wwPDB EM Validation Summary Report (i)

Apr 22, 2024 – 05:42 pm BST

PDB ID	:	7NHQ
EMDB ID	:	EMD-12337
Title	:	Structure of PSII-I prime (PSII with Psb28, and Psb34)
Authors	:	Zabret, J.; Bohn, S.; Schuller, S.K.; Arnolds, O.; Chan, A.; Tajkhorshid, E.; Stoll, R.; Engel, B.D.; Rudack, T.; Schuller, J.M.; Nowaczyk, M.M.
Deposited on	:	2021-02-11
Resolution	:	2.68 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:

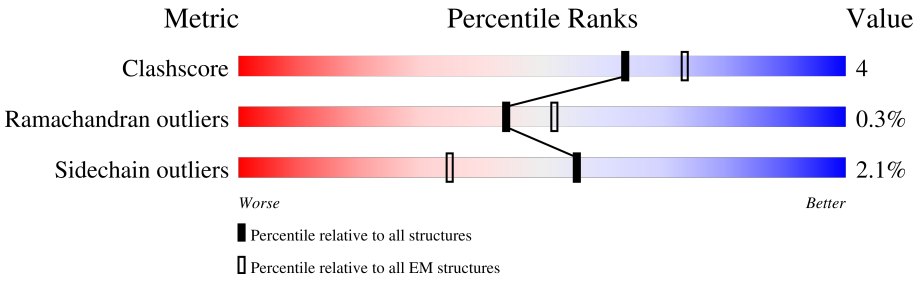
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.68 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	360	6% 86% 6% · 7%
2	B	510	· 94% · ·
3	C	461	5% 84% 9% · 6%
4	D	352	· 89% 8% · ·
5	E	84	17% 80% 11% · 8%
6	F	45	16% 71% 11% · 16%
7	H	66	· 94% · · ·
8	I	38	· 61% 5% · 32%

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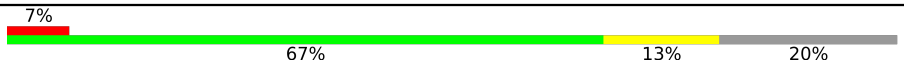
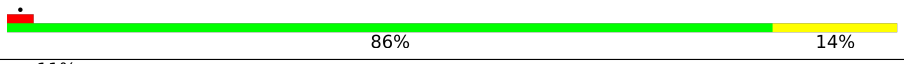
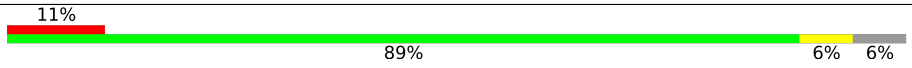
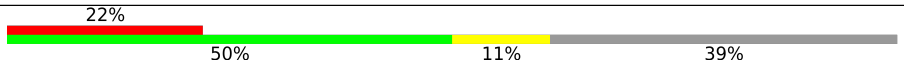
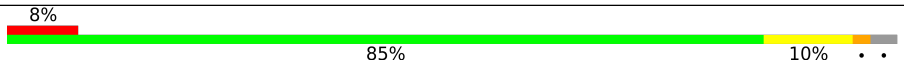
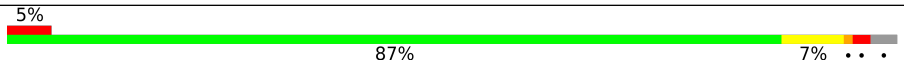
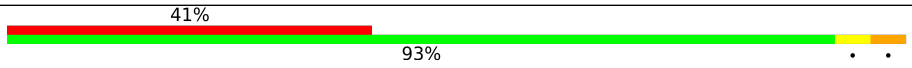
Mol	Chain	Length	Quality of chain
9	K	46	
10	L	37	
11	M	36	
12	T	32	
13	X	41	
14	y	46	
15	Z	62	
16	2	116	
17	3	56	

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
21	PHO	A	404	X	-	-	-
21	PHO	D	406	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	605	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	609	X	-	-	-
22	CLA	B	610	X	-	-	-
22	CLA	B	611	X	-	-	-
22	CLA	B	612	X	-	-	-
22	CLA	B	613	X	-	-	-
22	CLA	B	614	X	-	-	-
22	CLA	B	615	X	-	-	-
22	CLA	B	616	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	507	X	-	-	-
22	CLA	C	508	X	-	-	-
22	CLA	C	509	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	511	X	-	-	-
22	CLA	C	512	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	X	-	-	-
22	CLA	C	517	X	-	-	-
22	CLA	D	402	X	-	-	-
22	CLA	D	407	X	-	-	-
22	CLA	D	408	X	-	-	-

2 Entry composition (i)

There are 27 unique types of molecules in this entry. The entry contains 20946 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	335	Total	C	N	O	S	0	0
			2627	1720	432	460	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	496	Total	C	N	O	S	0	0
			3909	2569	649	678	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	432	Total	C	N	O	S	0	0
			3345	2197	561	575	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	0	0
			2717	1800	444	461	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	77	Total	C	N	O	0	0
			635	417	103	115		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	38	Total	C	N	O	S	0	0
			307	207	50	49	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	65	Total	C	N	O	S	0	0
			511	341	82	86	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	26	Total	C	N	O	S	0	0
			211	150	27	33	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	37	Total	C	N	O	0	0
			293	204	43	46		

- 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	34	Total	C	N	O	S	0	0
			267	178	40	48	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	28	Total	C	N	O	S	0	0
			241	170	34	35	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	X	35	Total	C	N	O	0	0
			254	172	38	44		

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	y	28	Total	C	N	O	S	0	0
			208	137	36	32	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	60	Total	C	N	O	S	0	0
			463	318	70	74	1		

- Molecule 16 is a protein called Photosystem II reaction center Psb28 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	112	Total	C	N	O	S	0	0
			897	562	156	173	6		

- Molecule 17 is a protein called Tsl0063 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	3	56	Total	C	N	O	S	0	0
			419	269	74	75	1		

- Molecule 18 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

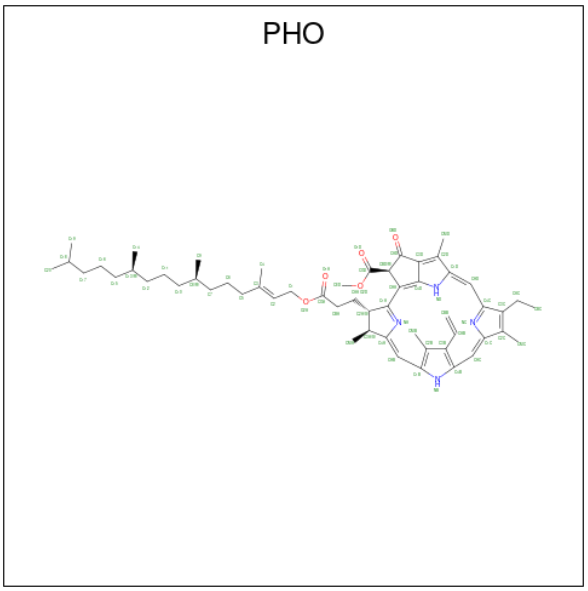
- Molecule 19 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		AltConf
19	A	1	Total	Mn	0
			1	1	

- Molecule 20 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

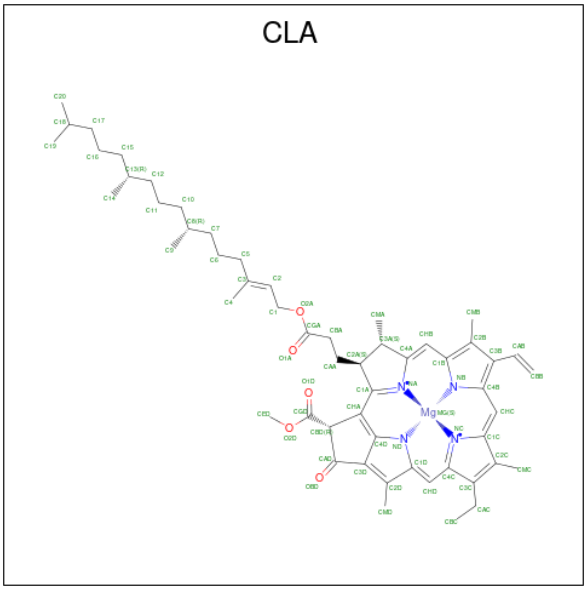
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Cl	0
			1	1	

- Molecule 21 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	B	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0

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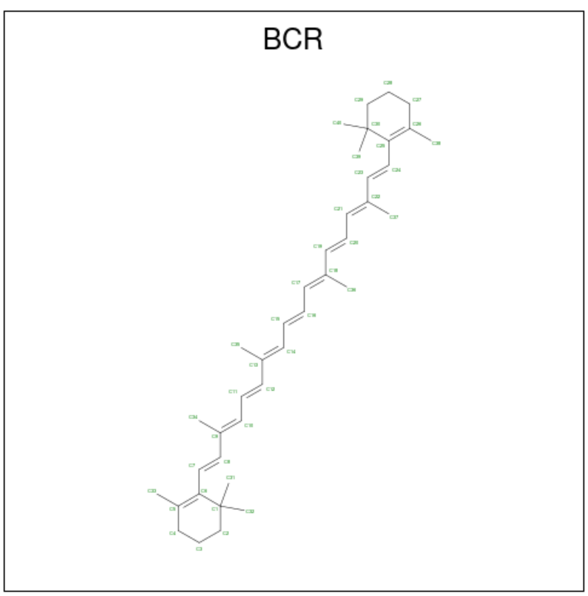
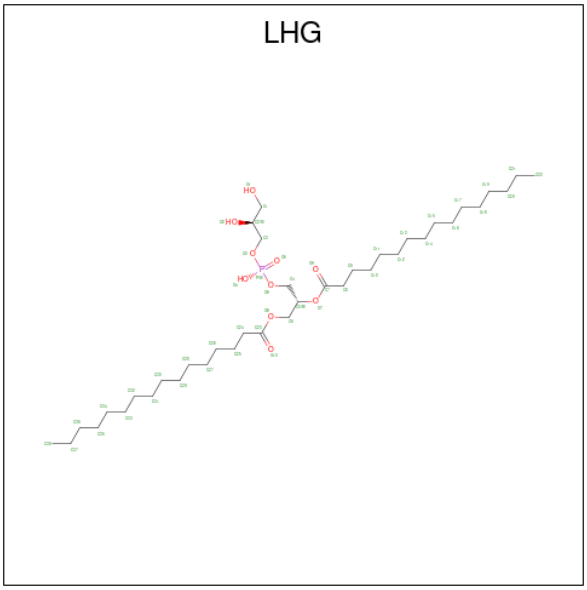
Mol	Chain	Residues	Atoms	AltConf
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	D	1	Total C Mg N O 65 55 1 4 5	0
22	D	1	Total C Mg N O 65 55 1 4 5	0
22	D	1	Total C Mg N O 65 55 1 4 5	0
22	D	1	Total C Mg N O 65 55 1 4 5	0

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



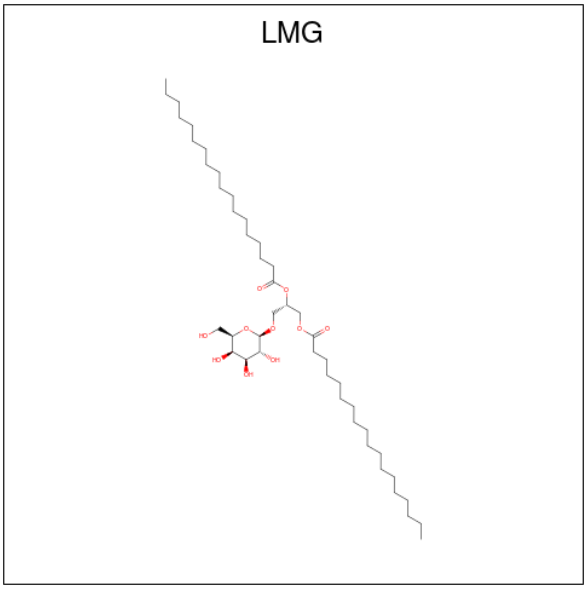
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	H	1	Total C 40 40	0
23	K	1	Total C 40 40	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



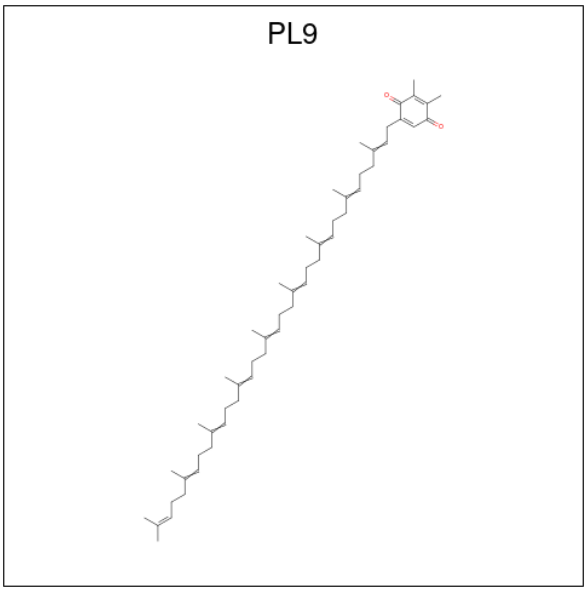
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C O P 49 38 10 1	0

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



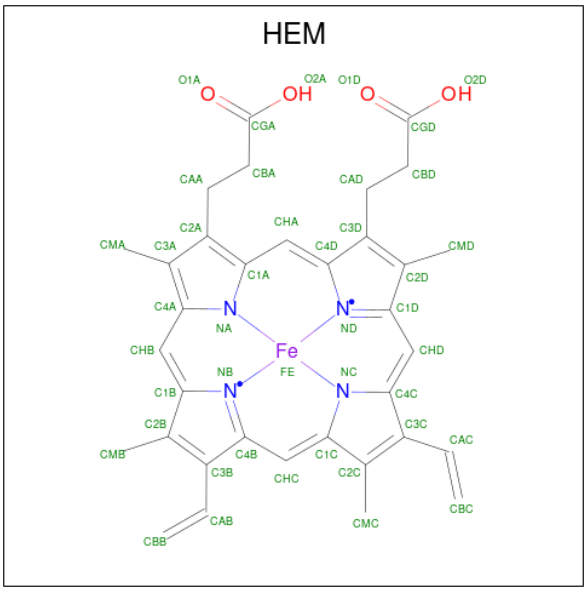
Mol	Chain	Residues	Atoms	AltConf
25	C	1	Total C O 55 45 10	0
25	C	1	Total C O 55 45 10	0
25	D	1	Total C O 55 45 10	0
25	D	1	Total C O 55 45 10	0
25	F	1	Total C O 55 45 10	0
25	I	1	Total C O 55 45 10	0
25	3	1	Total C O 55 45 10	0

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



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

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

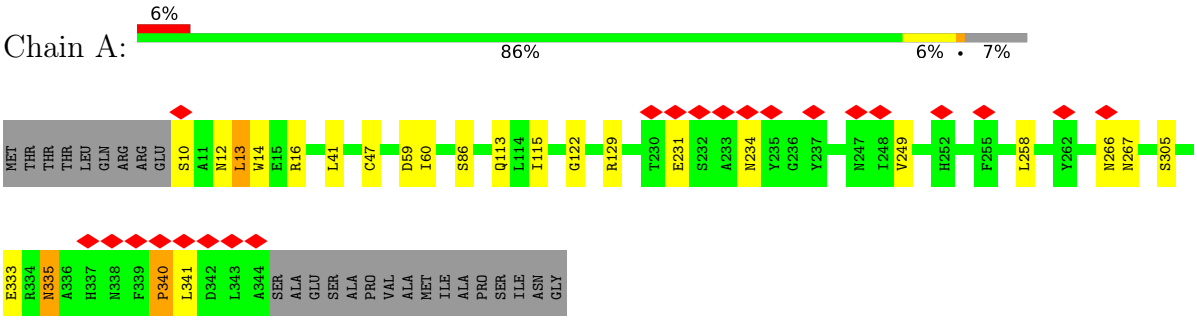


Mol	Chain	Residues	Atoms					AltConf
27	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

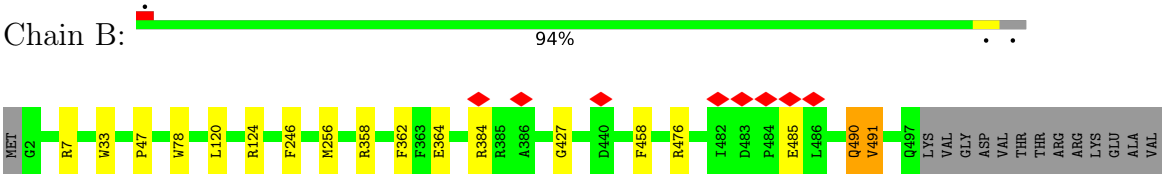
3 Residue-property plots (i)

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.

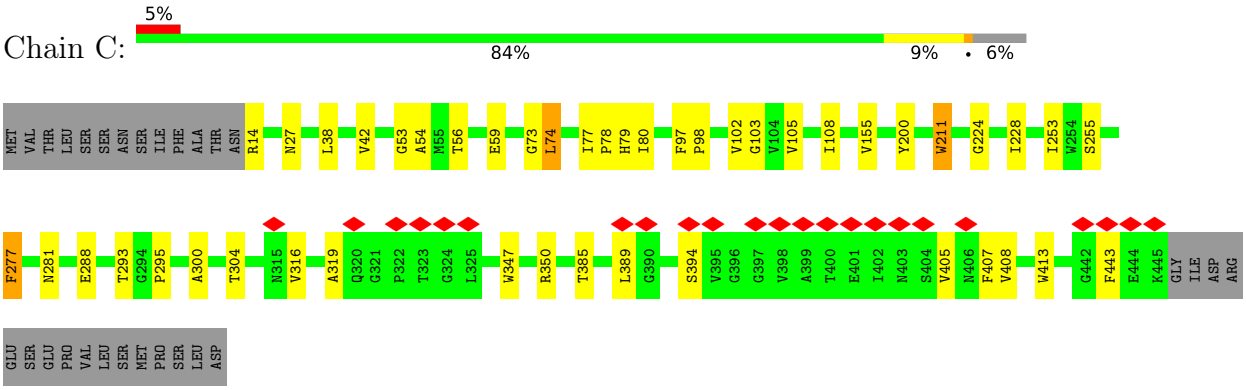
• Molecule 1: Photosystem II protein D1 1



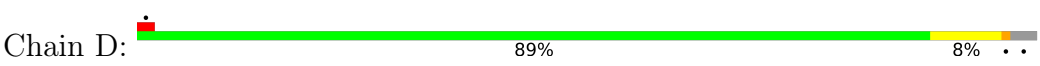
• Molecule 2: Photosystem II CP47 reaction center protein

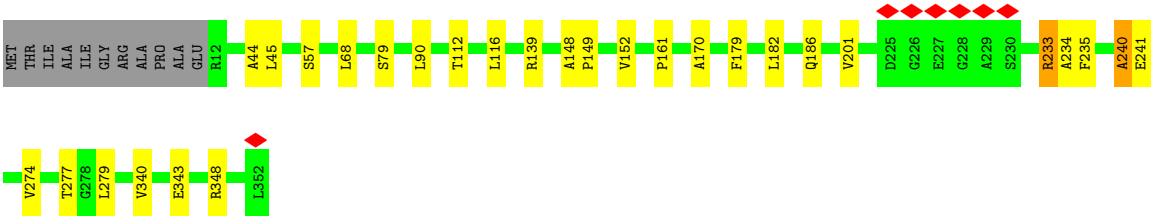


• Molecule 3: Photosystem II CP43 reaction center protein

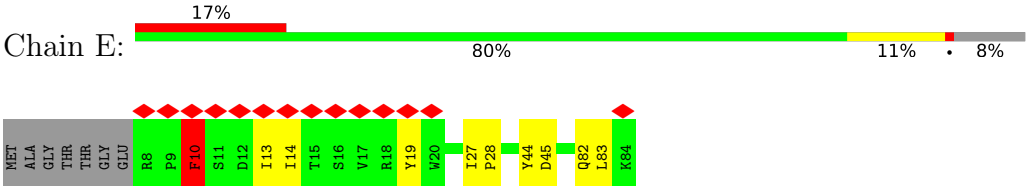


• Molecule 4: Photosystem II D2 protein

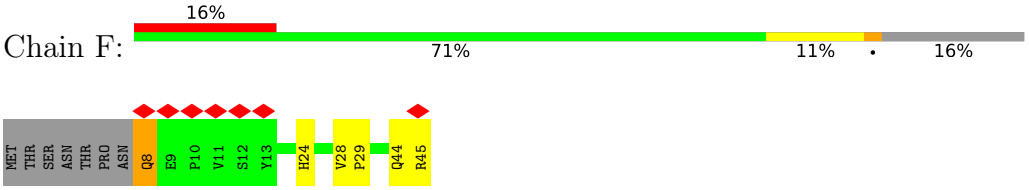




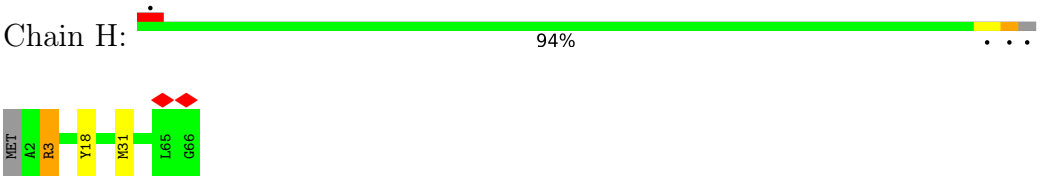
• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 6: Cytochrome b559 subunit beta

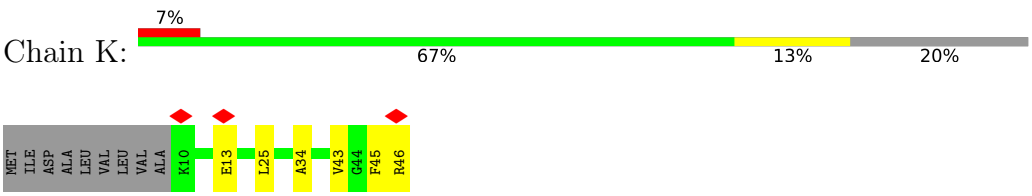


• Molecule 7: Photosystem II reaction center protein H

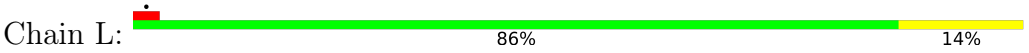


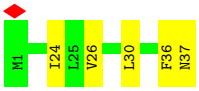
• Molecule 8: Photosystem II reaction center protein I

• Molecule 9: Photosystem II reaction center protein K



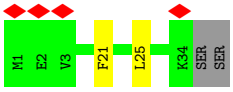
• Molecule 10: Photosystem II reaction center protein L





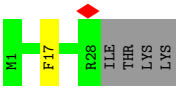
• Molecule 11: Photosystem II reaction center protein M

Chain M:



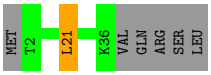
• Molecule 12: Photosystem II reaction center protein T

Chain T:



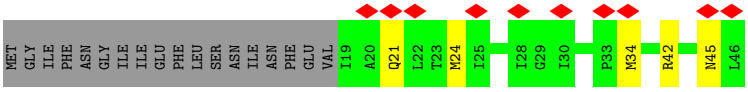
• Molecule 13: Photosystem II reaction center X protein

Chain X:



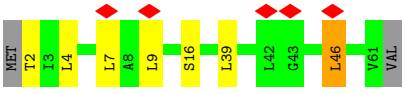
• Molecule 14: Photosystem II reaction center protein Ycf12

Chain y:



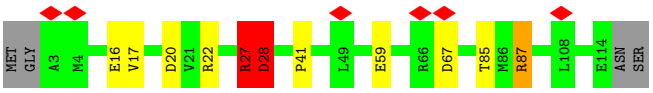
• Molecule 15: Photosystem II reaction center protein Z

Chain Z:



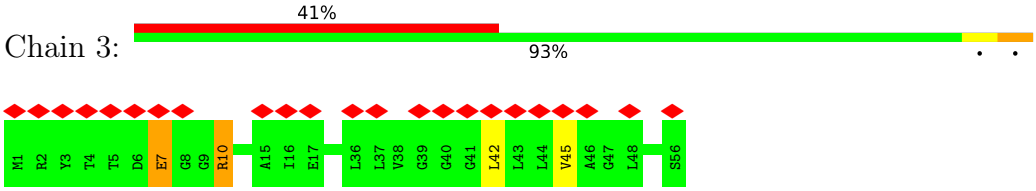
• Molecule 16: Photosystem II reaction center Psb28 protein

Chain 2:



• Molecule 17: Tsl0063 protein

Chain 3:


41%
93%
M1
R2
Y3
T4
T5
D6
E7
G8
G9
R10
A15
I16
E17
L36
L37
V38
G39
G40
G41
L42
L43
L44
V45
A46
G47
L48
S56

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91479	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 ($e^-/Å^2$)	55	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.065	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	283.4, 283.4, 283.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, PL9, CL, MN, PHO, LMG, CLA, HEM, LHG, FE

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	0.43	0/2712	0.75	1/3700 (0.0%)
2	B	0.45	0/4049	0.76	2/5519 (0.0%)
3	C	0.44	0/3456	0.75	5/4706 (0.1%)
4	D	0.43	0/2812	0.77	1/3832 (0.0%)
5	E	0.44	0/654	0.80	1/891 (0.1%)
6	F	0.57	0/317	0.96	1/433 (0.2%)
7	H	0.41	0/524	0.81	1/713 (0.1%)
8	I	0.52	0/216	0.91	0/292
9	K	0.50	0/303	0.72	0/416
10	L	0.43	0/311	0.79	0/422
11	M	0.46	0/270	0.83	0/367
12	T	0.55	0/250	0.84	1/338 (0.3%)
13	X	0.48	0/257	0.97	1/348 (0.3%)
14	y	0.52	0/209	1.01	1/279 (0.4%)
15	Z	0.48	0/474	0.99	3/649 (0.5%)
16	2	0.52	0/914	0.93	0/1231
17	3	0.57	1/426 (0.2%)	1.11	3/578 (0.5%)
All	All	0.45	1/18154 (0.0%)	0.80	21/24714 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	3
4	D	0	1
5	E	0	1
14	y	0	1
16	2	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	3	7	GLU	CB-CG	-5.73	1.41	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	3	7	GLU	CA-CB-CG	9.35	133.98	113.40
15	Z	46	LEU	CB-CG-CD1	7.83	124.31	111.00
1	A	249	VAL	CG1-CB-CG2	-7.13	99.49	110.90
4	D	45	LEU	CA-CB-CG	6.99	131.37	115.30
5	E	10	PHE	CB-CG-CD1	-6.88	115.98	120.80

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	335	ASN	Sidechain
2	B	364	GLU	Sidechain
2	B	485	GLU	Sidechain
2	B	490	GLN	Mainchain
4	D	233	ARG	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	2627	0	2524	14	0
2	B	3909	0	3763	8	0
3	C	3345	0	3273	33	0
4	D	2717	0	2621	19	0
5	E	635	0	625	5	0
6	F	307	0	312	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	511	0	532	2	0
8	I	211	0	227	2	0
9	K	293	0	305	7	0
10	L	304	0	316	4	0
11	M	267	0	289	2	0
12	T	241	0	244	0	0
13	X	254	0	282	0	0
14	y	208	0	237	0	0
15	Z	463	0	495	2	0
16	2	897	0	859	4	0
17	3	419	0	438	4	0
18	A	1	0	0	0	0
19	A	1	0	0	0	0
20	A	1	0	0	0	0
21	A	64	0	73	2	0
21	D	64	0	73	3	0
22	A	130	0	140	2	0
22	B	1040	0	1121	32	0
22	C	845	0	909	22	0
22	D	260	0	279	10	0
23	A	40	0	56	1	0
23	B	120	0	168	3	0
23	C	120	0	168	8	0
23	F	40	0	56	1	0
23	H	40	0	56	15	0
23	K	40	0	56	11	0
24	A	49	0	74	0	0
25	3	55	0	86	2	0
25	C	110	0	172	0	0
25	D	110	0	172	2	0
25	F	55	0	86	0	0
25	I	55	0	86	2	0
26	D	55	0	80	4	0
27	E	43	0	30	3	0
All	All	20946	0	21283	181	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 181 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)
22:B:609:CLA:C4B	23:H:101:BCR:H333	1.79	1.12
23:C:515:BCR:H353	23:K:101:BCR:H332	1.25	1.08
22:B:609:CLA:C3B	23:H:101:BCR:H333	1.95	0.96
23:K:101:BCR:C38	23:K:101:BCR:H23C	2.02	0.90
23:H:101:BCR:C38	23:H:101:BCR:H23C	2.03	0.89

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	333/360 (92%)	314 (94%)	17 (5%)	2 (1%)	25 47
2	B	494/510 (97%)	470 (95%)	23 (5%)	1 (0%)	47 71
3	C	430/461 (93%)	405 (94%)	25 (6%)	0	100 100
4	D	339/352 (96%)	321 (95%)	17 (5%)	1 (0%)	41 64
5	E	75/84 (89%)	71 (95%)	4 (5%)	0	100 100
6	F	36/45 (80%)	32 (89%)	4 (11%)	0	100 100
7	H	63/66 (96%)	57 (90%)	5 (8%)	1 (2%)	9 22
8	I	24/38 (63%)	24 (100%)	0	0	100 100
9	K	35/46 (76%)	33 (94%)	2 (6%)	0	100 100
10	L	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
11	M	32/36 (89%)	32 (100%)	0	0	100 100
12	T	26/32 (81%)	24 (92%)	2 (8%)	0	100 100
13	X	33/41 (80%)	32 (97%)	1 (3%)	0	100 100
14	y	26/46 (56%)	22 (85%)	4 (15%)	0	100 100
15	Z	58/62 (94%)	57 (98%)	1 (2%)	0	100 100
16	2	110/116 (95%)	102 (93%)	6 (6%)	2 (2%)	8 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	3	54/56 (96%)	53 (98%)	1 (2%)	0	100 100
All	All	2203/2388 (92%)	2083 (95%)	113 (5%)	7 (0%)	44 64

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	491	VAL
4	D	240	ALA
16	2	28	ASP
1	A	13	LEU
16	2	27	ARG

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	271/291 (93%)	264 (97%)	7 (3%)	46 73
2	B	395/407 (97%)	391 (99%)	4 (1%)	76 90
3	C	335/362 (92%)	330 (98%)	5 (2%)	65 84
4	D	276/283 (98%)	273 (99%)	3 (1%)	73 89
5	E	69/73 (94%)	68 (99%)	1 (1%)	67 85
6	F	32/39 (82%)	31 (97%)	1 (3%)	40 67
7	H	54/55 (98%)	54 (100%)	0	100 100
8	I	24/35 (69%)	22 (92%)	2 (8%)	11 23
9	K	30/37 (81%)	29 (97%)	1 (3%)	38 64
10	L	35/35 (100%)	35 (100%)	0	100 100
11	M	31/33 (94%)	31 (100%)	0	100 100
12	T	25/29 (86%)	25 (100%)	0	100 100
13	X	28/34 (82%)	27 (96%)	1 (4%)	35 61
14	y	21/37 (57%)	18 (86%)	3 (14%)	3 7
15	Z	50/52 (96%)	48 (96%)	2 (4%)	31 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	2	94/97 (97%)	88 (94%)	6 (6%)	17 36
17	3	42/42 (100%)	40 (95%)	2 (5%)	25 49
All	All	1812/1941 (93%)	1774 (98%)	38 (2%)	56 78

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	Z	16	SER
16	2	87	ARG
15	Z	46	LEU
16	2	22	ARG
17	3	10	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 60 ligands modelled in this entry, 3 are monoatomic - leaving 57 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	$\#\|Z\| > 2$
23	BCR	K	101	-	41,41,41	2.83	10 (24%)	56,56,56	3.77	31 (55%)
22	CLA	B	607	-	65,73,73	1.58	9 (13%)	76,113,113	2.23	25 (32%)
23	BCR	H	101	-	41,41,41	3.05	11 (26%)	56,56,56	3.99	30 (53%)
25	LMG	C	502	-	55,55,55	1.06	3 (5%)	63,63,63	0.99	5 (7%)
23	BCR	C	516	-	41,41,41	0.93	1 (2%)	56,56,56	1.20	9 (16%)
22	CLA	D	402	-	65,73,73	1.62	10 (15%)	76,113,113	2.44	26 (34%)
22	CLA	B	604	-	65,73,73	1.61	9 (13%)	76,113,113	2.77	19 (25%)
22	CLA	B	614	-	65,73,73	1.73	12 (18%)	76,113,113	2.65	23 (30%)
22	CLA	D	401	-	65,73,73	1.55	9 (13%)	76,113,113	2.13	22 (28%)
22	CLA	C	513	-	65,73,73	1.65	9 (13%)	76,113,113	2.80	24 (31%)
23	BCR	A	407	-	41,41,41	0.91	2 (4%)	56,56,56	1.08	3 (5%)
24	LHG	A	408	-	48,48,48	0.82	1 (2%)	51,54,54	0.90	2 (3%)
25	LMG	C	501	-	55,55,55	0.91	0	63,63,63	1.13	5 (7%)
25	LMG	3	101	-	55,55,55	0.92	1 (1%)	63,63,63	1.08	5 (7%)
25	LMG	I	101	-	55,55,55	0.98	2 (3%)	63,63,63	1.09	3 (4%)
22	CLA	B	606	-	65,73,73	1.57	11 (16%)	76,113,113	2.30	26 (34%)
22	CLA	C	505	-	65,73,73	1.58	10 (15%)	76,113,113	2.90	27 (35%)
27	HEM	E	101	6,5	41,50,50	1.45	3 (7%)	45,82,82	1.08	1 (2%)
21	PHO	D	406	-	51,69,69	1.08	5 (9%)	47,99,99	1.28	6 (12%)
22	CLA	B	608	-	65,73,73	1.72	11 (16%)	76,113,113	2.62	23 (30%)
22	CLA	C	514	-	65,73,73	1.77	10 (15%)	76,113,113	2.35	19 (25%)
22	CLA	B	612	-	65,73,73	1.66	15 (23%)	76,113,113	2.88	26 (34%)
22	CLA	B	601	-	65,73,73	1.66	10 (15%)	76,113,113	2.54	19 (25%)
22	CLA	A	405	-	65,73,73	1.62	9 (13%)	76,113,113	2.18	21 (27%)
22	CLA	C	512	-	65,73,73	1.79	11 (16%)	76,113,113	2.75	23 (30%)
22	CLA	C	510	22	65,73,73	1.79	13 (20%)	76,113,113	2.70	22 (28%)
22	CLA	C	503	-	65,73,73	1.69	11 (16%)	76,113,113	1.90	24 (31%)
23	BCR	B	619	-	41,41,41	0.92	2 (4%)	56,56,56	1.26	8 (14%)
22	CLA	C	504	-	65,73,73	1.59	12 (18%)	76,113,113	2.19	17 (22%)
25	LMG	D	404	-	55,55,55	0.97	2 (3%)	63,63,63	1.08	4 (6%)
23	BCR	B	618	-	41,41,41	1.00	1 (2%)	56,56,56	1.14	5 (8%)
22	CLA	C	517	22	65,73,73	1.76	12 (18%)	76,113,113	2.94	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	BCR	C	515	-	41,41,41	1.01	2 (4%)	56,56,56	1.45	12 (21%)
22	CLA	B	613	-	65,73,73	1.72	10 (15%)	76,113,113	2.81	25 (32%)
22	CLA	B	603	-	65,73,73	1.54	8 (12%)	76,113,113	2.33	20 (26%)
23	BCR	B	617	-	41,41,41	0.98	2 (4%)	56,56,56	1.27	7 (12%)
23	BCR	C	518	-	41,41,41	0.99	2 (4%)	56,56,56	1.53	13 (23%)
22	CLA	B	602	-	65,73,73	1.62	9 (13%)	76,113,113	2.53	21 (27%)
22	CLA	B	609	-	65,73,73	1.79	9 (13%)	76,113,113	2.75	20 (26%)
22	CLA	B	615	-	65,73,73	1.71	8 (12%)	76,113,113	2.64	23 (30%)
22	CLA	B	616	-	65,73,73	1.80	12 (18%)	76,113,113	3.08	22 (28%)
22	CLA	A	406	-	65,73,73	1.57	9 (13%)	76,113,113	2.27	19 (25%)
22	CLA	C	508	-	65,73,73	1.78	12 (18%)	76,113,113	2.13	18 (23%)
22	CLA	C	507	-	65,73,73	1.83	13 (20%)	76,113,113	2.82	25 (32%)
22	CLA	C	511	-	65,73,73	1.64	9 (13%)	76,113,113	2.64	21 (27%)
23	BCR	F	102	-	41,41,41	0.84	0	56,56,56	1.18	8 (14%)
22	CLA	B	611	-	65,73,73	1.70	9 (13%)	76,113,113	2.42	23 (30%)
21	PHO	A	404	-	51,69,69	1.04	5 (9%)	47,99,99	1.22	5 (10%)
25	LMG	F	101	-	55,55,55	1.02	2 (3%)	63,63,63	1.00	3 (4%)
22	CLA	C	506	-	65,73,73	1.57	12 (18%)	76,113,113	2.44	18 (23%)
22	CLA	B	610	-	65,73,73	1.67	13 (20%)	76,113,113	2.84	24 (31%)
22	CLA	D	407	-	65,73,73	1.62	10 (15%)	76,113,113	2.05	21 (27%)
25	LMG	D	403	-	55,55,55	0.96	2 (3%)	63,63,63	1.05	3 (4%)
22	CLA	B	605	-	65,73,73	1.50	11 (16%)	76,113,113	2.35	17 (22%)
26	PL9	D	405	-	55,55,55	1.12	3 (5%)	68,69,69	1.41	11 (16%)
22	CLA	D	408	-	65,73,73	1.67	9 (13%)	76,113,113	2.08	16 (21%)
22	CLA	C	509	-	65,73,73	1.61	11 (16%)	76,113,113	2.49	15 (19%)

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
23	BCR	K	101	-	-	15/29/63/63	0/2/2/2
22	CLA	B	607	-	2/2/15/20	12/37/115/115	-
23	BCR	H	101	-	-	15/29/63/63	0/2/2/2
25	LMG	C	502	-	-	7/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	C	516	-	-	14/29/63/63	0/2/2/2
22	CLA	D	402	-	2/2/15/20	9/37/115/115	-
22	CLA	B	604	-	1/1/15/20	7/37/115/115	-
22	CLA	B	614	-	3/3/15/20	9/37/115/115	-
22	CLA	D	401	-	-	13/37/115/115	-
22	CLA	C	513	-	3/3/15/20	4/37/115/115	-
23	BCR	A	407	-	-	8/29/63/63	0/2/2/2
24	LHG	A	408	-	-	7/53/53/53	-
25	LMG	C	501	-	-	18/50/70/70	0/1/1/1
25	LMG	3	101	-	-	8/50/70/70	0/1/1/1
25	LMG	I	101	-	-	5/50/70/70	0/1/1/1
22	CLA	B	606	-	2/2/15/20	14/37/115/115	-
22	CLA	C	505	-	1/1/15/20	17/37/115/115	-
27	HEM	E	101	6,5	-	4/12/54/54	-
21	PHO	D	406	-	1/1/17/22	6/37/103/103	0/5/6/6
22	CLA	B	608	-	-	6/37/115/115	-
22	CLA	C	514	-	3/3/15/20	10/37/115/115	-
22	CLA	B	612	-	4/4/15/20	12/37/115/115	-
22	CLA	B	601	-	3/3/15/20	9/37/115/115	-
22	CLA	A	405	-	2/2/15/20	12/37/115/115	-
22	CLA	C	512	-	1/1/15/20	9/37/115/115	-
22	CLA	C	510	22	1/1/15/20	12/37/115/115	-
22	CLA	C	503	-	-	7/37/115/115	-
23	BCR	B	619	-	-	6/29/63/63	0/2/2/2
22	CLA	C	504	-	2/2/15/20	13/37/115/115	-
25	LMG	D	404	-	-	11/50/70/70	0/1/1/1
23	BCR	B	618	-	-	5/29/63/63	0/2/2/2
22	CLA	C	517	22	3/3/15/20	11/37/115/115	-
23	BCR	C	515	-	-	9/29/63/63	0/2/2/2
22	CLA	B	613	-	3/3/15/20	8/37/115/115	-
22	CLA	B	603	-	3/3/15/20	10/37/115/115	-
23	BCR	B	617	-	-	14/29/63/63	0/2/2/2
23	BCR	C	518	-	-	9/29/63/63	0/2/2/2
22	CLA	B	602	-	2/2/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	609	-	2/2/15/20	7/37/115/115	-
22	CLA	B	615	-	3/3/15/20	10/37/115/115	-
22	CLA	B	616	-	4/4/15/20	9/37/115/115	-
22	CLA	A	406	-	2/2/15/20	10/37/115/115	-
22	CLA	C	508	-	1/1/15/20	3/37/115/115	-
22	CLA	C	507	-	2/2/15/20	11/37/115/115	-
22	CLA	C	511	-	3/3/15/20	9/37/115/115	-
23	BCR	F	102	-	-	3/29/63/63	0/2/2/2
22	CLA	B	611	-	1/1/15/20	13/37/115/115	-
21	PHO	A	404	-	1/1/17/22	7/37/103/103	0/5/6/6
25	LMG	F	101	-	-	7/50/70/70	0/1/1/1
22	CLA	C	506	-	3/3/15/20	11/37/115/115	-
22	CLA	B	610	-	2/2/15/20	9/37/115/115	-
22	CLA	D	407	-	2/2/15/20	9/37/115/115	-
25	LMG	D	403	-	-	5/50/70/70	0/1/1/1
22	CLA	B	605	-	2/2/15/20	9/37/115/115	-
26	PL9	D	405	-	-	14/53/73/73	0/1/1/1
22	CLA	D	408	-	3/3/15/20	5/37/115/115	-
22	CLA	C	509	-	2/2/15/20	8/37/115/115	-

The worst 5 of 429 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	101	BCR	C1-C6	-9.89	1.40	1.53
23	H	101	BCR	C5-C6	-9.63	1.17	1.34
22	B	615	CLA	C4B-NB	9.42	1.43	1.35
22	C	514	CLA	C4B-NB	9.37	1.43	1.35
22	C	512	CLA	C4B-NB	9.23	1.43	1.35

The worst 5 of 941 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	604	CLA	C4A-NA-C1A	15.59	113.71	106.71
22	C	505	CLA	C4A-NA-C1A	15.19	113.53	106.71
23	H	101	BCR	C33-C5-C6	-13.26	109.64	124.53
22	B	616	CLA	C4A-NA-C1A	13.21	112.64	106.71
22	B	605	CLA	C4A-NA-C1A	12.70	112.42	106.71

5 of 75 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	404	PHO	C8
21	D	406	PHO	C8
22	A	405	CLA	ND
22	A	405	CLA	C2A
22	A	406	CLA	ND

5 of 535 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	404	PHO	O2A-C1-C2-C3
22	A	405	CLA	C3A-C2A-CAA-CBA
22	A	406	CLA	C3A-C2A-CAA-CBA
22	A	406	CLA	C11-C10-C8-C7
22	B	601	CLA	C11-C10-C8-C9

There are no ring outliers.

47 monomers are involved in 109 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	K	101	BCR	11	0
22	B	607	CLA	2	0
23	H	101	BCR	15	0
23	C	516	BCR	3	0
22	D	402	CLA	2	0
22	B	604	CLA	2	0
22	B	614	CLA	3	0
22	D	401	CLA	2	0
22	C	513	CLA	3	0
23	A	407	BCR	1	0
25	3	101	LMG	2	0
25	I	101	LMG	2	0
22	B	606	CLA	1	0
22	C	505	CLA	4	0
27	E	101	HEM	3	0
21	D	406	PHO	3	0
22	B	608	CLA	1	0
22	C	514	CLA	1	0
22	B	612	CLA	2	0
22	B	601	CLA	2	0
22	C	510	CLA	3	0
22	C	503	CLA	4	0

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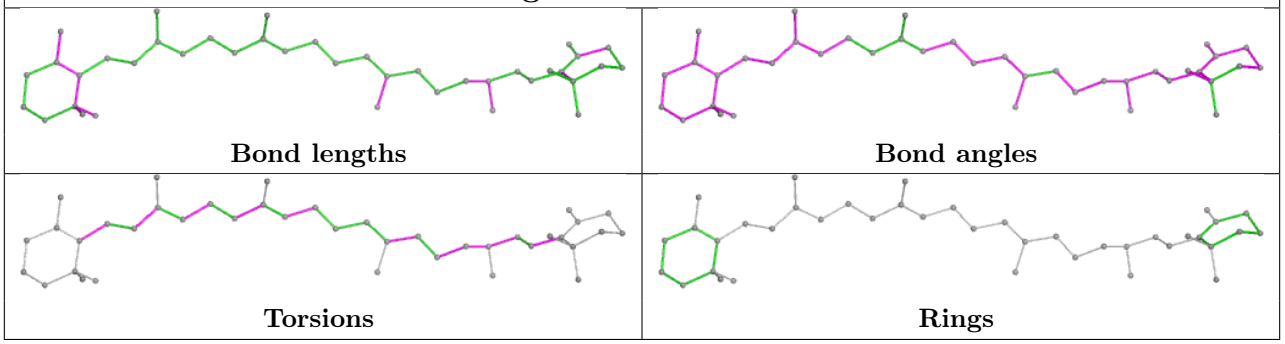
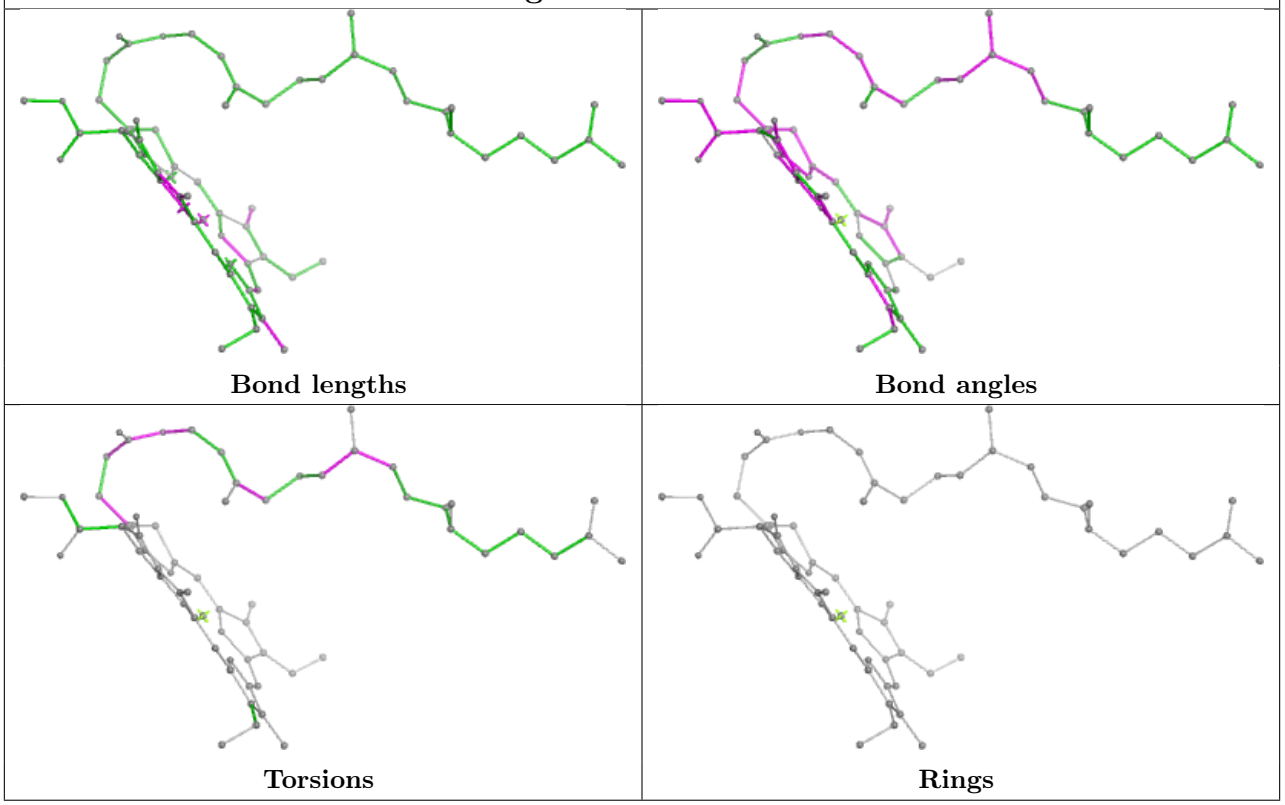
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	619	BCR	1	0
22	C	504	CLA	3	0
25	D	404	LMG	1	0
22	C	517	CLA	4	0
23	C	515	BCR	4	0
22	B	613	CLA	4	0
22	B	603	CLA	4	0
23	B	617	BCR	2	0
23	C	518	BCR	1	0
22	B	602	CLA	2	0
22	B	609	CLA	11	0
22	B	615	CLA	1	0
22	A	406	CLA	2	0
22	C	511	CLA	5	0
23	F	102	BCR	1	0
22	B	611	CLA	1	0
21	A	404	PHO	2	0
22	C	506	CLA	1	0
22	B	610	CLA	2	0
22	D	407	CLA	3	0
25	D	403	LMG	1	0
22	B	605	CLA	2	0
26	D	405	PL9	4	0
22	D	408	CLA	3	0
22	C	509	CLA	2	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 BCR K 101

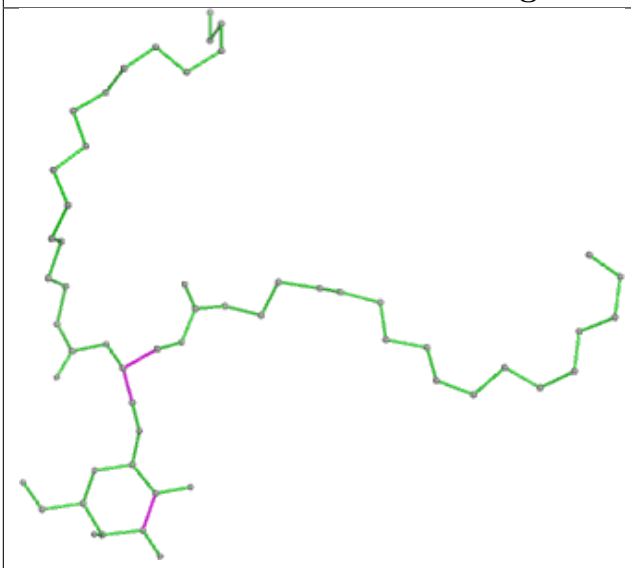


Ligand CLA B 607

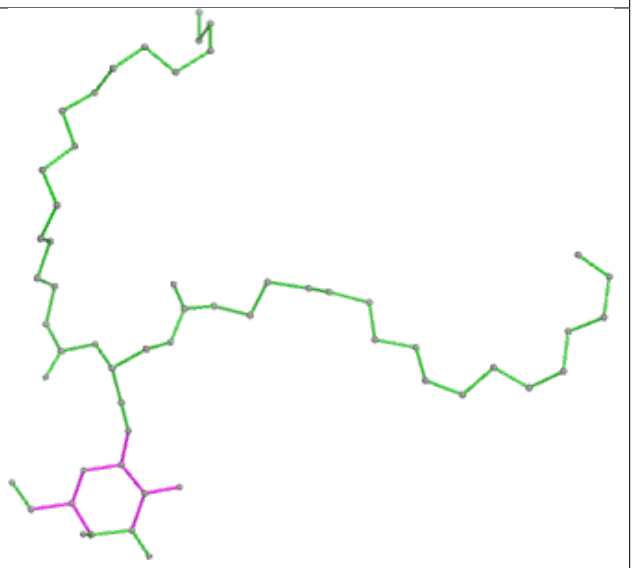


Ligand BCR H 101

Ligand LMG C 502

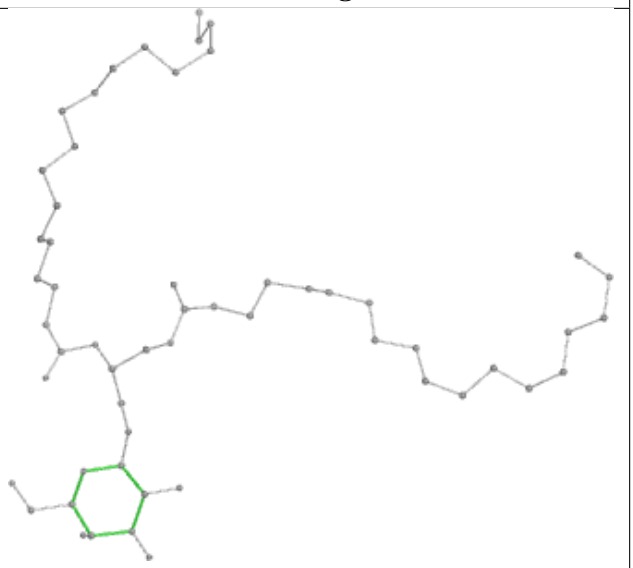


Bond lengths



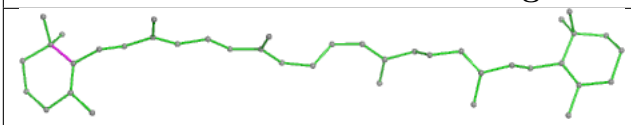
Bond angles

Torsions

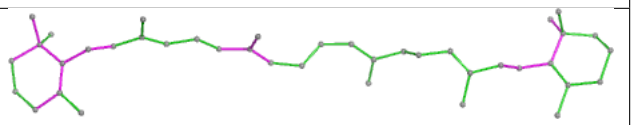


Rings

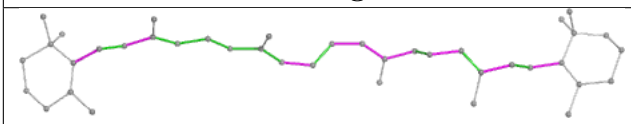
Ligand BCR C 516



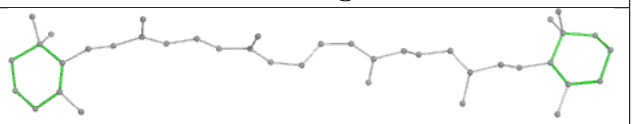
Bond lengths



Bond angles

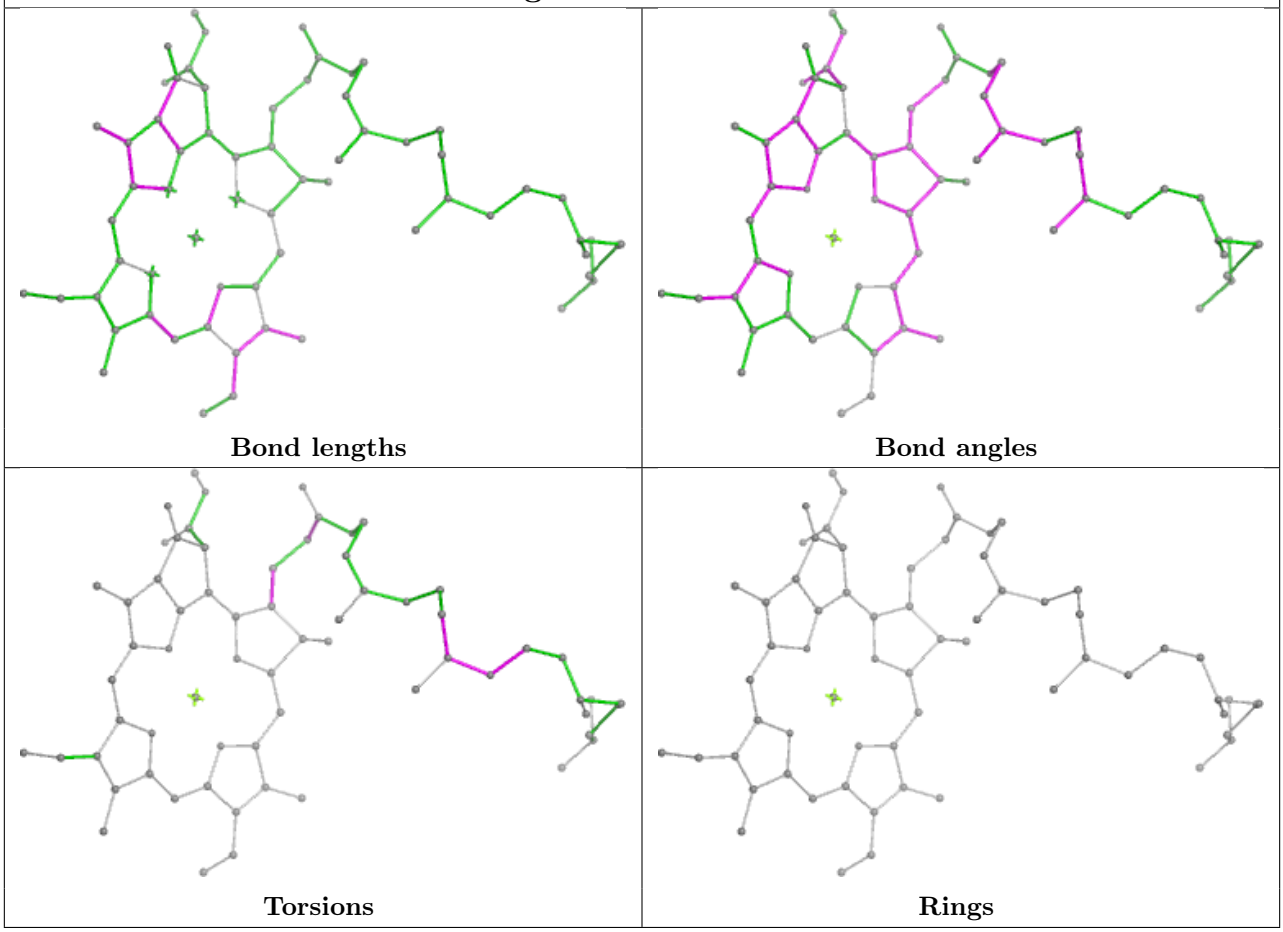


Torsions



Rings

Ligand CLA D 402



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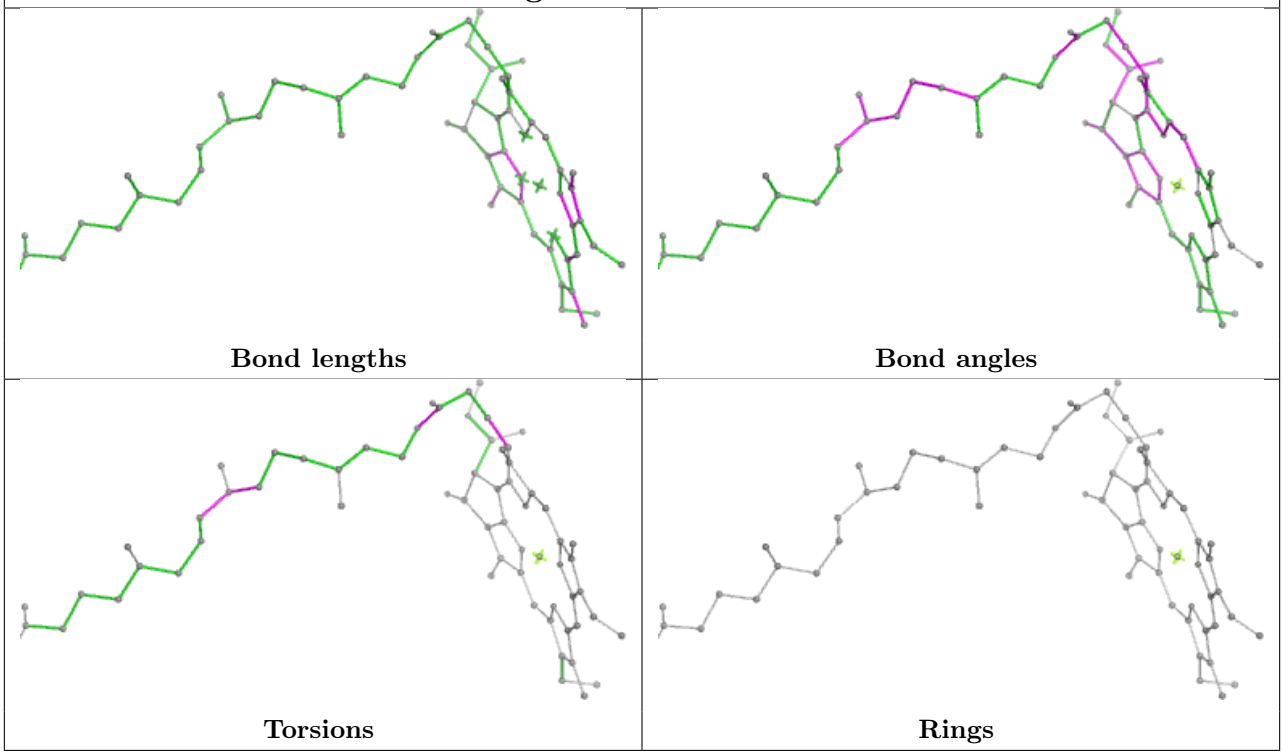
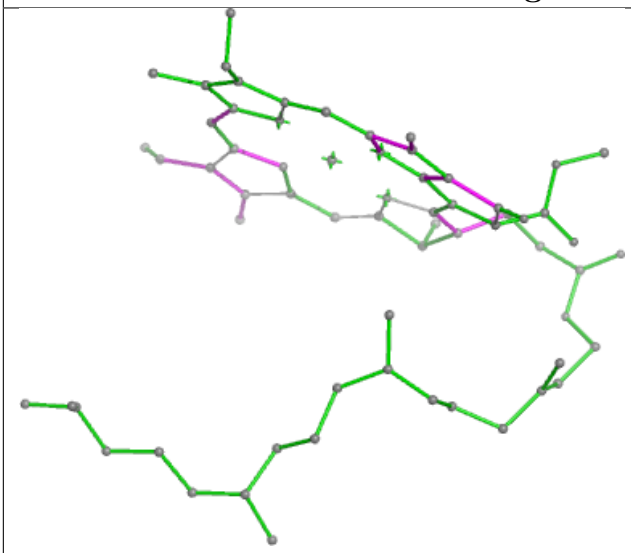
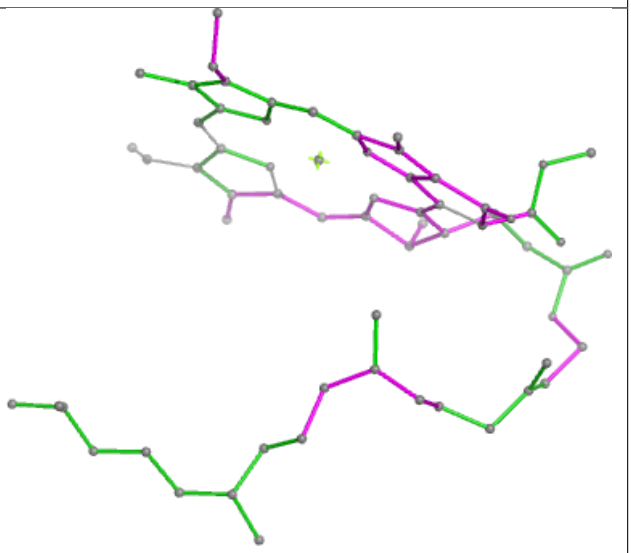


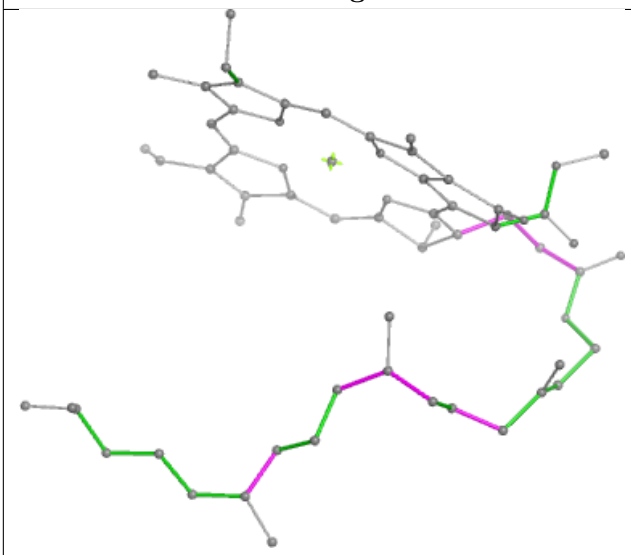
Ligand CLA B 614



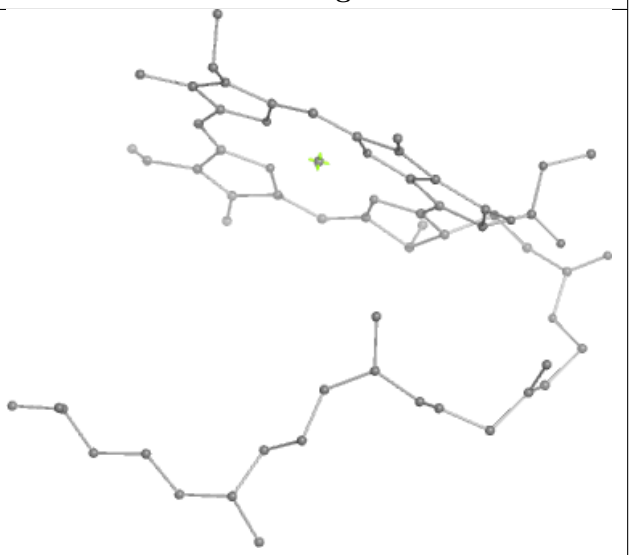
Bond lengths



Bond angles

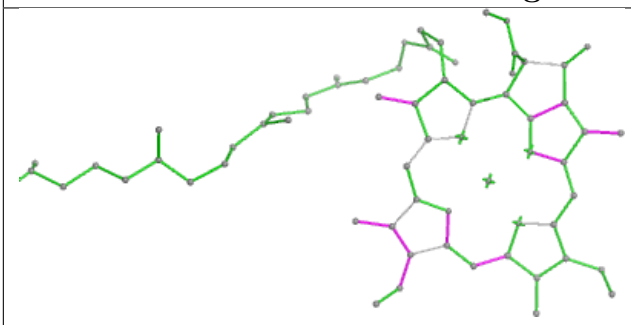


Torsions

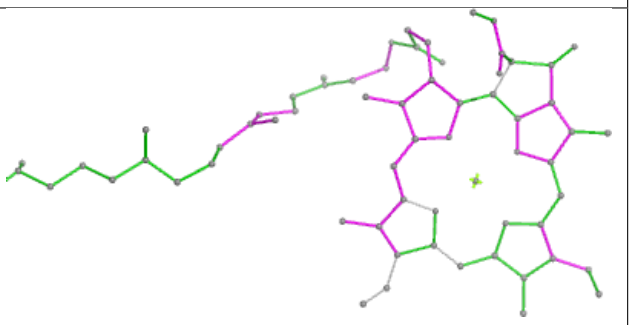


Rings

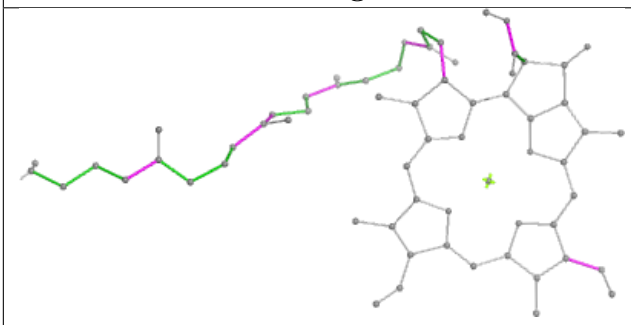
Ligand CLA D 401



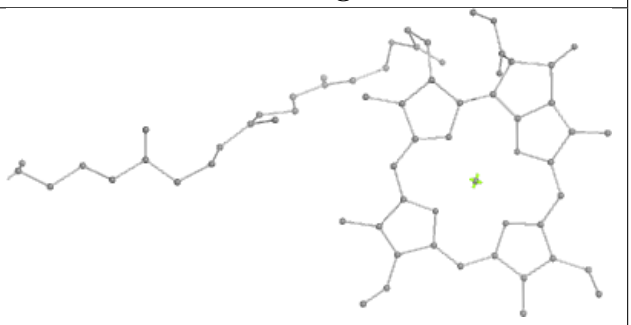
Bond lengths



Bond angles

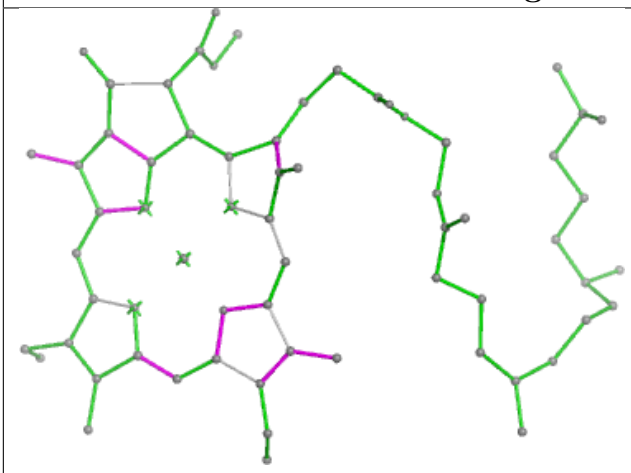


Torsions

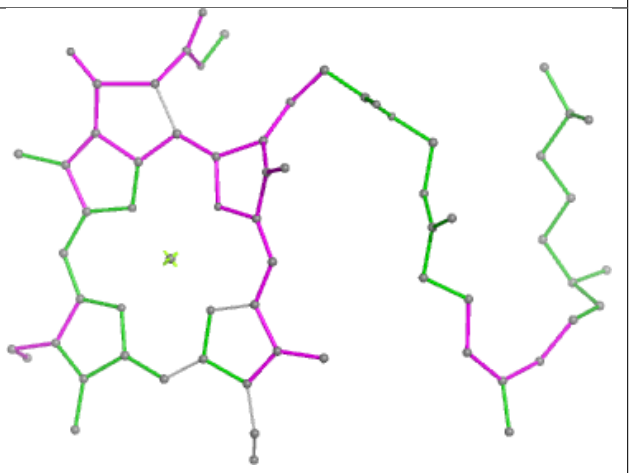


Rings

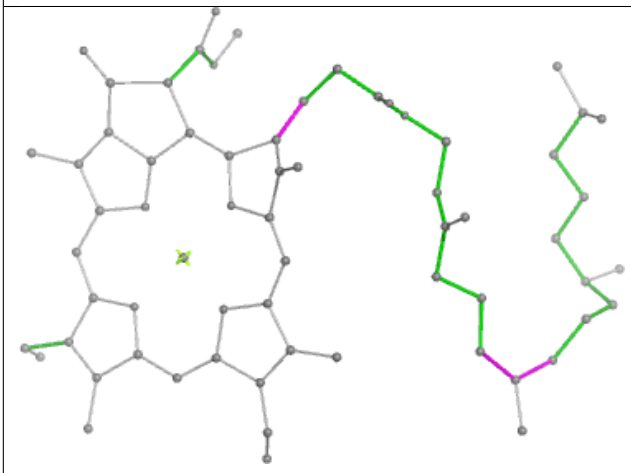
Ligand CLA C 513



Bond lengths



Bond angles



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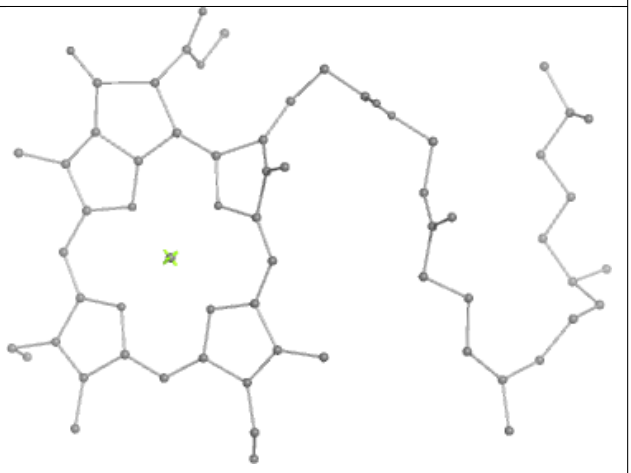
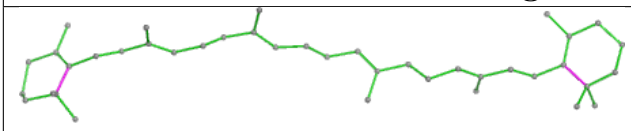
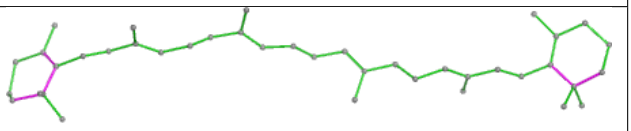


Rings

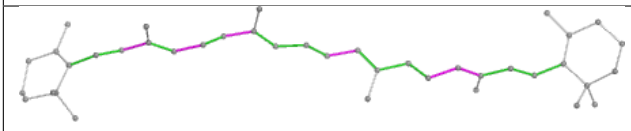
Ligand BCR A 407



Bond lengths



Bond angles



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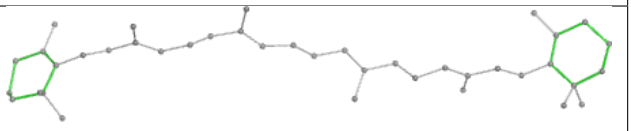


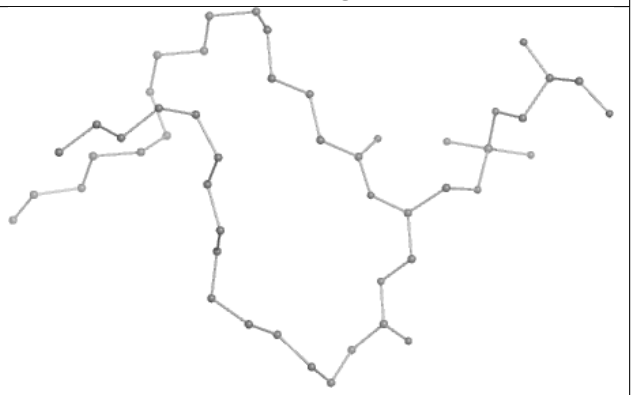
Rings

Ligand LHG A 408

Bond lengths

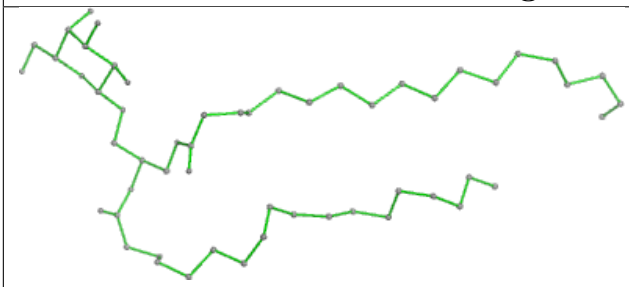
Bond angles

Torsions

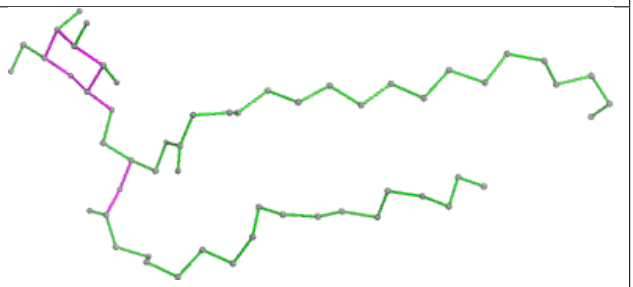


Rings

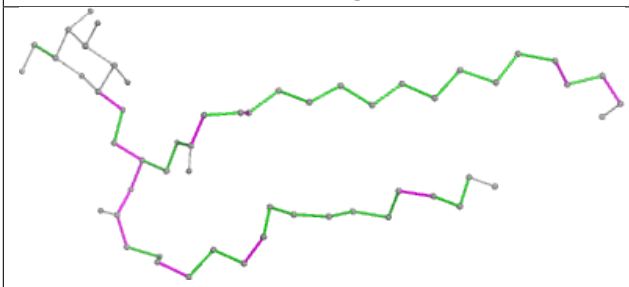
Ligand LMG C 501



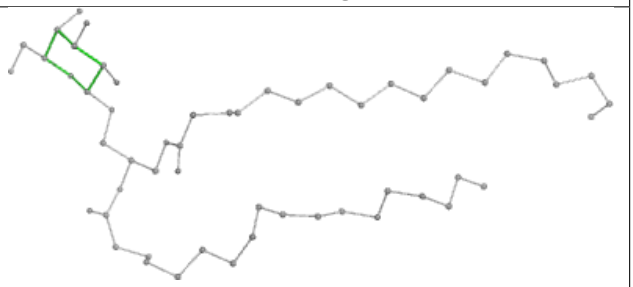
Bond lengths



Bond angles

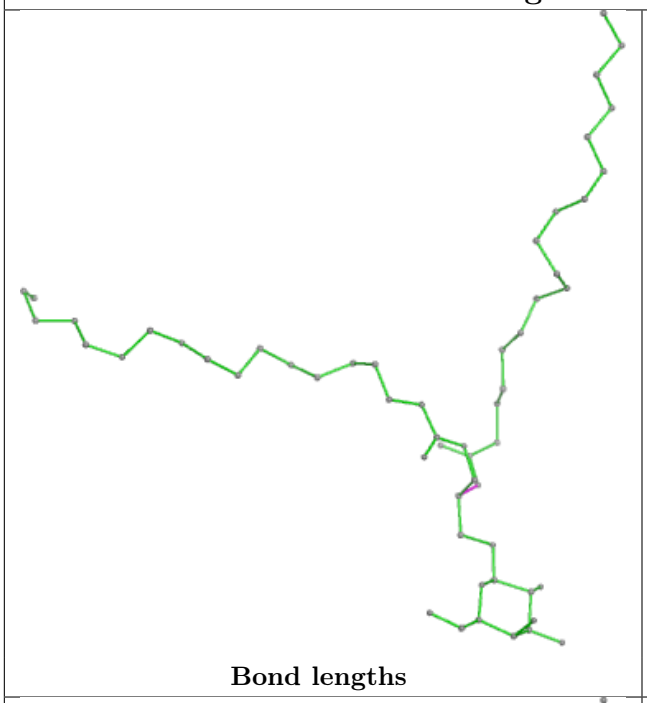


Torsions

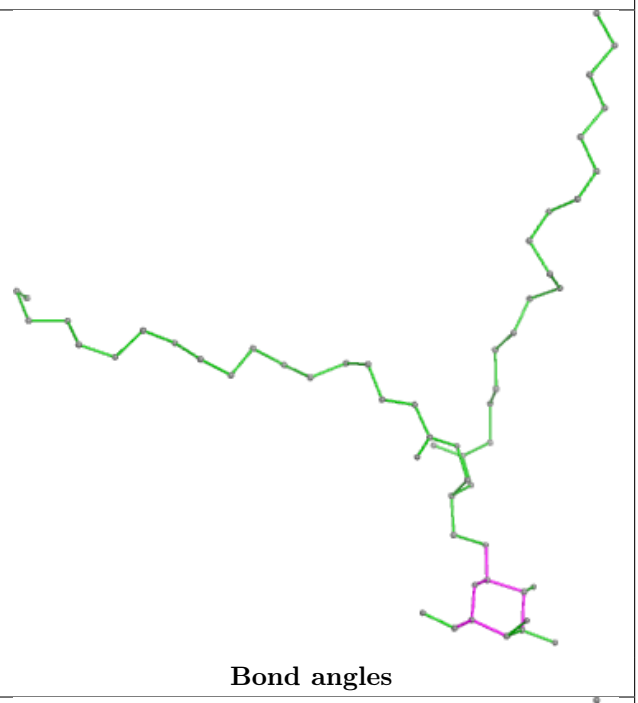


Rings

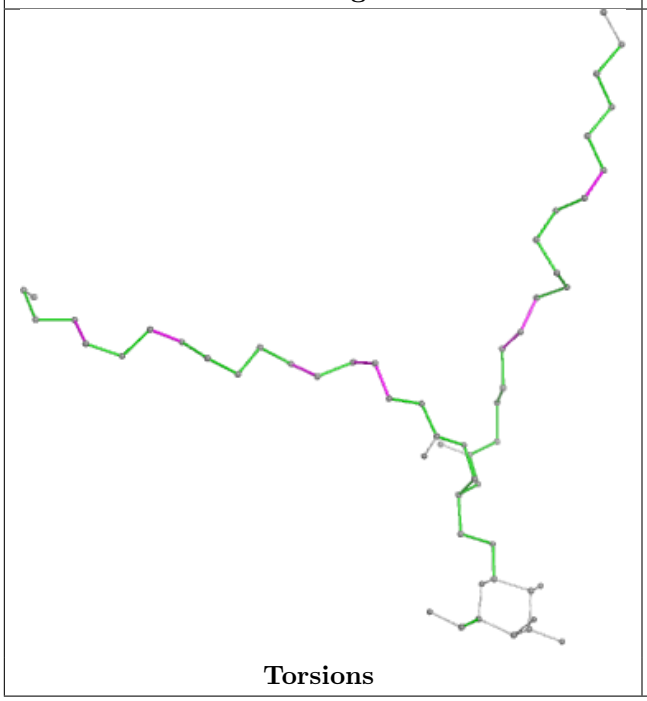
Ligand LMG 3 101



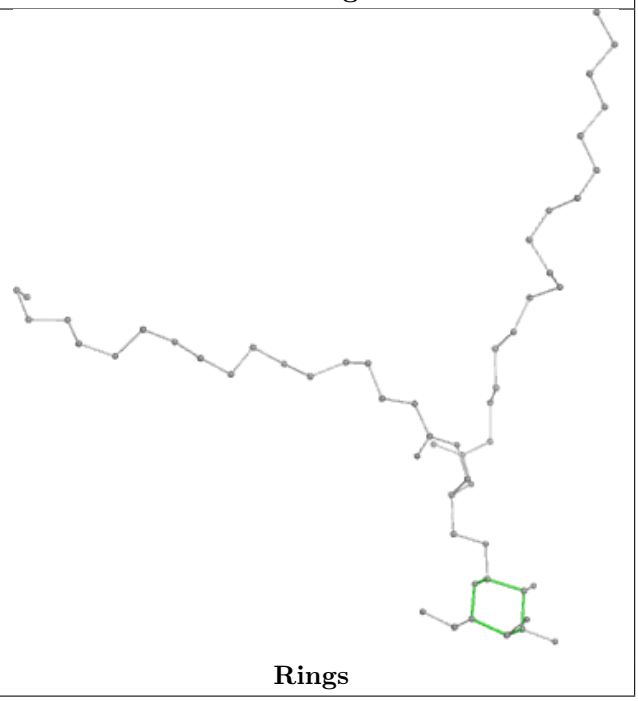
Bond lengths



Bond angles

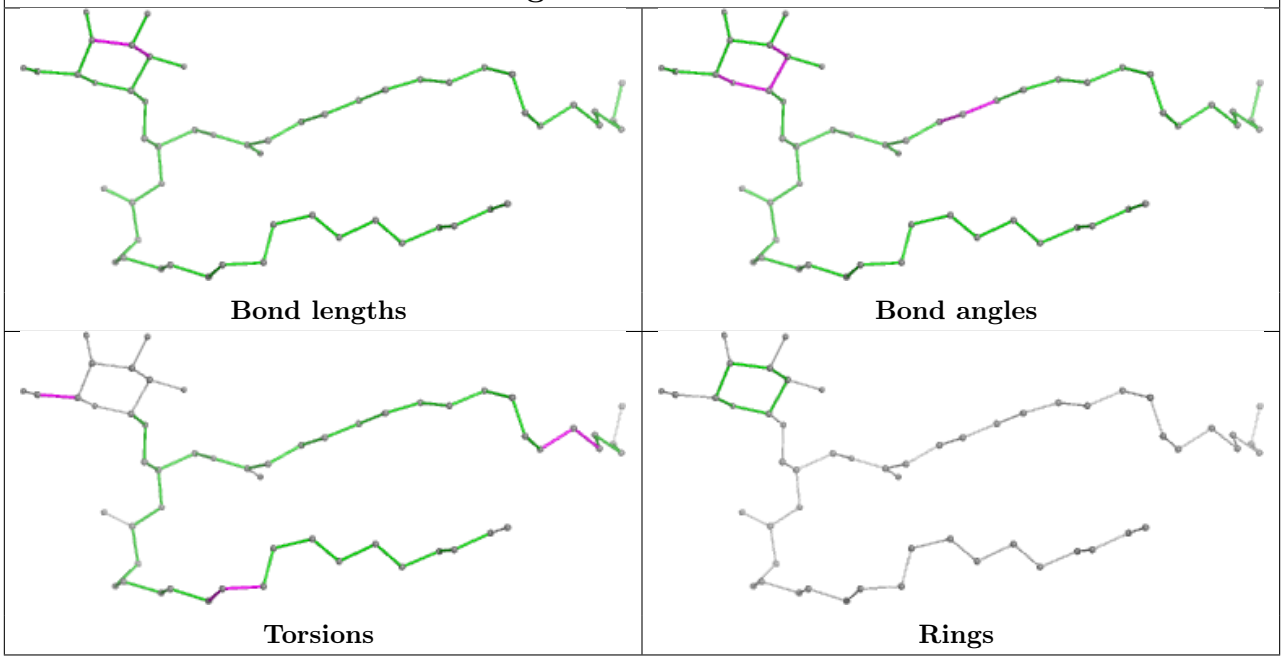


Torsions

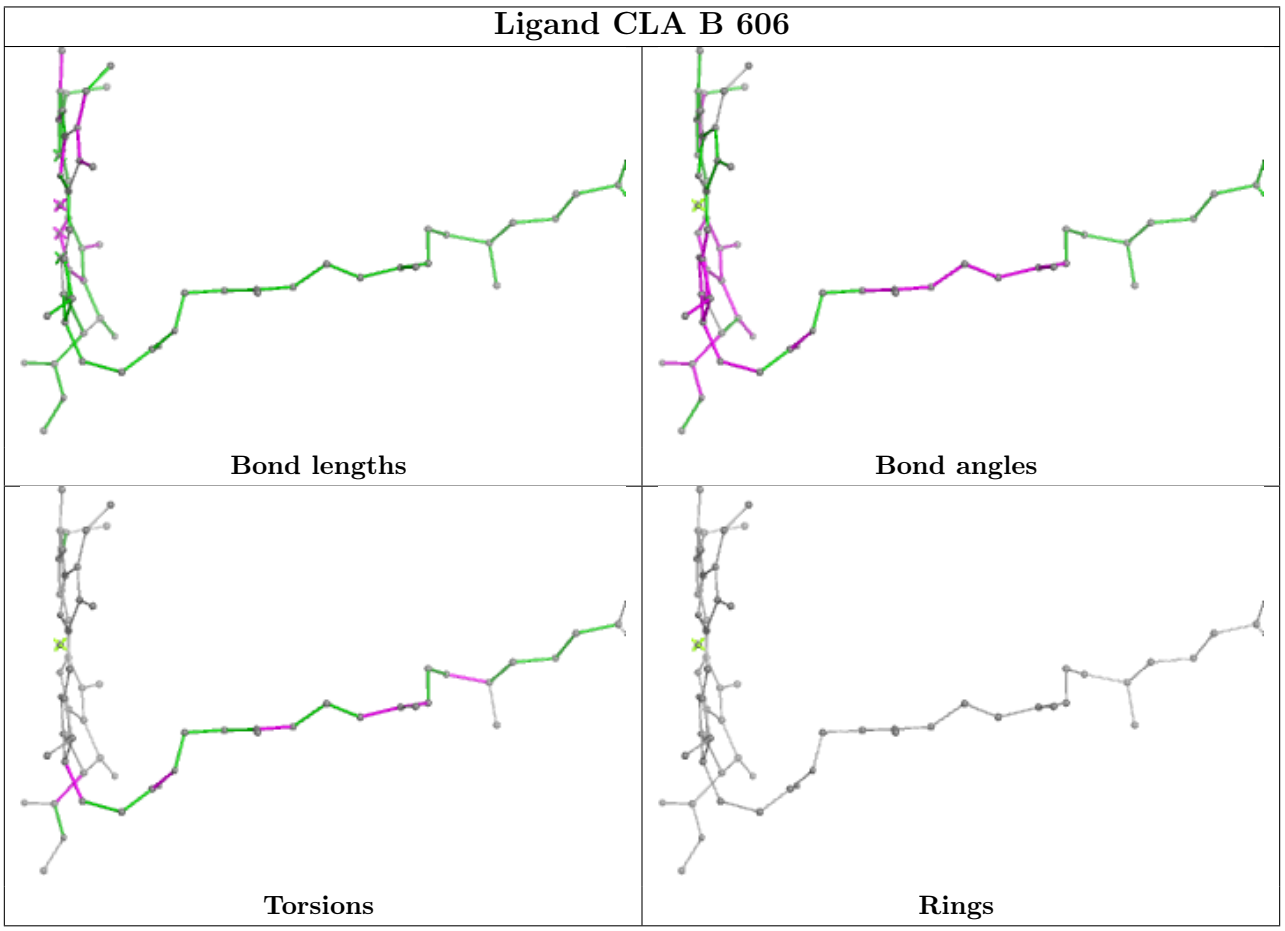


Rings

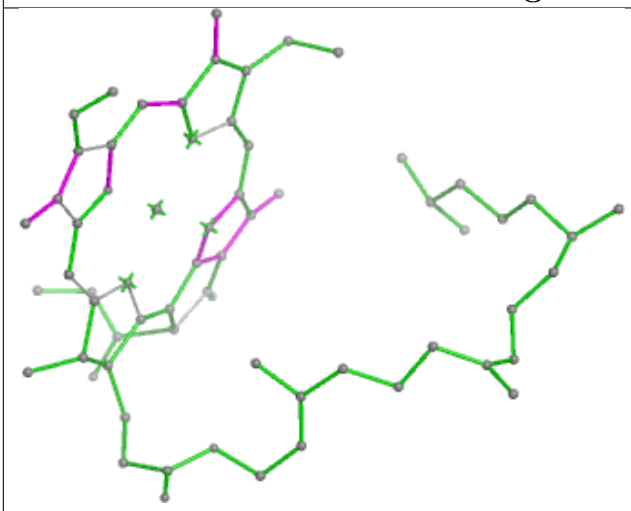
Ligand LMG I 101



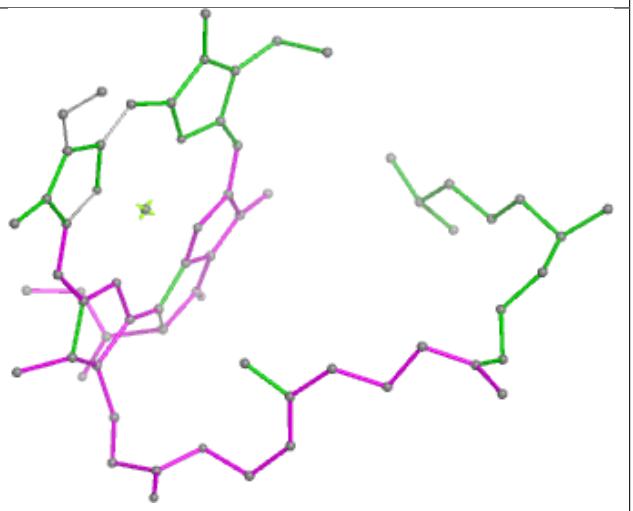
Ligand CLA B 606



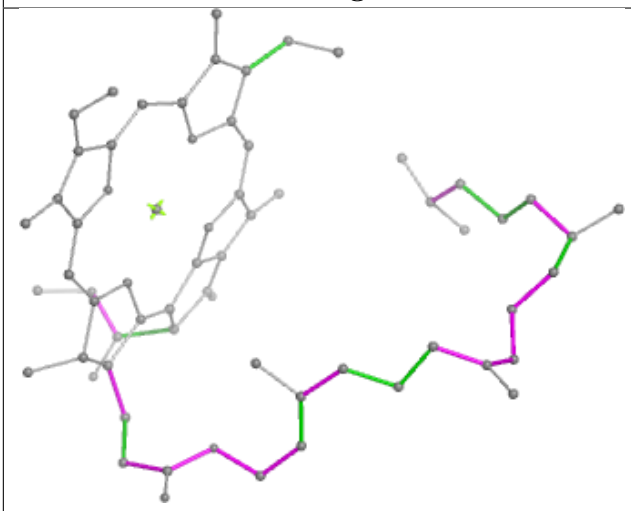
Ligand CLA C 505



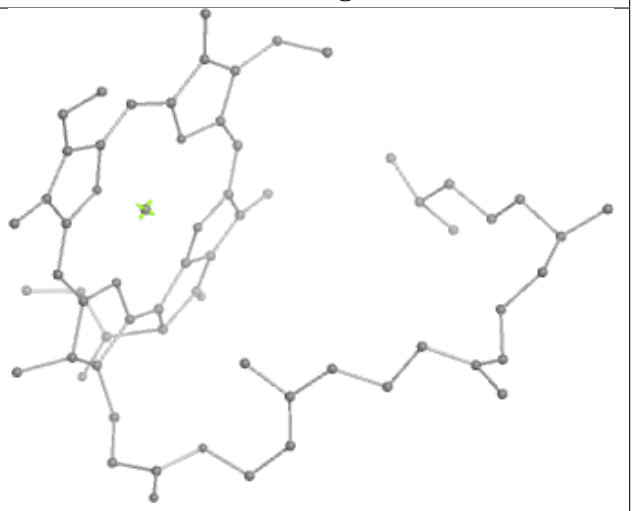
Bond lengths



Bond angles

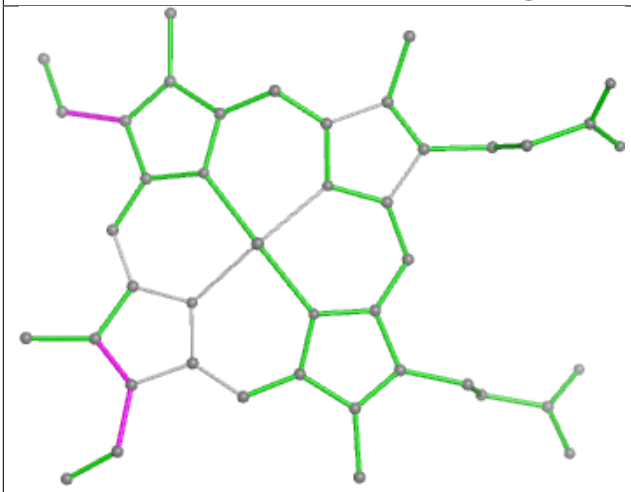


Torsions

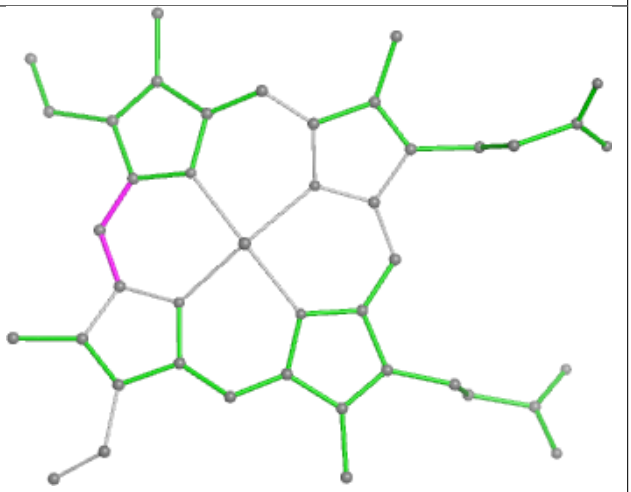


Rings

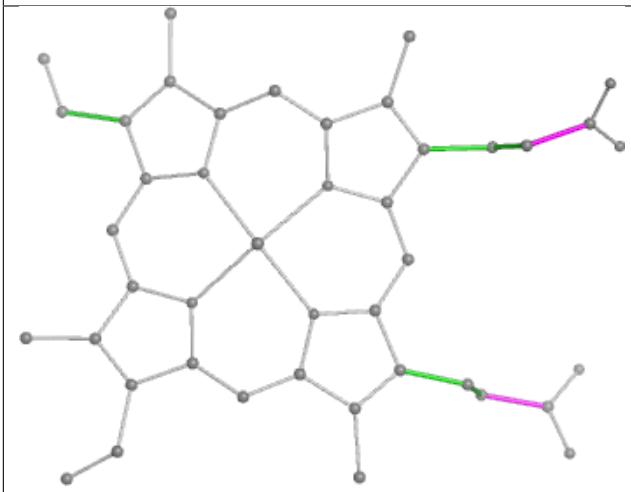
Ligand HEM E 101



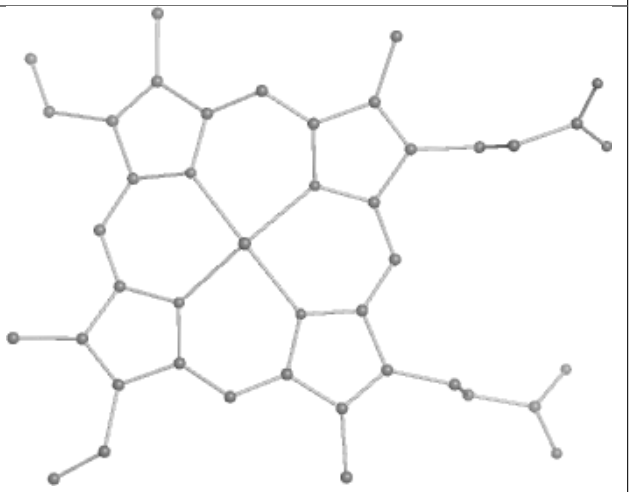
Bond lengths



Bond angles

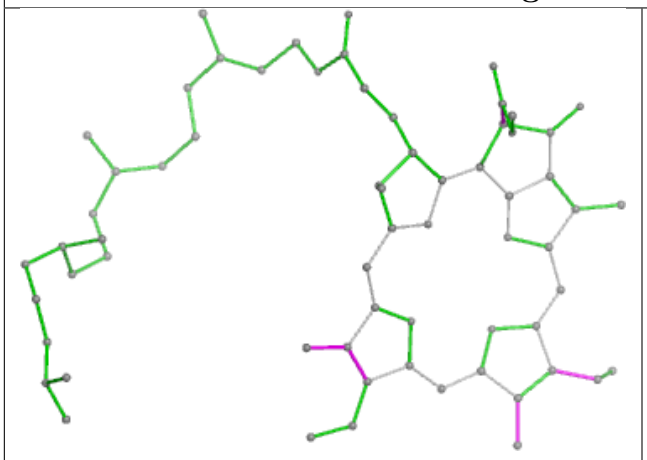


Torsions

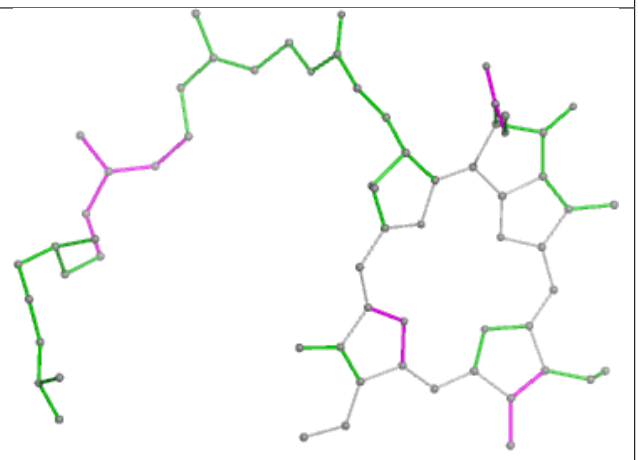


Rings

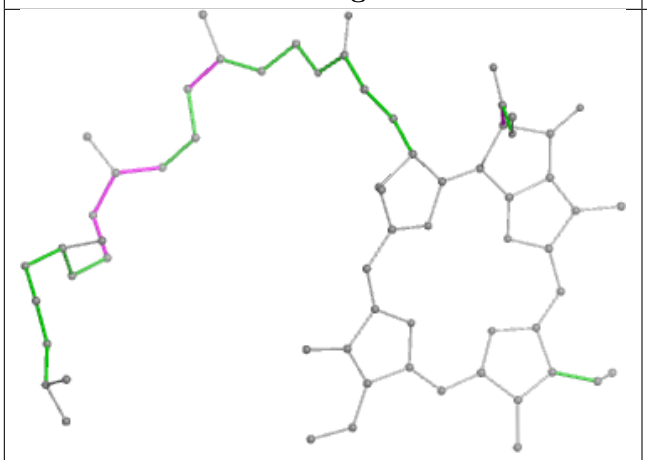
Ligand PHO D 406



Bond lengths



Bond angles



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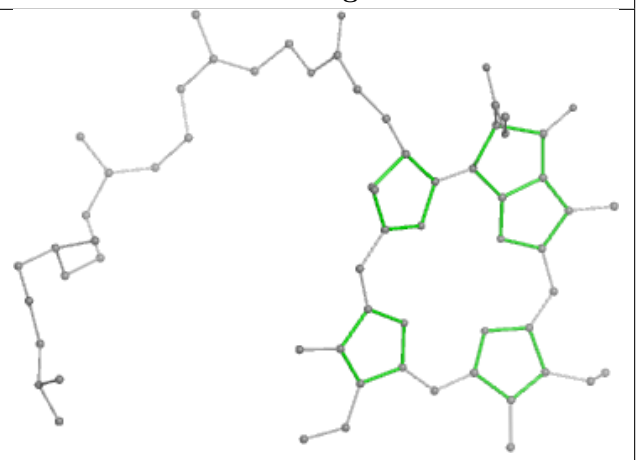
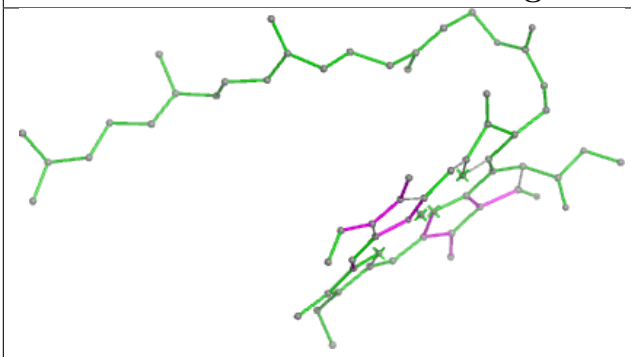
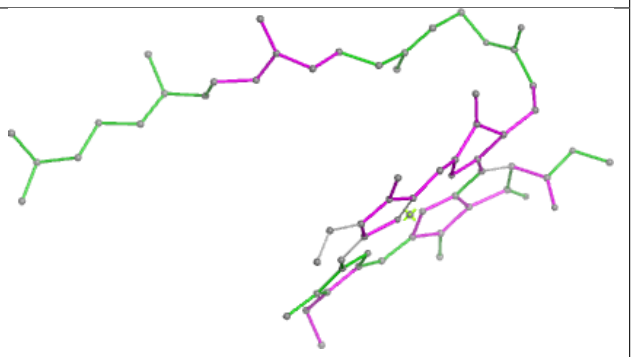


Rings

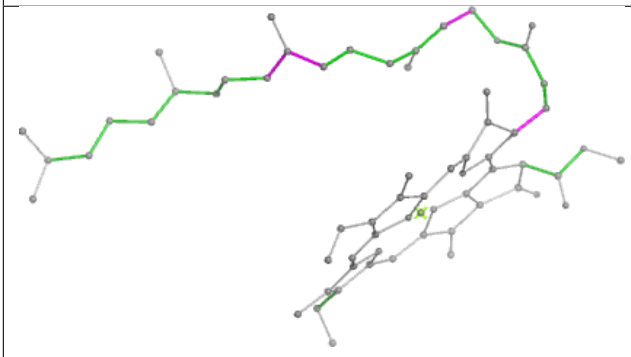
Ligand CLA B 608



Bond lengths



Bond angles



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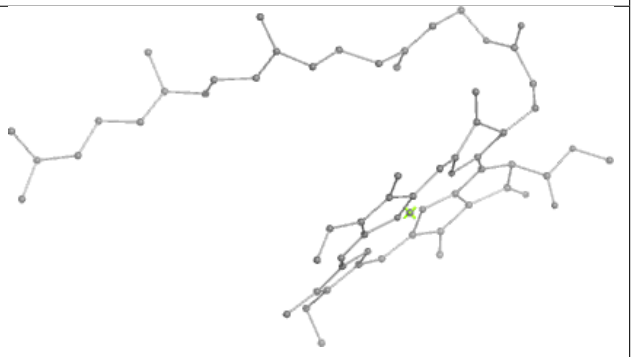
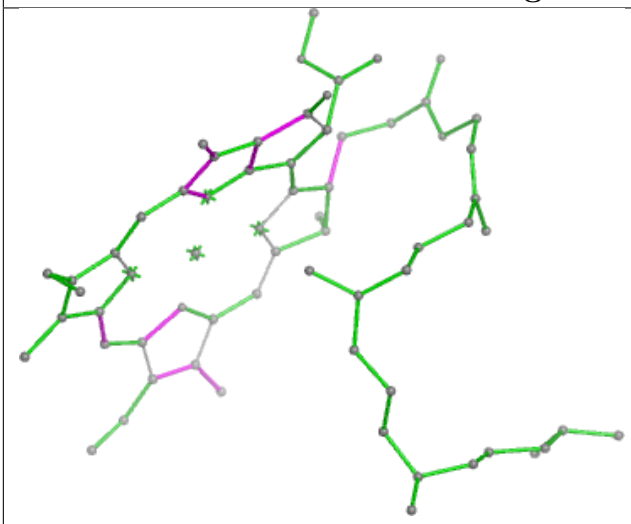
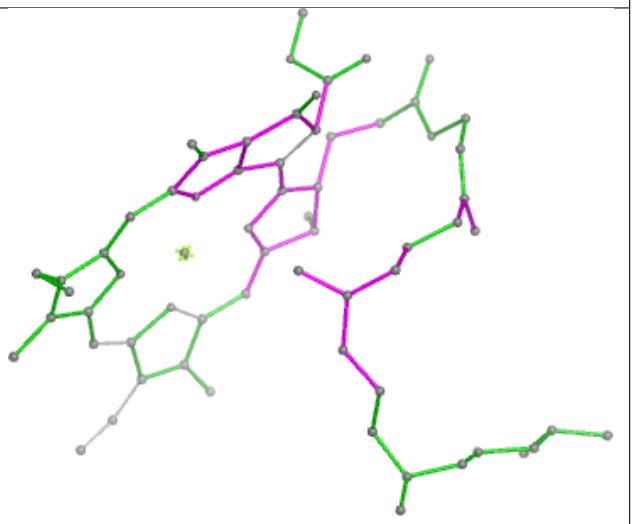


Rings

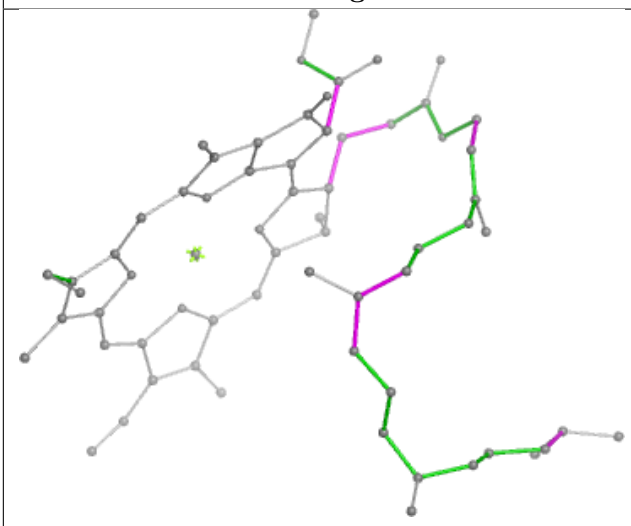
Ligand CLA C 514



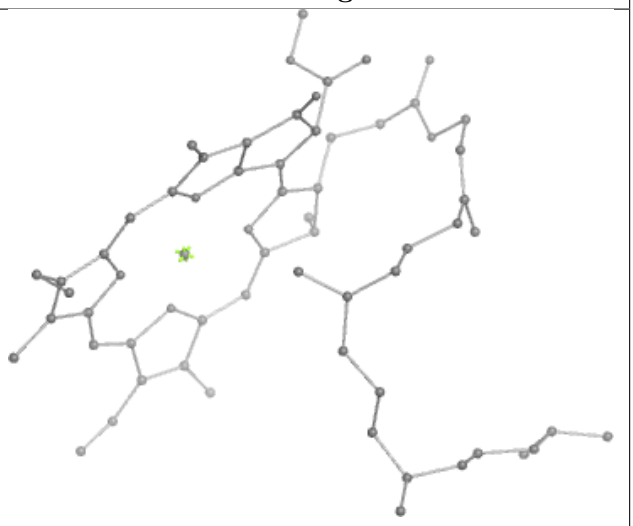
Bond lengths



Bond angles

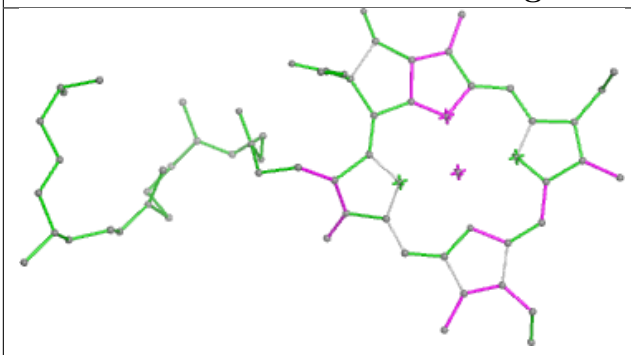


Torsions

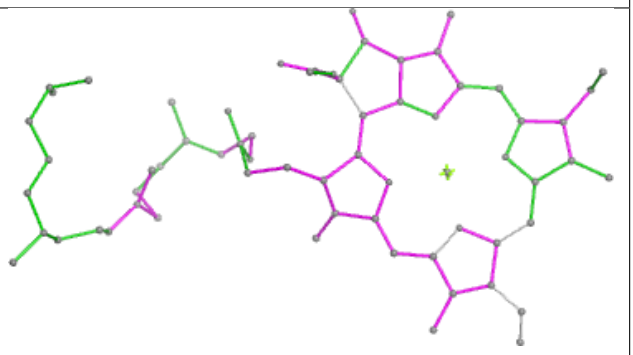


Rings

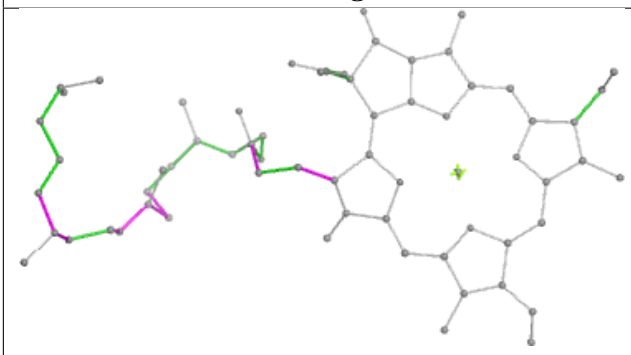
Ligand CLA B 612



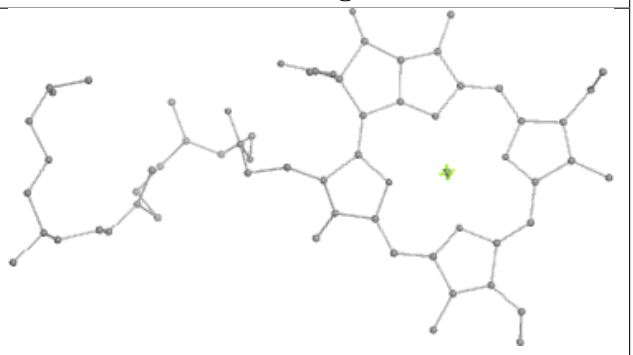
Bond lengths



Bond angles

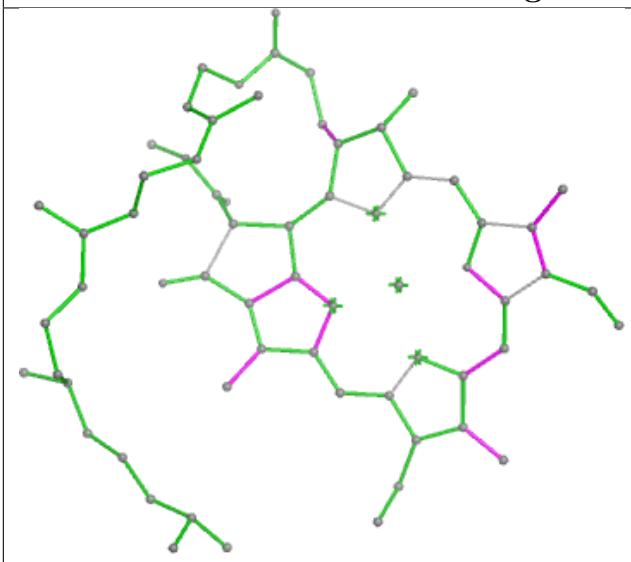


Torsions

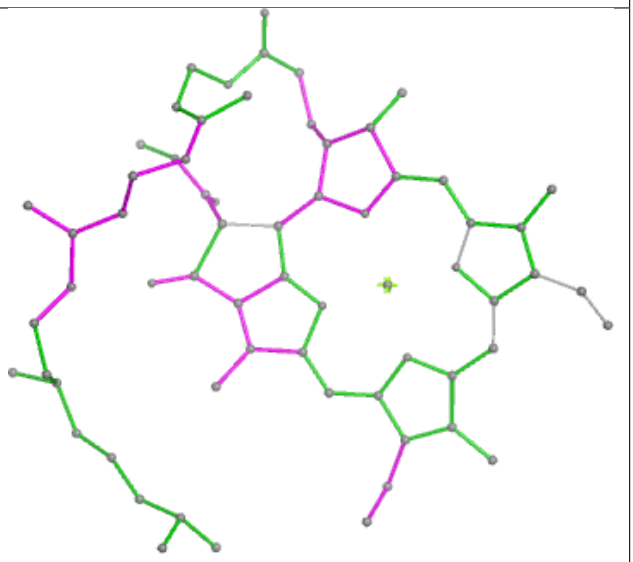


Rings

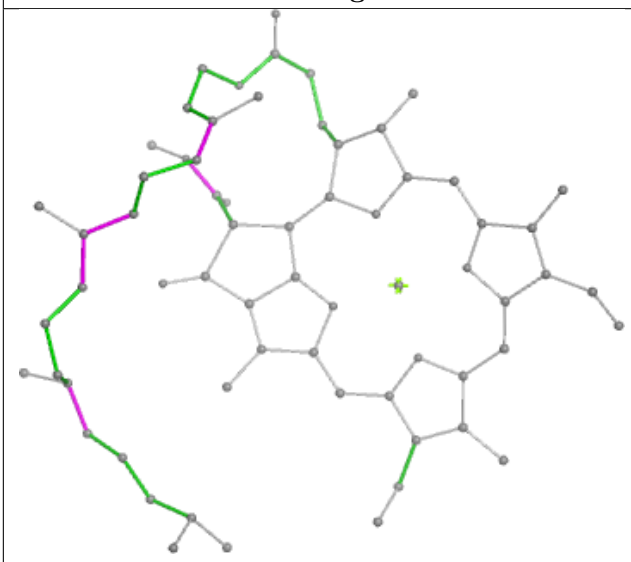
Ligand CLA B 601



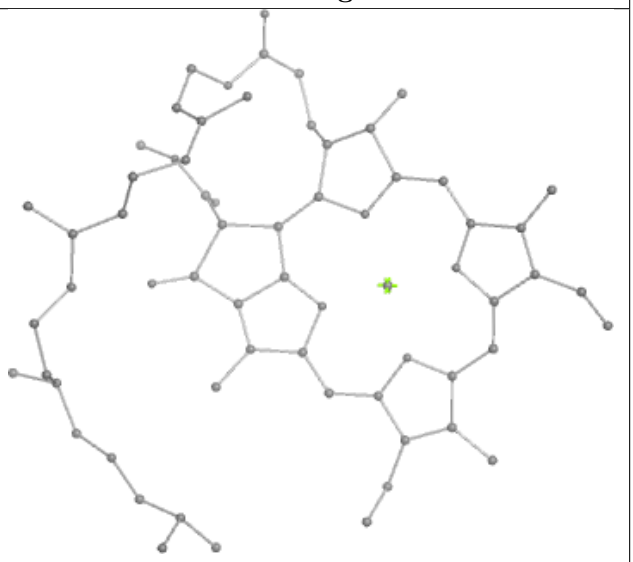
Bond lengths



Bond angles

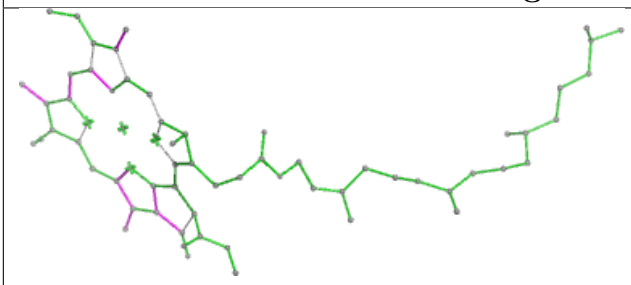


Torsions

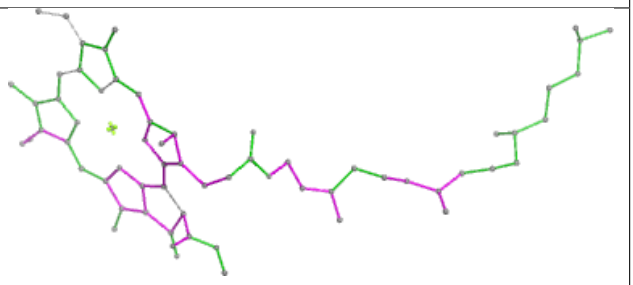


Rings

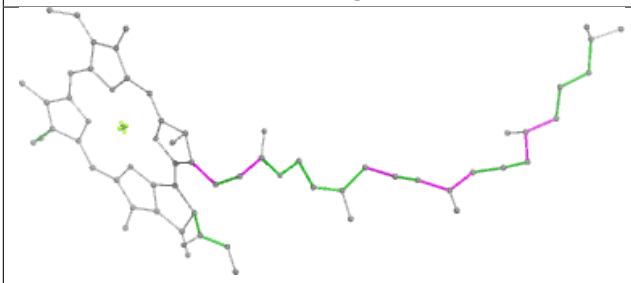
Ligand CLA A 405



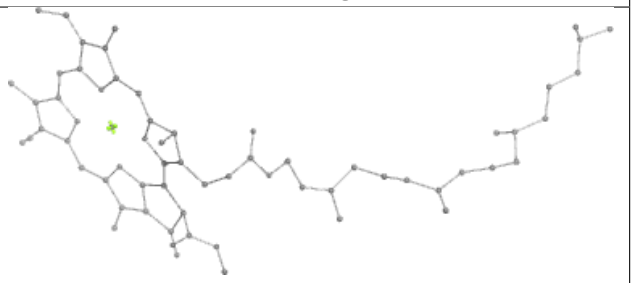
Bond lengths



Bond angles

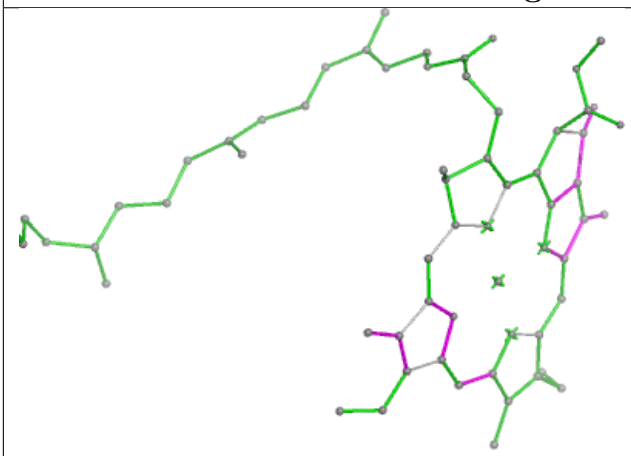


Torsions

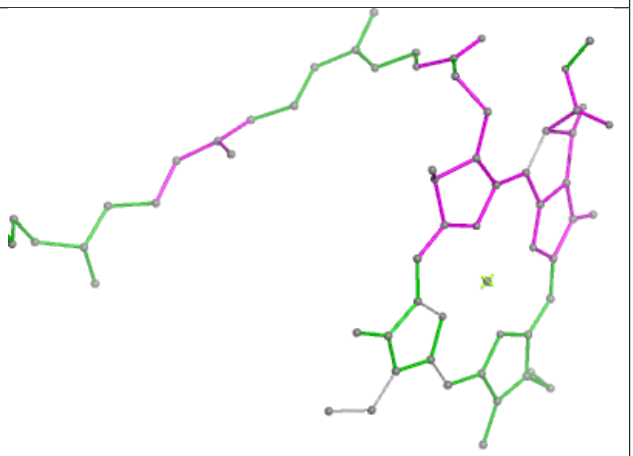


Rings

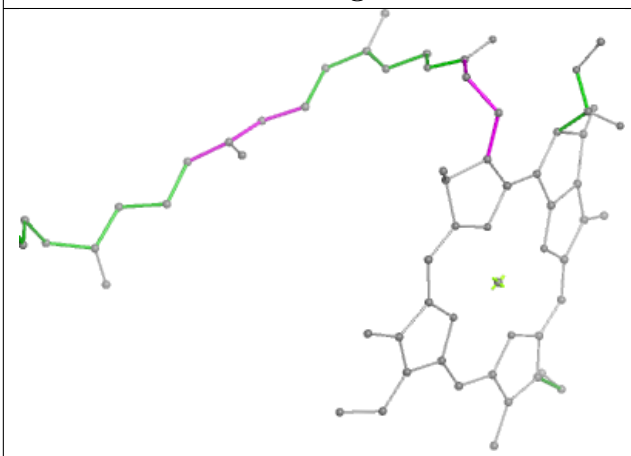
Ligand CLA C 512



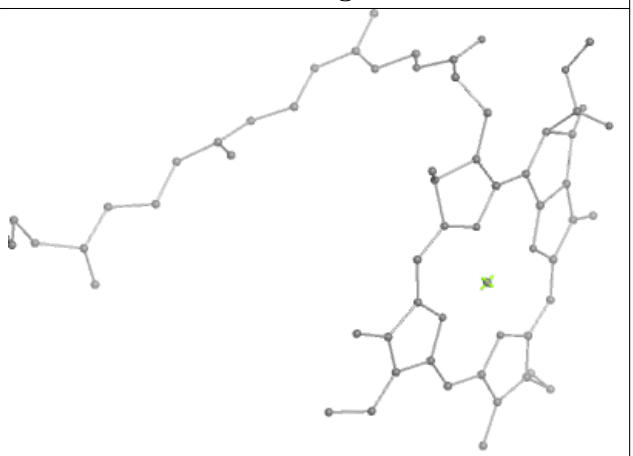
Bond lengths



Bond angles

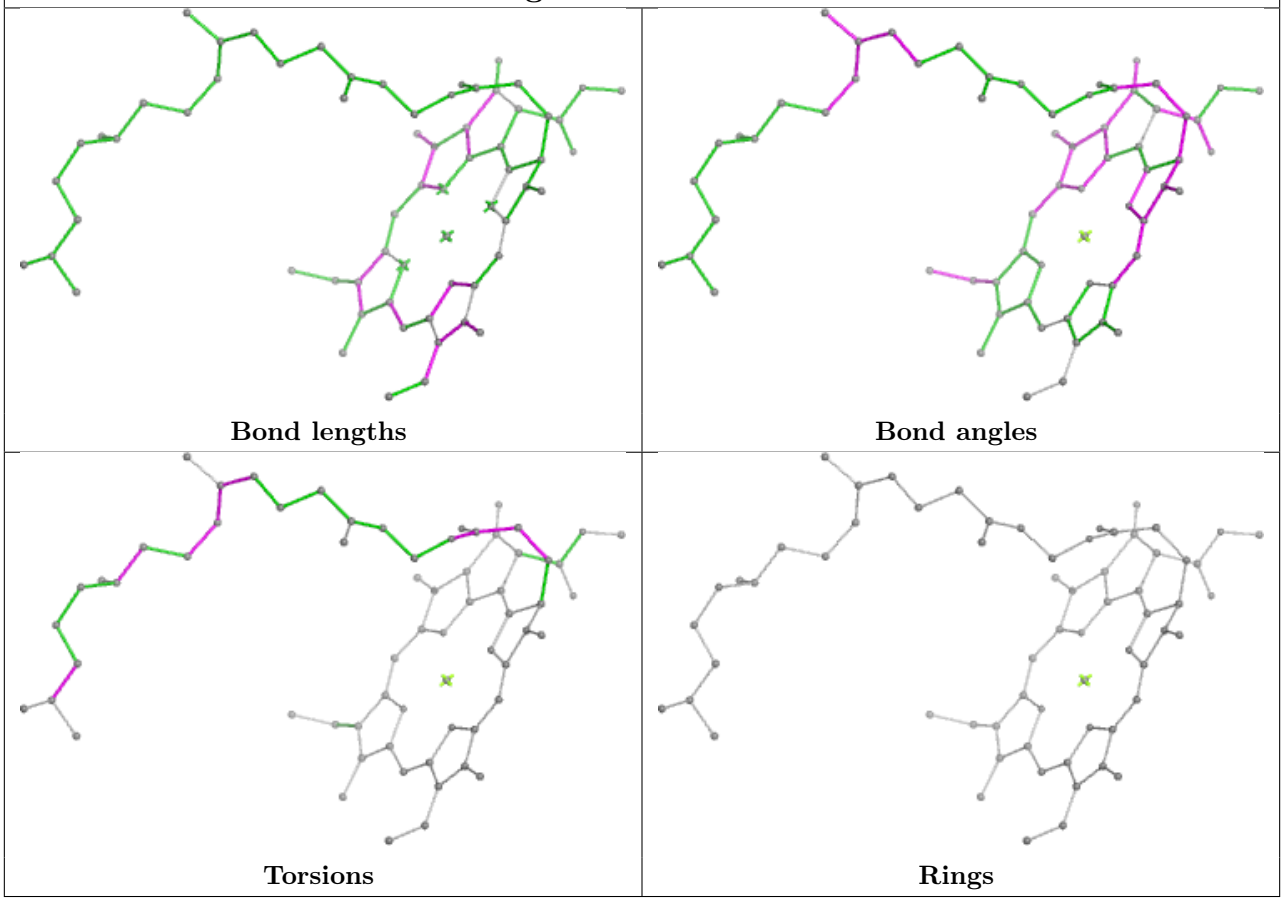


Torsions

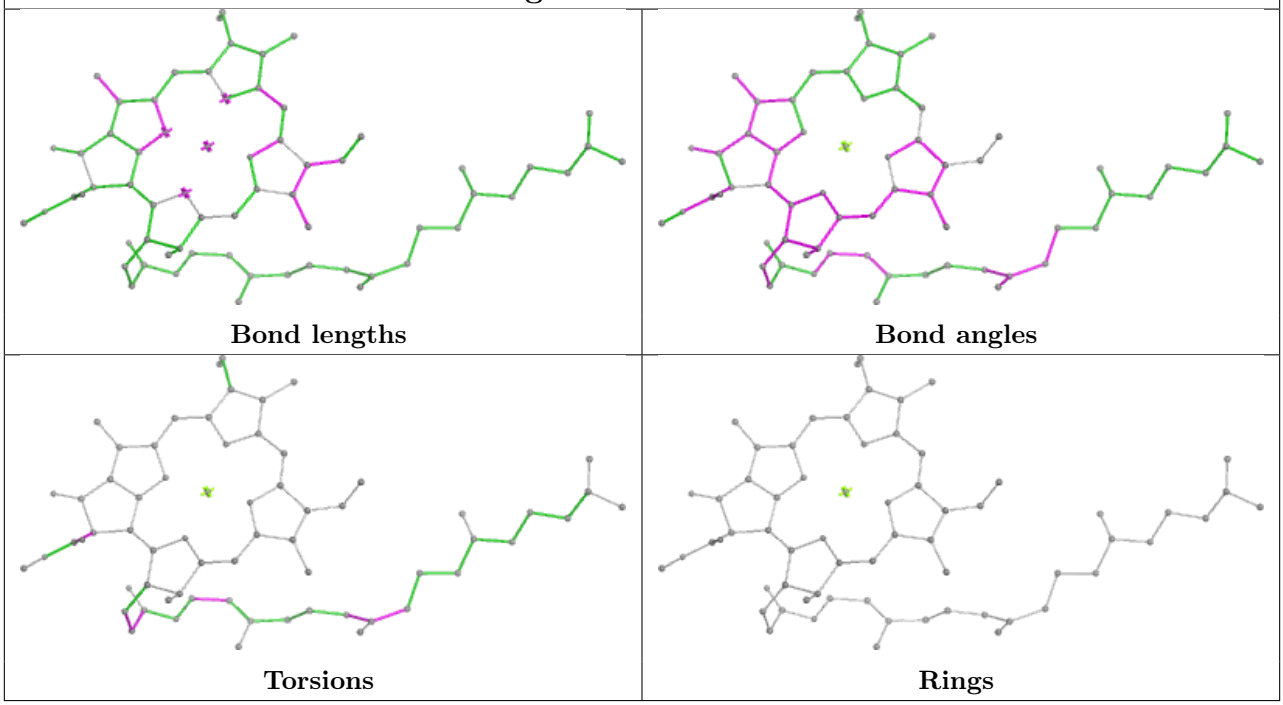


Rings

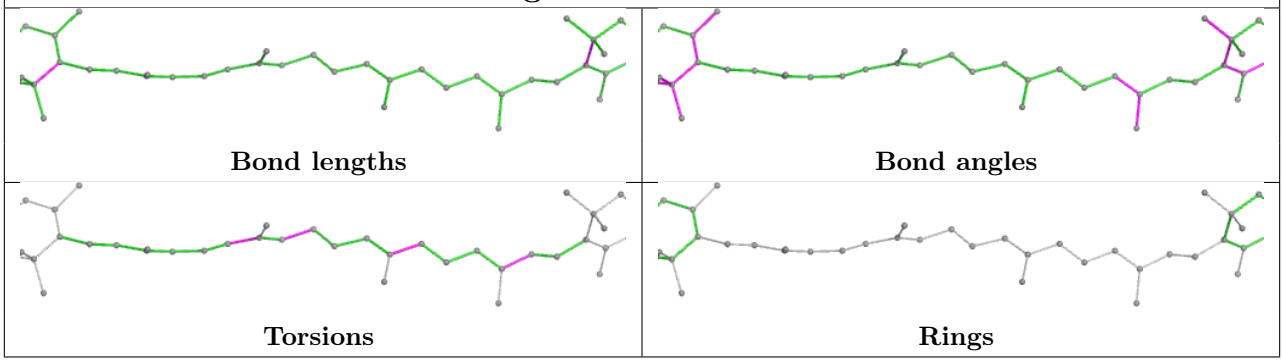
Ligand CLA C 510



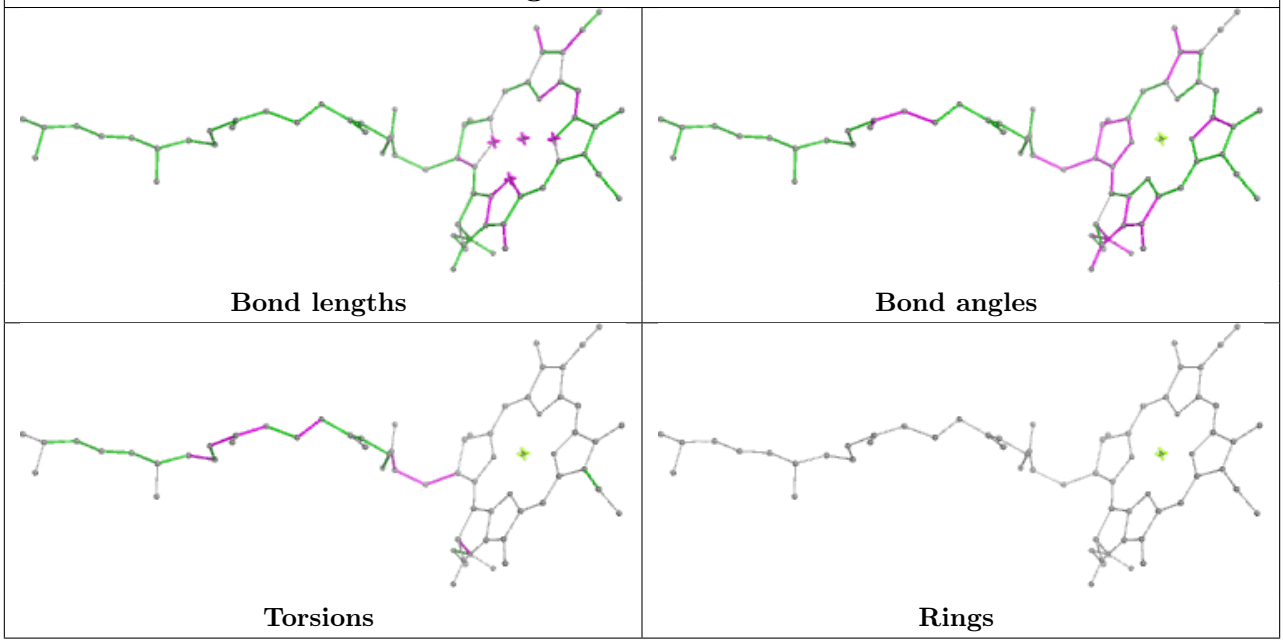
Ligand CLA C 503



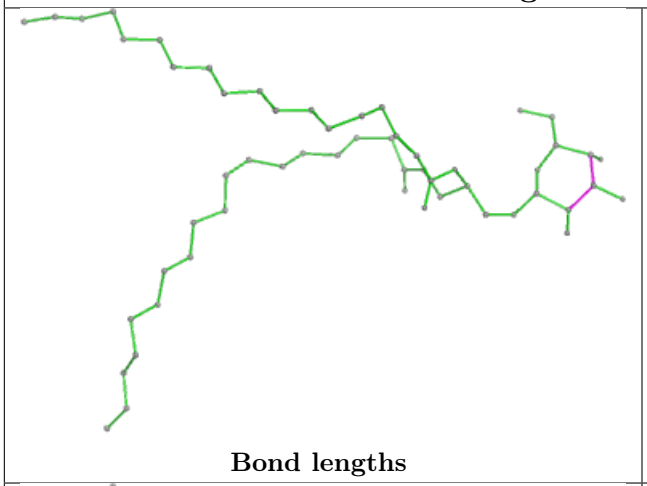
Ligand BCR B 619



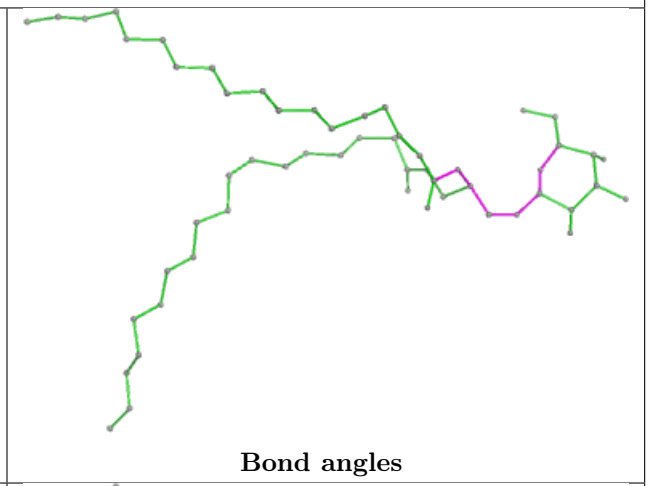
Ligand CLA C 504



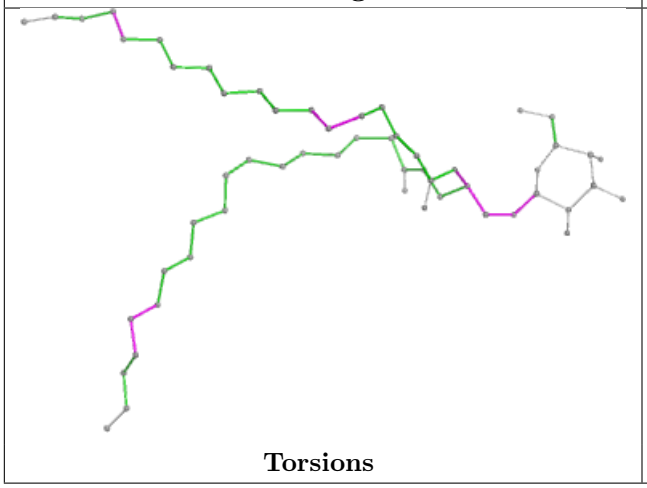
Ligand LMG D 404



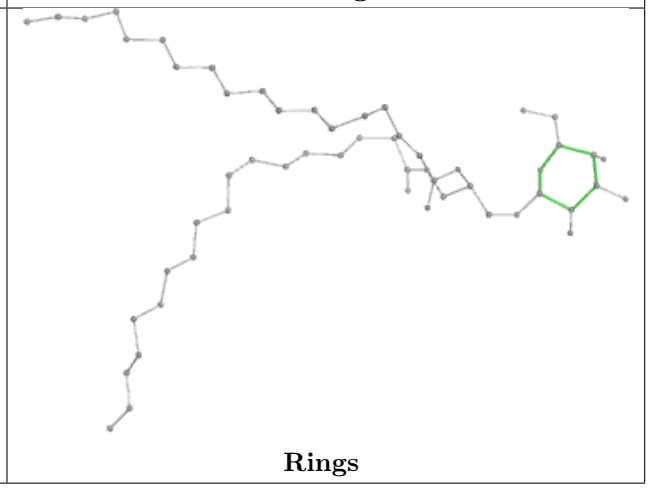
Bond lengths



Bond angles

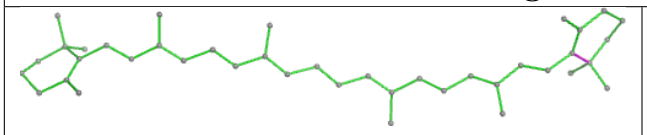


Torsions

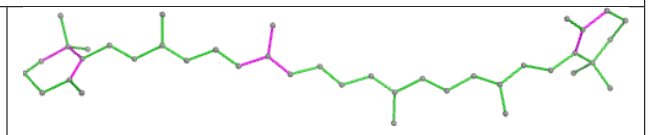


Rings

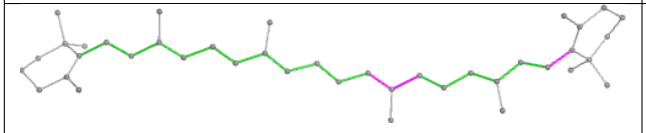
Ligand BCR B 618



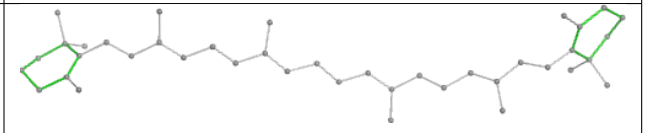
Bond lengths



Bond angles

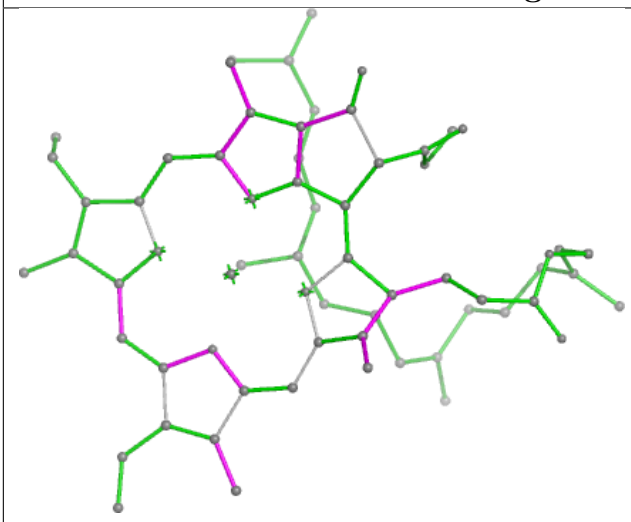


Torsions

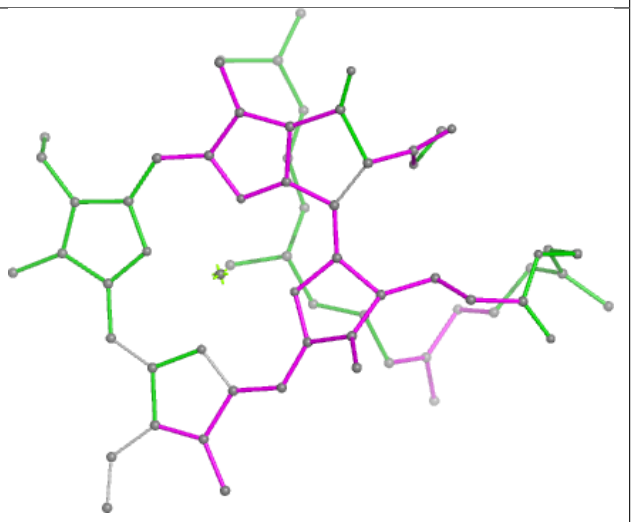


Rings

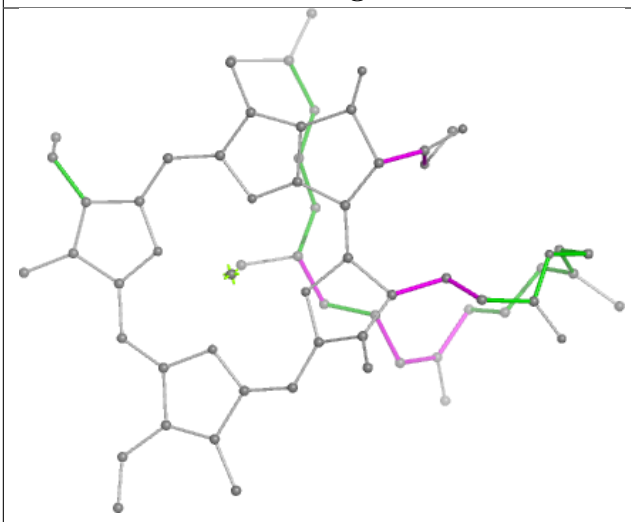
Ligand CLA C 517



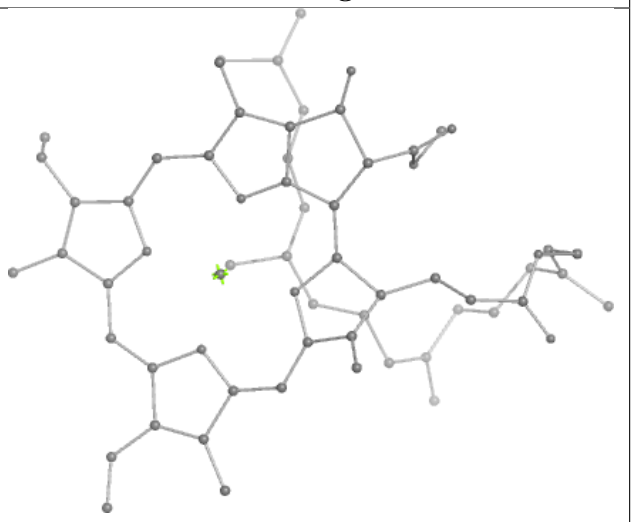
Bond lengths



Bond angles

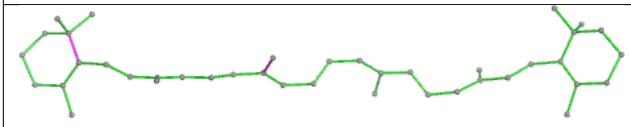


Torsions

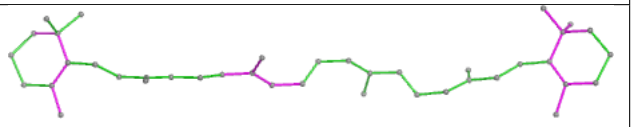


Rings

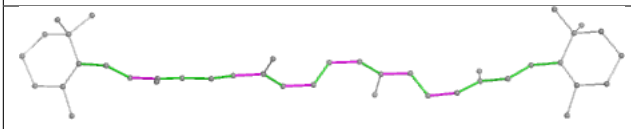
Ligand BCR C 515



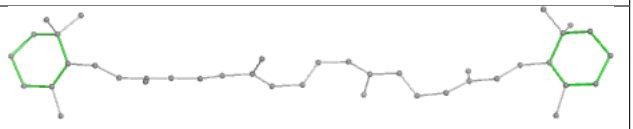
Bond lengths



Bond angles

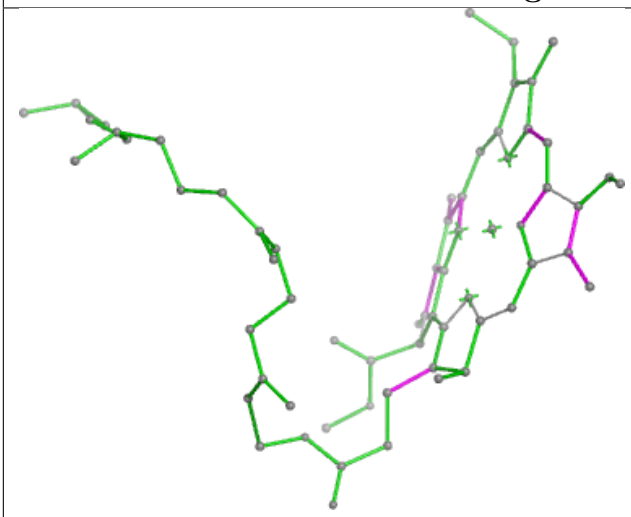


Torsions

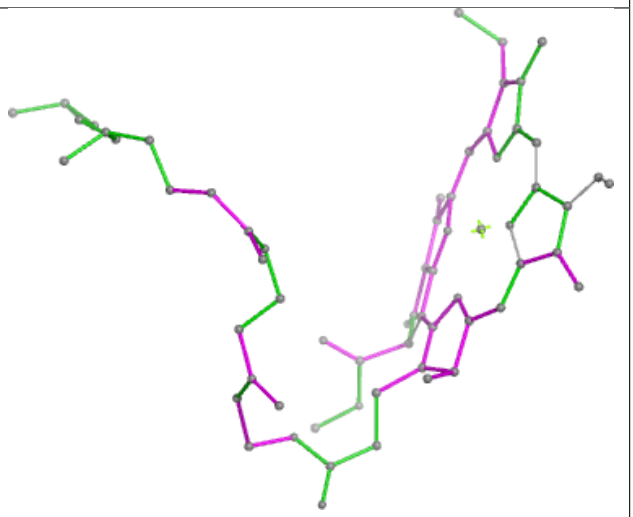


Rings

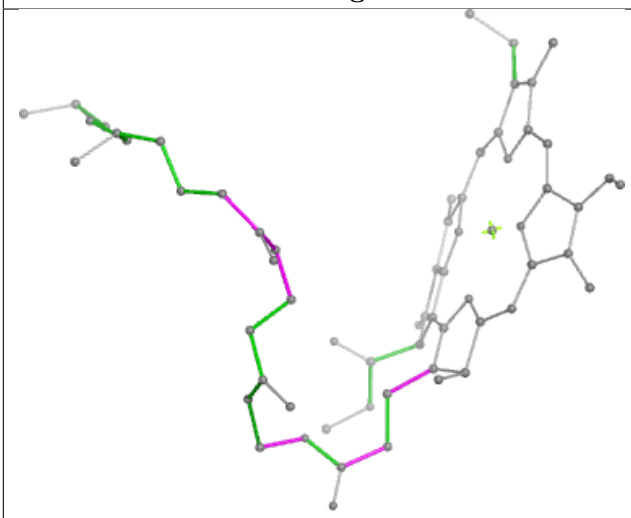
Ligand CLA B 613



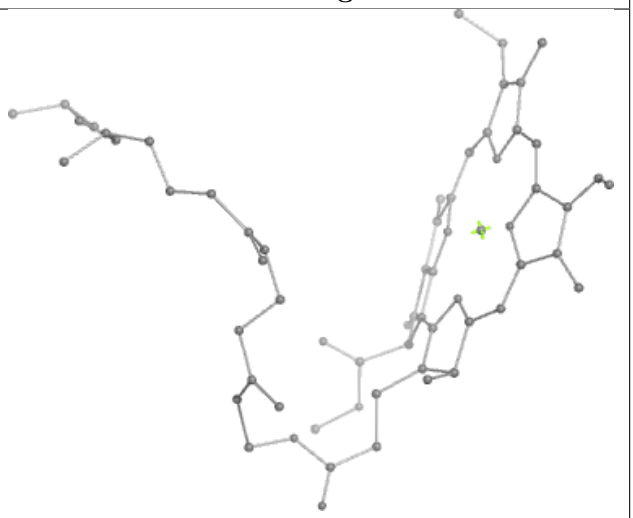
Bond lengths



Bond angles

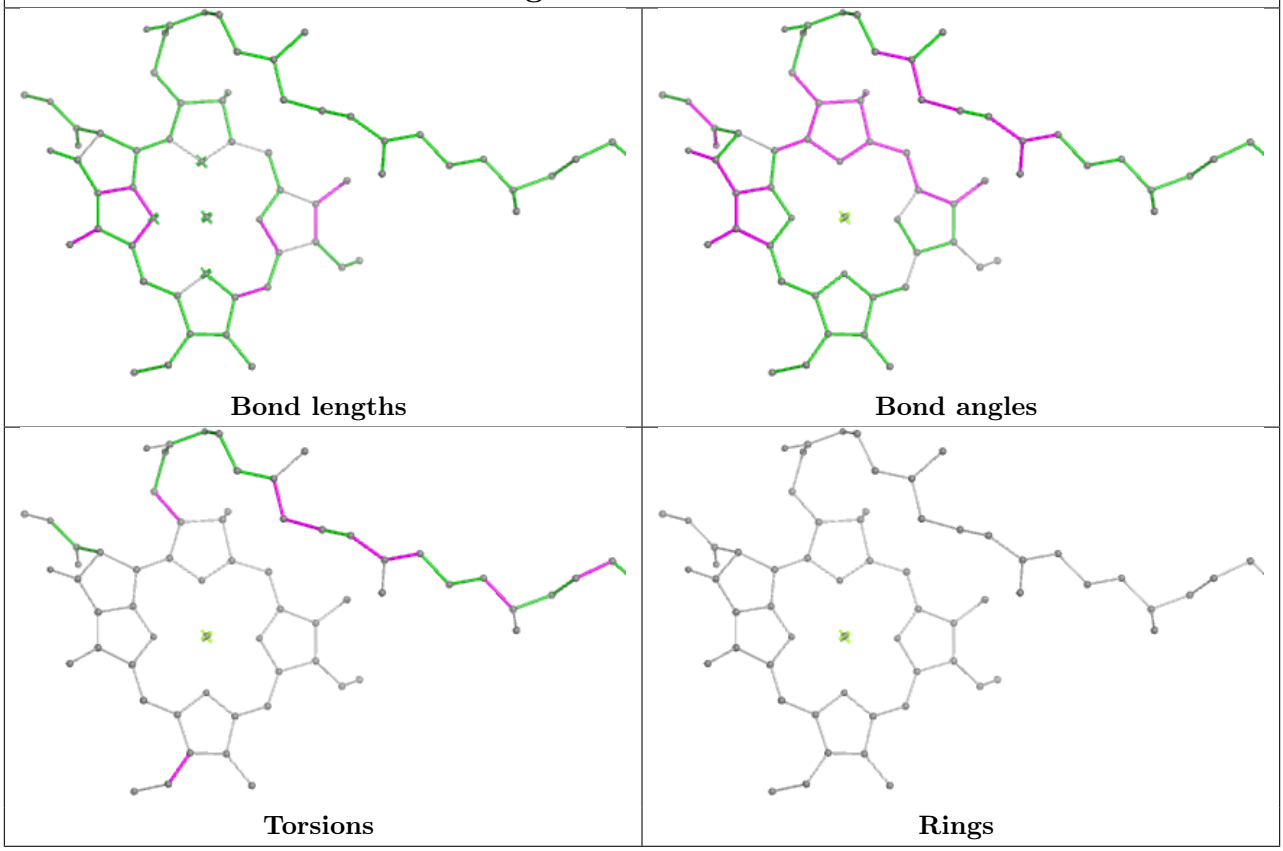


Torsions

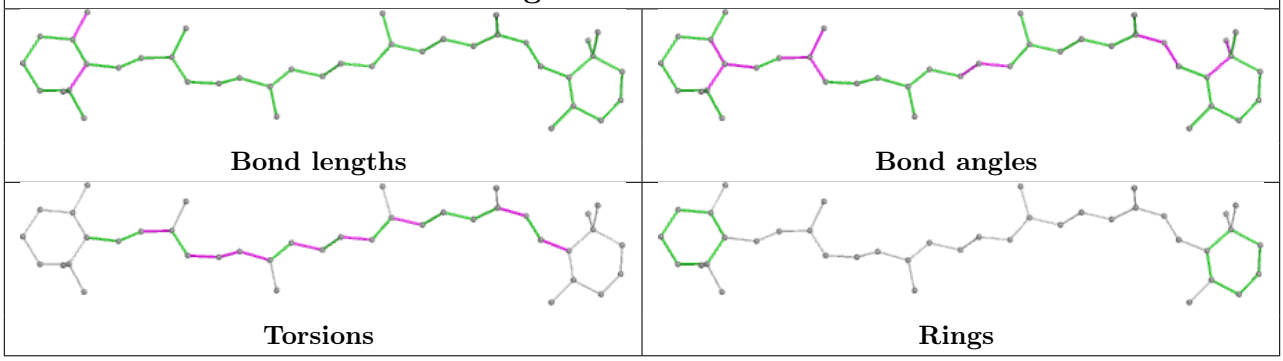


Rings

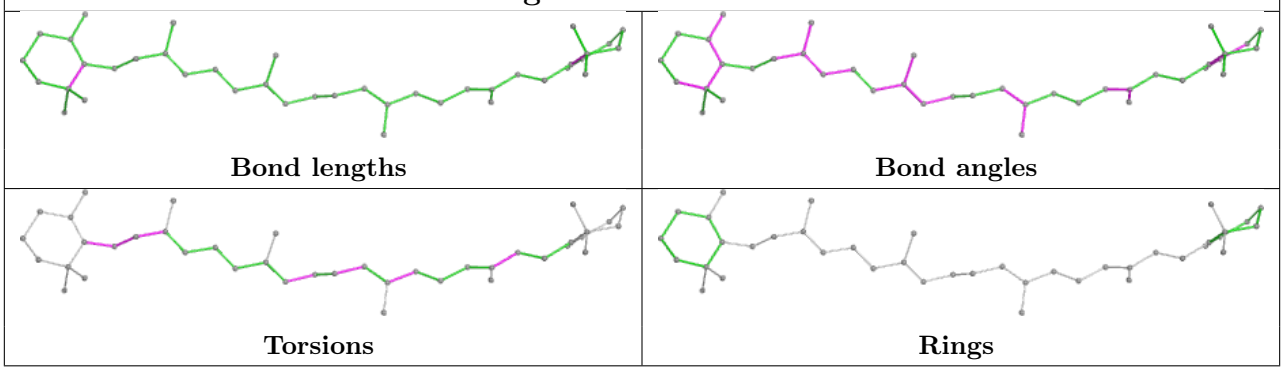
Ligand CLA B 603



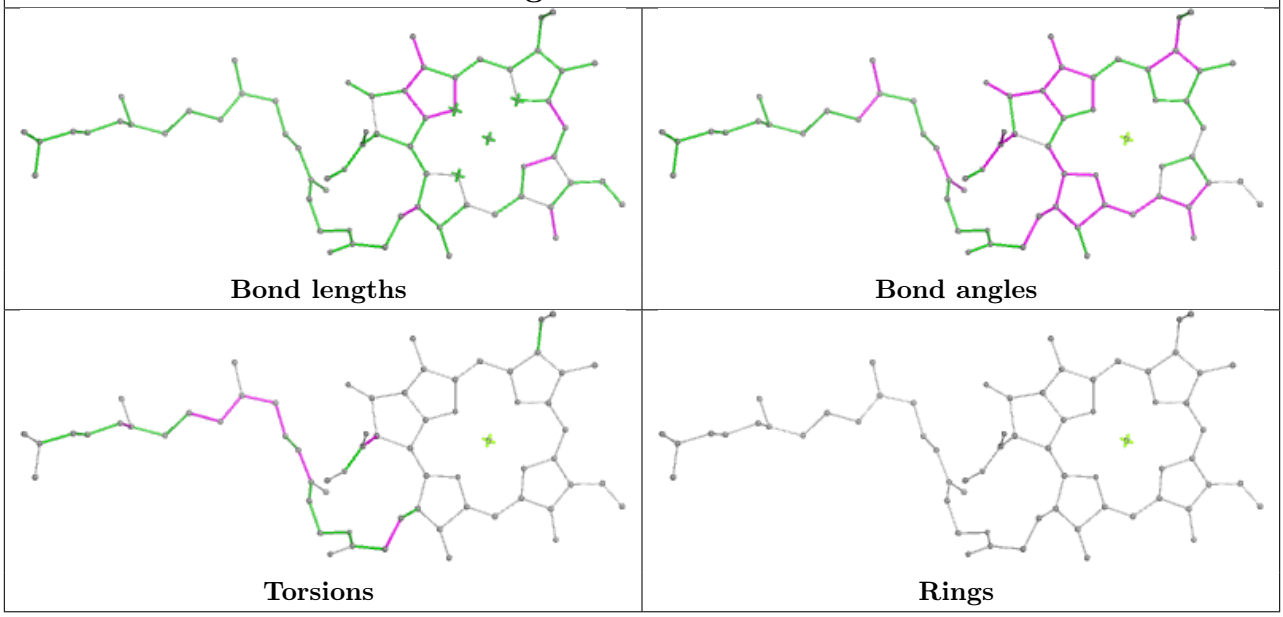
Ligand BCR B 617



Ligand BCR C 518



Ligand CLA B 602



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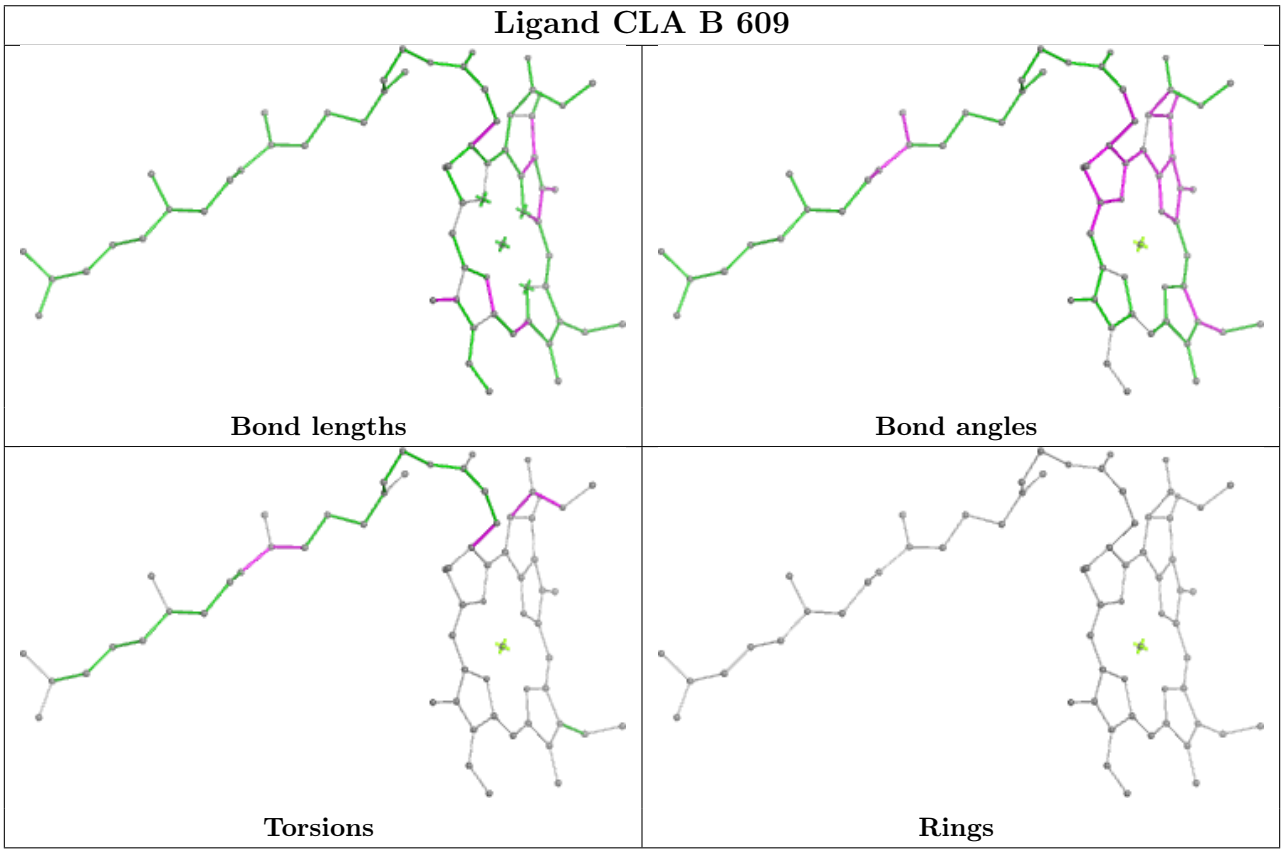
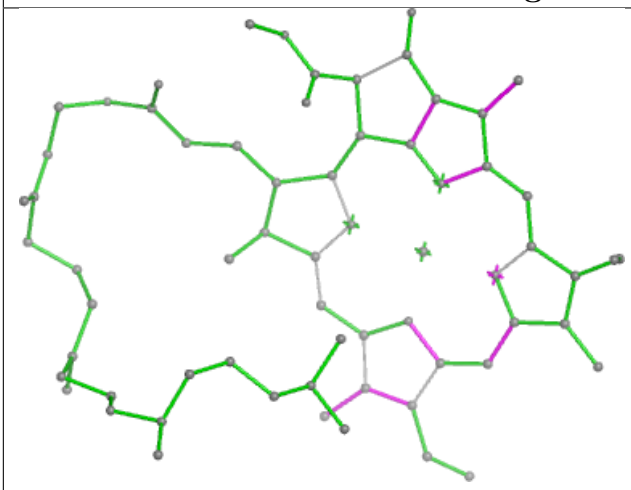
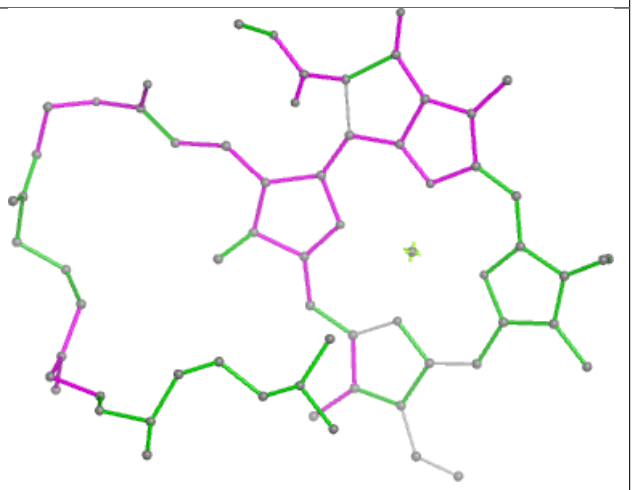


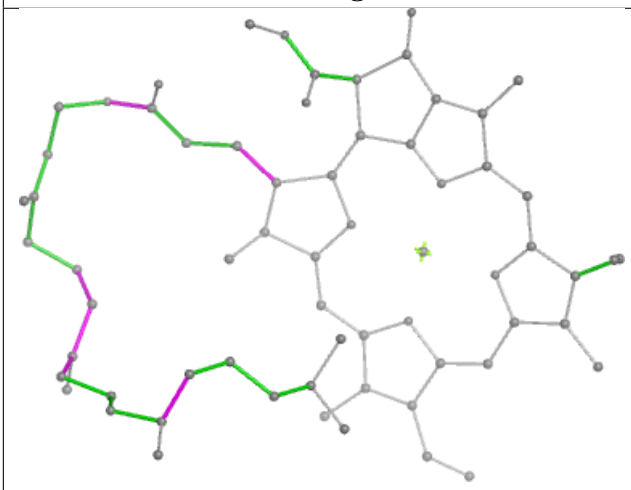
Ligand CLA B 615



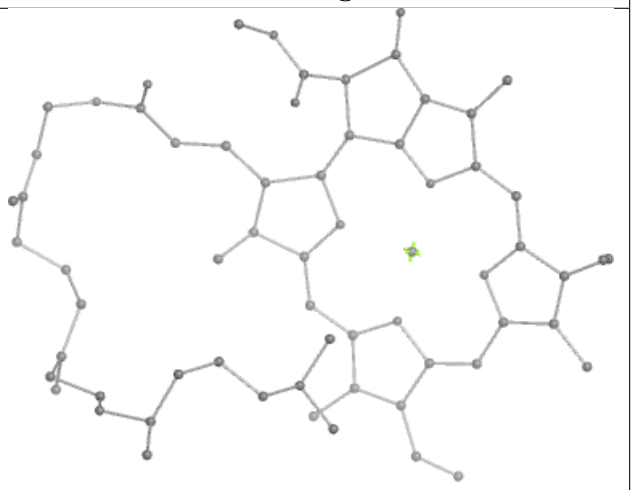
Bond lengths



Bond angles

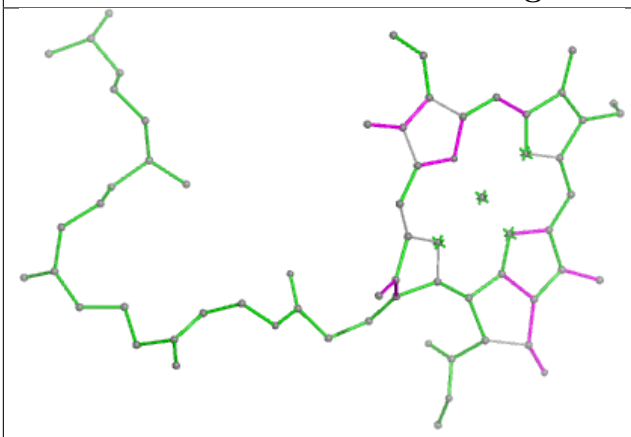


Torsions

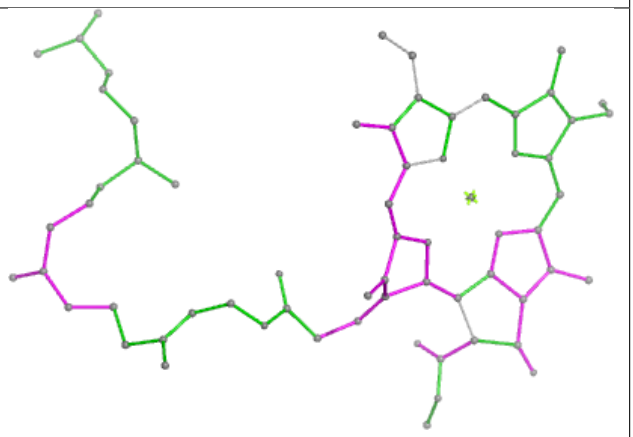


Rings

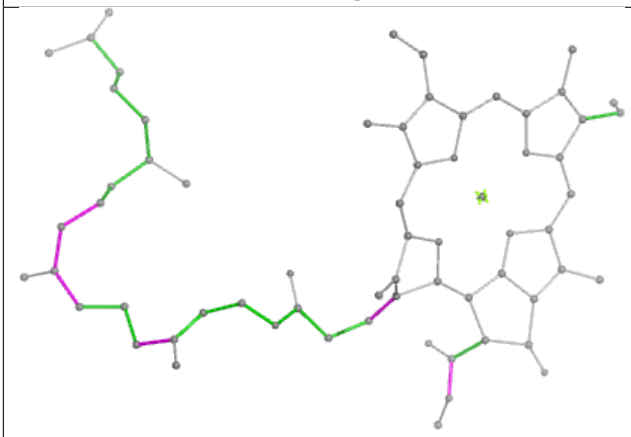
Ligand CLA B 616



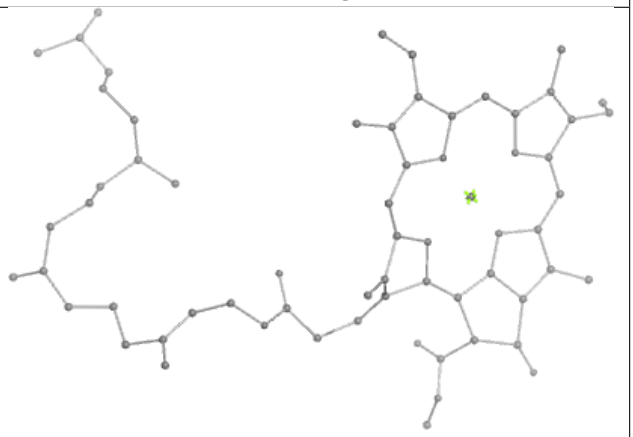
Bond lengths



Bond angles

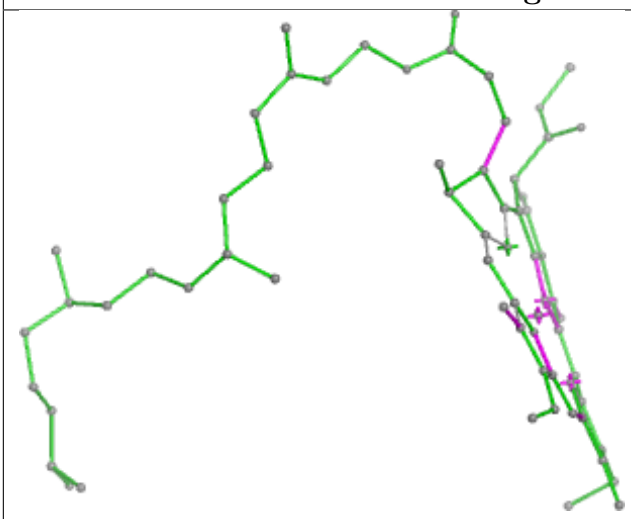


Torsions

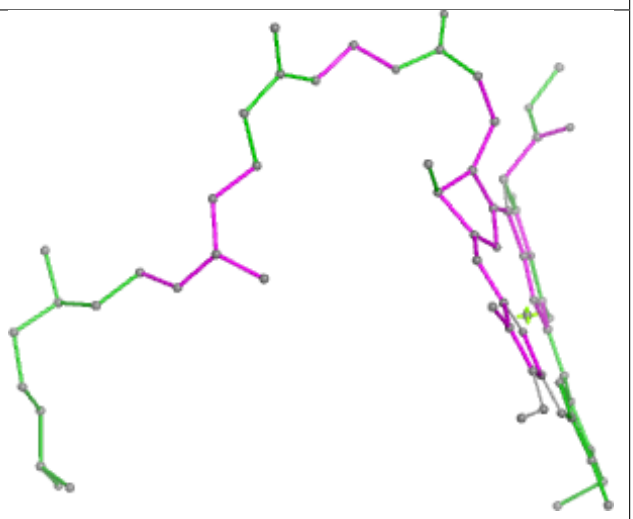


Rings

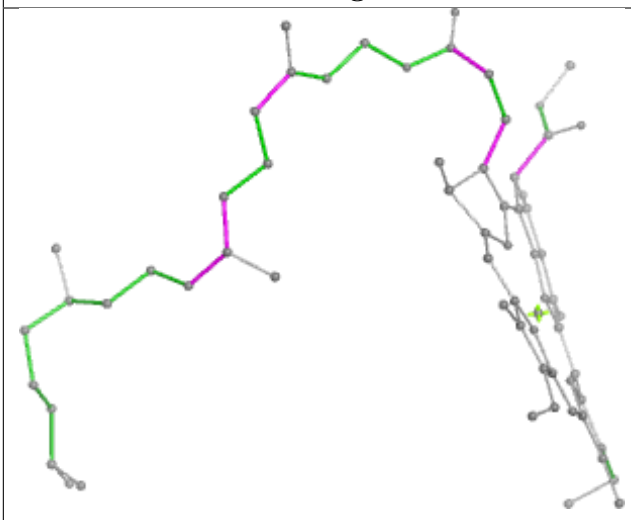
Ligand CLA A 406



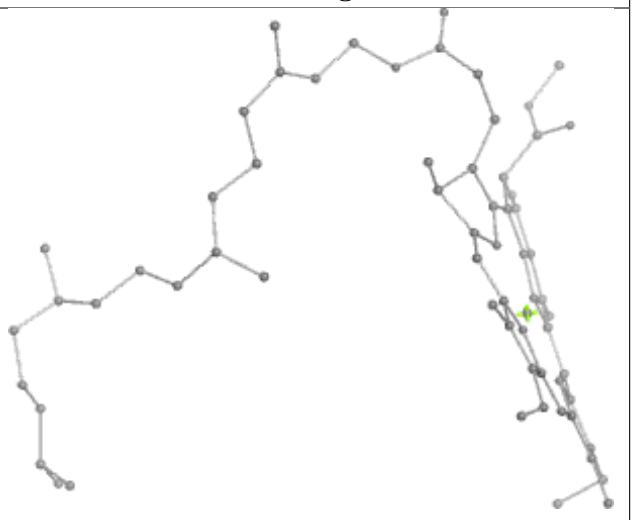
Bond lengths



Bond angles

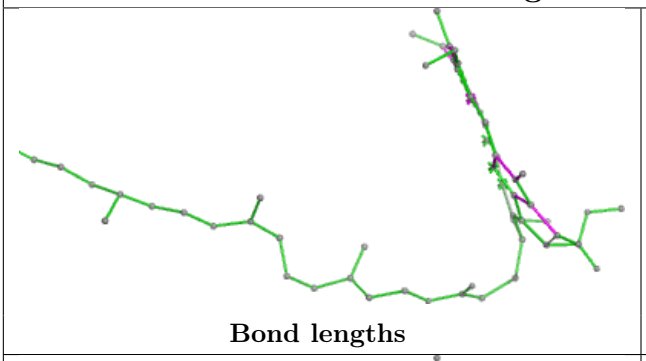


Torsions

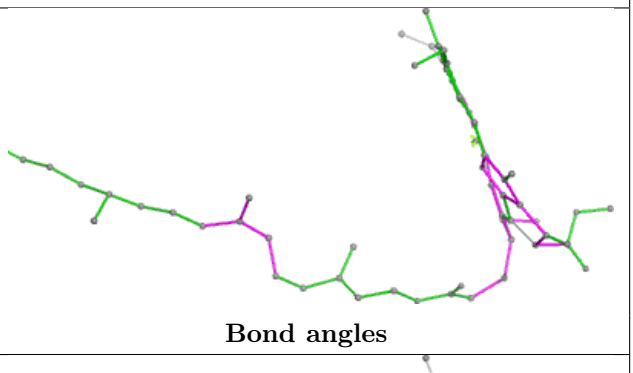


Rings

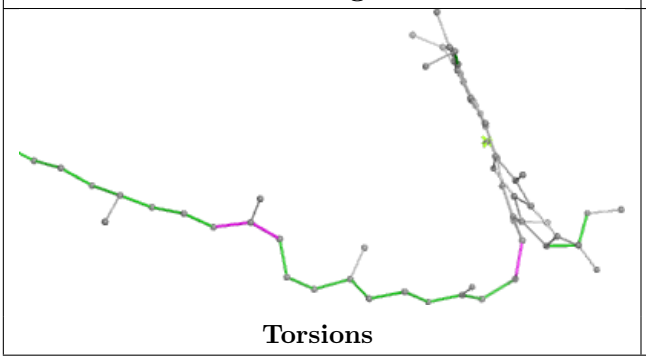
Ligand CLA C 508



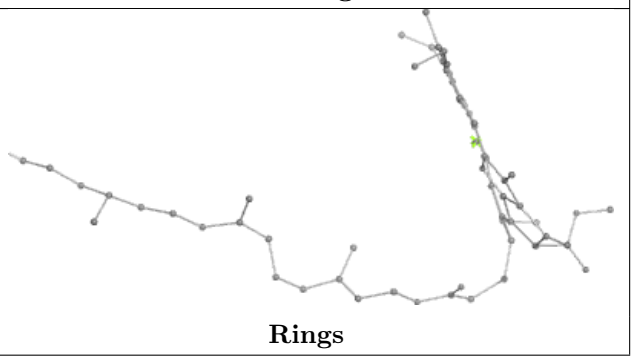
Bond lengths



Bond angles

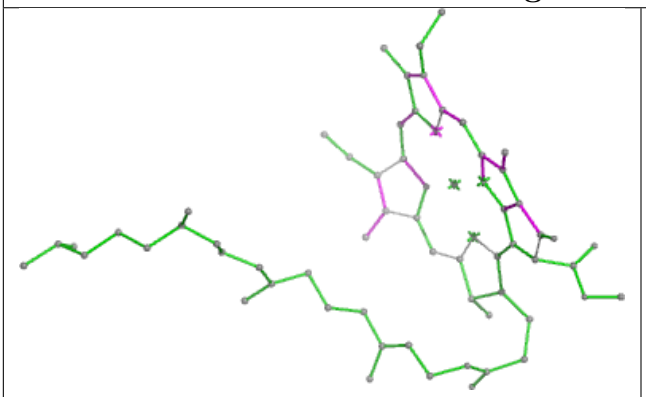


Torsions

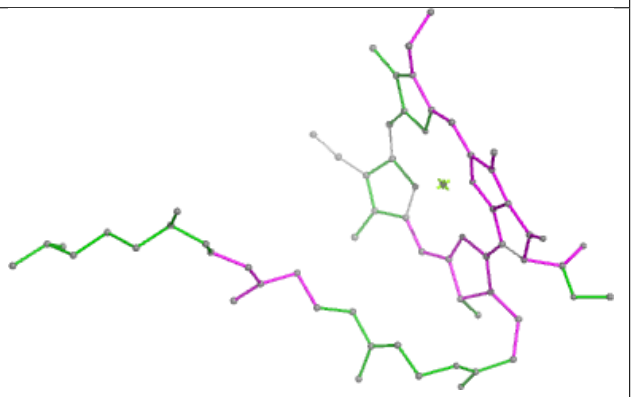


Rings

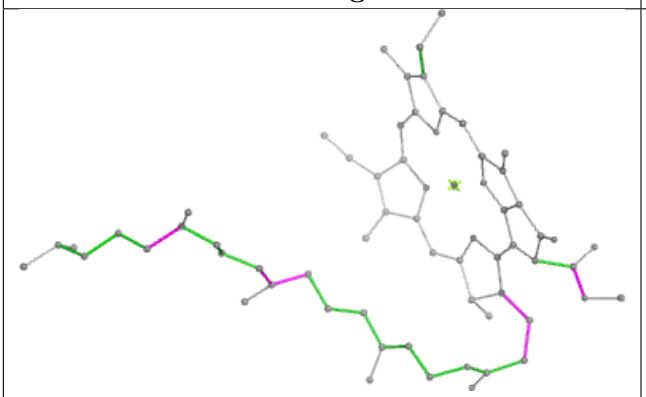
Ligand CLA C 507



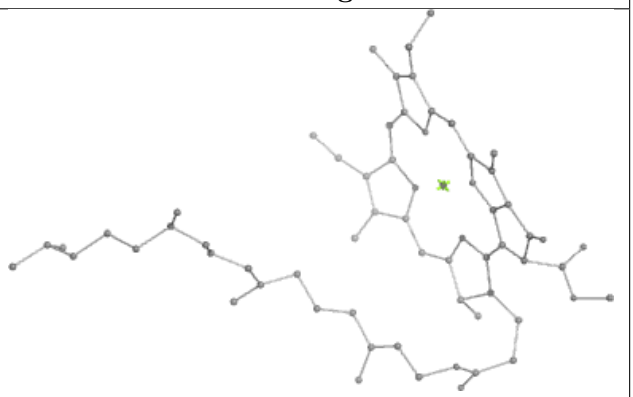
Bond lengths



Bond angles

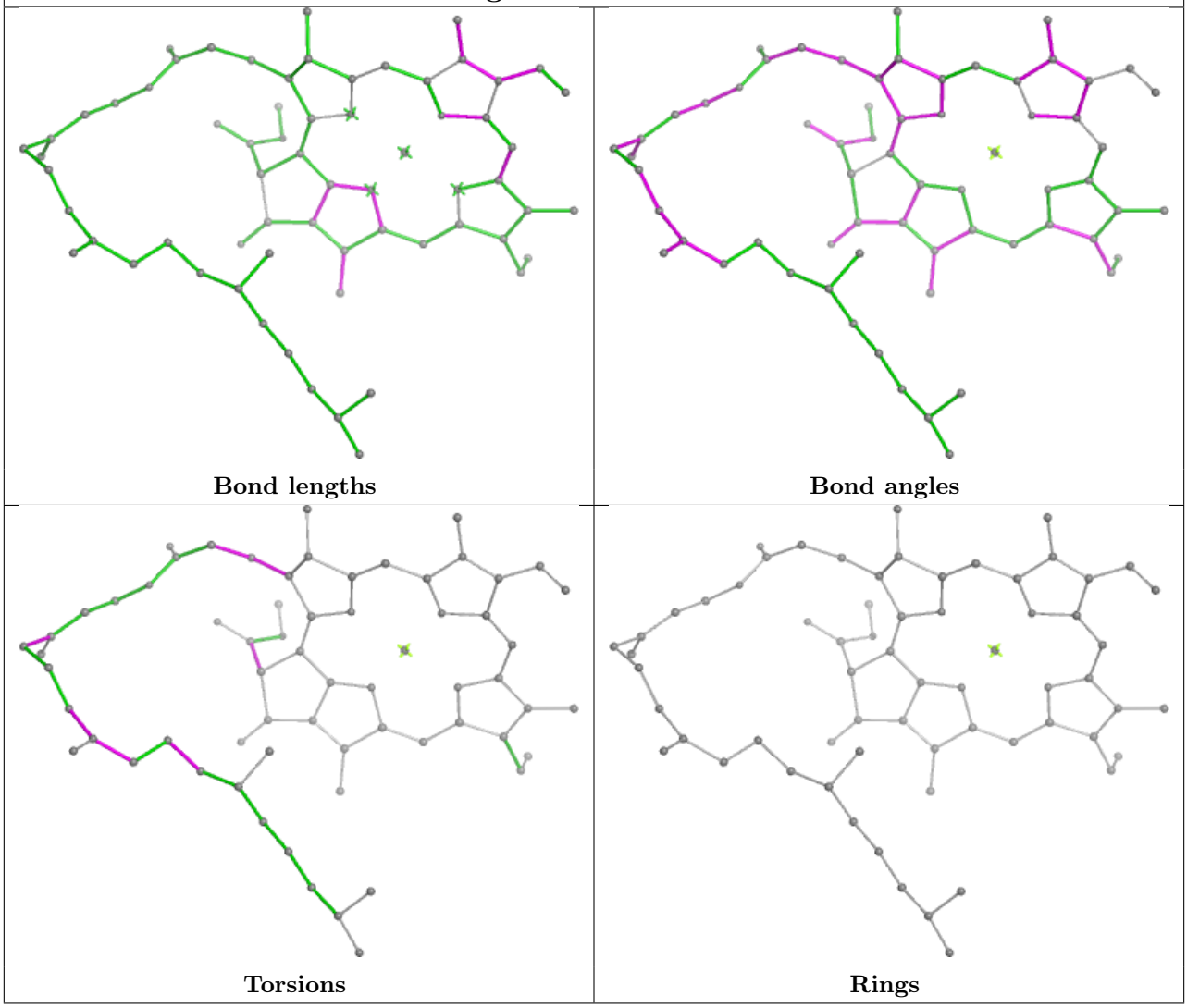


Torsions

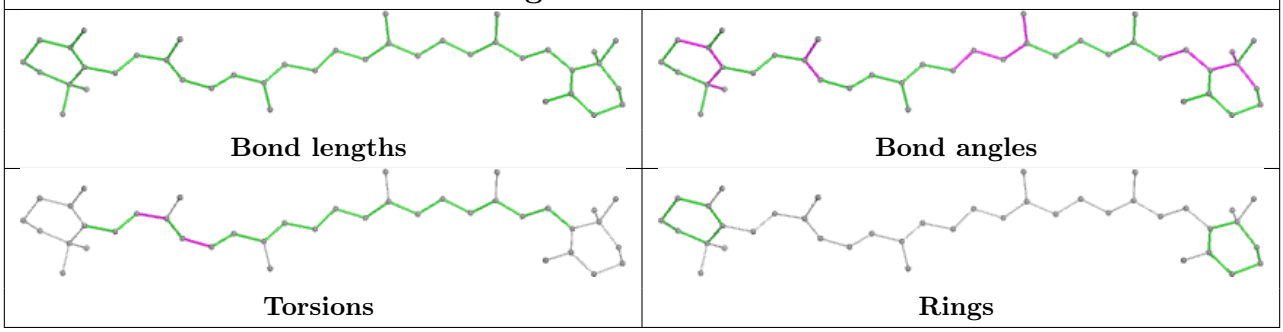


Rings

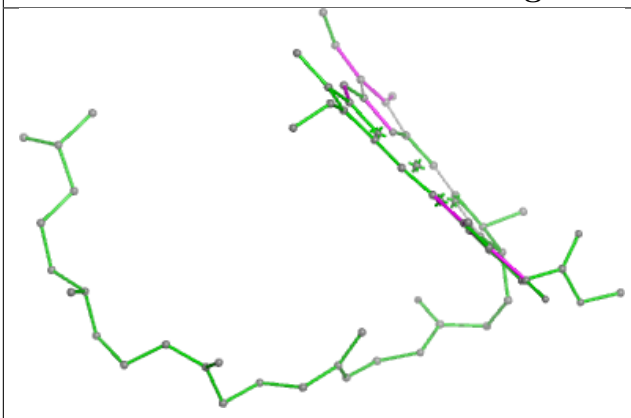
Ligand CLA C 511



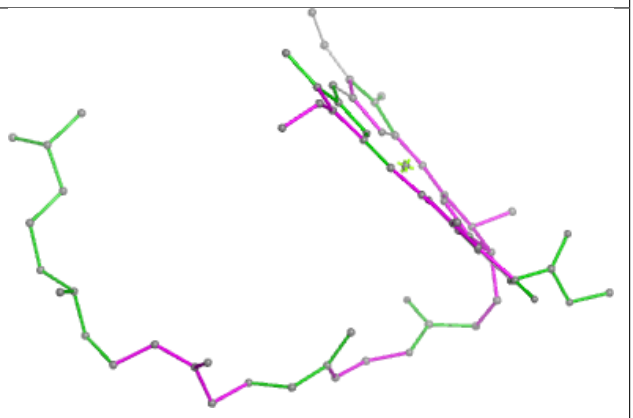
Ligand BCR F 102



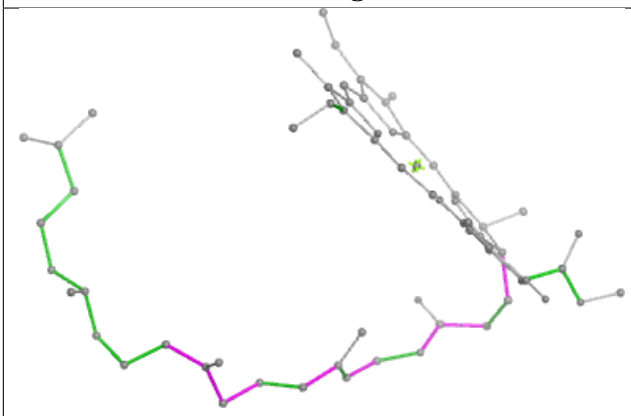
Ligand CLA B 611



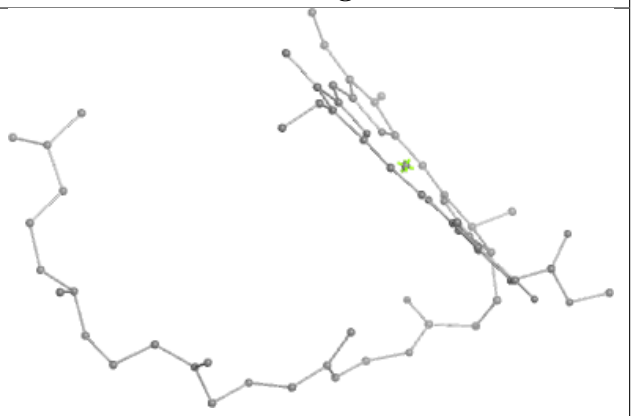
Bond lengths



Bond angles

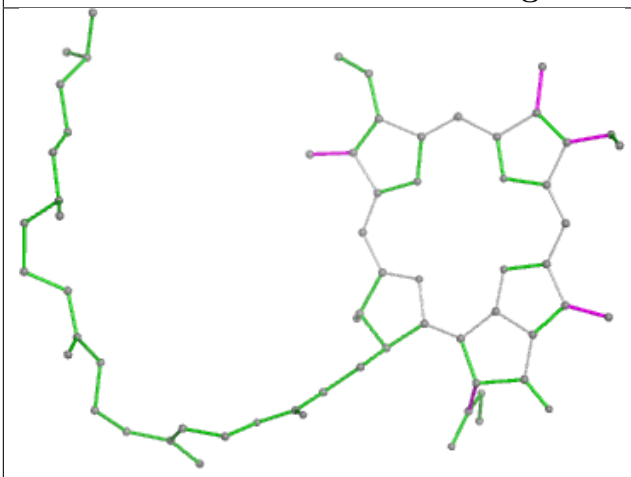


Torsions

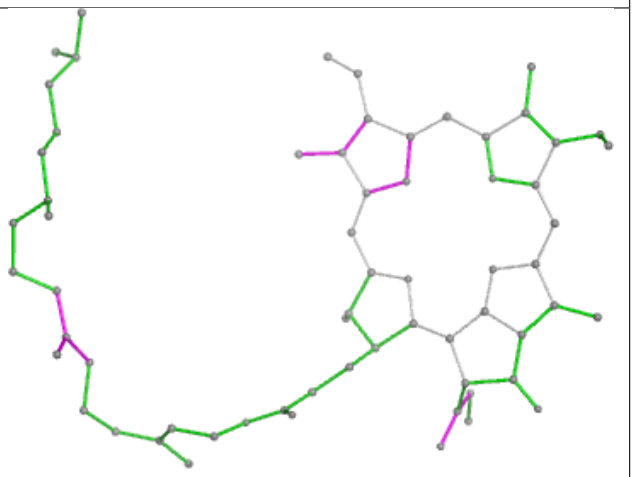


Rings

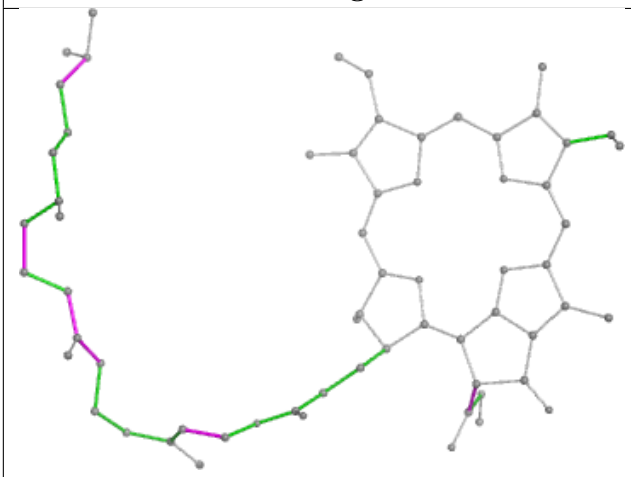
Ligand PHO A 404



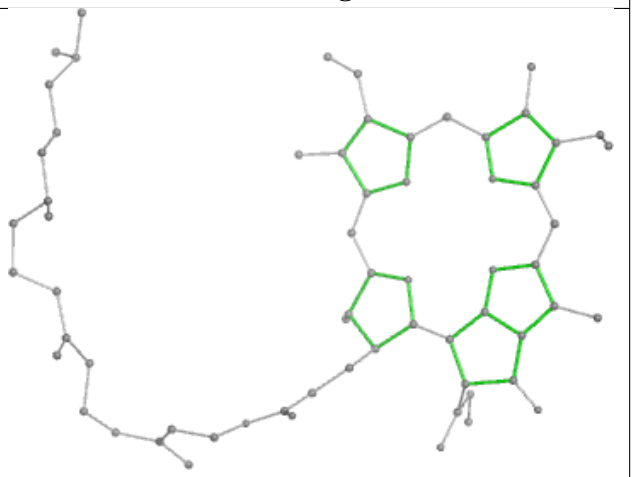
Bond lengths



Bond angles

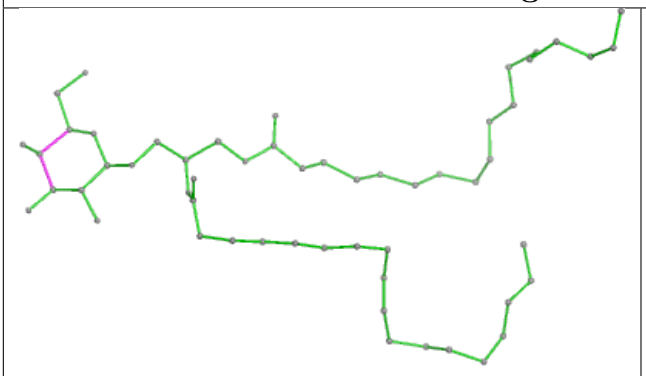


Torsions

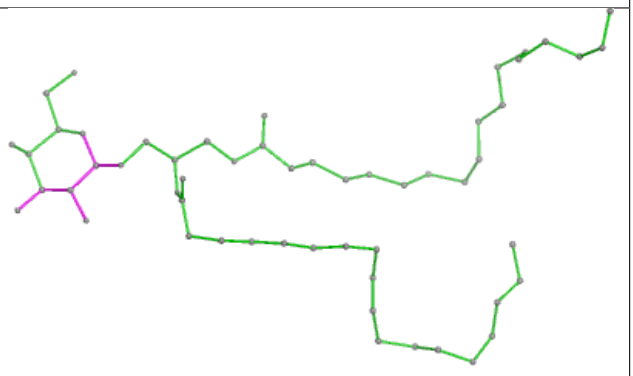


Rings

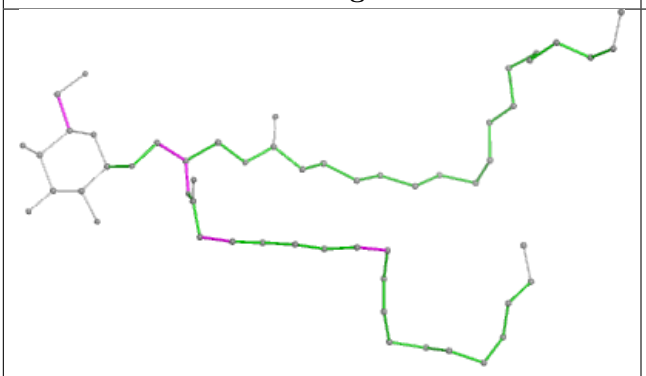
Ligand LMG F 101



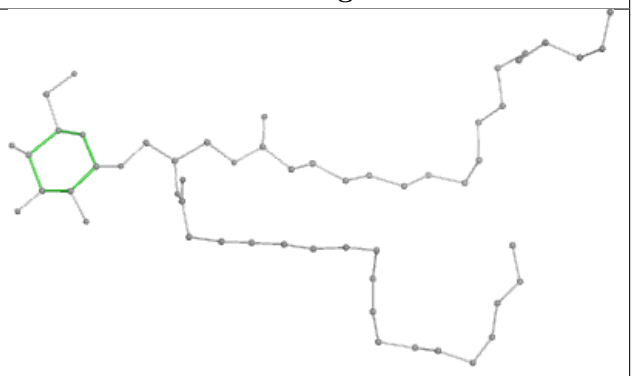
Bond lengths



Bond angles

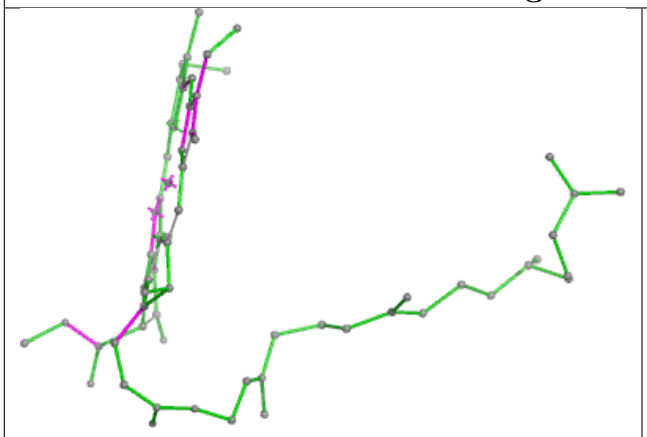


Torsions

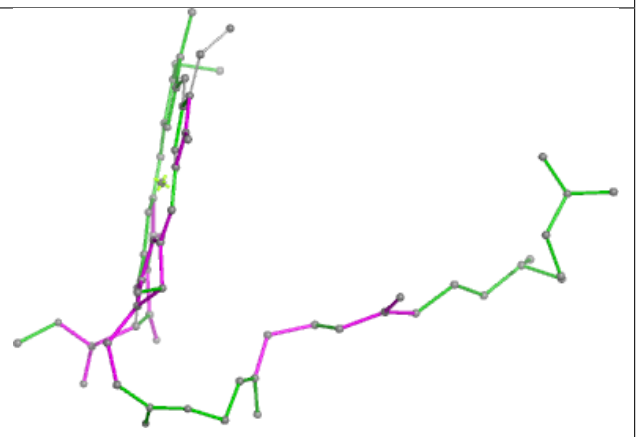


Rings

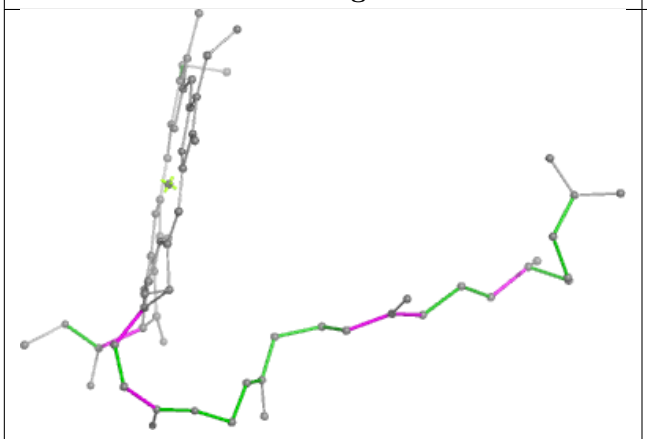
Ligand CLA C 506



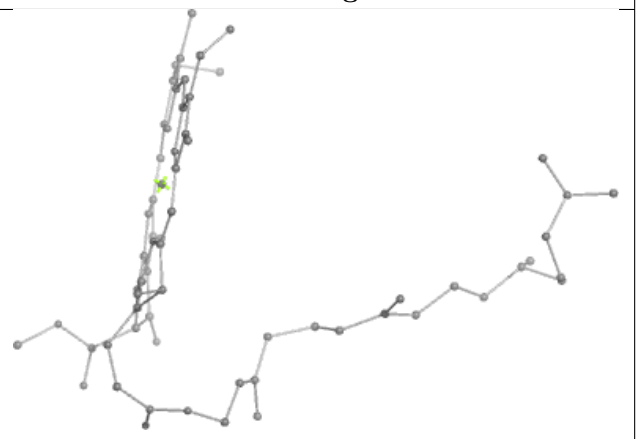
Bond lengths



Bond angles

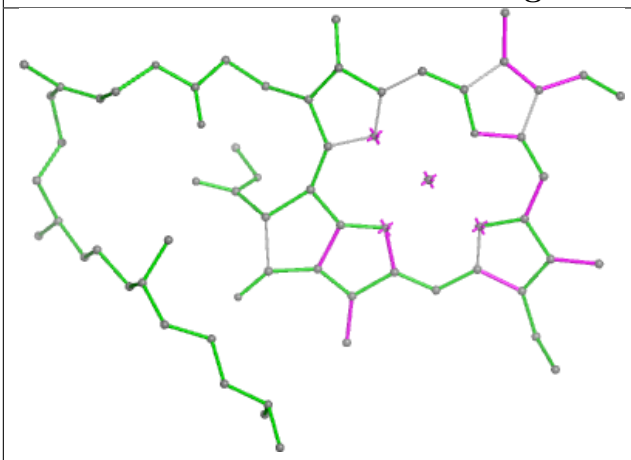


Torsions

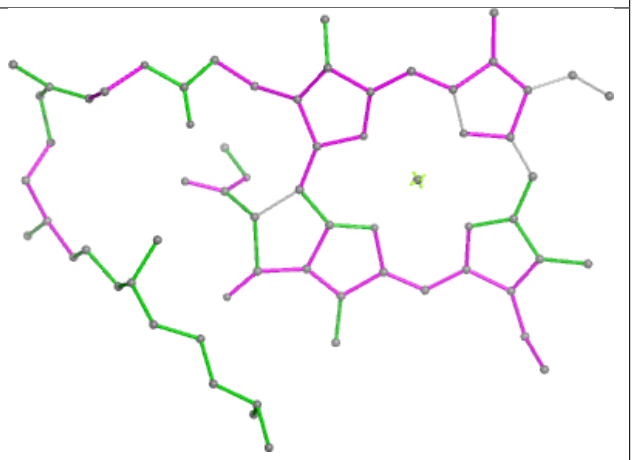


Rings

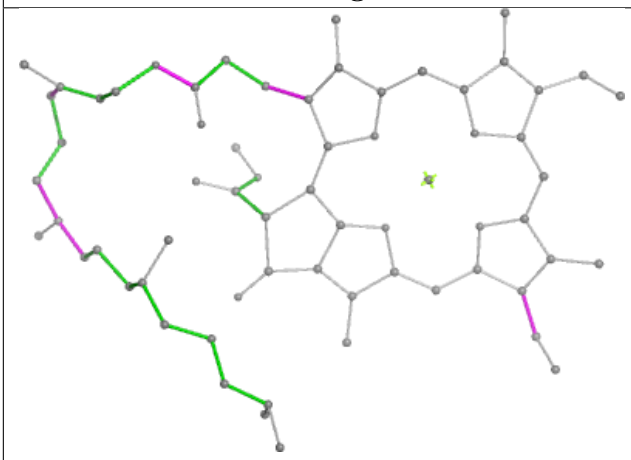
Ligand CLA B 610



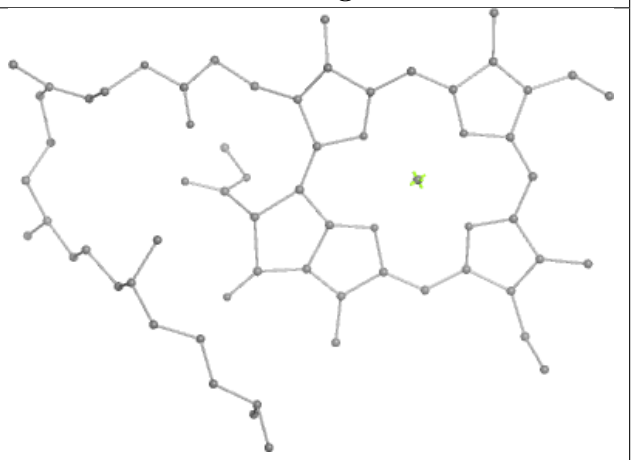
Bond lengths



Bond angles

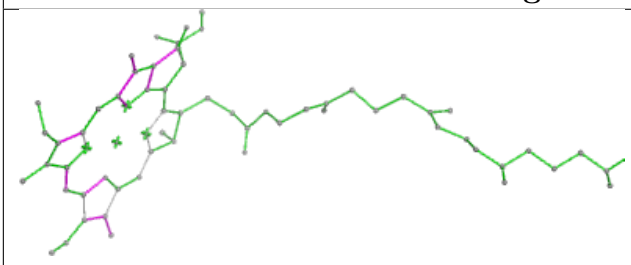


Torsions

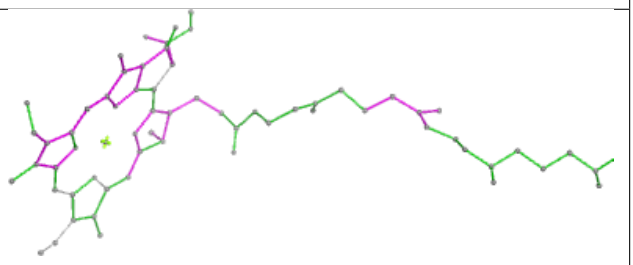


Rings

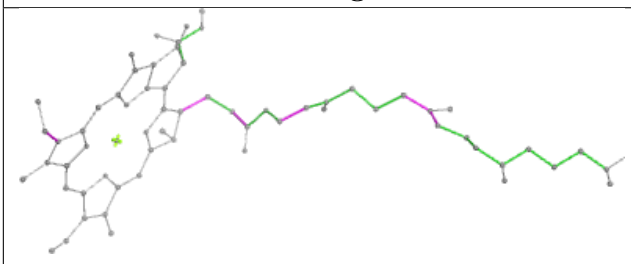
Ligand CLA D 407



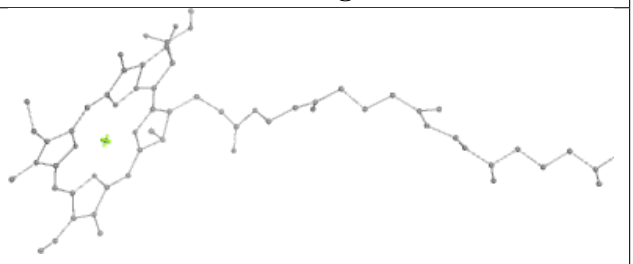
Bond lengths



Bond angles

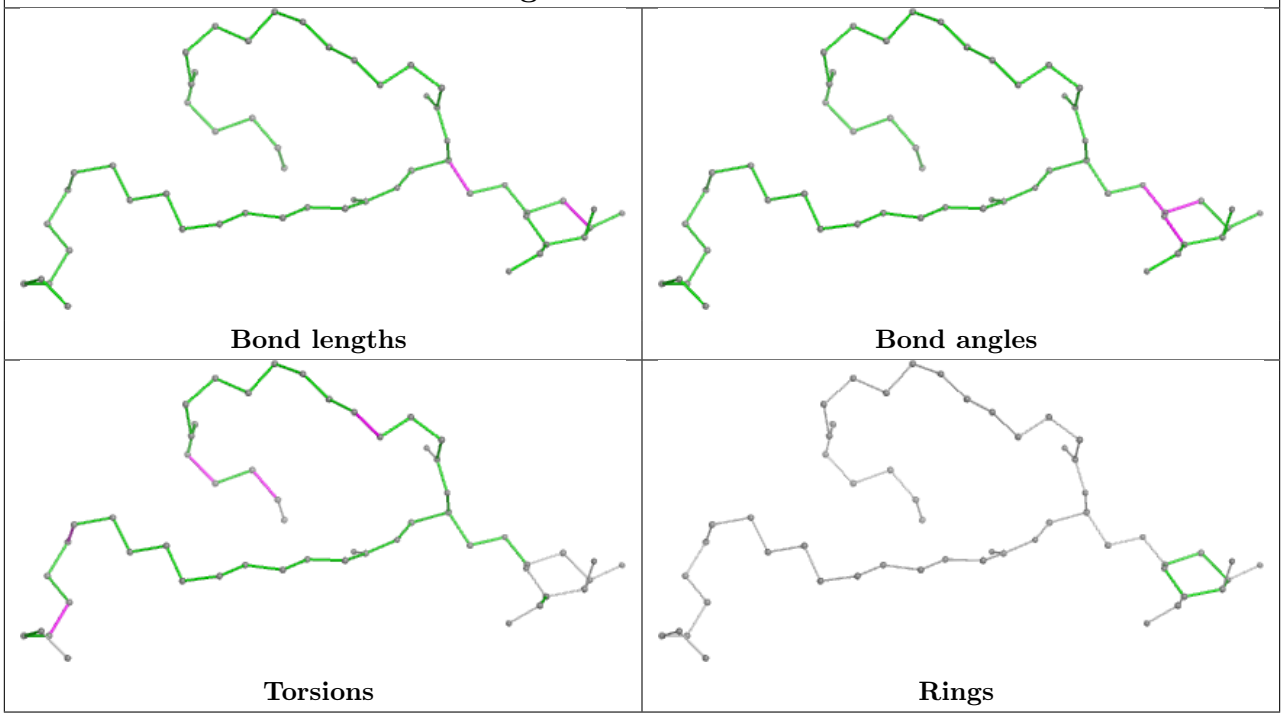


Torsions

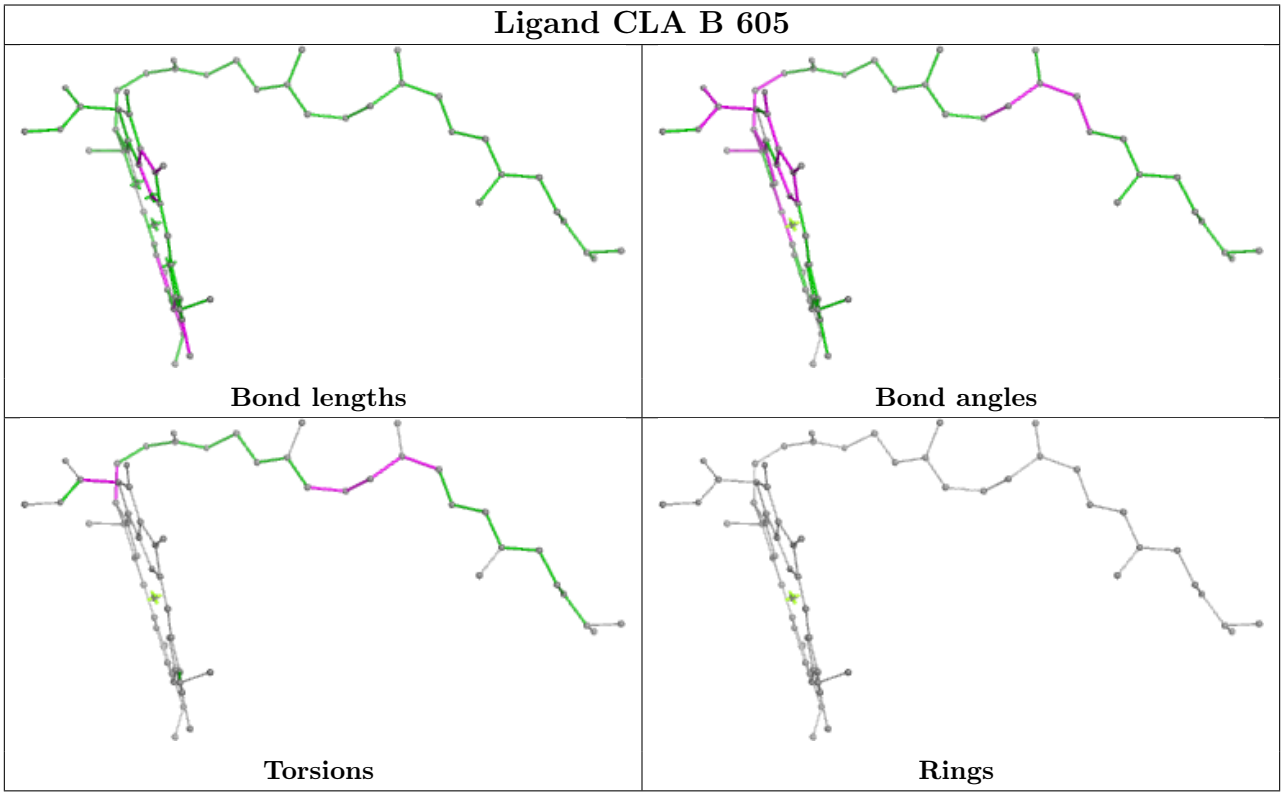


Rings

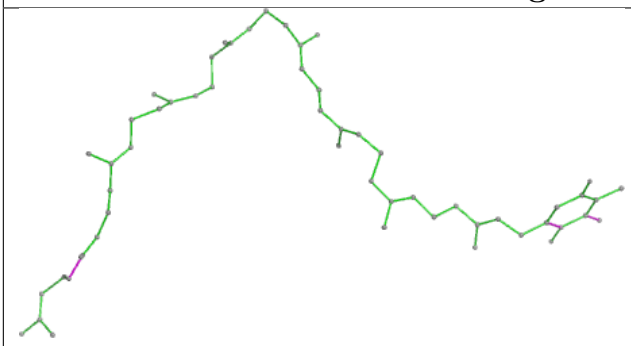
Ligand LMG D 403



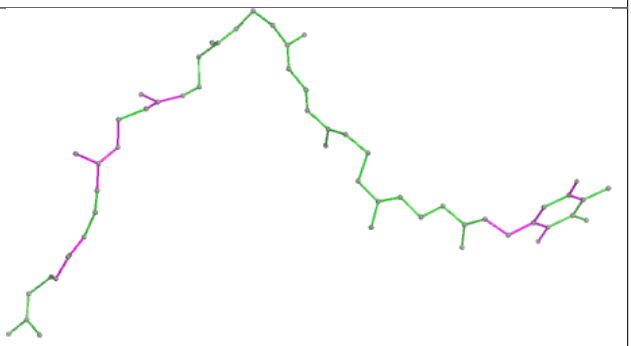
Ligand CLA B 605



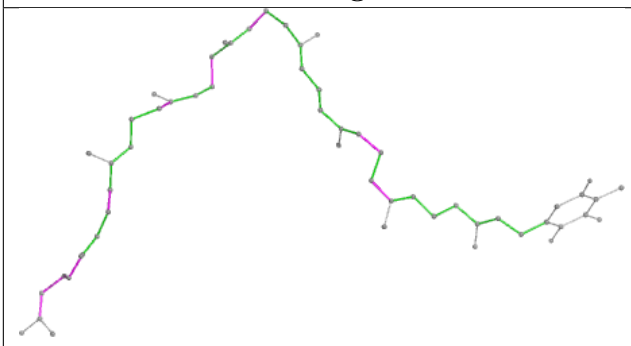
Ligand PL9 D 405



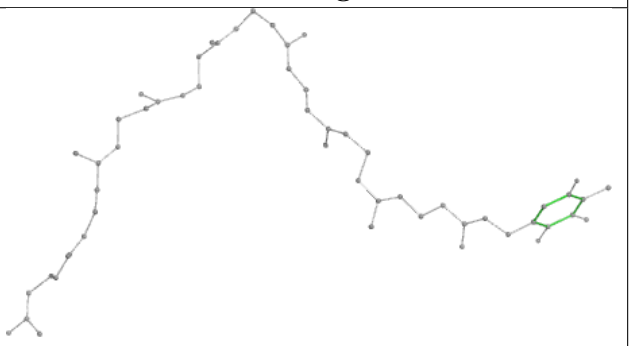
Bond lengths



Bond angles

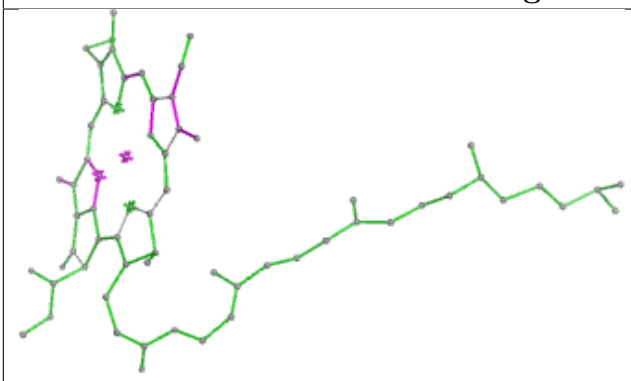


Torsions

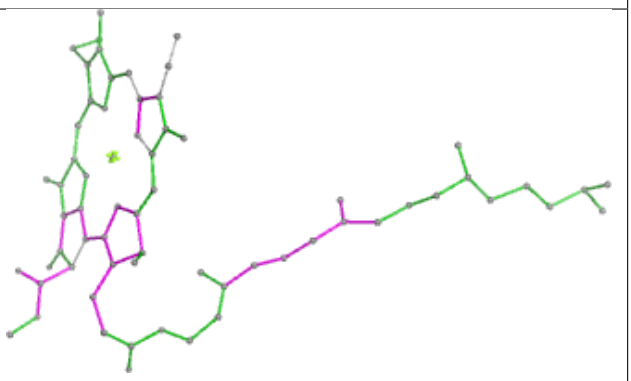


Rings

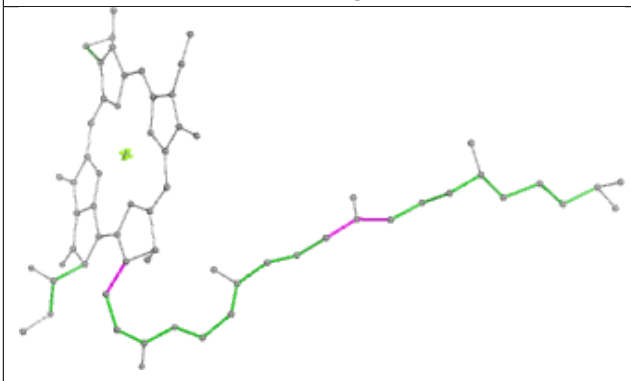
Ligand CLA D 408



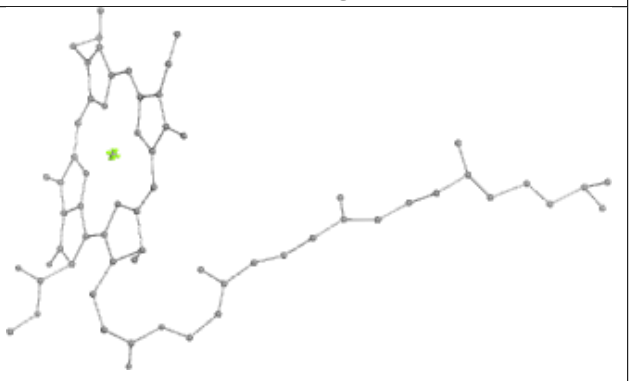
Bond lengths



Bond angles

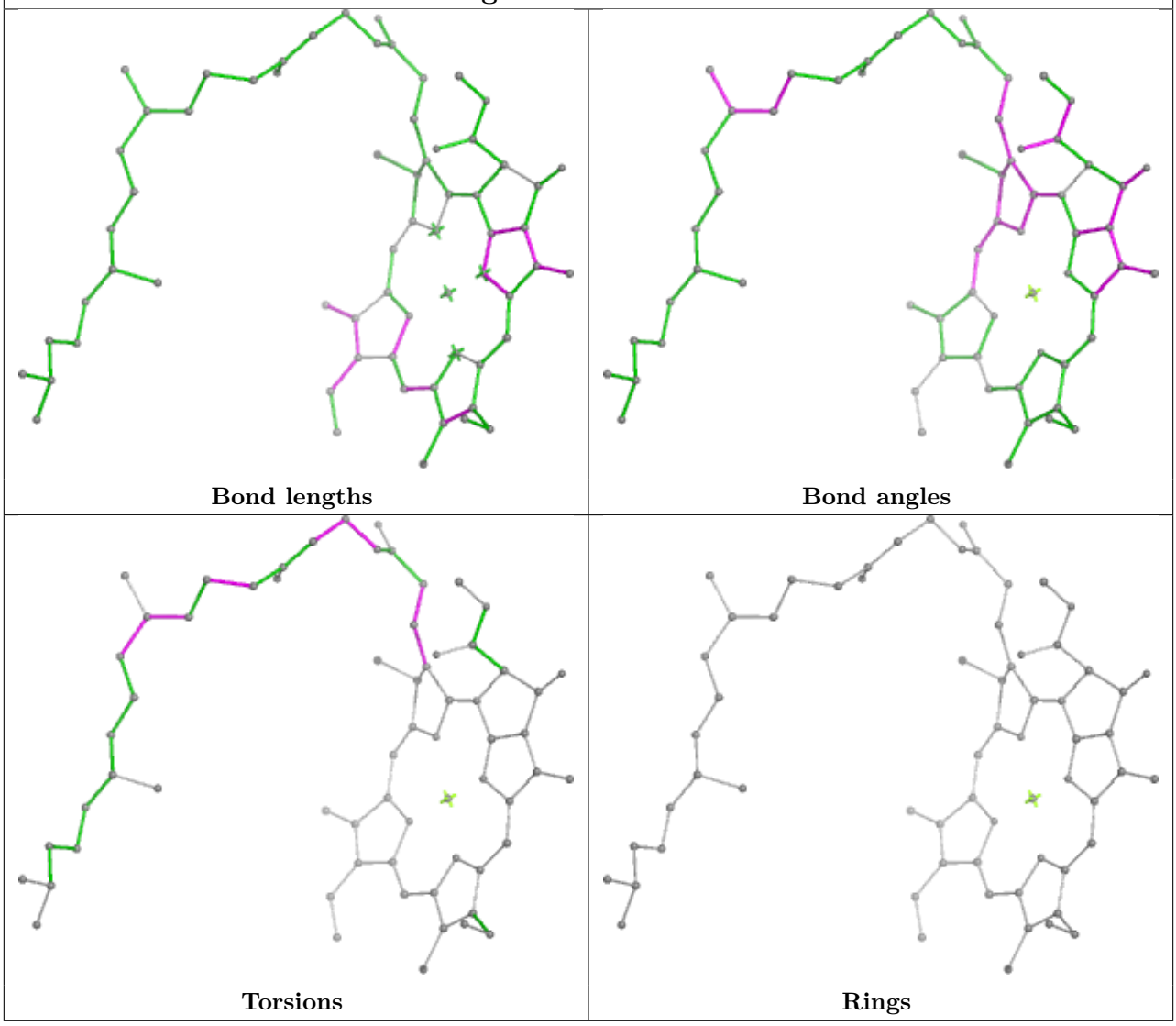


Torsions



Rings

Ligand CLA C 509



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.

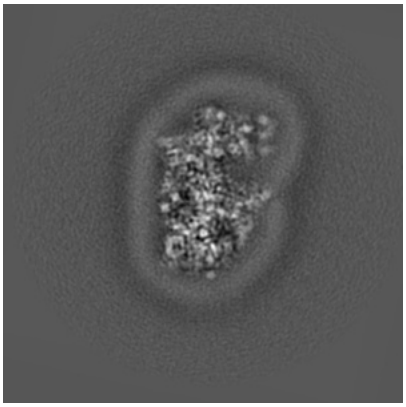
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12337. These allow visual inspection of the internal detail of the map and identification of artifacts.

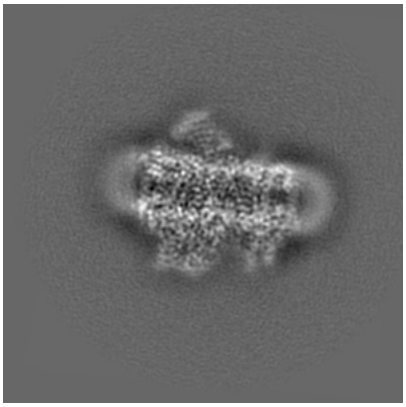
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

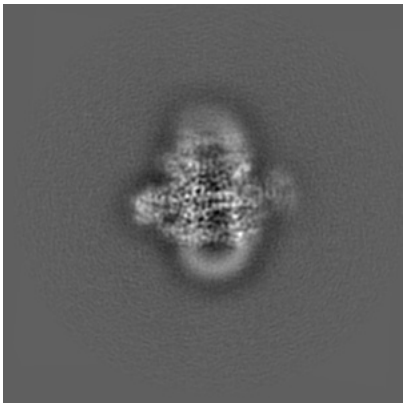
6.1.1 Primary map



X



Y

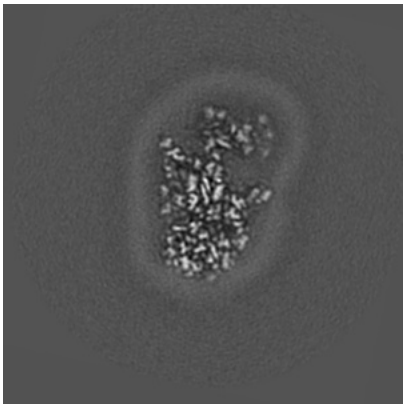


Z

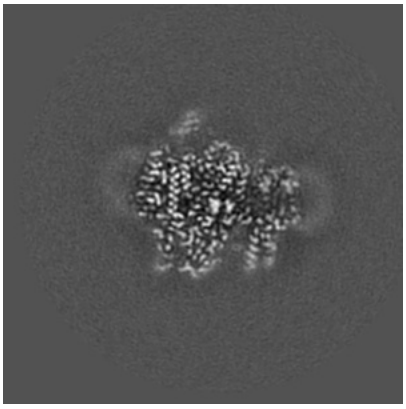
The images above show the map projected in three orthogonal directions.

6.2 Central slices

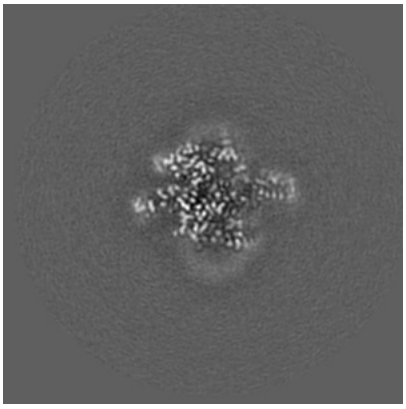
6.2.1 Primary map



X Index: 130



Y Index: 130

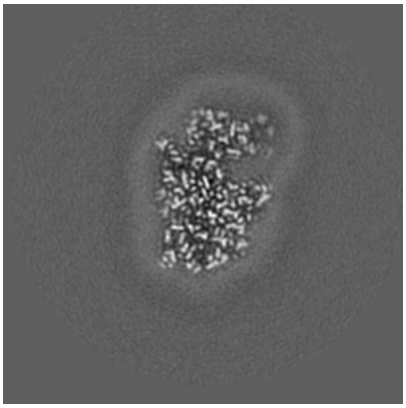


Z Index: 130

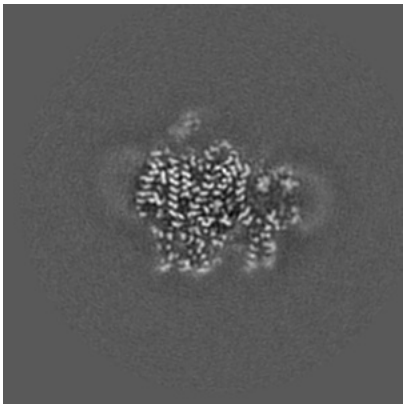
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

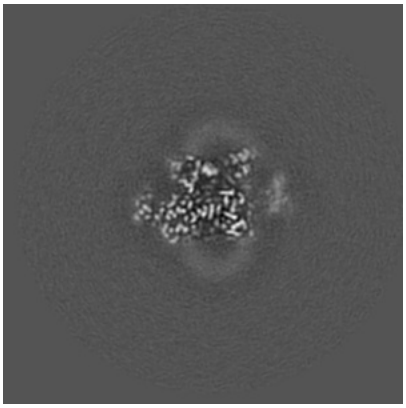
6.3.1 Primary map



X Index: 125



Y Index: 129

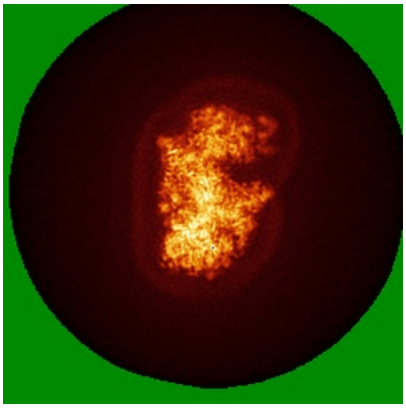


Z Index: 116

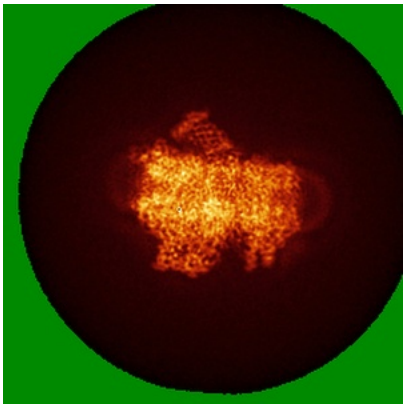
The images above show the largest variance slices of the map in three orthogonal directions.

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

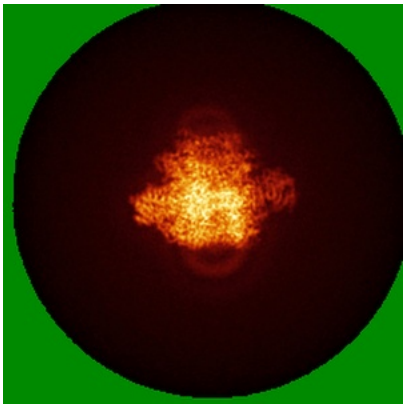
6.4.1 Primary map



X



Y



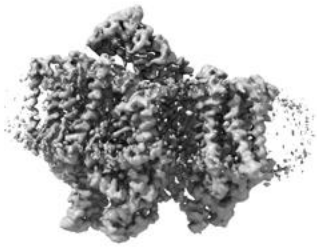
Z

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.

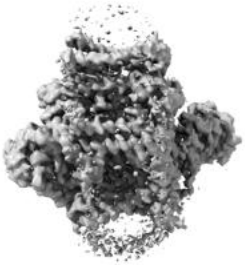
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

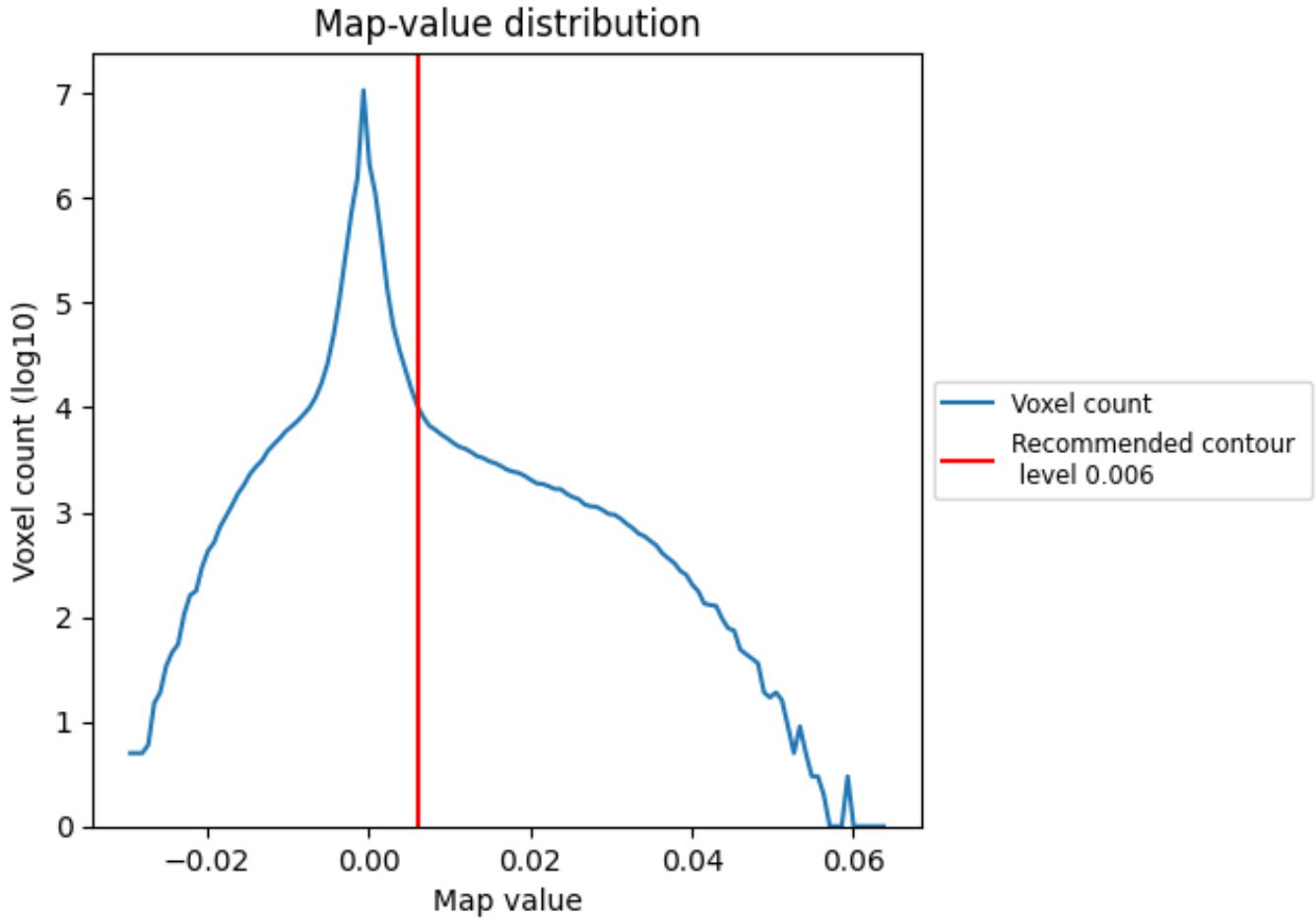
6.6 Mask visualisation (i)

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

7 Map analysis

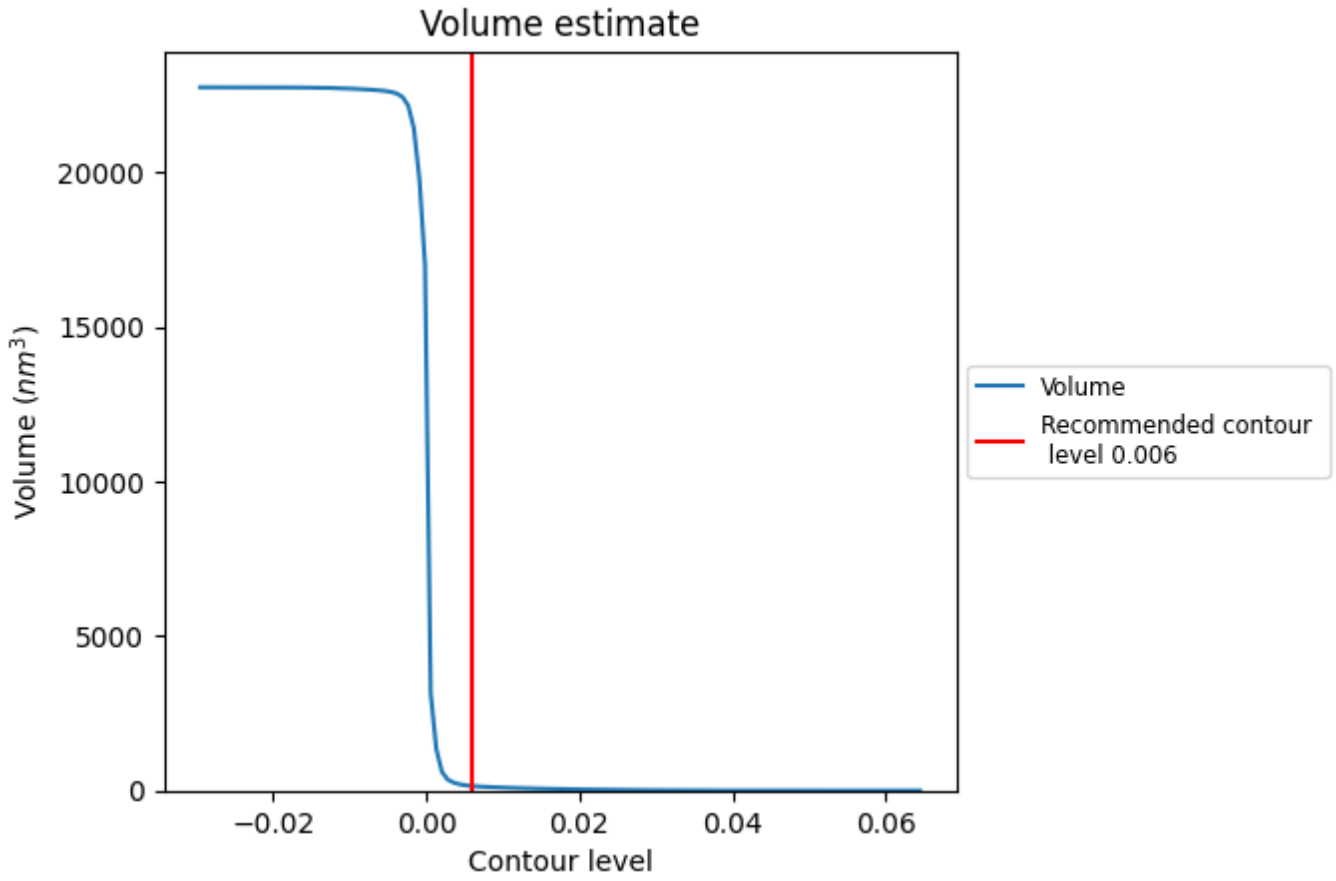
This section contains the results of statistical analysis of the map.

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.

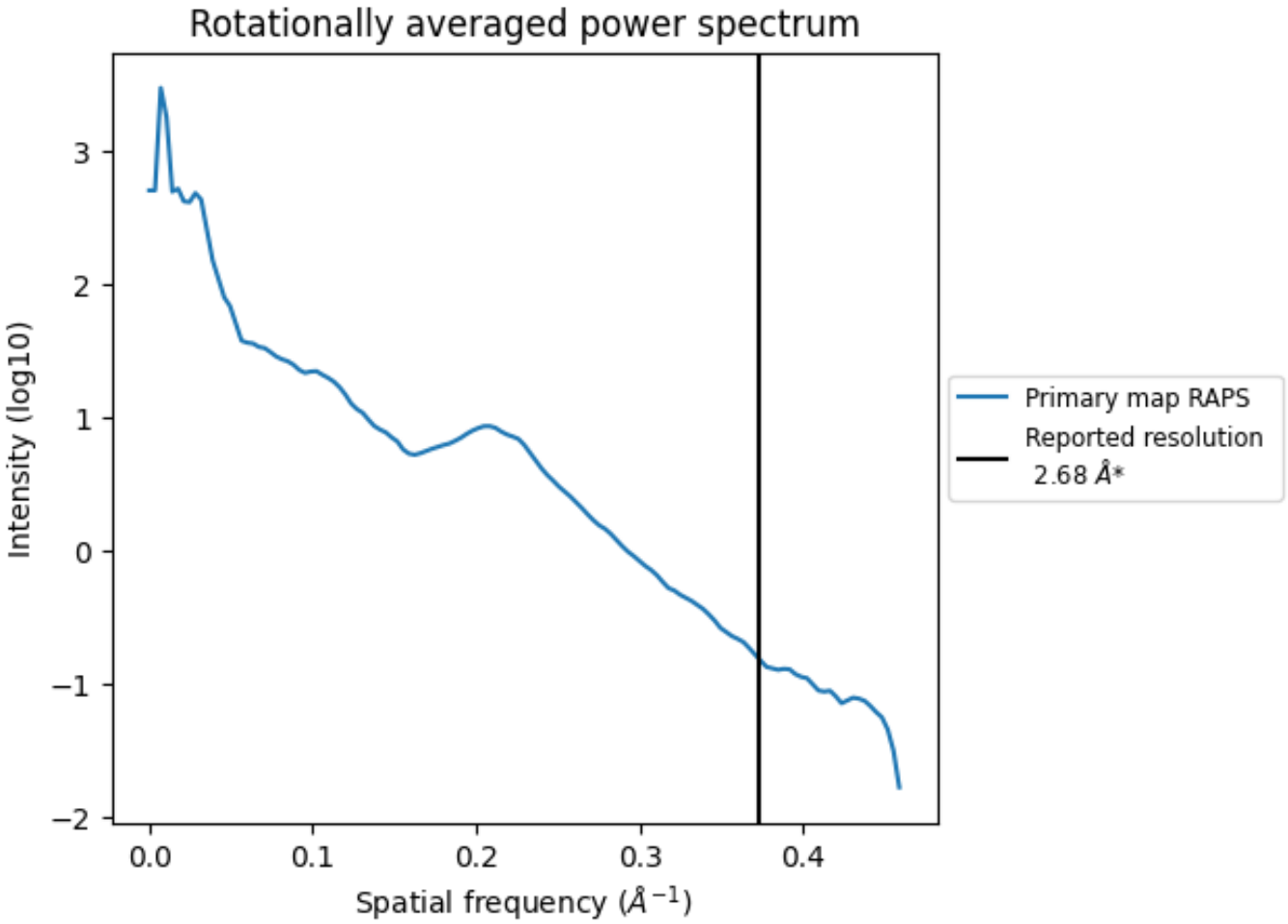
7.2 Volume estimate (i)



The volume at the recommended contour level is 147 nm^3; this corresponds to an approximate mass of 133 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 0.373 $Å^{-1}$

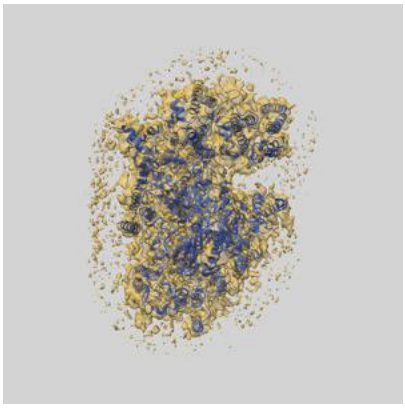
8 Fourier-Shell correlation (i)

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

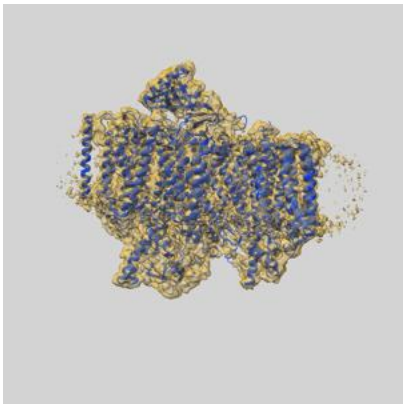
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12337 and PDB model 7NHQ. Per-residue inclusion information can be found in section 3 on page 14.

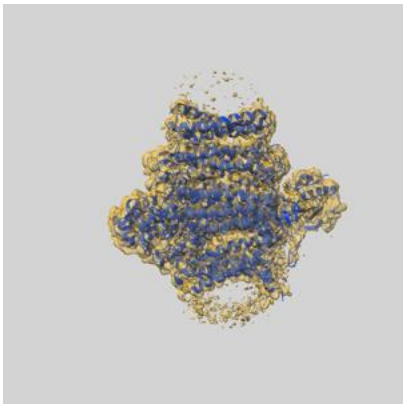
9.1 Map-model overlay



X



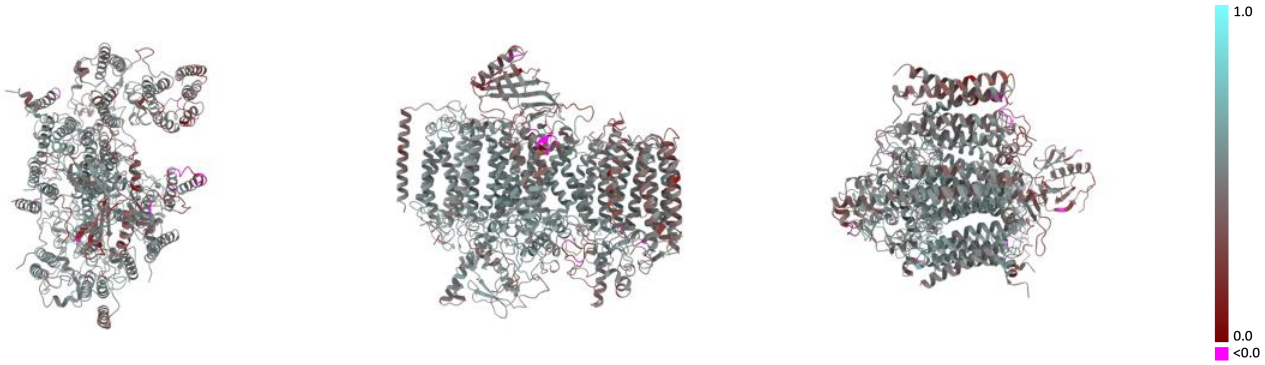
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 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.

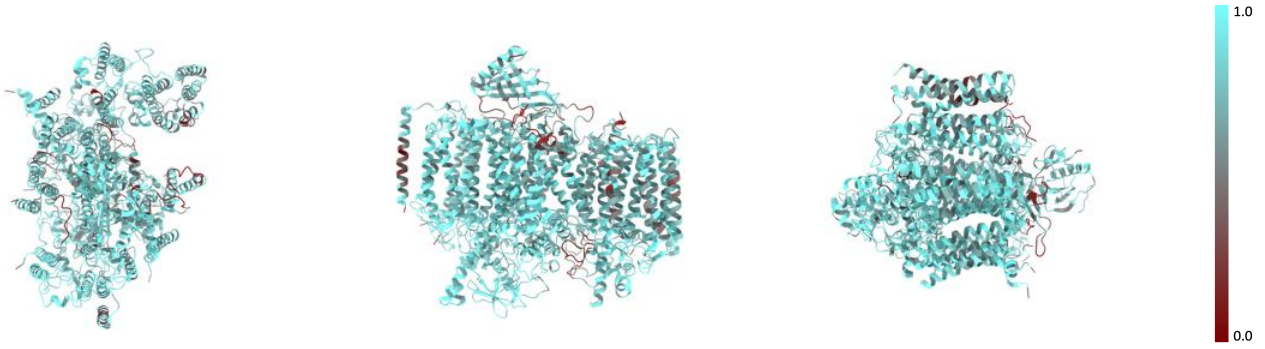
9.2 Q-score mapped to coordinate model



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.

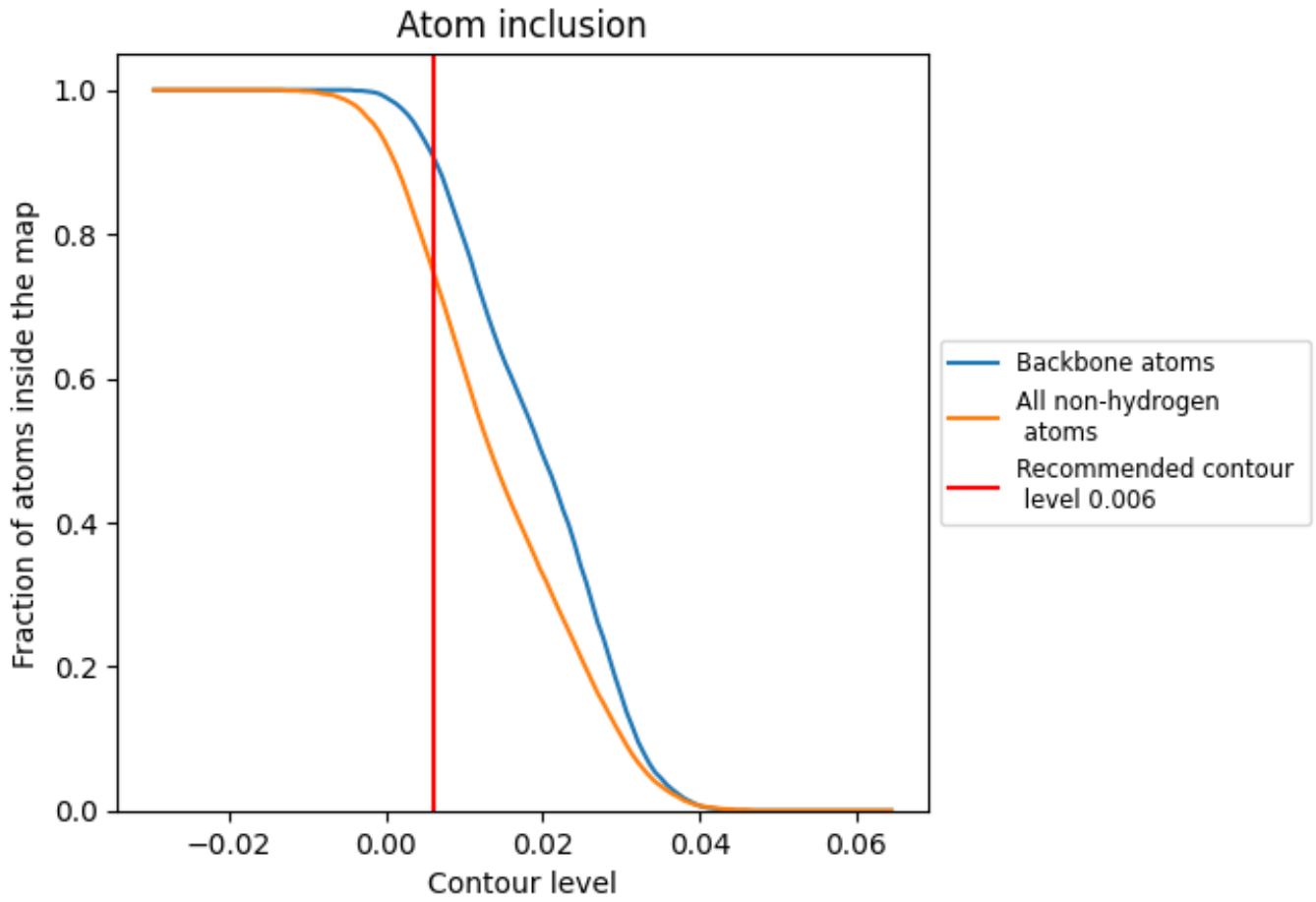
9.3 Atom inclusion mapped to coordinate model



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 (0.006).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 75% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7510	0.4650
2	0.7490	0.3980
3	0.4990	0.4070
A	0.7660	0.4900
B	0.8120	0.4970
C	0.7050	0.4280
D	0.8150	0.5250
E	0.7010	0.3620
F	0.5680	0.3920
H	0.8410	0.4930
I	0.6230	0.3870
K	0.5780	0.3990
L	0.8020	0.5130
M	0.6800	0.4440
T	0.7420	0.4800
X	0.7790	0.4710
Z	0.6720	0.3760
y	0.5240	0.3410