wwPDB EM Validation Summary Report ⓘ

Apr 22, 2024 – 03:48 pm BST

PDB ID	:	7NHP
EMDB ID	:	EMD-12336
Title	:	Structure of PSII-I (PSII with Psb27, 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	:	2.72 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

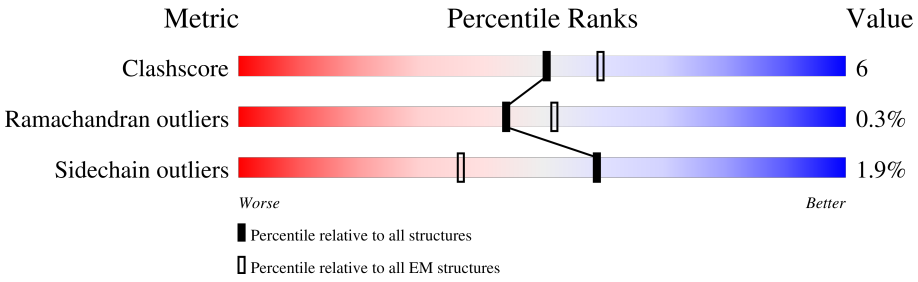
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.72 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	8% 84% 9% 7%
2	B	510	91% 6%
3	C	461	7% 80% 13% 6%
4	D	352	89% 7%
5	E	84	14% 85% 7% 8%
6	F	45	13% 82% 16%
7	H	66	94% 5%
8	I	38	58% 11% 32%

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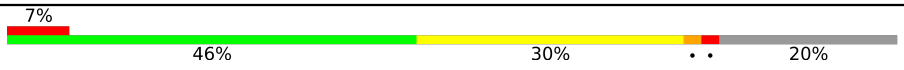
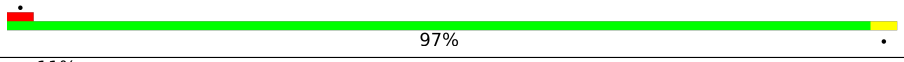
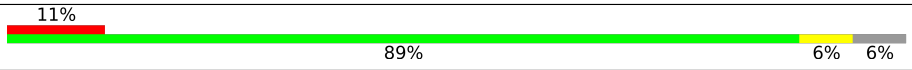
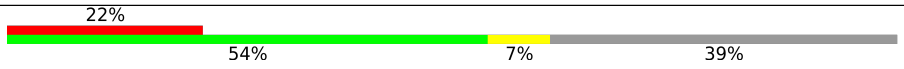
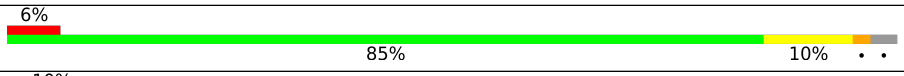
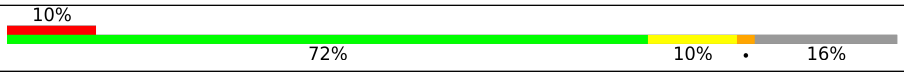
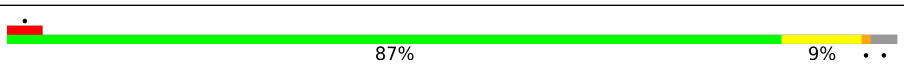
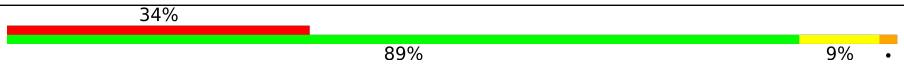
Mol	Chain	Length	Quality of chain
9	K	46	
10	L	37	
11	M	36	
12	T	32	
13	X	41	
14	y	46	
15	Z	62	
16	1	134	
17	2	116	
18	3	56	

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	403	X	-	-	-
21	PHO	D	407	X	-	-	-
22	CLA	A	404	X	-	-	-
22	CLA	A	405	X	-	-	-
22	CLA	A	406	X	-	-	-
22	CLA	A	407	X	-	-	-
22	CLA	B	601	X	-	-	-
22	CLA	B	602	X	-	-	-
22	CLA	B	603	X	-	-	-
22	CLA	B	604	X	-	-	-
22	CLA	B	606	X	-	-	-
22	CLA	B	607	X	-	-	-
22	CLA	B	608	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	C	503	X	-	-	-
22	CLA	C	504	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	506	X	-	-	-
22	CLA	C	507	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	408	X	-	-	-
22	CLA	D	409	X	-	-	-
23	BCR	K	101	-	-	X	-

2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 21839 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
			Total	C	N	O	S		
1	A	335	2627	1720	432	460	15	0	0

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

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

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

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

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

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

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

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

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

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

- 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 lipoprotein Psb27.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1	113	Total	C	N	O	S	0	0
			893	556	161	173	3		

- Molecule 17 is a protein called Photosystem II reaction center Psb28 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	2	112	Total	C	N	O	S	0	0
			897	562	156	173	6		

- Molecule 18 is a protein called Tsl0063 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	3	56	Total	C	N	O	S	0	0
			419	269	74	75	1		

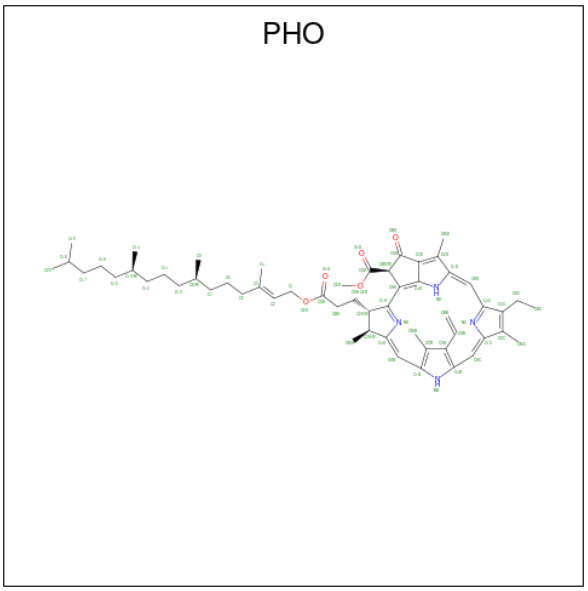
- Molecule 19 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

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

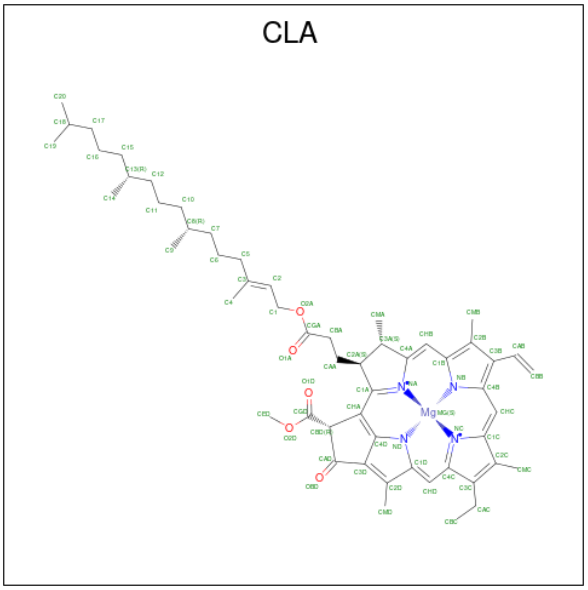
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Cl	0
			1	1	

- 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	A	1	Total C Mg N O 65 55 1 4 5	0
22	A	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	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

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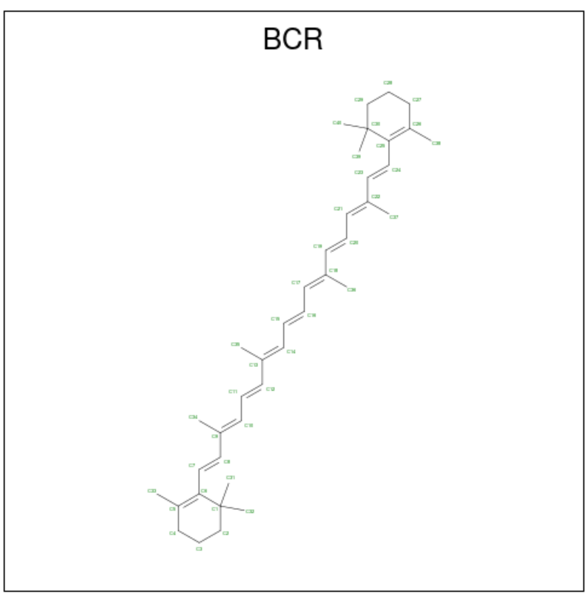
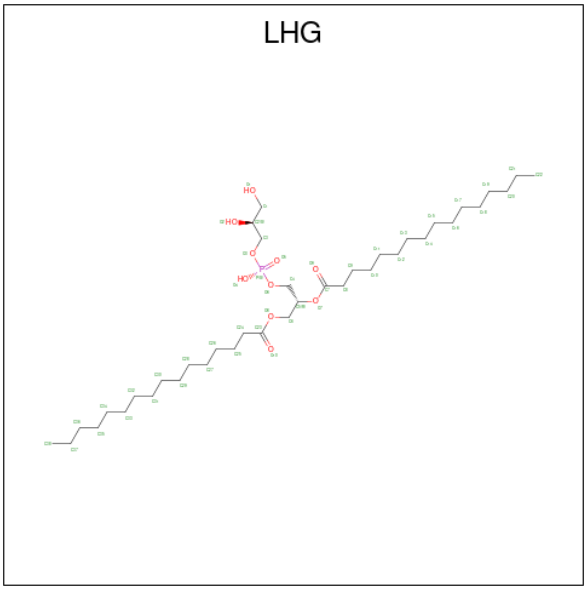
Mol	Chain	Residues	Atoms	AltConf
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg N O 65 55 1 4 5	0
22	C	1	Total C Mg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

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



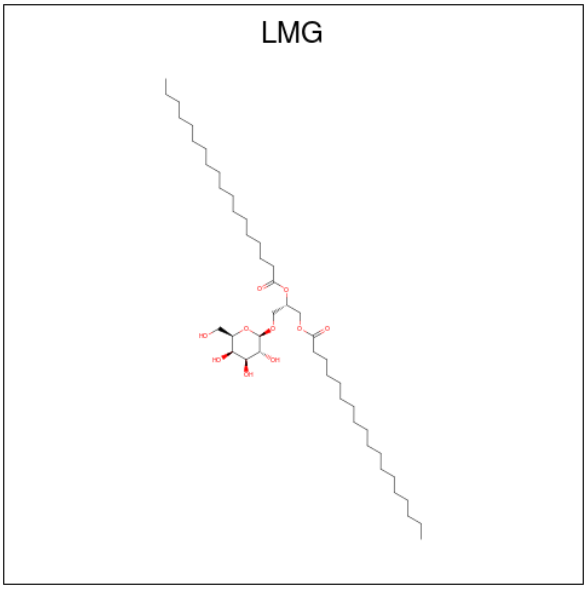
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	C	1	Total C 40 40	0
23	D	1	Total C 40 40	0
23	H	1	Total C 40 40	0
23	K	1	Total C 40 40	0

- 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: $C_{45}H_{86}O_{10}$).

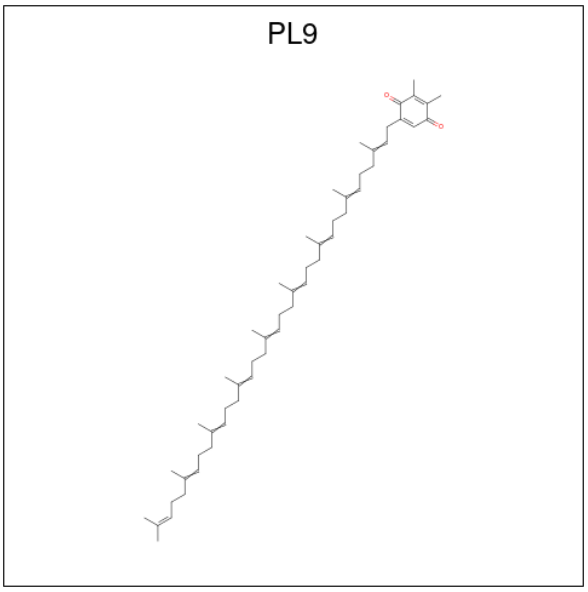


Mol	Chain	Residues	Atoms	AltConf
25	C	1	Total C O 55 45 10	0
25	C	1	Total C O 55 45 10	0
25	D	1	Total C O 55 45 10	0
25	D	1	Total C O 55 45 10	0
25	D	1	Total C O 55 45 10	0
25	D	1	Total C O 55 45 10	0
25	I	1	Total C O 55 45 10	0

- Molecule 26 is FE (III) ION (three-letter code: FE) (formula: Fe).

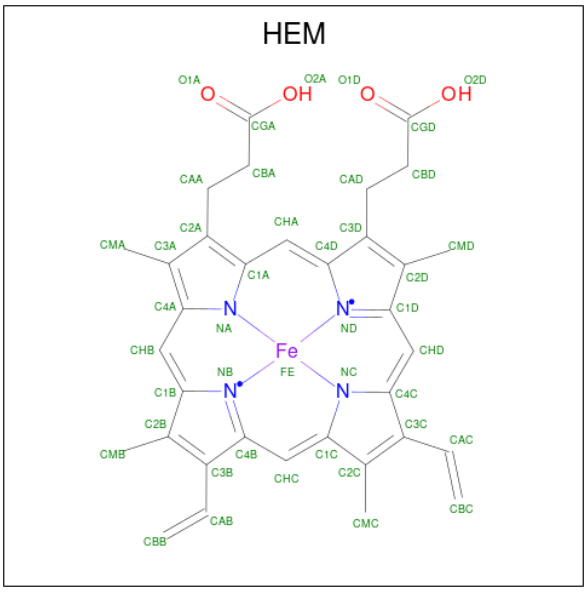
Mol	Chain	Residues	Atoms	AltConf
26	D	1	Total Fe 1 1	0

- Molecule 27 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
27	D	1	Total	C	O	0
			55	53	2	

- Molecule 28 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

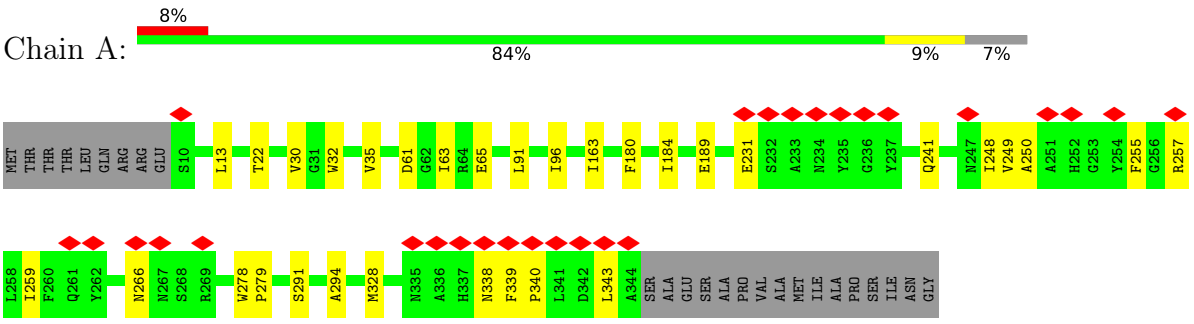


Mol	Chain	Residues	Atoms					AltConf
28	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

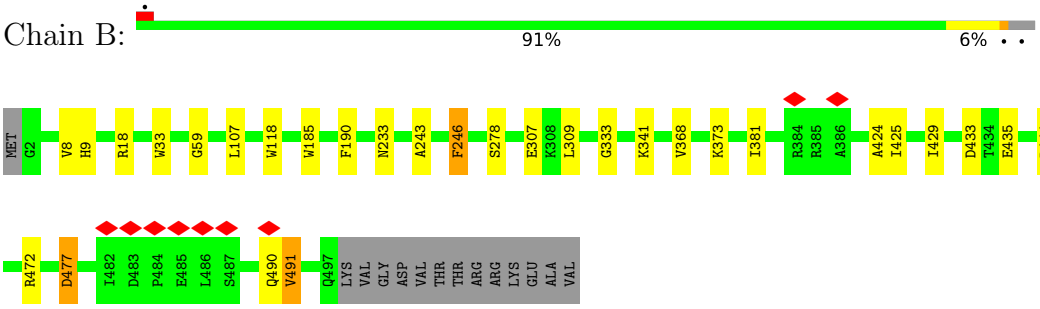
3 Residue-property plots (i)

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.

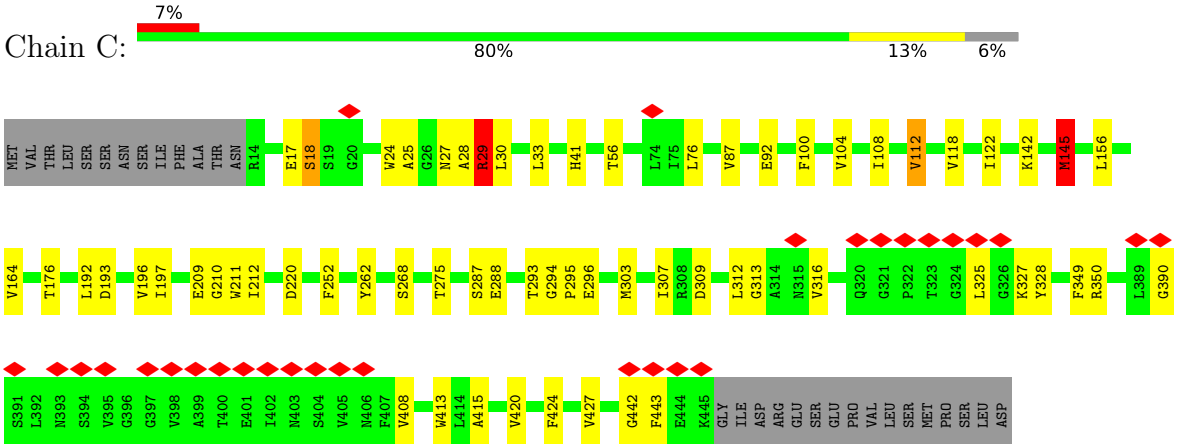
• Molecule 1: Photosystem II protein D1 1



• Molecule 2: Photosystem II CP47 reaction center protein

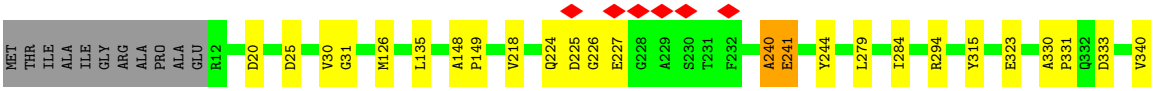


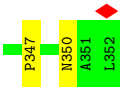
• Molecule 3: Photosystem II CP43 reaction center protein



• Molecule 4: Photosystem II D2 protein

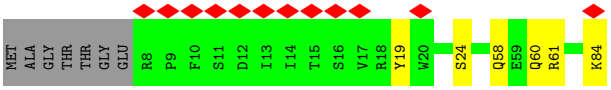
Chain D:





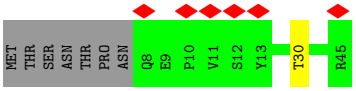
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



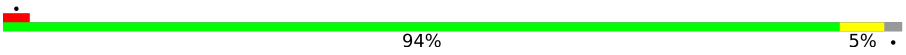
• Molecule 6: Cytochrome b559 subunit beta

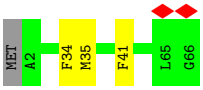
Chain F:



• Molecule 7: Photosystem II reaction center protein H

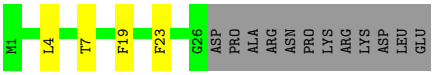
Chain H:





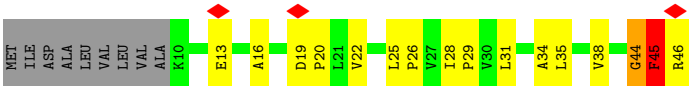
• Molecule 8: Photosystem II reaction center protein I

Chain I:



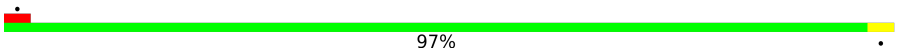
• Molecule 9: Photosystem II reaction center protein K

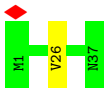
Chain K:



• Molecule 10: Photosystem II reaction center protein L

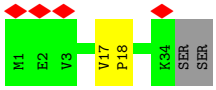
Chain L:





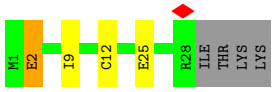
• Molecule 11: Photosystem II reaction center protein M

Chain M:



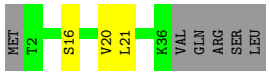
• Molecule 12: Photosystem II reaction center protein T

Chain T:



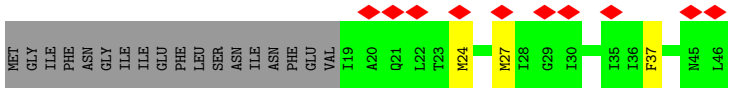
• Molecule 13: Photosystem II reaction center X protein

Chain X:



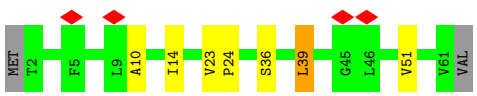
• Molecule 14: Photosystem II reaction center protein Ycf12

Chain y:



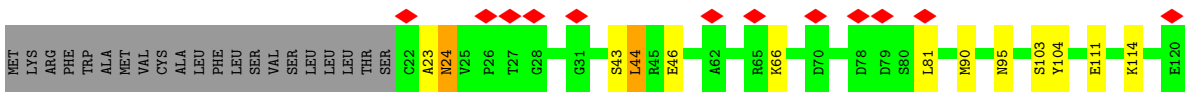
• Molecule 15: Photosystem II reaction center protein Z

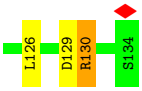
Chain Z:



• Molecule 16: Photosystem II lipoprotein Psb27

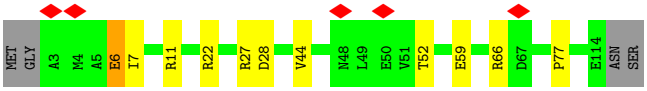
Chain 1:





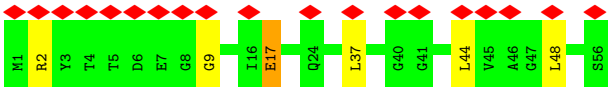
• Molecule 17: Photosystem II reaction center Psb28 protein

Chain 2:



• Molecule 18: Tsl0063 protein

Chain 3:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	57268	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	0.062	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	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: HEM, PL9, MN, BCR, CLA, PHO, CL, LHG, LMG, 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	0.44	0/2712	0.76	3/3700 (0.1%)
2	B	0.45	0/4049	0.77	2/5519 (0.0%)
3	C	0.45	0/3456	0.79	7/4706 (0.1%)
4	D	0.42	0/2812	0.74	1/3832 (0.0%)
5	E	0.43	0/654	0.74	1/891 (0.1%)
6	F	0.48	0/317	0.76	0/433
7	H	0.43	0/524	0.82	0/713
8	I	0.57	0/216	0.87	0/292
9	K	0.44	0/303	0.80	1/416 (0.2%)
10	L	0.47	0/311	0.79	0/422
11	M	0.44	0/270	0.68	0/367
12	T	0.50	0/250	0.81	0/338
13	X	0.43	0/257	0.92	2/348 (0.6%)
14	y	0.56	0/209	0.97	0/279
15	Z	0.44	0/474	0.77	0/649
16	1	0.44	0/907	0.81	1/1220 (0.1%)
17	2	0.45	0/914	0.87	1/1231 (0.1%)
18	3	0.45	0/426	0.83	0/578
All	All	0.45	0/19061	0.78	19/25934 (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	4
2	B	0	3
3	C	0	2
4	D	0	3
9	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	1	0	2
17	2	0	1
18	3	0	2
All	All	0	19

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	X	21	LEU	CB-CG-CD2	-8.09	97.25	111.00
3	C	145	MET	CB-CG-SD	8.00	136.40	112.40
17	2	22	ARG	NE-CZ-NH2	6.70	123.65	120.30
3	C	420	VAL	CG1-CB-CG2	-6.59	100.36	110.90
3	C	29	ARG	NE-CZ-NH2	6.26	123.43	120.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	GLU	Sidechain
1	A	266	ASN	Sidechain
1	A	338	ASN	Sidechain
1	A	343	LEU	Peptide
2	B	477	ASP	Sidechain

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	19	0
2	B	3909	0	3763	24	0
3	C	3345	0	3273	66	0
4	D	2717	0	2621	18	0
5	E	635	0	625	4	0
6	F	307	0	312	1	0
7	H	511	0	532	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	211	0	227	4	0
9	K	293	0	305	25	0
10	L	304	0	316	2	0
11	M	267	0	289	1	0
12	T	241	0	244	2	0
13	X	254	0	282	1	0
14	y	208	0	237	0	0
15	Z	463	0	495	5	0
16	1	893	0	896	6	0
17	2	897	0	859	3	0
18	3	419	0	438	2	0
19	A	1	0	0	0	0
20	A	1	0	0	0	0
21	A	64	0	73	1	0
21	D	64	0	73	0	0
22	A	260	0	281	9	0
22	B	1040	0	1127	38	0
22	C	845	0	918	44	0
22	D	130	0	140	8	0
23	A	40	0	56	2	0
23	B	120	0	168	5	0
23	C	120	0	168	20	0
23	D	40	0	56	0	0
23	H	40	0	56	18	0
23	K	40	0	56	24	0
24	A	49	0	74	0	0
25	C	110	0	172	0	0
25	D	220	0	344	3	0
25	I	55	0	86	0	0
26	D	1	0	0	0	0
27	D	55	0	80	4	0
28	E	43	0	30	0	0
All	All	21839	0	22196	258	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 6.

The worst 5 of 258 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)
23:C:515:BCR:H353	23:K:101:BCR:C33	1.74	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:ILE:HD11	22:C:512:CLA:H92	1.17	1.09
23:C:515:BCR:H353	23:K:101:BCR:H332	1.39	1.05
3:C:30:LEU:HD21	22:C:512:CLA:H2A	1.39	1.03
3:C:122:ILE:CD1	22:C:512:CLA:H92	1.88	1.03

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%)	312 (94%)	19 (6%)	2 (1%)	25 48
2	B	494/510 (97%)	469 (95%)	24 (5%)	1 (0%)	47 72
3	C	430/461 (93%)	396 (92%)	33 (8%)	1 (0%)	47 72
4	D	339/352 (96%)	316 (93%)	22 (6%)	1 (0%)	41 65
5	E	75/84 (89%)	72 (96%)	3 (4%)	0	100 100
6	F	36/45 (80%)	34 (94%)	2 (6%)	0	100 100
7	H	63/66 (96%)	58 (92%)	5 (8%)	0	100 100
8	I	24/38 (63%)	24 (100%)	0	0	100 100
9	K	35/46 (76%)	30 (86%)	4 (11%)	1 (3%)	4 10
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%)	33 (100%)	0	0	100 100
14	y	26/46 (56%)	23 (88%)	3 (12%)	0	100 100
15	Z	58/62 (94%)	57 (98%)	1 (2%)	0	100 100
16	1	111/134 (83%)	104 (94%)	6 (5%)	1 (1%)	17 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	2	110/116 (95%)	101 (92%)	8 (7%)	1 (1%)	17 38
18	3	54/56 (96%)	52 (96%)	2 (4%)	0	100 100
All	All	2314/2522 (92%)	2171 (94%)	135 (6%)	8 (0%)	44 65

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	491	VAL
4	D	240	ALA
9	K	45	PHE
17	2	28	ASP
1	A	13	LEU

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%)	270 (100%)	1 (0%)	91 96
2	B	395/407 (97%)	391 (99%)	4 (1%)	76 90
3	C	335/362 (92%)	327 (98%)	8 (2%)	49 76
4	D	276/283 (98%)	271 (98%)	5 (2%)	59 82
5	E	69/73 (94%)	68 (99%)	1 (1%)	67 85
6	F	32/39 (82%)	32 (100%)	0	100 100
7	H	54/55 (98%)	54 (100%)	0	100 100
8	I	24/35 (69%)	24 (100%)	0	100 100
9	K	30/37 (81%)	30 (100%)	0	100 100
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%)	23 (92%)	2 (8%)	12 26
13	X	28/34 (82%)	28 (100%)	0	100 100
14	y	21/37 (57%)	18 (86%)	3 (14%)	3 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	Z	50/52 (96%)	49 (98%)	1 (2%)	55 80
16	1	96/115 (84%)	89 (93%)	7 (7%)	14 31
17	2	94/97 (97%)	91 (97%)	3 (3%)	39 67
18	3	42/42 (100%)	40 (95%)	2 (5%)	25 51
All	All	1908/2056 (93%)	1871 (98%)	37 (2%)	59 81

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	1	81	LEU
18	3	2	ARG
16	1	90	MET
17	2	6	GLU
3	C	350	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	HIS
2	B	9	HIS
2	B	14	ASN
10	L	6	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	B	619	-	41,41,41	0.95	2 (4%)	56,56,56	1.17	5 (8%)
23	BCR	C	515	-	41,41,41	1.07	2 (4%)	56,56,56	1.59	9 (16%)
22	CLA	B	602	-	65,73,73	1.58	8 (12%)	76,113,113	2.51	24 (31%)
22	CLA	B	601	-	65,73,73	1.47	8 (12%)	76,113,113	2.89	26 (34%)
22	CLA	C	513	-	65,73,73	1.67	13 (20%)	76,113,113	2.34	28 (36%)
22	CLA	B	616	-	65,73,73	1.80	8 (12%)	76,113,113	2.84	22 (28%)
22	CLA	C	517	-	65,73,73	1.73	9 (13%)	76,113,113	2.44	21 (27%)
22	CLA	A	406	-	65,73,73	1.57	10 (15%)	76,113,113	1.98	23 (30%)
22	CLA	B	613	-	65,73,73	1.62	9 (13%)	76,113,113	2.23	17 (22%)
22	CLA	D	408	-	65,73,73	1.75	12 (18%)	76,113,113	1.86	20 (26%)
22	CLA	A	404	-	65,73,73	1.65	10 (15%)	76,113,113	1.96	22 (28%)
22	CLA	B	608	-	65,73,73	1.65	11 (16%)	76,113,113	2.46	25 (32%)
22	CLA	C	509	-	65,73,73	1.62	11 (16%)	76,113,113	2.44	25 (32%)
22	CLA	C	510	-	65,73,73	1.76	9 (13%)	76,113,113	2.55	15 (19%)
25	LMG	C	502	-	55,55,55	1.03	0	63,63,63	1.05	4 (6%)
28	HEM	E	101	5	41,50,50	1.44	3 (7%)	45,82,82	1.22	4 (8%)
27	PL9	D	406	-	55,55,55	1.16	1 (1%)	68,69,69	1.55	8 (11%)
22	CLA	B	603	-	65,73,73	1.59	12 (18%)	76,113,113	2.05	16 (21%)
23	BCR	C	518	-	41,41,41	1.04	2 (4%)	56,56,56	1.11	5 (8%)
22	CLA	C	506	-	65,73,73	1.63	14 (21%)	76,113,113	1.98	15 (19%)
21	PHO	A	403	-	51,69,69	1.03	4 (7%)	47,99,99	1.15	5 (10%)
22	CLA	B	614	-	65,73,73	1.73	9 (13%)	76,113,113	2.53	25 (32%)
23	BCR	B	617	-	41,41,41	0.99	2 (4%)	56,56,56	1.17	3 (5%)
25	LMG	D	405	-	55,55,55	0.97	0	63,63,63	1.11	3 (4%)
22	CLA	B	611	-	65,73,73	1.68	10 (15%)	76,113,113	2.36	22 (28%)
21	PHO	D	407	-	51,69,69	1.08	6 (11%)	47,99,99	1.41	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	CLA	B	604	-	65,73,73	1.60	9 (13%)	76,113,113	2.26	25 (32%)
22	CLA	B	607	-	65,73,73	1.67	13 (20%)	76,113,113	2.05	21 (27%)
23	BCR	A	408	-	41,41,41	1.11	2 (4%)	56,56,56	1.33	9 (16%)
25	LMG	D	404	-	55,55,55	0.93	0	63,63,63	1.14	3 (4%)
25	LMG	I	101	-	55,55,55	0.99	2 (3%)	63,63,63	1.06	4 (6%)
23	BCR	D	410	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)
22	CLA	C	514	-	65,73,73	1.77	13 (20%)	76,113,113	2.14	17 (22%)
25	LMG	C	501	-	55,55,55	1.11	3 (5%)	63,63,63	1.00	3 (4%)
25	LMG	D	403	-	55,55,55	0.92	2 (3%)	63,63,63	1.14	5 (7%)
22	CLA	B	605	-	65,73,73	1.68	10 (15%)	76,113,113	2.07	21 (27%)
22	CLA	B	609	-	65,73,73	1.88	12 (18%)	76,113,113	2.36	21 (27%)
23	BCR	C	516	-	41,41,41	1.12	3 (7%)	56,56,56	1.34	4 (7%)
22	CLA	D	409	-	65,73,73	1.61	9 (13%)	76,113,113	1.72	16 (21%)
22	CLA	C	504	-	65,73,73	1.56	10 (15%)	76,113,113	1.96	18 (23%)
23	BCR	H	101	-	41,41,41	3.44	14 (34%)	56,56,56	4.30	30 (53%)
23	BCR	K	101	-	41,41,41	3.43	14 (34%)	56,56,56	4.27	29 (51%)
23	BCR	B	618	-	41,41,41	1.02	2 (4%)	56,56,56	1.24	9 (16%)
22	CLA	C	503	-	65,73,73	1.52	9 (13%)	76,113,113	2.05	16 (21%)
22	CLA	C	512	-	65,73,73	1.85	9 (13%)	76,113,113	2.52	23 (30%)
22	CLA	C	508	-	65,73,73	1.78	8 (12%)	76,113,113	2.25	22 (28%)
22	CLA	B	615	-	65,73,73	1.64	11 (16%)	76,113,113	2.36	17 (22%)
25	LMG	D	402	-	55,55,55	0.98	0	63,63,63	1.09	4 (6%)
22	CLA	B	612	-	65,73,73	1.67	9 (13%)	76,113,113	2.51	27 (35%)
22	CLA	C	511	-	65,73,73	1.67	11 (16%)	76,113,113	2.40	22 (28%)
22	CLA	C	505	-	65,73,73	1.66	11 (16%)	76,113,113	2.32	24 (31%)
22	CLA	C	507	-	65,73,73	1.80	10 (15%)	76,113,113	2.54	21 (27%)
24	LHG	A	409	-	48,48,48	0.79	1 (2%)	51,54,54	0.89	1 (1%)
22	CLA	B	606	-	65,73,73	1.55	5 (7%)	76,113,113	1.82	21 (27%)
22	CLA	B	610	-	65,73,73	1.58	9 (13%)	76,113,113	2.47	22 (28%)
22	CLA	A	405	-	65,73,73	1.65	8 (12%)	76,113,113	1.93	21 (27%)
22	CLA	A	407	-	65,73,73	1.77	9 (13%)	76,113,113	1.63	16 (21%)

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	B	619	-	-	4/29/63/63	0/2/2/2
23	BCR	C	515	-	-	7/29/63/63	0/2/2/2
22	CLA	B	602	-	1/1/15/20	13/37/115/115	-
22	CLA	B	601	-	3/3/15/20	9/37/115/115	-
22	CLA	C	513	-	2/2/15/20	10/37/115/115	-
22	CLA	C	517	-	1/1/15/20	10/37/115/115	-
22	CLA	B	616	-	-	9/37/115/115	-
22	CLA	A	406	-	1/1/15/20	10/37/115/115	-
22	CLA	B	613	-	1/1/15/20	11/37/115/115	-
22	CLA	D	408	-	1/1/15/20	12/37/115/115	-
22	CLA	A	404	-	1/1/15/20	6/37/115/115	-
22	CLA	B	608	-	2/2/15/20	9/37/115/115	-
22	CLA	C	509	-	1/1/15/20	13/37/115/115	-
22	CLA	C	510	-	2/2/15/20	12/37/115/115	-
25	LMG	C	502	-	-	7/50/70/70	0/1/1/1
28	HEM	E	101	5	-	5/12/54/54	-
27	PL9	D	406	-	-	9/53/73/73	0/1/1/1
22	CLA	B	603	-	2/2/15/20	12/37/115/115	-
23	BCR	C	518	-	-	12/29/63/63	0/2/2/2
22	CLA	C	506	-	1/1/15/20	11/37/115/115	-
21	PHO	A	403	-	1/1/17/22	6/37/103/103	0/5/6/6
22	CLA	B	614	-	2/2/15/20	4/37/115/115	-
23	BCR	B	617	-	-	6/29/63/63	0/2/2/2
25	LMG	D	405	-	-	13/50/70/70	0/1/1/1
22	CLA	B	611	-	1/1/15/20	11/37/115/115	-
21	PHO	D	407	-	1/1/17/22	7/37/103/103	0/5/6/6
22	CLA	B	604	-	2/2/15/20	11/37/115/115	-
22	CLA	B	607	-	2/2/15/20	12/37/115/115	-
23	BCR	A	408	-	-	7/29/63/63	0/2/2/2
25	LMG	D	404	-	-	8/50/70/70	0/1/1/1
25	LMG	I	101	-	-	8/50/70/70	0/1/1/1
23	BCR	D	410	-	-	6/29/63/63	0/2/2/2
22	CLA	C	514	-	2/2/15/20	10/37/115/115	-
25	LMG	C	501	-	-	12/50/70/70	0/1/1/1
25	LMG	D	403	-	-	14/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	605	-	-	10/37/115/115	-
22	CLA	B	609	-	2/2/15/20	9/37/115/115	-
23	BCR	C	516	-	-	8/29/63/63	0/2/2/2
22	CLA	D	409	-	1/1/15/20	3/37/115/115	-
22	CLA	C	504	-	1/1/15/20	9/37/115/115	-
23	BCR	H	101	-	-	15/29/63/63	0/2/2/2
23	BCR	K	101	-	-	15/29/63/63	0/2/2/2
23	BCR	B	618	-	-	3/29/63/63	0/2/2/2
22	CLA	C	503	-	1/1/15/20	8/37/115/115	-
22	CLA	C	512	-	1/1/15/20	10/37/115/115	-
22	CLA	C	508	-	-	7/37/115/115	-
22	CLA	B	615	-	1/1/15/20	8/37/115/115	-
25	LMG	D	402	-	-	7/50/70/70	0/1/1/1
22	CLA	B	612	-	1/1/15/20	14/37/115/115	-
22	CLA	C	511	-	1/1/15/20	13/37/115/115	-
22	CLA	C	505	-	1/1/15/20	15/37/115/115	-
22	CLA	C	507	-	1/1/15/20	4/37/115/115	-
24	LHG	A	409	-	-	15/53/53/53	-
22	CLA	B	606	-	2/2/15/20	11/37/115/115	-
22	CLA	B	610	-	2/2/15/20	11/37/115/115	-
22	CLA	A	405	-	1/1/15/20	12/37/115/115	-
22	CLA	A	407	-	2/2/15/20	7/37/115/115	-

The worst 5 of 415 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	H	101	BCR	C1-C6	-10.18	1.39	1.53
23	K	101	BCR	C1-C6	-9.95	1.40	1.53
22	B	616	CLA	C4B-NB	9.89	1.44	1.35
22	B	609	CLA	C4B-NB	9.83	1.44	1.35
23	K	101	BCR	C5-C6	-9.67	1.17	1.34

The worst 5 of 897 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	B	601	CLA	C4A-NA-C1A	14.35	113.16	106.71
23	H	101	BCR	C33-C5-C6	-13.58	109.28	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	C	510	CLA	C4A-NA-C1A	13.10	112.60	106.71
22	B	616	CLA	C4A-NA-C1A	12.90	112.50	106.71
23	K	101	BCR	C33-C5-C6	-12.66	110.31	124.53

5 of 48 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	403	PHO	C8
21	D	407	PHO	C8
22	A	404	CLA	ND
22	A	405	CLA	C8
22	A	406	CLA	ND

5 of 540 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	403	PHO	O2A-C1-C2-C3
22	A	404	CLA	C1A-C2A-CAA-CBA
22	A	404	CLA	C6-C7-C8-C9
22	A	405	CLA	C1A-C2A-CAA-CBA
22	A	405	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

45 monomers are involved in 145 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	619	BCR	2	0
23	C	515	BCR	14	0
22	B	601	CLA	5	0
22	C	513	CLA	3	0
22	B	616	CLA	1	0
22	C	517	CLA	4	0
22	A	406	CLA	2	0
22	B	613	CLA	2	0
22	D	408	CLA	2	0
22	B	608	CLA	5	0
22	C	509	CLA	4	0
22	C	510	CLA	11	0
27	D	406	PL9	4	0
22	B	603	CLA	3	0
23	C	518	BCR	2	0
22	C	506	CLA	1	0

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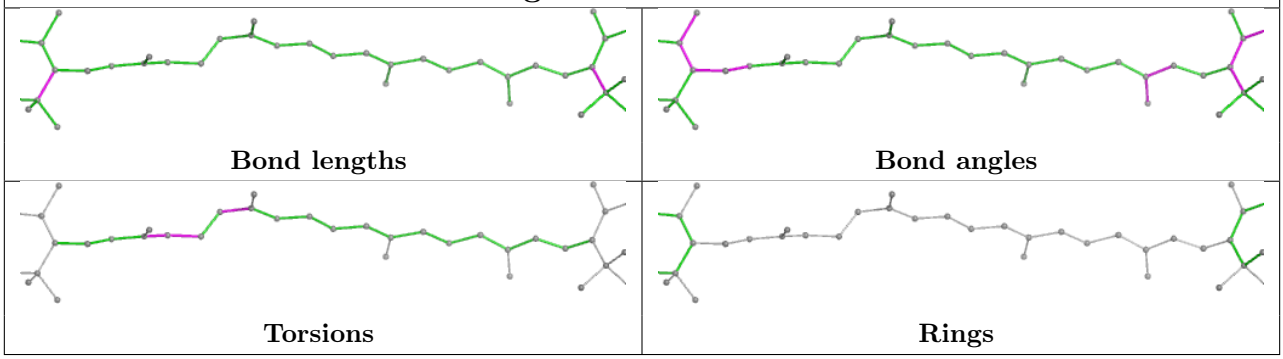
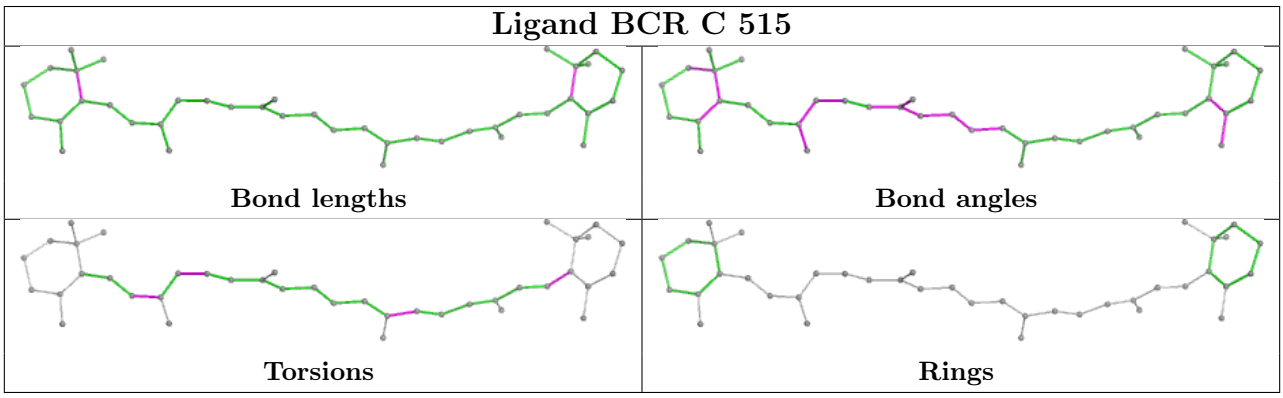
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	403	PHO	1	0
22	B	614	CLA	2	0
23	B	617	BCR	1	0
22	B	611	CLA	3	0
22	B	604	CLA	2	0
22	B	607	CLA	2	0
23	A	408	BCR	2	0
25	D	404	LMG	1	0
22	C	514	CLA	1	0
25	D	403	LMG	1	0
22	B	605	CLA	1	0
22	B	609	CLA	8	0
23	C	516	BCR	4	0
22	D	409	CLA	6	0
22	C	504	CLA	2	0
23	H	101	BCR	18	0
23	K	101	BCR	24	0
23	B	618	BCR	2	0
22	C	503	CLA	4	0
22	C	512	CLA	12	0
22	B	615	CLA	1	0
25	D	402	LMG	1	0
22	B	612	CLA	3	0
22	C	511	CLA	4	0
22	C	505	CLA	3	0
22	B	606	CLA	2	0
22	B	610	CLA	3	0
22	A	405	CLA	5	0
22	A	407	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.

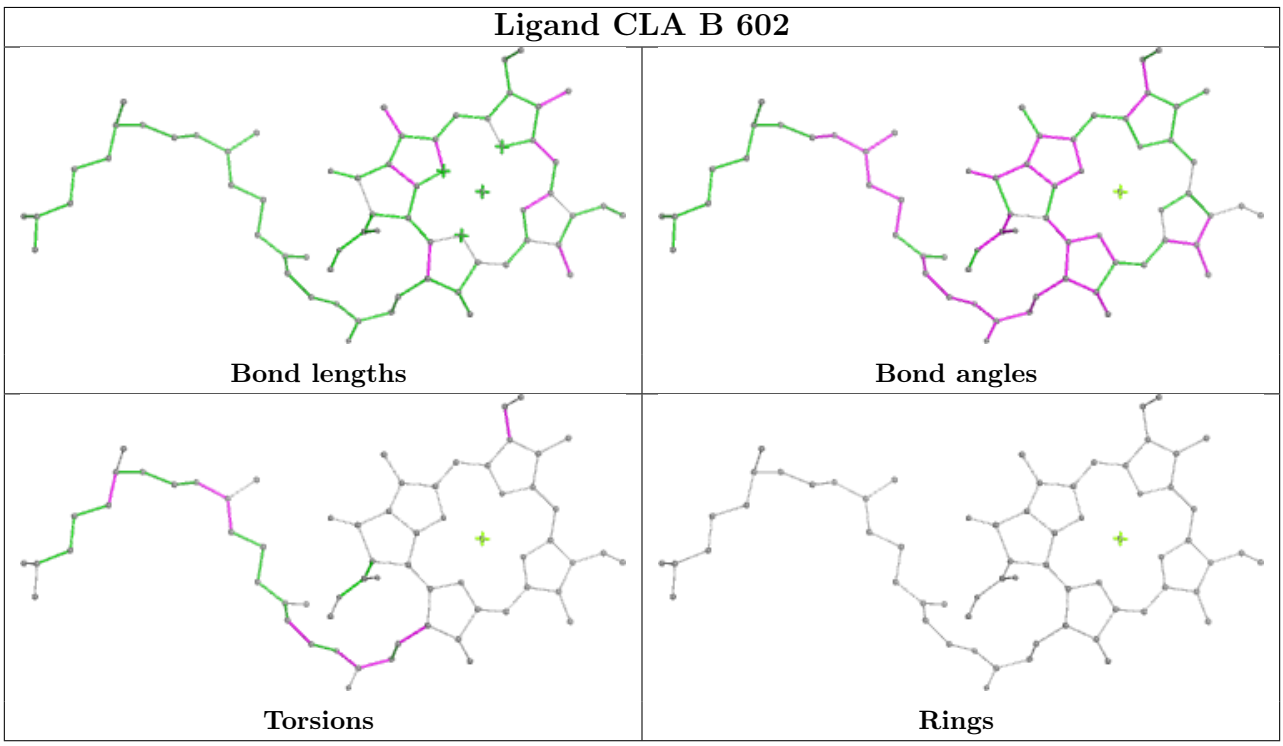
Ligand BCR B 619



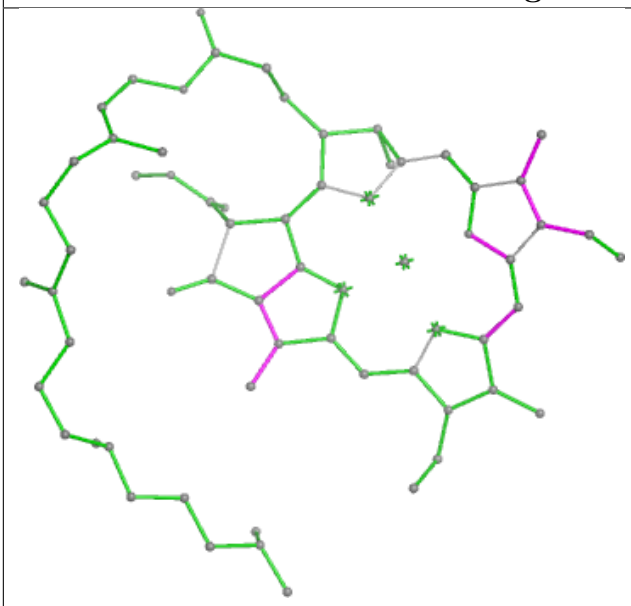
Ligand BCR C 515



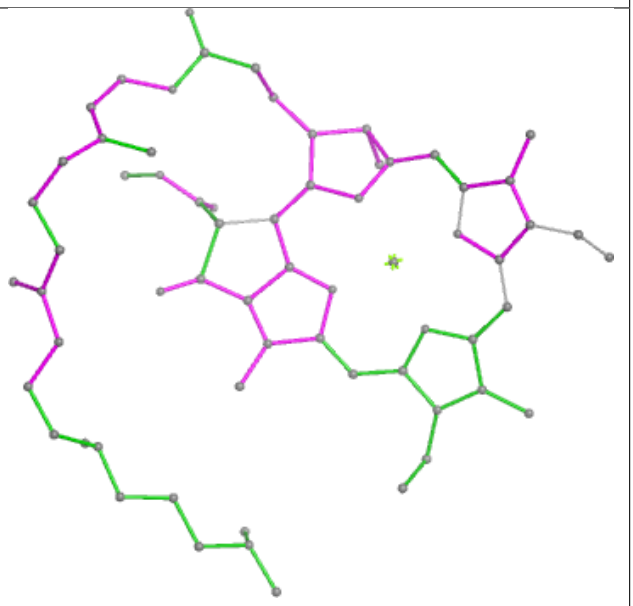
Ligand CLA B 602



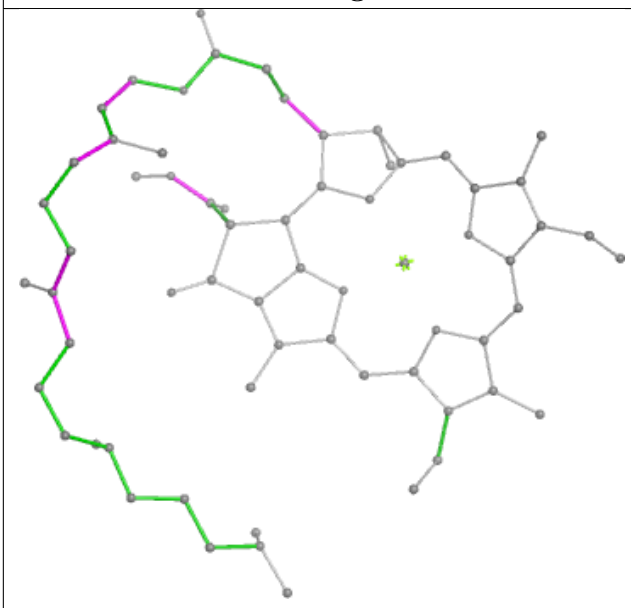
Ligand CLA B 601



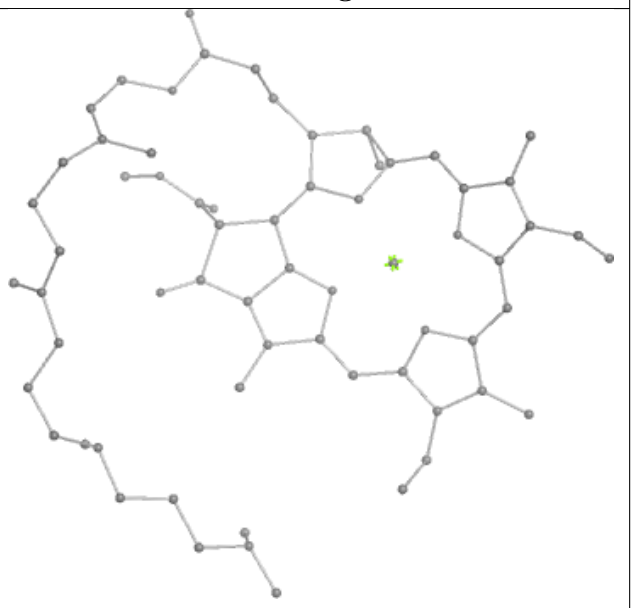
Bond lengths



Bond angles

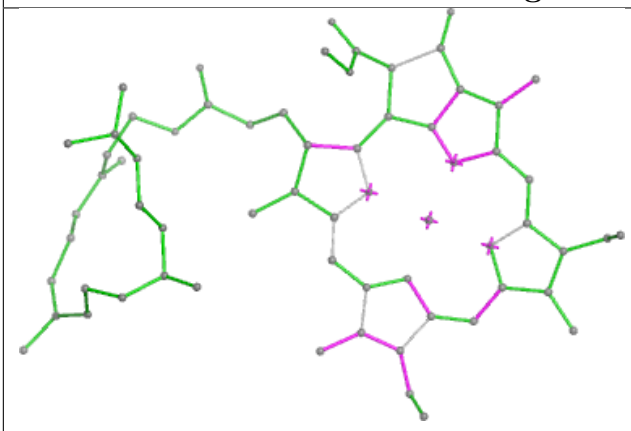


Torsions

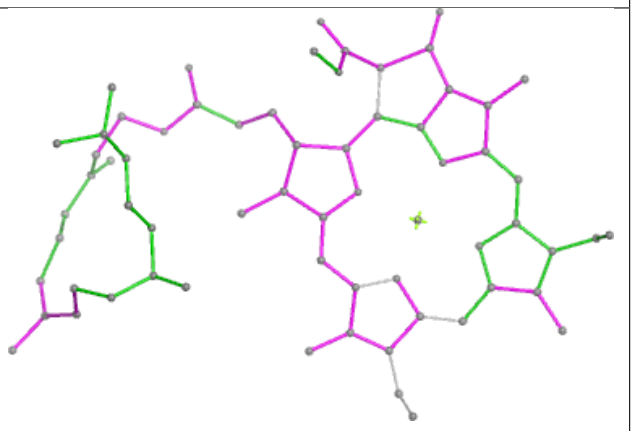


Rings

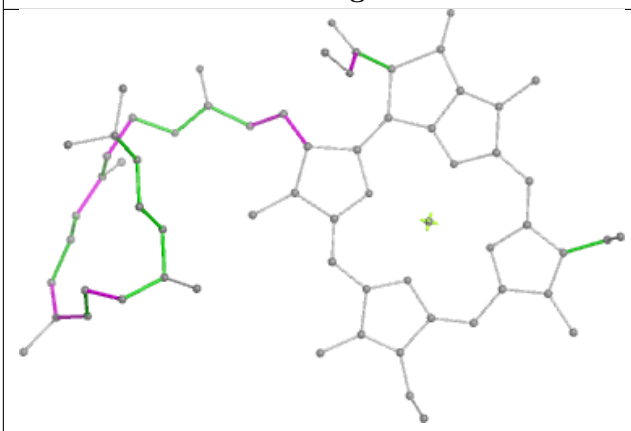
Ligand CLA C 513



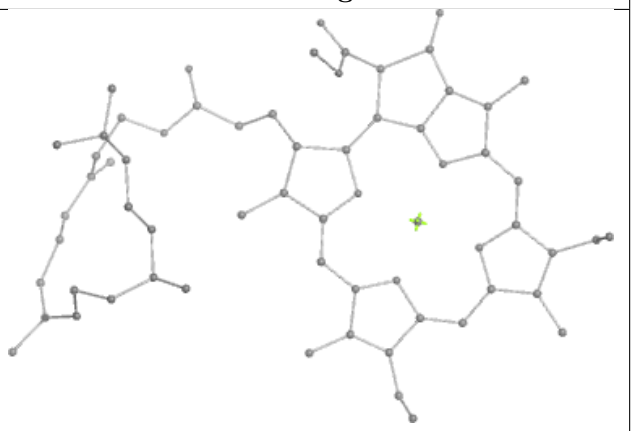
Bond lengths



Bond angles

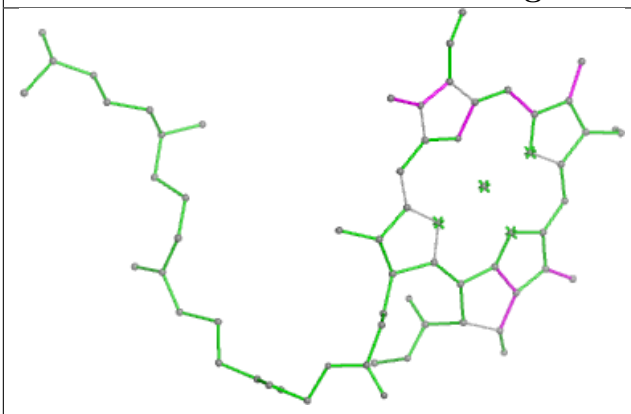


Torsions

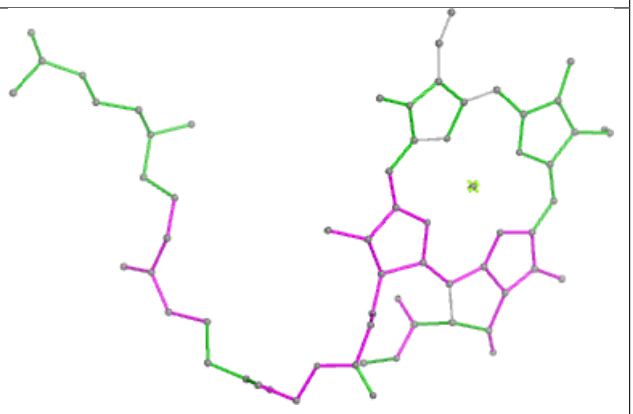


Rings

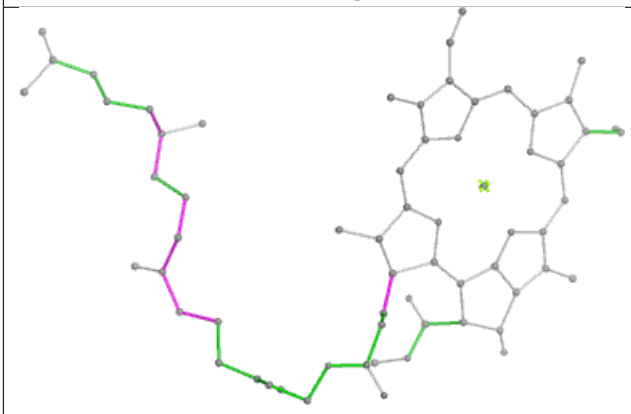
Ligand CLA B 616



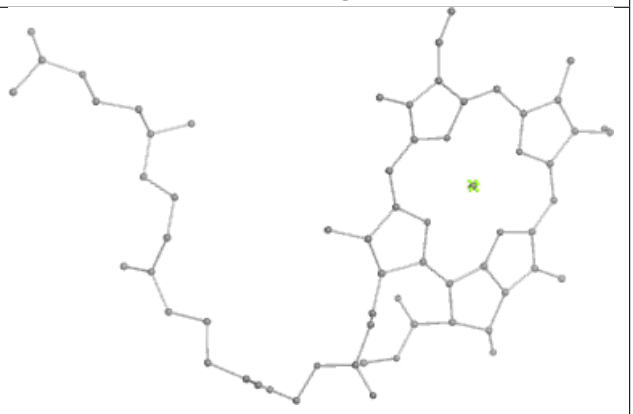
Bond lengths



Bond angles

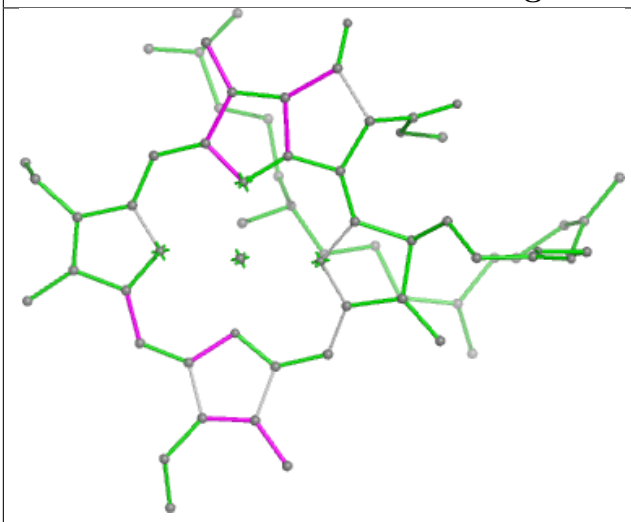


Torsions

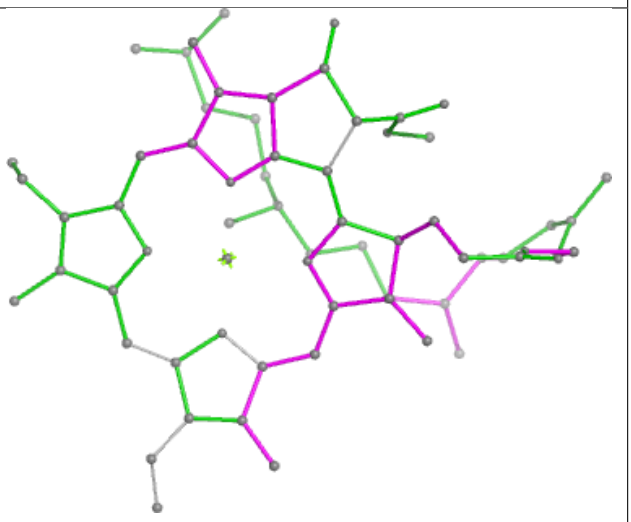


Rings

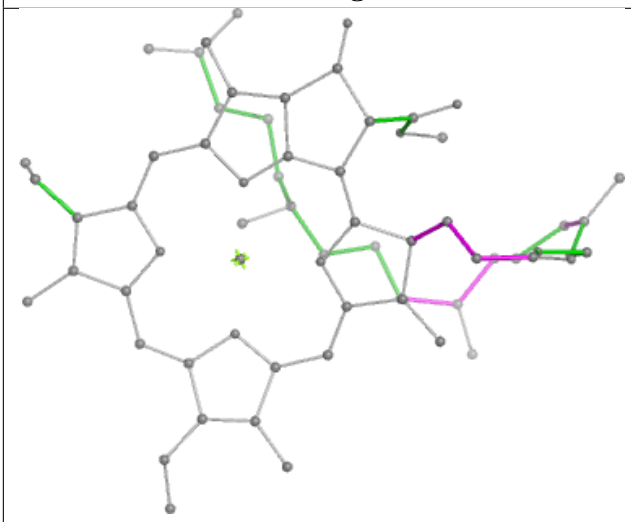
Ligand CLA C 517



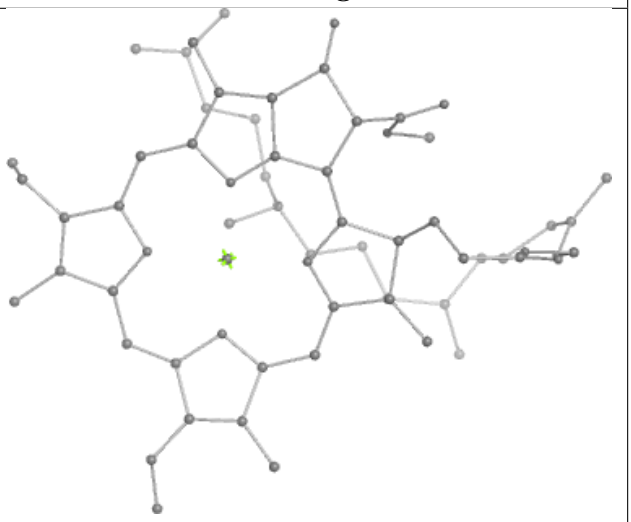
Bond lengths



Bond angles

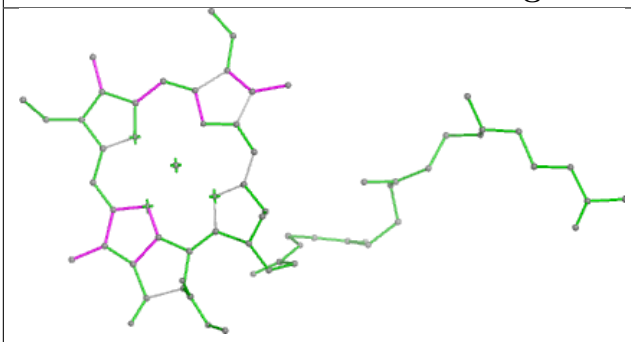


Torsions

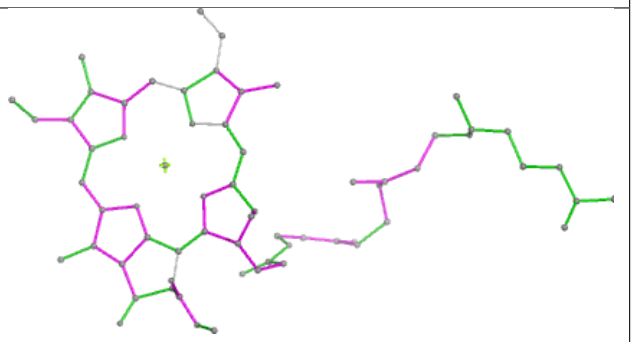


Rings

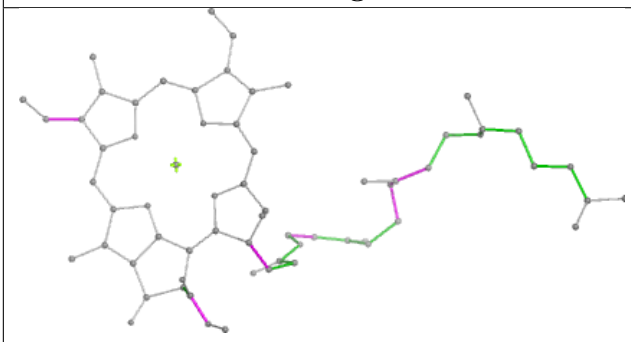
Ligand CLA A 406



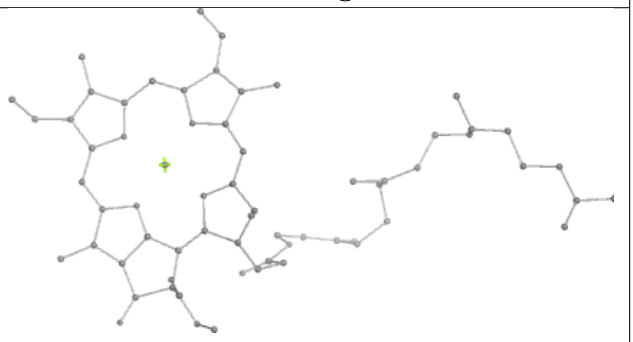
Bond lengths



Bond angles

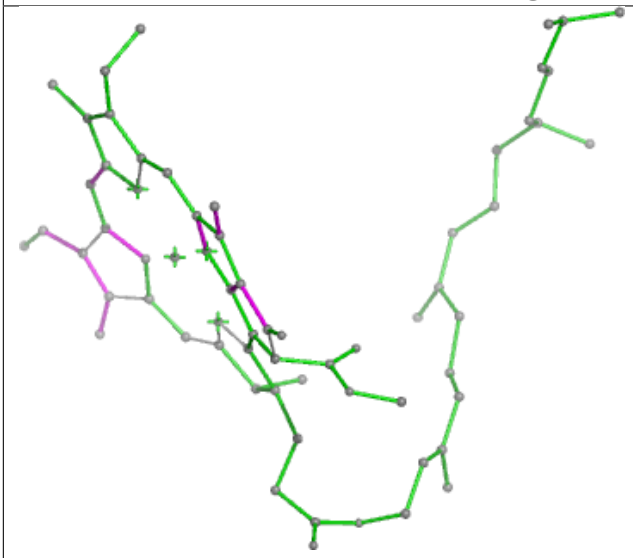


Torsions

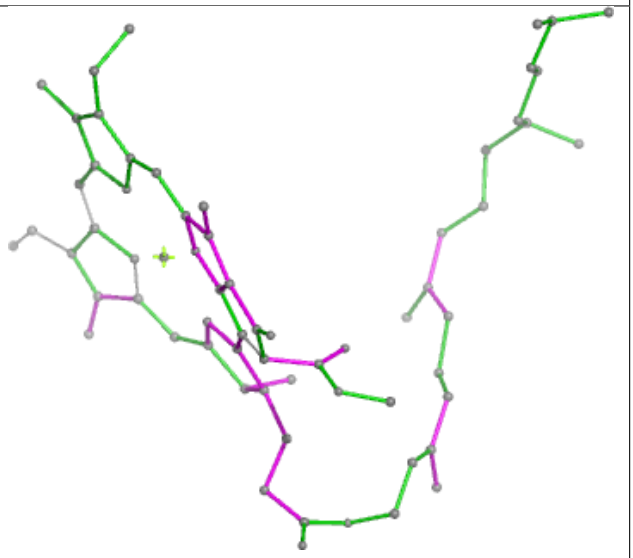


Rings

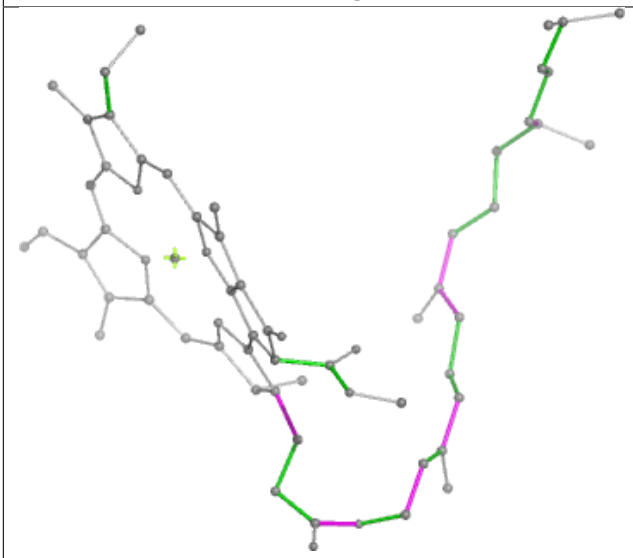
Ligand CLA B 613



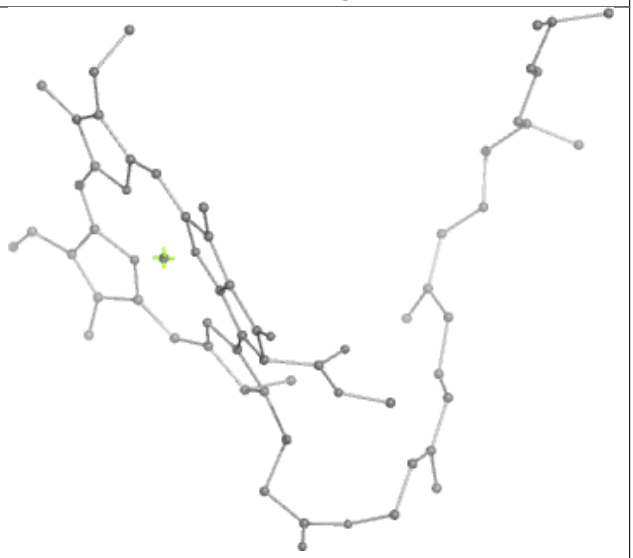
Bond lengths



Bond angles

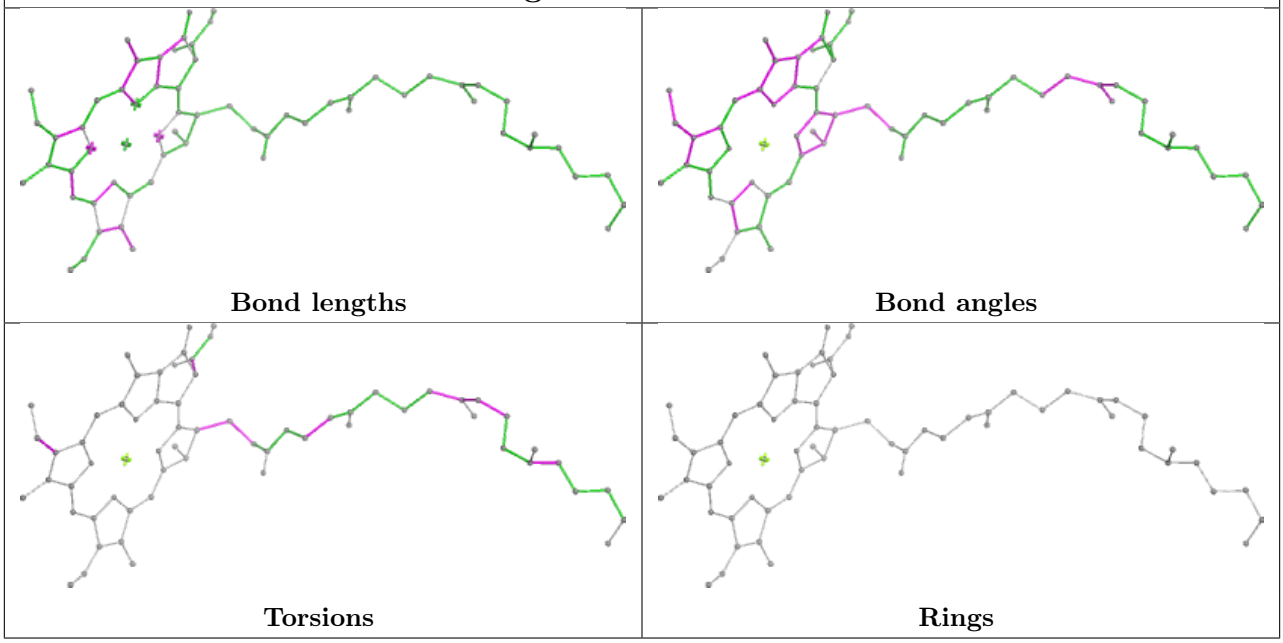


Torsions

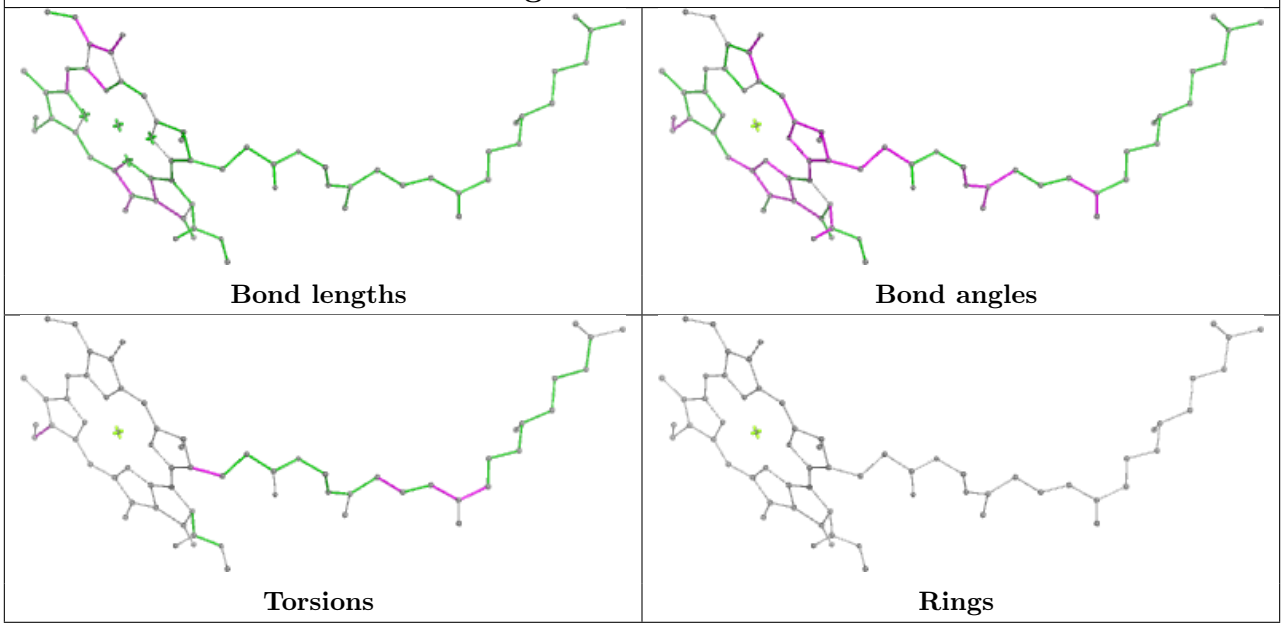


Rings

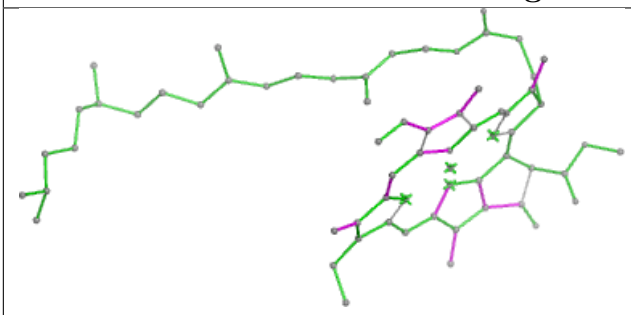
Ligand CLA D 408



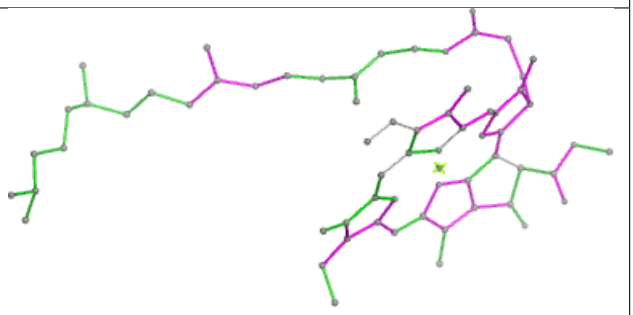
Ligand CLA A 404



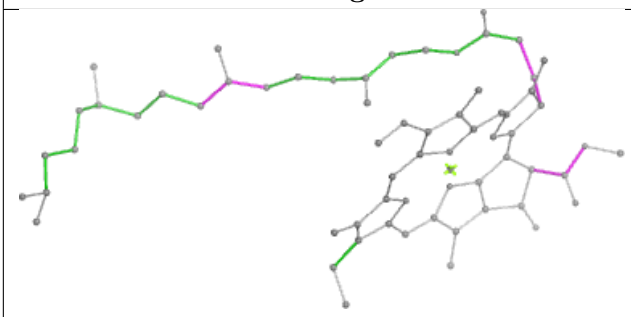
Ligand CLA B 608



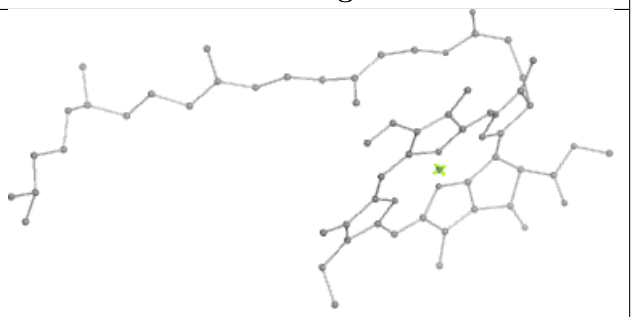
Bond lengths



Bond angles

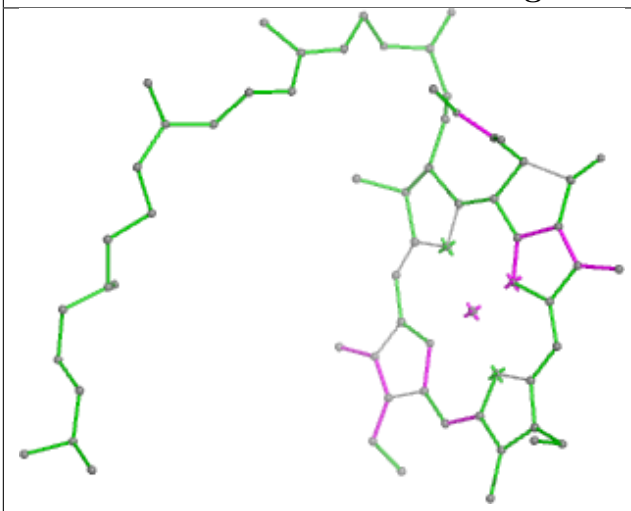


Torsions

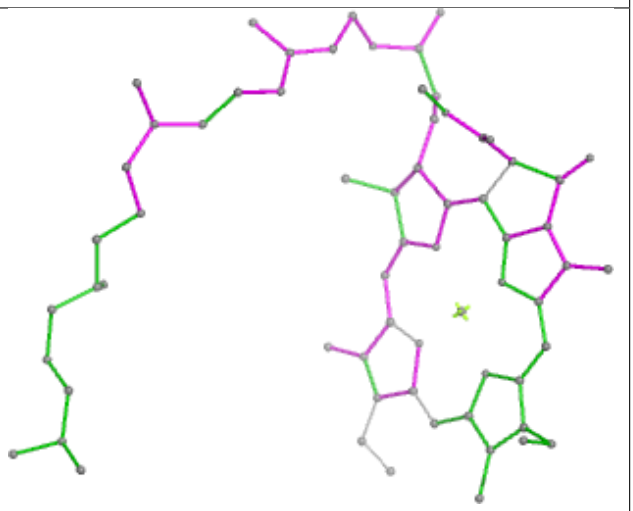


Rings

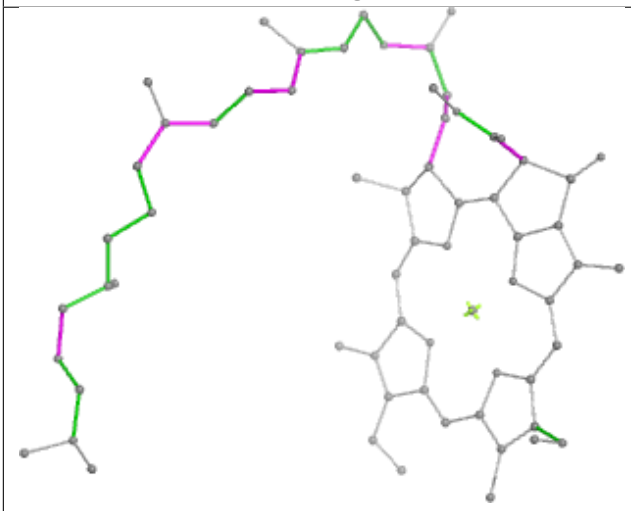
Ligand CLA C 509



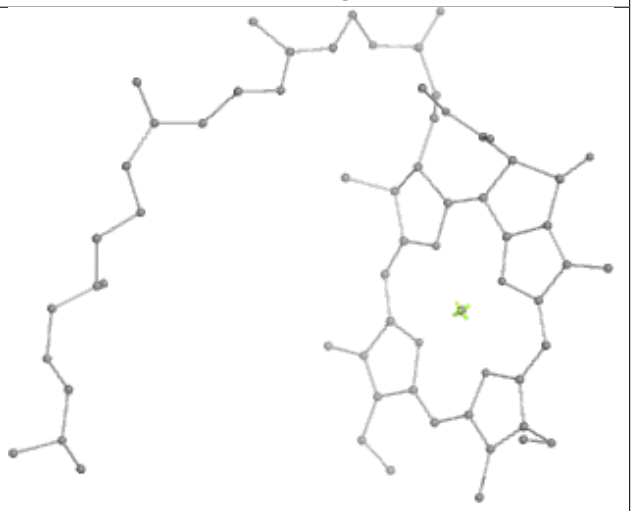
Bond lengths



Bond angles

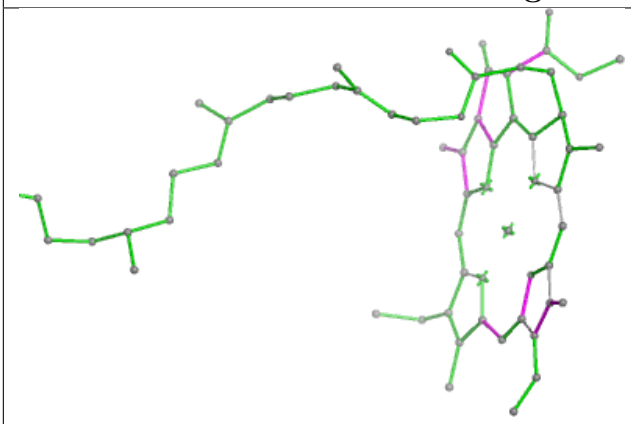


Torsions

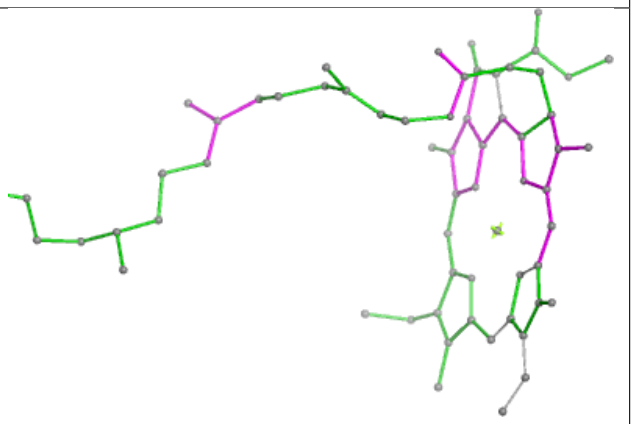


Rings

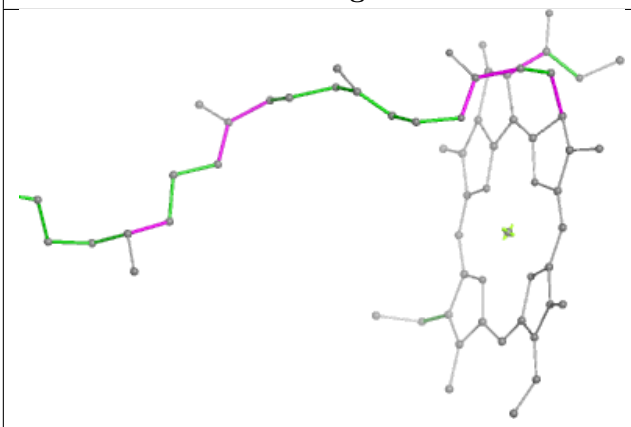
Ligand CLA C 510



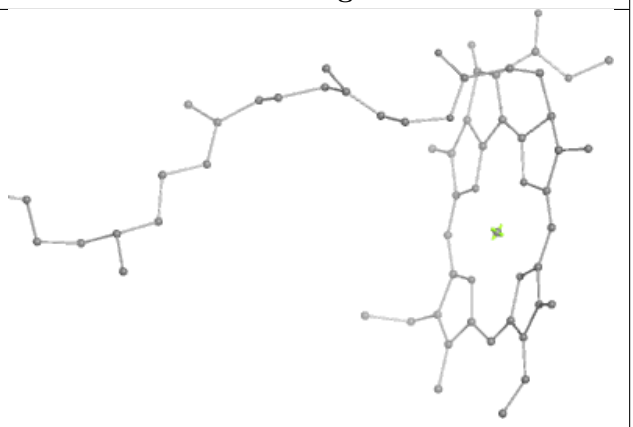
Bond lengths



Bond angles

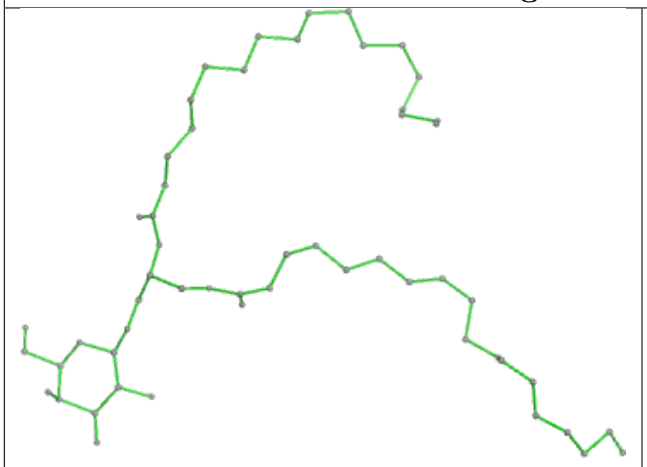


Torsions

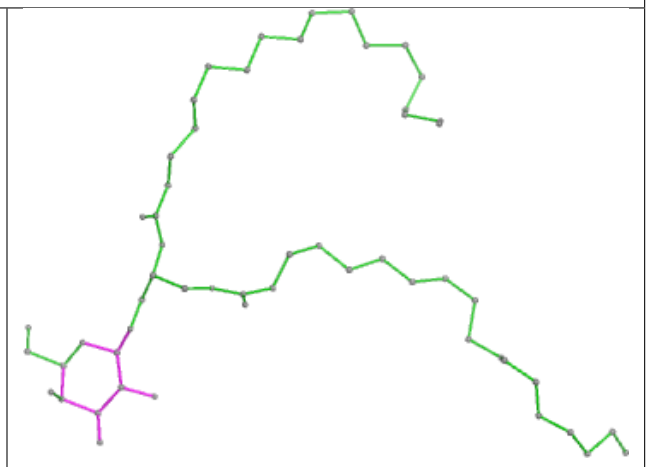


Rings

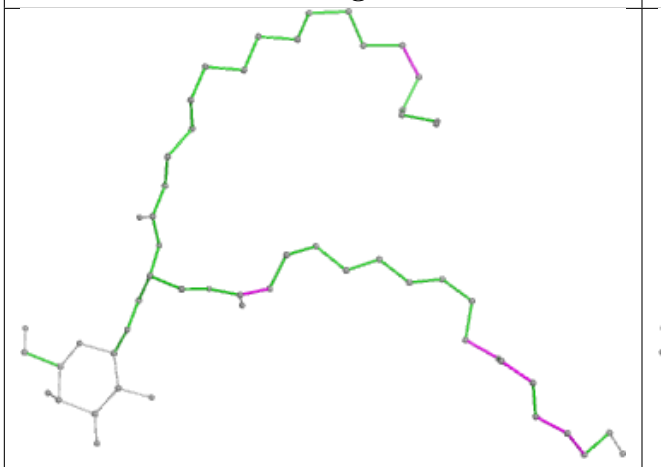
Ligand LMG C 502



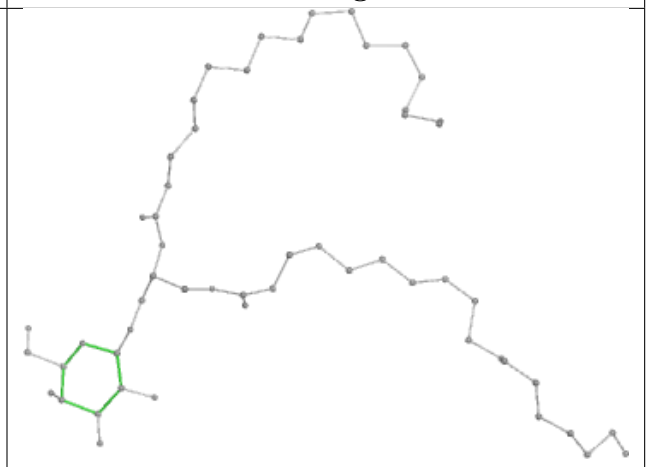
Bond lengths



Bond angles

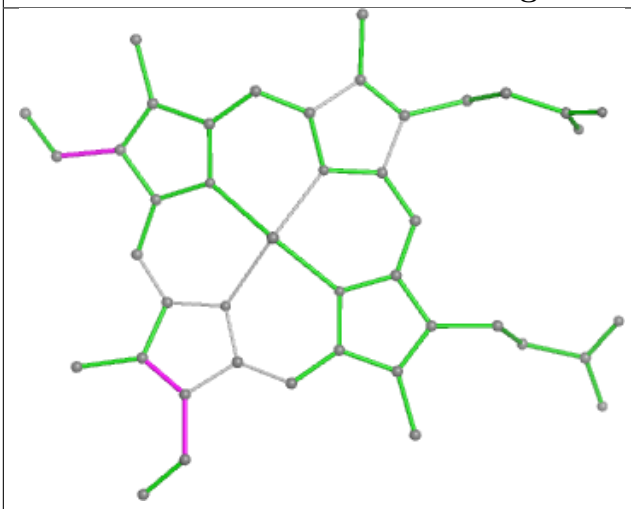


Torsions

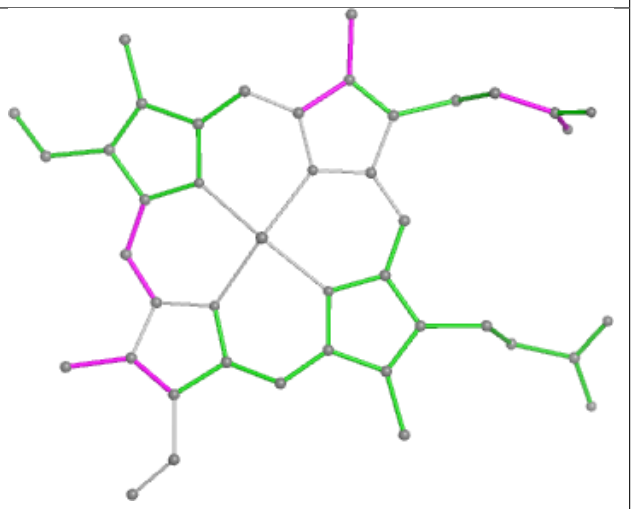


Rings

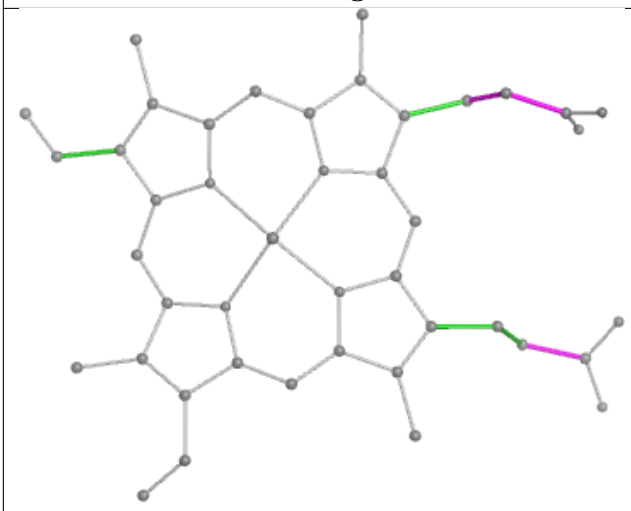
Ligand HEM E 101



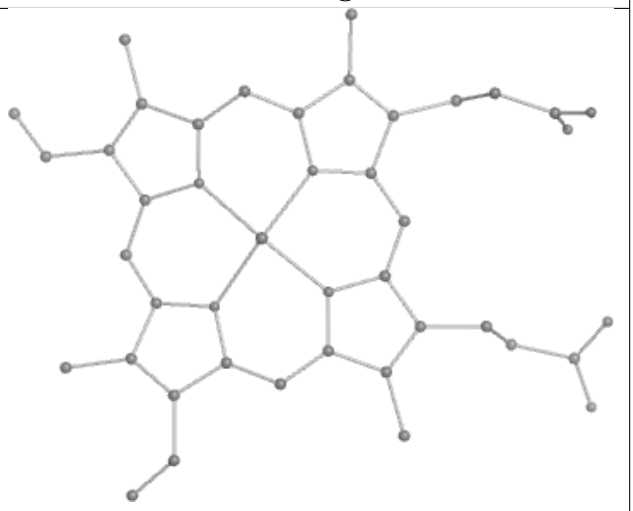
Bond lengths



Bond angles

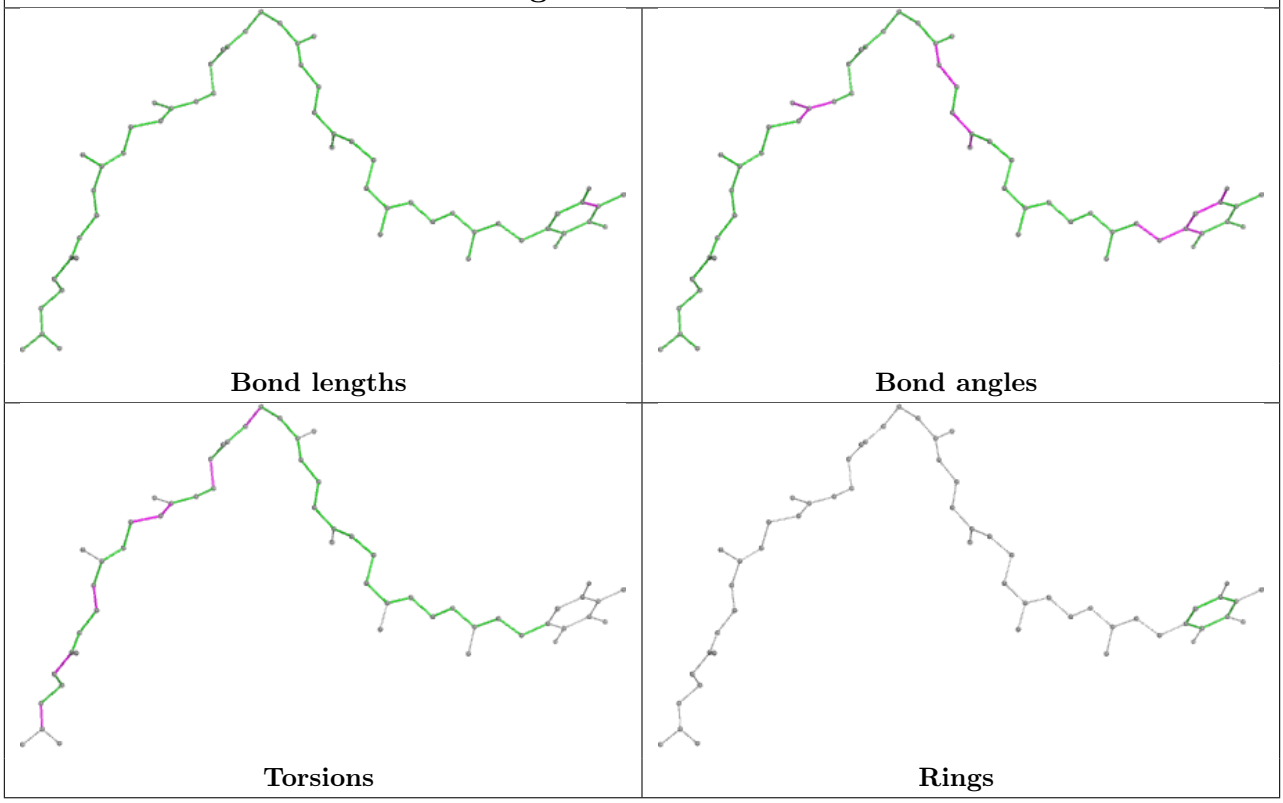


Torsions

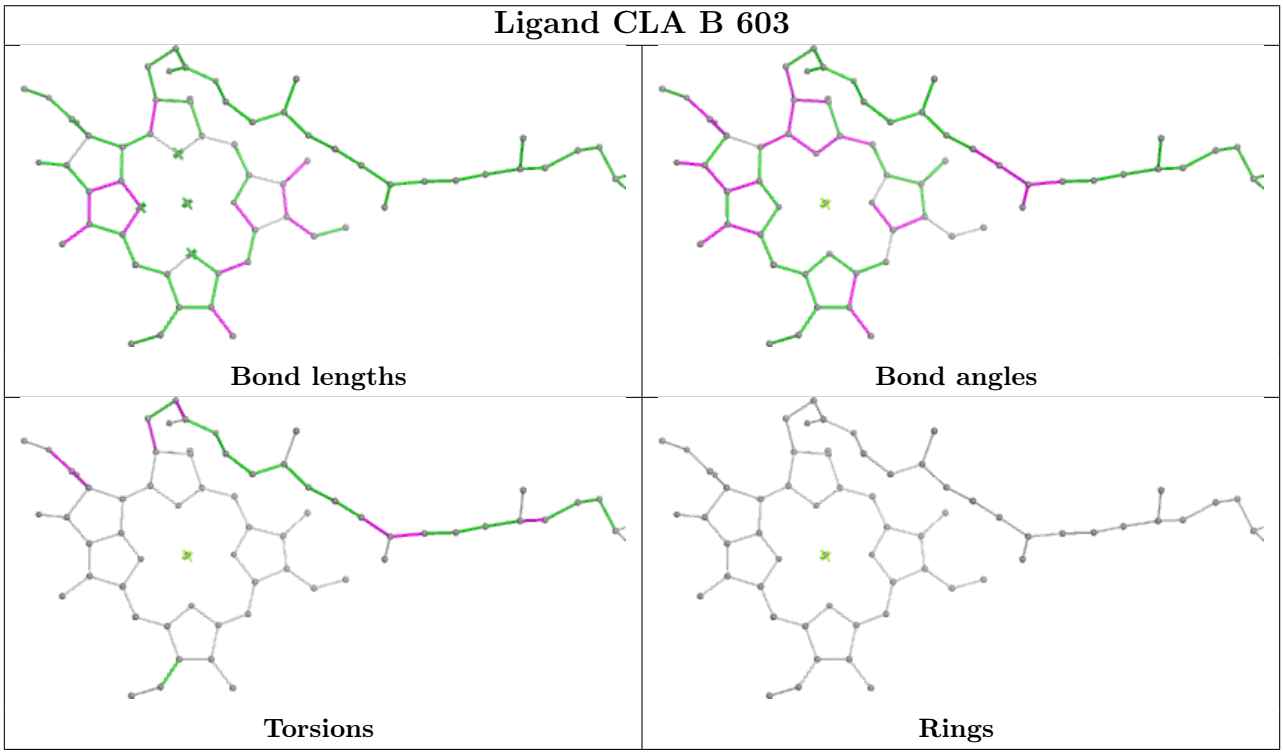


Rings

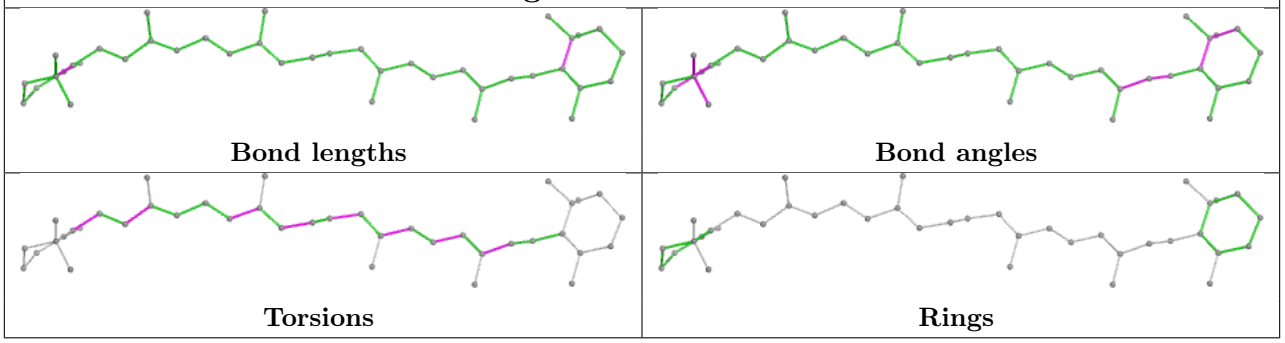
Ligand PL9 D 406



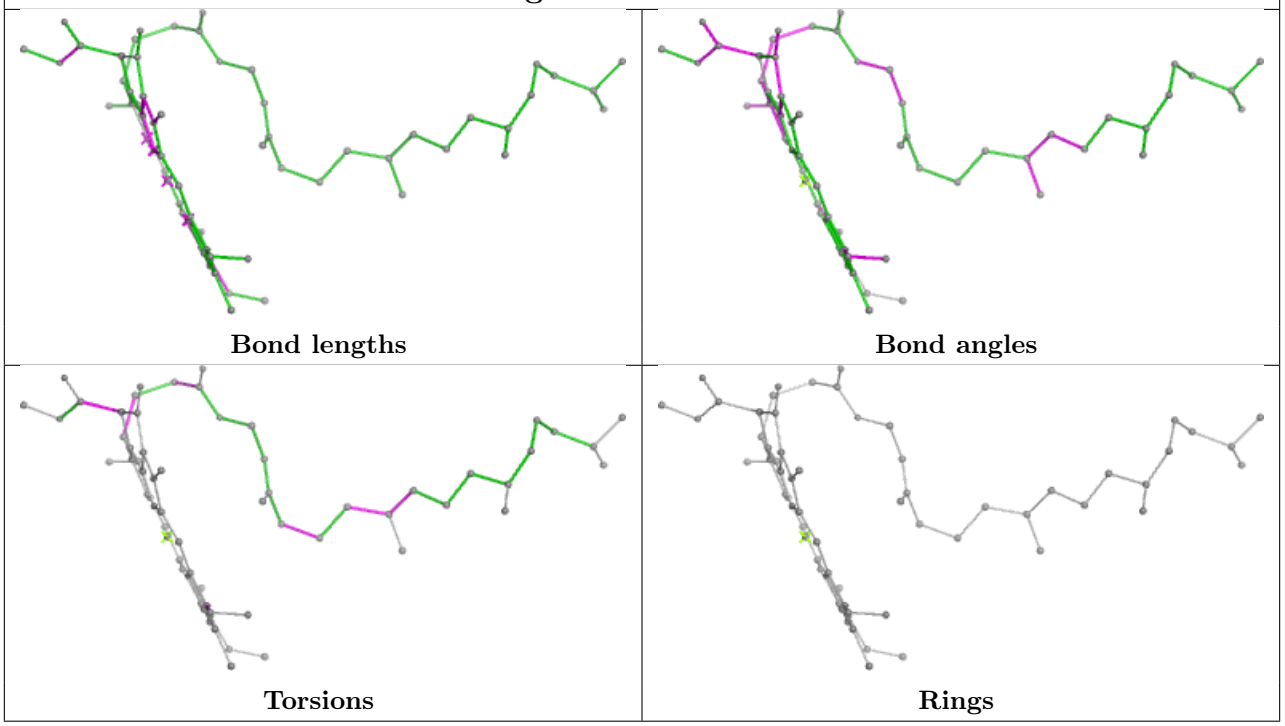
Ligand CLA B 603



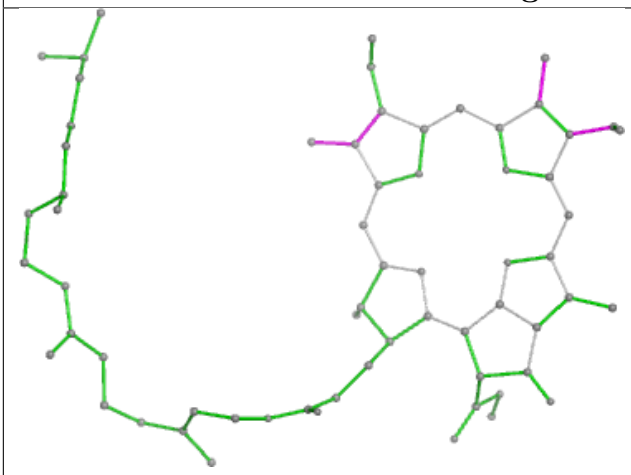
Ligand BCR C 518



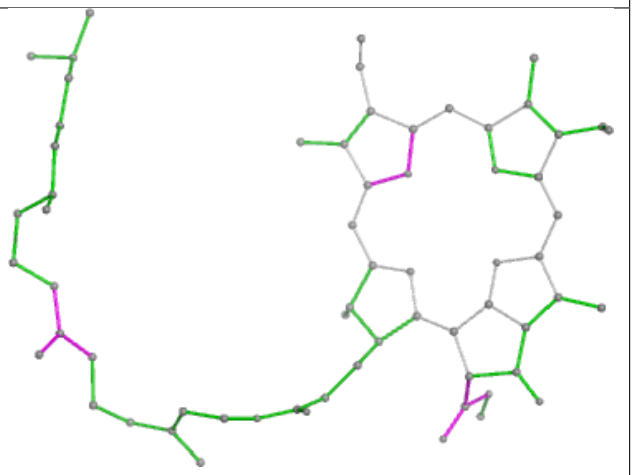
Ligand CLA C 506



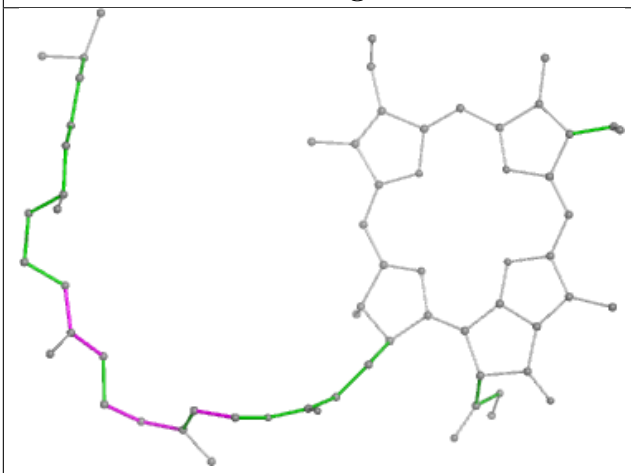
Ligand PHO A 403



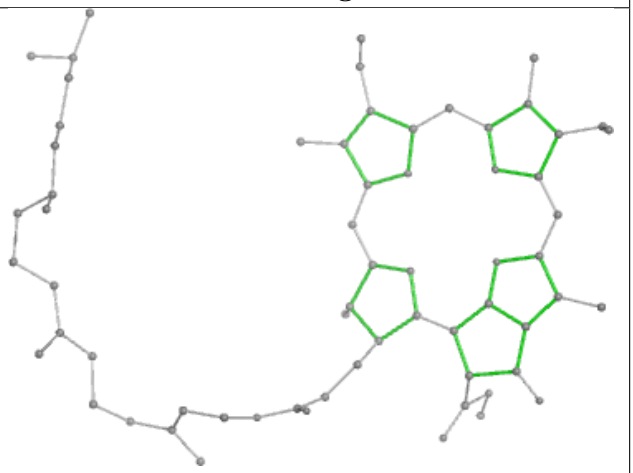
Bond lengths



Bond angles

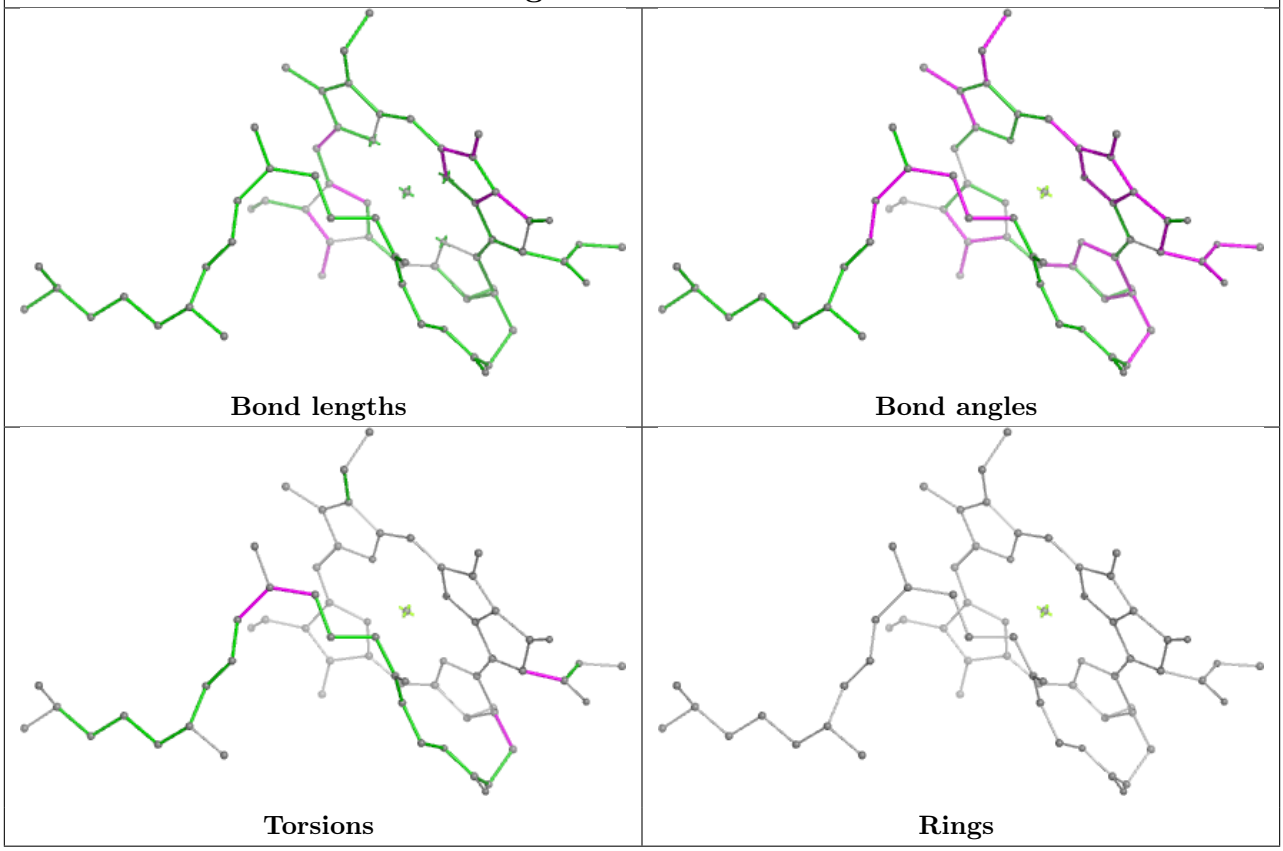


Torsions

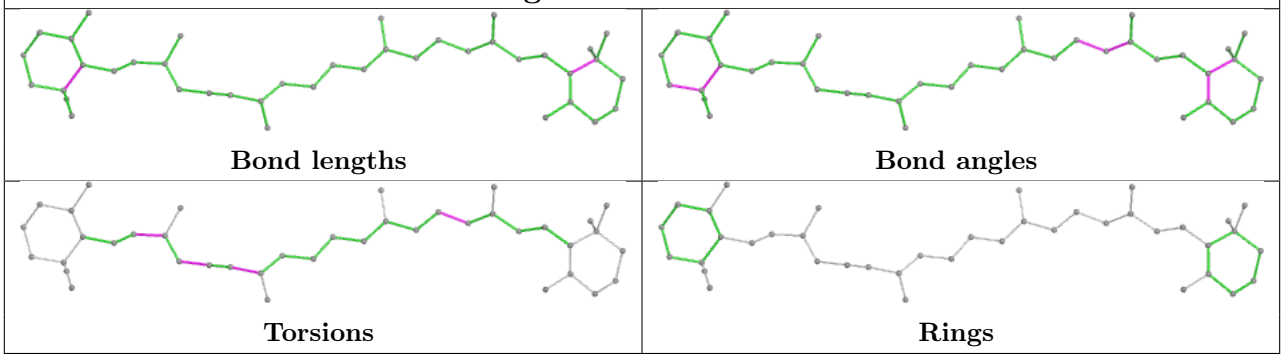


Rings

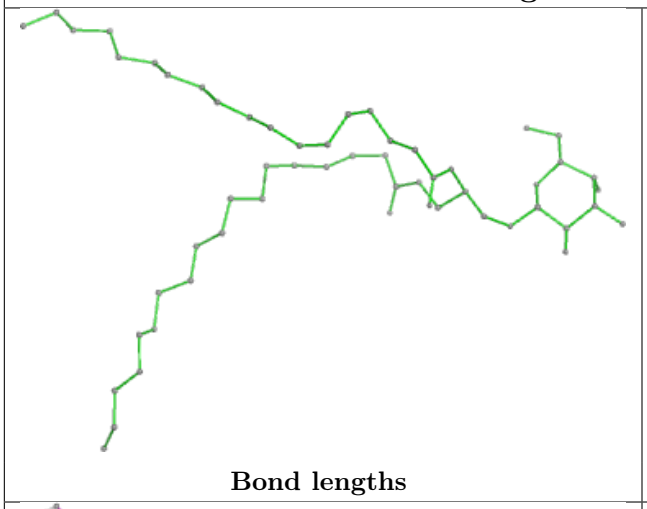
Ligand CLA B 614



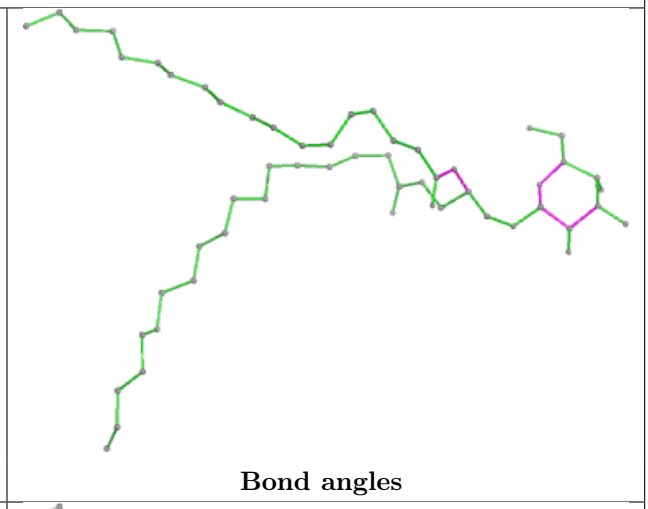
Ligand BCR B 617



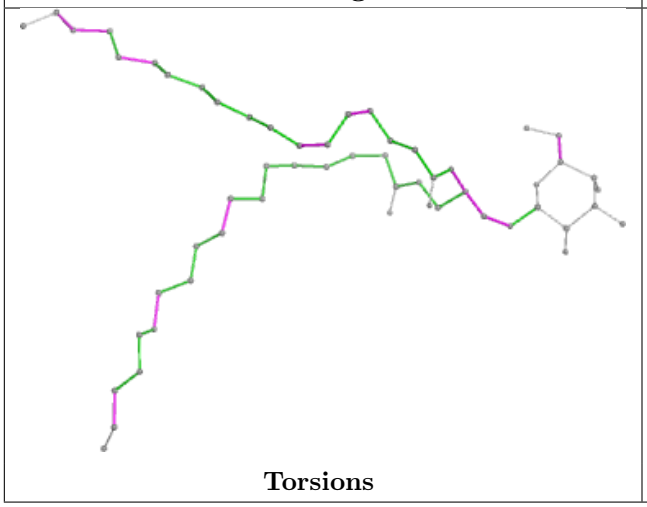
Ligand LMG D 405



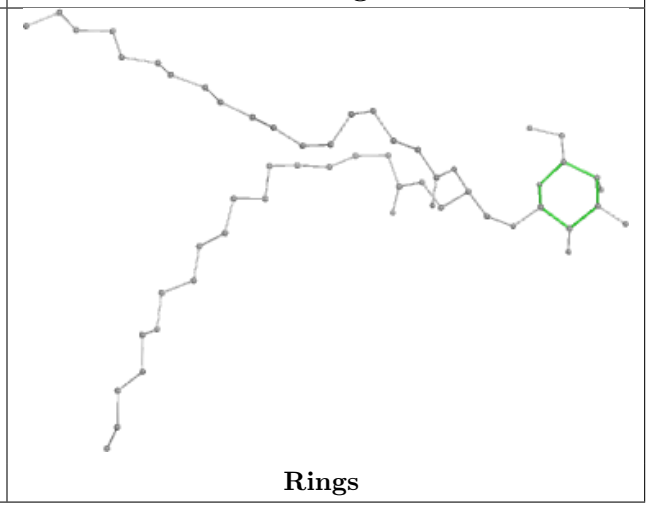
Bond lengths



Bond angles

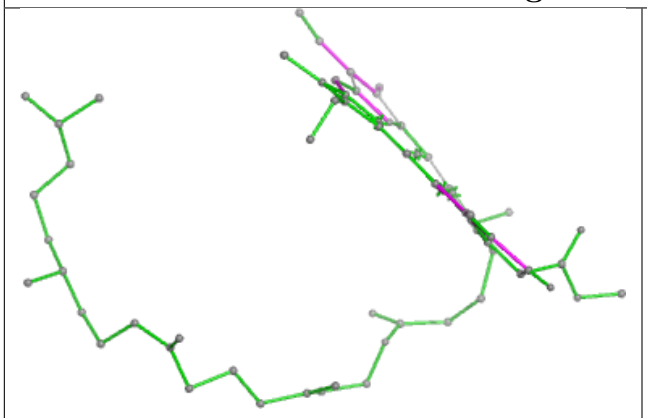


Torsions

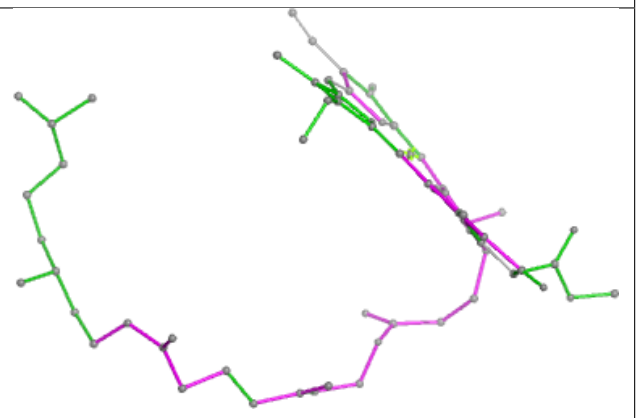


Rings

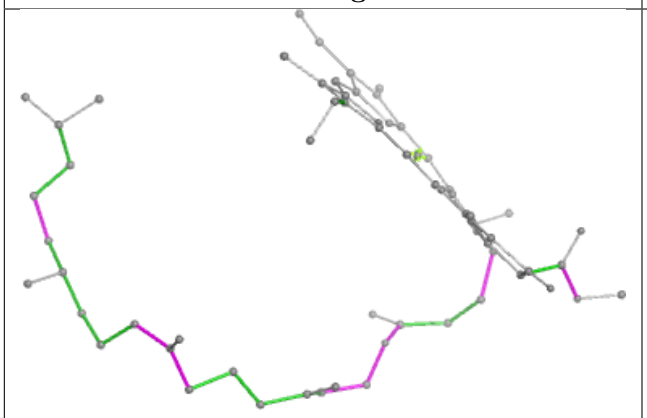
Ligand CLA B 611



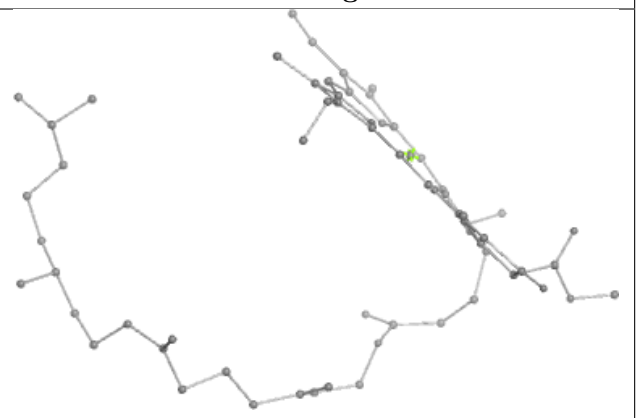
Bond lengths



Bond angles

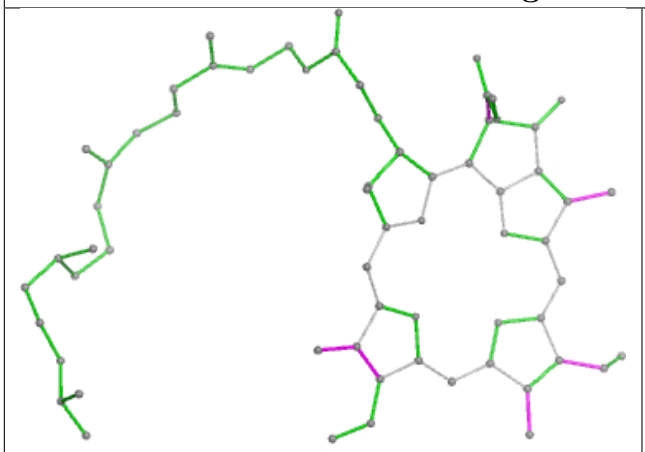


Torsions

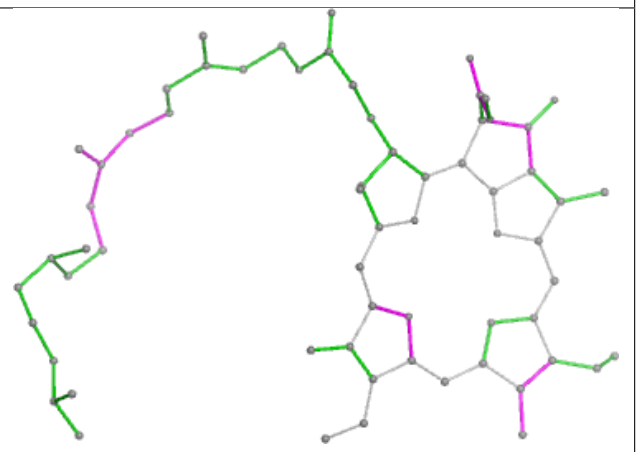


Rings

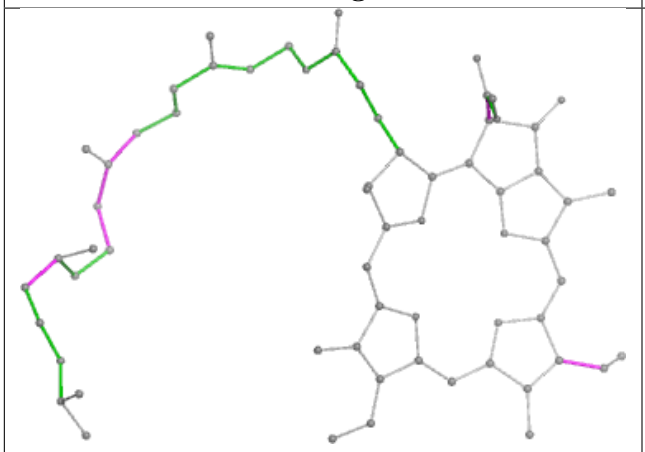
Ligand PHO D 407



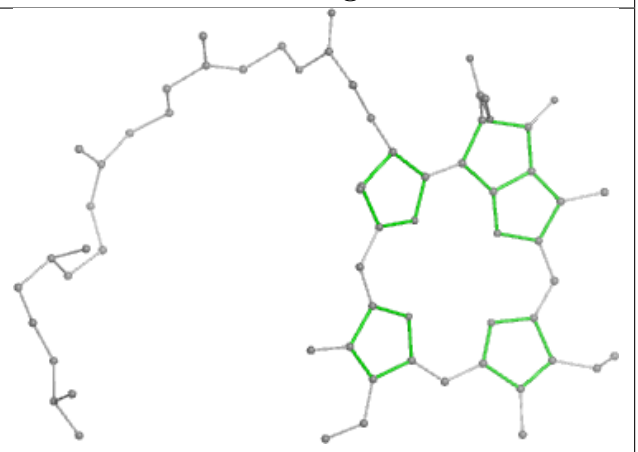
Bond lengths



Bond angles

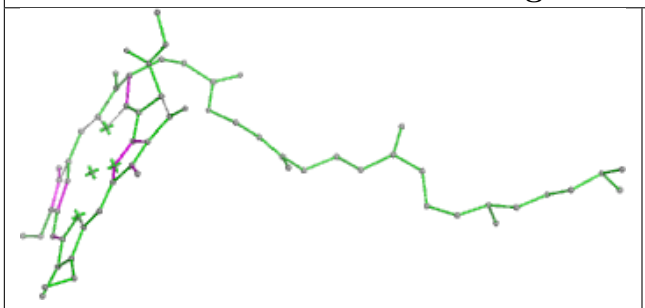


Torsions

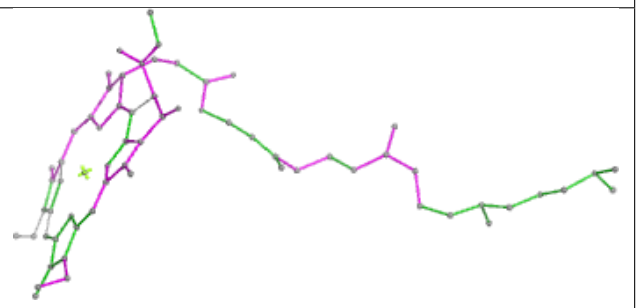


Rings

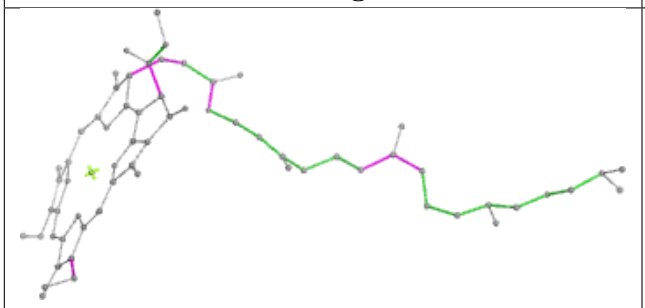
Ligand CLA B 604



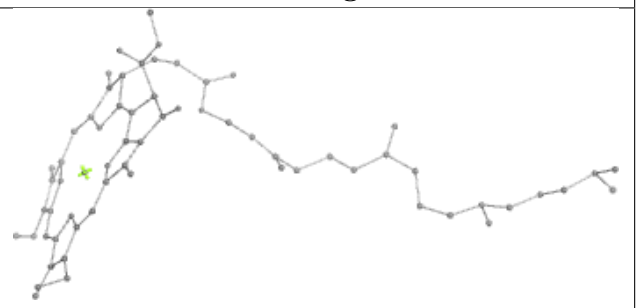
Bond lengths



Bond angles

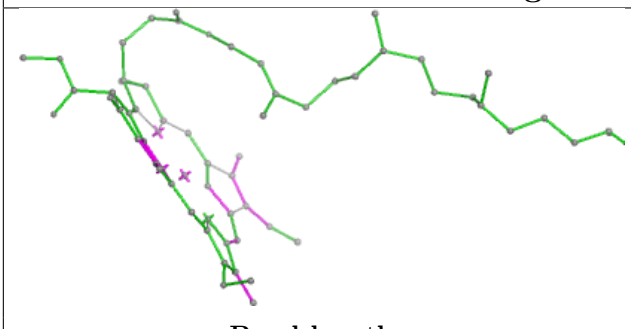


Torsions

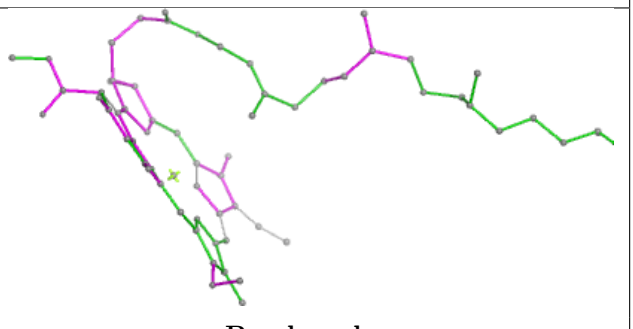


Rings

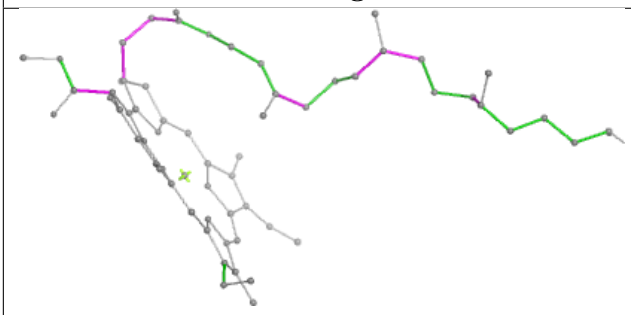
Ligand CLA B 607



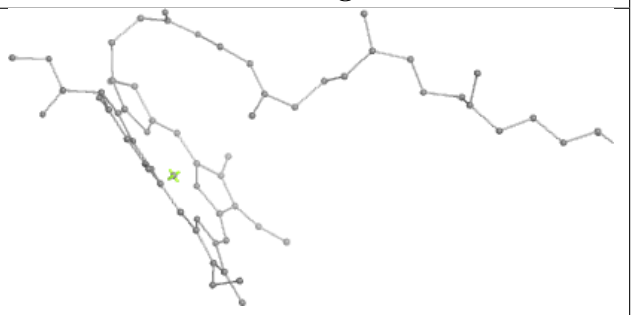
Bond lengths



Bond angles

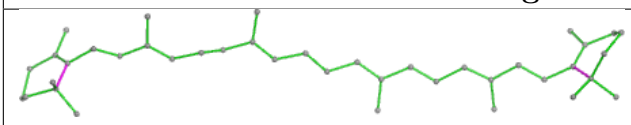


Torsions

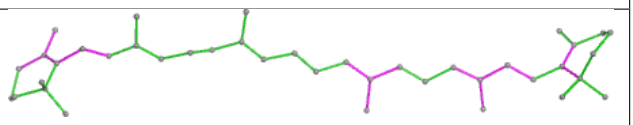


Rings

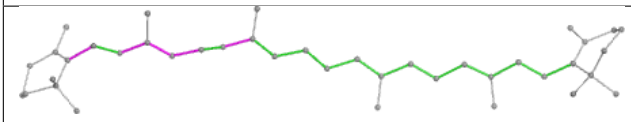
Ligand BCR A 408



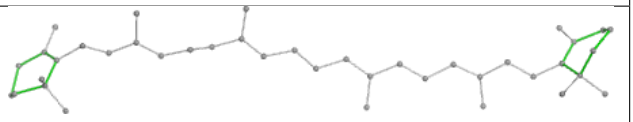
Bond lengths



Bond angles

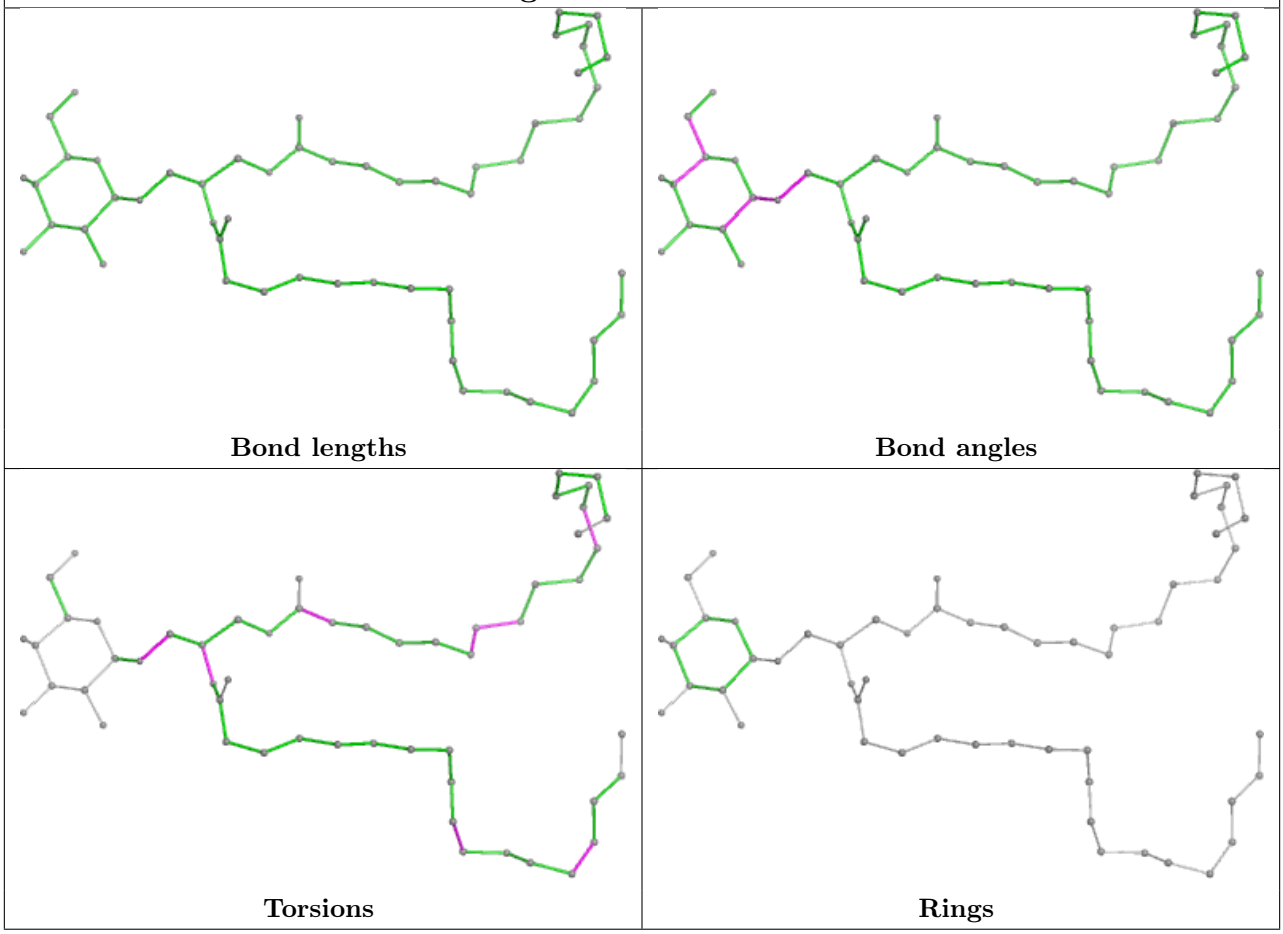


Torsions

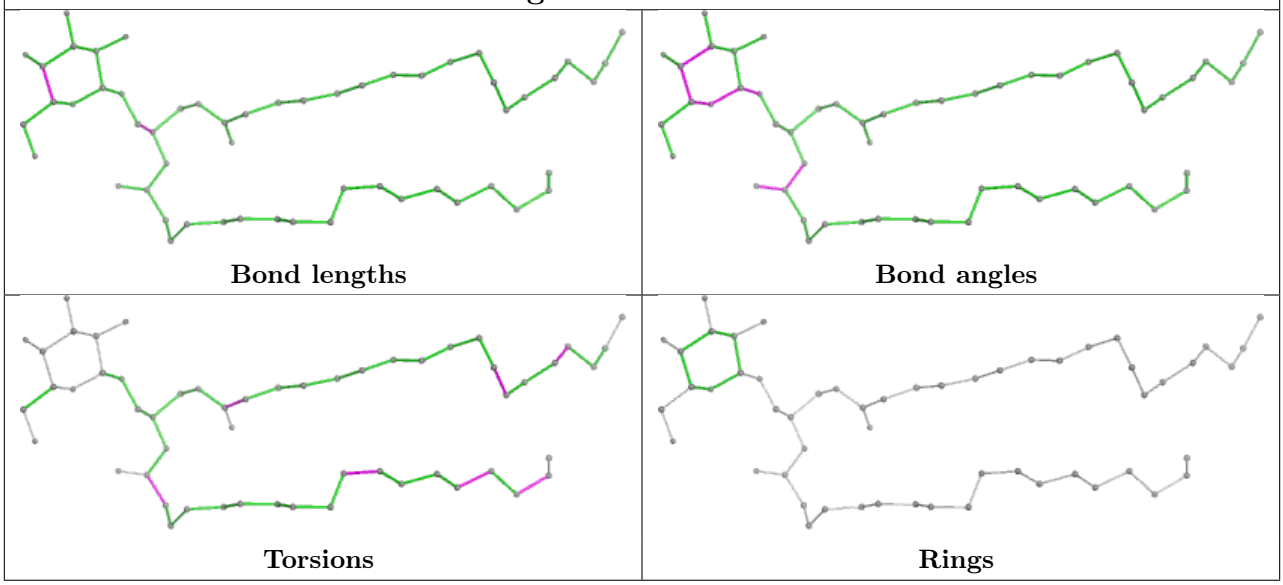


Rings

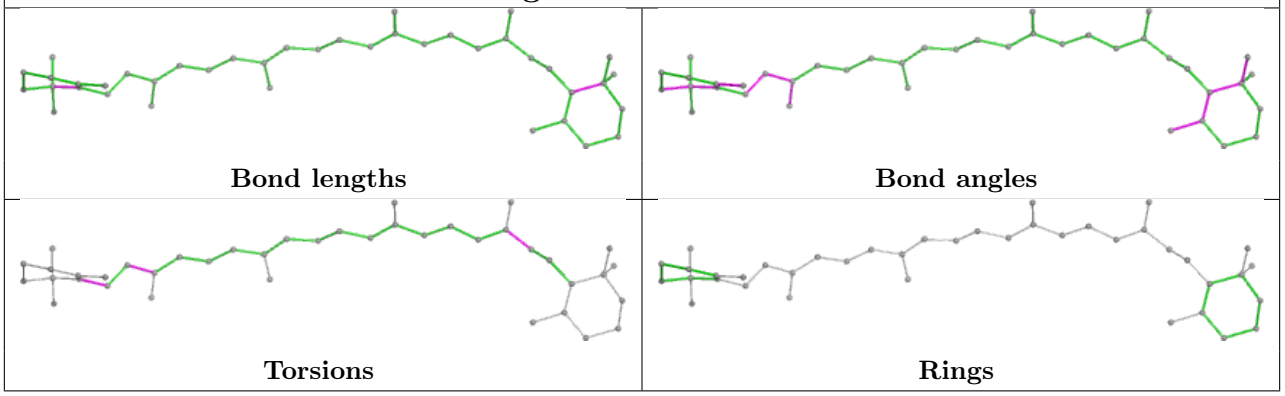
Ligand LMG D 404



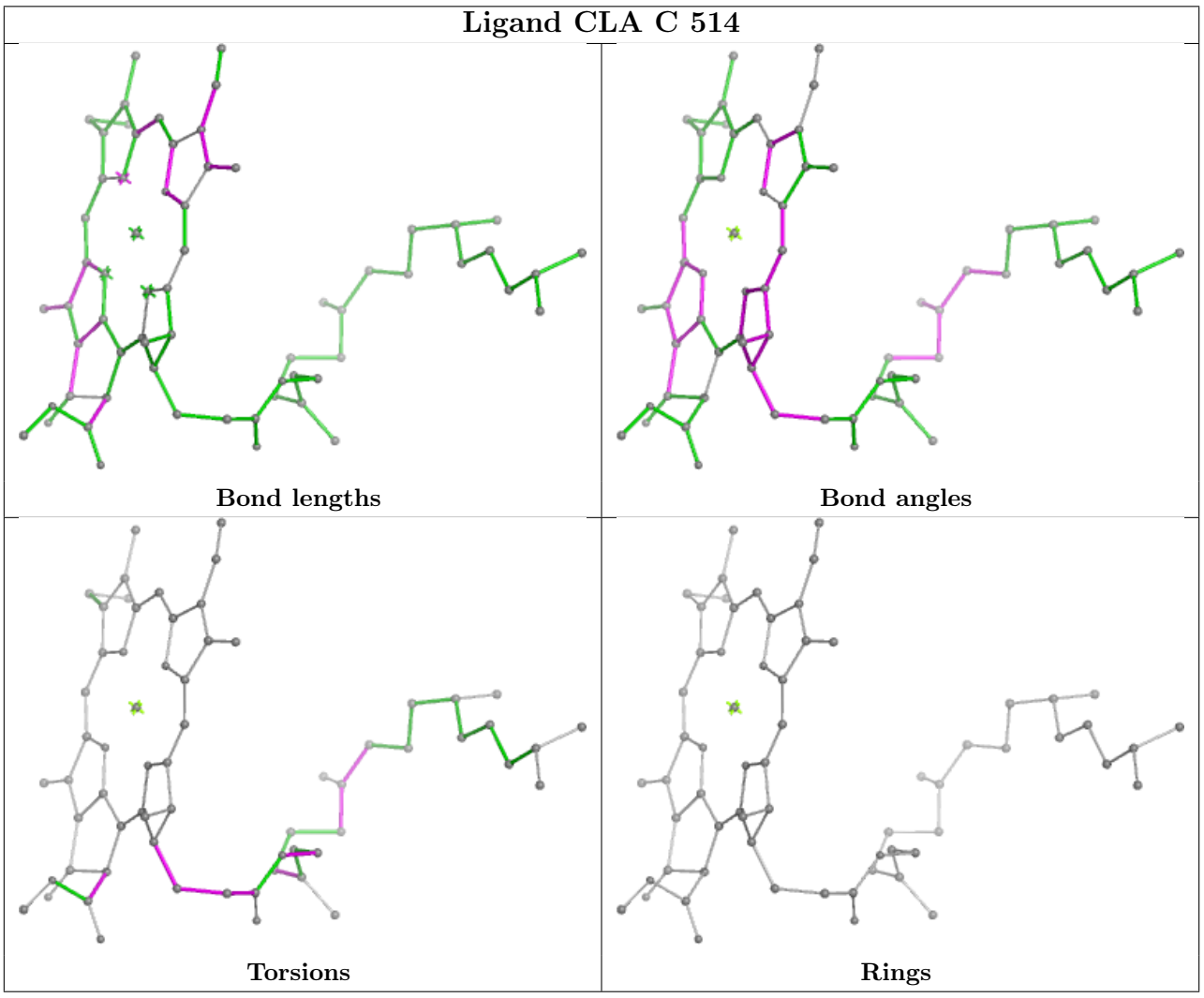
Ligand LMG I 101



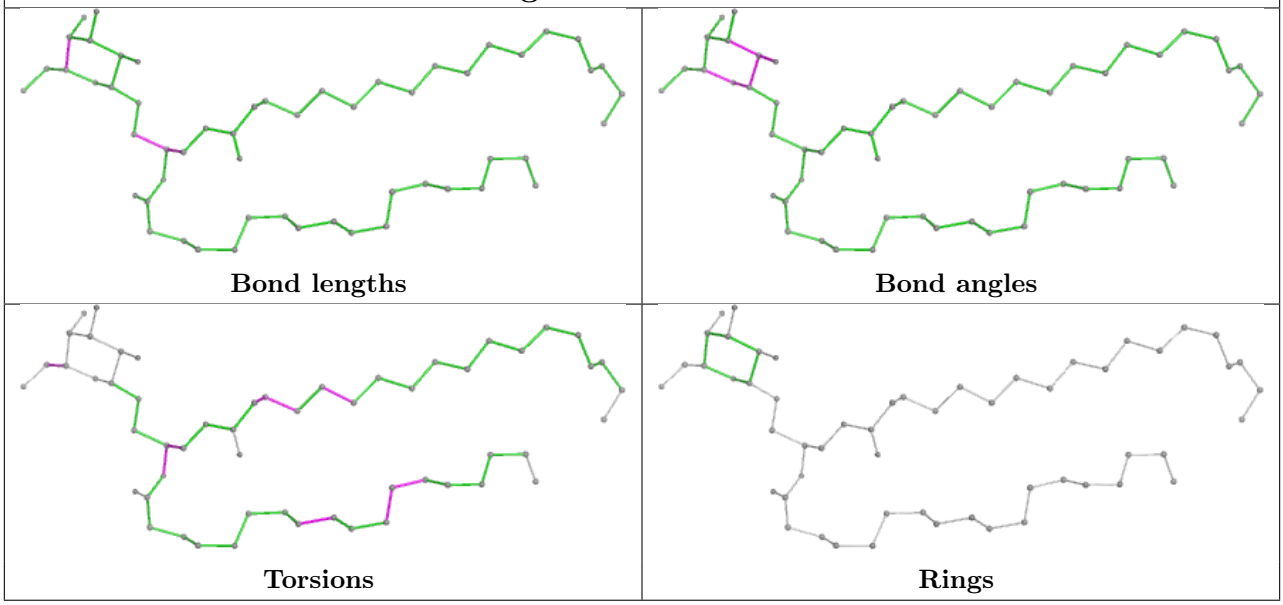
Ligand BCR D 410



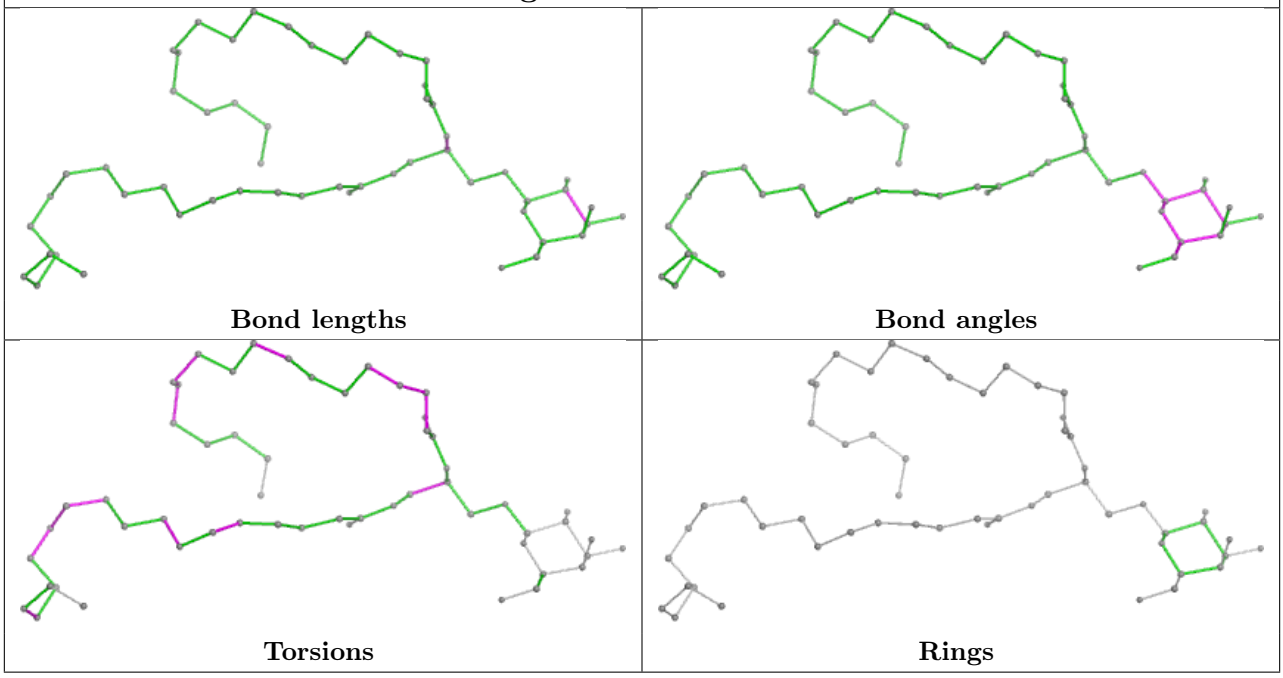
Ligand CLA C 514



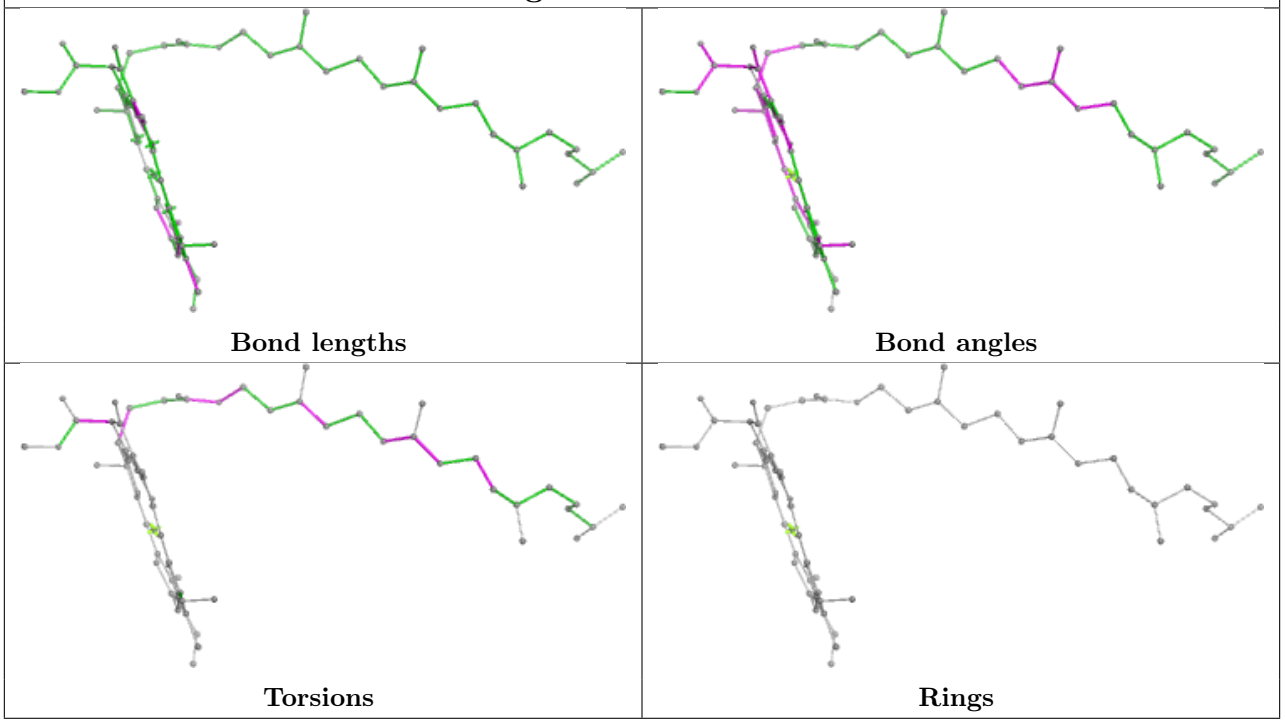
Ligand LMG C 501



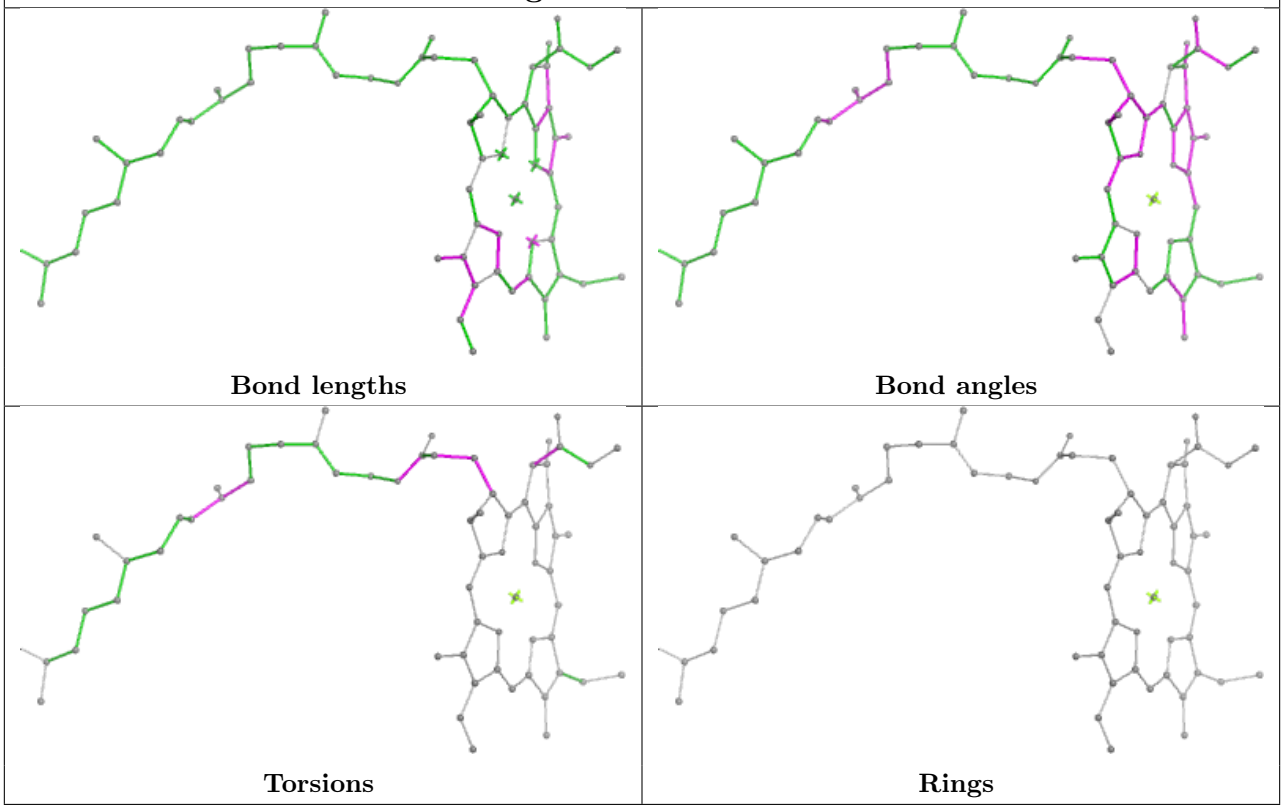
Ligand LMG D 403



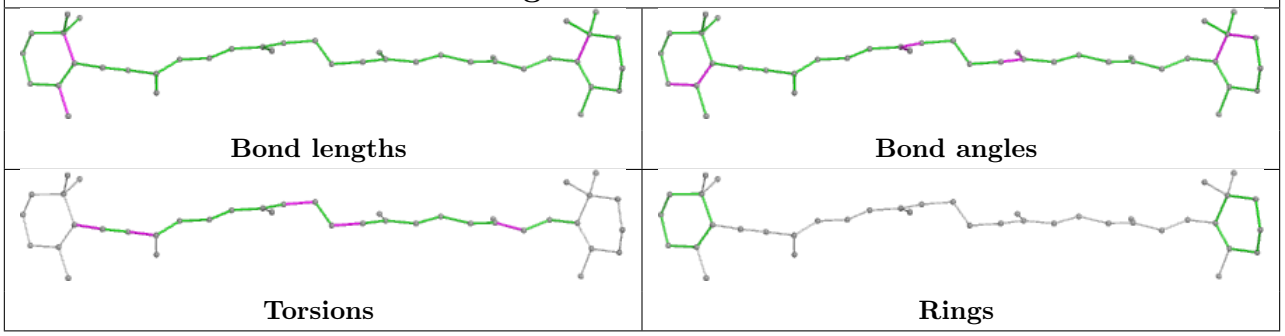
Ligand CLA B 605



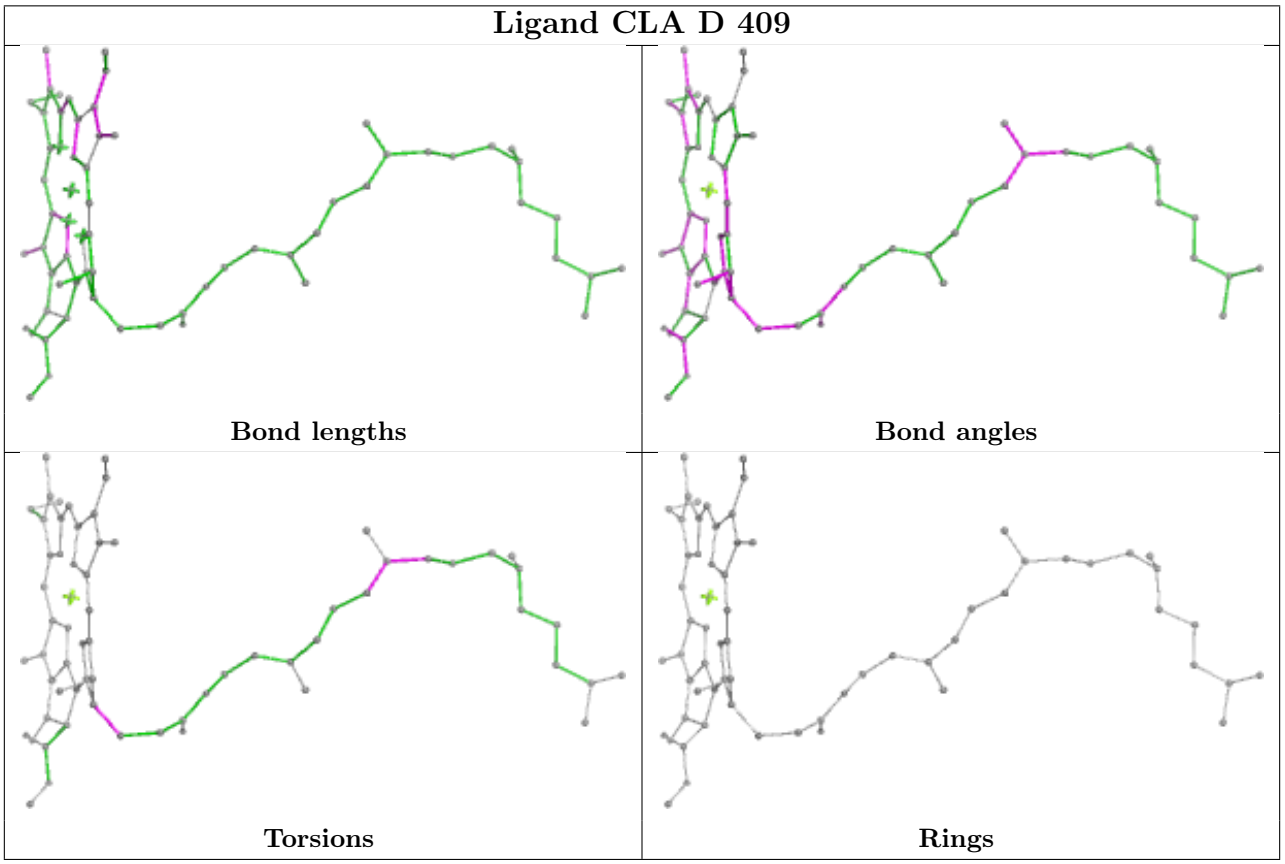
Ligand CLA B 609



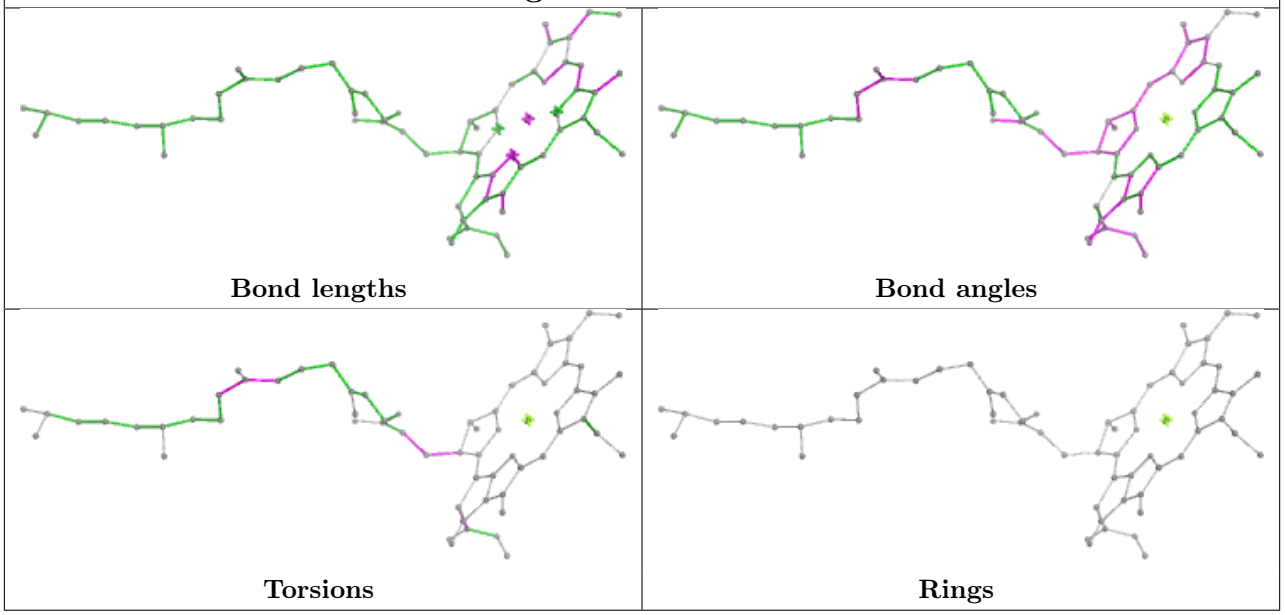
Ligand BCR C 516



Ligand CLA D 409

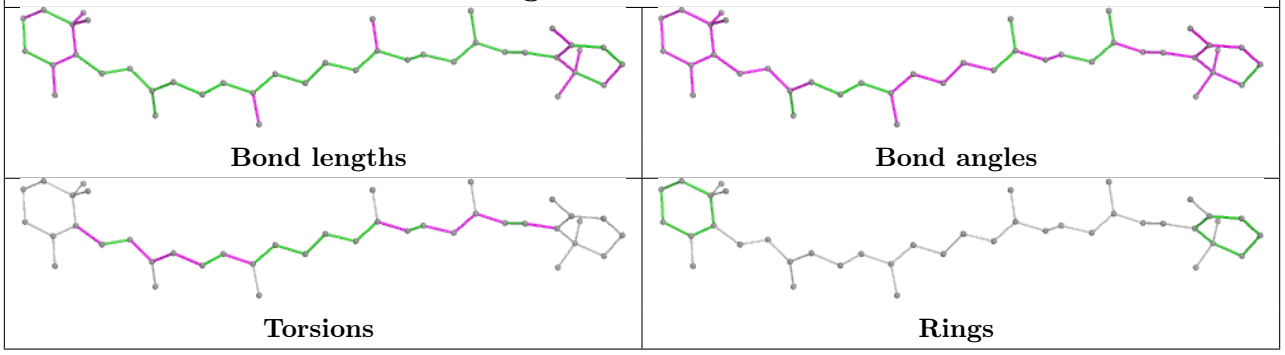


Ligand CLA C 504

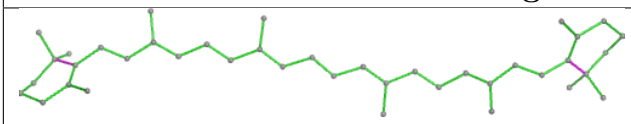


Ligand BCR H 101

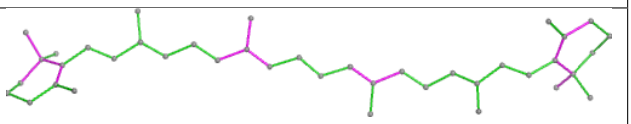
Ligand BCR K 101



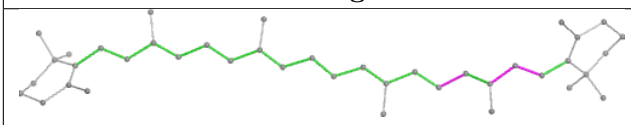
Ligand BCR B 618



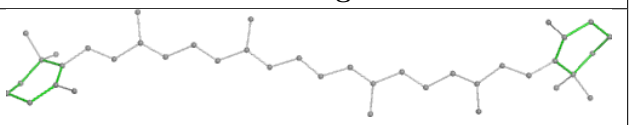
Bond lengths



Bond angles

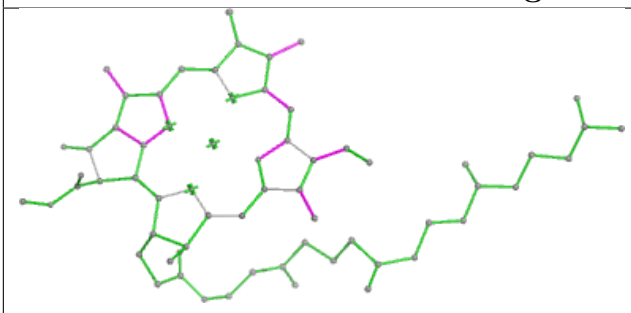


Torsions

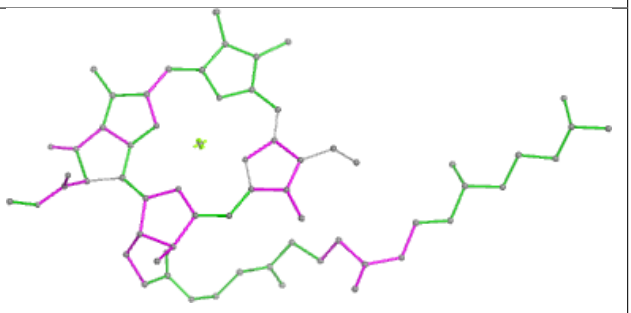


Rings

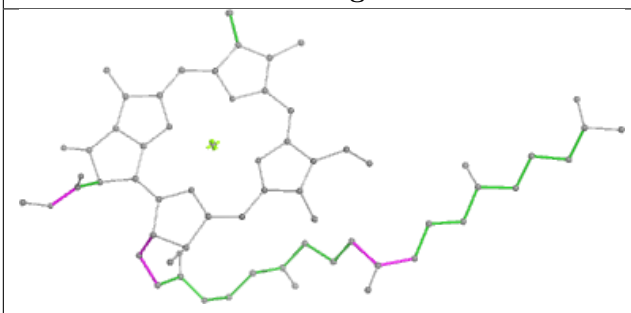
Ligand CLA C 503



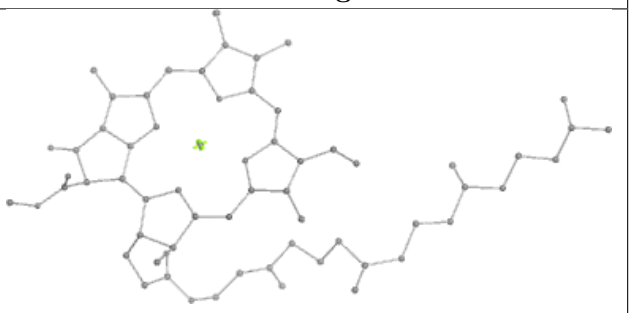
Bond lengths



Bond angles

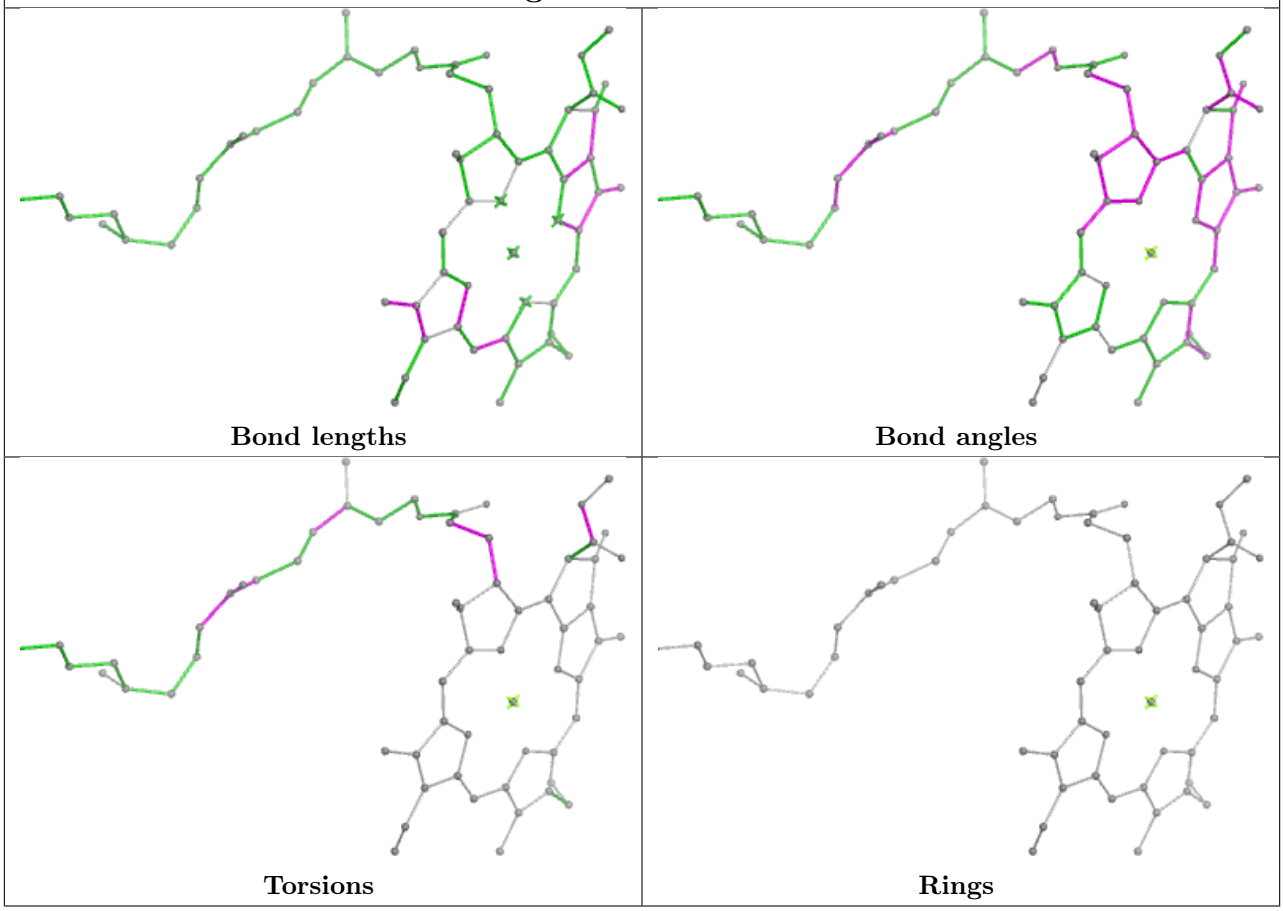


Torsions

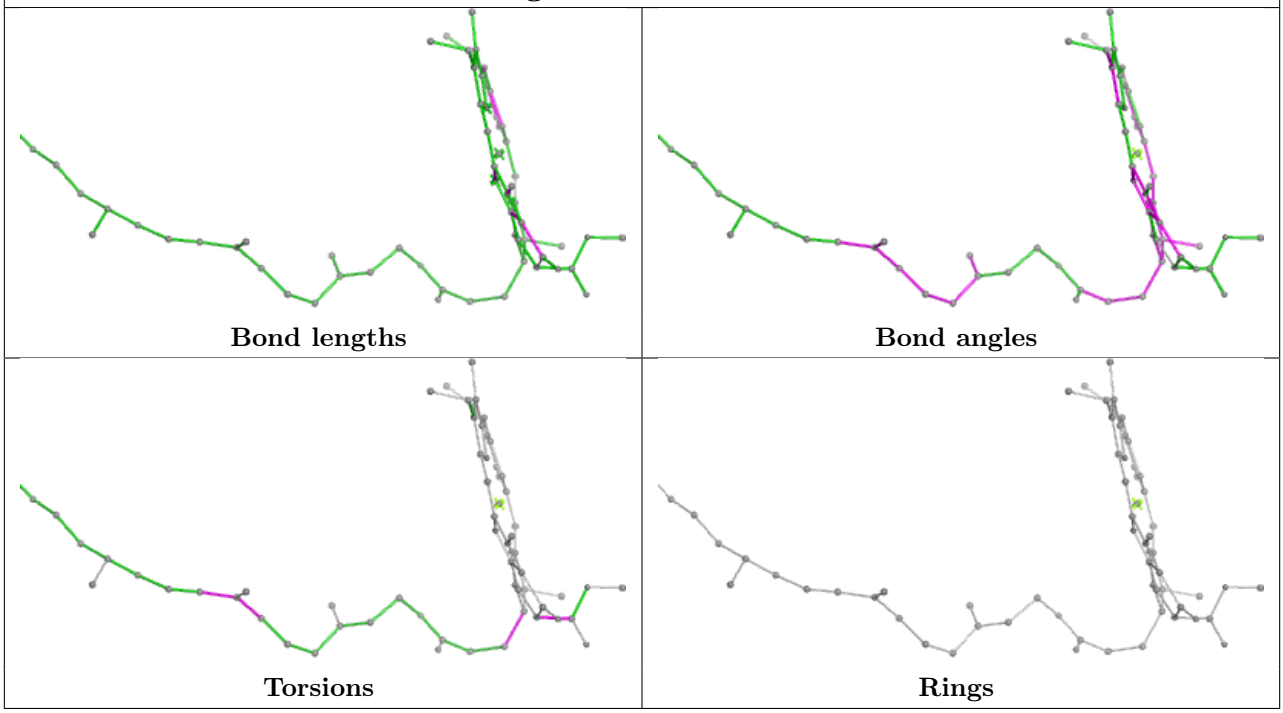


Rings

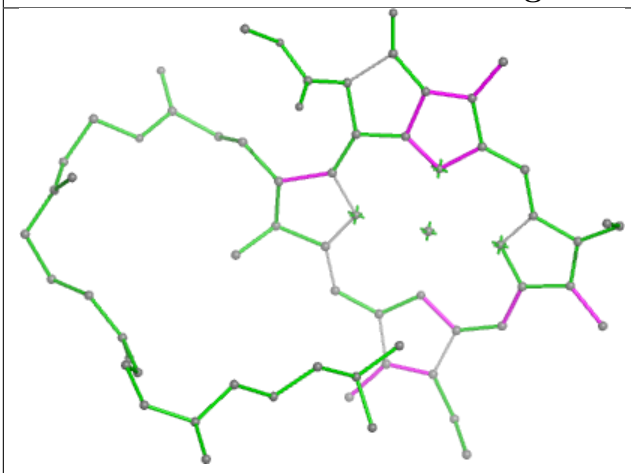
Ligand CLA C 512



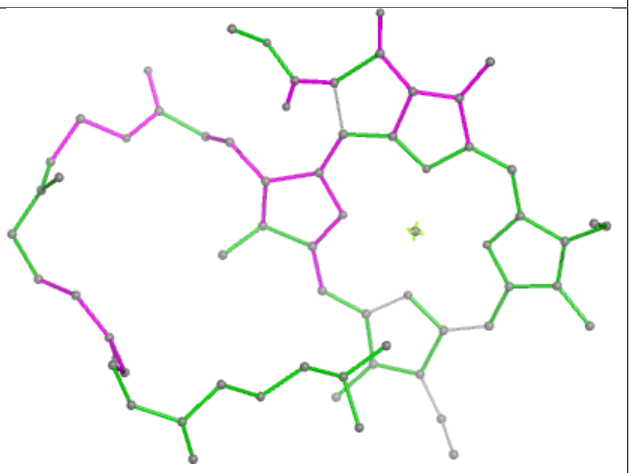
Ligand CLA C 508



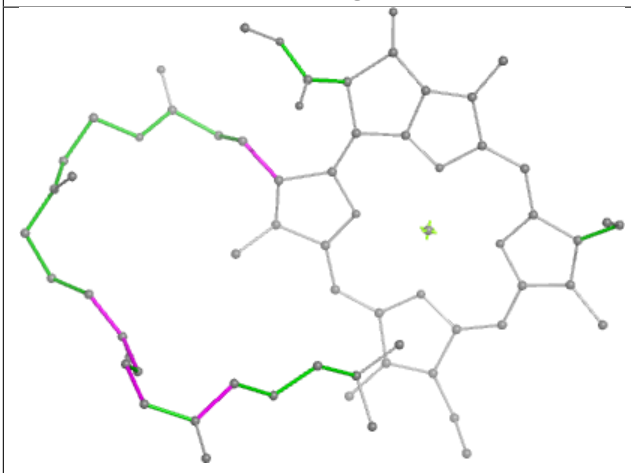
Ligand CLA B 615



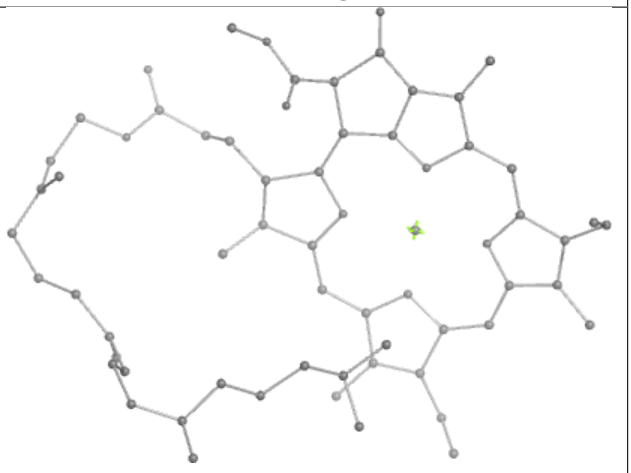
Bond lengths



Bond angles

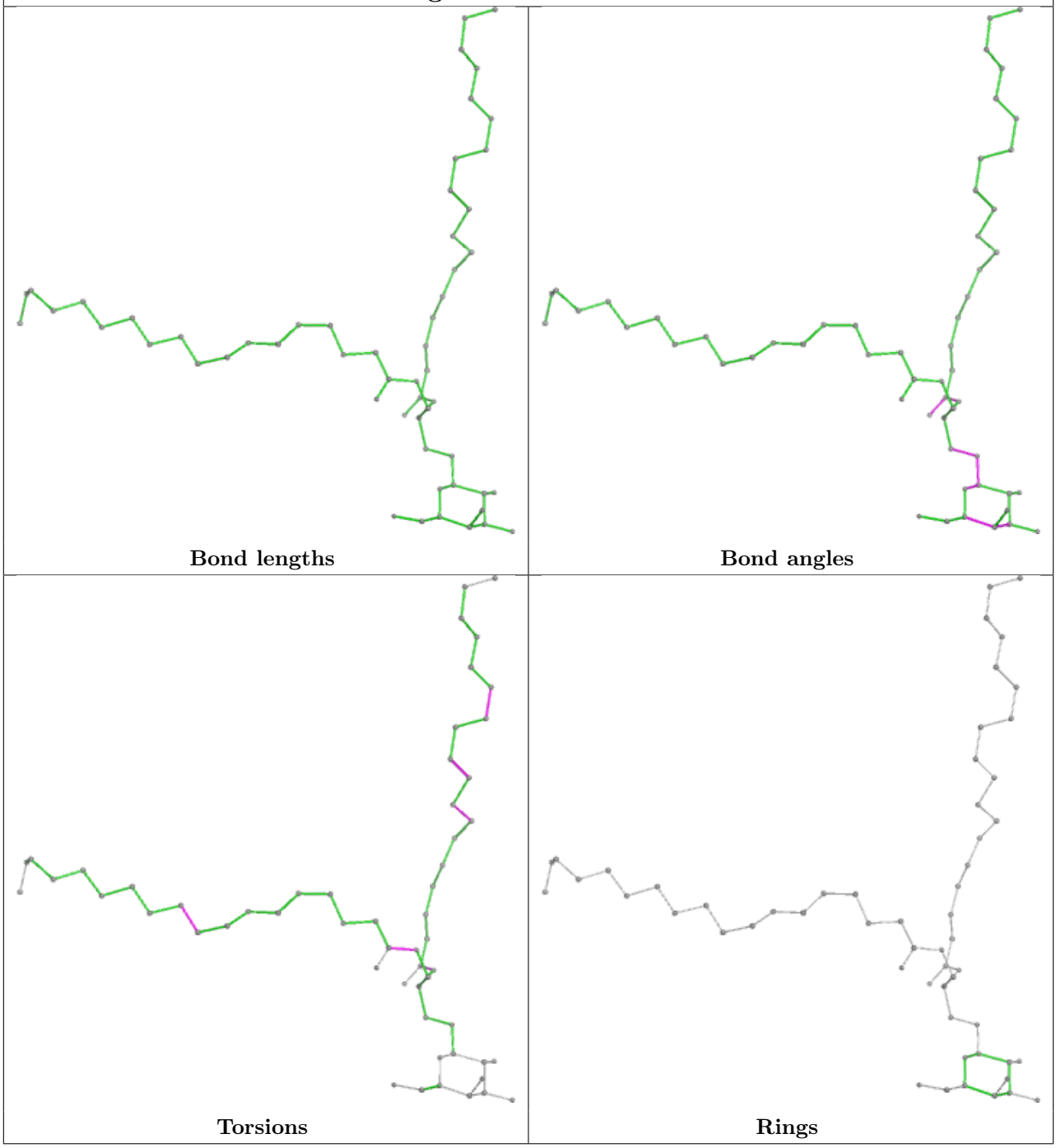


Torsions

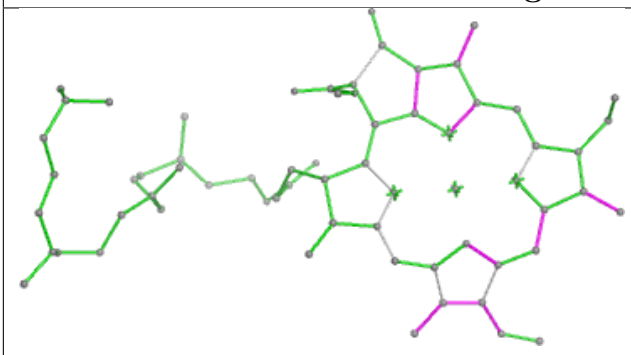


Rings

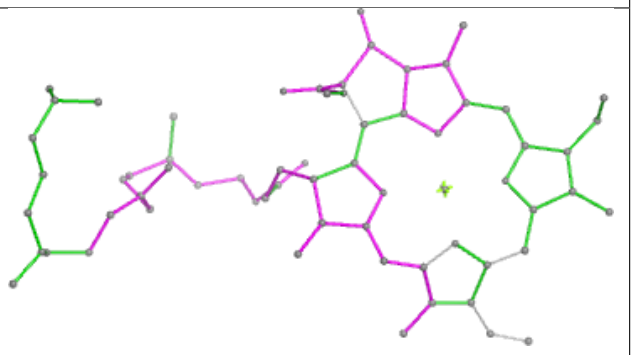
Ligand LMG D 402



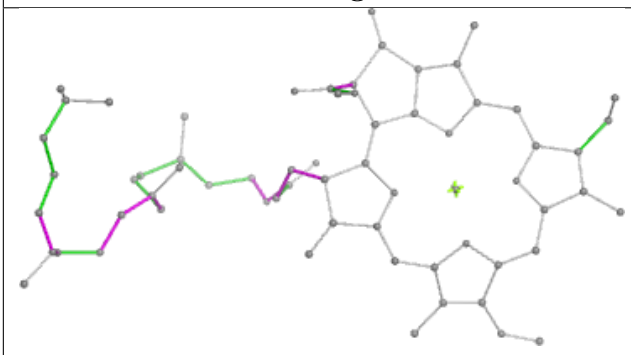
Ligand CLA B 612



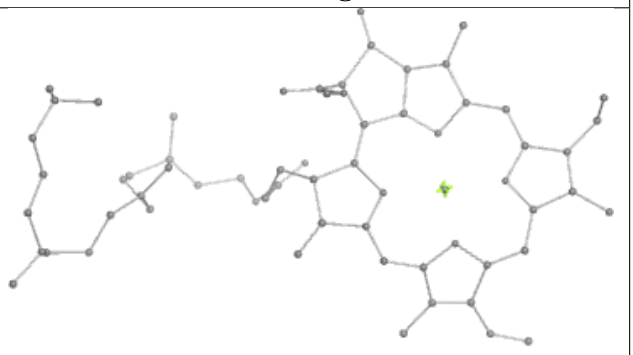
Bond lengths



Bond angles

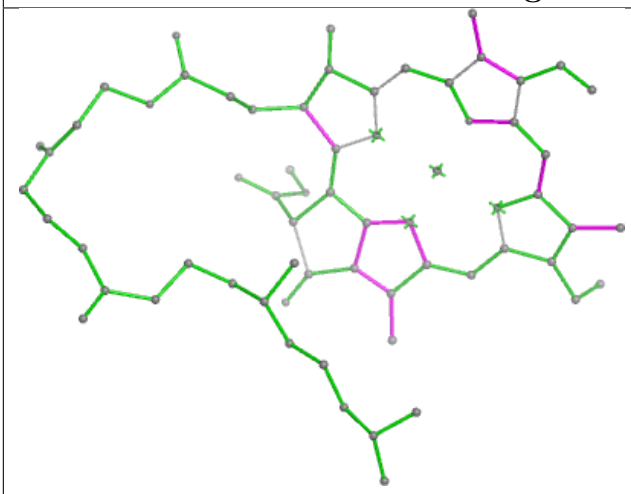


Torsions

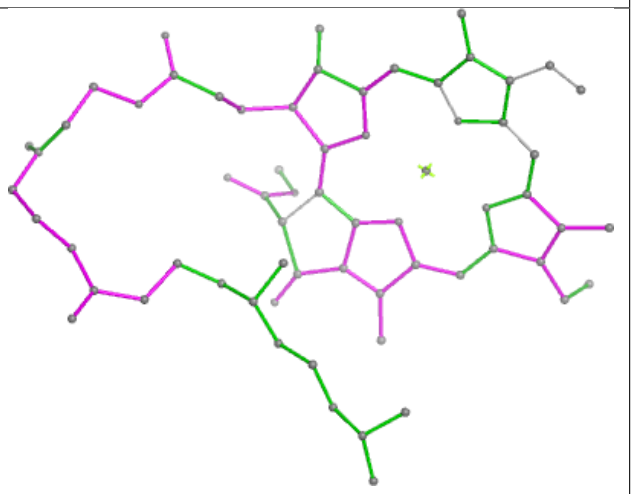


Rings

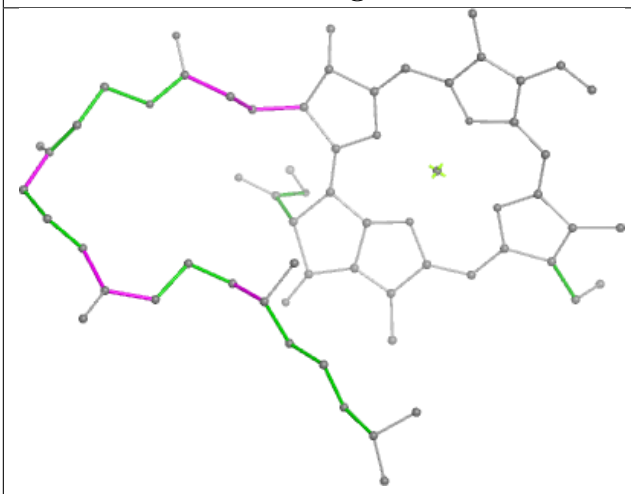
Ligand CLA C 511



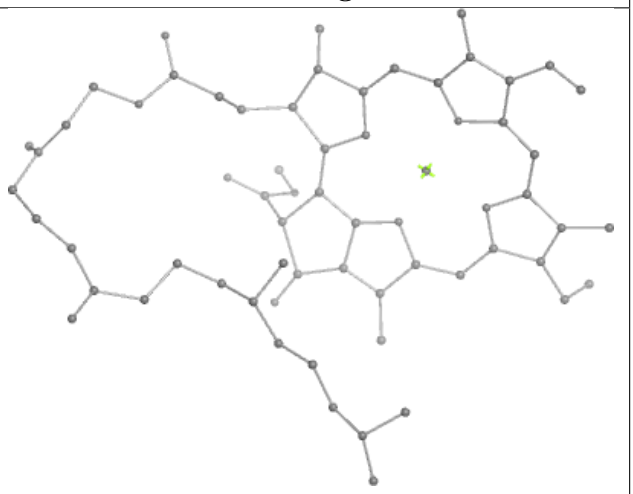
Bond lengths



Bond angles

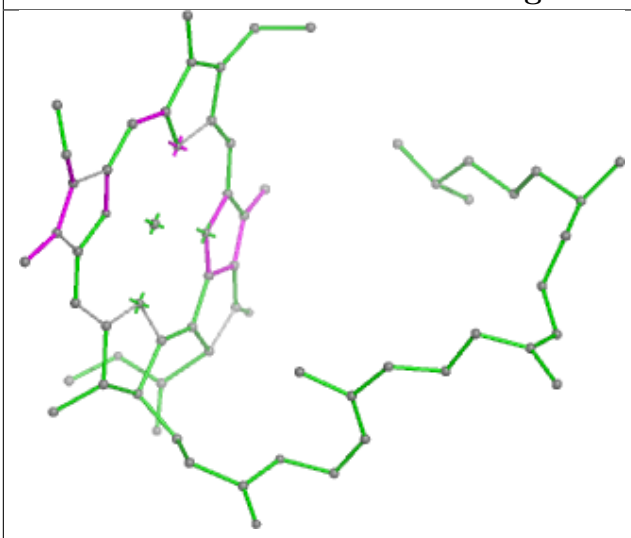


Torsions

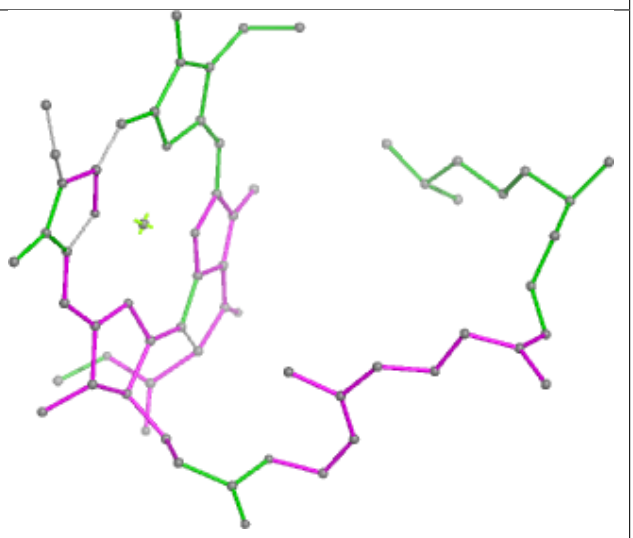


Rings

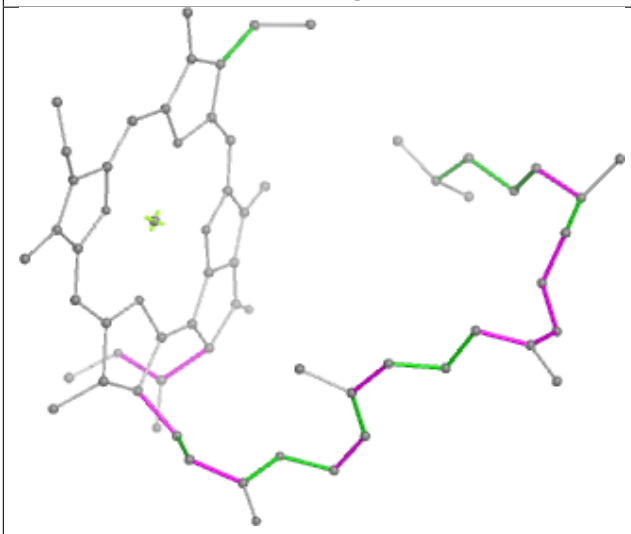
Ligand CLA C 505



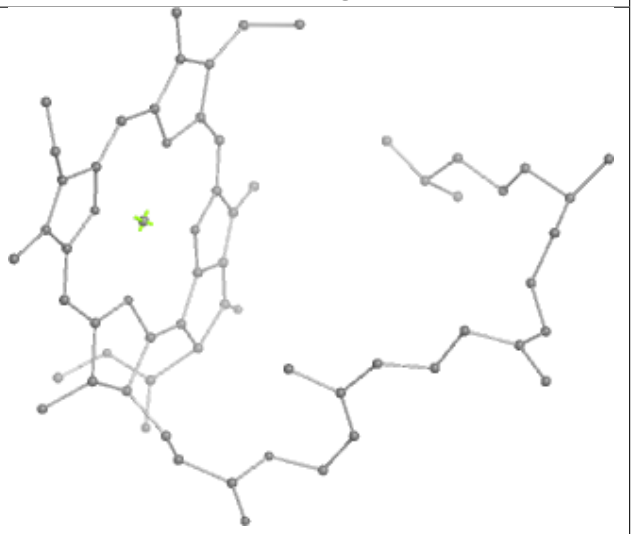
Bond lengths



Bond angles

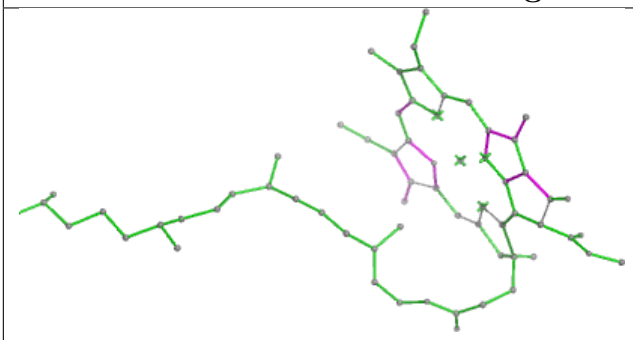


Torsions

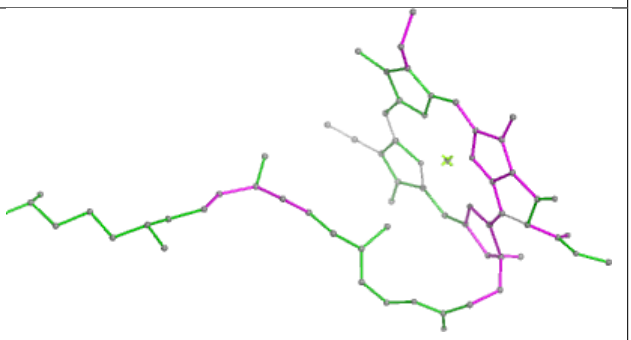


Rings

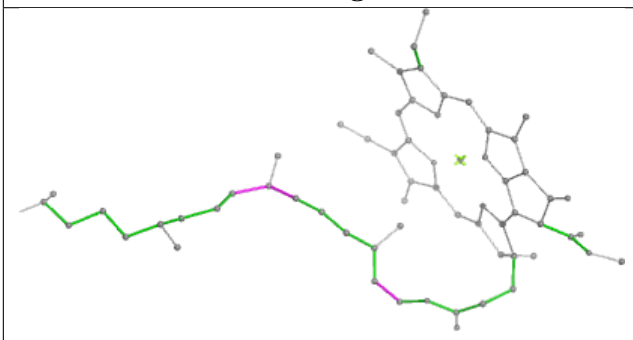
Ligand CLA C 507



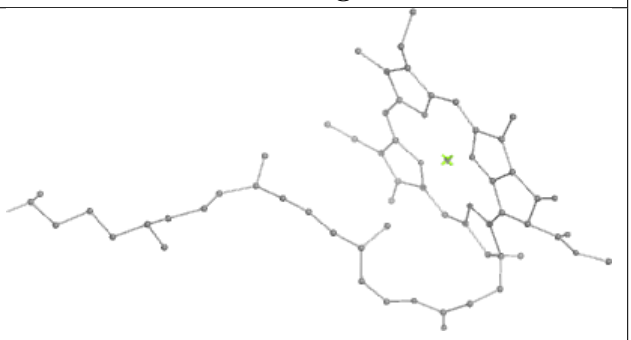
Bond lengths



Bond angles

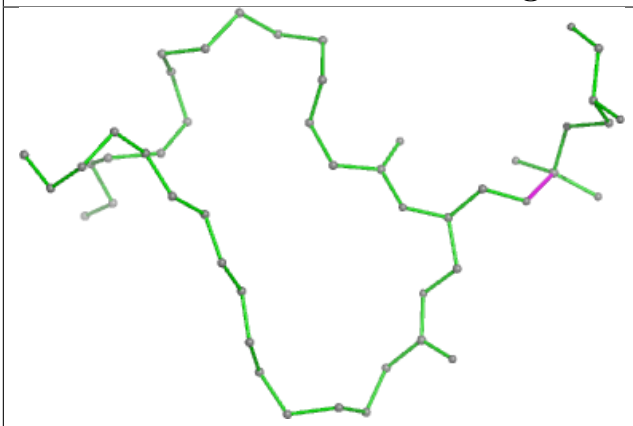


Torsions

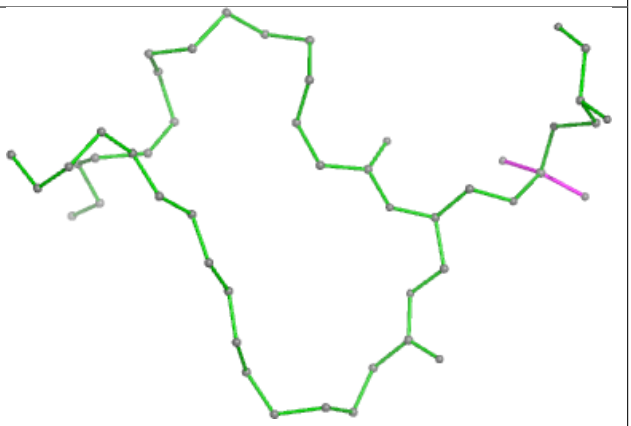


Rings

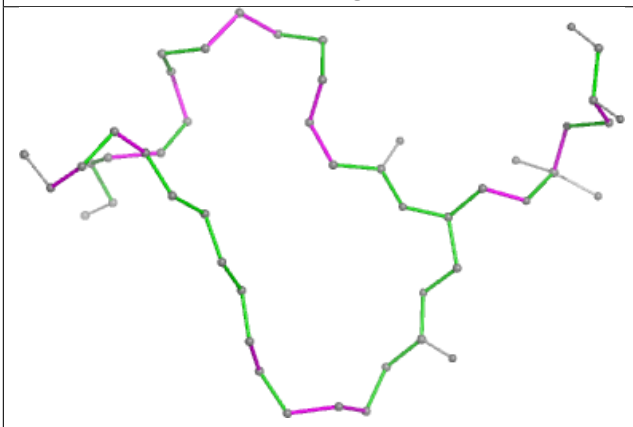
Ligand LHG A 409



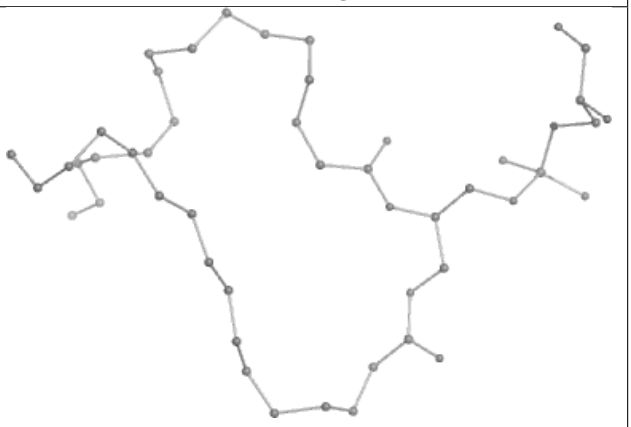
Bond lengths



Bond angles

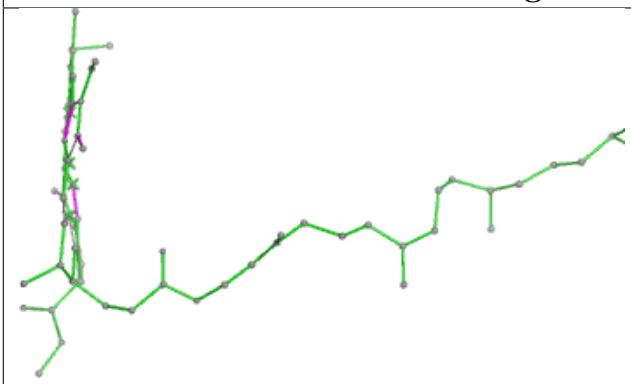


Torsions

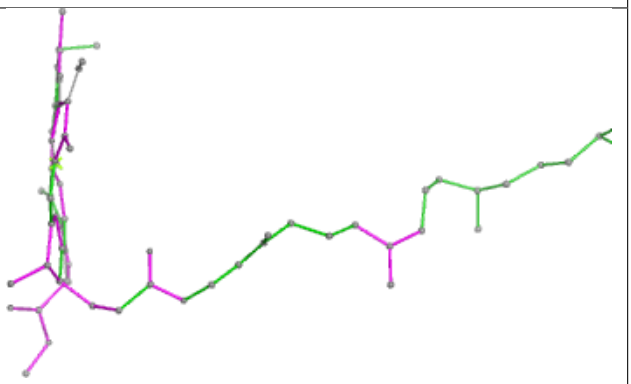


Rings

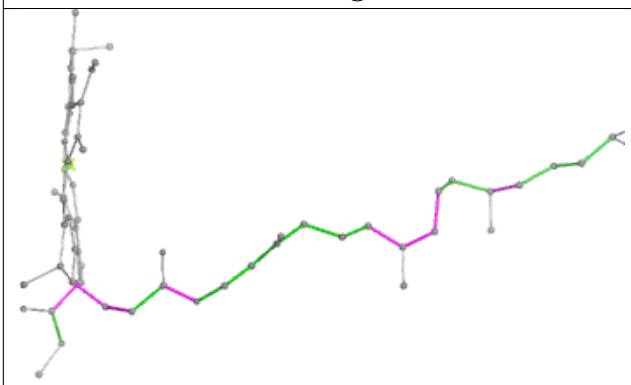
Ligand CLA B 606



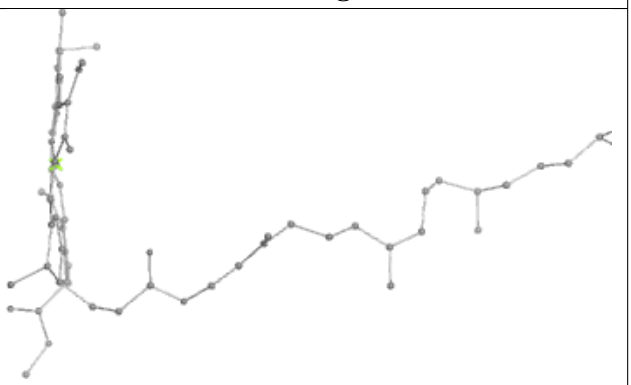
Bond lengths



Bond angles

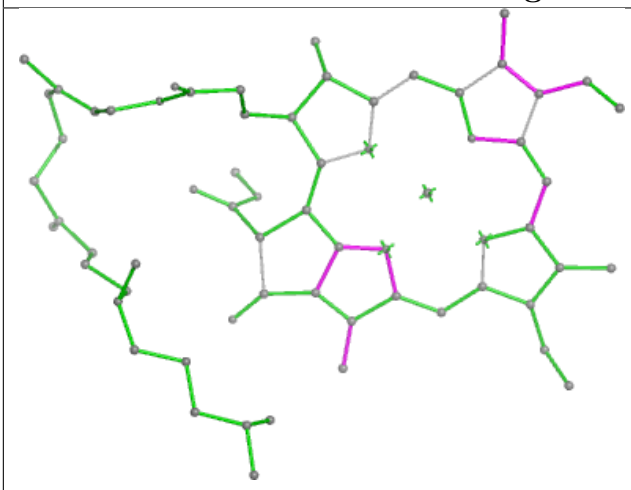


Torsions

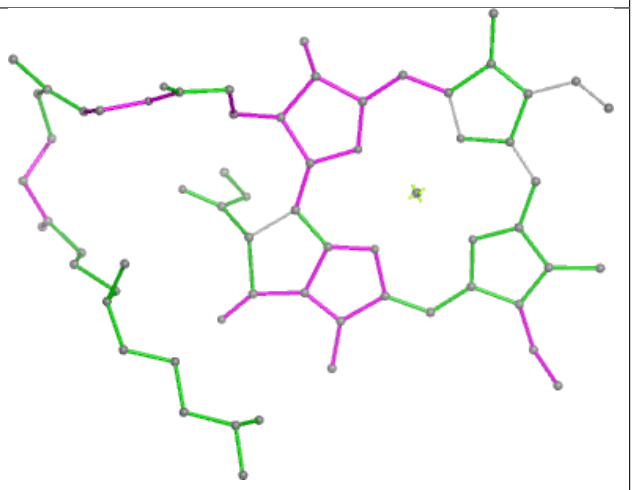


Rings

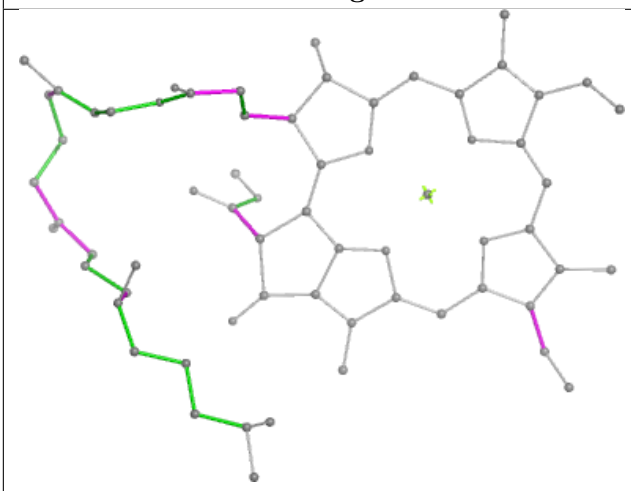
Ligand CLA B 610



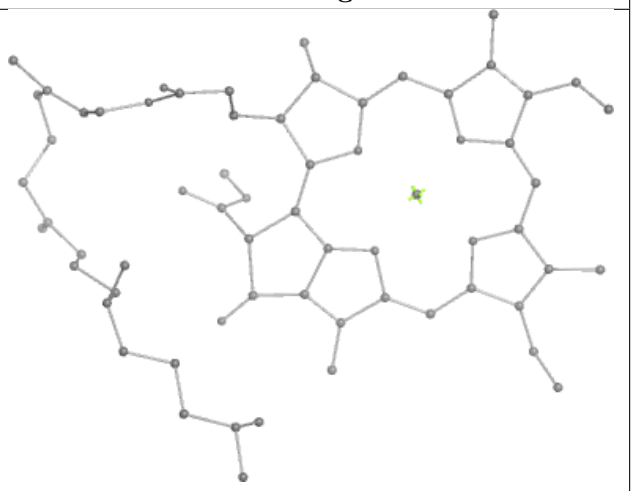
Bond lengths



Bond angles

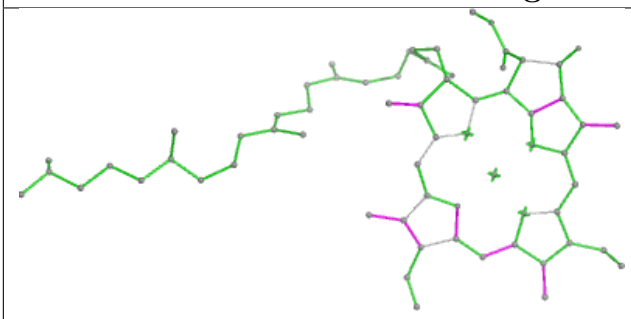


Torsions

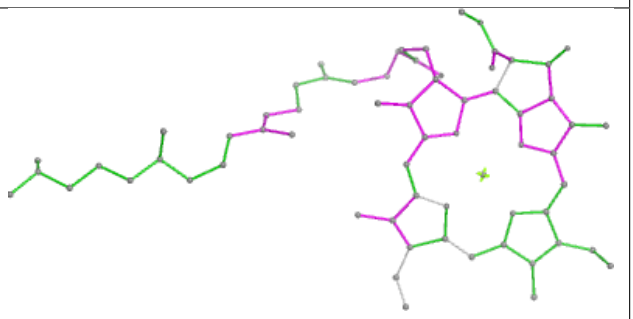


Rings

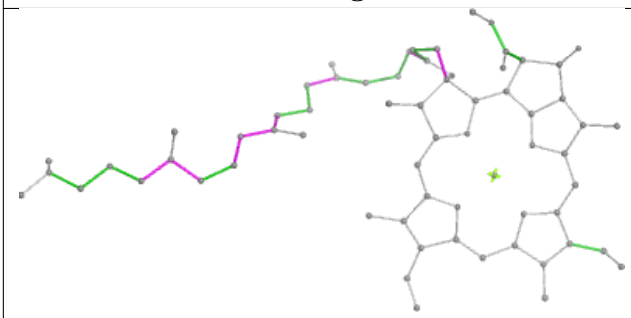
Ligand CLA A 405



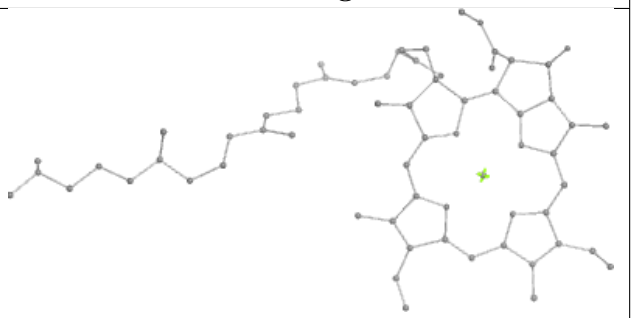
Bond lengths



Bond angles

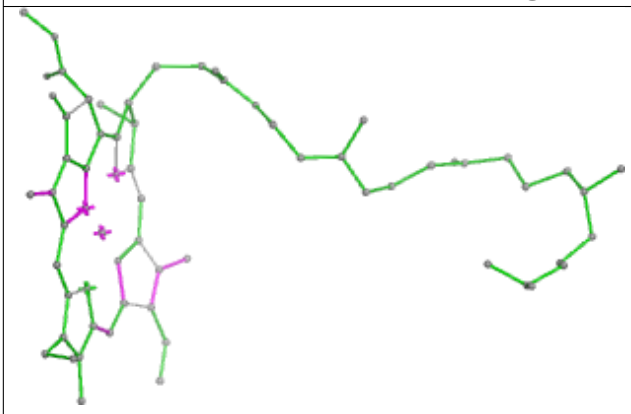


Torsions

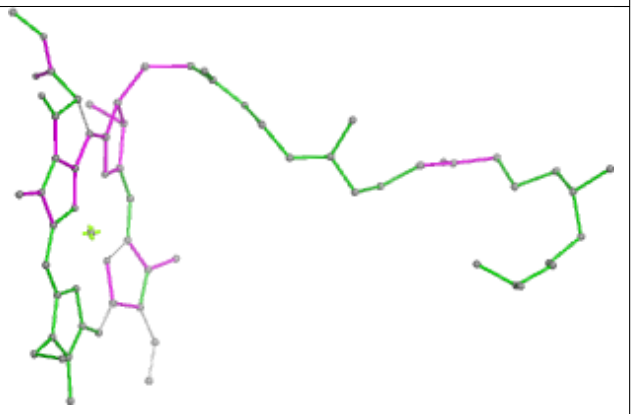


Rings

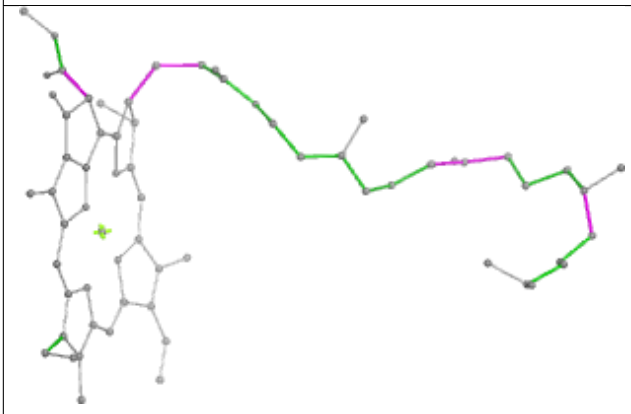
Ligand CLA A 407



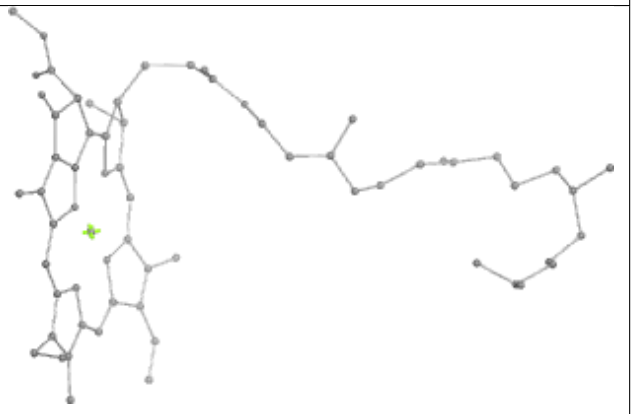
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

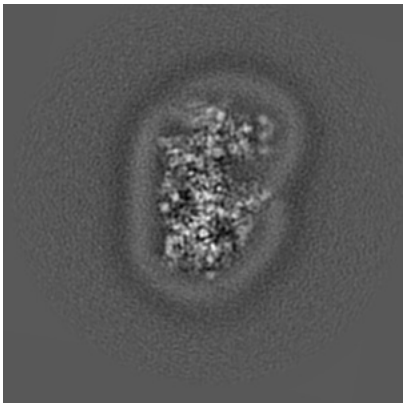
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12336. These allow visual inspection of the internal detail of the map and identification of artifacts.

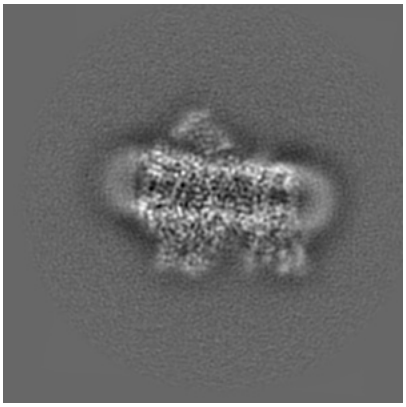
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

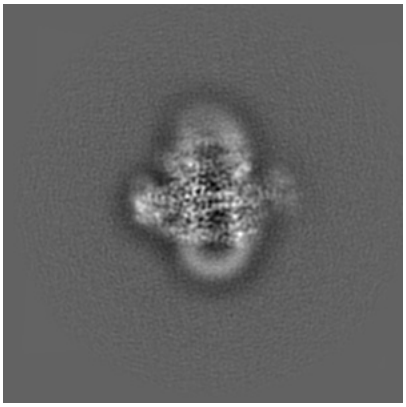
6.1.1 Primary map



X



Y

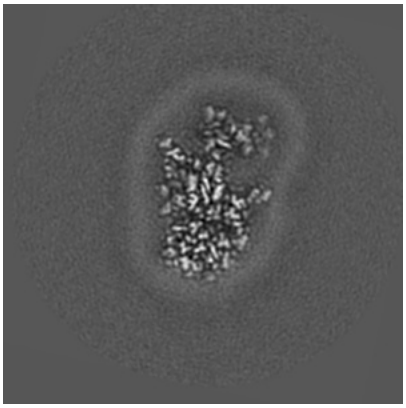


Z

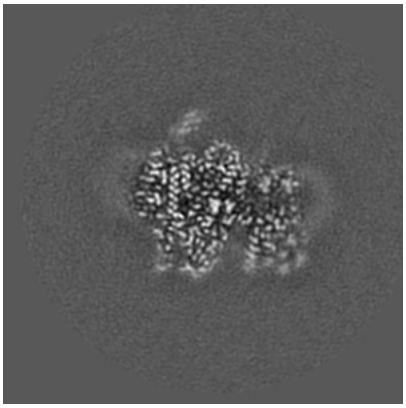
The images above show the map projected in three orthogonal directions.

6.2 Central slices

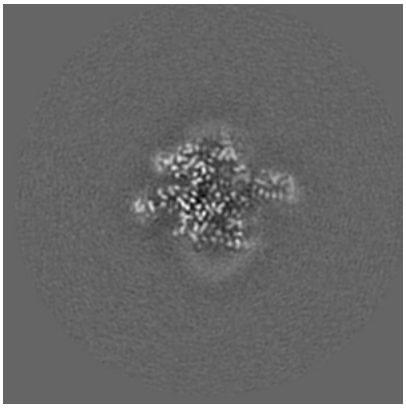
6.2.1 Primary map



X Index: 130



Y Index: 130

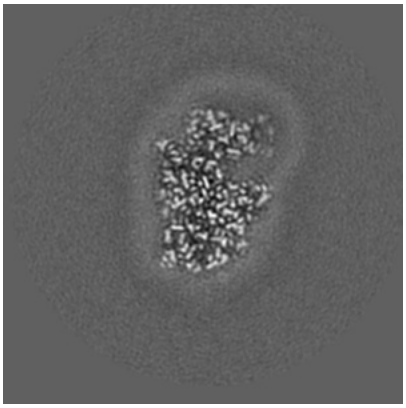


Z Index: 130

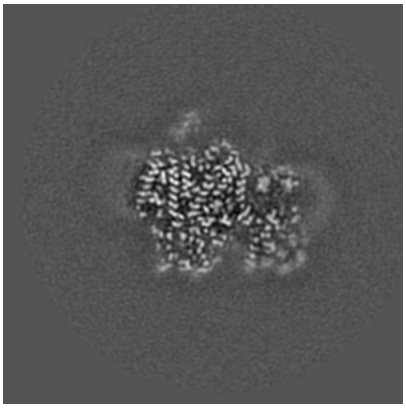
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

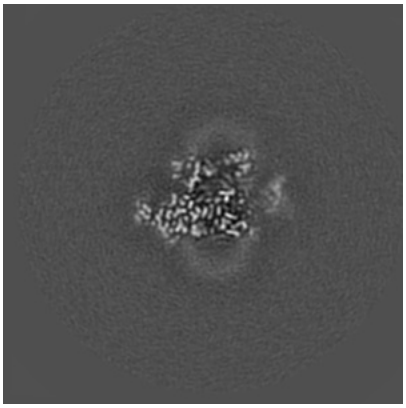
6.3.1 Primary map



X Index: 125



Y Index: 129

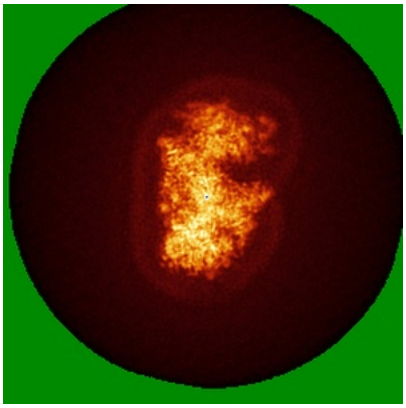


Z Index: 115

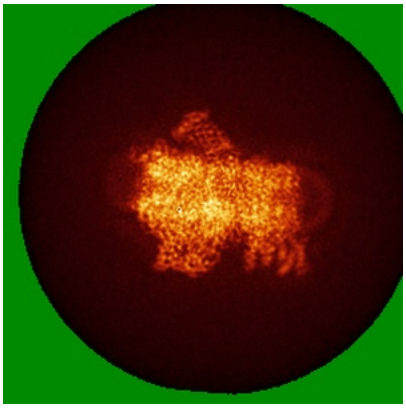
The images above show the largest variance slices of the map in three orthogonal directions.

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

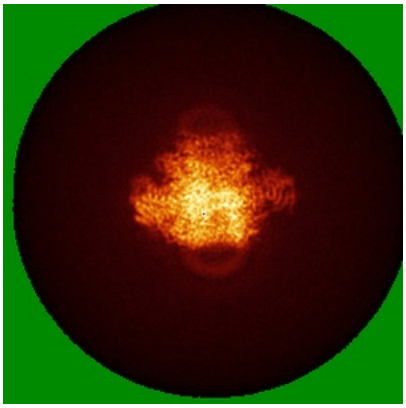
6.4.1 Primary map



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 0.007. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

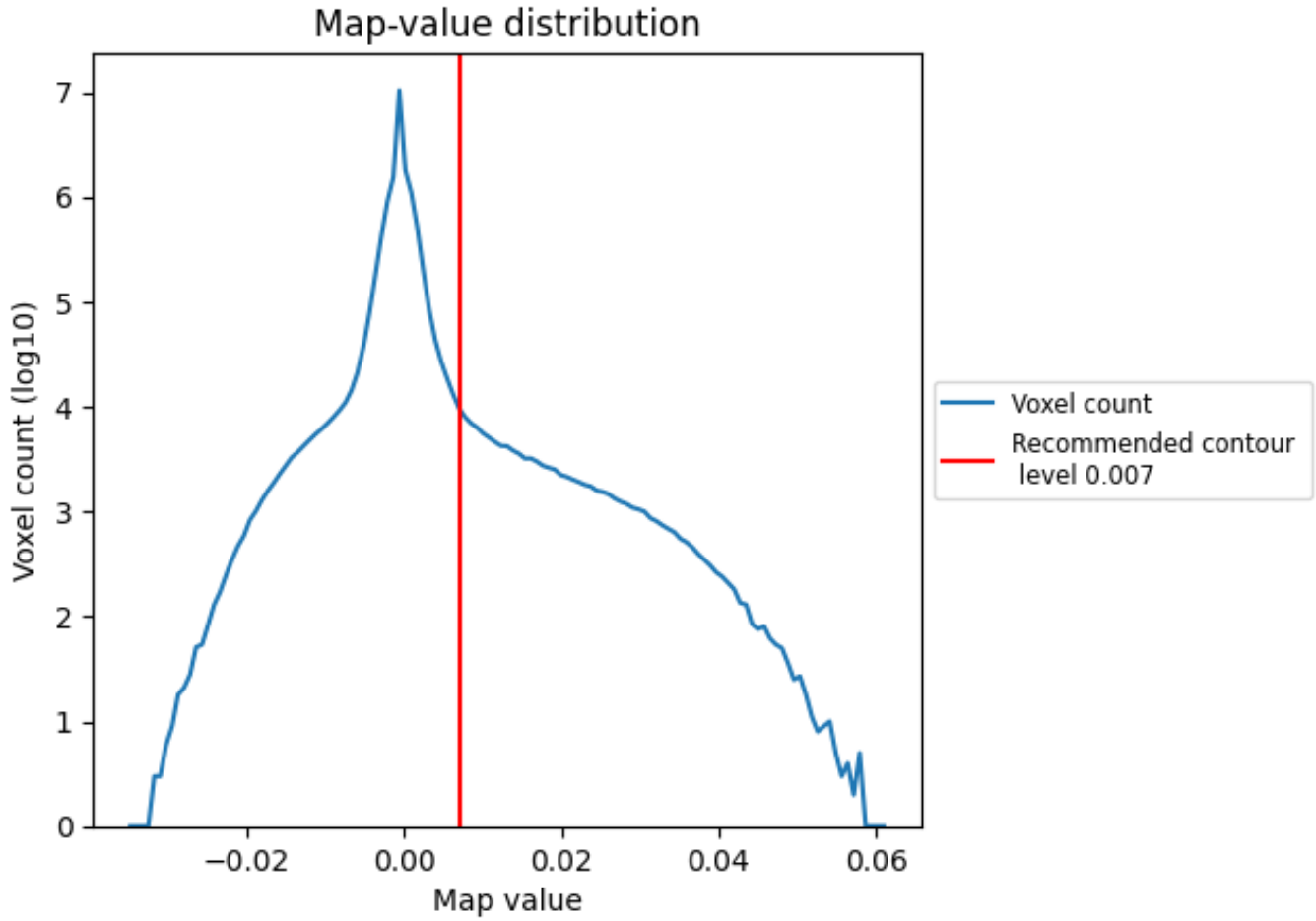
6.6 Mask visualisation (i)

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

7 Map analysis

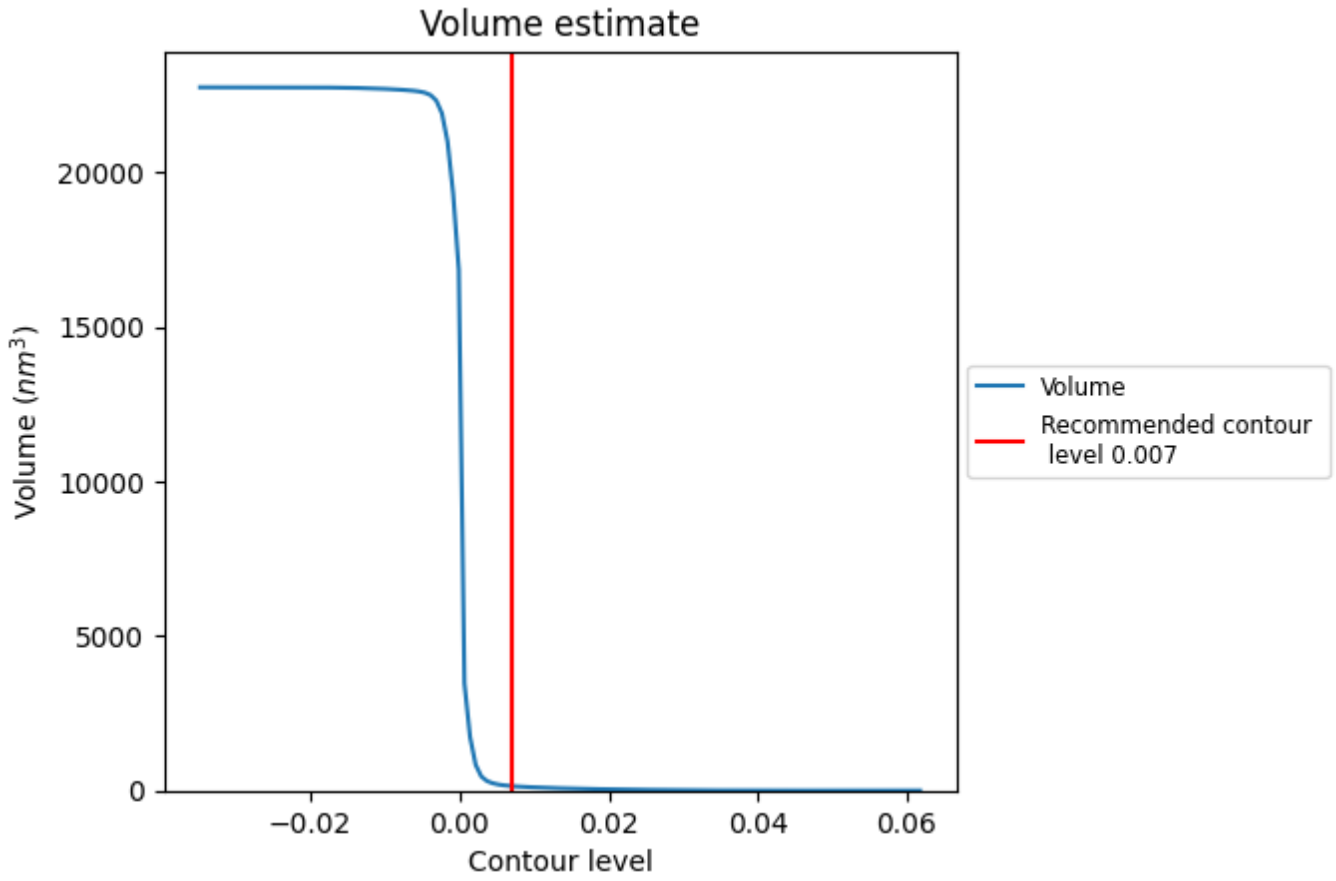
This section contains the results of statistical analysis of the map.

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.

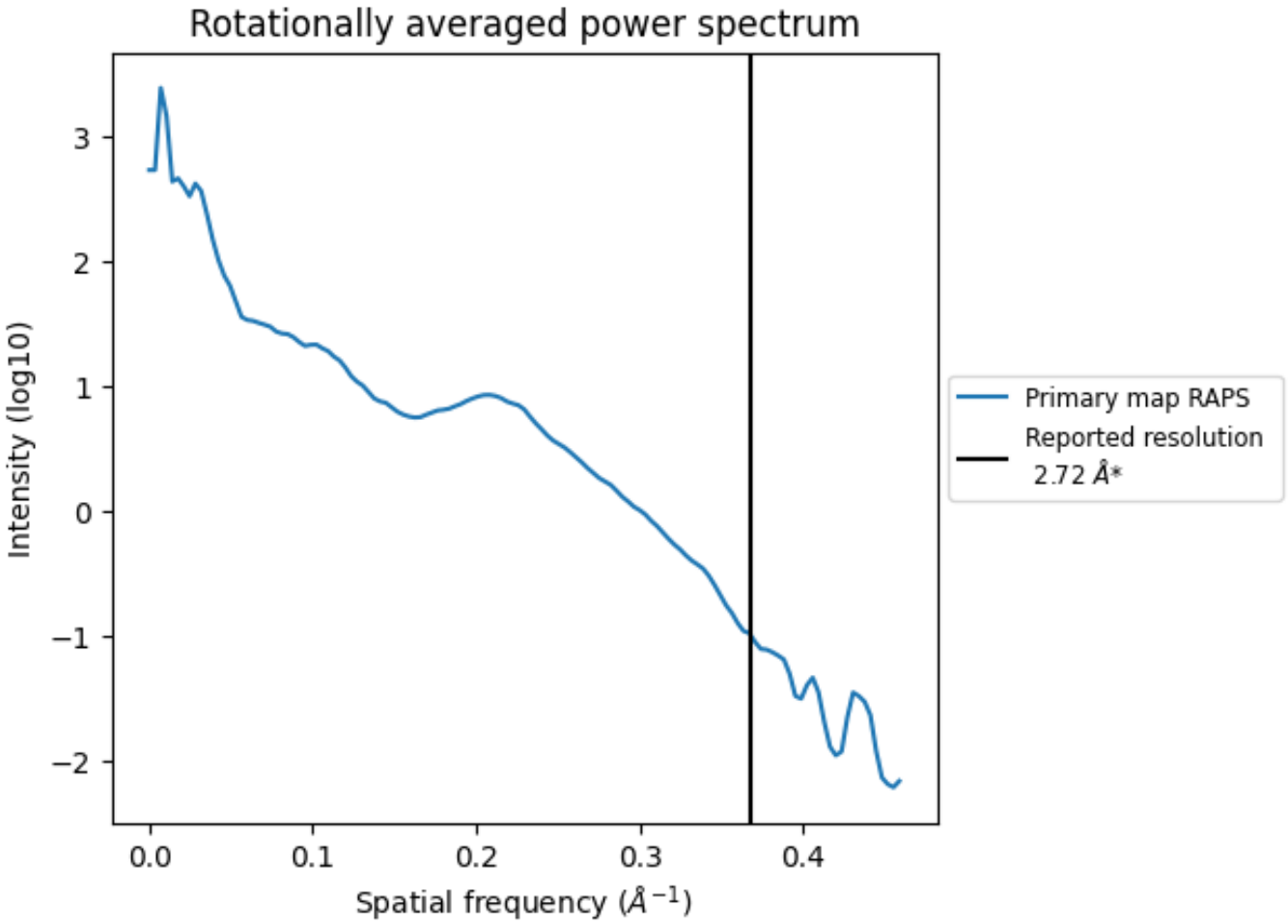
7.2 Volume estimate (i)



The volume at the recommended contour level is 144 nm^3; this corresponds to an approximate mass of 130 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 0.368 Å^{-1}

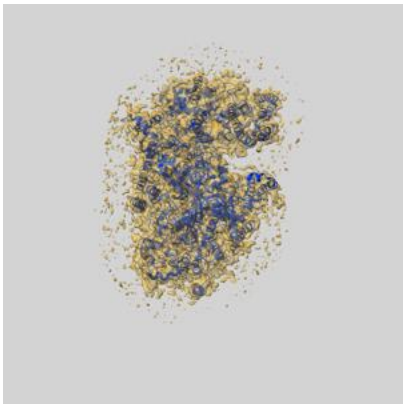
8 Fourier-Shell correlation (i)

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

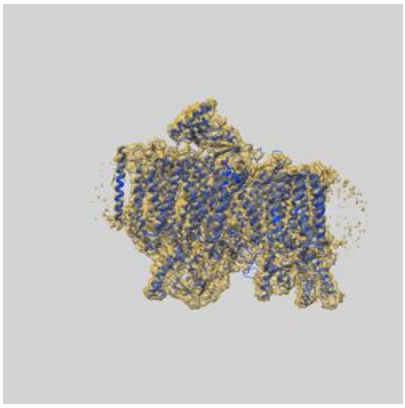
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12336 and PDB model 7NHP. Per-residue inclusion information can be found in section 3 on page 14.

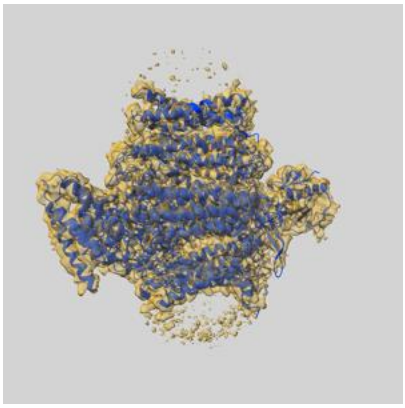
9.1 Map-model overlay



X



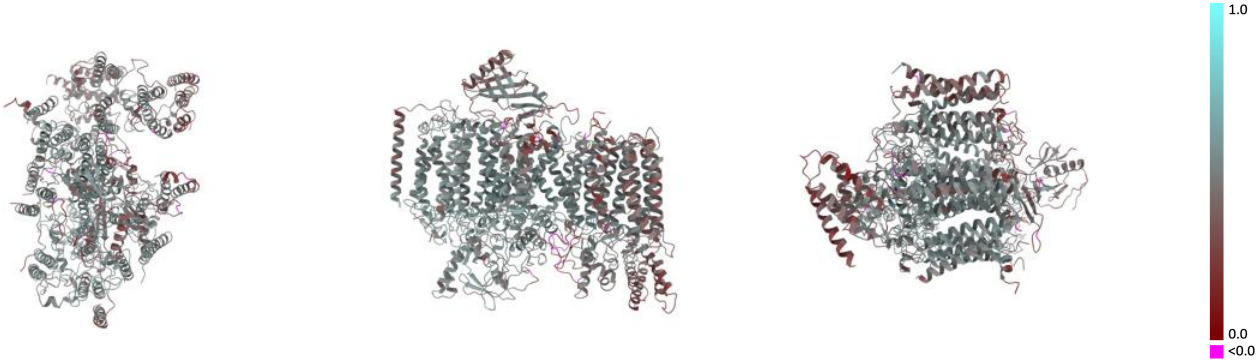
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

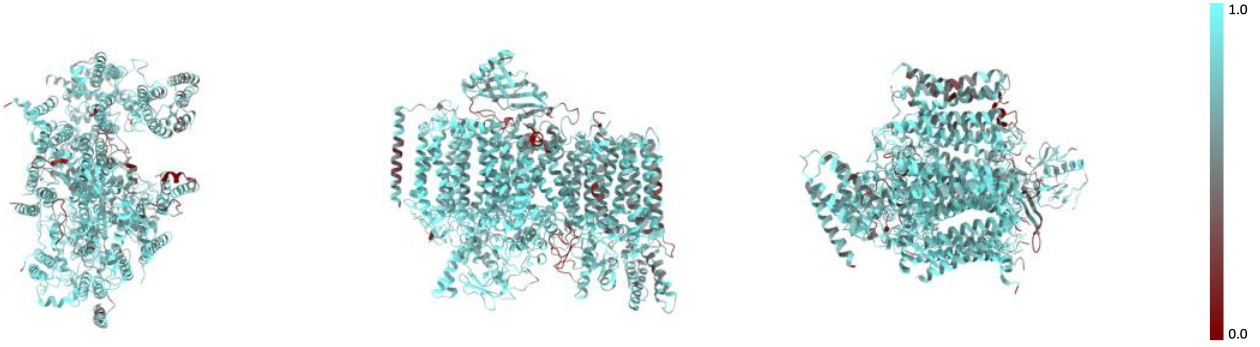
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

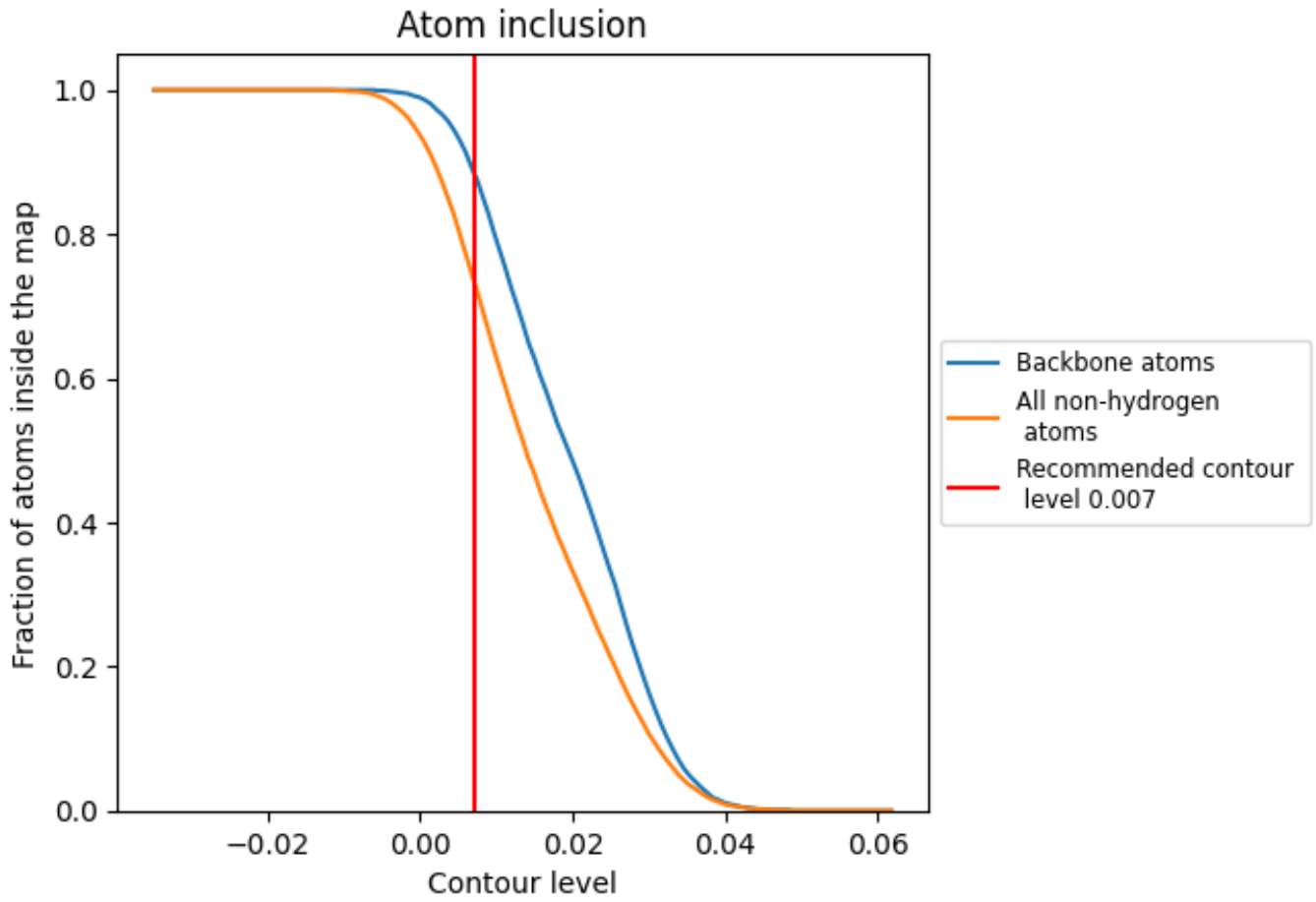
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.007).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 74% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7370	0.4690
1	0.6620	0.3400
2	0.7440	0.4250
3	0.5100	0.3840
A	0.7410	0.4840
B	0.8140	0.5100
C	0.6900	0.4410
D	0.7850	0.5250
E	0.7020	0.4240
F	0.6280	0.4010
H	0.8300	0.4890
I	0.6230	0.4120
K	0.6200	0.4340
L	0.7950	0.5040
M	0.6580	0.4600
T	0.7290	0.4740
X	0.7520	0.4890
Z	0.6250	0.3790
y	0.4750	0.3120