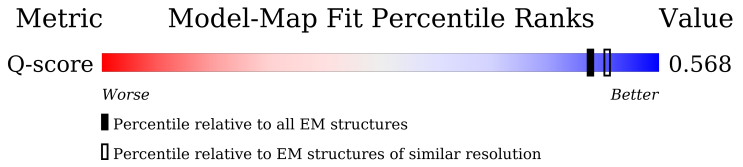
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.14 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14483 (2.64 - 3.64)

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	116	52% 34% 9% 6%
2	B	56	68% 14% 7% 11%
3	a	360	64% 15% 17%
4	b	505	78% 18%
5	d	342	76% 21%

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Mol	Chain	Length	Quality of chain
6	e	84	5% 57% 15% 25%
7	f	45	53% 7% 38%
8	h	65	75% 18% 5%
9	i	38	61% 16% 24%
10	l	37	5% 76% 24%
11	m	36	72% 14% 14%
12	t	32	6% 88% 6% 6%
13	x	40	72% 18% 10%
14	C	23	17% 87% 13%

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
16	CLA	b	606	-	-	X	-
16	CLA	d	404	X	-	-	-
19	CL	a	408	-	-	X	-

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 15162 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 reaction center Psb28 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	109	875	549	153	168	5	0	0

- Molecule 2 is a protein called Tsl0063 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	50	365	237	65	63	0	0

- Molecule 3 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	a	298	2311	1520	382	394	15	0	0

- Molecule 4 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	b	494	3886	2554	646	673	13	0	0

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	d	339	2694	1787	439	456	12	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	e	63	509	334	81	94	0	0

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	f	28	Total	C	N	O	S	0	0
			219	149	36	33	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	62	Total	C	N	O	S	0	0
			493	330	79	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	29	Total	C	N	O	S	0	0
			231	162	30	38	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	37	Total	C	N	O	S	0	0
			304	202	48	53	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	m	31	Total	C	N	O	0	0
			244	165	36	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	t	30	Total	C	N	O	S	0	0
			254	179	36	37	2		

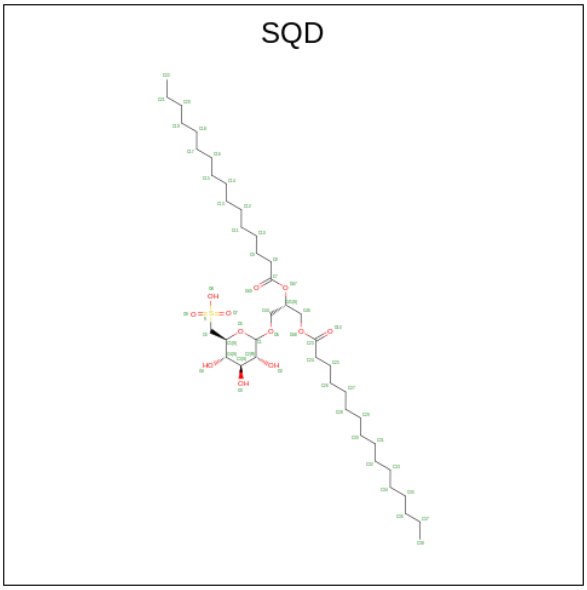
- Molecule 13 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	x	36	Total	C	N	O	0	0
			261	177	39	45		

- Molecule 14 is a protein called unidentified transmembrane protein.

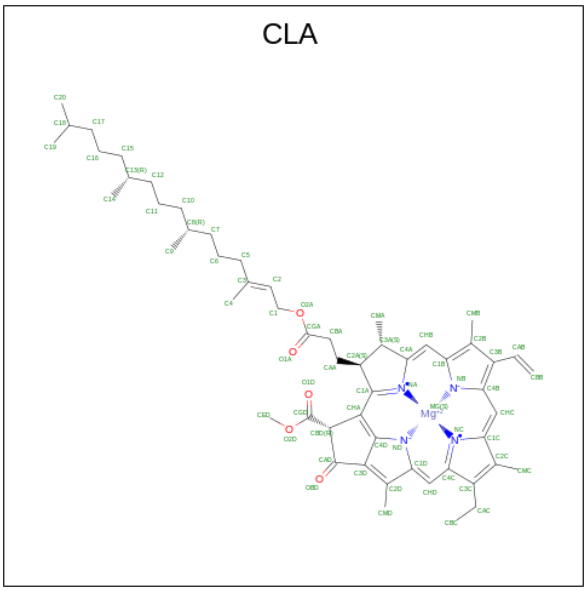
Mol	Chain	Residues	Atoms				AltConf	Trace
14	C	23	Total	C	N	O	0	0
			115	69	23	23		

- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
15	a	1	Total	C	O	S	0
			26	13	12	1	
15	l	1	Total	C	O	S	0
			47	34	12	1	

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



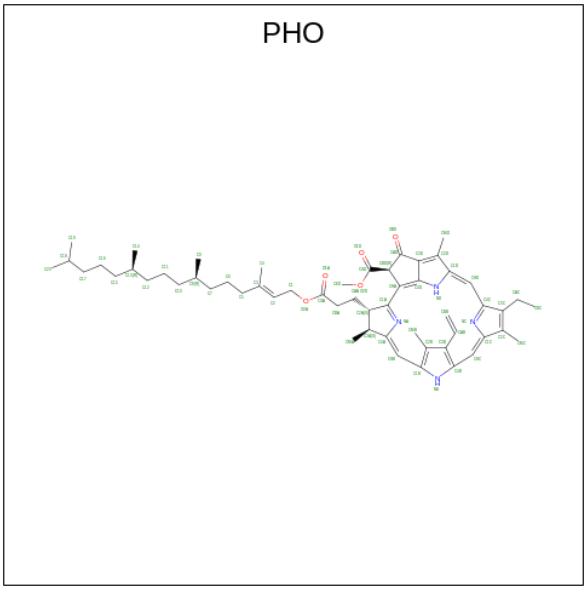
Mol	Chain	Residues	Atoms					AltConf
16	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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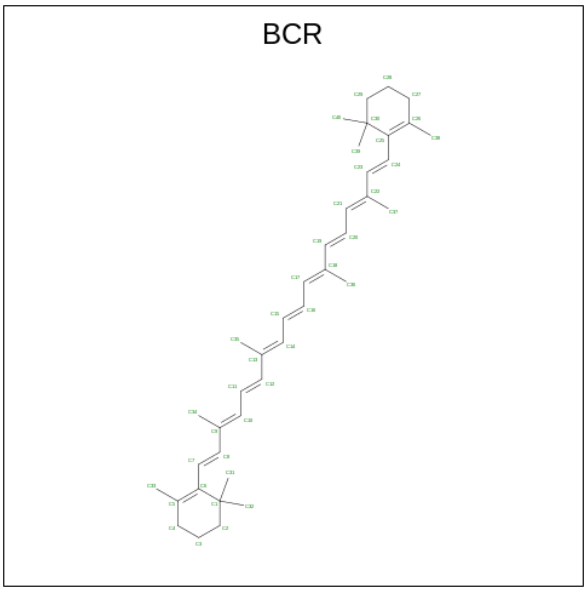
Mol	Chain	Residues	Atoms					AltConf
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
16	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
16	d	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
16	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 17 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



Mol	Chain	Residues	Atoms				AltConf
17	a	1	Total	C	N	O	0
			64	55	4	5	
17	a	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).

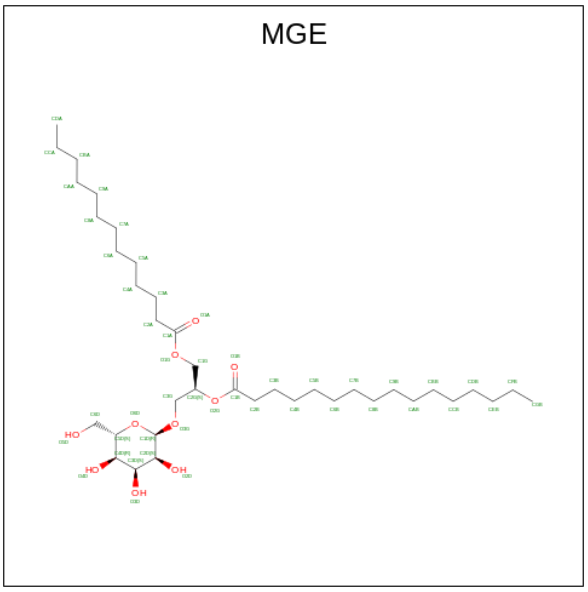


Mol	Chain	Residues	Atoms	AltConf
18	a	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	d	1	Total C 40 40	0
18	h	1	Total C 40 40	0

- Molecule 19 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
19	a	1	Total Cl 1 1	0

- Molecule 20 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: $C_{38}H_{72}O_{10}$).

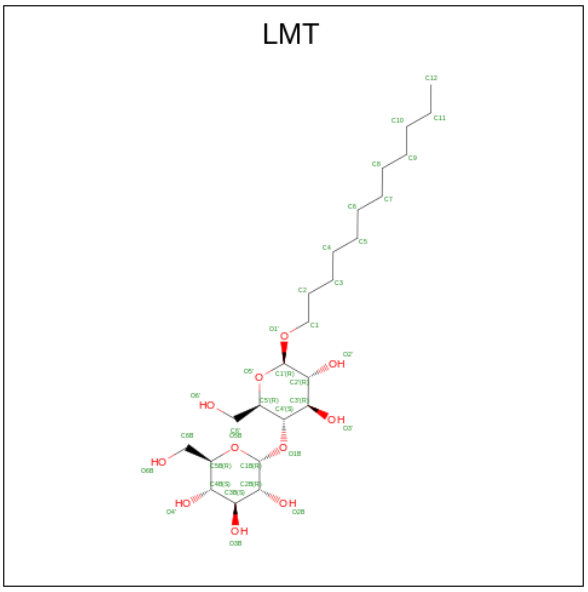


Mol	Chain	Residues	Atoms	AltConf
20	a	1	Total C O 48 38 10	0
20	b	1	Total C O 48 38 10	0
20	b	1	Total C O 48 38 10	0
20	d	1	Total C O 47 37 10	0
20	d	1	Total C O 41 31 10	0
20	d	1	Total C O 48 38 10	0
20	m	1	Total C O 48 38 10	0

- Molecule 21 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms	AltConf
21	b	1	Total C O 36 31 5	0
21	x	1	Total C O 17 16 1	0

- Molecule 22 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).

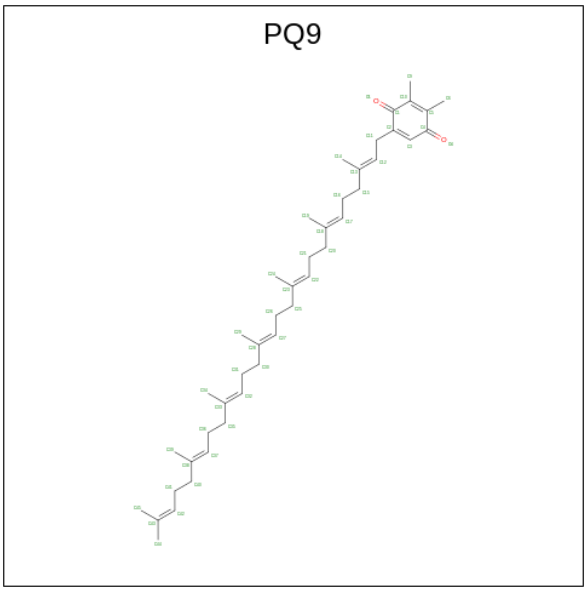


Mol	Chain	Residues	Atoms	AltConf
22	b	1	Total C O 35 24 11	0
22	d	1	Total C O 35 24 11	0
22	t	1	Total C O 35 24 11	0

- Molecule 23 is FE (II) ION (CCD ID: FE2) (formula: Fe).

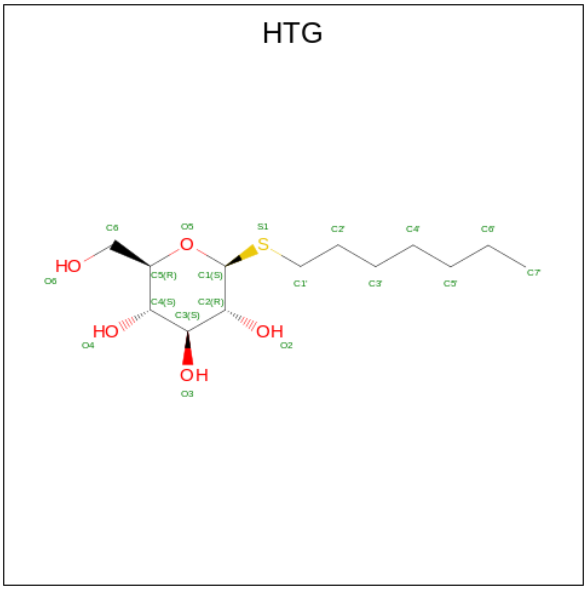
Mol	Chain	Residues	Atoms	AltConf
23	d	1	Total Fe 1 1	0

- Molecule 24 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACOSA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula: $C_{43}H_{64}O_2$).



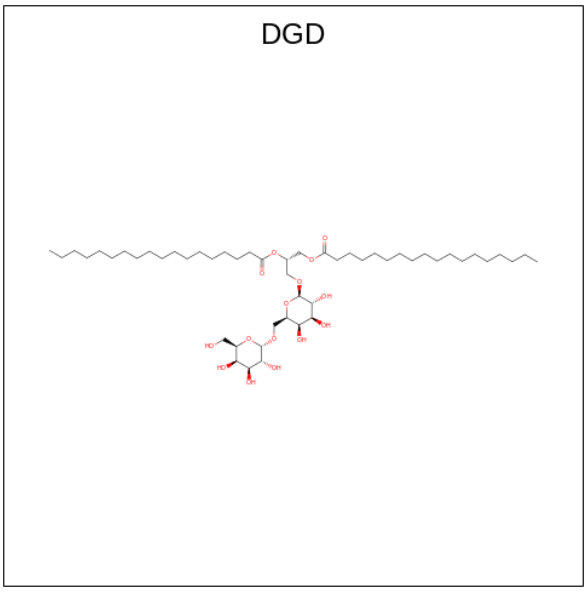
Mol	Chain	Residues	Atoms			AltConf
24	d	1	Total	C	O	0
			45	43	2	

- Molecule 25 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



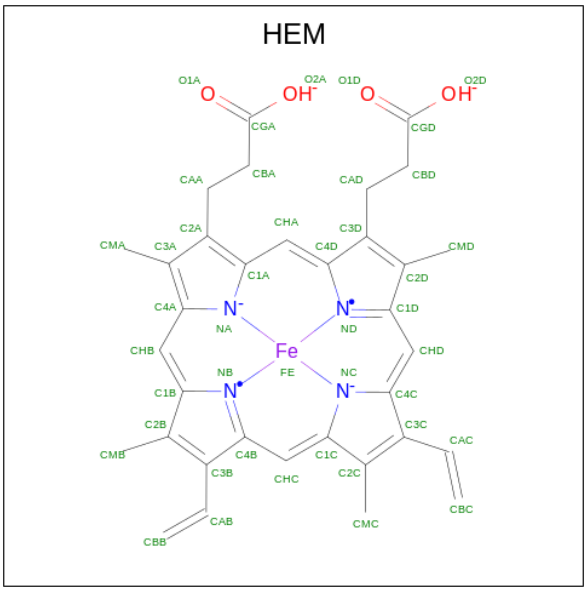
Mol	Chain	Residues	Atoms				AltConf
25	d	1	Total	C	O	S	0
			16	10	5	1	

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	d	1	54	39	15	0

- Molecule 27 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



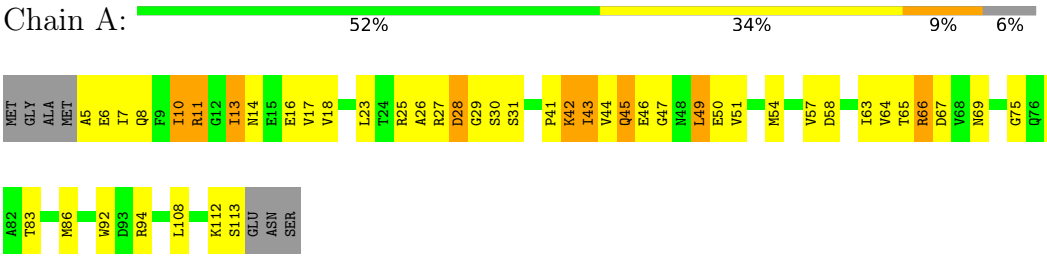
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
27	e	1	43	34	1	4	4	0

3 Residue-property plots (i)

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

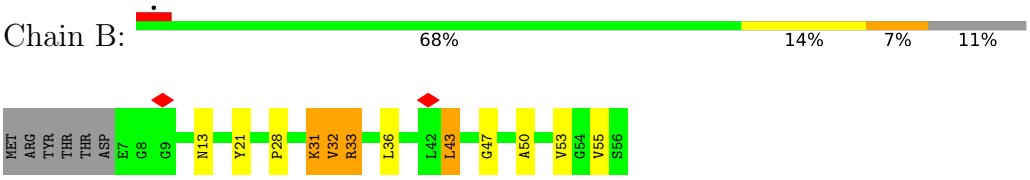
• Molecule 1: Photosystem II reaction center Psb28 protein

Chain A:



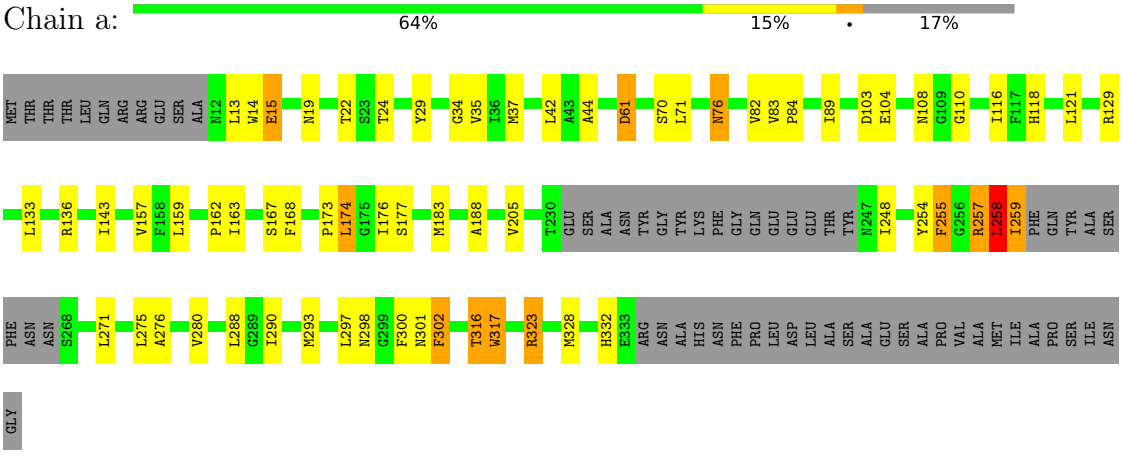
• Molecule 2: Tsl0063 protein

Chain B:



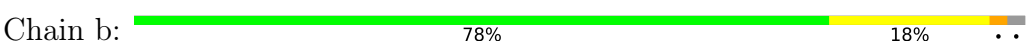
• Molecule 3: Photosystem II protein D1

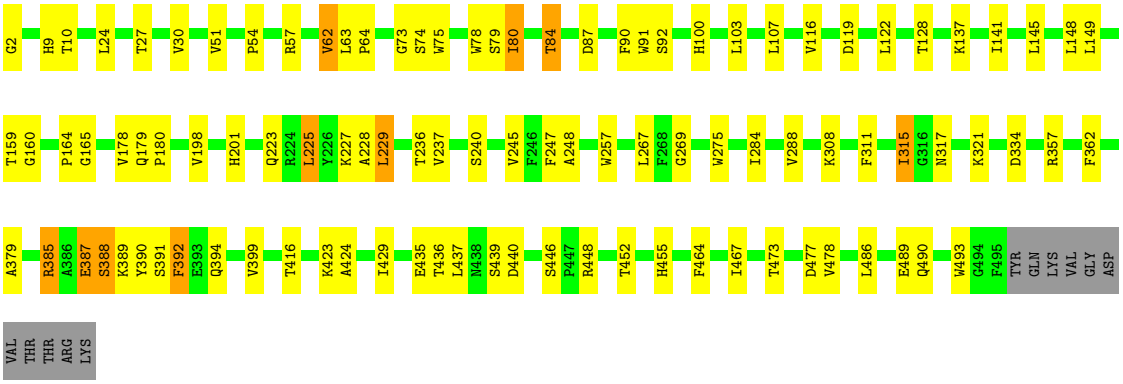
Chain a:



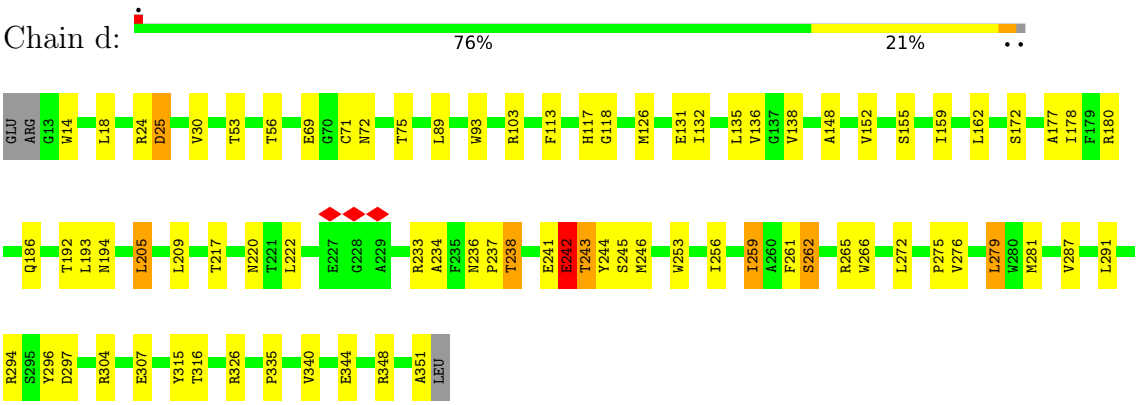
• Molecule 4: Photosystem II CP47 reaction center protein

Chain b:

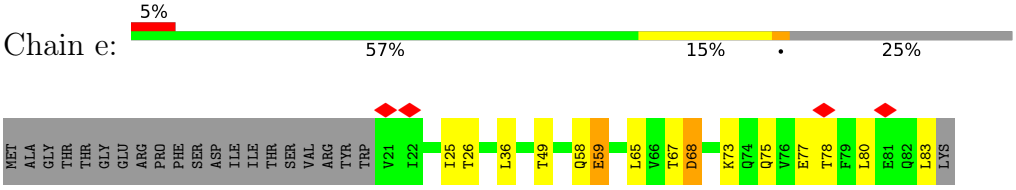




• Molecule 5: Photosystem II D2 protein



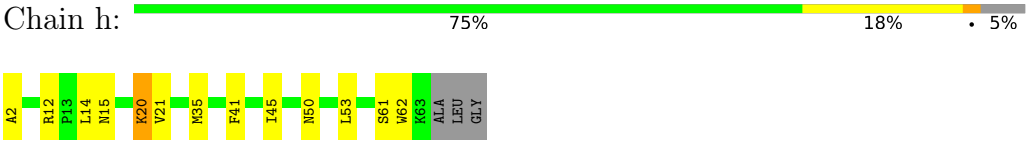
• Molecule 6: Cytochrome b559 subunit alpha



• Molecule 7: Cytochrome b559 subunit beta

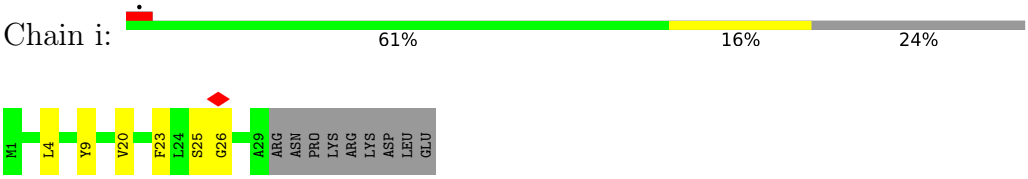


• Molecule 8: Photosystem II reaction center protein H



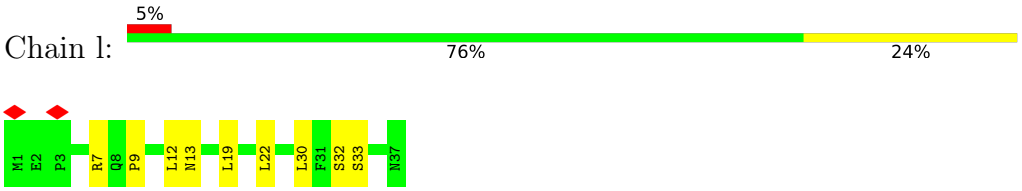
• Molecule 9: Photosystem II reaction center protein I

Chain i:



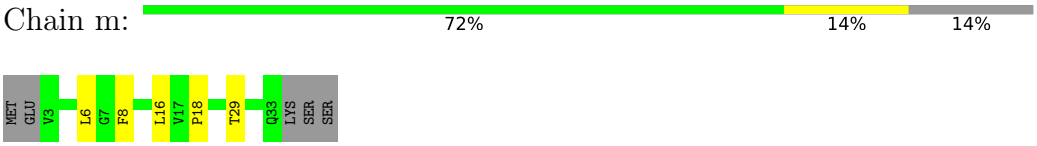
• Molecule 10: Photosystem II reaction center protein L

Chain l:



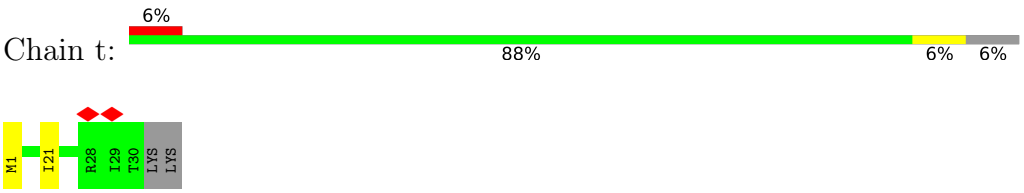
• Molecule 11: Photosystem II reaction center protein M

Chain m:



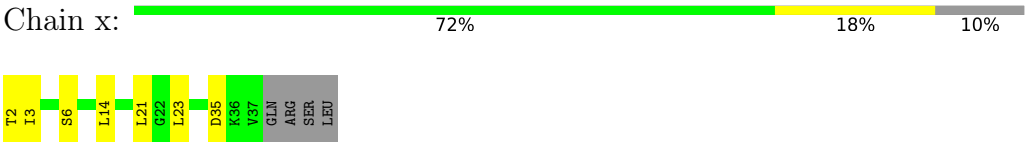
• Molecule 12: Photosystem II reaction center protein T

Chain t:



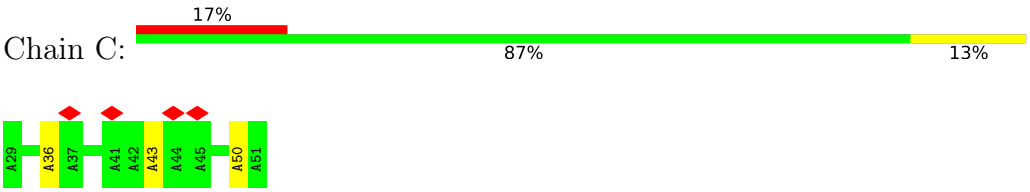
• Molecule 13: Photosystem II reaction center protein X

Chain x:



• Molecule 14: unidentified transmembrane protein

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	241790	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.236	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	261.308, 261.308, 261.308	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PQ9, MGE, LMT, UNL, SQD, PHO, BCR, CL, HTG, DGD, FE2, HEM, CLA

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	0.61	0/892	0.85	0/1202
2	B	0.38	0/371	0.71	0/505
3	a	0.49	0/2383	0.77	3/3249 (0.1%)
4	b	0.48	0/4025	0.72	2/5486 (0.0%)
5	d	0.51	0/2789	0.74	0/3803
6	e	0.36	0/523	0.79	3/714 (0.4%)
7	f	0.36	0/225	0.73	0/308
8	h	0.45	0/506	0.82	0/690
9	i	0.31	0/237	0.70	0/322
10	l	0.40	0/311	0.66	0/422
11	m	0.36	0/248	0.85	0/339
12	t	0.30	0/263	0.52	0/356
13	x	0.28	0/264	0.61	0/358
14	C	0.40	0/114	0.99	0/158
All	All	0.48	0/13151	0.75	8/17912 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	d	0	1
6	e	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	435	GLU	CA-C-N	6.04	133.08	121.54
4	b	435	GLU	C-N-CA	6.04	133.08	121.54
6	e	67	THR	CA-C-N	5.66	129.75	121.31
6	e	67	THR	C-N-CA	5.66	129.75	121.31
3	a	258	LEU	CA-C-N	5.38	131.39	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	d	93	TRP	Peptide
6	e	68	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	875	0	839	64	0
2	B	365	0	386	34	0
3	a	2311	0	2244	64	0
4	b	3886	0	3741	76	0
5	d	2694	0	2588	75	0
6	e	509	0	499	7	0
7	f	219	0	228	3	0
8	h	493	0	513	14	0
9	i	231	0	243	1	0
10	l	304	0	316	6	0
11	m	244	0	256	13	0
12	t	254	0	257	9	0
13	x	261	0	291	4	0
14	C	115	0	114	10	0
15	a	26	0	16	0	0
15	l	47	0	61	2	0
16	a	165	0	150	10	0
16	b	973	0	1017	73	0
16	d	176	0	172	18	0
17	a	128	0	148	11	0
18	a	40	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	b	120	0	168	21	0
18	d	40	0	56	4	0
18	h	40	0	56	4	0
19	a	1	0	0	2	0
20	a	48	0	72	0	0
20	b	96	0	144	3	0
20	d	136	0	193	14	0
20	m	48	0	72	2	0
21	b	36	0	0	0	0
21	x	17	0	0	1	0
22	b	35	0	46	0	0
22	d	35	0	46	1	0
22	t	35	0	46	1	0
23	d	1	0	0	0	0
24	d	45	0	64	6	0
25	d	16	0	17	6	0
26	d	54	0	66	1	0
27	e	43	0	30	0	0
All	All	15162	0	15211	381	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 13.

The worst 5 of 381 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:28:PRO:HA	2:B:31:LYS:CG	1.25	1.62
16:b:606:CLA:H71	18:b:619:BCR:C34	1.52	1.39
16:b:606:CLA:C7	18:b:619:BCR:H342	1.60	1.29
16:b:607:CLA:H191	20:d:409:MGE:C6A	1.63	1.29
2:B:28:PRO:HA	2:B:31:LYS:CD	1.71	1.20

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	107/116 (92%)	91 (85%)	15 (14%)	1 (1%)	14 41
2	B	48/56 (86%)	47 (98%)	1 (2%)	0	100 100
3	a	292/360 (81%)	272 (93%)	20 (7%)	0	100 100
4	b	492/505 (97%)	466 (95%)	25 (5%)	1 (0%)	43 70
5	d	337/342 (98%)	323 (96%)	13 (4%)	1 (0%)	36 64
6	e	61/84 (73%)	53 (87%)	8 (13%)	0	100 100
7	f	26/45 (58%)	26 (100%)	0	0	100 100
8	h	60/65 (92%)	57 (95%)	3 (5%)	0	100 100
9	i	27/38 (71%)	26 (96%)	1 (4%)	0	100 100
10	l	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
11	m	29/36 (81%)	27 (93%)	2 (7%)	0	100 100
12	t	28/32 (88%)	27 (96%)	1 (4%)	0	100 100
13	x	34/40 (85%)	34 (100%)	0	0	100 100
14	C	21/23 (91%)	20 (95%)	1 (5%)	0	100 100
All	All	1597/1779 (90%)	1502 (94%)	92 (6%)	3 (0%)	44 70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	d	242	GLU
1	A	47	GLY
4	b	387	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	92/97 (95%)	70 (76%)	22 (24%)	1 3
2	B	36/42 (86%)	31 (86%)	5 (14%)	3 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	a	237/290 (82%)	200 (84%)	37 (16%)	2 11
4	b	392/403 (97%)	357 (91%)	35 (9%)	9 29
5	d	272/277 (98%)	245 (90%)	27 (10%)	7 26
6	e	55/73 (75%)	52 (94%)	3 (6%)	19 46
7	f	22/39 (56%)	21 (96%)	1 (4%)	24 52
8	h	53/54 (98%)	51 (96%)	2 (4%)	29 56
9	i	26/35 (74%)	22 (85%)	4 (15%)	2 11
10	l	35/35 (100%)	32 (91%)	3 (9%)	10 31
11	m	28/33 (85%)	26 (93%)	2 (7%)	13 37
12	t	26/29 (90%)	26 (100%)	0	100 100
13	x	29/33 (88%)	27 (93%)	2 (7%)	14 38
All	All	1303/1440 (90%)	1160 (89%)	143 (11%)	8 21

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	d	245	SER
5	d	279	LEU
8	h	20	LYS
3	a	248	ILE
3	a	205	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
4	b	58	GLN
5	d	236	ASN
4	b	289	GLN
5	d	332	GLN
5	d	129	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 50 ligands modelled in this entry, 2 are monoatomic and 2 are unknown - leaving 46 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	$\#\|Z\| > 2$
16	CLA	b	610	-	69,73,73	2.16	18 (26%)	83,113,113	2.65	25 (30%)
24	PQ9	d	406	-	45,45,45	0.75	1 (2%)	56,57,57	1.44	10 (17%)
16	CLA	a	402	3	69,73,73	1.92	17 (24%)	83,113,113	2.43	28 (33%)
16	CLA	b	607	-	69,73,73	2.32	18 (26%)	83,113,113	2.12	26 (31%)
22	LMT	t	101	-	36,36,36	0.46	0	47,47,47	1.09	4 (8%)
16	CLA	b	603	-	69,73,73	2.08	19 (27%)	83,113,113	2.70	29 (34%)
16	CLA	b	612	4	69,73,73	2.22	18 (26%)	83,113,113	2.58	27 (32%)
18	BCR	b	617	-	41,41,41	0.76	0	56,56,56	1.70	16 (28%)
27	HEM	e	101	-	50,50,50	1.56	8 (16%)	66,82,82	1.72	13 (19%)
17	PHO	a	404	-	58,69,69	2.00	10 (17%)	56,99,99	2.03	12 (21%)
15	SQD	a	401	-	25,26,54	1.70	4 (16%)	34,37,65	5.07	11 (32%)
20	MGE	b	620	-	48,48,48	0.96	2 (4%)	56,56,56	1.37	5 (8%)
18	BCR	a	407	-	41,41,41	0.72	0	56,56,56	2.37	20 (35%)
16	CLA	b	611	-	69,73,73	2.06	16 (23%)	83,113,113	2.37	30 (36%)
18	BCR	h	101	-	41,41,41	0.81	0	56,56,56	2.03	16 (28%)
22	LMT	d	402	-	36,36,36	0.41	0	47,47,47	0.87	1 (2%)
20	MGE	a	409	-	48,48,48	0.98	2 (4%)	56,56,56	1.05	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
20	MGE	b	622	-	48,48,48	0.96	2 (4%)	56,56,56	1.38	8 (14%)
16	CLA	d	405	-	54,58,73	2.15	16 (29%)	65,95,113	4.50	32 (49%)
16	CLA	b	614	-	56,60,73	2.10	16 (28%)	67,97,113	3.24	38 (56%)
16	CLA	d	404	-	65,69,73	1.95	12 (18%)	78,108,113	4.10	36 (46%)
16	CLA	b	609	-	69,73,73	2.39	22 (31%)	83,113,113	2.09	23 (27%)
17	PHO	a	405	3	58,69,69	1.96	9 (15%)	56,99,99	2.07	16 (28%)
20	MGE	d	410	5	48,48,48	0.98	3 (6%)	56,56,56	1.56	11 (19%)
20	MGE	m	101	-	48,48,48	1.01	3 (6%)	56,56,56	1.10	3 (5%)
16	CLA	b	604	-	69,73,73	2.13	20 (28%)	83,113,113	2.58	28 (33%)
15	SQD	l	101	-	46,47,54	1.31	4 (8%)	55,58,65	3.92	10 (18%)
20	MGE	d	408	-	47,47,48	0.96	2 (4%)	55,55,56	1.20	6 (10%)
18	BCR	b	619	-	41,41,41	0.73	0	56,56,56	1.99	16 (28%)
26	DGD	d	412	-	55,55,67	0.93	2 (3%)	69,69,81	1.18	4 (5%)
16	CLA	b	615	4	69,73,73	2.06	18 (26%)	83,113,113	2.57	30 (36%)
18	BCR	d	407	-	41,41,41	0.71	0	56,56,56	1.60	12 (21%)
16	CLA	a	406	-	54,58,73	2.23	15 (27%)	65,95,113	4.73	35 (53%)
16	CLA	b	602	-	69,73,73	2.14	17 (24%)	83,113,113	2.33	29 (34%)
16	CLA	b	605	-	69,73,73	1.99	18 (26%)	83,113,113	2.61	29 (34%)
16	CLA	d	401	-	69,73,73	2.00	21 (30%)	83,113,113	2.37	26 (31%)
16	CLA	b	608	-	69,73,73	2.12	18 (26%)	83,113,113	2.21	24 (28%)
16	CLA	a	403	-	54,58,73	2.10	11 (20%)	65,95,113	4.74	35 (53%)
16	CLA	b	616	4	50,54,73	2.54	19 (38%)	60,90,113	2.88	26 (43%)
18	BCR	b	618	-	41,41,41	0.68	0	56,56,56	1.87	16 (28%)
16	CLA	b	606	-	69,73,73	2.32	20 (28%)	83,113,113	2.56	28 (33%)
25	HTG	d	411	-	16,16,19	1.18	2 (12%)	20,21,24	1.68	1 (5%)
22	LMT	b	623	-	36,36,36	0.44	0	47,47,47	0.84	1 (2%)
20	MGE	d	409	-	41,41,48	1.06	2 (4%)	49,49,56	1.46	9 (18%)
16	CLA	b	613	4	58,62,73	2.12	18 (31%)	69,99,113	2.60	24 (34%)
16	CLA	b	601	-	45,49,73	2.43	17 (37%)	54,84,113	4.99	29 (53%)

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
16	CLA	b	610	-	-	4/39/115/115	-
24	PQ9	d	406	-	-	8/41/61/61	0/1/1/1
16	CLA	a	402	3	-	5/39/115/115	-
16	CLA	b	607	-	-	2/39/115/115	-
22	LMT	t	101	-	-	7/21/61/61	0/2/2/2
16	CLA	b	603	-	-	4/39/115/115	-
16	CLA	b	612	4	-	7/39/115/115	-
18	BCR	b	617	-	-	0/29/63/63	0/2/2/2
27	HEM	e	101	-	-	6/14/54/54	-
17	PHO	a	404	-	-	13/37/103/103	0/5/6/6
15	SQD	a	401	-	-	4/19/39/69	0/1/1/1
20	MGE	b	620	-	-	13/43/63/63	0/1/1/1
18	BCR	a	407	-	-	9/29/63/63	0/2/2/2
16	CLA	b	611	-	-	6/39/115/115	-
18	BCR	h	101	-	-	11/29/63/63	0/2/2/2
22	LMT	d	402	-	-	4/21/61/61	0/2/2/2
20	MGE	a	409	-	-	13/43/63/63	0/1/1/1
20	MGE	b	622	-	-	15/43/63/63	0/1/1/1
16	CLA	d	405	-	-	6/21/97/115	-
16	CLA	d	404	-	1/1/14/20	9/35/111/115	-
16	CLA	b	614	-	-	9/24/100/115	-
16	CLA	b	609	-	-	2/39/115/115	-
17	PHO	a	405	3	-	10/37/103/103	0/5/6/6
20	MGE	d	410	5	-	13/43/63/63	0/1/1/1
20	MGE	m	101	-	-	8/43/63/63	0/1/1/1
16	CLA	b	604	-	-	7/39/115/115	-
15	SQD	l	101	-	-	14/42/62/69	0/1/1/1
20	MGE	d	408	-	-	7/42/62/63	0/1/1/1
18	BCR	b	619	-	-	0/29/63/63	0/2/2/2
26	DGD	d	412	-	-	9/43/83/95	0/2/2/2
16	CLA	b	615	4	-	9/39/115/115	-
18	BCR	d	407	-	-	8/29/63/63	0/2/2/2
16	CLA	a	406	-	-	6/21/97/115	-
16	CLA	b	602	-	-	4/39/115/115	-
16	CLA	b	605	-	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	d	401	-	-	5/39/115/115	-
16	CLA	b	608	-	-	1/39/115/115	-
16	CLA	a	403	-	-	5/21/97/115	-
16	CLA	b	616	4	-	2/17/93/115	-
18	BCR	b	618	-	-	2/29/63/63	0/2/2/2
16	CLA	b	606	-	-	12/39/115/115	-
25	HTG	d	411	-	-	0/7/27/30	0/1/1/1
22	LMT	b	623	-	-	1/21/61/61	0/2/2/2
20	MGE	d	409	-	-	6/36/56/63	0/1/1/1
16	CLA	b	613	4	-	0/26/102/115	-
16	CLA	b	601	-	-	4/10/86/115	-

The worst 5 of 440 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	b	612	CLA	MG-NA	10.40	2.31	2.06
16	b	606	CLA	MG-NA	10.30	2.30	2.06
17	a	405	PHO	C1B-C2B	9.35	1.49	1.39
16	a	406	CLA	C1D-ND	8.86	1.48	1.37
17	a	404	PHO	C1B-C2B	8.78	1.49	1.39

The worst 5 of 862 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	a	401	SQD	O9-S-C6	-20.30	82.82	106.94
15	l	101	SQD	O9-S-C6	-20.03	83.13	106.94
16	a	406	CLA	C1D-ND-C4D	-18.90	92.91	106.33
16	a	403	CLA	C1D-ND-C4D	-17.71	93.75	106.33
16	d	404	CLA	C1D-ND-C4D	-16.62	94.53	106.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	d	404	CLA	C8

5 of 294 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	a	401	SQD	O5-C5-C6-S
15	a	401	SQD	C5-C6-S-O8

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Mol	Chain	Res	Type	Atoms
15	l	101	SQD	C5-C6-S-O7
15	l	101	SQD	C5-C6-S-O9
16	a	403	CLA	C2B-C3B-CAB-CBB

There are no ring outliers.

41 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	b	610	CLA	3	0
24	d	406	PQ9	6	0
16	a	402	CLA	8	0
16	b	607	CLA	10	0
22	t	101	LMT	1	0
16	b	603	CLA	2	0
16	b	612	CLA	1	0
18	b	617	BCR	1	0
17	a	404	PHO	8	0
20	b	620	MGE	1	0
18	a	407	BCR	4	0
16	b	611	CLA	1	0
18	h	101	BCR	4	0
22	d	402	LMT	1	0
20	b	622	MGE	2	0
16	d	405	CLA	1	0
16	b	614	CLA	1	0
16	d	404	CLA	7	0
16	b	609	CLA	1	0
17	a	405	PHO	3	0
20	d	410	MGE	6	0
20	m	101	MGE	2	0
16	b	604	CLA	7	0
15	l	101	SQD	2	0
20	d	408	MGE	2	0
18	b	619	BCR	17	0
26	d	412	DGD	1	0
16	b	615	CLA	5	0
18	d	407	BCR	4	0
16	b	602	CLA	8	0
16	b	605	CLA	5	0
16	d	401	CLA	10	0
16	b	608	CLA	3	0
16	a	403	CLA	2	0

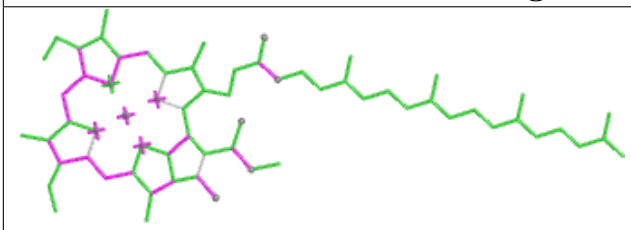
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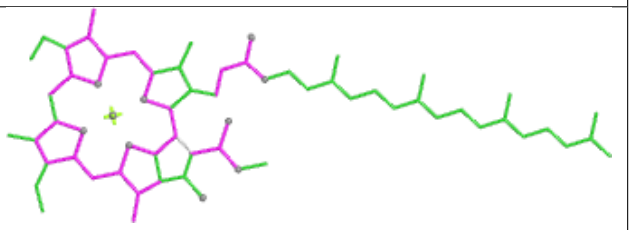
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	b	616	CLA	2	0
18	b	618	BCR	3	0
16	b	606	CLA	25	0
25	d	411	HTG	6	0
20	d	409	MGE	6	0
16	b	613	CLA	3	0
16	b	601	CLA	1	0

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.

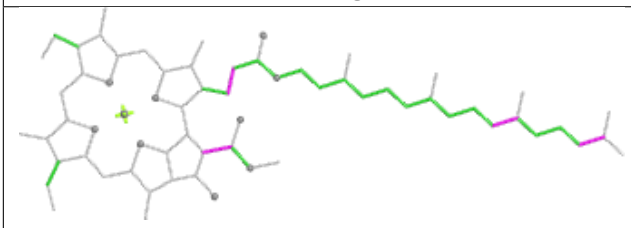
Ligand CLA b 610



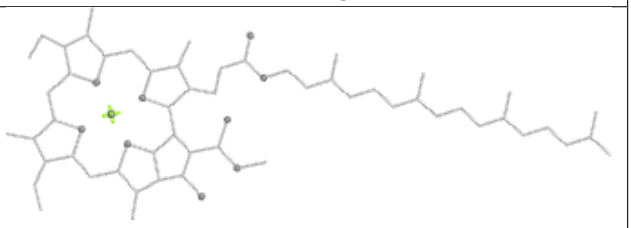
Bond lengths



Bond angles

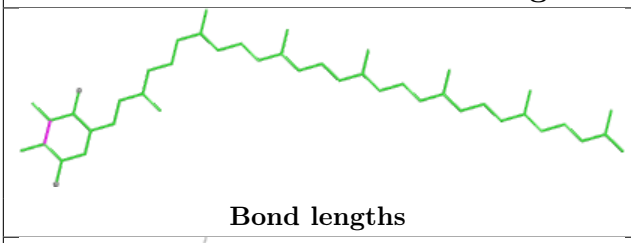


Torsions

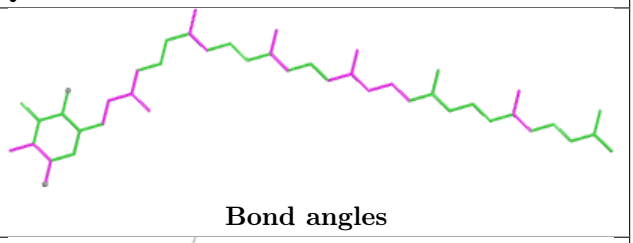


Rings

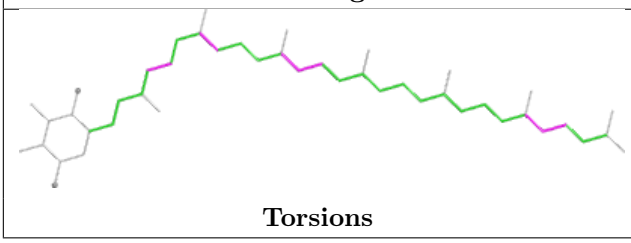
Ligand PQ9 d 406



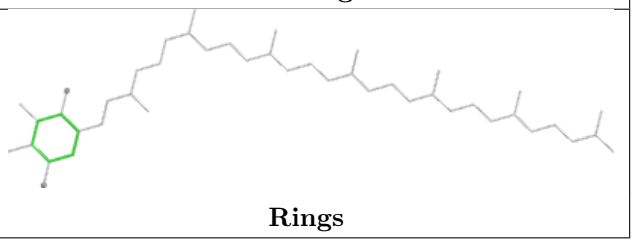
Bond lengths



Bond angles

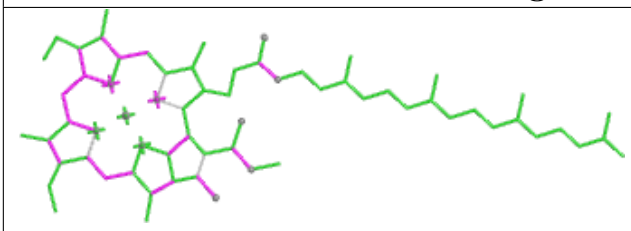


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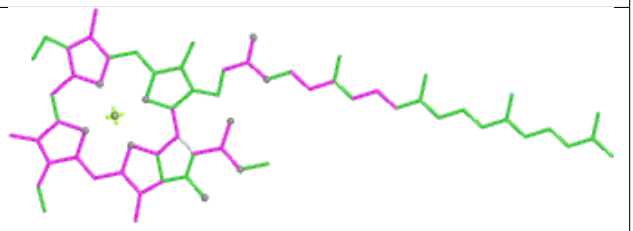


Rings

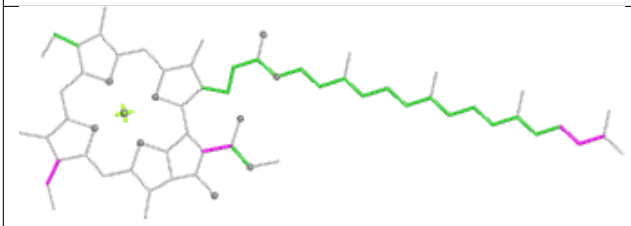
Ligand CLA a 402



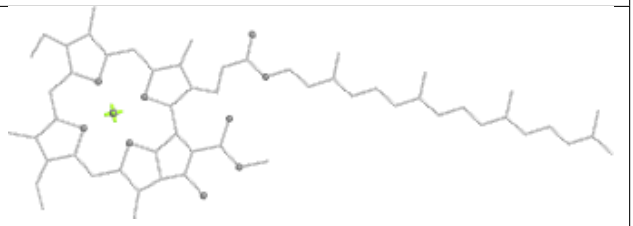
Bond lengths



Bond angles

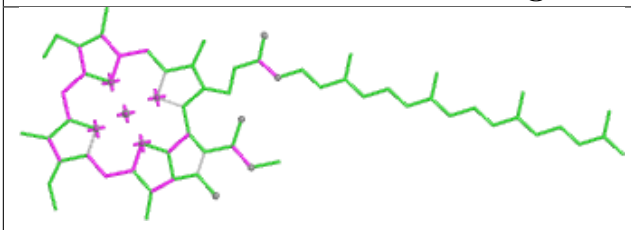


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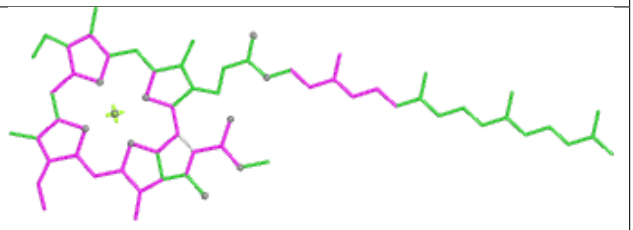


Rings

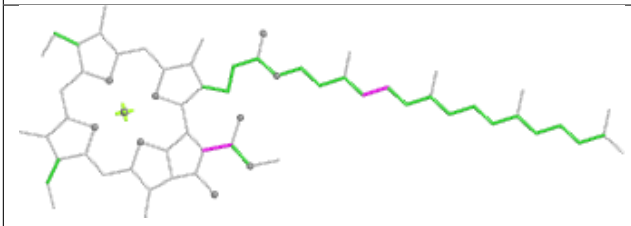
Ligand CLA b 607



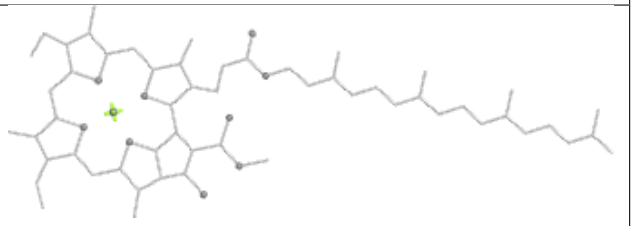
Bond lengths



Bond angles

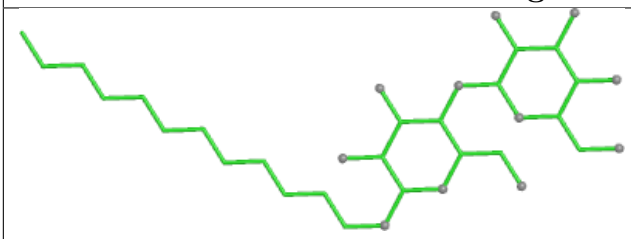


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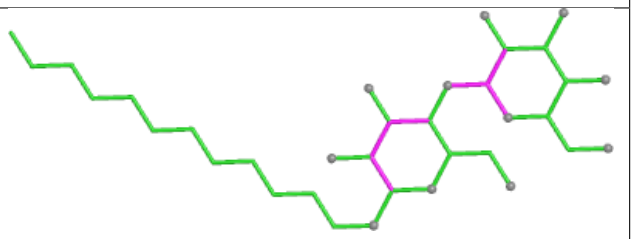


Rings

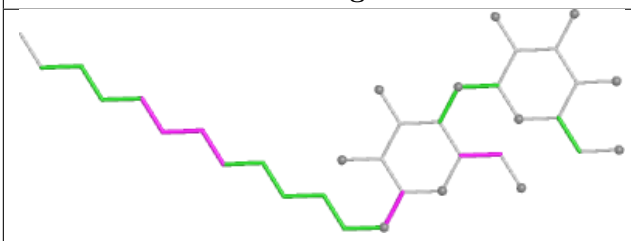
Ligand LMT t 101



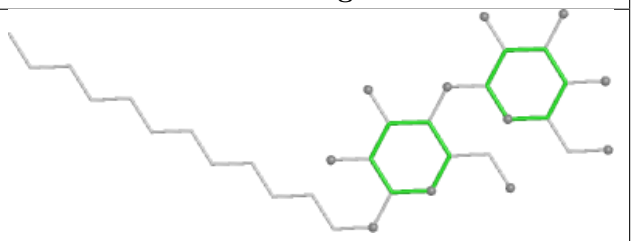
Bond lengths



Bond angles

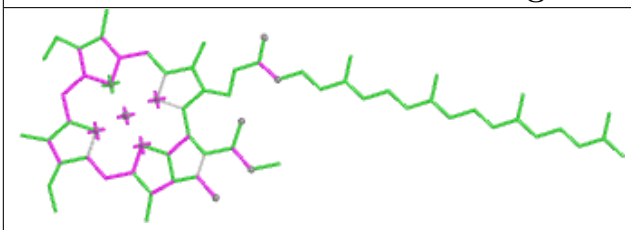


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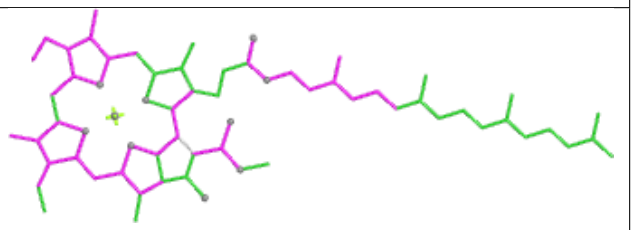


Rings

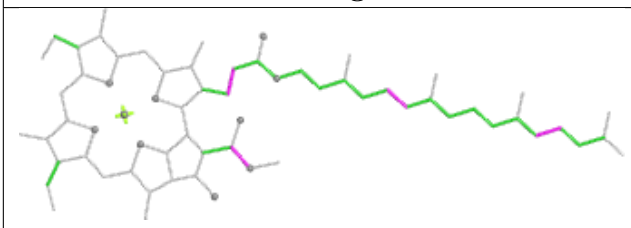
Ligand CLA b 603



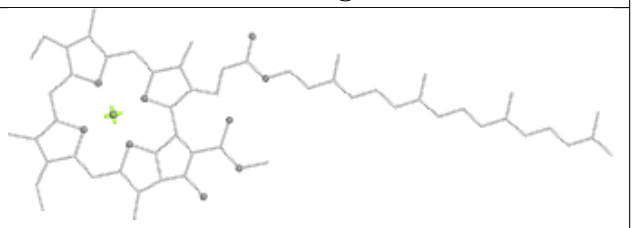
Bond lengths



Bond angles

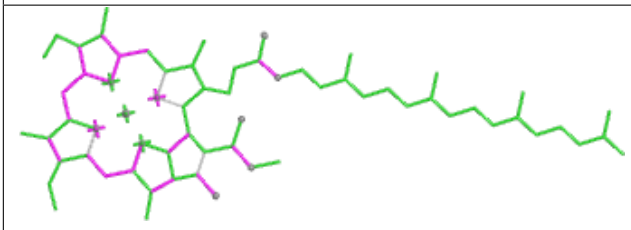


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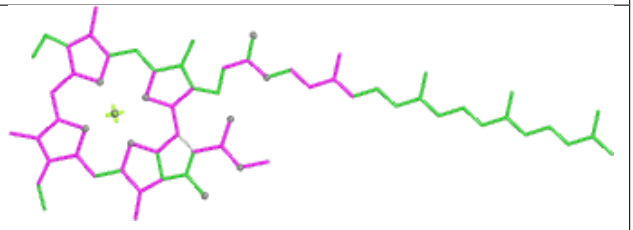


Rings

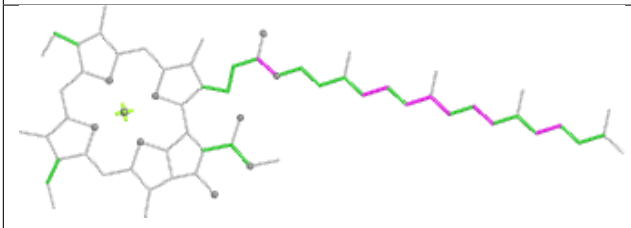
Ligand CLA b 612



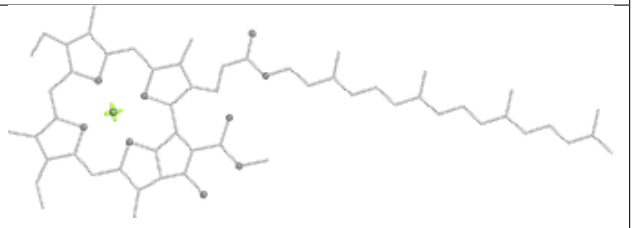
Bond lengths



Bond angles

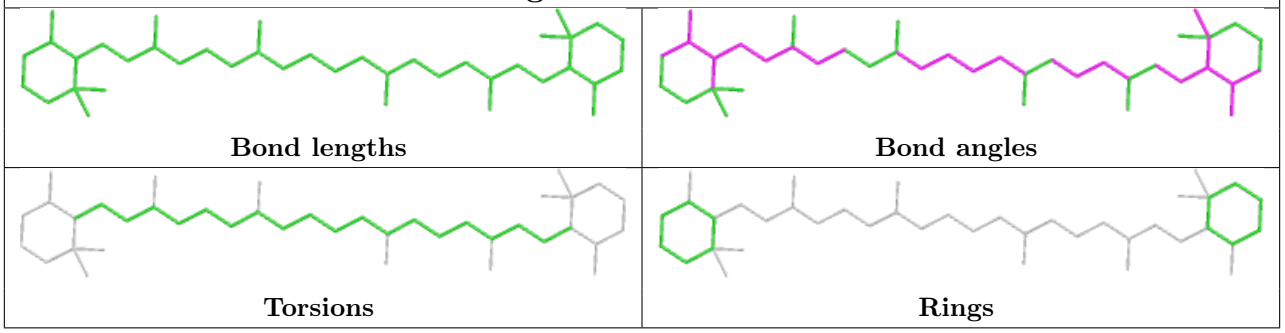


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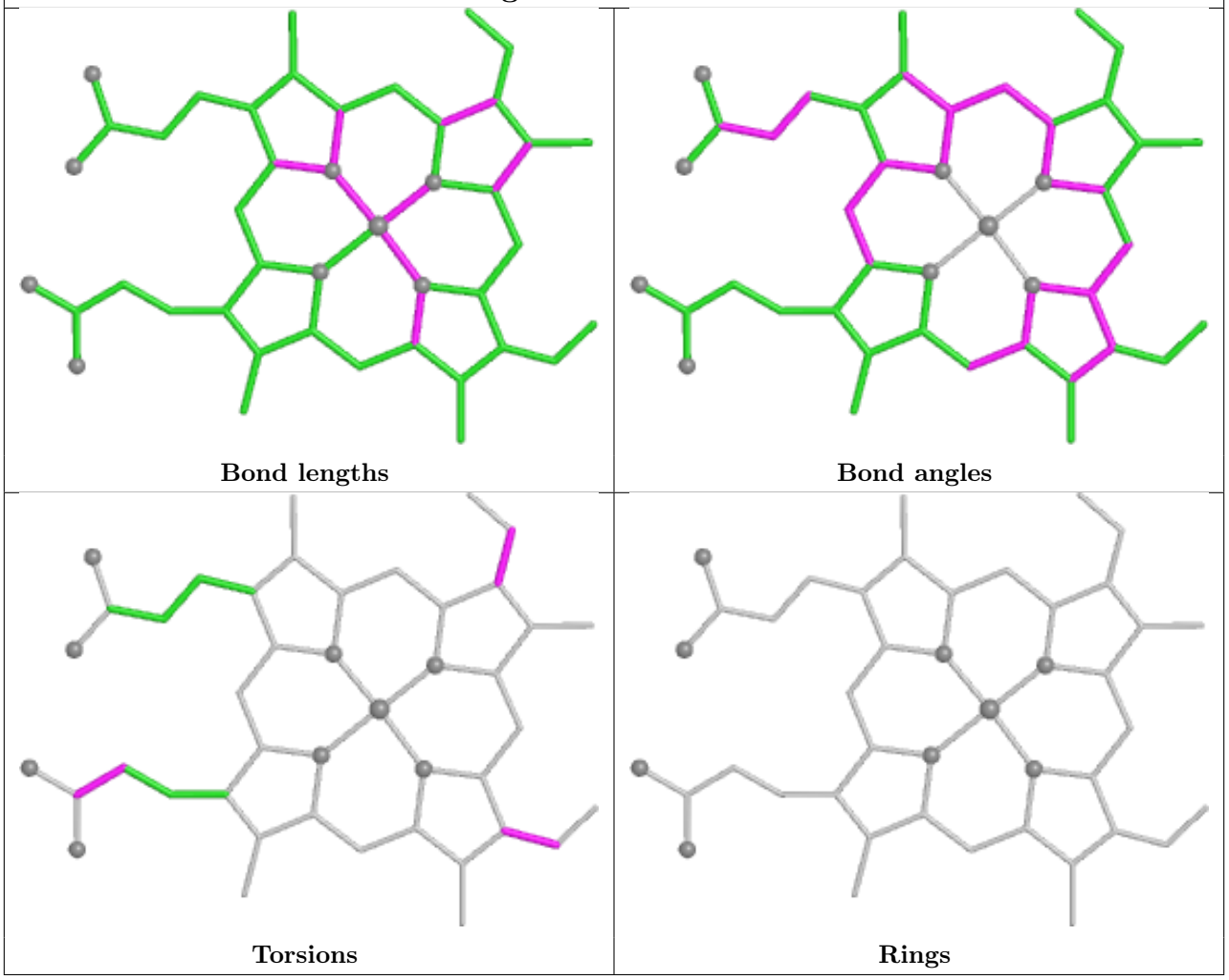


Rings

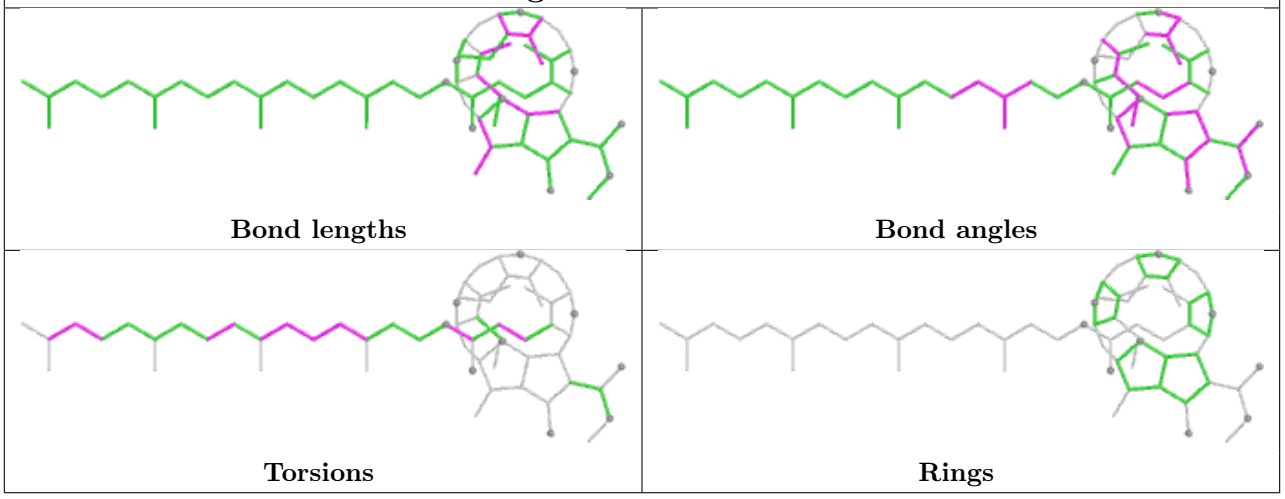
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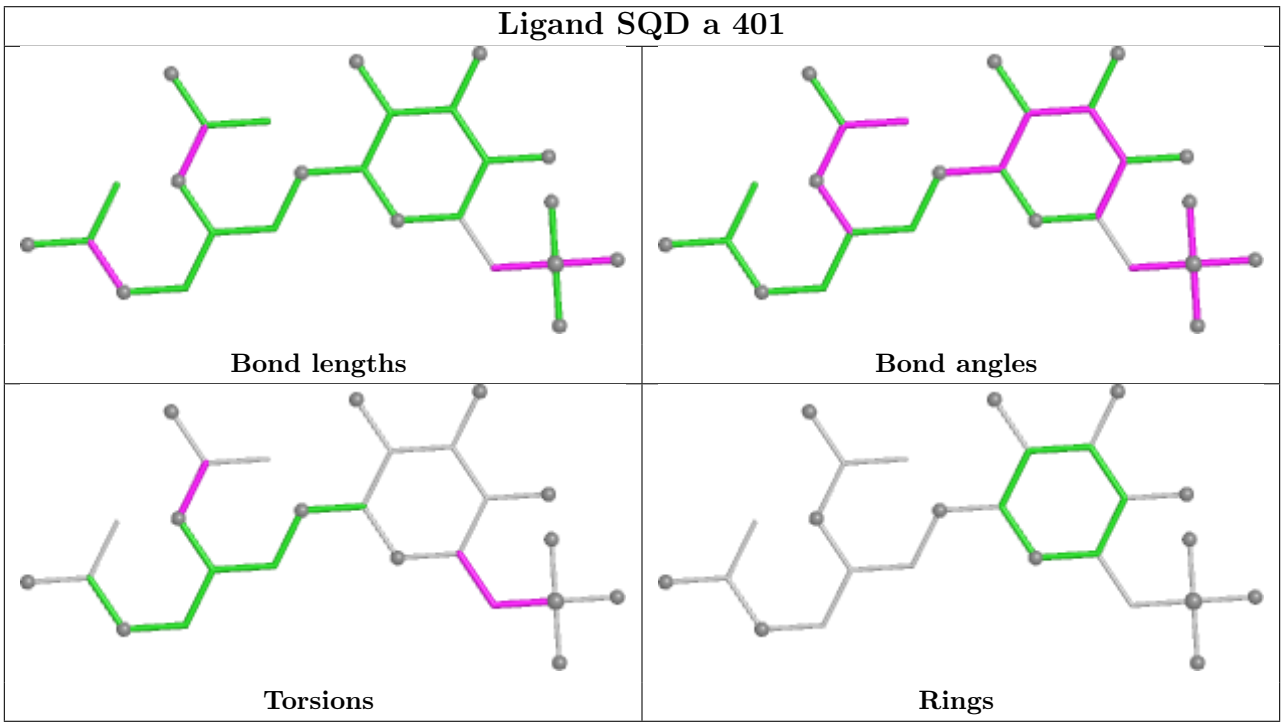
Ligand HEM e 101



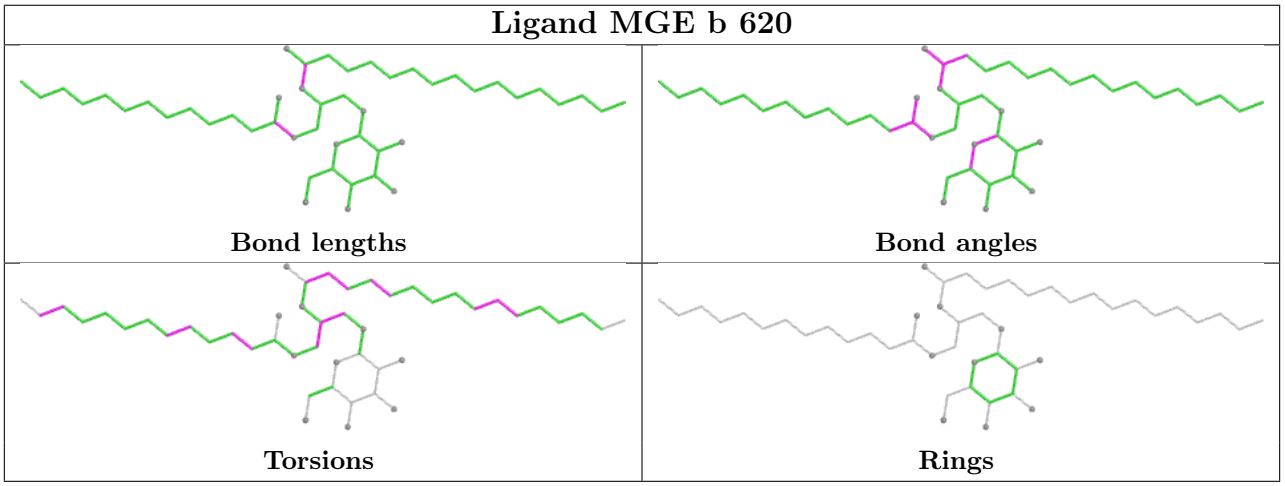
Ligand PHO a 404



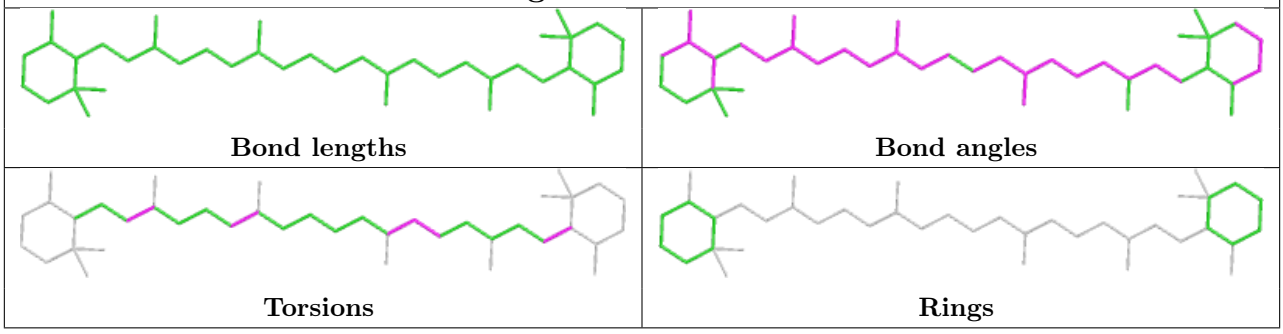
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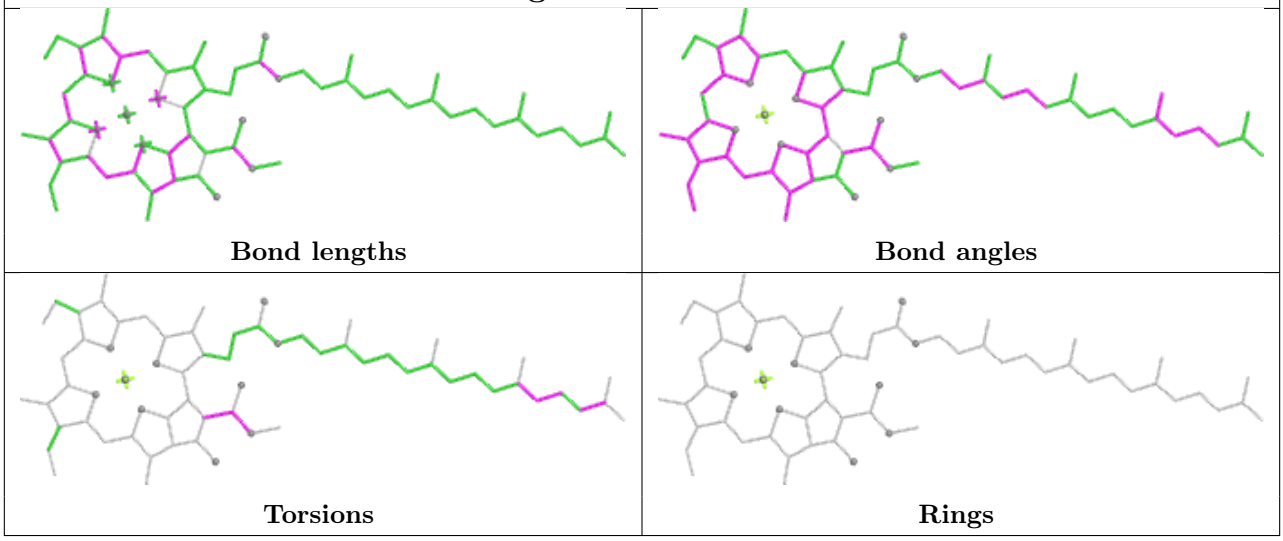
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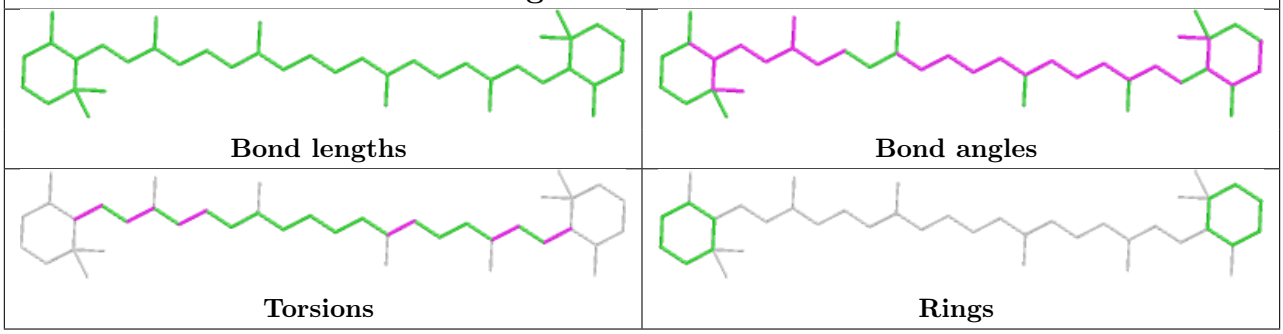
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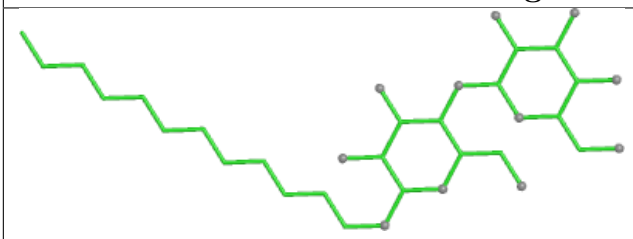
Ligand CLA b 611



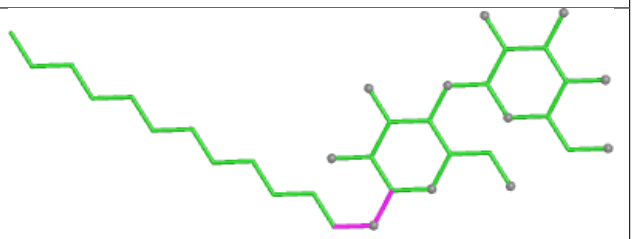
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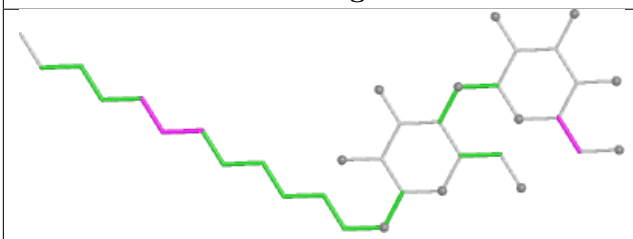
Ligand LMT d 402



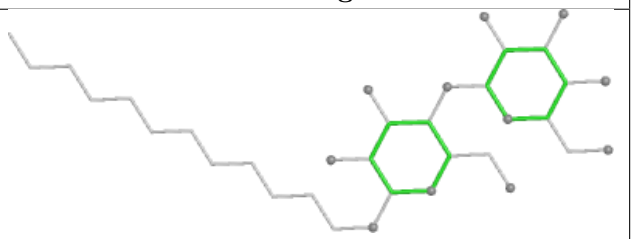
Bond lengths



Bond angles

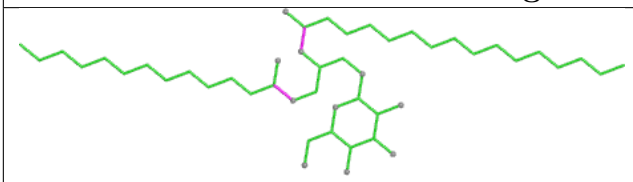


Torsions

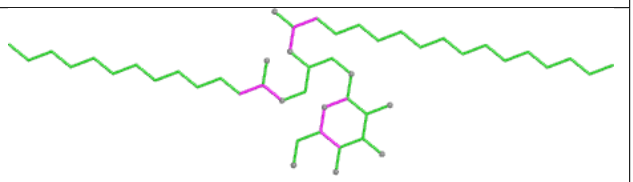


Rings

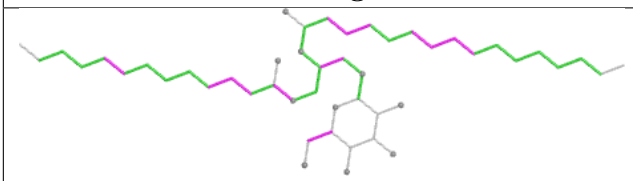
Ligand MGE a 409



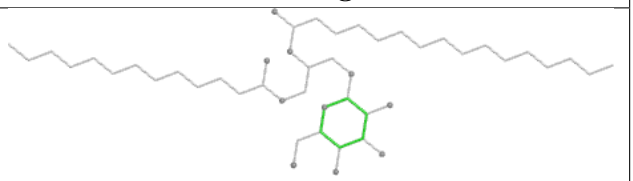
Bond lengths



Bond angles

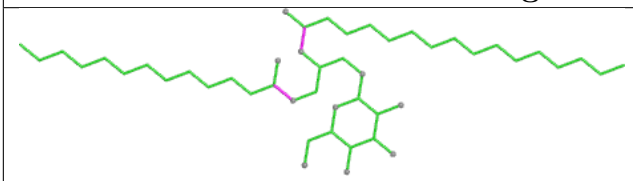


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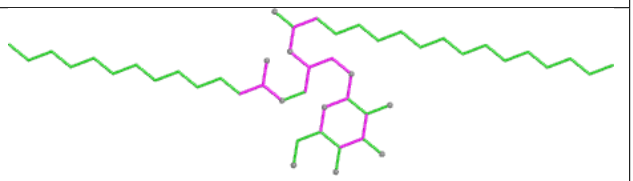


Rings

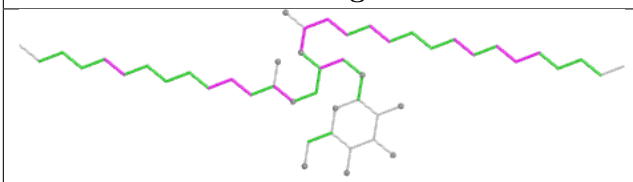
Ligand MGE b 622



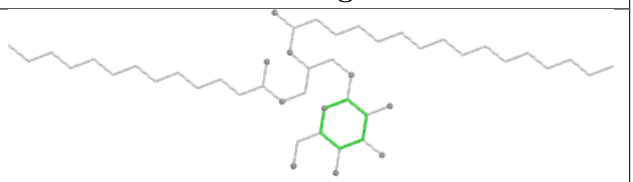
Bond lengths



Bond angles

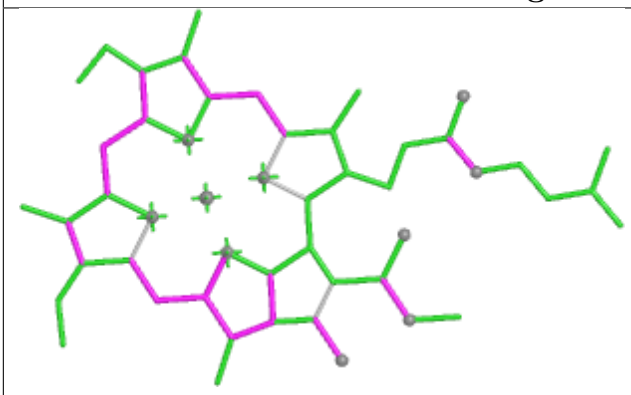


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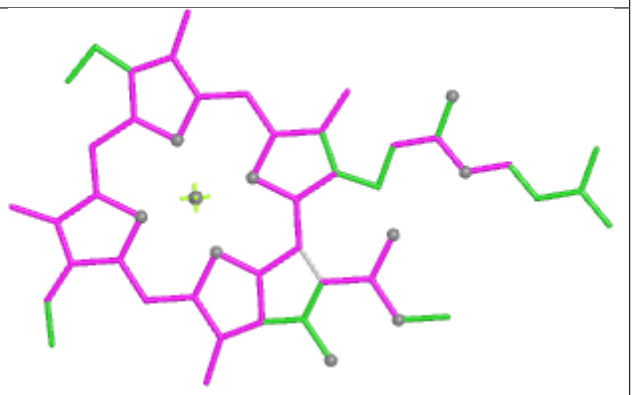


Rings

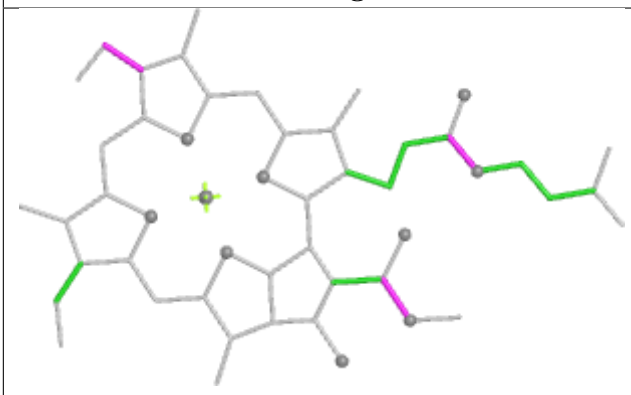
Ligand CLA d 405



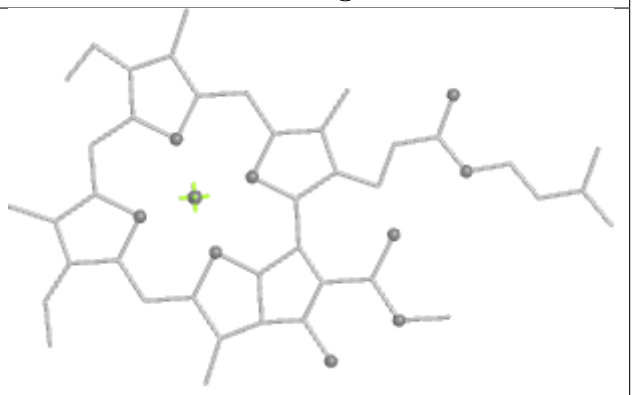
Bond lengths



Bond angles

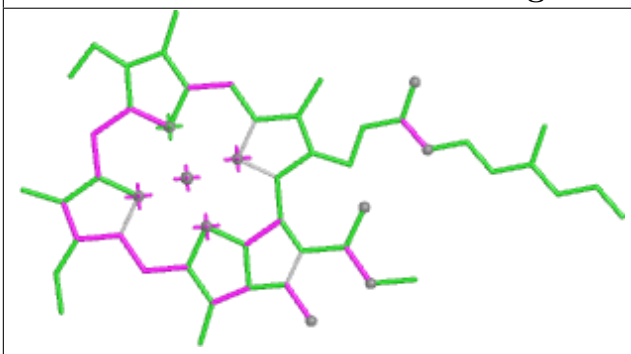


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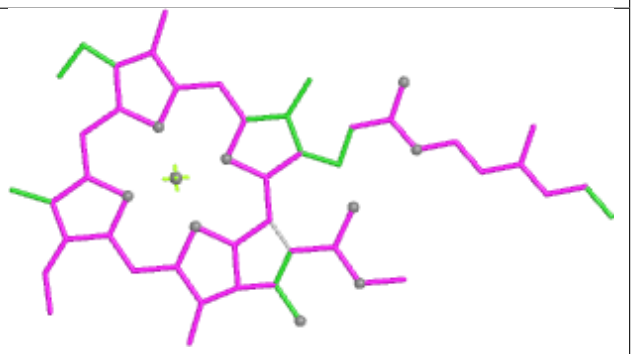


Rings

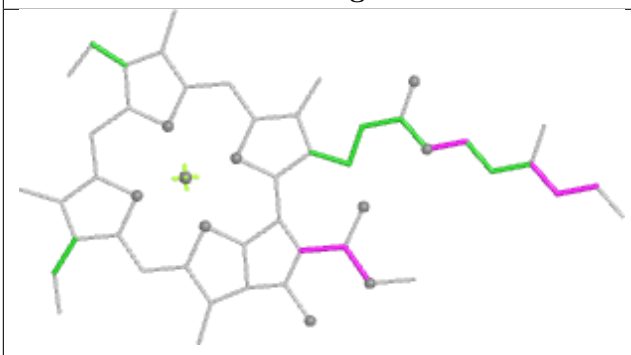
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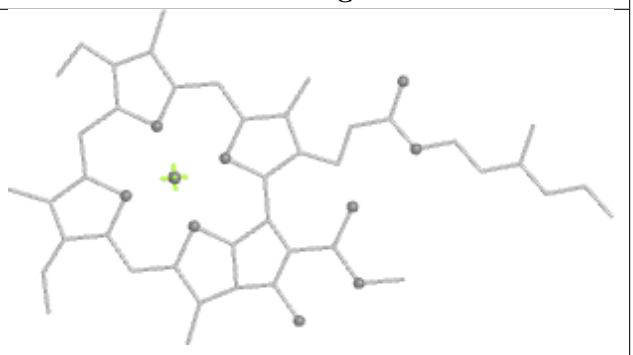
Bond lengths



Bond angles

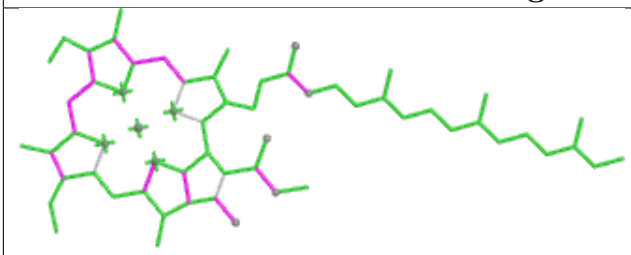


Torsions

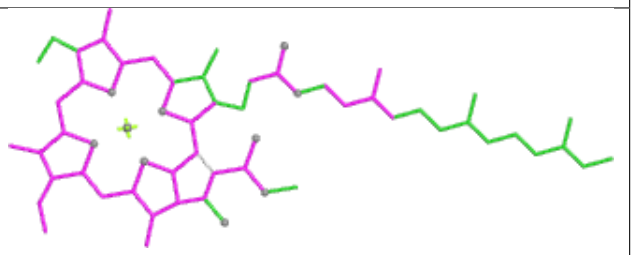


Rings

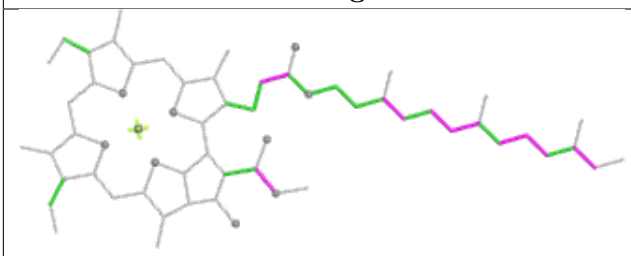
Ligand CLA d 404



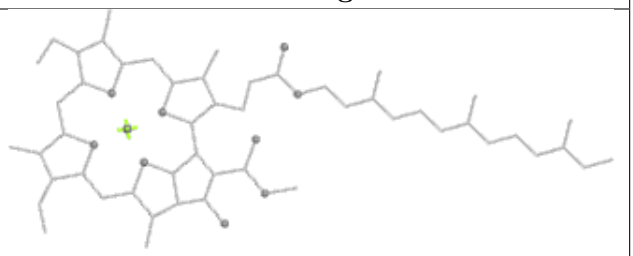
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Bond angles

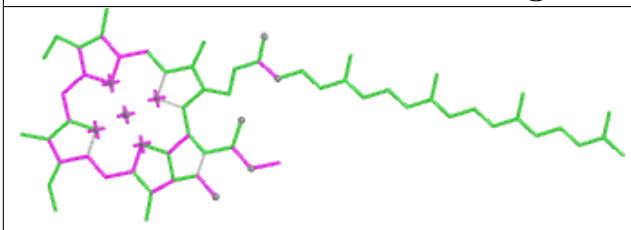


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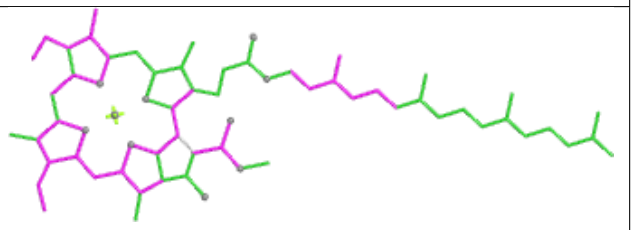


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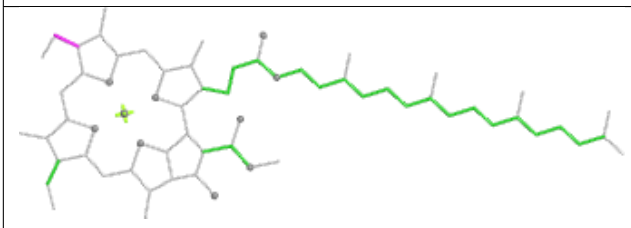
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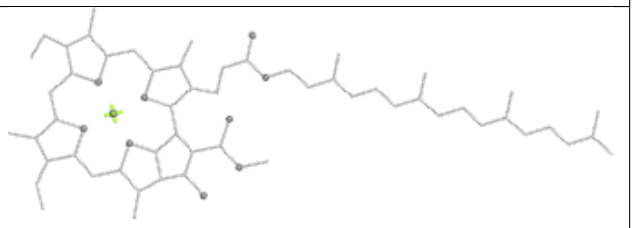
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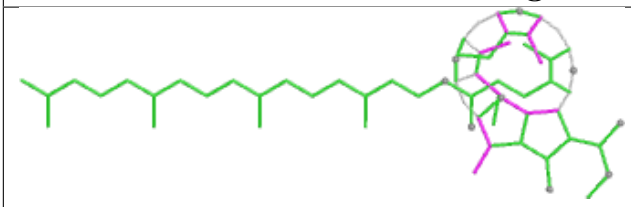


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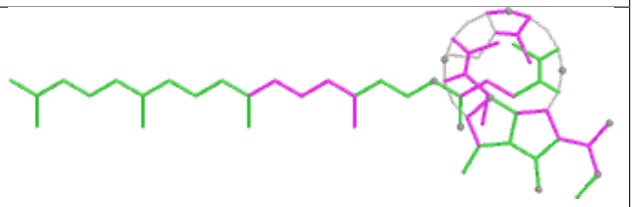


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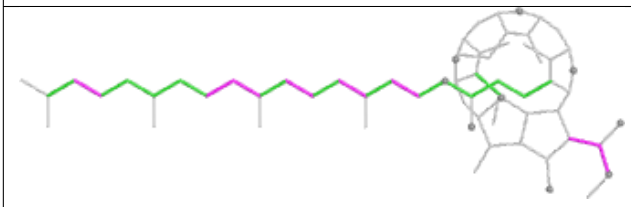
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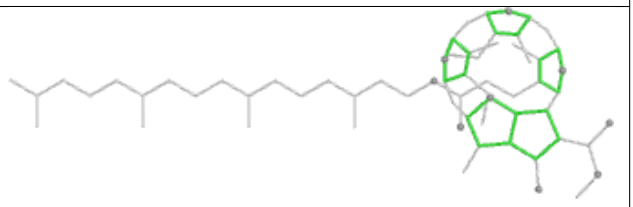
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Bond angles

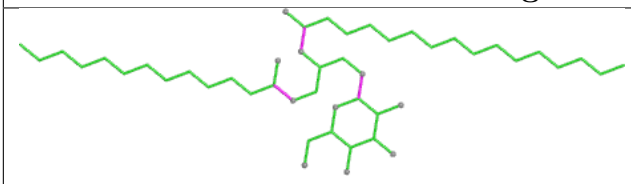


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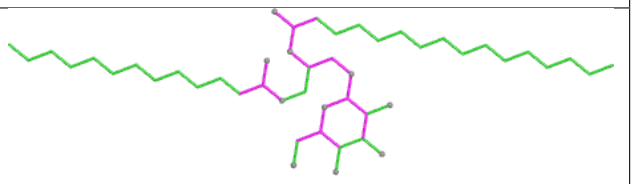


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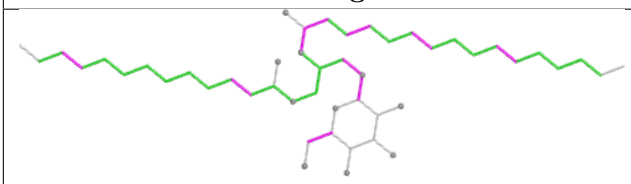
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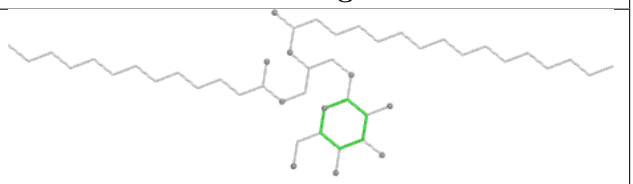
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Bond angles

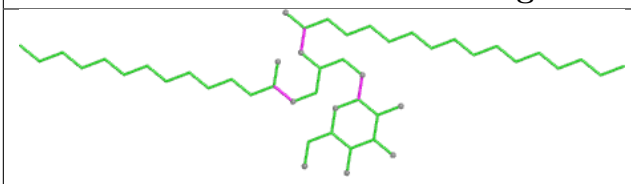


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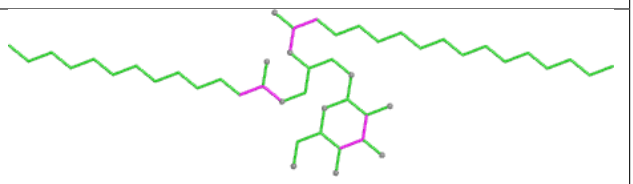


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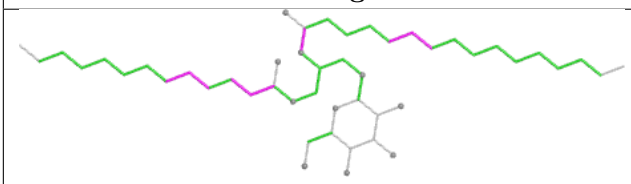
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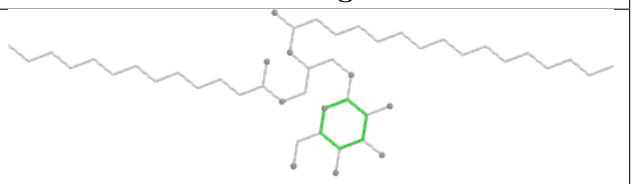
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Bond angles

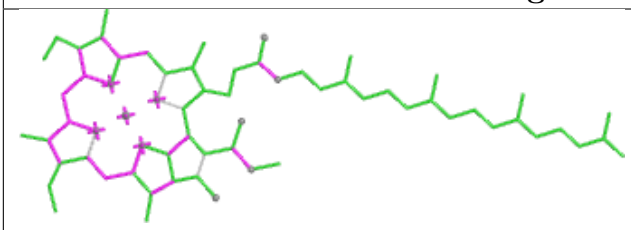


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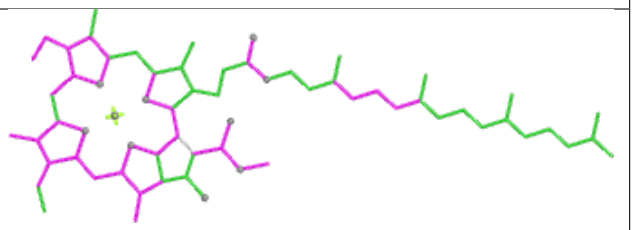


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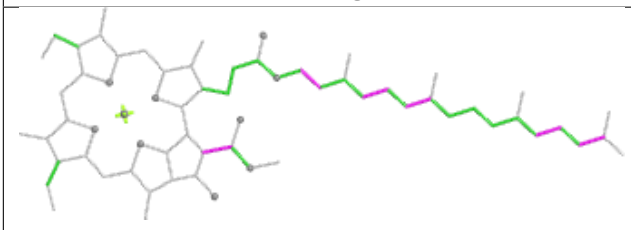
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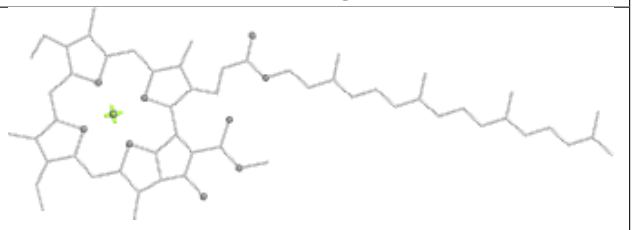
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Bond angles

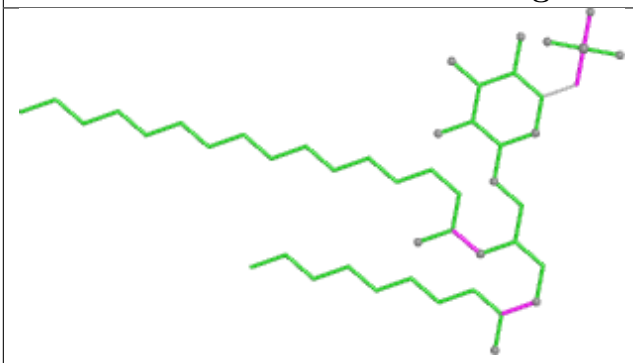


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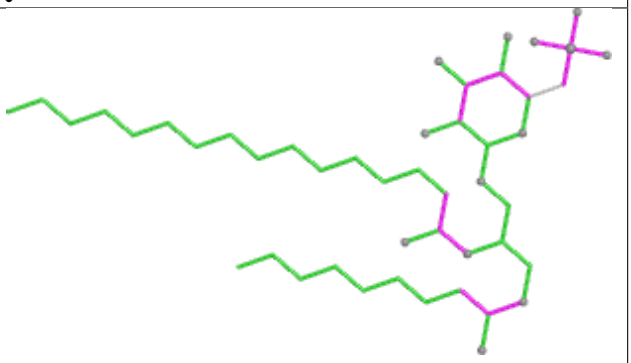


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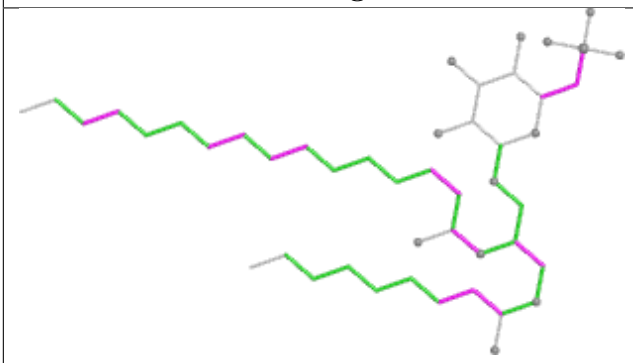
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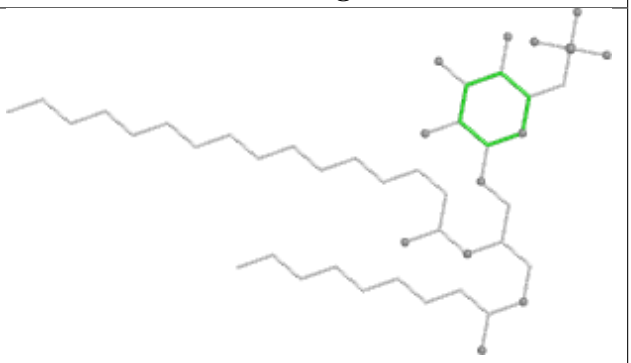
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Bond angles

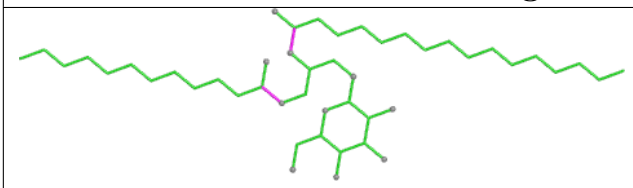


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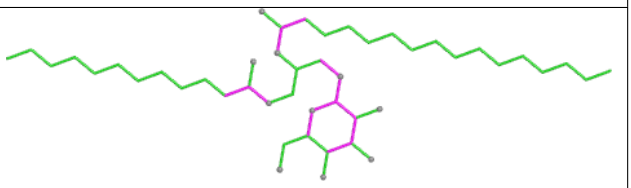


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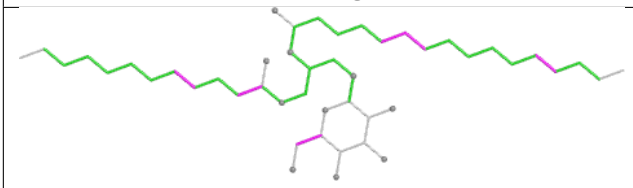
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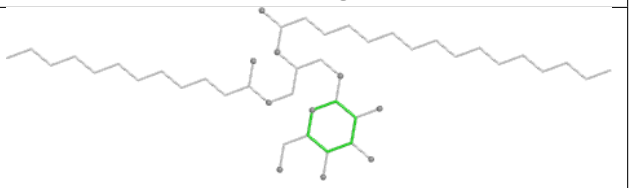
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Bond angles

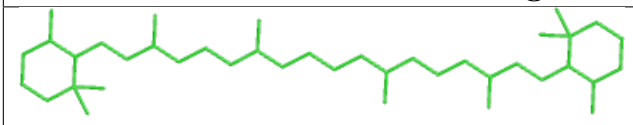


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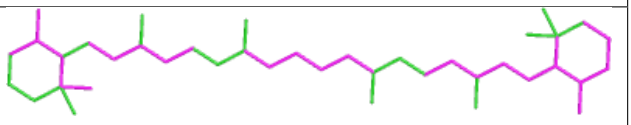


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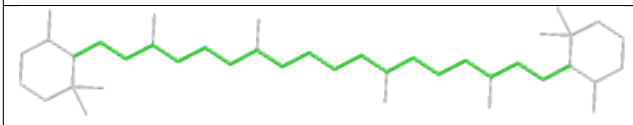
Ligand BCR b 619



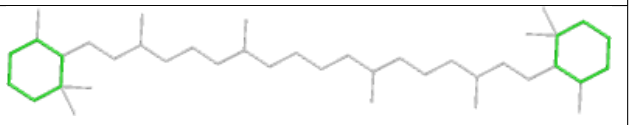
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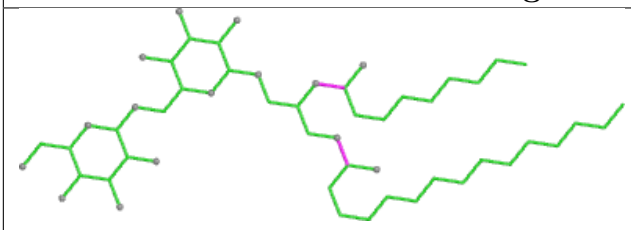


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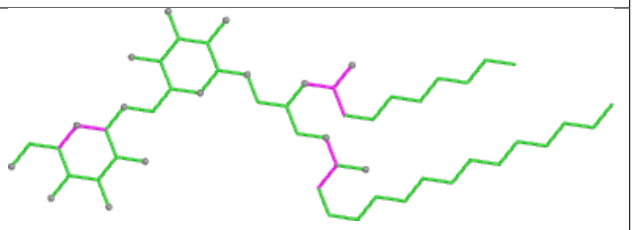


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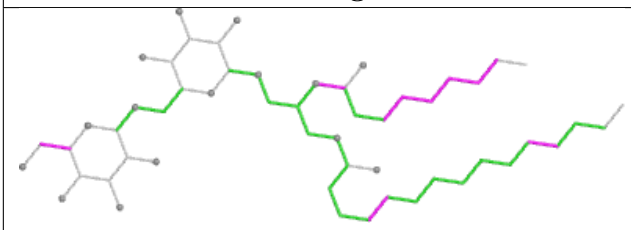
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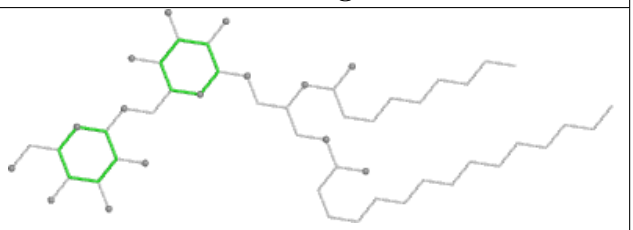
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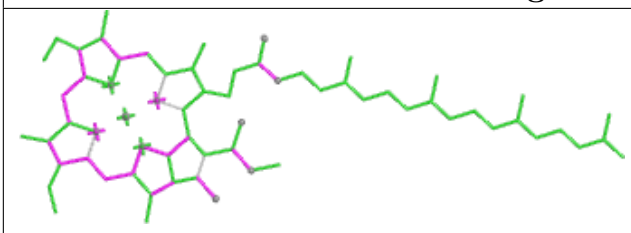


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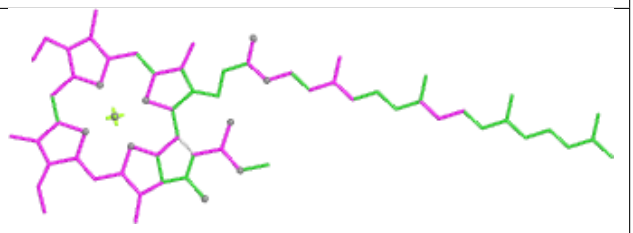


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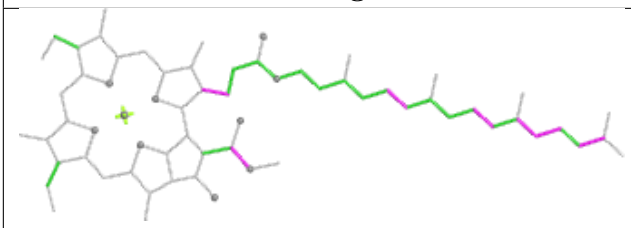
Ligand CLA b 615



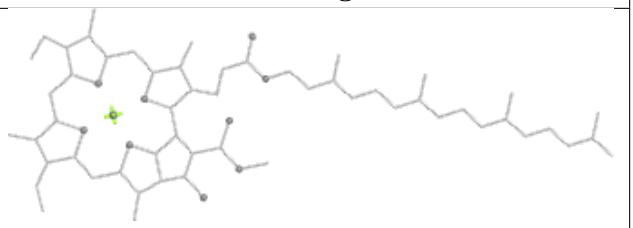
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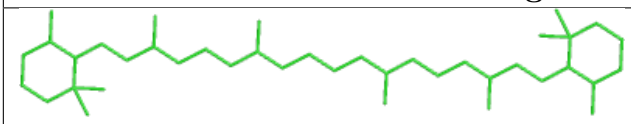


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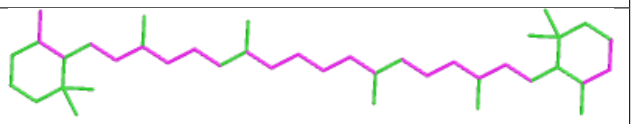


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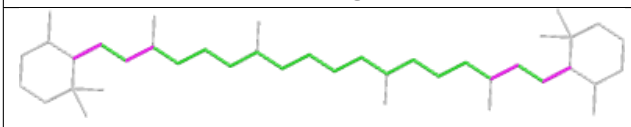
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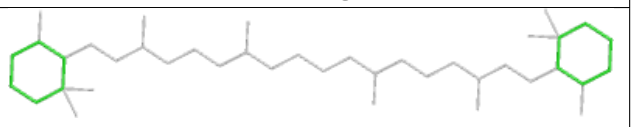
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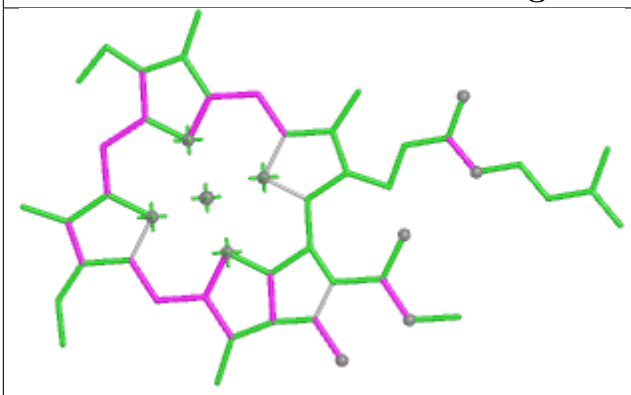


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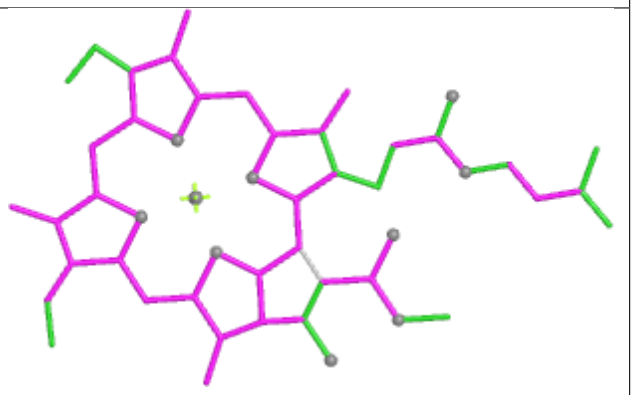


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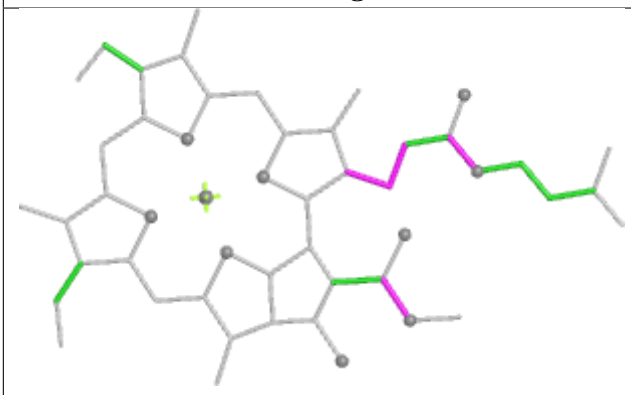
Ligand CLA a 406



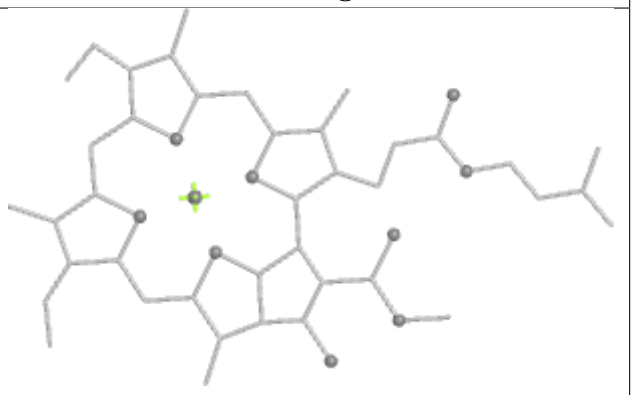
Bond lengths



Bond angles

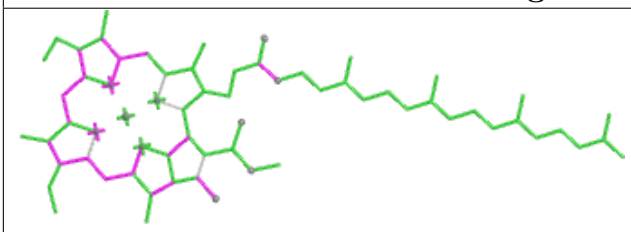


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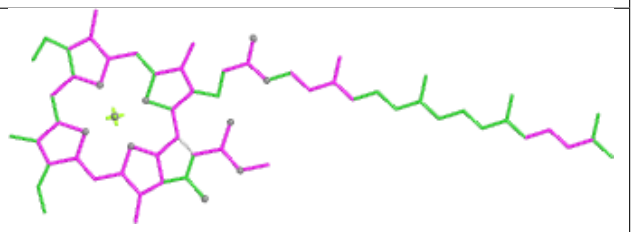


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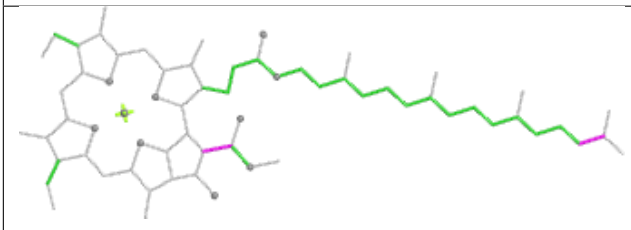
Ligand CLA b 602



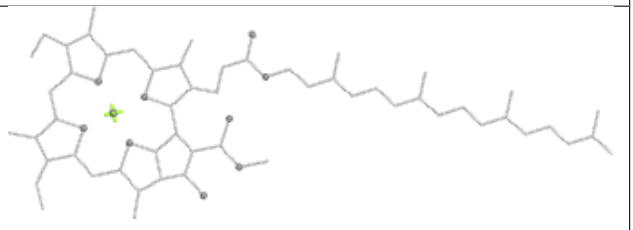
Bond lengths



Bond angles

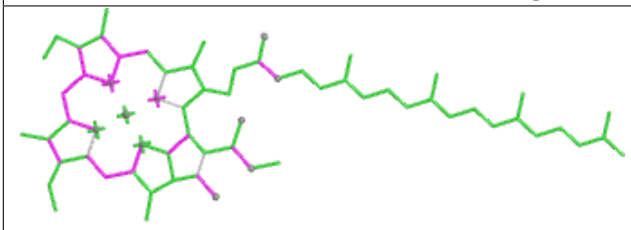


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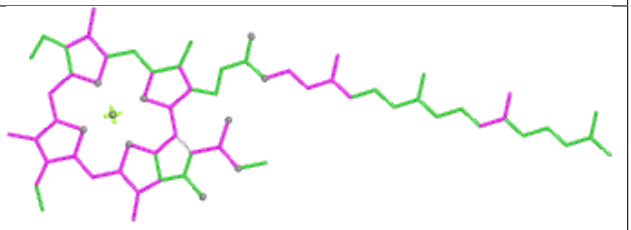


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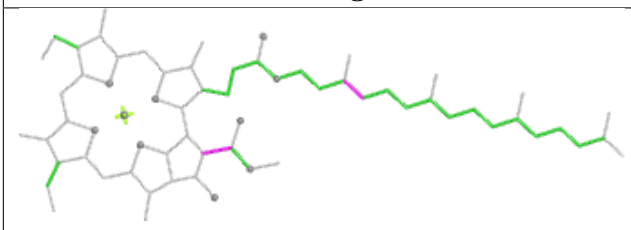
Ligand CLA b 605



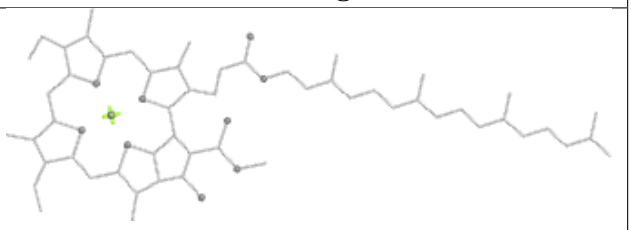
Bond lengths



Bond angles

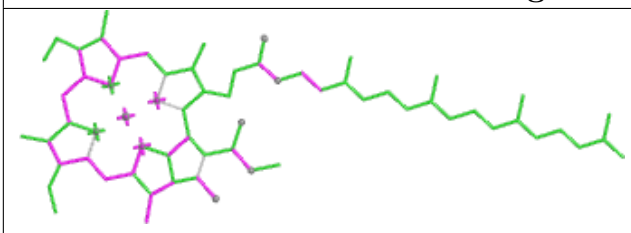


Torsions

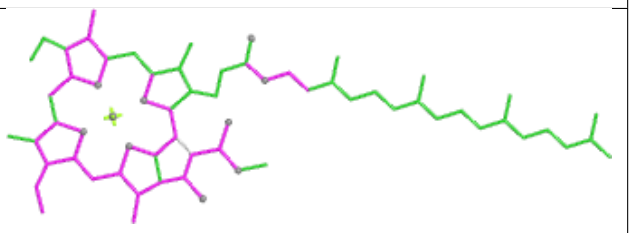


Rings

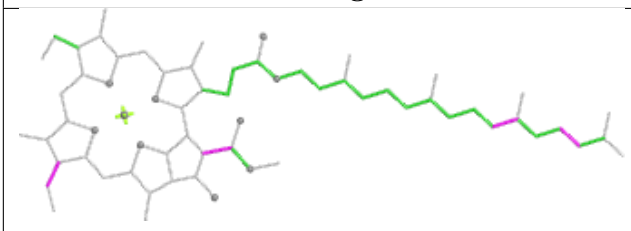
Ligand CLA d 401



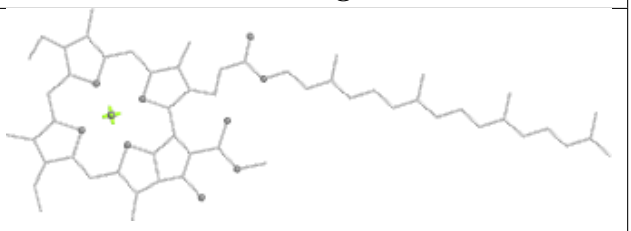
Bond lengths



Bond angles

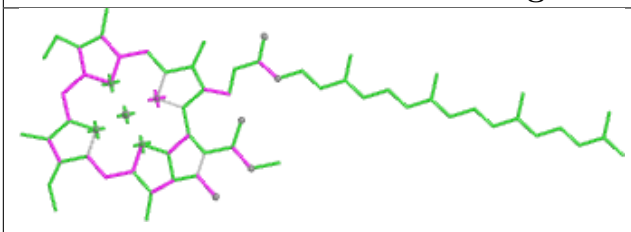


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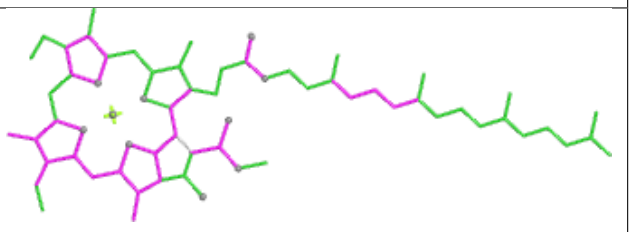


Rings

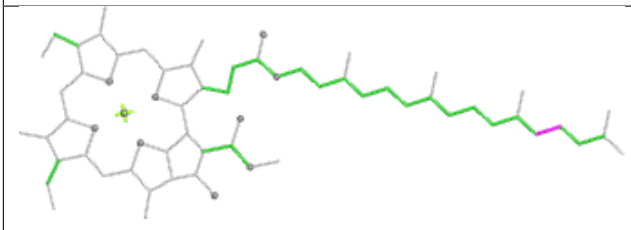
Ligand CLA b 608



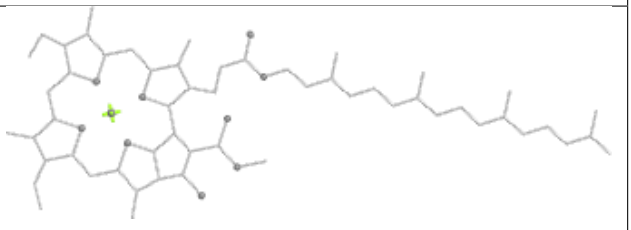
Bond lengths



Bond angles

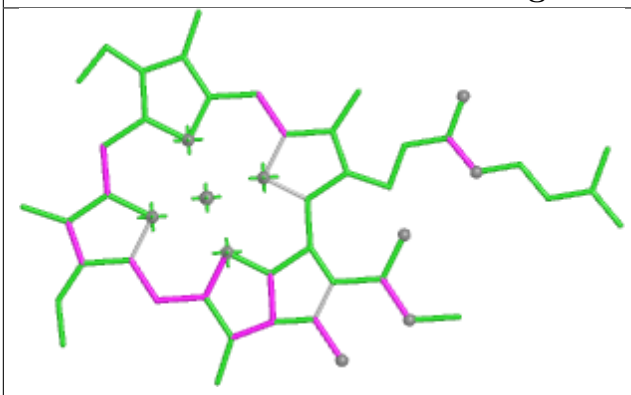


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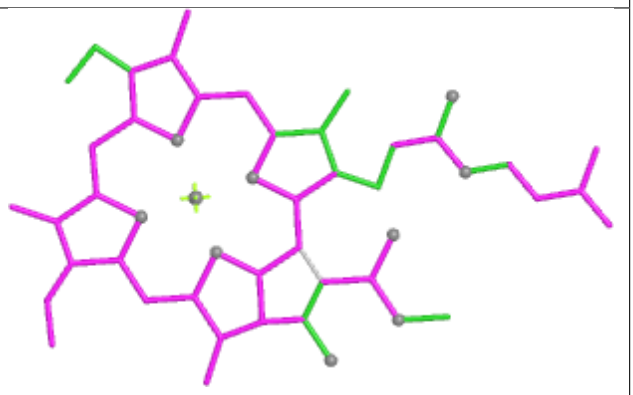


Rings

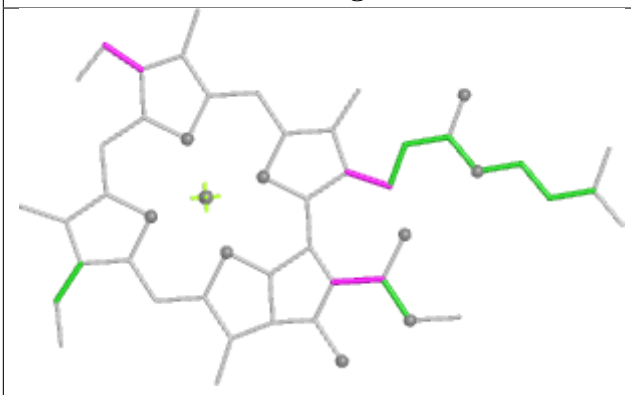
Ligand CLA a 403



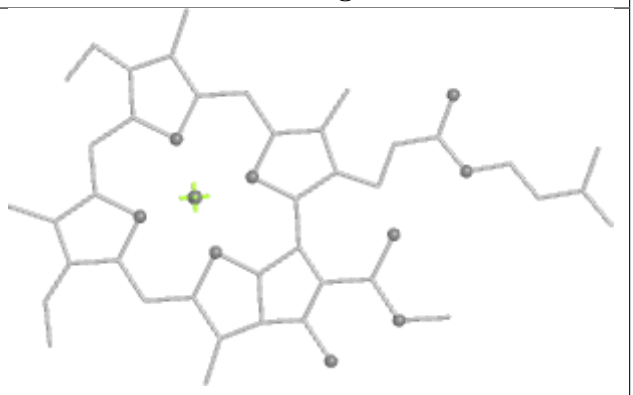
Bond lengths



Bond angles

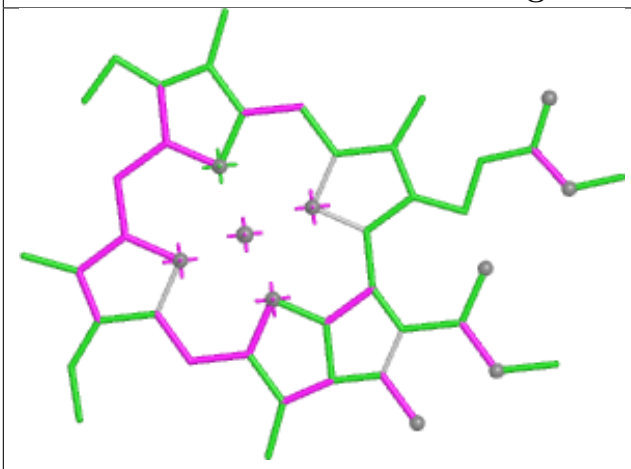


Torsions

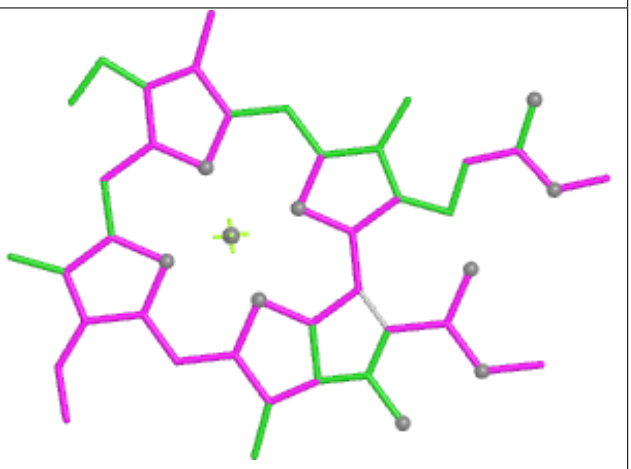


Rings

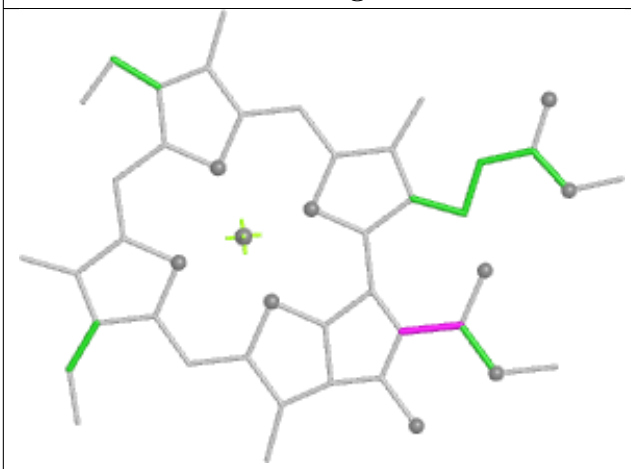
Ligand CLA b 616



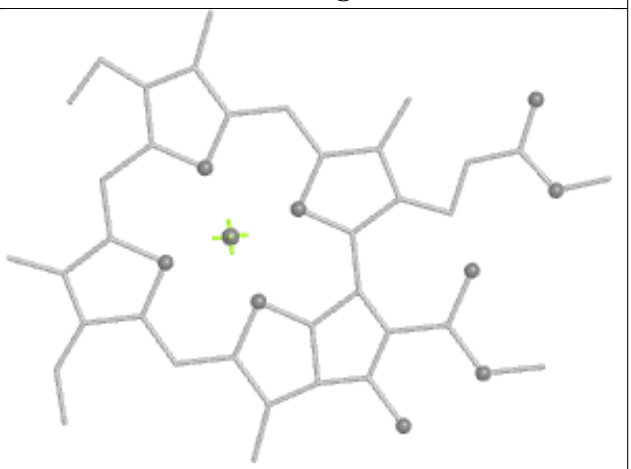
Bond lengths



Bond angles



Torsions

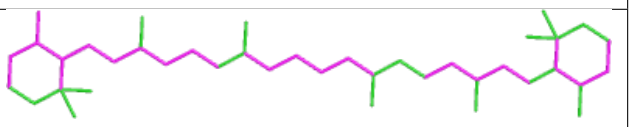


Rings

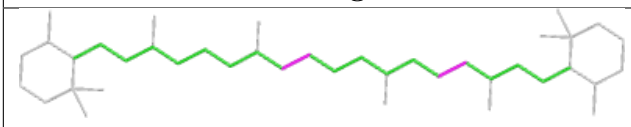
Ligand BCR b 618



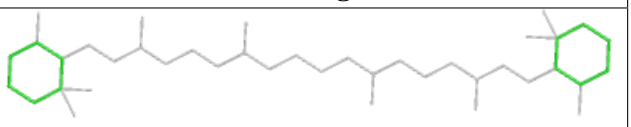
Bond lengths



Bond angles

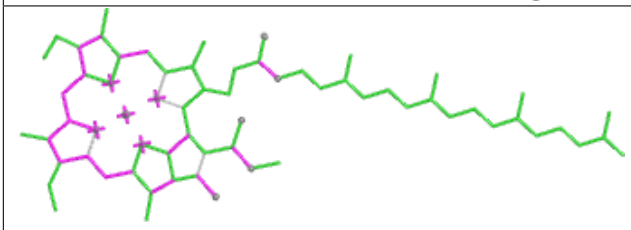


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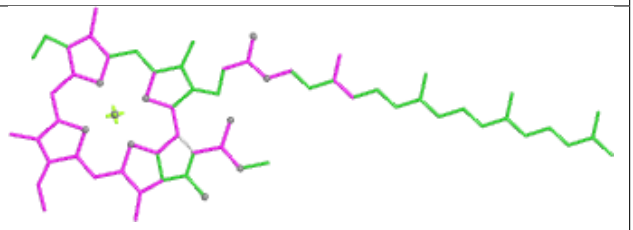


Rings

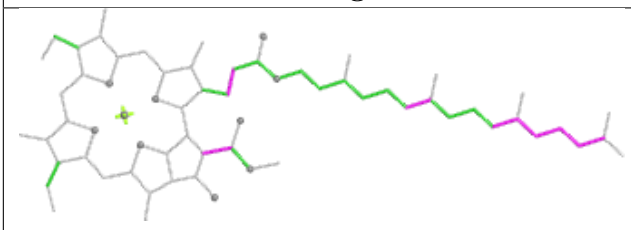
Ligand CLA b 606



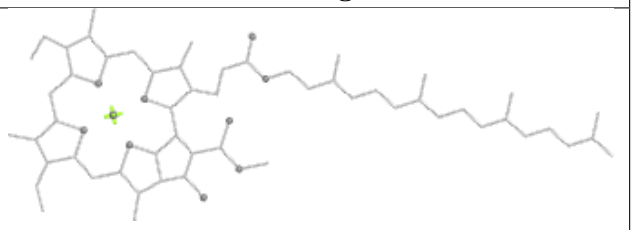
Bond lengths



Bond angles

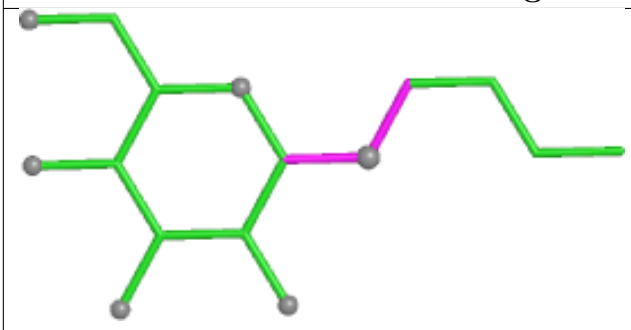


Torsions

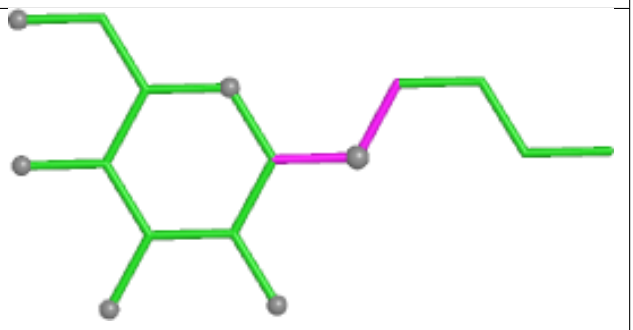


Rings

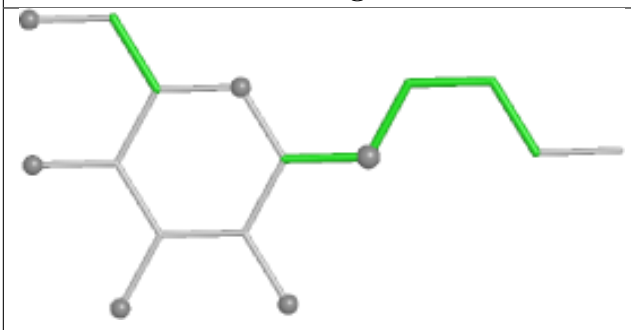
Ligand HTG d 411



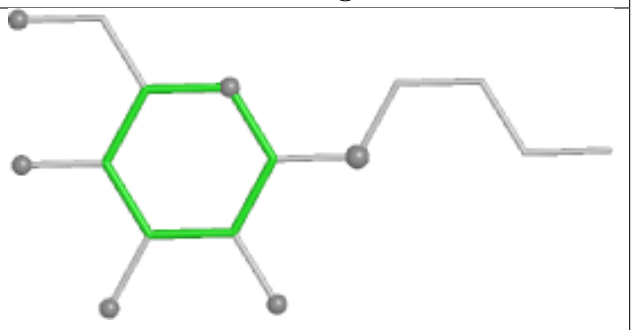
Bond lengths



Bond angles

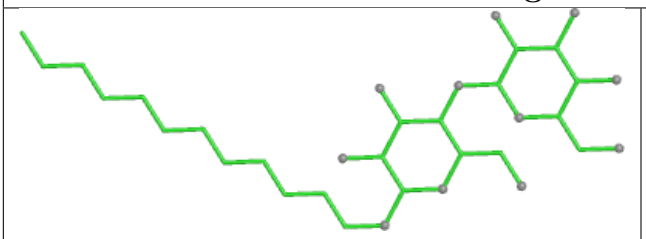


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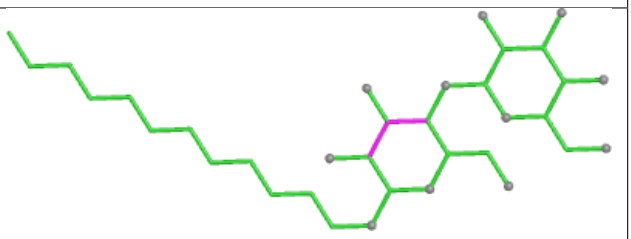


Rings

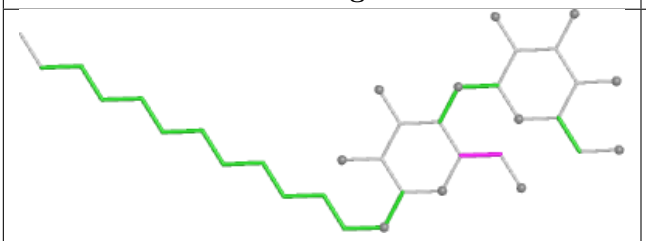
Ligand LMT b 623



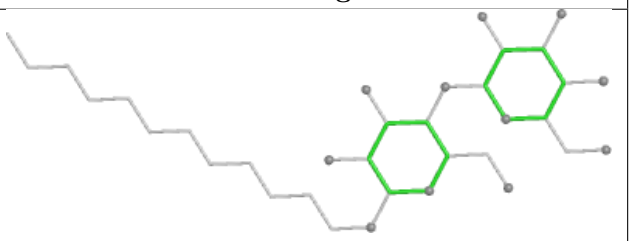
Bond lengths



Bond angles

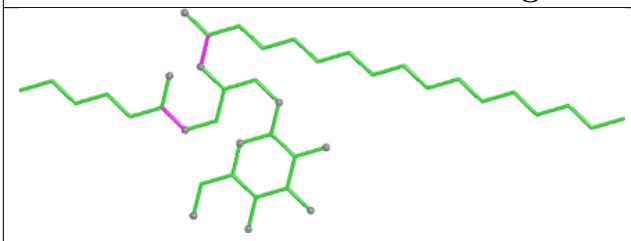


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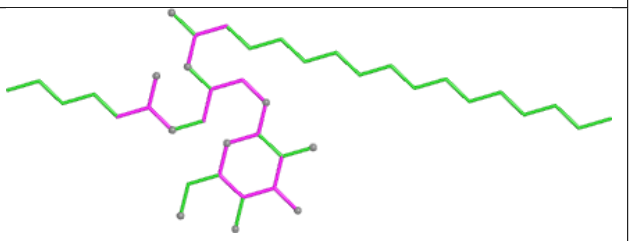


Rings

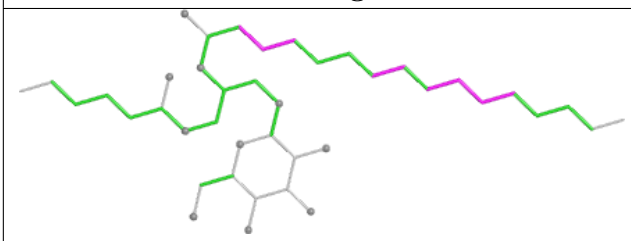
Ligand MGE d 409



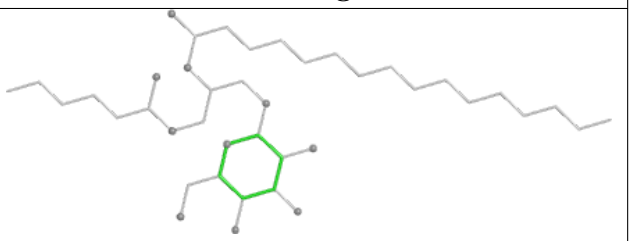
Bond lengths



Bond angles

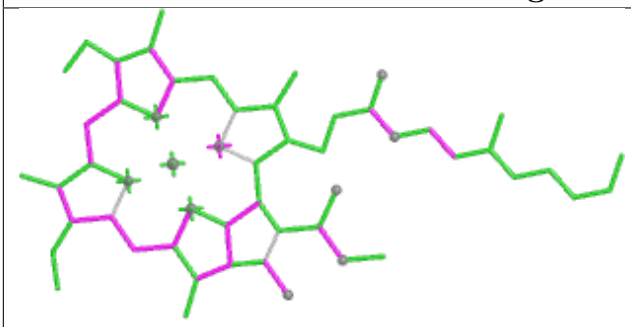


Torsions

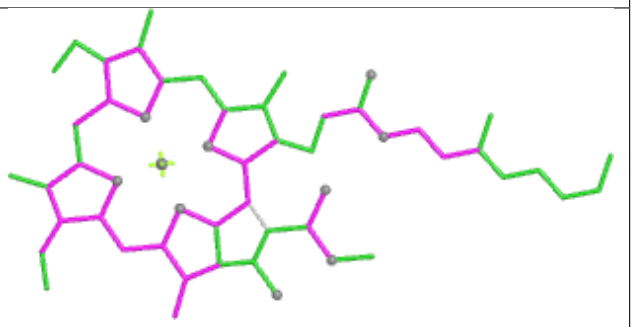


Rings

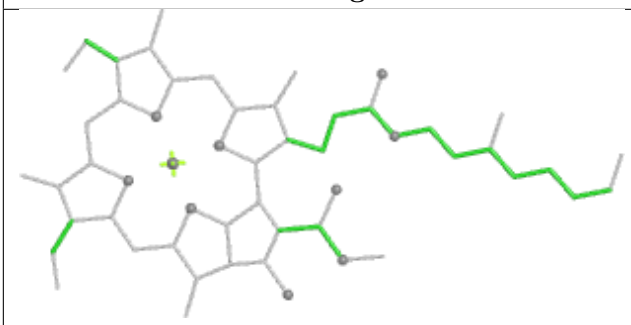
Ligand CLA b 613



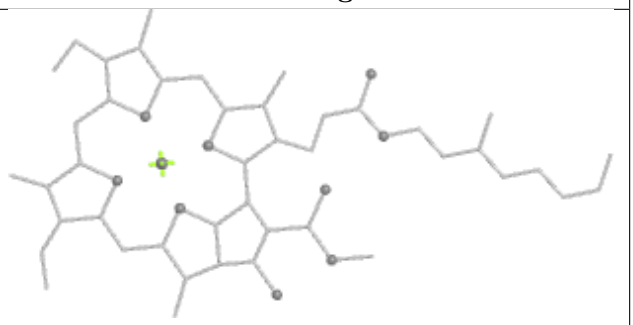
Bond lengths



Bond angles

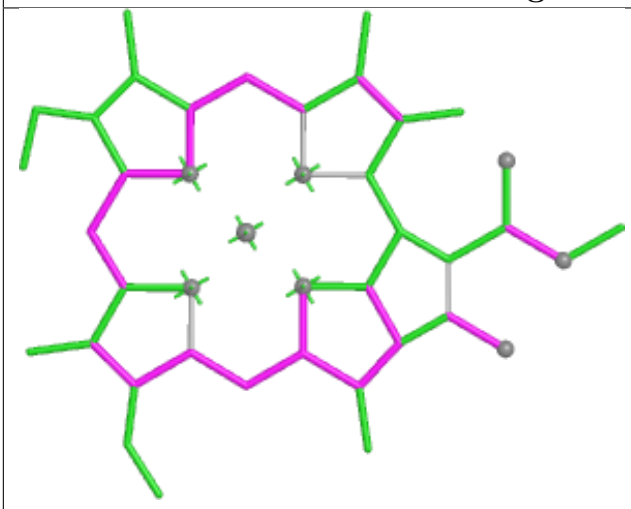


Torsions

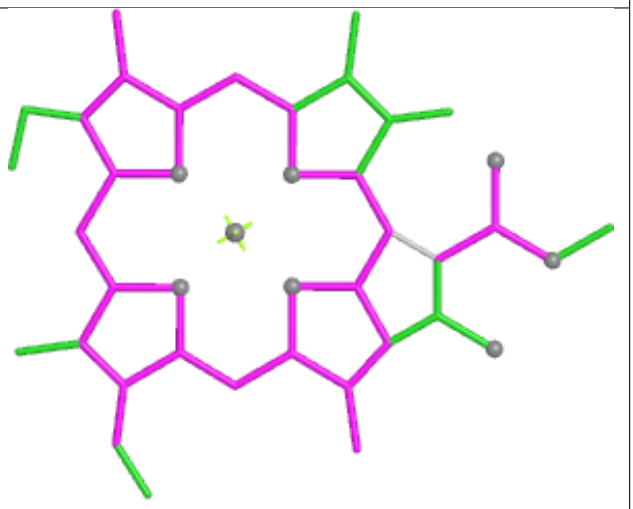


Rings

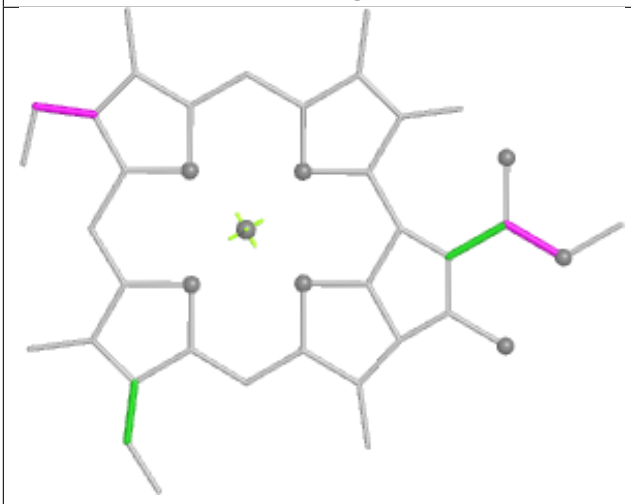
Ligand CLA b 601



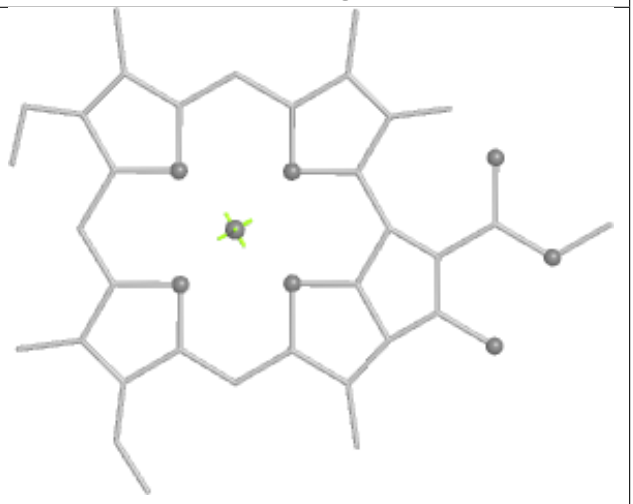
Bond lengths



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.

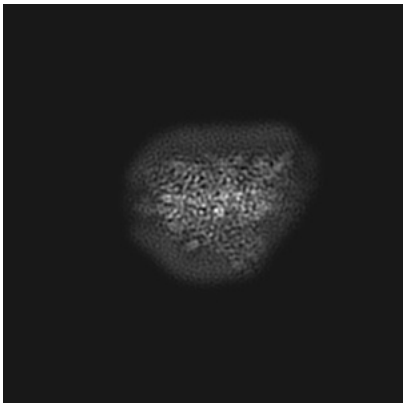
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30902. These allow visual inspection of the internal detail of the map and identification of artifacts.

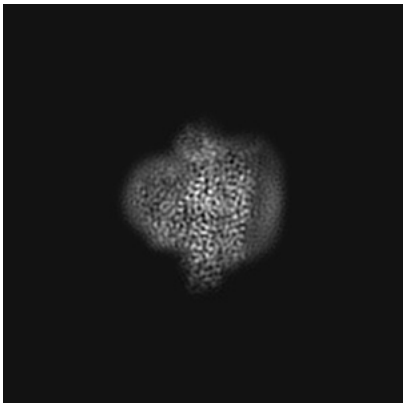
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

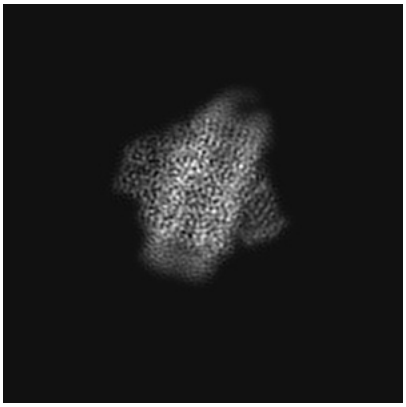
6.1.1 Primary map



X



Y

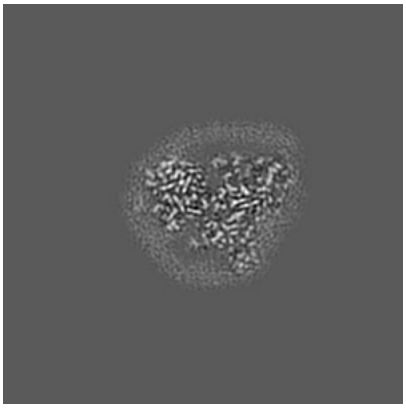


Z

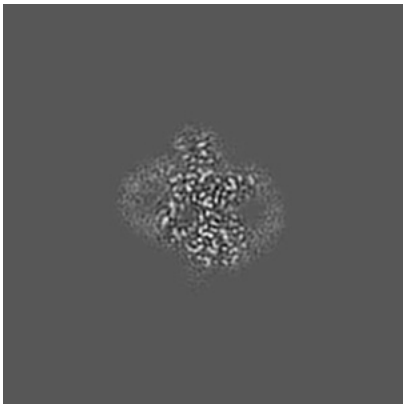
The images above show the map projected in three orthogonal directions.

6.2 Central slices

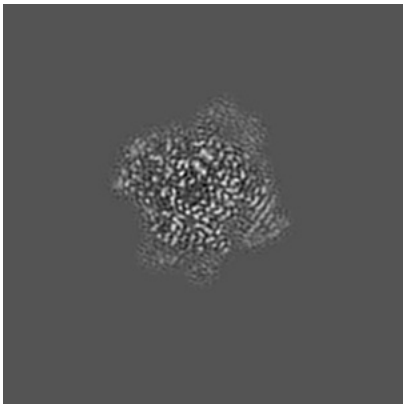
6.2.1 Primary map



X Index: 100



Y Index: 100

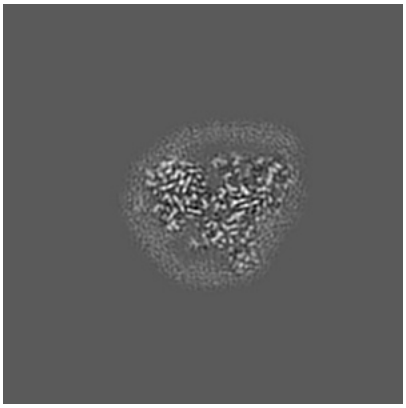


Z Index: 100

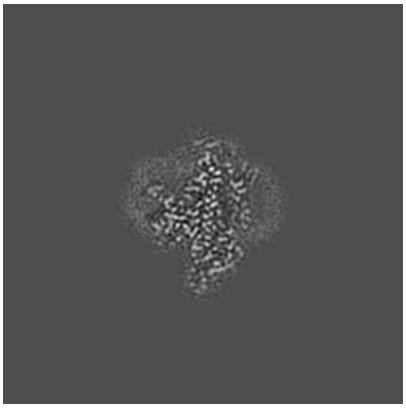
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

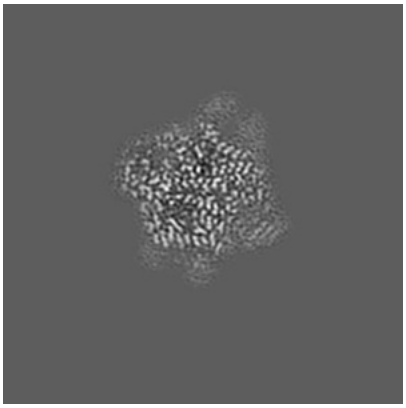
6.3.1 Primary map



X Index: 100



Y Index: 110

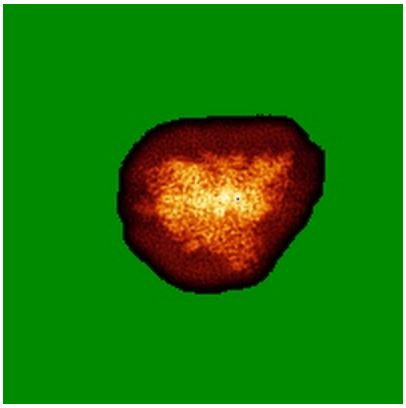


Z Index: 103

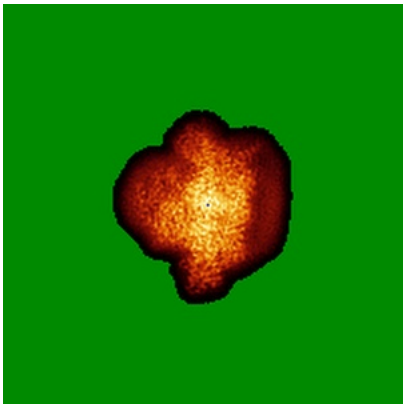
The images above show the largest variance slices of the map in three orthogonal directions.

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

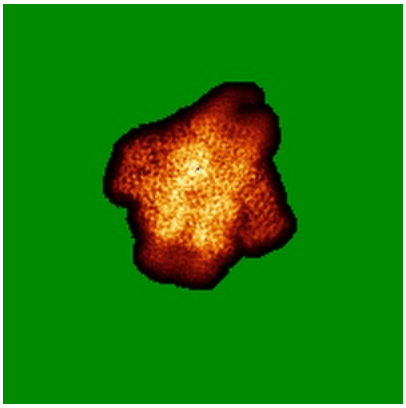
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

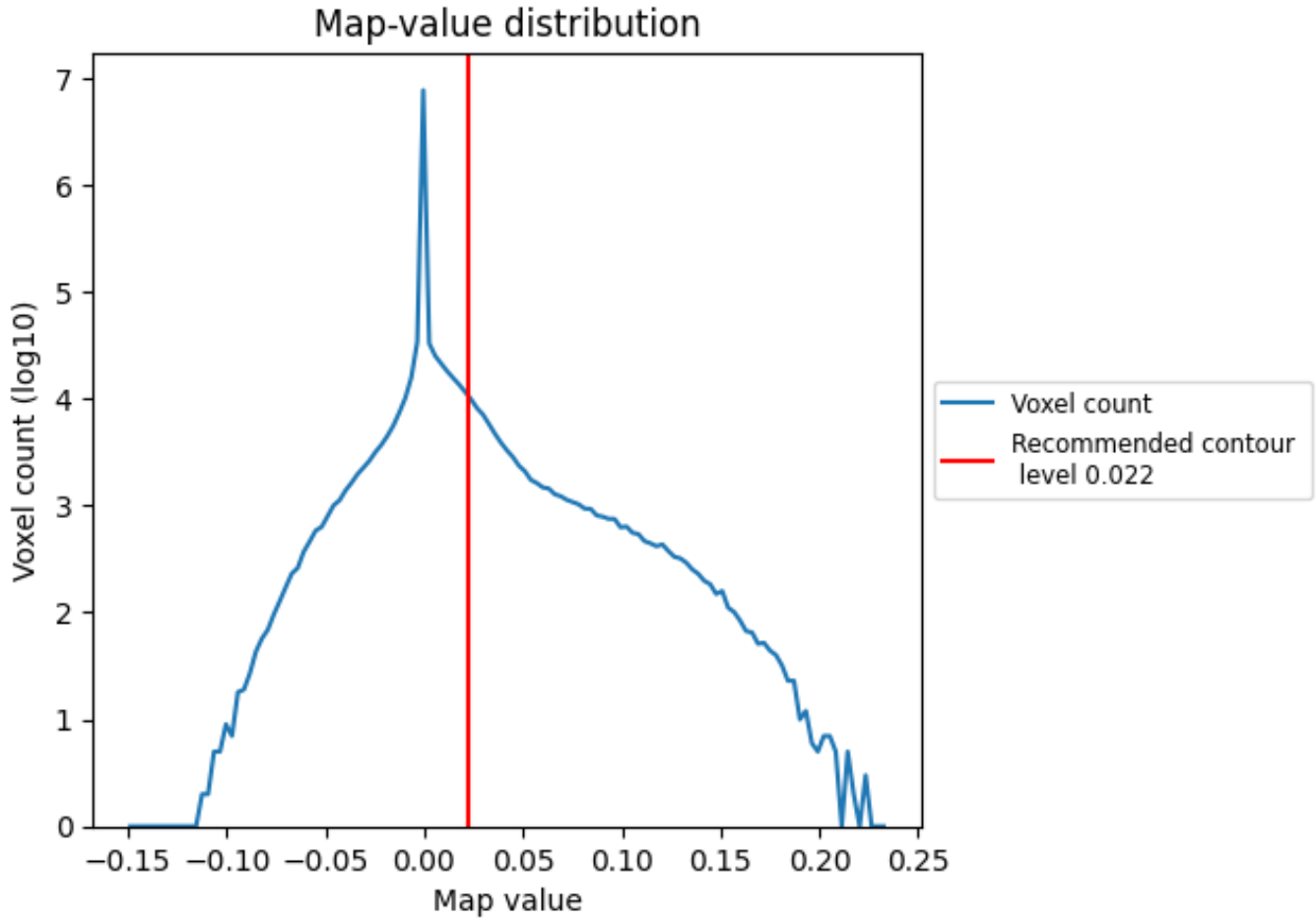
6.6 Mask visualisation (i)

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

7 Map analysis

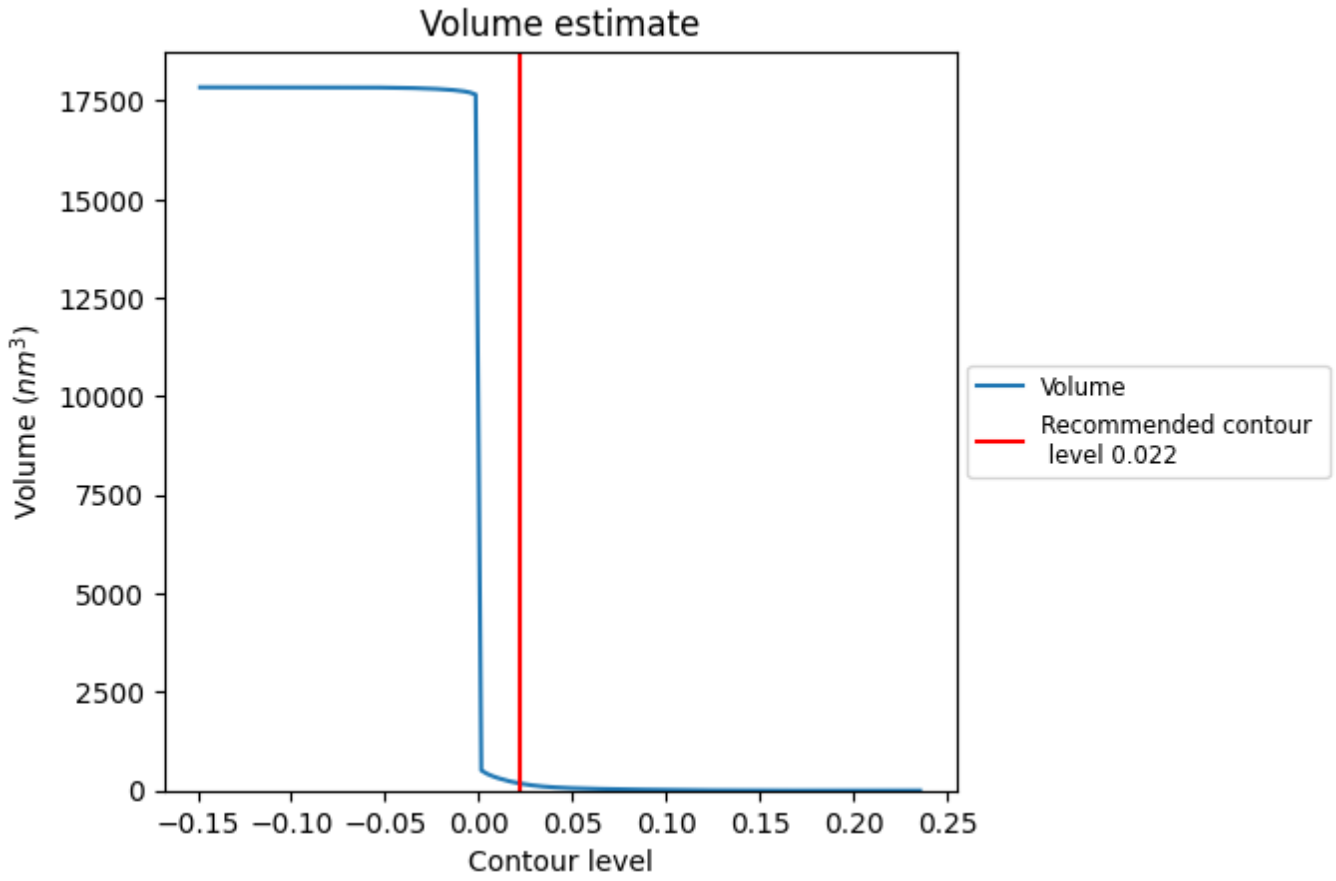
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

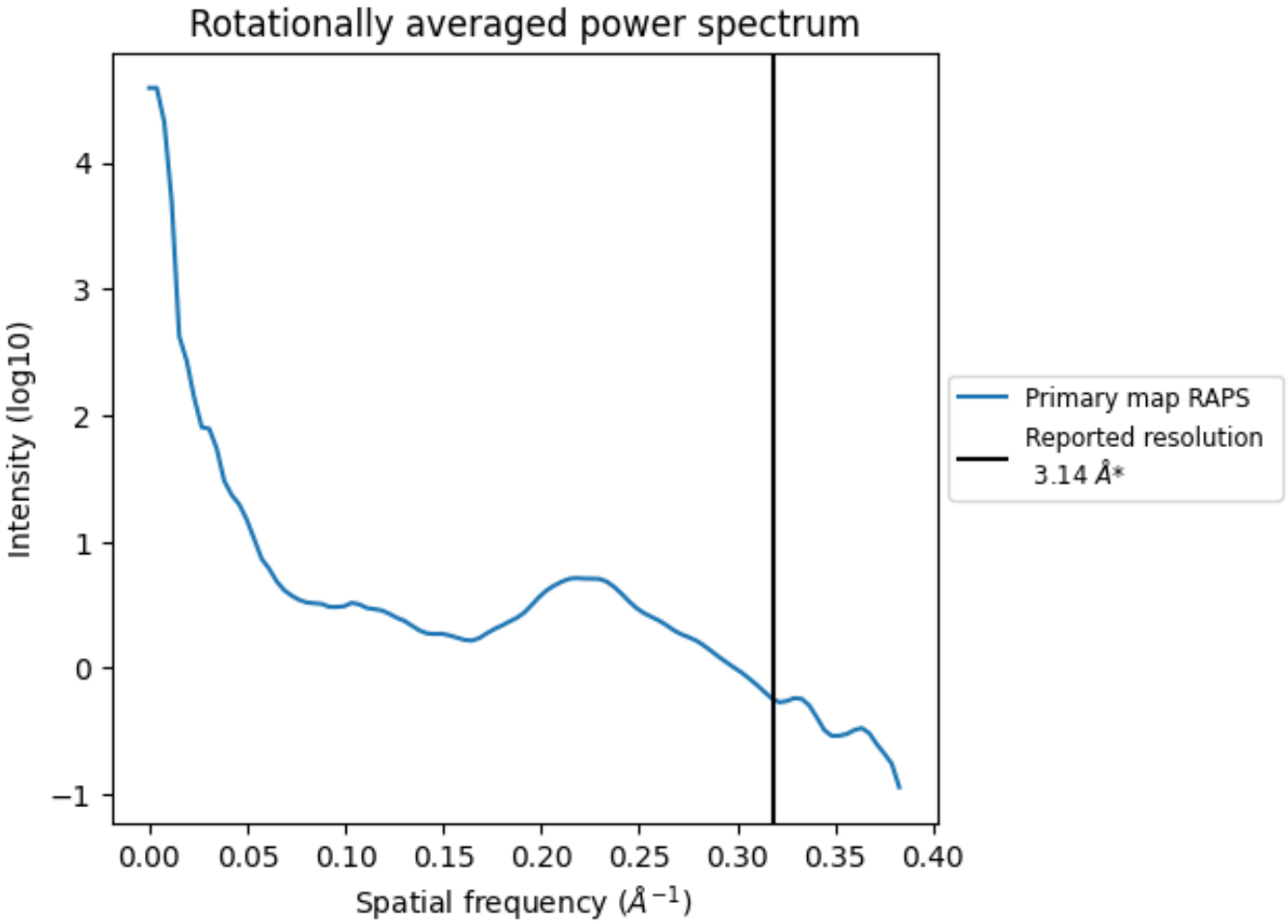
7.2 Volume estimate (i)



The volume at the recommended contour level is 181 nm^3; this corresponds to an approximate mass of 163 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 0.318 Å^{-1}

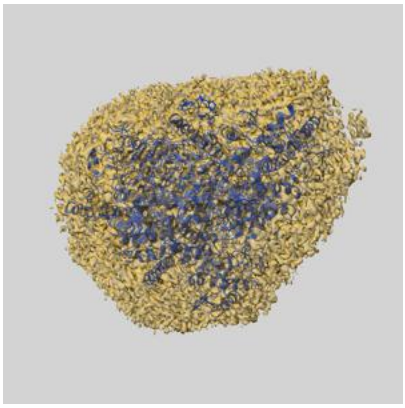
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

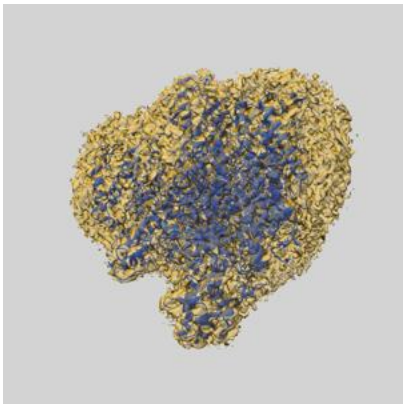
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30902 and PDB model 7DXA. Per-residue inclusion information can be found in section 3 on page 14.

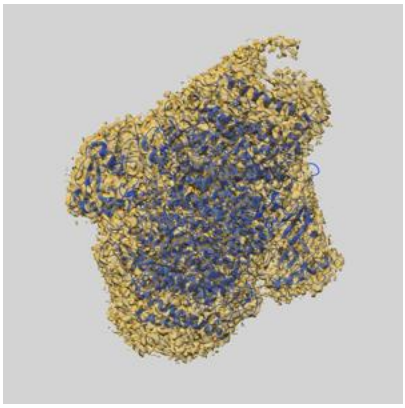
9.1 Map-model overlay



X



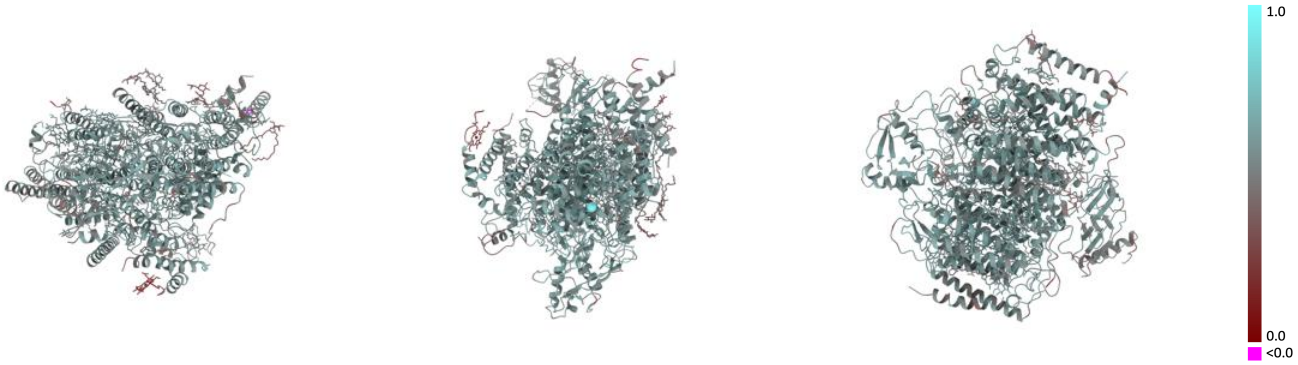
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 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.

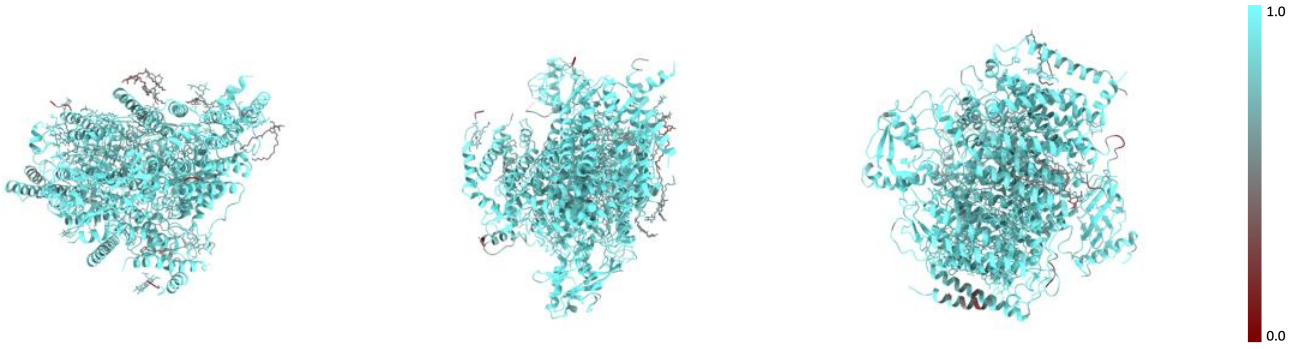
9.2 Q-score mapped to coordinate model (i)



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.

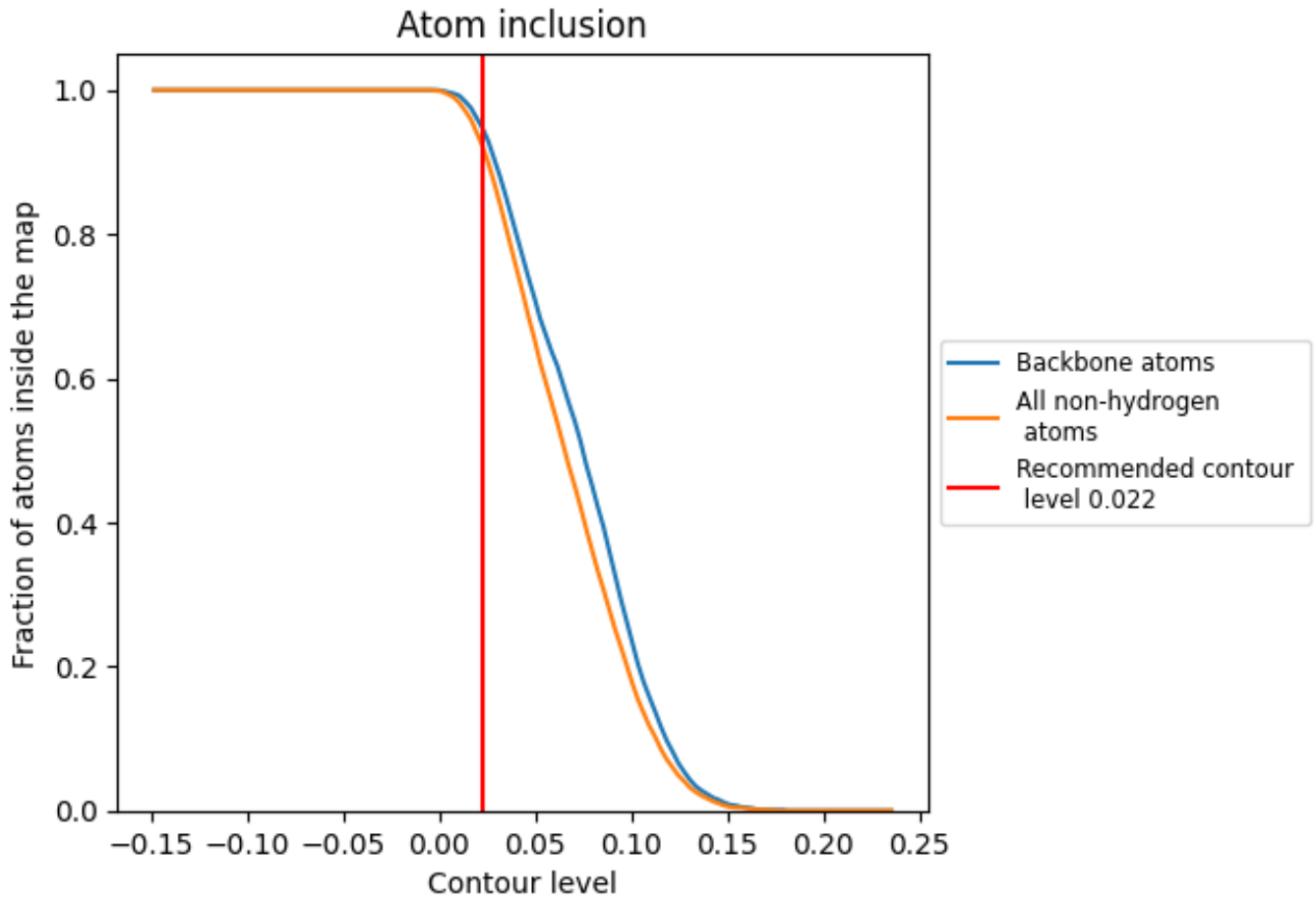
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.022).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9240	0.5680
A	0.9200	0.5280
B	0.8660	0.5290
C	0.7300	0.4980
a	0.9400	0.5640
b	0.9440	0.5840
d	0.9500	0.5940
e	0.8070	0.4830
f	0.9540	0.5290
h	0.9660	0.5830
i	0.8440	0.4770
l	0.8350	0.5560
m	0.7870	0.5070
t	0.7920	0.5400
x	0.8810	0.5480

