wwPDB EM Validation Summary Report (i)

Sep 8, 2026 – 05:01 am BST

PDB ID	:	7NHP / pdb_00007nhp
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 (i) symbol.

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

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

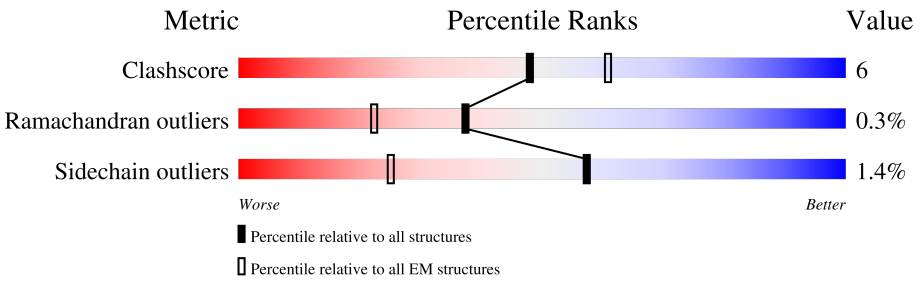
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

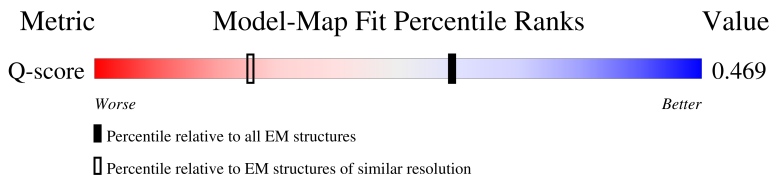
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10355 (2.22 - 3.22)

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% 83% 9% 7%
2	B	510	• 90% 6% •
3	C	461	7% 81% 12% • 6%
4	D	352	• 89% 7% • •

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Mol	Chain	Length	Quality of chain
5	E	84	14% 85% 7% 8%
6	F	45	13% 82% • 16%
7	H	66	• 92% 6% •
8	I	38	58% 11% 32%
9	K	46	7% 46% 30% • • 20%
10	L	37	• 97% •
11	M	36	11% 89% 6% 6%
12	T	32	• 75% 12% 12%
13	X	41	80% 5% 15%
14	y	46	22% 57% • • 39%
15	Z	62	6% 82% 13% • •
16	1	134	10% 70% 13% • 16%
17	2	116	• 89% 8% •
18	3	56	34% 91% 7% •

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	405	X	-	-	-
22	CLA	A	407	X	-	-	-
22	CLA	B	601	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	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	614	X	-	-	-
22	CLA	C	505	X	-	-	-
22	CLA	C	510	X	-	-	-
22	CLA	C	513	X	-	-	-
22	CLA	C	514	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
			Total	C	N	O	S		
7	H	65	511	341	82	86	2	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	34	267	178	40	48	1	0	0

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

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

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

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

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

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

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

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

- Molecule 16 is a protein called Photosystem II lipoprotein Psb27.

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

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

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

- Molecule 18 is a protein called Tsl0063 protein.

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

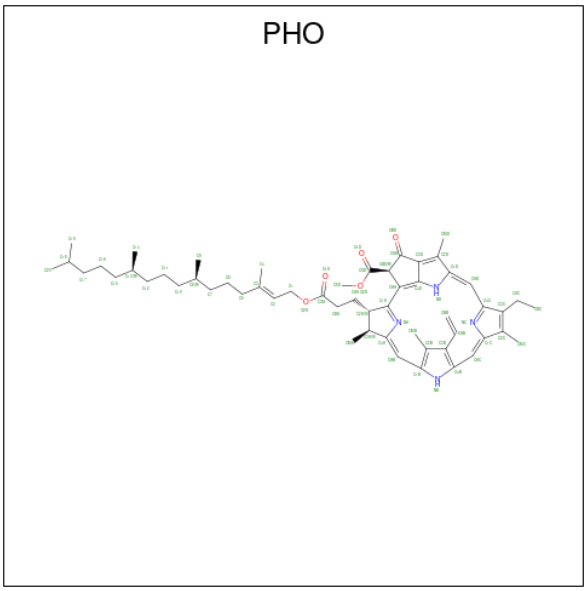
- Molecule 19 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 20 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

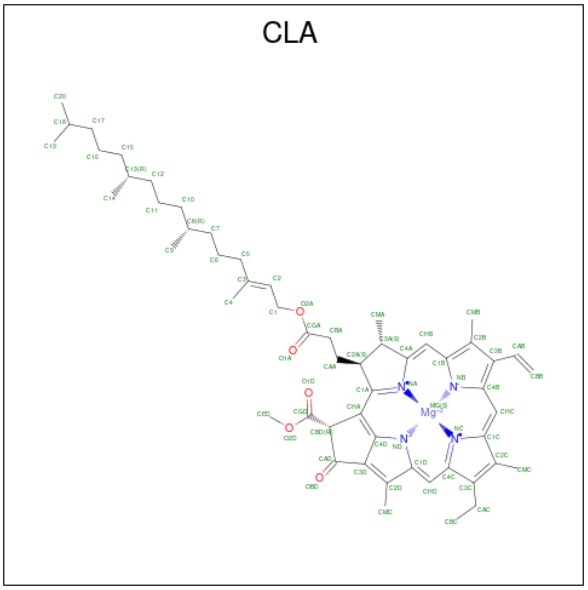
Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
20	A	1	1	1	0

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



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

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



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

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

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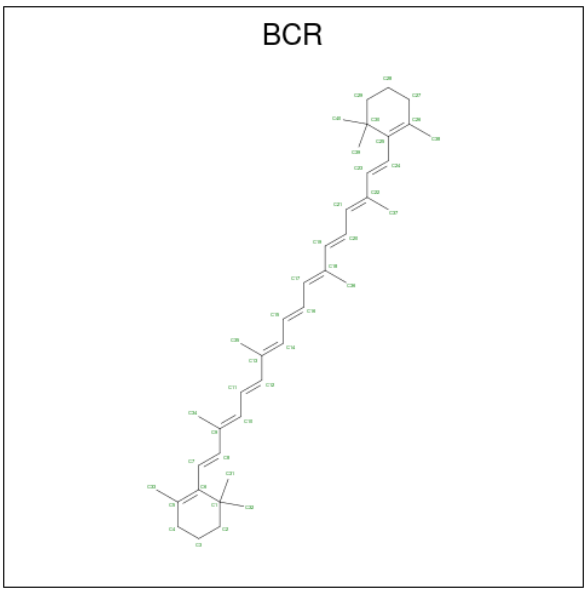
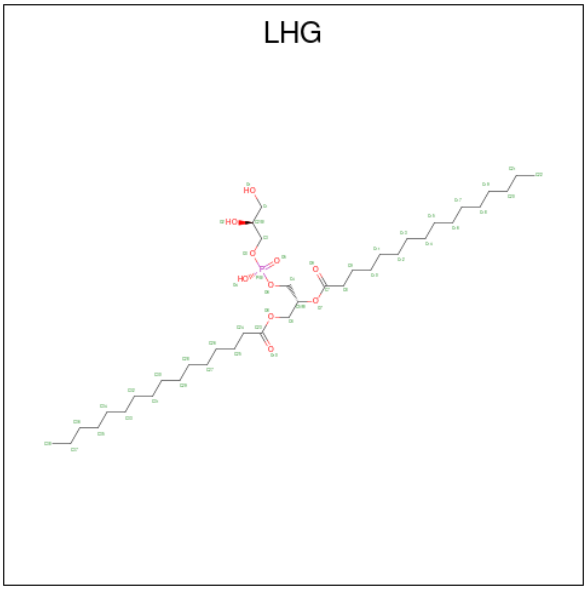
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
22	C	1	65	55	1	4	5	0
22	C	1	65	55	1	4	5	0
22	C	1	65	55	1	4	5	0
22	C	1	65	55	1	4	5	0
22	C	1	65	55	1	4	5	0
22	C	1	65	55	1	4	5	0
22	C	1	65	55	1	4	5	0
22	C	1	65	55	1	4	5	0
22	C	1	65	55	1	4	5	0
22	C	1	65	55	1	4	5	0
22	D	1	65	55	1	4	5	0
22	D	1	65	55	1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

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



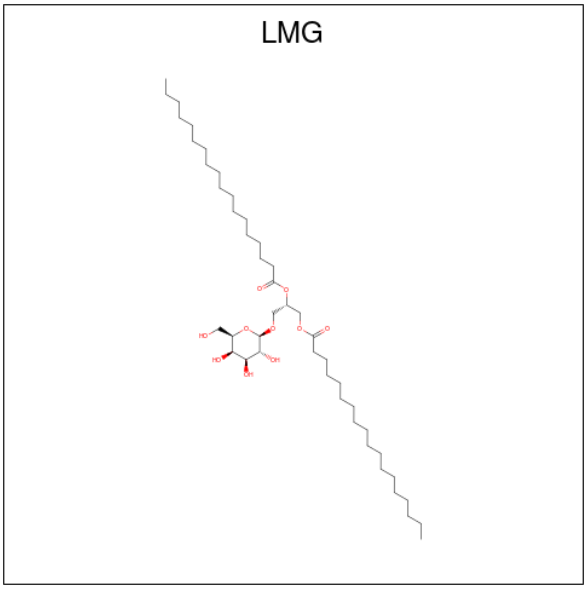
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
23	A	1	40	40	0
23	B	1	40	40	0
23	B	1	40	40	0
23	B	1	40	40	0
23	C	1	40	40	0
23	C	1	40	40	0
23	C	1	40	40	0
23	D	1	40	40	0
23	H	1	40	40	0
23	K	1	40	40	0

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



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

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

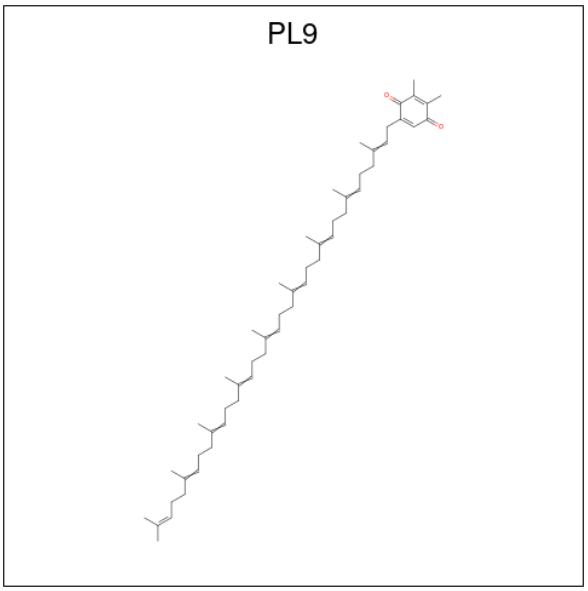


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
25	C	1	55	45	10	0
25	C	1	55	45	10	0
25	D	1	55	45	10	0
25	D	1	55	45	10	0
25	D	1	55	45	10	0
25	D	1	55	45	10	0
25	I	1	55	45	10	0

- Molecule 26 is FE (III) ION (CCD ID: FE) (formula: Fe).

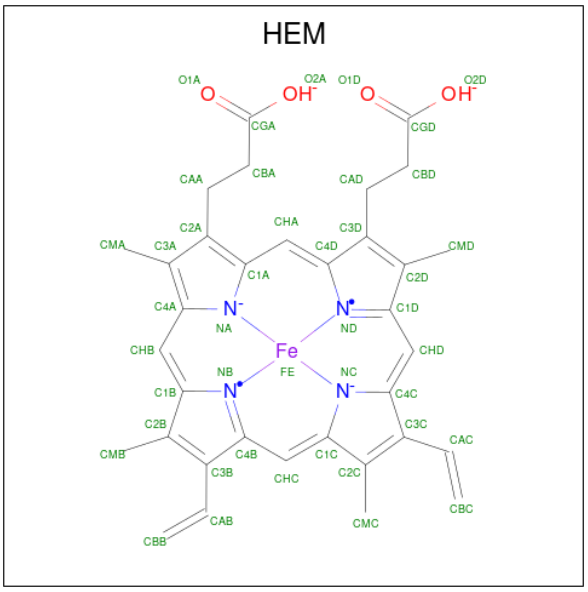
Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
26	D	1	1	1	0

- 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 (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).



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

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



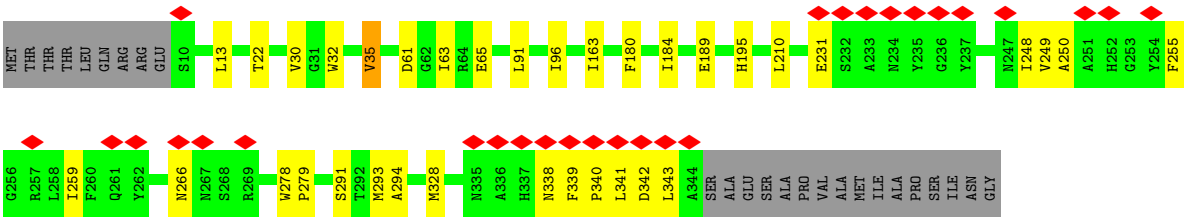
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
28	E	1	43	34	1	4	4	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

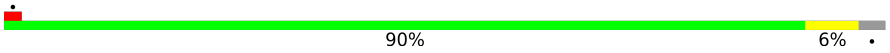
- Molecule 1: Photosystem II protein D1 1

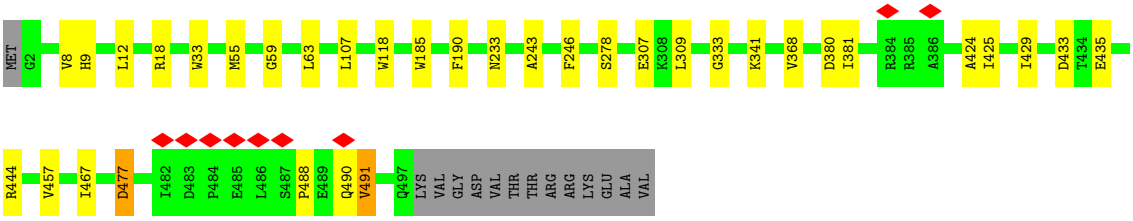
Chain A:



- Molecule 2: Photosystem II CP47 reaction center protein

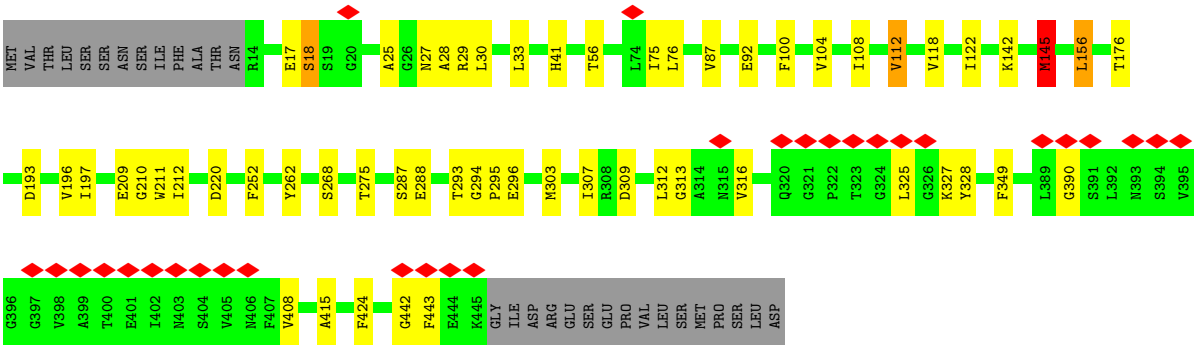
Chain B:





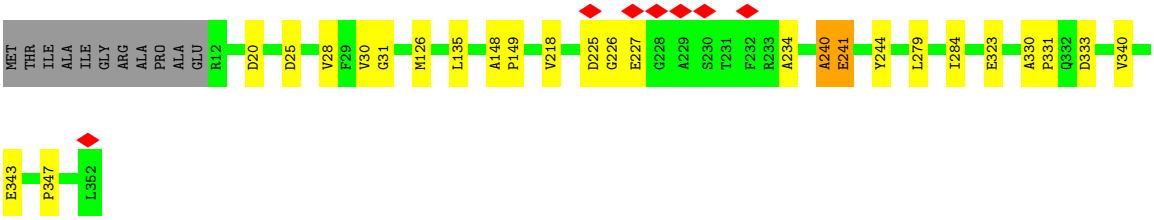
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



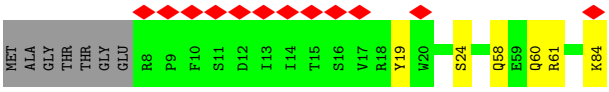
- Molecule 4: Photosystem II D2 protein

Chain D:



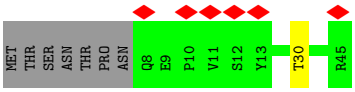
- Molecule 5: Cytochrome b559 subunit alpha

Chain E:



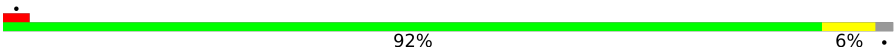
- Molecule 6: Cytochrome b559 subunit beta

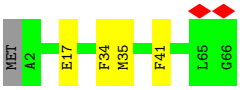
Chain F:



- Molecule 7: Photosystem II reaction center protein H

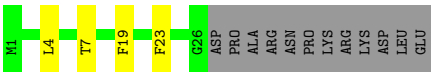
Chain H:





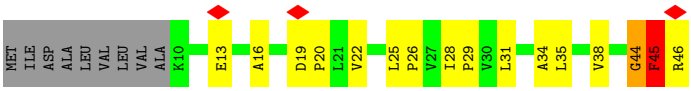
- Molecule 8: Photosystem II reaction center protein I

Chain I:



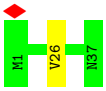
- Molecule 9: Photosystem II reaction center protein K

Chain K:



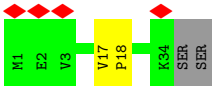
- Molecule 10: Photosystem II reaction center protein L

Chain L: 97%



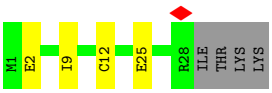
• Molecule 11: Photosystem II reaction center protein M

Chain M: 11% 89% 6% 6%



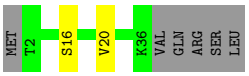
• Molecule 12: Photosystem II reaction center protein T

Chain T: 75% 12% 12%



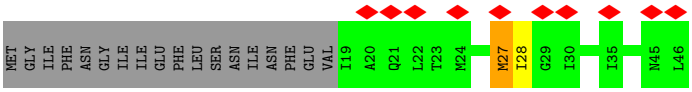
• Molecule 13: Photosystem II reaction center X protein

Chain X: 80% 5% 15%



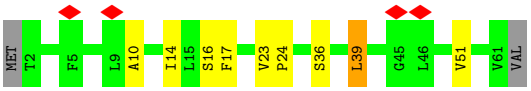
• Molecule 14: Photosystem II reaction center protein Ycf12

Chain y: 22% 57% 39%



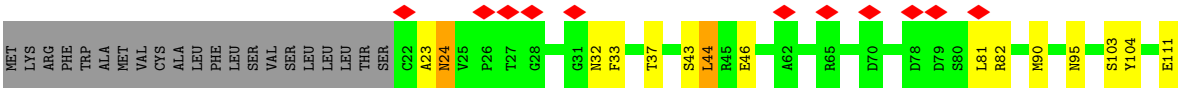
• Molecule 15: Photosystem II reaction center protein Z

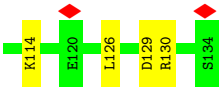
Chain Z: 6% 82% 13%



• Molecule 16: Photosystem II lipoprotein Psb27

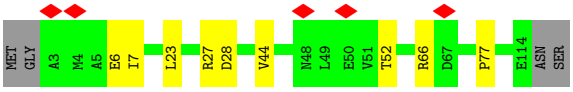
Chain 1: 10% 70% 13% 16%





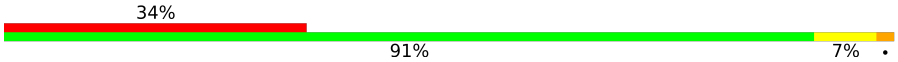
• Molecule 17: Photosystem II reaction center Psb28 protein

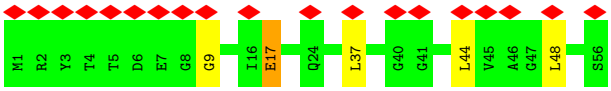
Chain 2:



• 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 (i)

5.1 Standard geometry (i)

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

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	0.41	0/2712	0.82	1/3700 (0.0%)
2	B	0.39	0/4049	0.80	1/5519 (0.0%)
3	C	0.42	0/3456	0.85	1/4706 (0.0%)
4	D	0.38	0/2812	0.80	2/3832 (0.1%)
5	E	0.40	0/654	0.77	1/891 (0.1%)
6	F	0.47	0/317	0.85	0/433
7	H	0.41	0/524	0.88	2/713 (0.3%)
8	I	0.52	0/216	0.94	0/292
9	K	0.45	0/303	0.92	1/416 (0.2%)
10	L	0.41	0/311	0.79	0/422
11	M	0.41	0/270	0.72	0/367
12	T	0.49	0/250	0.84	0/338
13	X	0.44	0/257	0.90	0/348
14	y	0.59	0/209	1.11	0/279
15	Z	0.45	0/474	0.91	0/649
16	1	0.42	0/907	0.89	3/1220 (0.2%)
17	2	0.42	0/914	0.92	0/1231
18	3	0.44	0/426	0.89	0/578
All	All	0.41	0/19061	0.84	12/25934 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	145	MET	CB-CG-SD	7.90	136.40	112.70
9	K	45	PHE	N-CA-C	-6.61	96.72	110.80
16	1	104	TYR	CA-CB-CG	5.88	124.49	113.90
2	B	491	VAL	N-CA-C	-5.76	97.36	109.34
1	A	328	MET	CB-CG-SD	5.66	129.67	112.70

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	21	0
2	B	3909	0	3763	26	0
3	C	3345	0	3273	67	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	3	0
15	Z	463	0	495	6	0
16	1	893	0	896	8	0
17	2	897	0	859	4	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	7	0
22	B	1040	0	1127	33	0
22	C	845	0	918	44	0
22	D	130	0	140	6	0
23	A	40	0	56	2	0
23	B	120	0	168	5	0
23	C	120	0	168	19	0
23	D	40	0	56	0	0
23	H	40	0	56	18	0
23	K	40	0	56	26	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	259	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 259 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%)	21	42
2	B	494/510 (97%)	469 (95%)	24 (5%)	1 (0%)	43	66
3	C	430/461 (93%)	396 (92%)	33 (8%)	1 (0%)	43	66
4	D	339/352 (96%)	316 (93%)	22 (6%)	1 (0%)	36	59
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%)	3	8
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%)	14	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	2	110/116 (95%)	101 (92%)	8 (7%)	1 (1%)	14	33
18	3	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
All	All	2314/2522 (92%)	2171 (94%)	135 (6%)	8 (0%)	37	59

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%)	269 (99%)	2 (1%)	76	89
2	B	395/407 (97%)	392 (99%)	3 (1%)	73	87
3	C	335/362 (92%)	329 (98%)	6 (2%)	51	76
4	D	276/283 (98%)	273 (99%)	3 (1%)	65	84
5	E	69/73 (94%)	68 (99%)	1 (1%)	59	80
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%)	24 (96%)	1 (4%)	28	55
13	X	28/34 (82%)	28 (100%)	0	100	100
14	y	21/37 (57%)	20 (95%)	1 (5%)	23	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	Z	50/52 (96%)	48 (96%)	2 (4%)	28	55
16	1	96/115 (84%)	90 (94%)	6 (6%)	16	37
17	2	94/97 (97%)	94 (100%)	0	100	100
18	3	42/42 (100%)	41 (98%)	1 (2%)	43	70
All	All	1908/2056 (93%)	1882 (99%)	26 (1%)	57	80

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	24	SER
15	Z	16	SER
16	1	103	SER
14	y	27	MET
15	Z	39	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	268	HIS
6	F	44	GLN
17	2	90	GLN
5	E	58	GLN
7	H	50	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 oligosaccharides 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	$\#\|Z\| > 2$
25	LMG	D	403	-	55,55,55	0.92	2 (3%)	63,63,63	1.14	5 (7%)
22	CLA	A	406	-	69,73,73	1.31	10 (14%)	83,113,113	1.93	23 (27%)
22	CLA	B	603	-	69,73,73	1.34	11 (15%)	83,113,113	2.01	16 (19%)
22	CLA	B	611	2	69,73,73	1.38	9 (13%)	83,113,113	2.31	23 (27%)
23	BCR	A	408	-	41,41,41	1.11	2 (4%)	56,56,56	1.33	9 (16%)
22	CLA	B	608	2	69,73,73	1.39	10 (14%)	83,113,113	2.35	25 (30%)
22	CLA	B	609	-	69,73,73	1.55	10 (14%)	83,113,113	2.33	23 (27%)
25	LMG	I	101	-	55,55,55	0.99	2 (3%)	63,63,63	1.06	4 (6%)
22	CLA	B	613	-	69,73,73	1.39	8 (11%)	83,113,113	2.14	17 (20%)
22	CLA	B	604	2	69,73,73	1.35	11 (15%)	83,113,113	2.21	26 (31%)
22	CLA	C	511	3	69,73,73	1.36	12 (17%)	83,113,113	2.32	23 (27%)
27	PL9	D	406	-	55,55,55	1.16	1 (1%)	68,69,69	1.55	8 (11%)
22	CLA	B	614	2	69,73,73	1.43	9 (13%)	83,113,113	2.42	25 (30%)
22	CLA	C	510	-	69,73,73	1.44	10 (14%)	83,113,113	2.45	16 (19%)
23	BCR	K	101	-	41,41,41	3.43	14 (34%)	56,56,56	4.27	29 (51%)
22	CLA	B	610	-	69,73,73	1.31	8 (11%)	83,113,113	2.40	22 (26%)
23	BCR	H	101	-	41,41,41	3.44	14 (34%)	56,56,56	4.30	30 (53%)
22	CLA	B	616	-	69,73,73	1.45	9 (13%)	83,113,113	2.75	24 (28%)
28	HEM	E	101	5	50,50,50	1.26	3 (6%)	66,82,82	1.01	2 (3%)
22	CLA	B	615	-	69,73,73	1.36	11 (15%)	83,113,113	2.29	18 (21%)
22	CLA	C	512	-	69,73,73	1.55	9 (13%)	83,113,113	2.40	23 (27%)
23	BCR	C	516	-	41,41,41	1.12	3 (7%)	56,56,56	1.34	4 (7%)
25	LMG	C	501	-	55,55,55	1.11	3 (5%)	63,63,63	1.00	3 (4%)
22	CLA	D	408	-	69,73,73	1.45	13 (18%)	83,113,113	1.85	22 (26%)
22	CLA	C	506	-	69,73,73	1.40	14 (20%)	83,113,113	1.99	18 (21%)
25	LMG	D	404	-	55,55,55	0.93	0	63,63,63	1.14	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	CLA	C	507	3	69,73,73	1.51	9 (13%)	83,113,113	2.49	23 (27%)
25	LMG	D	402	-	55,55,55	0.98	0	63,63,63	1.09	4 (6%)
25	LMG	D	405	-	55,55,55	0.97	0	63,63,63	1.11	3 (4%)
22	CLA	A	404	1	69,73,73	1.34	10 (14%)	83,113,113	1.92	23 (27%)
22	CLA	B	602	2	69,73,73	1.35	11 (15%)	83,113,113	2.43	25 (30%)
22	CLA	A	407	1	69,73,73	1.44	10 (14%)	83,113,113	1.70	17 (20%)
22	CLA	C	517	-	69,73,73	1.46	10 (14%)	83,113,113	2.34	20 (24%)
22	CLA	B	606	-	69,73,73	1.29	7 (10%)	83,113,113	1.80	22 (26%)
22	CLA	C	505	-	69,73,73	1.37	10 (14%)	83,113,113	2.28	24 (28%)
23	BCR	C	518	-	41,41,41	1.04	2 (4%)	56,56,56	1.11	5 (8%)
22	CLA	C	509	-	69,73,73	1.39	11 (15%)	83,113,113	2.46	26 (31%)
23	BCR	B	618	-	41,41,41	1.02	2 (4%)	56,56,56	1.24	9 (16%)
22	CLA	C	504	-	69,73,73	1.33	11 (15%)	83,113,113	1.95	18 (21%)
22	CLA	C	508	3	69,73,73	1.47	8 (11%)	83,113,113	2.16	22 (26%)
22	CLA	D	409	-	69,73,73	1.33	10 (14%)	83,113,113	1.70	17 (20%)
22	CLA	C	503	3	69,73,73	1.29	10 (14%)	83,113,113	2.02	17 (20%)
23	BCR	B	619	-	41,41,41	0.95	2 (4%)	56,56,56	1.17	5 (8%)
22	CLA	C	513	-	69,73,73	1.41	13 (18%)	83,113,113	2.39	29 (34%)
23	BCR	D	410	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)
22	CLA	A	405	-	69,73,73	1.34	9 (13%)	83,113,113	1.88	21 (25%)
22	CLA	B	605	-	69,73,73	1.39	11 (15%)	83,113,113	2.01	21 (25%)
22	CLA	C	514	-	69,73,73	1.48	11 (15%)	83,113,113	2.11	16 (19%)
21	PHO	A	403	-	58,69,69	2.09	10 (17%)	56,99,99	1.77	7 (12%)
24	LHG	A	409	-	48,48,48	0.79	1 (2%)	51,54,54	0.89	1 (1%)
25	LMG	C	502	-	55,55,55	1.03	0	63,63,63	1.05	4 (6%)
22	CLA	B	607	-	69,73,73	1.44	13 (18%)	83,113,113	2.05	21 (25%)
22	CLA	B	601	-	69,73,73	1.26	10 (14%)	83,113,113	2.89	25 (30%)
22	CLA	B	612	-	69,73,73	1.33	9 (13%)	83,113,113	2.57	28 (33%)
21	PHO	D	407	-	58,69,69	2.06	12 (20%)	56,99,99	2.20	10 (17%)
23	BCR	C	515	-	41,41,41	1.07	2 (4%)	56,56,56	1.59	9 (16%)
23	BCR	B	617	-	41,41,41	0.99	2 (4%)	56,56,56	1.17	3 (5%)

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
25	LMG	D	403	-	-	14/50/70/70	0/1/1/1
22	CLA	A	406	-	-	10/39/115/115	-
22	CLA	B	603	-	1/1/15/20	12/39/115/115	-
22	CLA	B	611	2	-	11/39/115/115	-
23	BCR	A	408	-	-	7/29/63/63	0/2/2/2
22	CLA	B	608	2	2/2/15/20	9/39/115/115	-
22	CLA	B	609	-	1/1/15/20	9/39/115/115	-
25	LMG	I	101	-	-	8/50/70/70	0/1/1/1
22	CLA	B	613	-	-	11/39/115/115	-
22	CLA	B	604	2	1/1/15/20	11/39/115/115	-
22	CLA	C	511	3	-	13/39/115/115	-
27	PL9	D	406	-	-	9/53/73/73	0/1/1/1
22	CLA	B	614	2	1/1/15/20	4/39/115/115	-
22	CLA	C	510	-	1/1/15/20	12/39/115/115	-
23	BCR	K	101	-	-	15/29/63/63	0/2/2/2
22	CLA	B	610	-	1/1/15/20	11/39/115/115	-
23	BCR	H	101	-	-	15/29/63/63	0/2/2/2
22	CLA	B	616	-	-	9/39/115/115	-
28	HEM	E	101	5	-	5/14/54/54	-
22	CLA	B	615	-	-	10/39/115/115	-
22	CLA	C	512	-	-	10/39/115/115	-
23	BCR	C	516	-	-	8/29/63/63	0/2/2/2
25	LMG	C	501	-	-	12/50/70/70	0/1/1/1
22	CLA	D	408	-	-	12/39/115/115	-
22	CLA	C	506	-	-	13/39/115/115	-
25	LMG	D	404	-	-	8/50/70/70	0/1/1/1
22	CLA	C	507	3	-	4/39/115/115	-
25	LMG	D	402	-	-	7/50/70/70	0/1/1/1
25	LMG	D	405	-	-	13/50/70/70	0/1/1/1
22	CLA	A	404	1	-	6/39/115/115	-
22	CLA	B	602	2	-	13/39/115/115	-
22	CLA	A	407	1	1/1/15/20	7/39/115/115	-
22	CLA	C	517	-	-	10/39/115/115	-
22	CLA	C	505	-	1/1/15/20	16/39/115/115	-
22	CLA	B	606	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	C	518	-	-	12/29/63/63	0/2/2/2
22	CLA	C	509	-	-	15/39/115/115	-
23	BCR	B	618	-	-	3/29/63/63	0/2/2/2
22	CLA	C	504	-	-	11/39/115/115	-
22	CLA	D	409	-	1/1/15/20	3/39/115/115	-
22	CLA	C	508	3	-	7/39/115/115	-
22	CLA	C	503	3	-	8/39/115/115	-
23	BCR	B	619	-	-	4/29/63/63	0/2/2/2
22	CLA	C	513	-	1/1/15/20	12/39/115/115	-
23	BCR	D	410	-	-	6/29/63/63	0/2/2/2
22	CLA	A	405	-	1/1/15/20	12/39/115/115	-
22	CLA	B	605	-	-	10/39/115/115	-
22	CLA	C	514	-	1/1/15/20	10/39/115/115	-
21	PHO	A	403	-	1/1/17/22	6/37/103/103	0/5/6/6
24	LHG	A	409	-	-	15/53/53/53	-
25	LMG	C	502	-	-	7/50/70/70	0/1/1/1
22	CLA	B	607	-	1/1/15/20	12/39/115/115	-
22	CLA	B	601	-	2/2/15/20	10/39/115/115	-
22	CLA	B	612	-	1/1/15/20	14/39/115/115	-
21	PHO	D	407	-	1/1/17/22	6/37/103/103	0/5/6/6
23	BCR	C	515	-	-	7/29/63/63	0/2/2/2
23	BCR	B	617	-	-	6/29/63/63	0/2/2/2

The worst 5 of 436 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
23	K	101	BCR	C5-C6	-9.67	1.17	1.34
21	D	407	PHO	C1B-C2B	9.57	1.50	1.39
23	H	101	BCR	C5-C6	-9.08	1.18	1.34

The worst 5 of 922 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 21 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	403	PHO	C8
21	D	407	PHO	C8
22	A	405	CLA	C8
22	A	407	CLA	C8
22	B	601	CLA	C2A

5 of 551 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.

43 monomers are involved in 138 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	D	403	LMG	1	0
22	A	406	CLA	1	0
22	B	603	CLA	1	0
22	B	611	CLA	2	0
23	A	408	BCR	2	0
22	B	608	CLA	5	0
22	B	609	CLA	8	0
22	B	613	CLA	2	0
22	B	604	CLA	2	0
22	C	511	CLA	3	0
27	D	406	PL9	4	0
22	B	614	CLA	2	0
22	C	510	CLA	12	0
23	K	101	BCR	26	0
22	B	610	CLA	3	0
23	H	101	BCR	18	0

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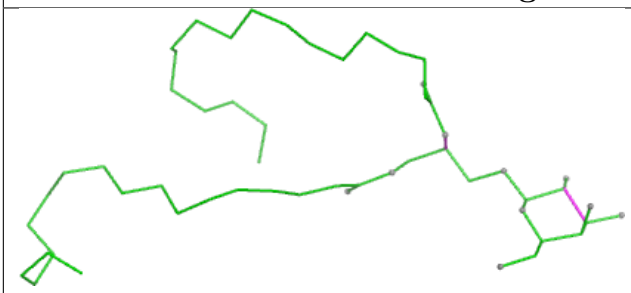
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	616	CLA	1	0
22	B	615	CLA	1	0
22	C	512	CLA	12	0
23	C	516	BCR	3	0
22	D	408	CLA	2	0
22	C	506	CLA	2	0
25	D	404	LMG	1	0
25	D	402	LMG	1	0
22	A	407	CLA	2	0
22	C	517	CLA	4	0
22	C	505	CLA	3	0
23	C	518	BCR	2	0
22	C	509	CLA	4	0
23	B	618	BCR	2	0
22	C	504	CLA	2	0
22	D	409	CLA	4	0
22	C	503	CLA	3	0
23	B	619	BCR	2	0
22	C	513	CLA	3	0
22	A	405	CLA	4	0
22	C	514	CLA	1	0
21	A	403	PHO	1	0
22	B	607	CLA	2	0
22	B	601	CLA	5	0
22	B	612	CLA	2	0
23	C	515	BCR	14	0
23	B	617	BCR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand LMG D 403



Bond lengths

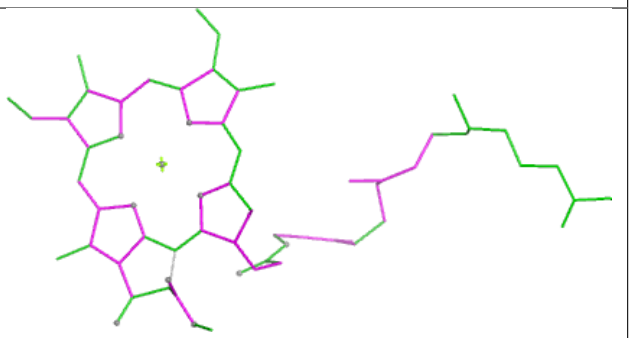
Bond angles

Torsions

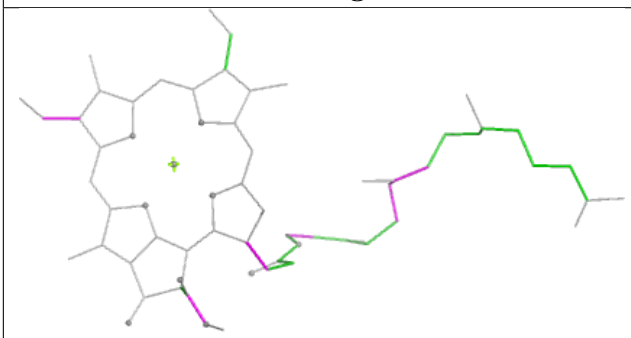
Rings

Ligand CLA A 406

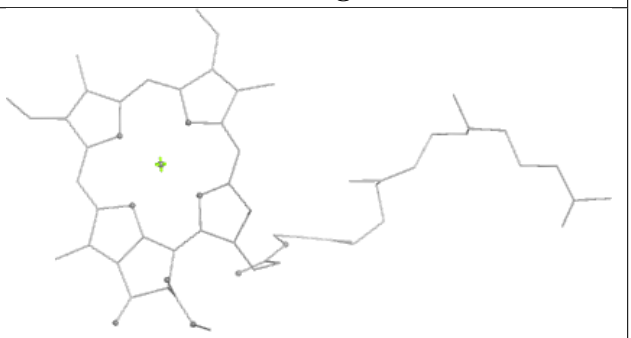
Bond lengths



Bond angles

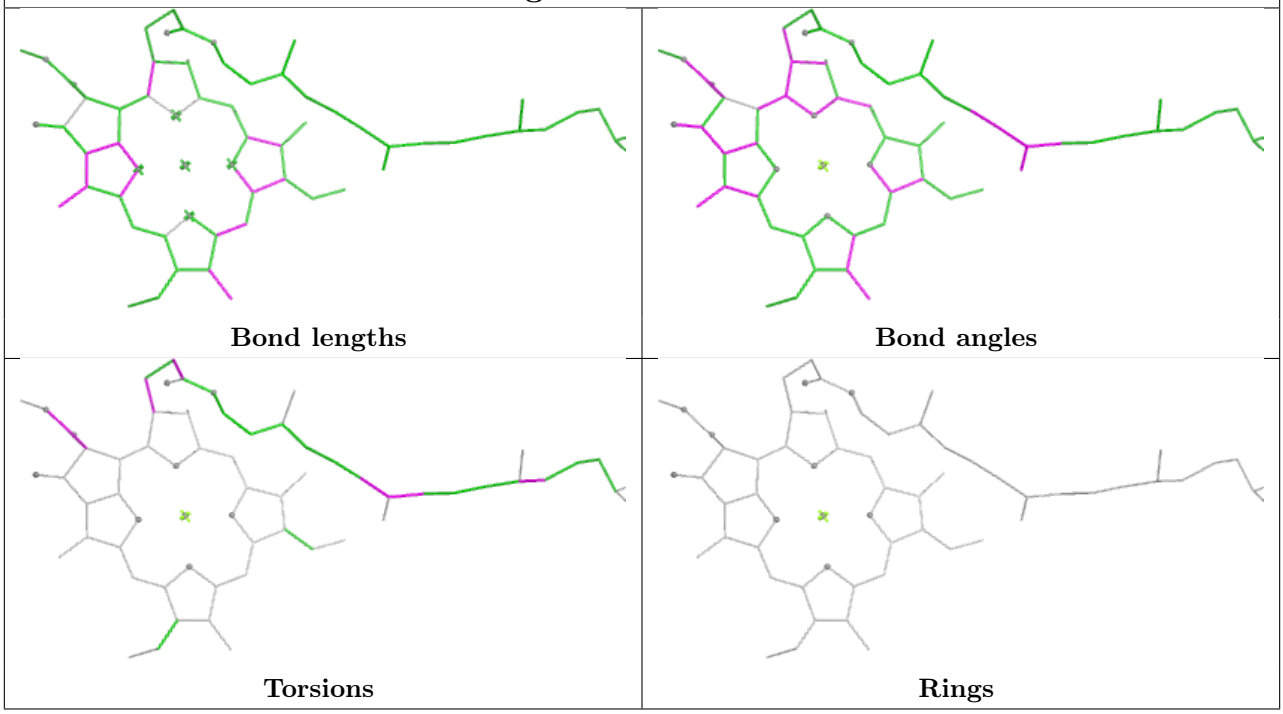


Torsions

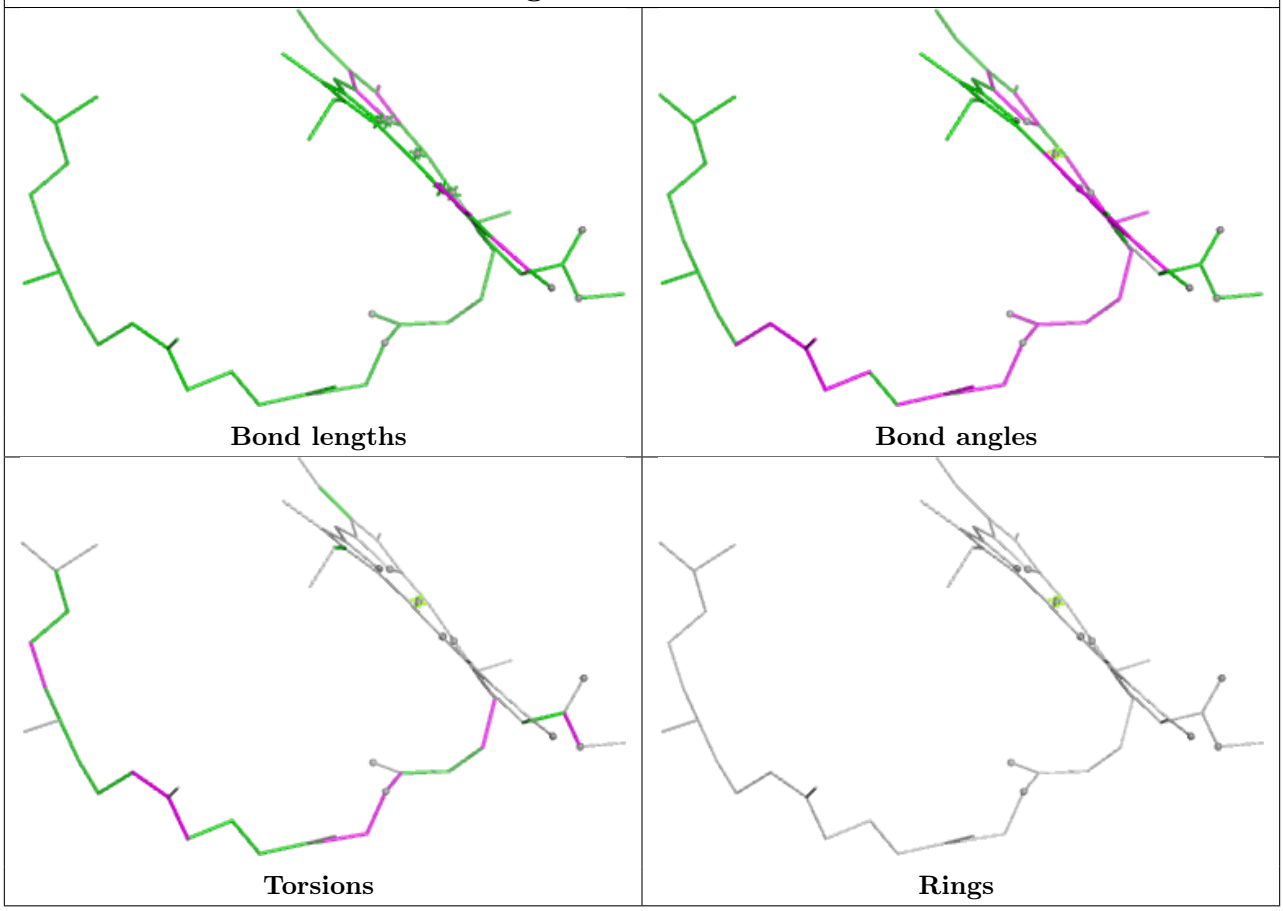


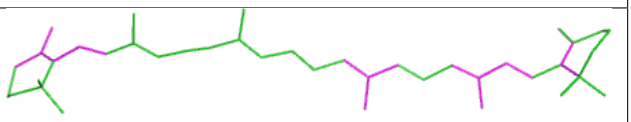
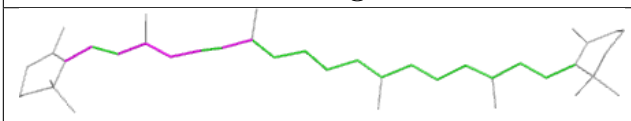
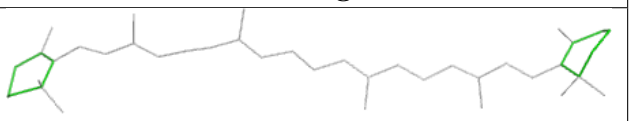
Rings

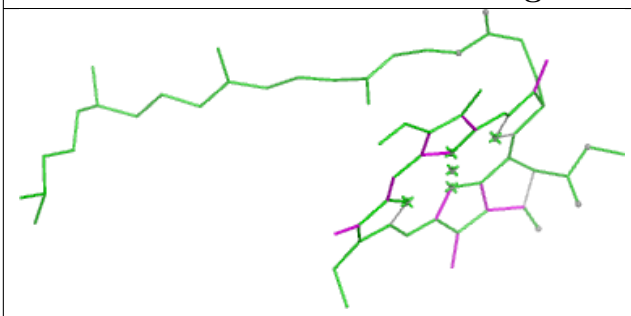
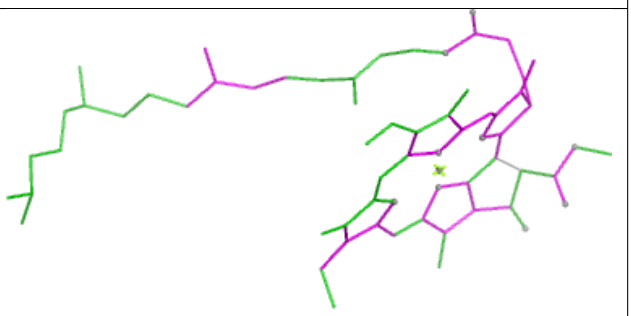
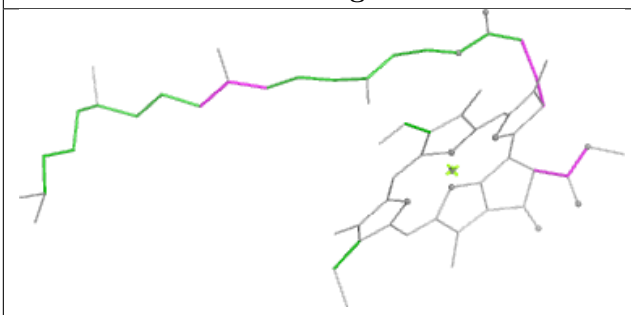
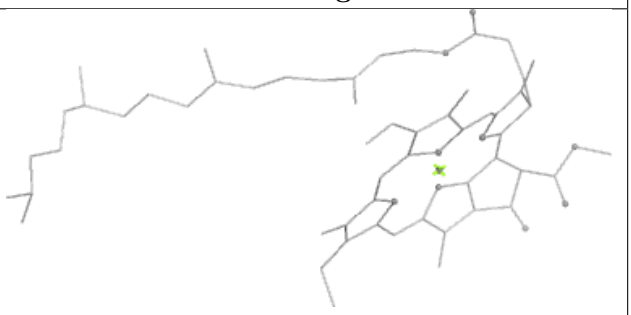
Ligand CLA B 603



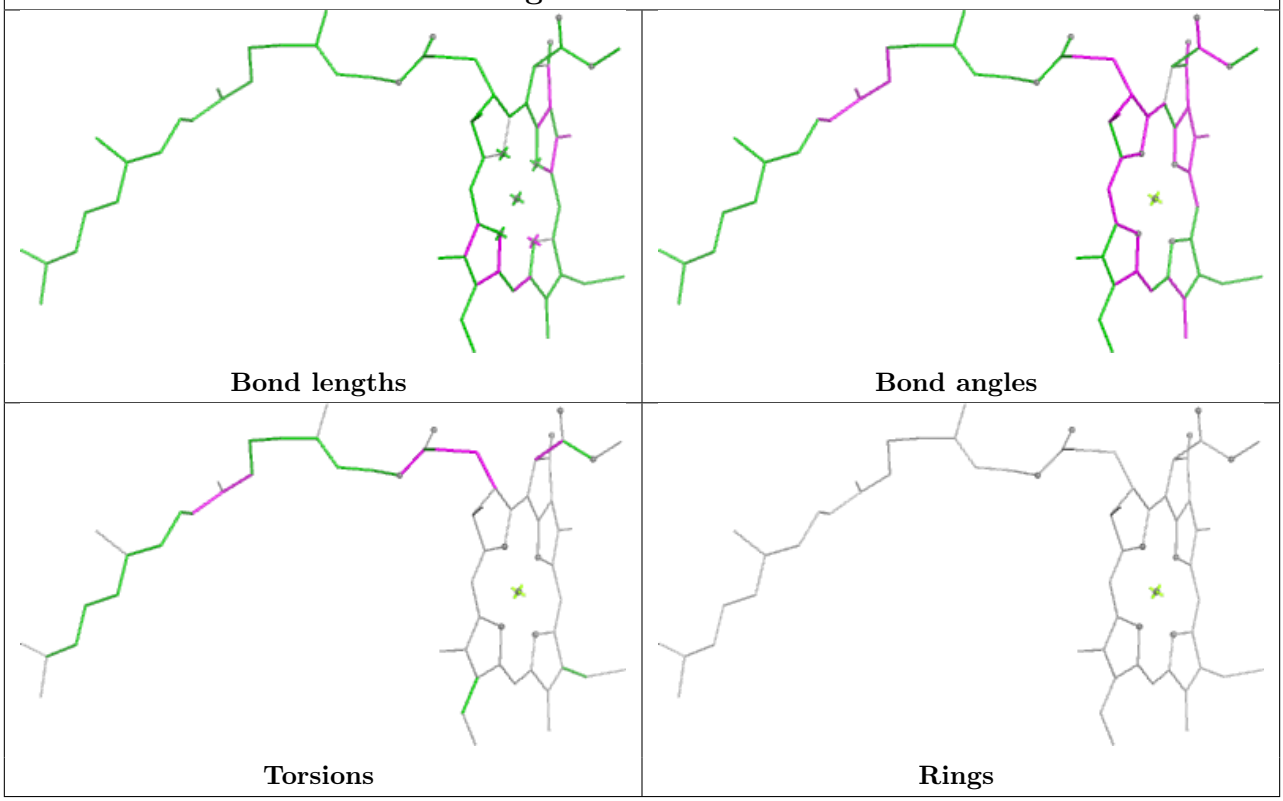
Ligand CLA B 611



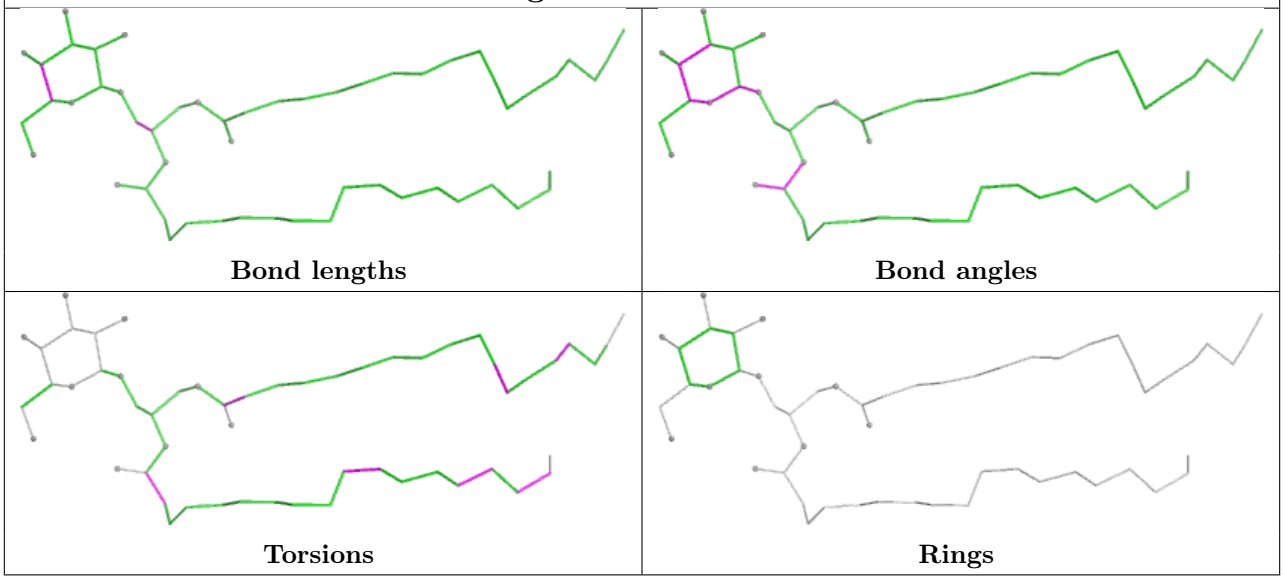
Ligand BCR A 408	
Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 608	
 Bond lengths	 Bond angles
 Torsions	 Rings

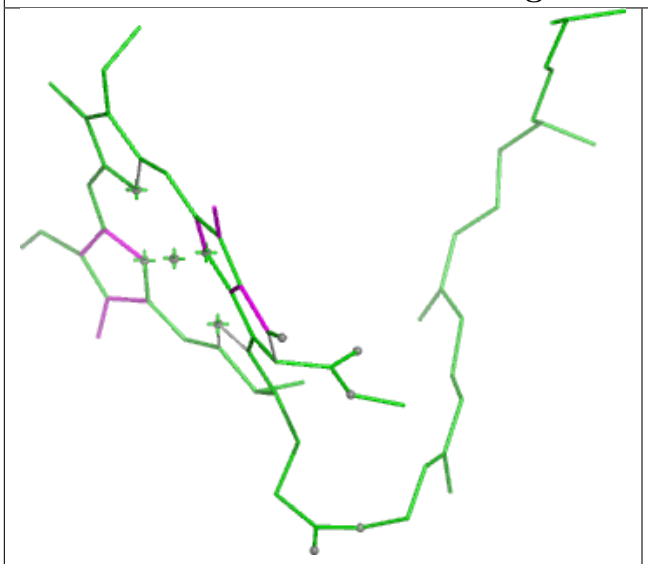
Ligand CLA B 609



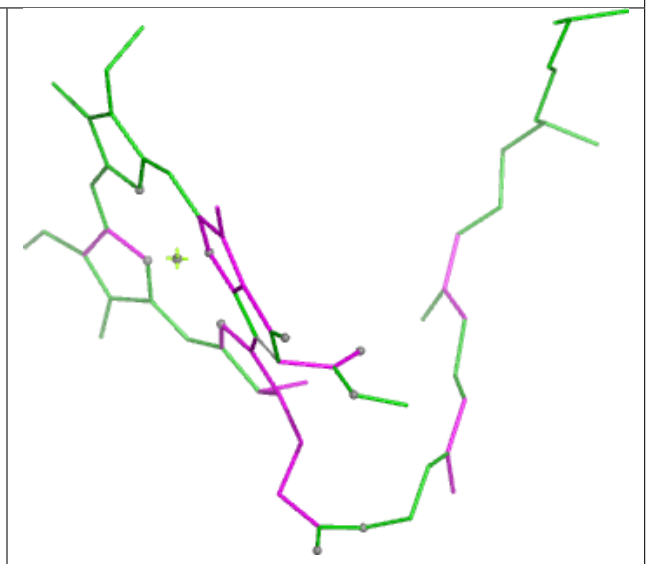
Ligand LMG I 101



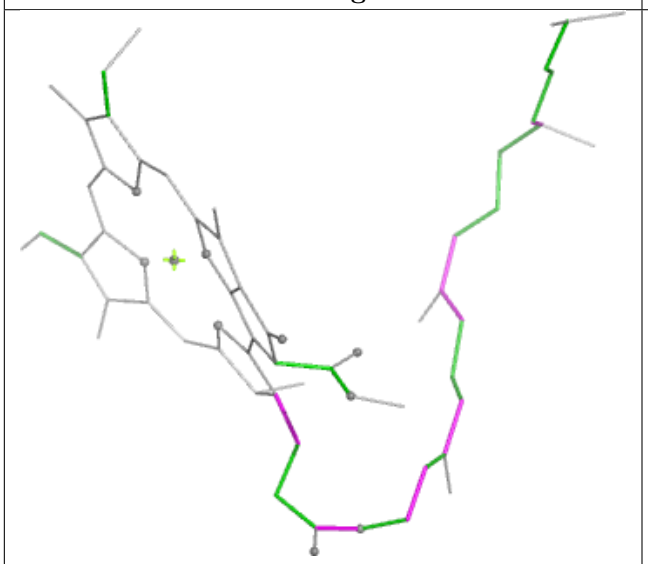
Ligand CLA B 613



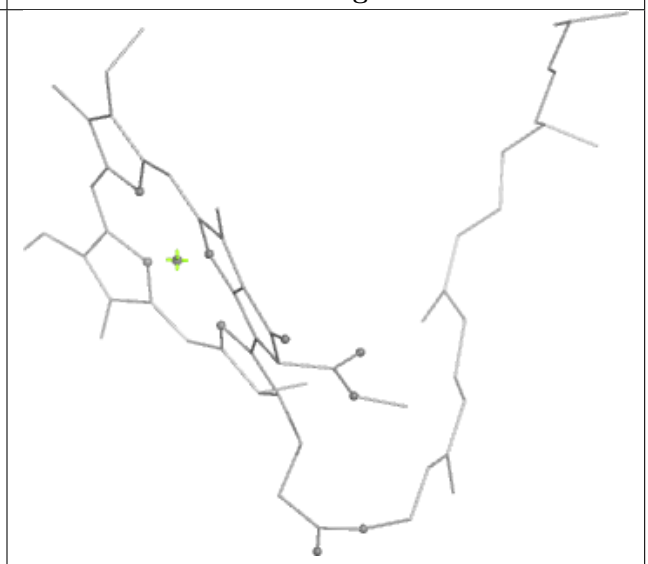
Bond lengths



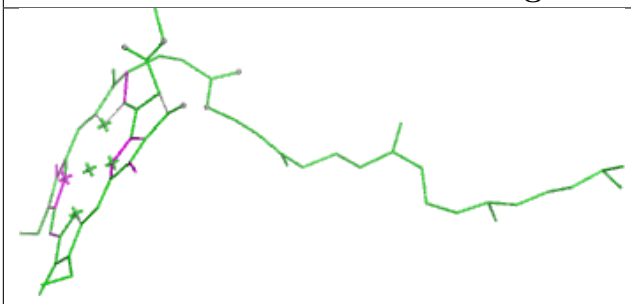
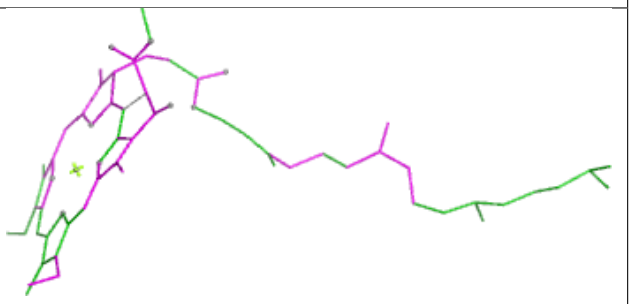
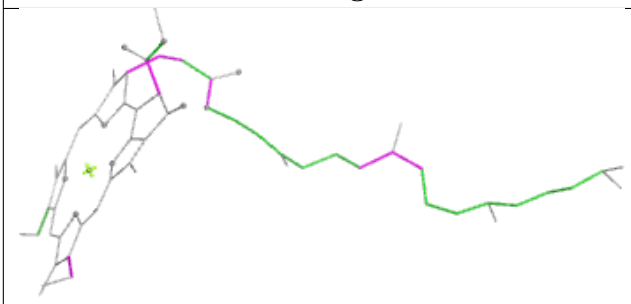
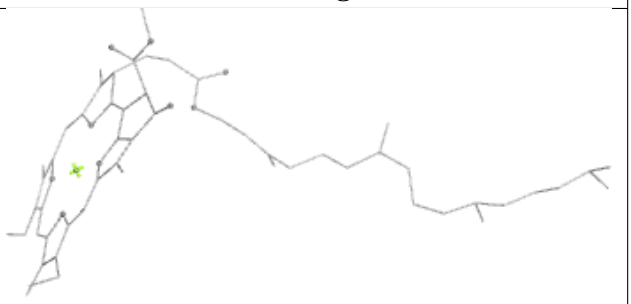
Bond angles



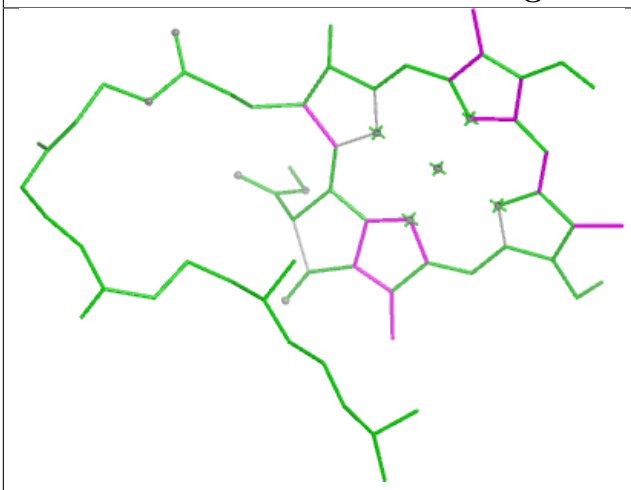
Torsions



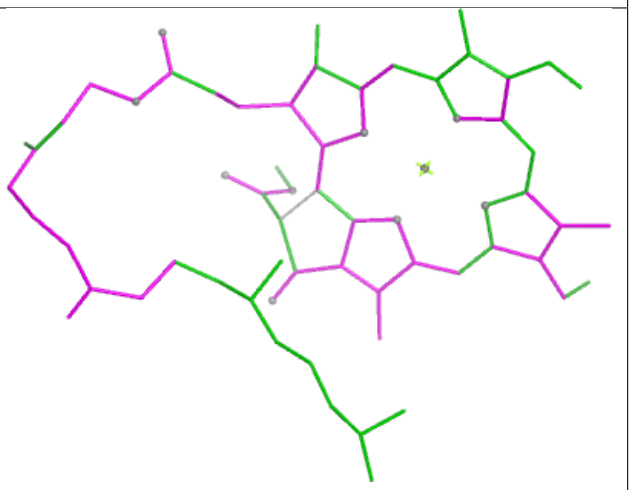
Rings

Ligand CLA B 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

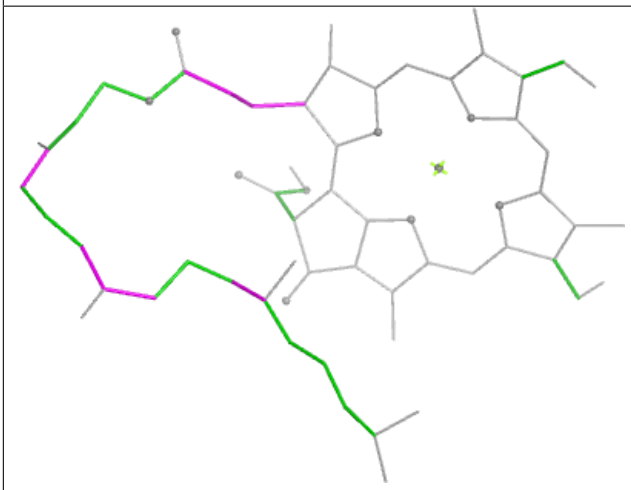
Ligand CLA C 511



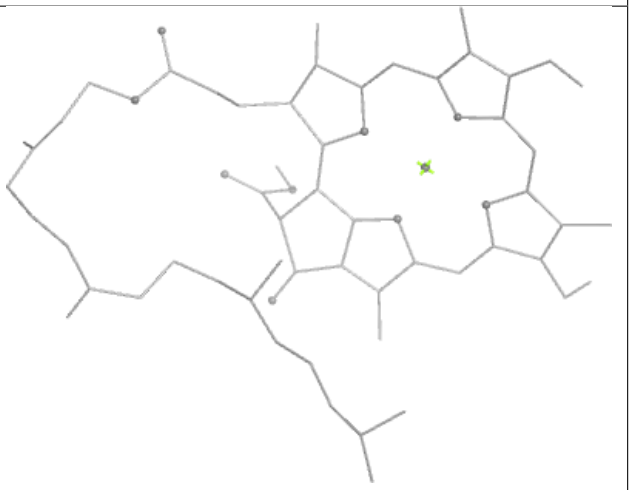
Bond lengths



Bond angles

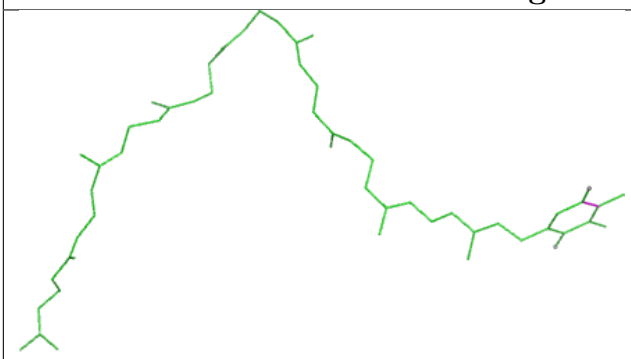


Torsions

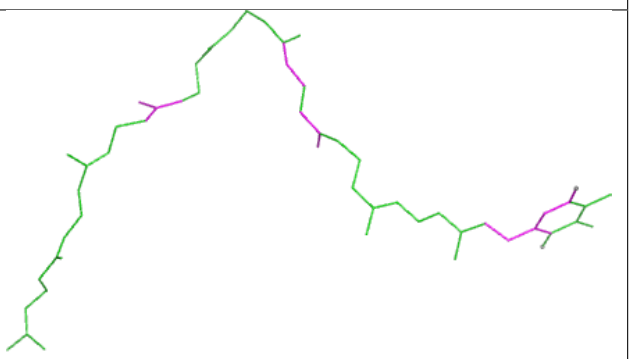


Rings

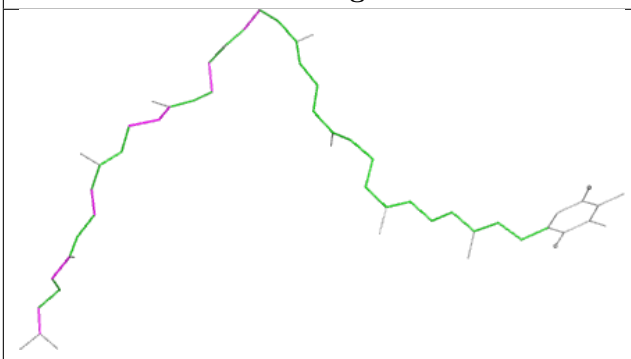
Ligand PL9 D 406



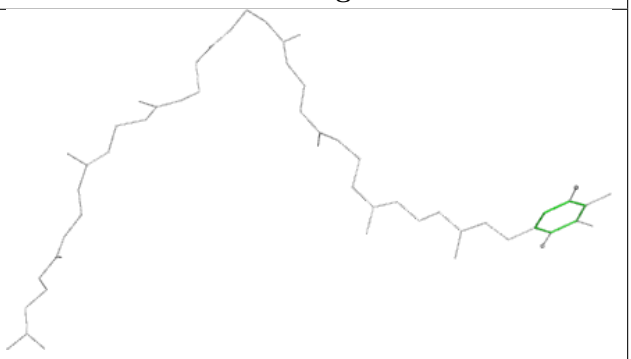
Bond lengths



Bond angles

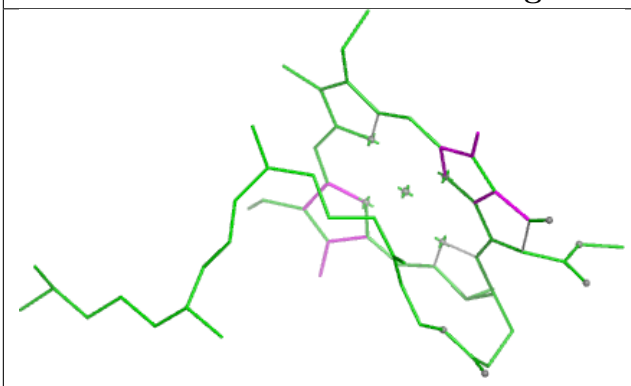


Torsions

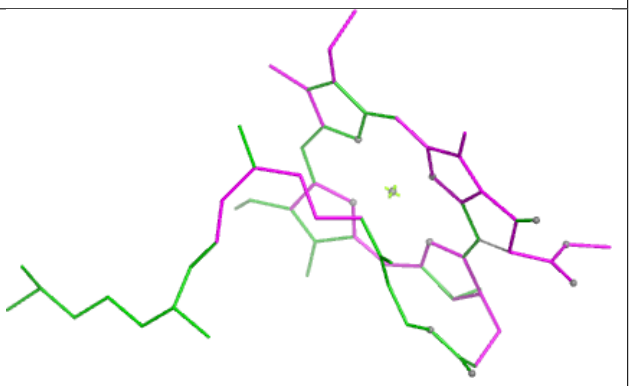


Rings

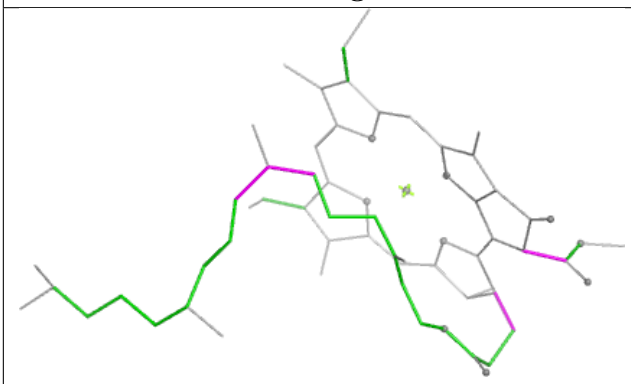
Ligand CLA B 614



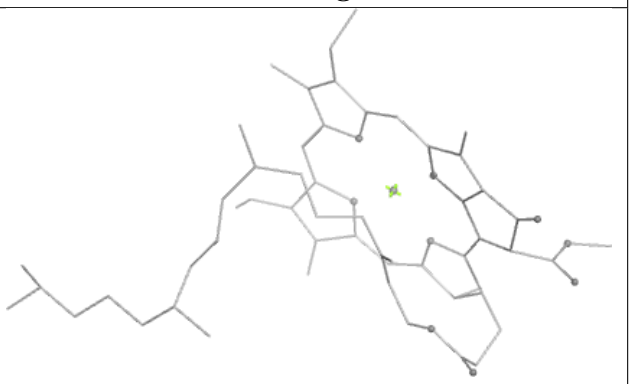
Bond lengths



Bond angles

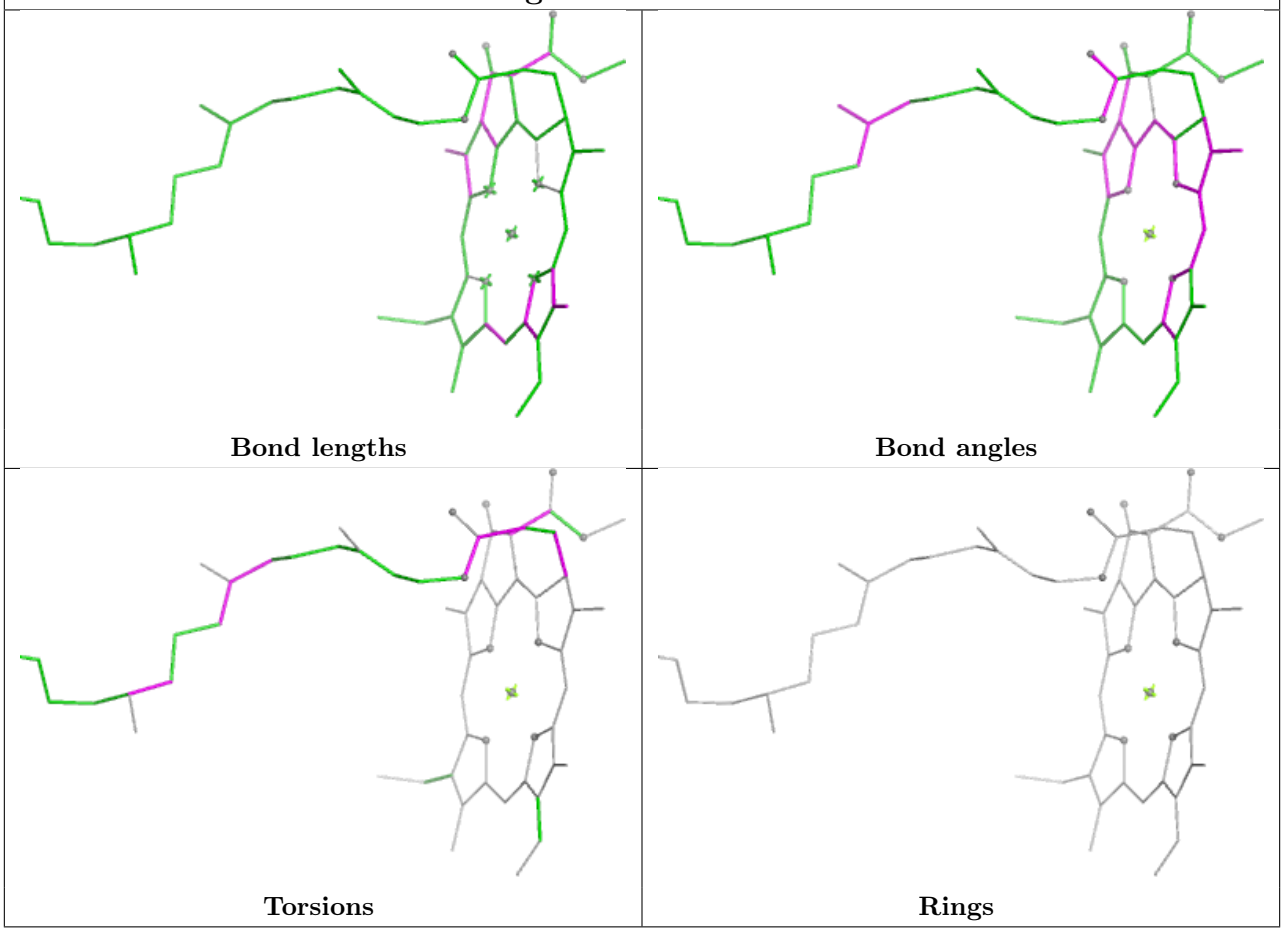


Torsions

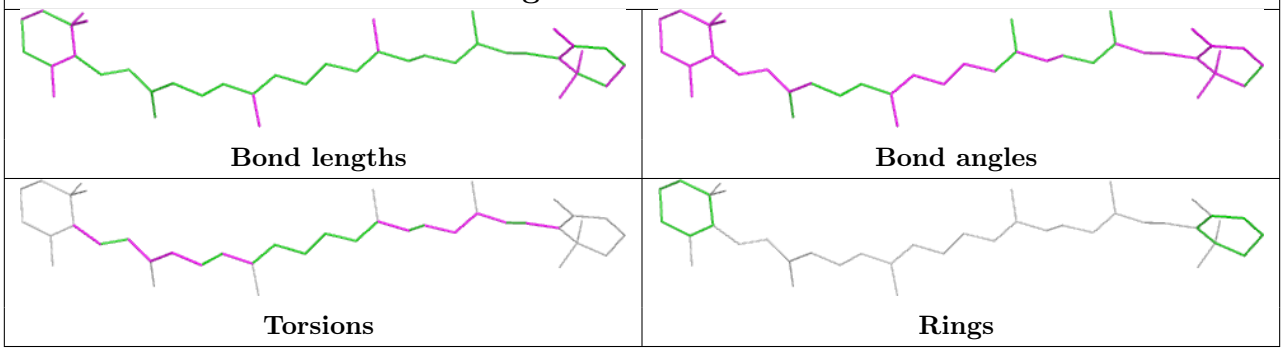


Rings

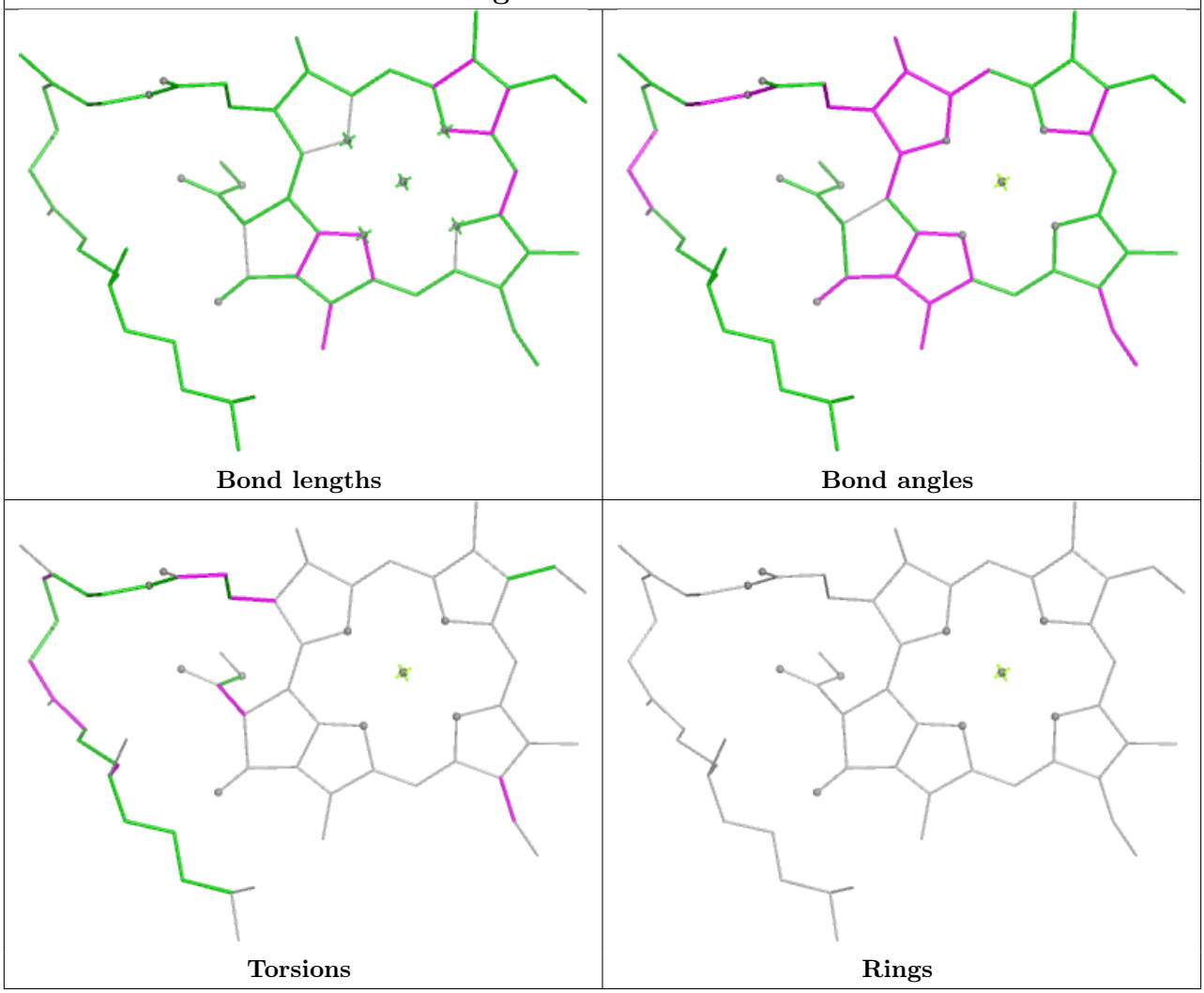
Ligand CLA C 510



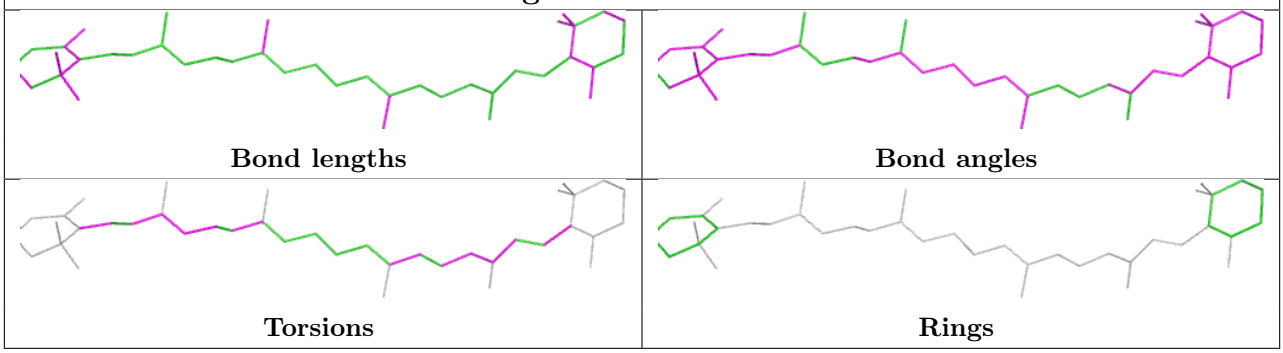
Ligand BCR K 101



Ligand CLA B 610



Ligand BCR H 101



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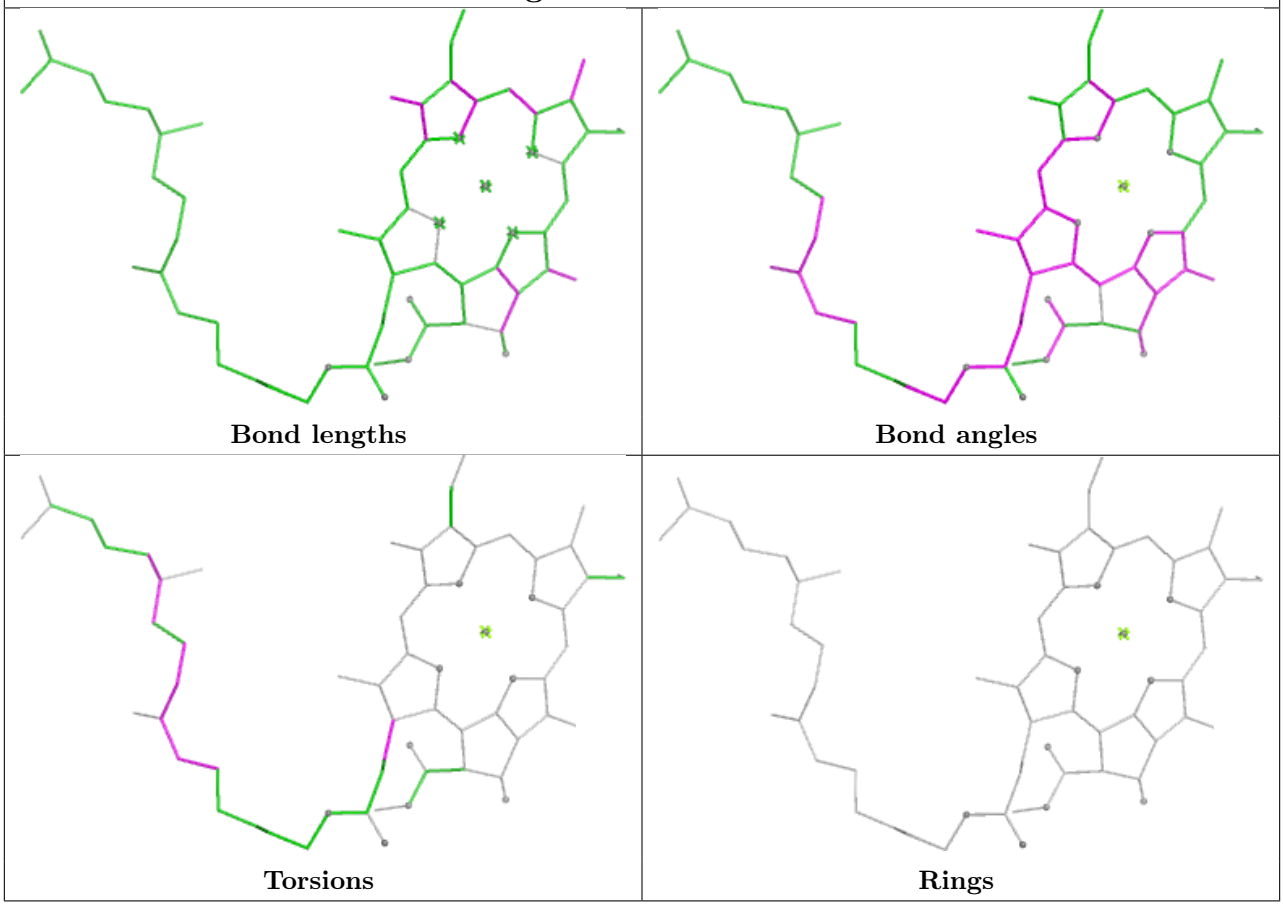
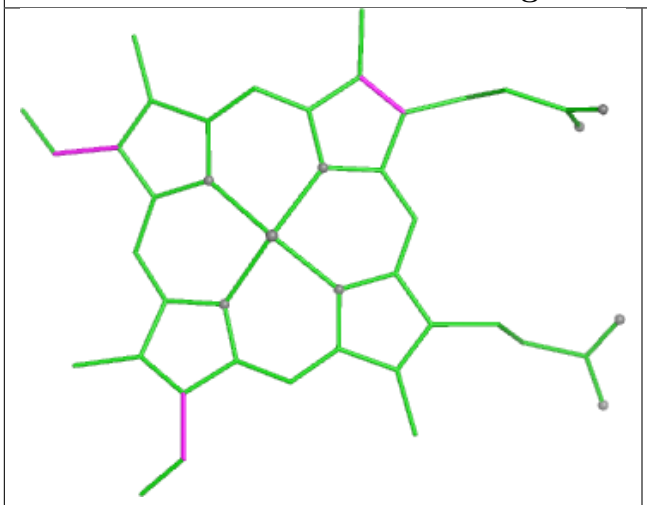
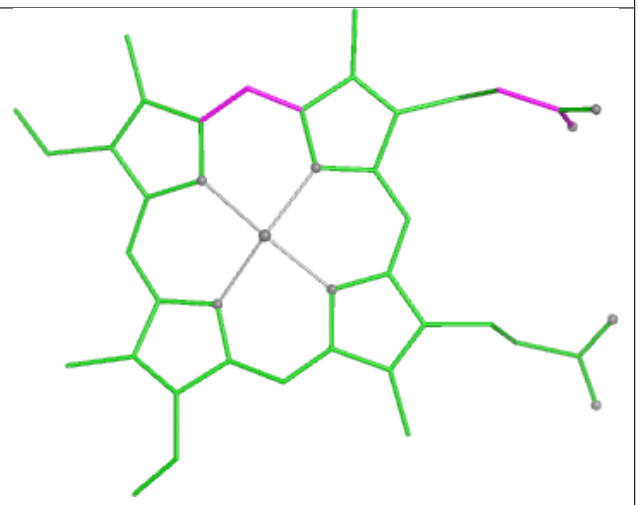


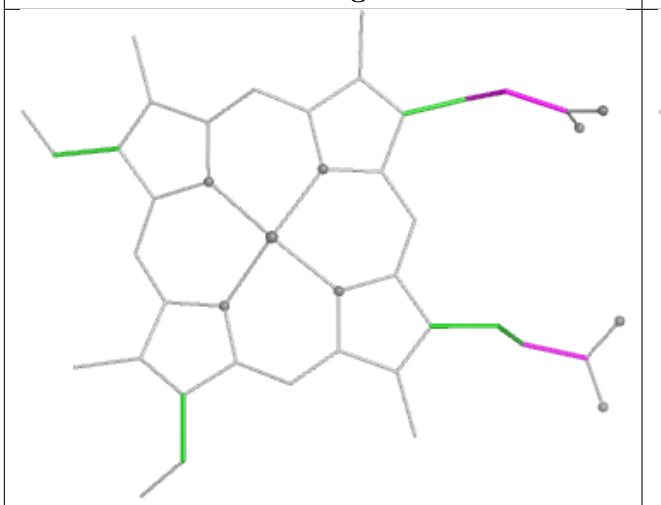
Ligand HEM E 101



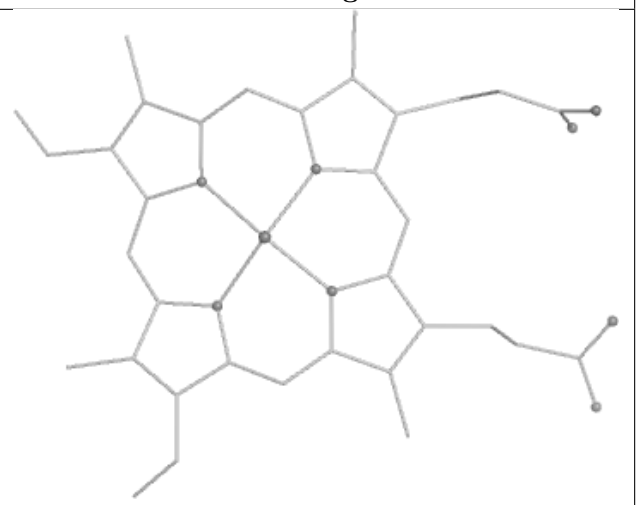
Bond lengths



Bond angles

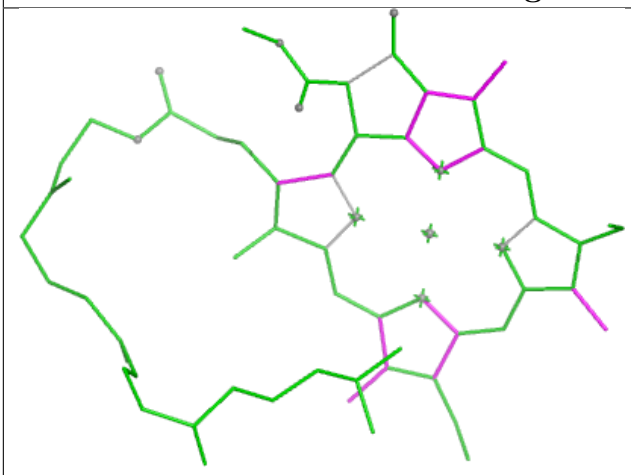


Torsions

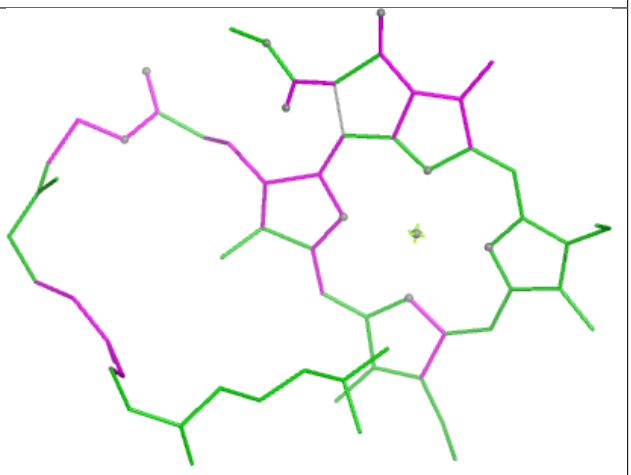


Rings

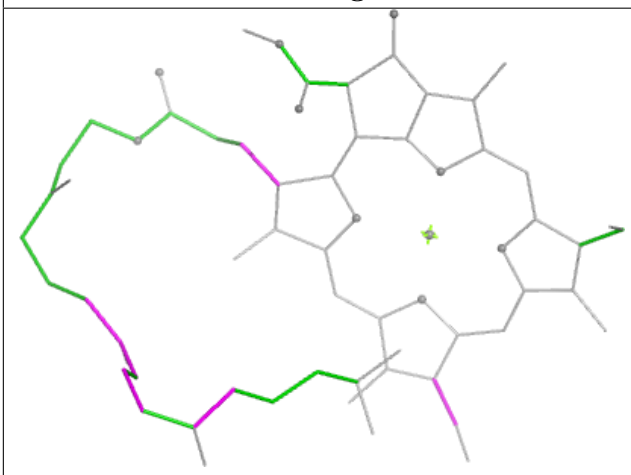
Ligand CLA B 615



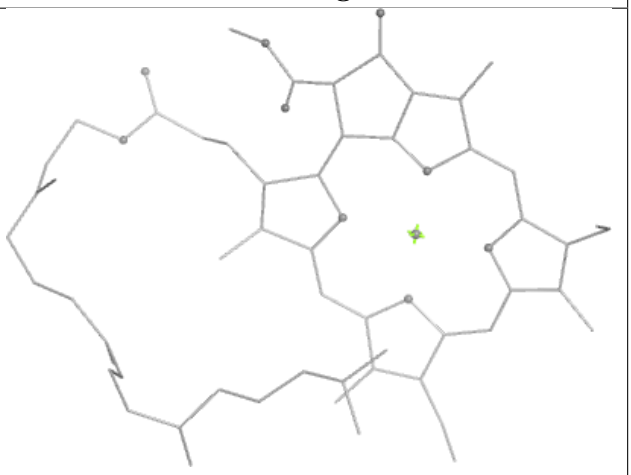
Bond lengths



Bond angles

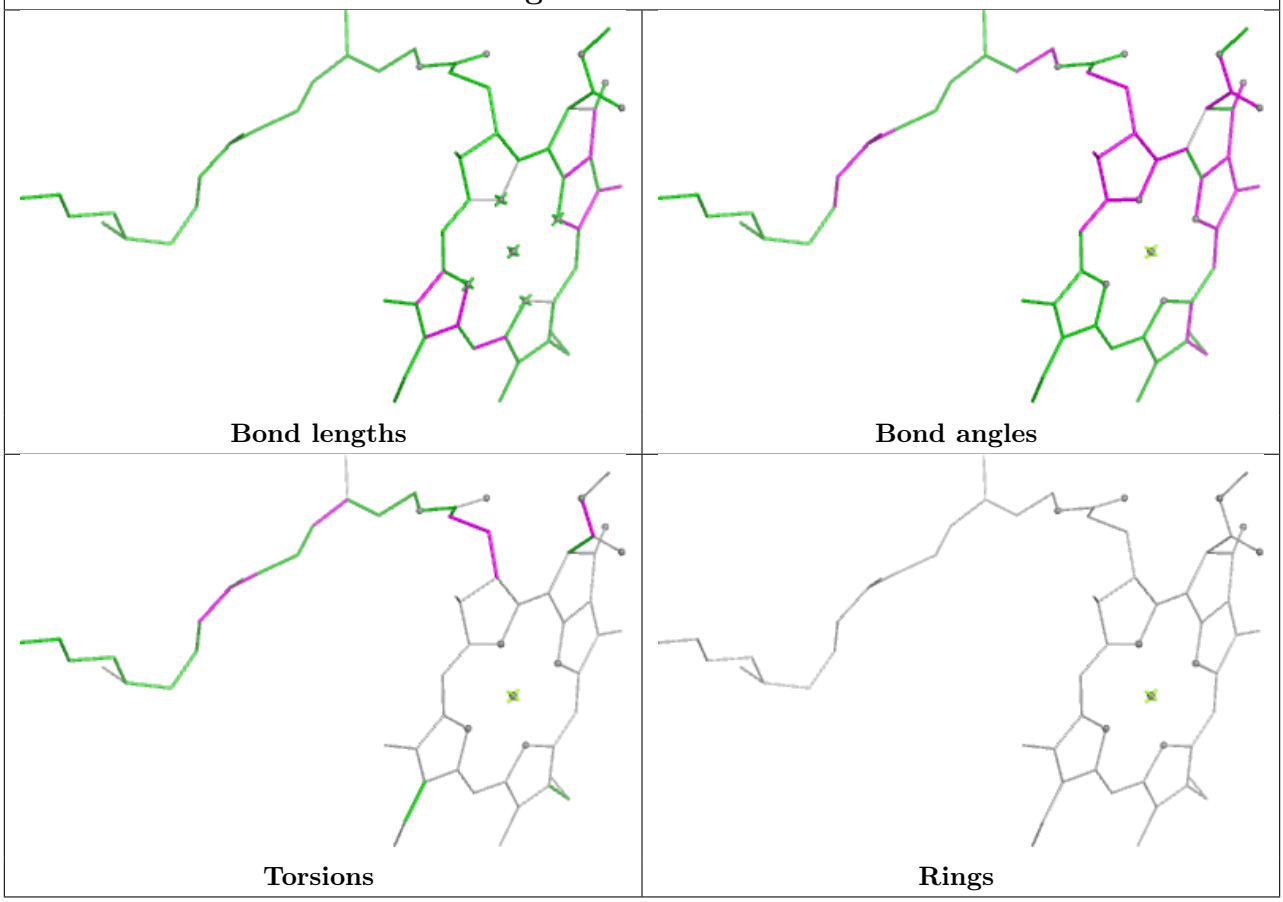


Torsions

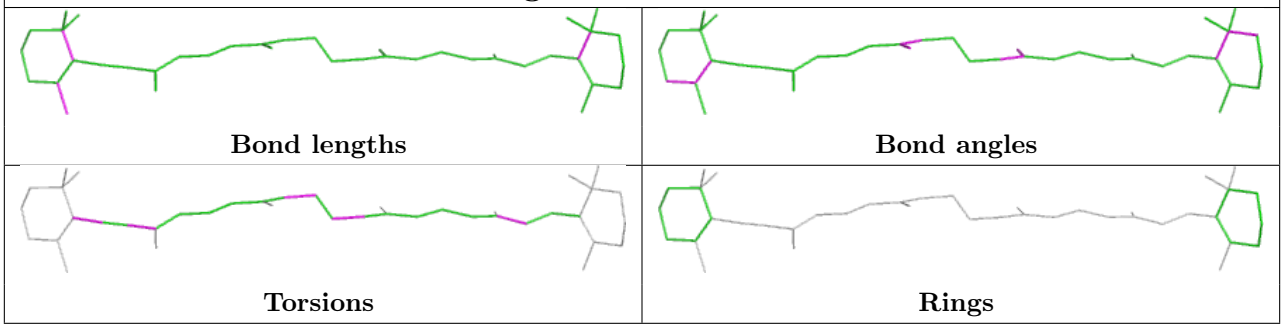


Rings

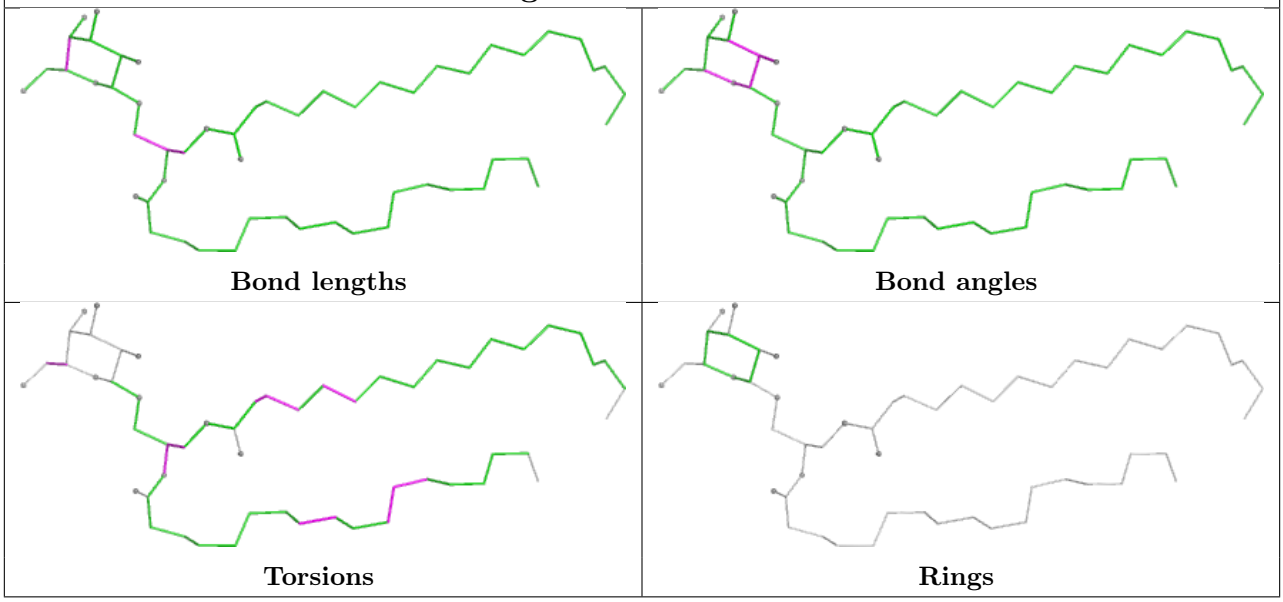
Ligand CLA C 512



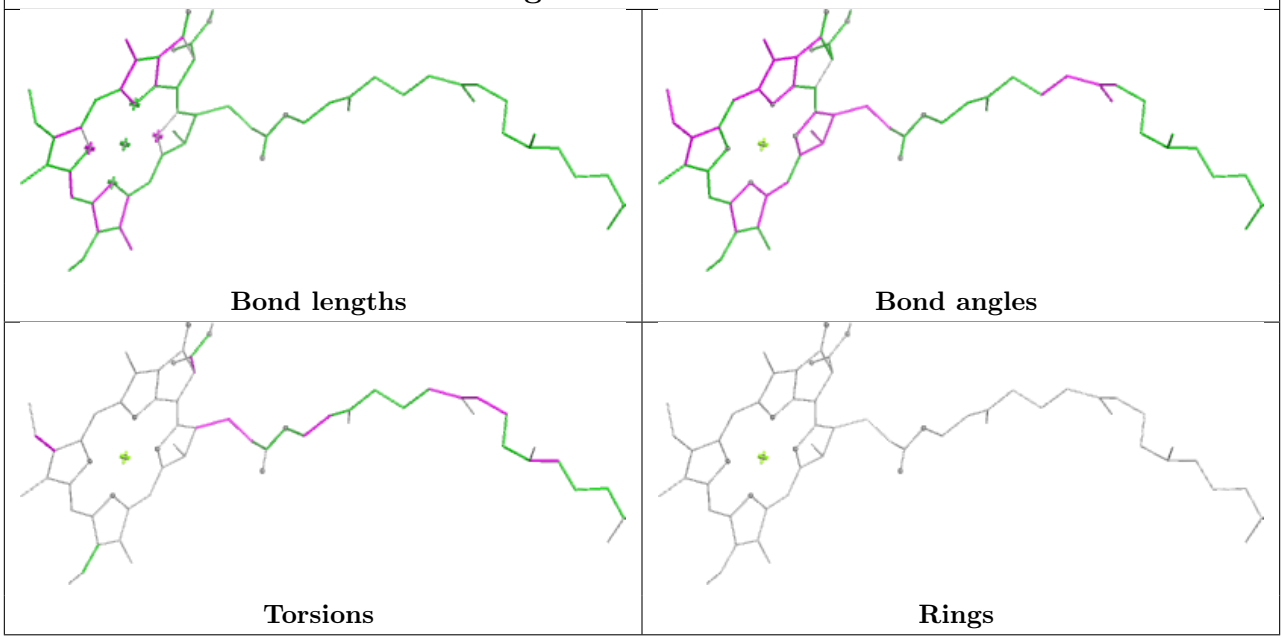
Ligand BCR C 516



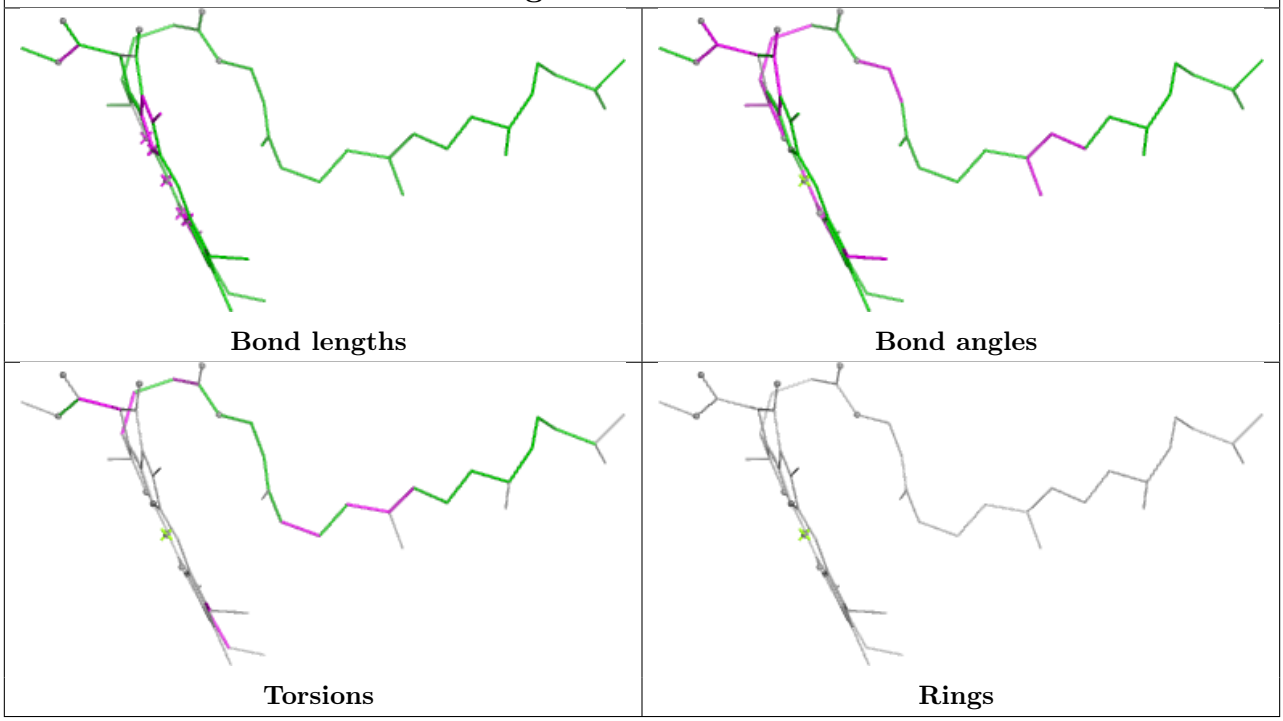
Ligand LMG C 501



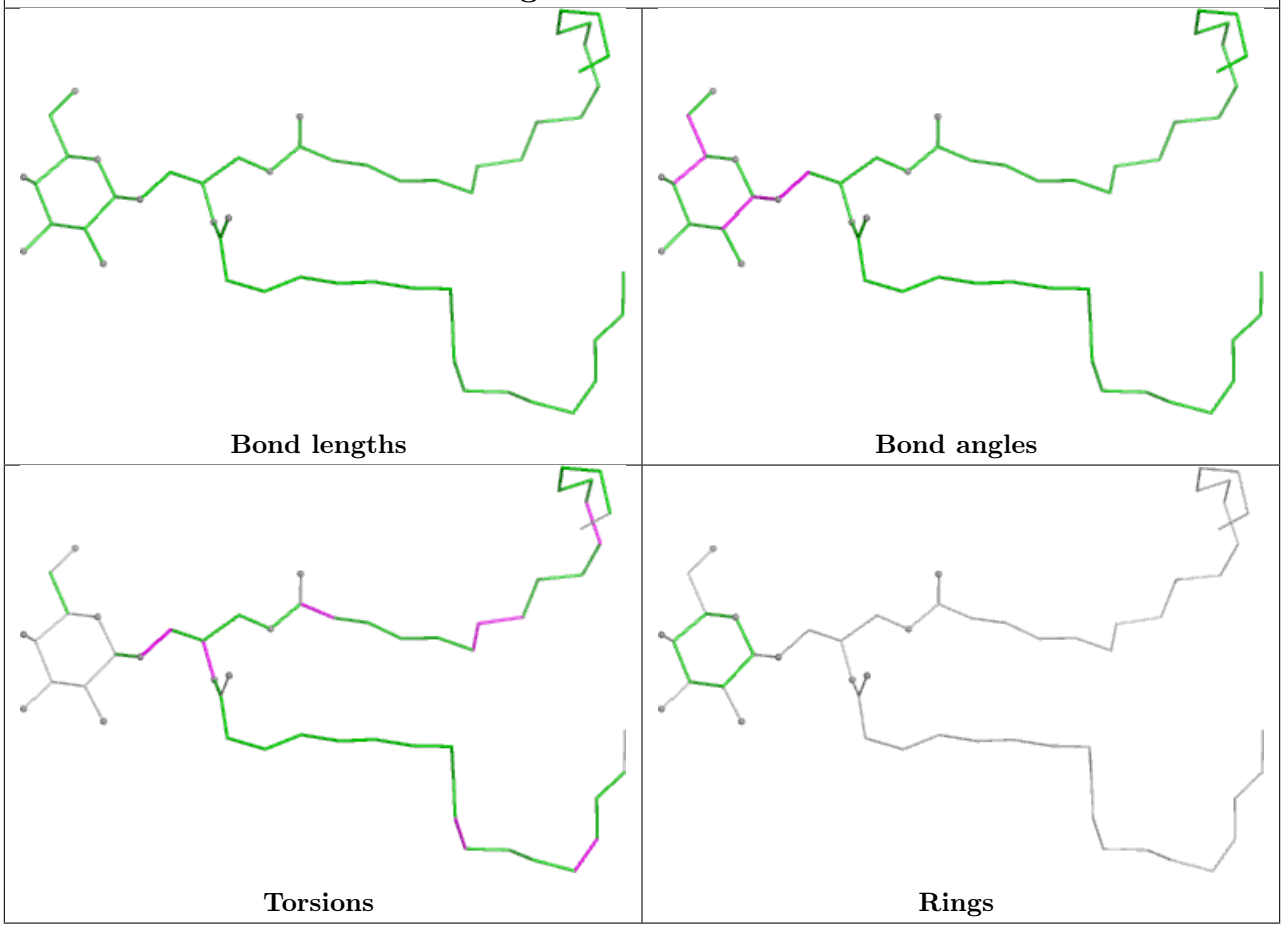
Ligand CLA D 408

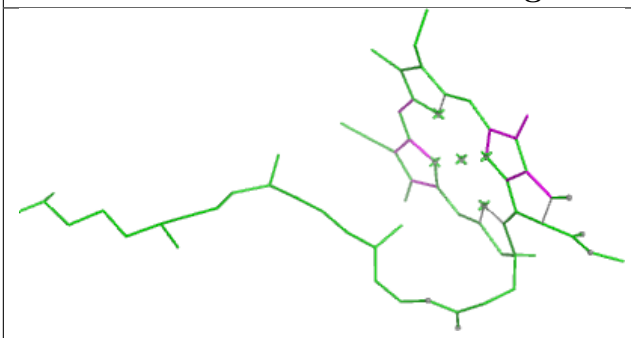
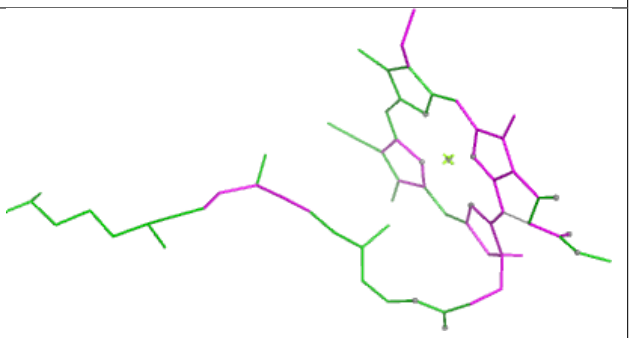
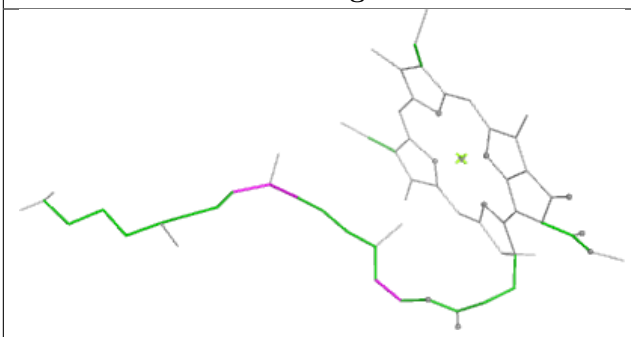
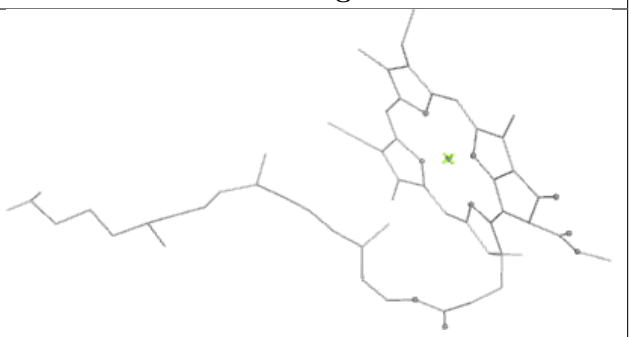


Ligand CLA C 506

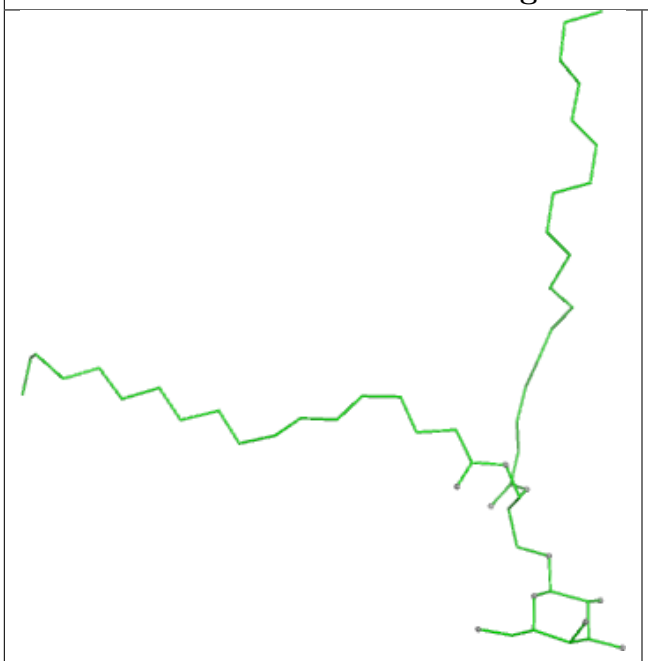


Ligand LMG D 404



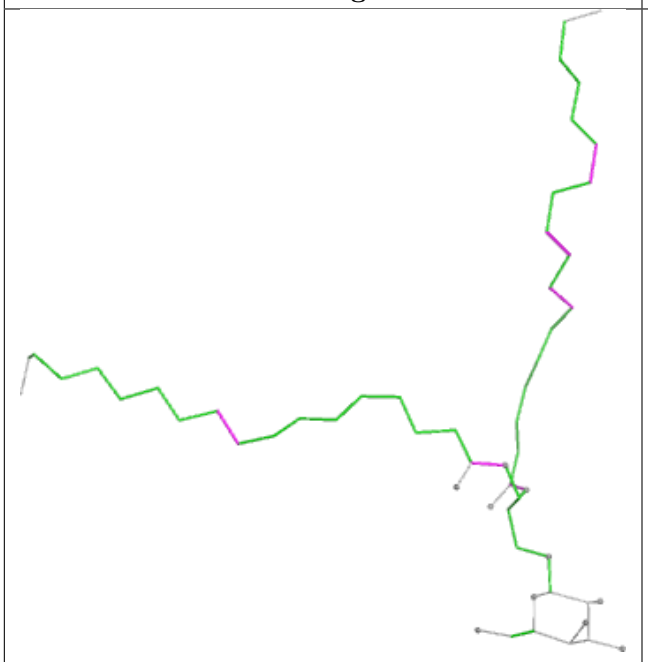
Ligand CLA C 507	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG D 402

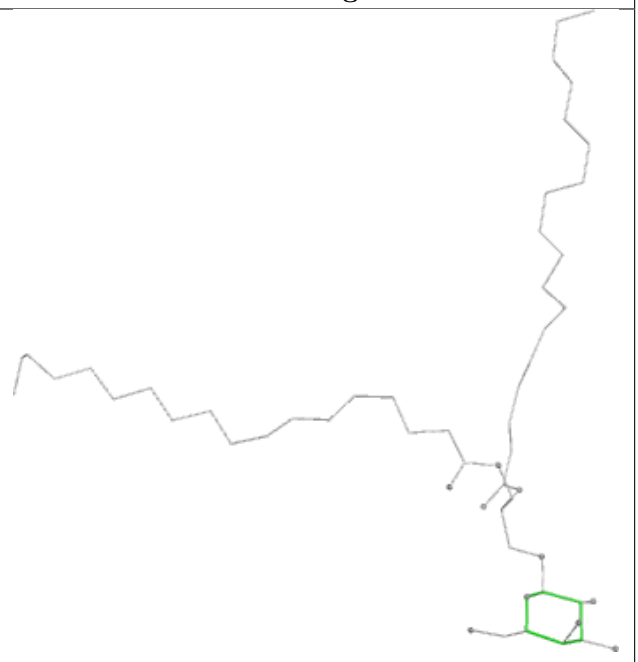


Bond lengths

Bond angles

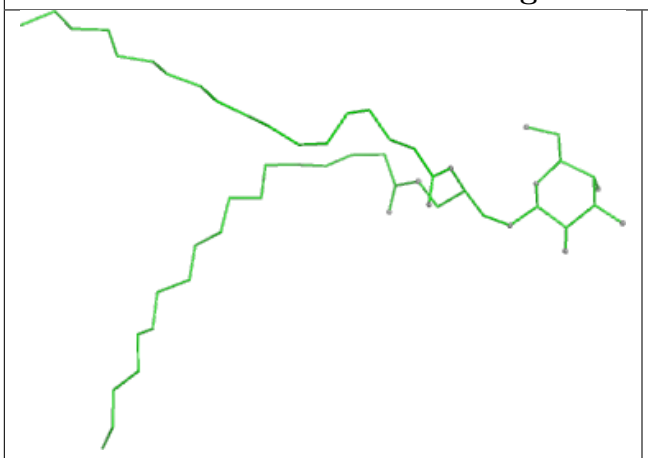


Torsions

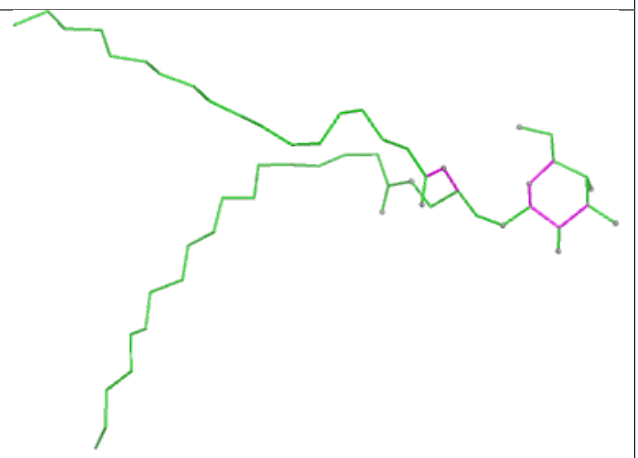


Rings

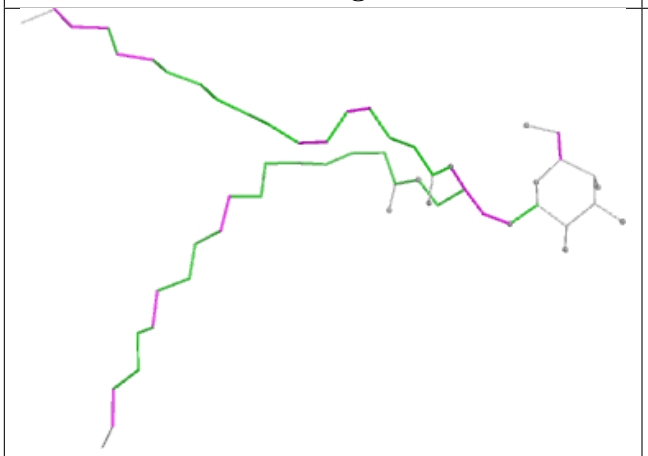
Ligand LMG D 405



Bond lengths



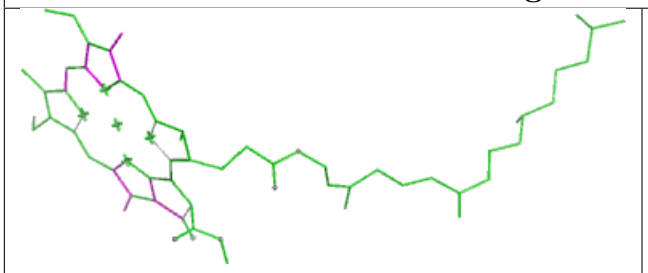
Bond angles



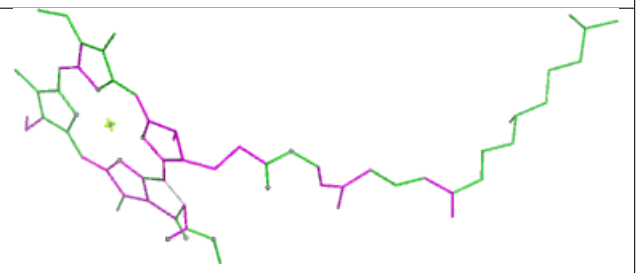
Torsions

Rings

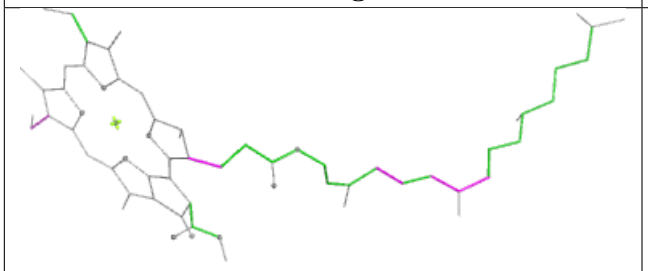
Ligand CLA A 404



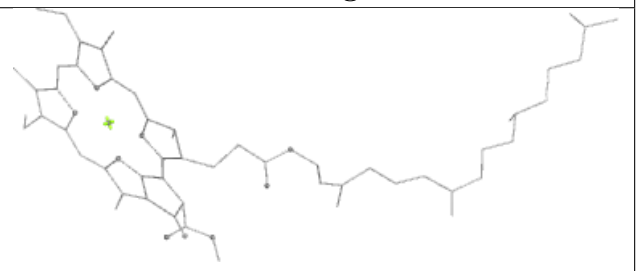
Bond lengths



Bond angles

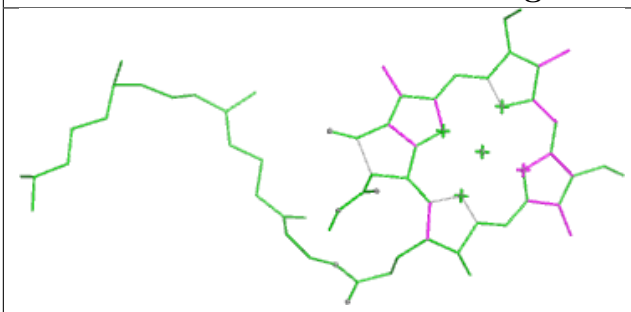


Torsions

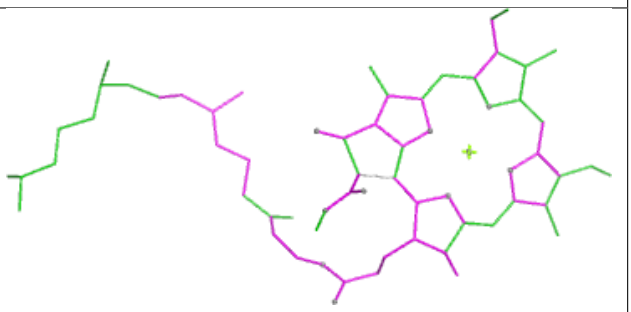


Rings

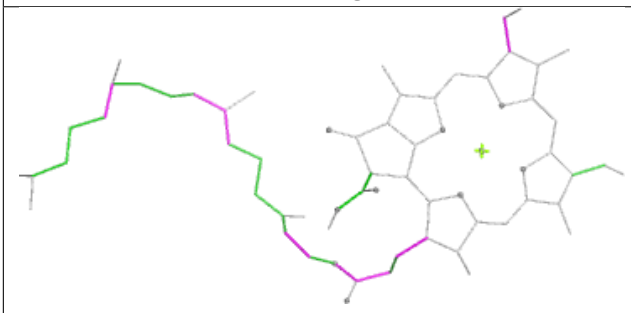
Ligand CLA B 602



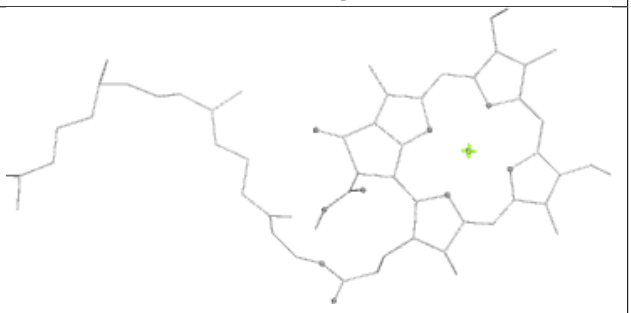
Bond lengths



Bond angles

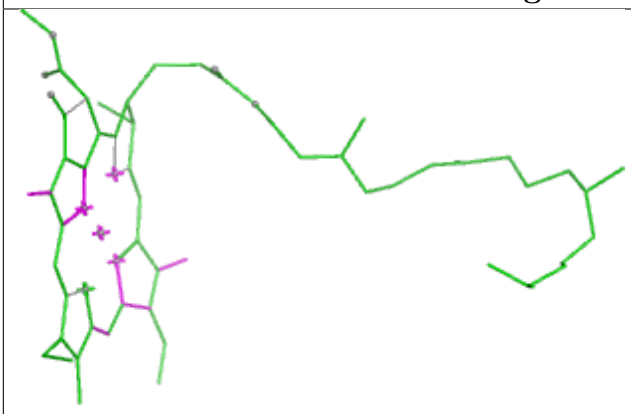


Torsions

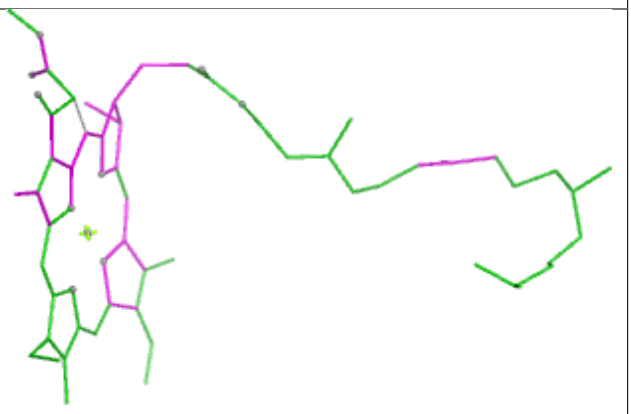


Rings

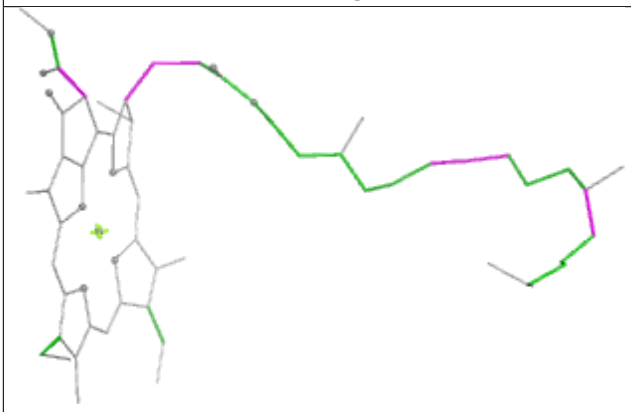
Ligand CLA A 407



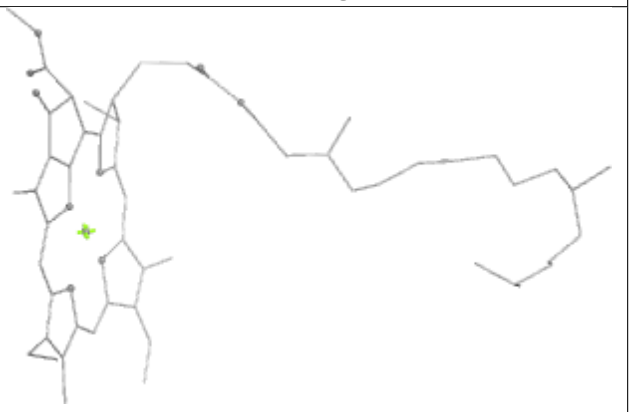
Bond lengths



Bond angles

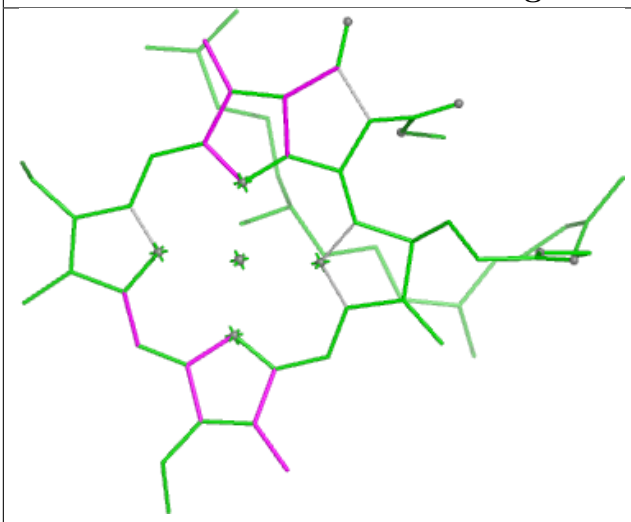


Torsions

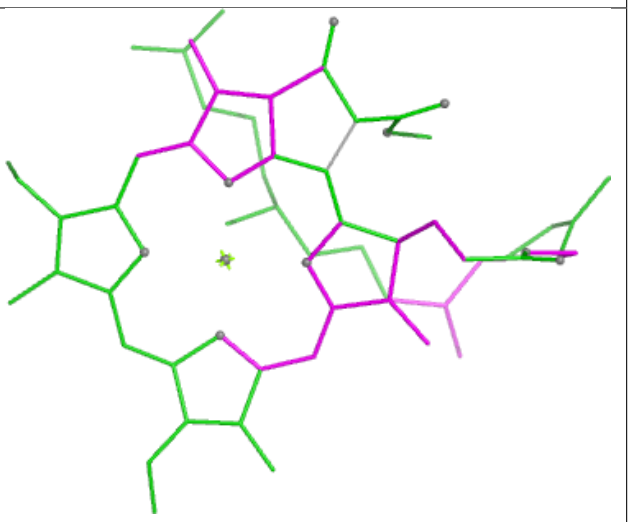


Rings

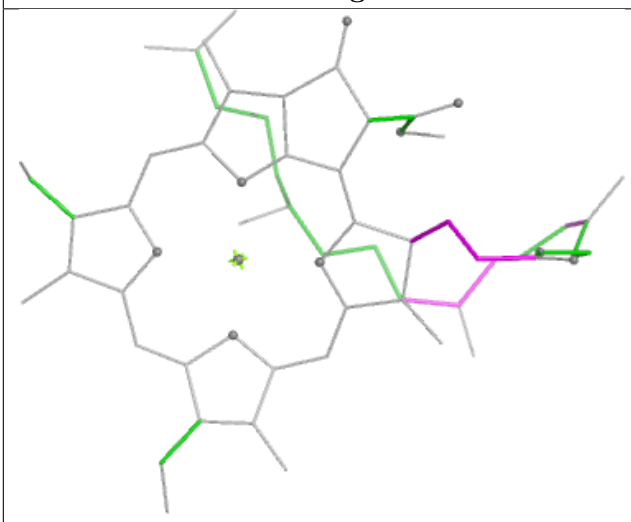
Ligand CLA C 517



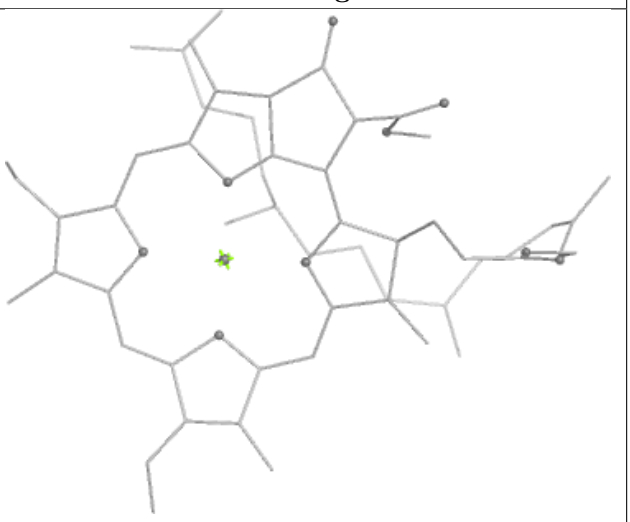
Bond lengths



Bond angles

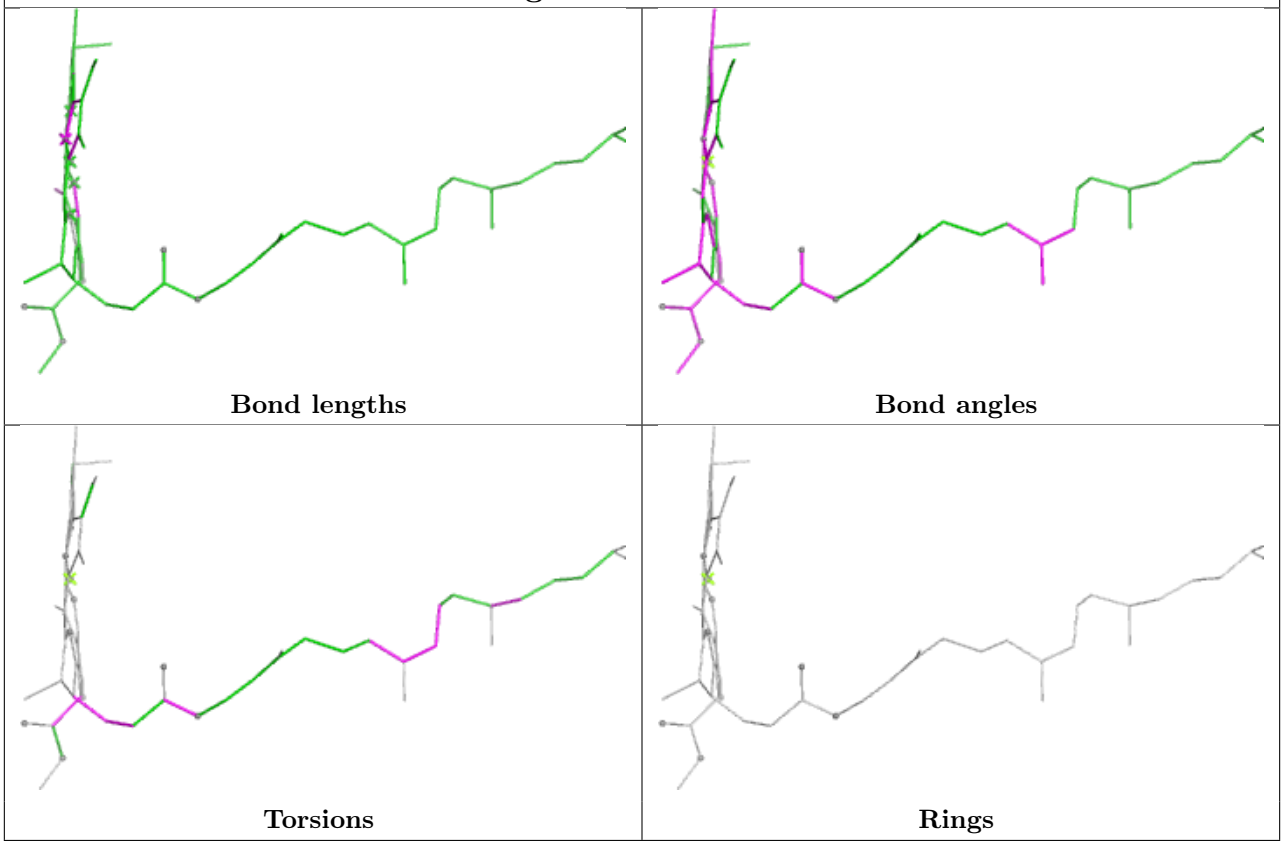


Torsions



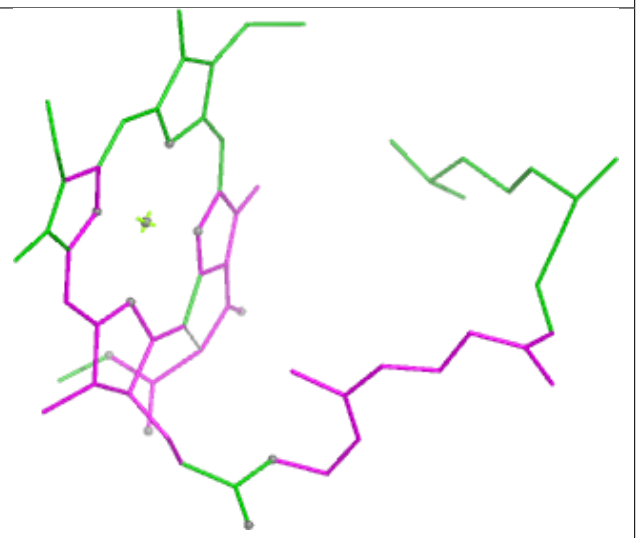
Rings

Ligand CLA B 606

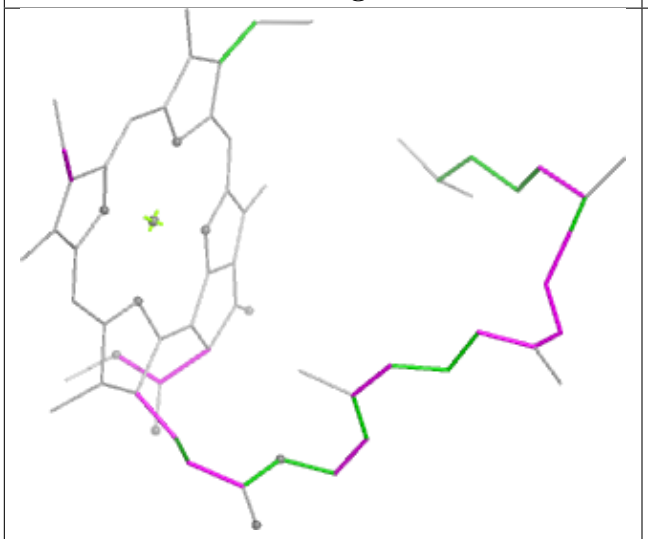


Ligand CLA C 505

Bond lengths



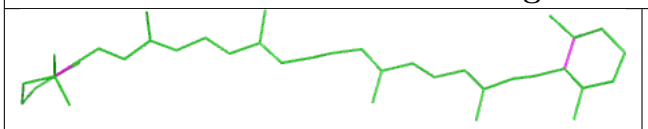
Bond angles



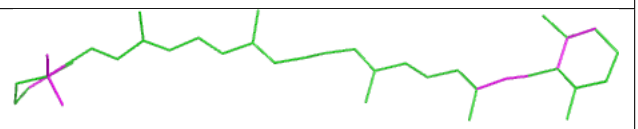
Torsions

Rings

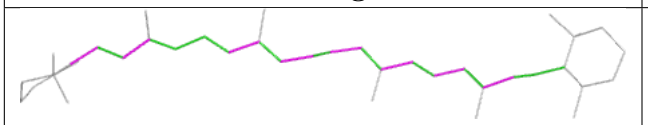
Ligand BCR C 518



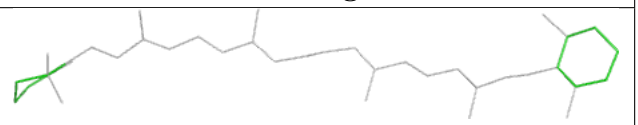
Bond lengths



Bond angles

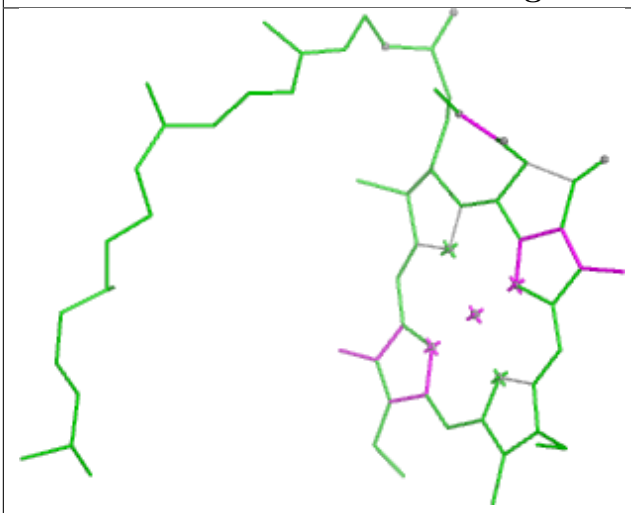


Torsions

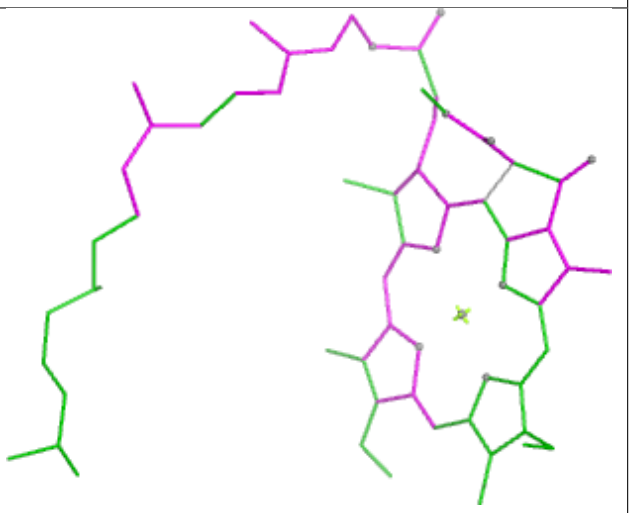


Rings

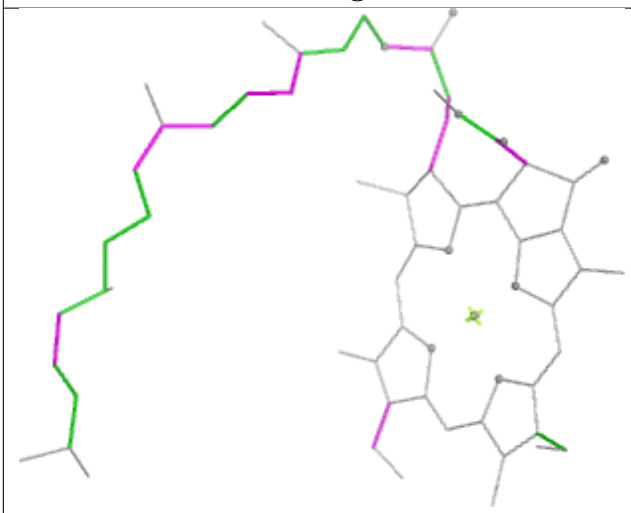
Ligand CLA C 509



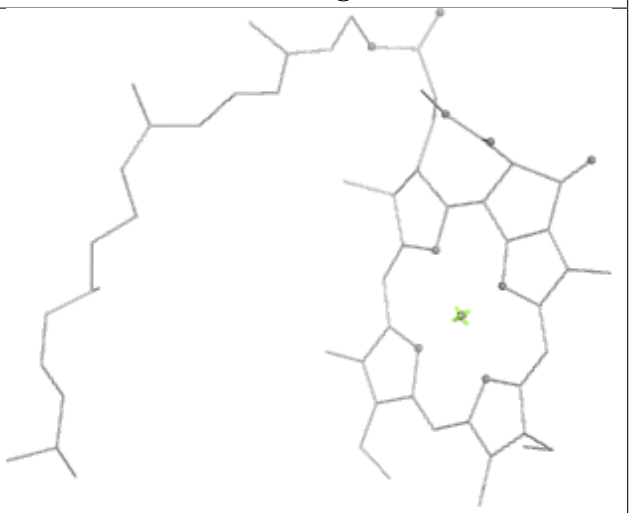
Bond lengths



Bond angles

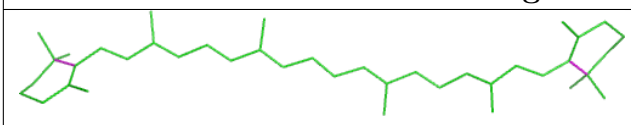


Torsions

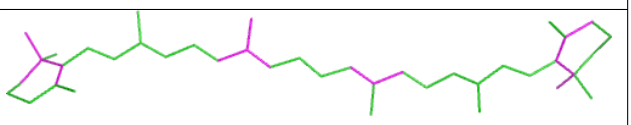


Rings

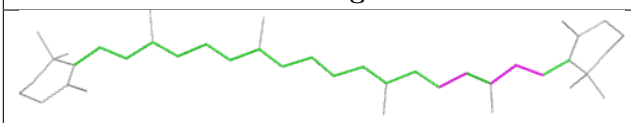
Ligand BCR B 618



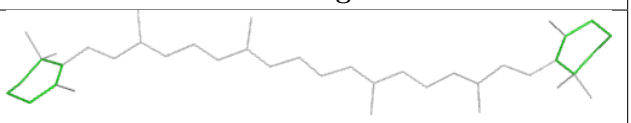
Bond lengths



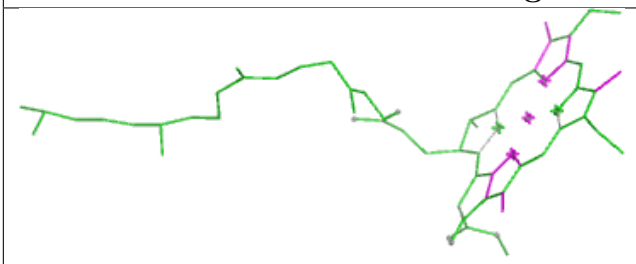
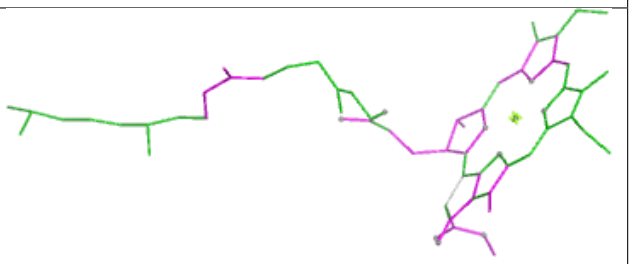
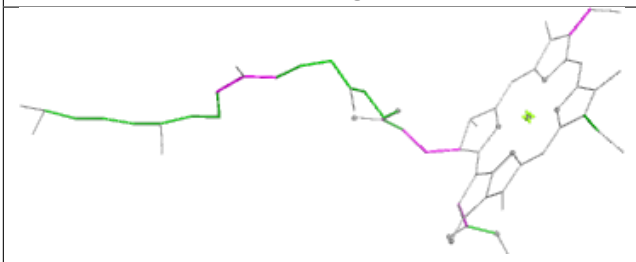
Bond angles



Torsions



Rings

Ligand CLA C 504	
 Bond lengths	 Bond angles
 Torsions	Rings

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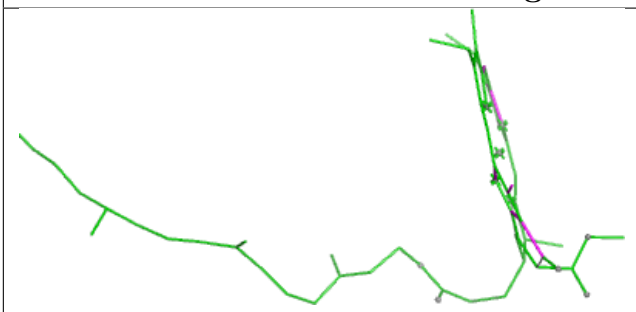
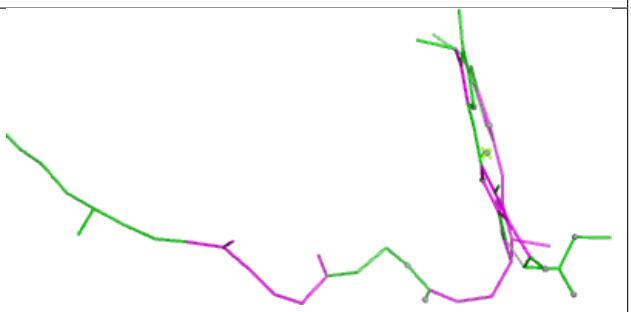
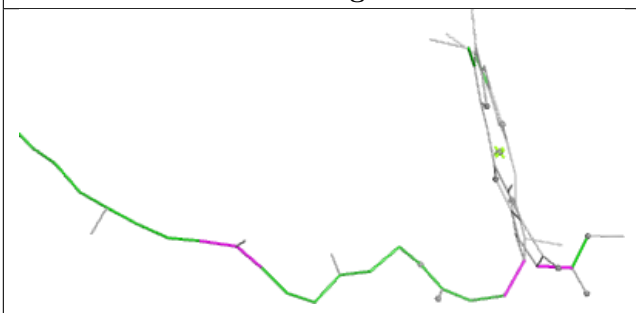
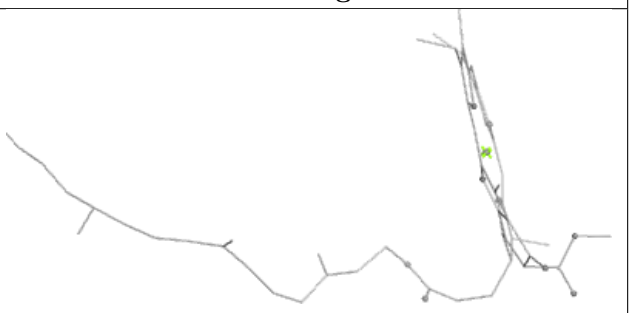
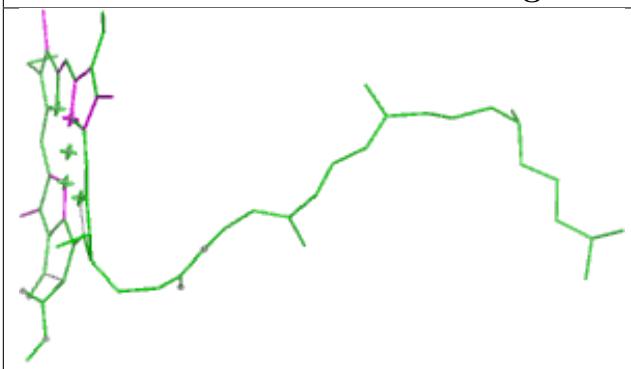
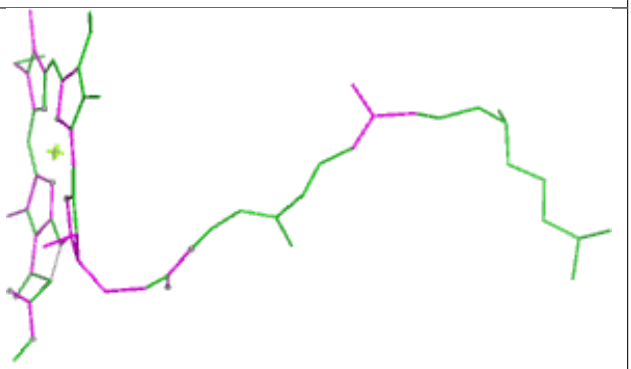
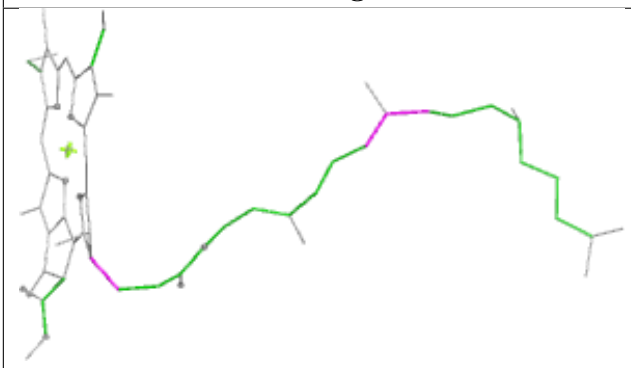
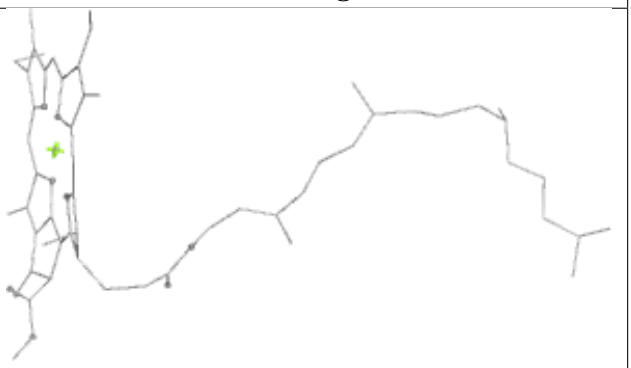
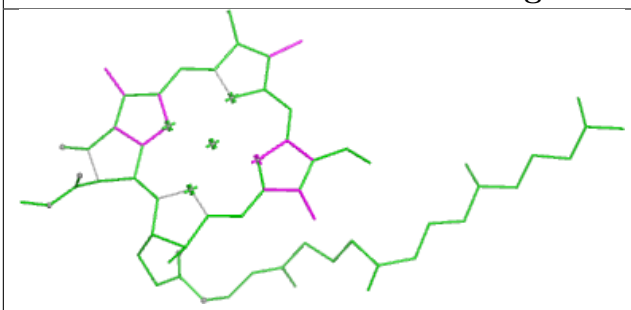
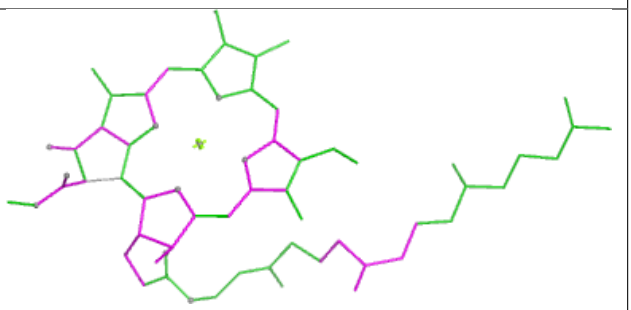
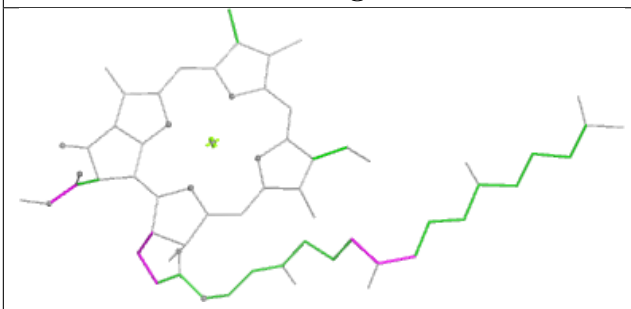
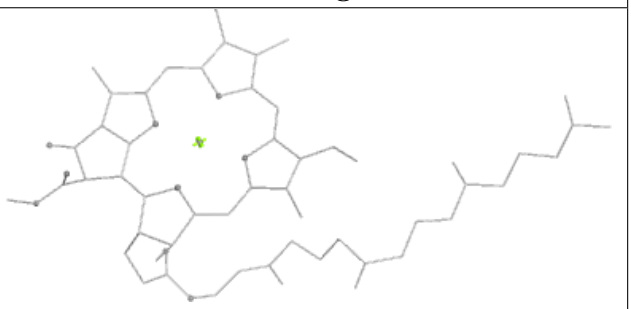
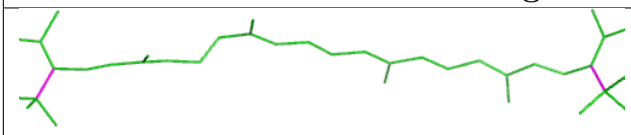
 Bond lengths	 Bond angles
 Torsions	 Rings

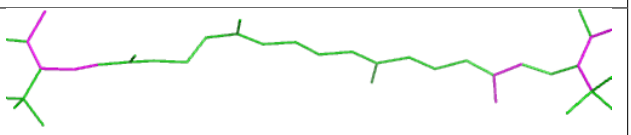
Ligand CLA D 409	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

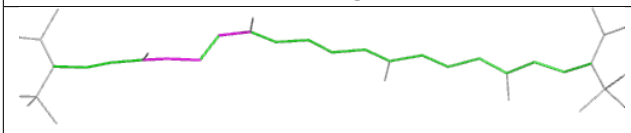
Ligand BCR B 619



Bond lengths



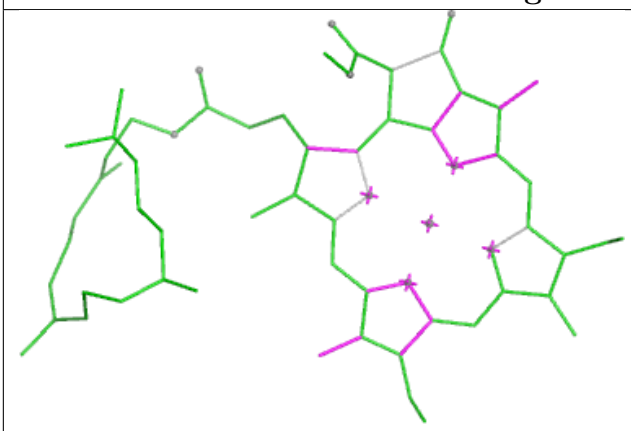
Bond angles



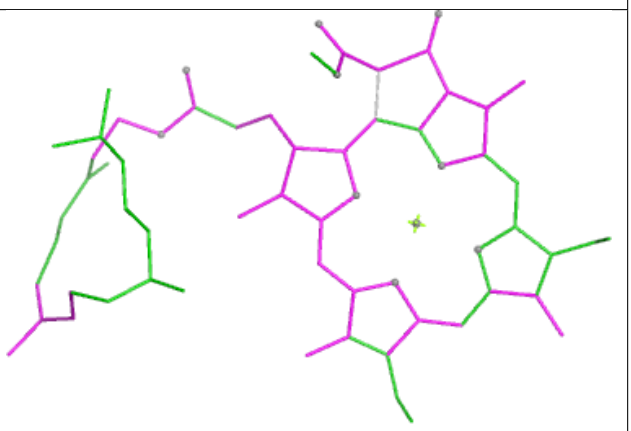
Torsions

Rings

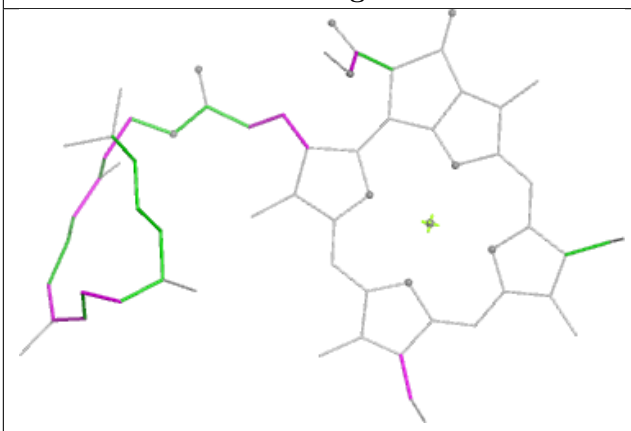
Ligand CLA C 513



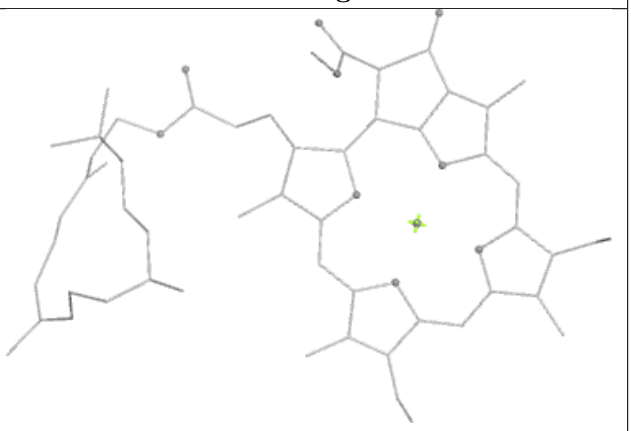
Bond lengths



Bond angles

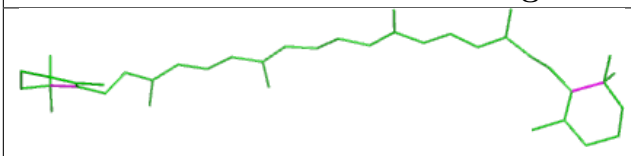


Torsions

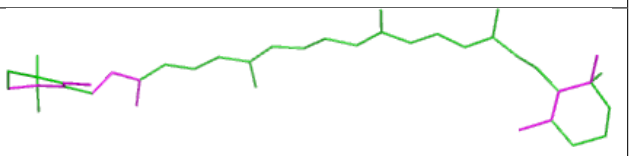


Rings

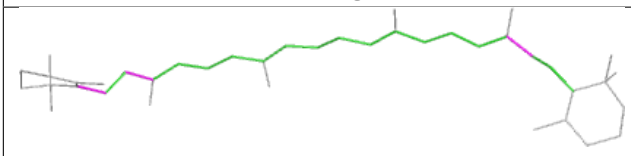
Ligand BCR D 410



Bond lengths



Bond angles



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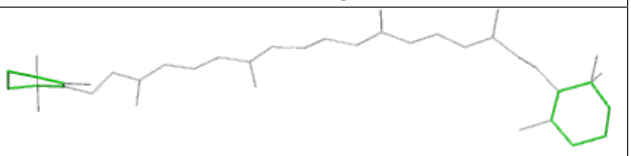
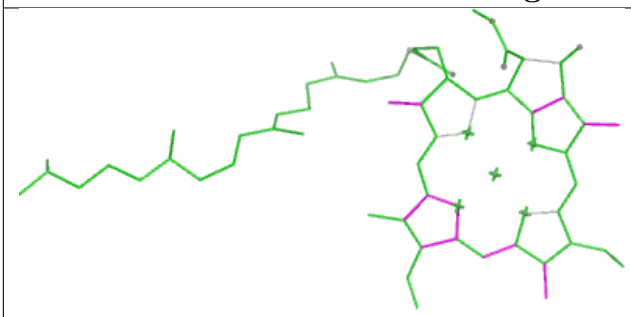


Rings

Ligand CLA A 405



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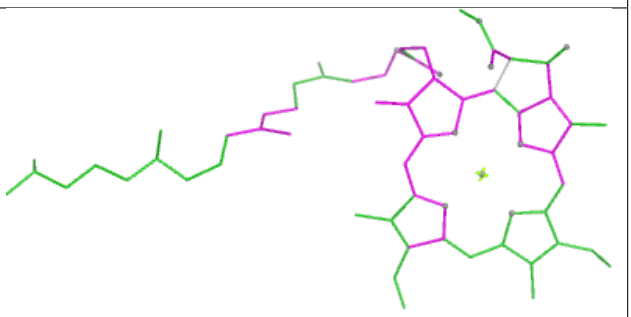
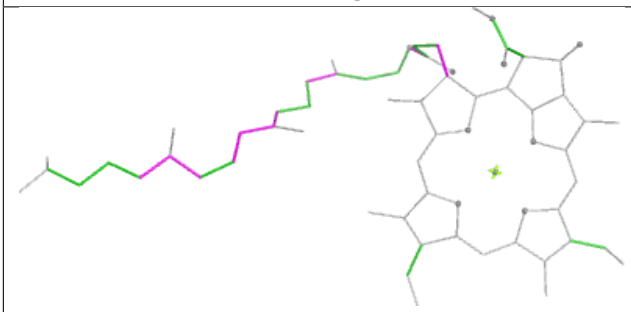
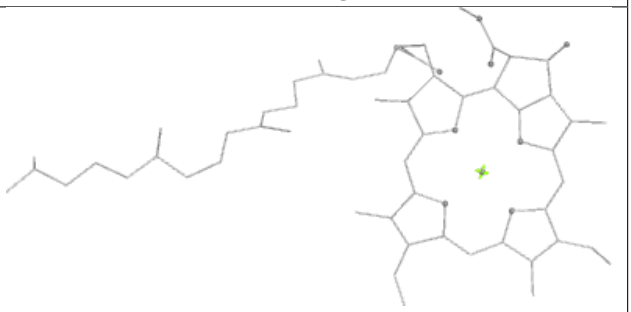


Bond angles

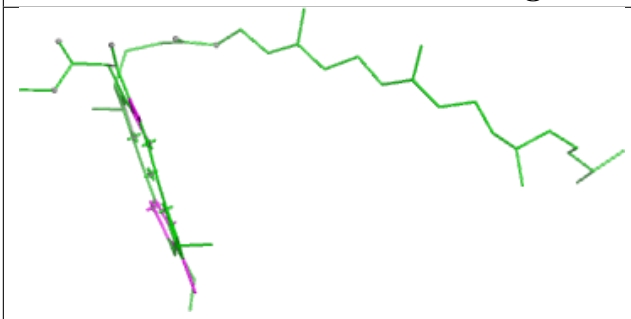


Torsions

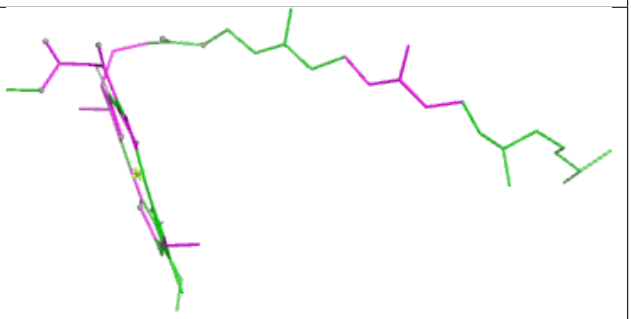


Rings

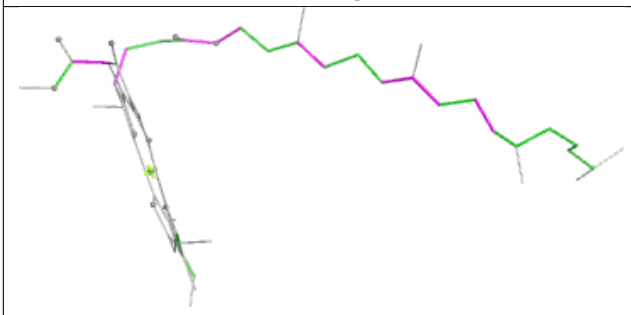
Ligand CLA B 605



Bond lengths



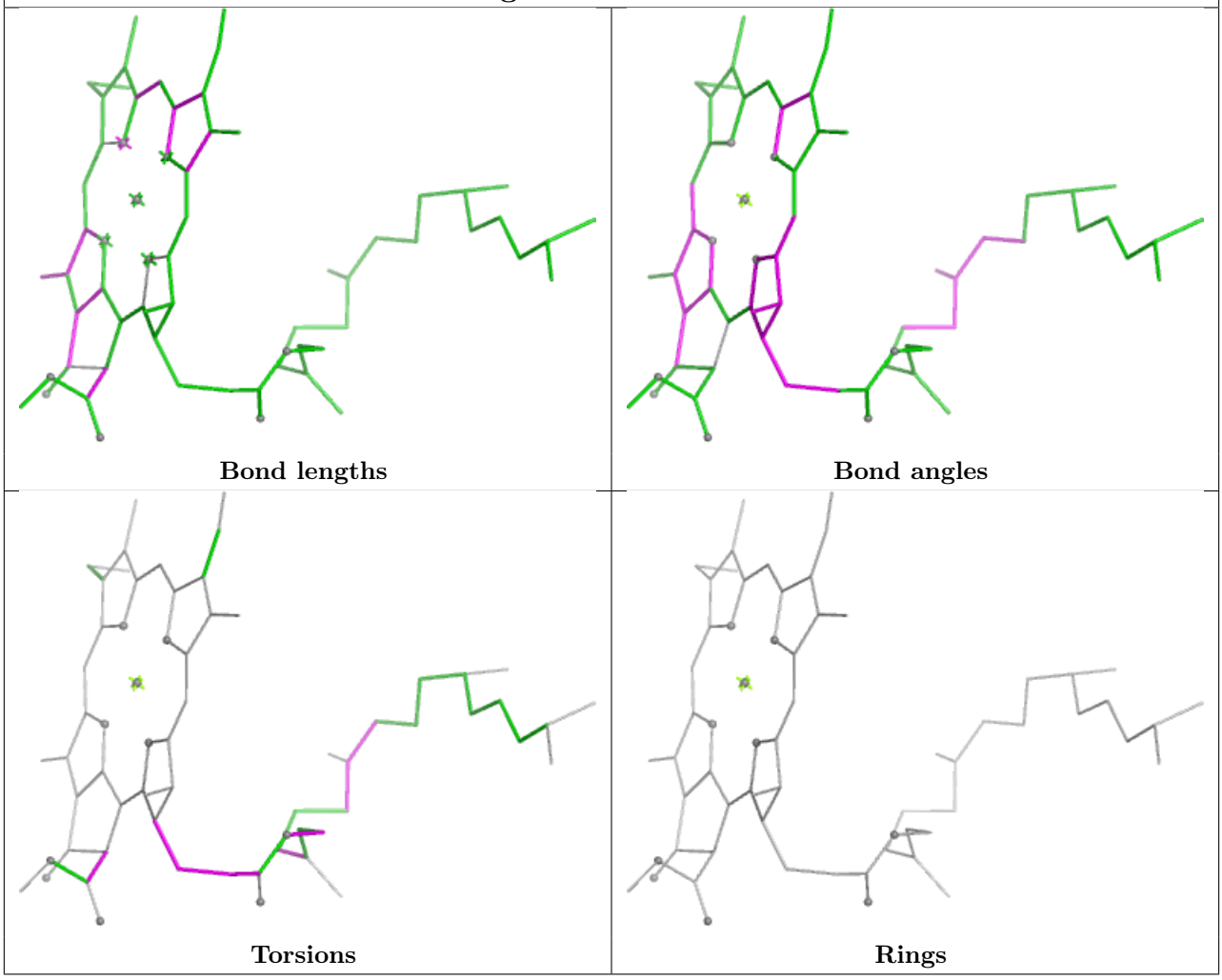
Bond angles



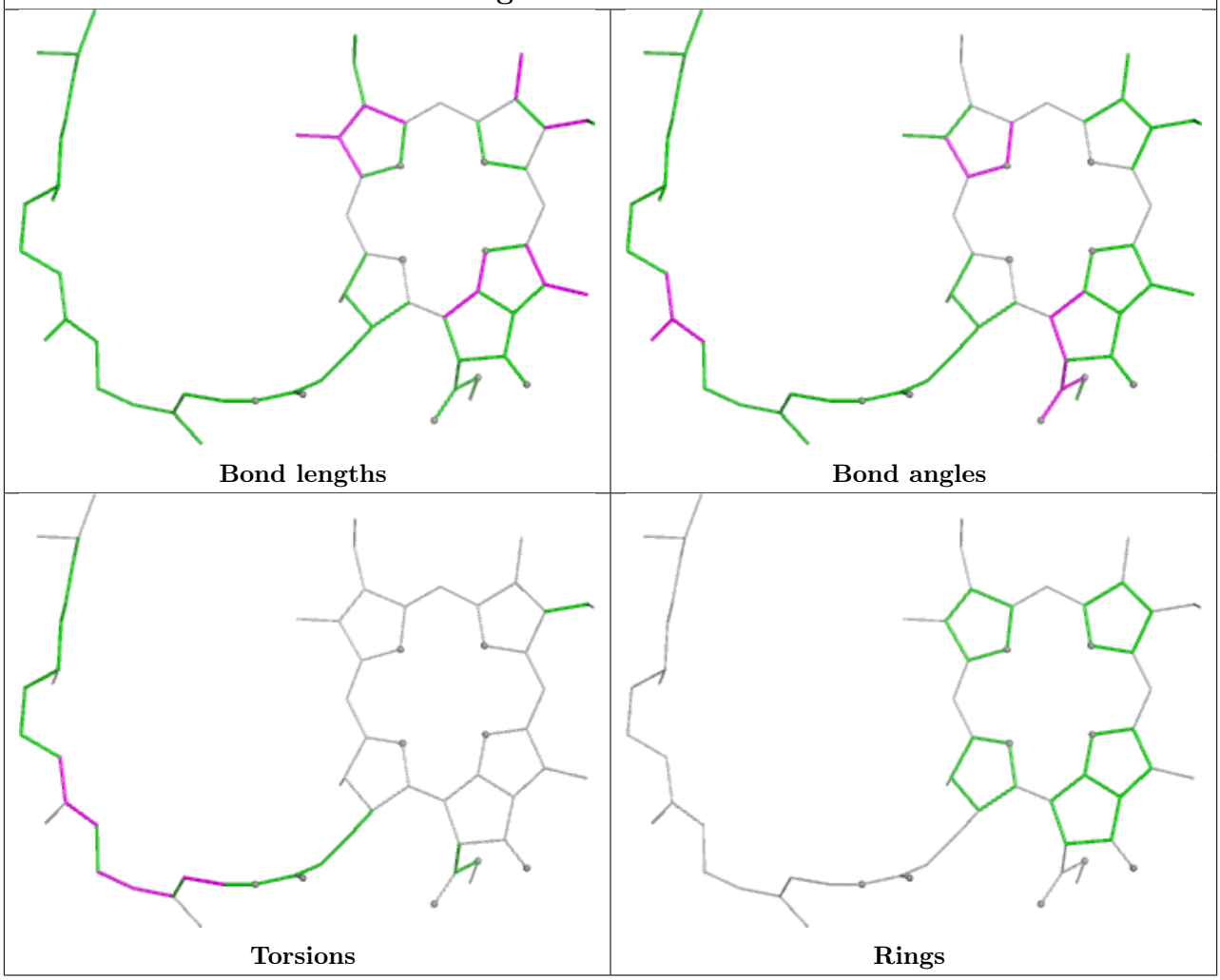
Torsions

Rings

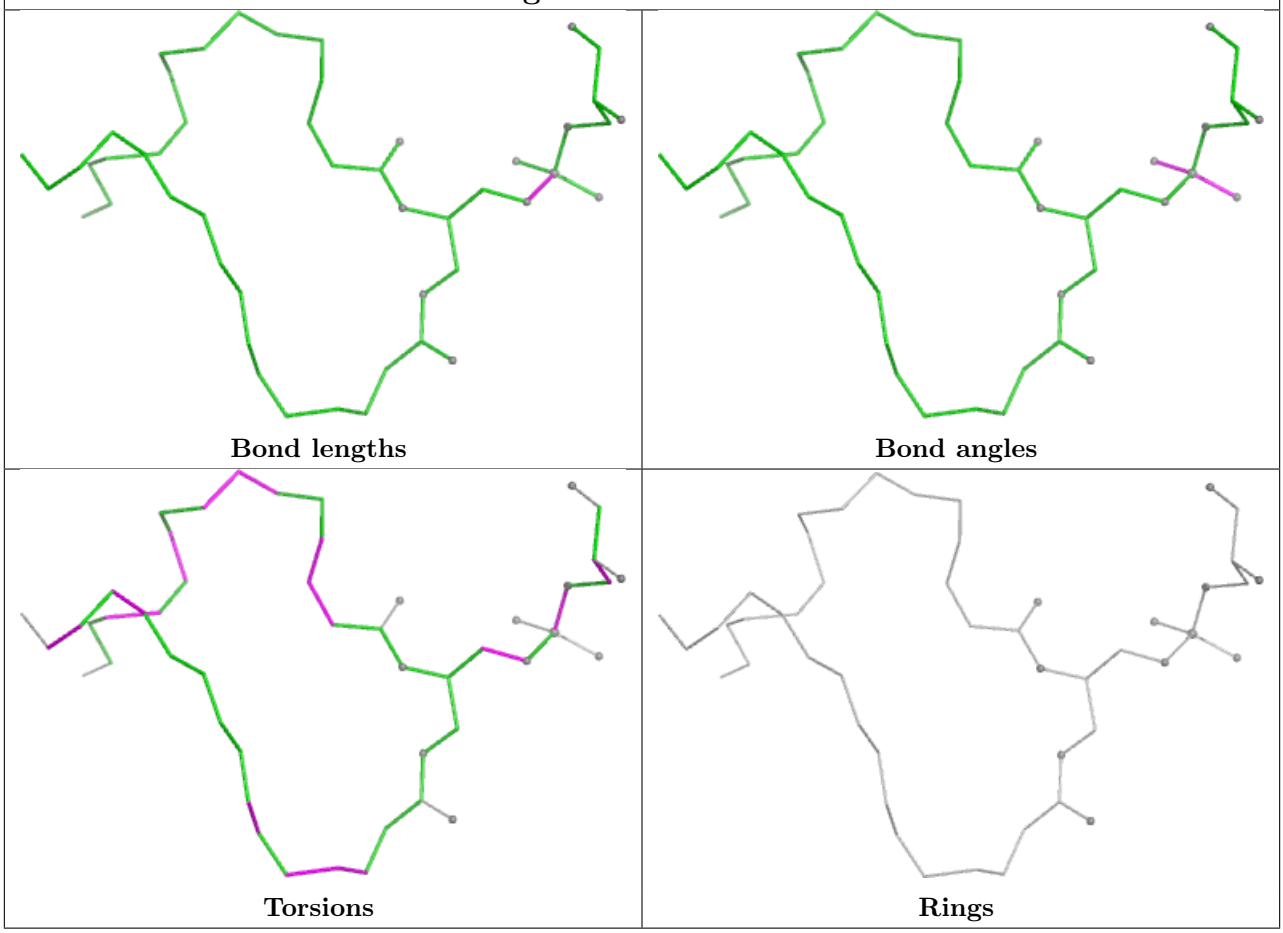
Ligand CLA C 514



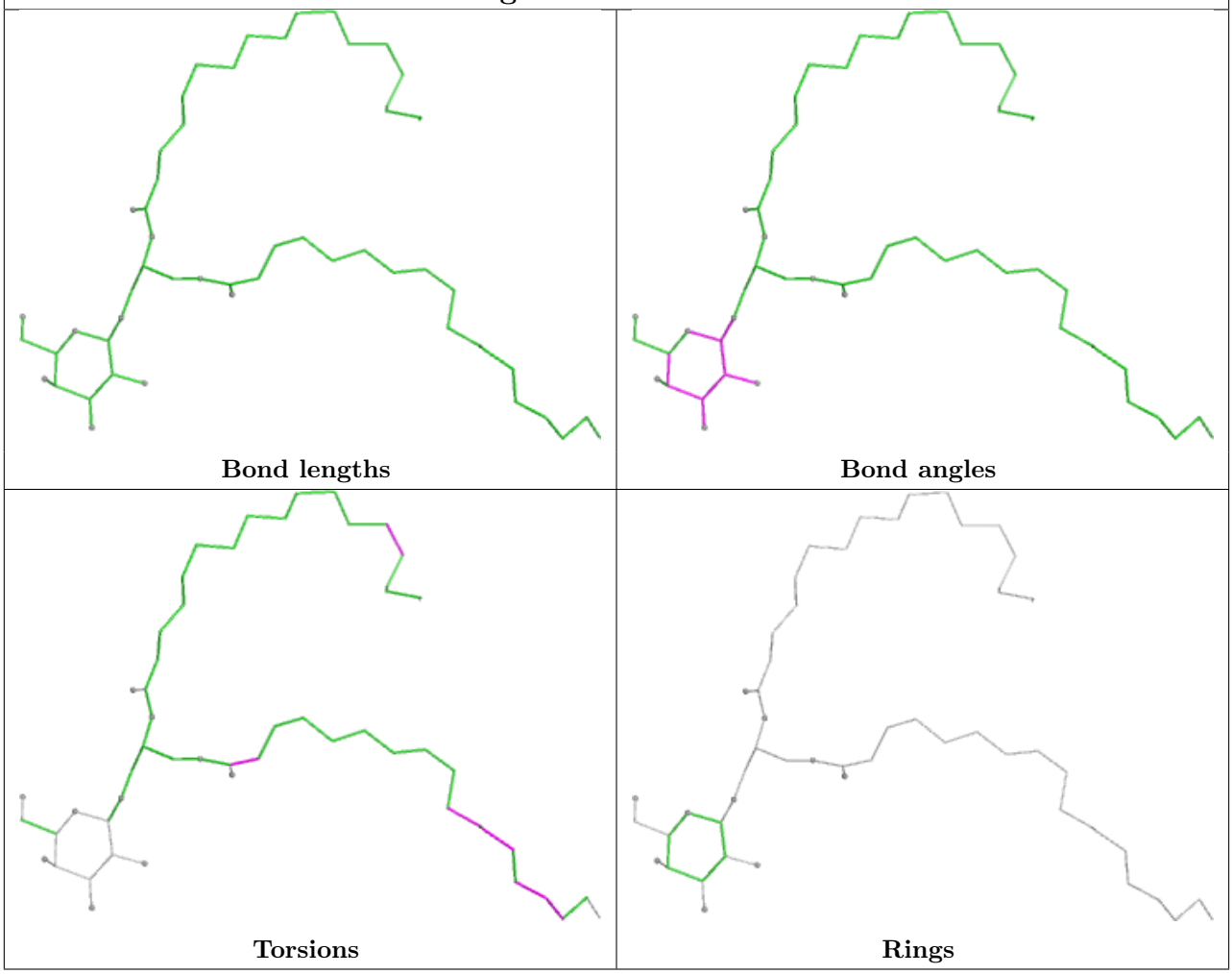
Ligand PHO A 403



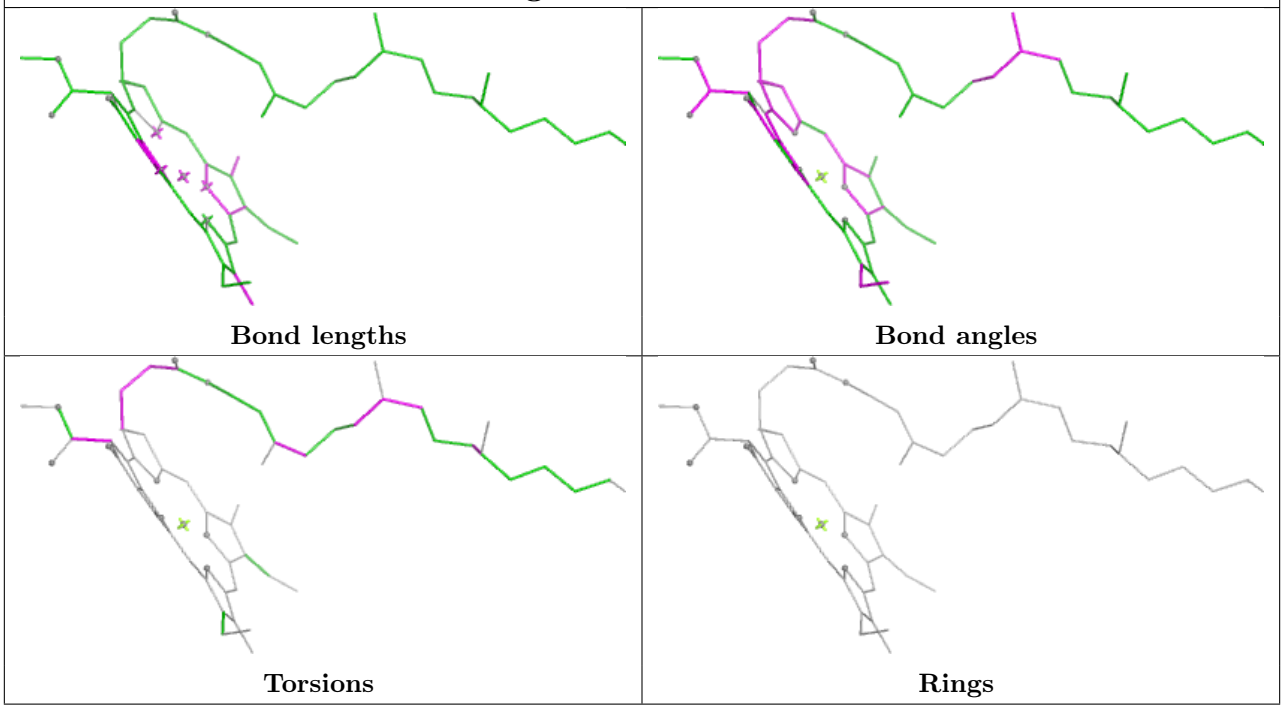
Ligand LHG A 409



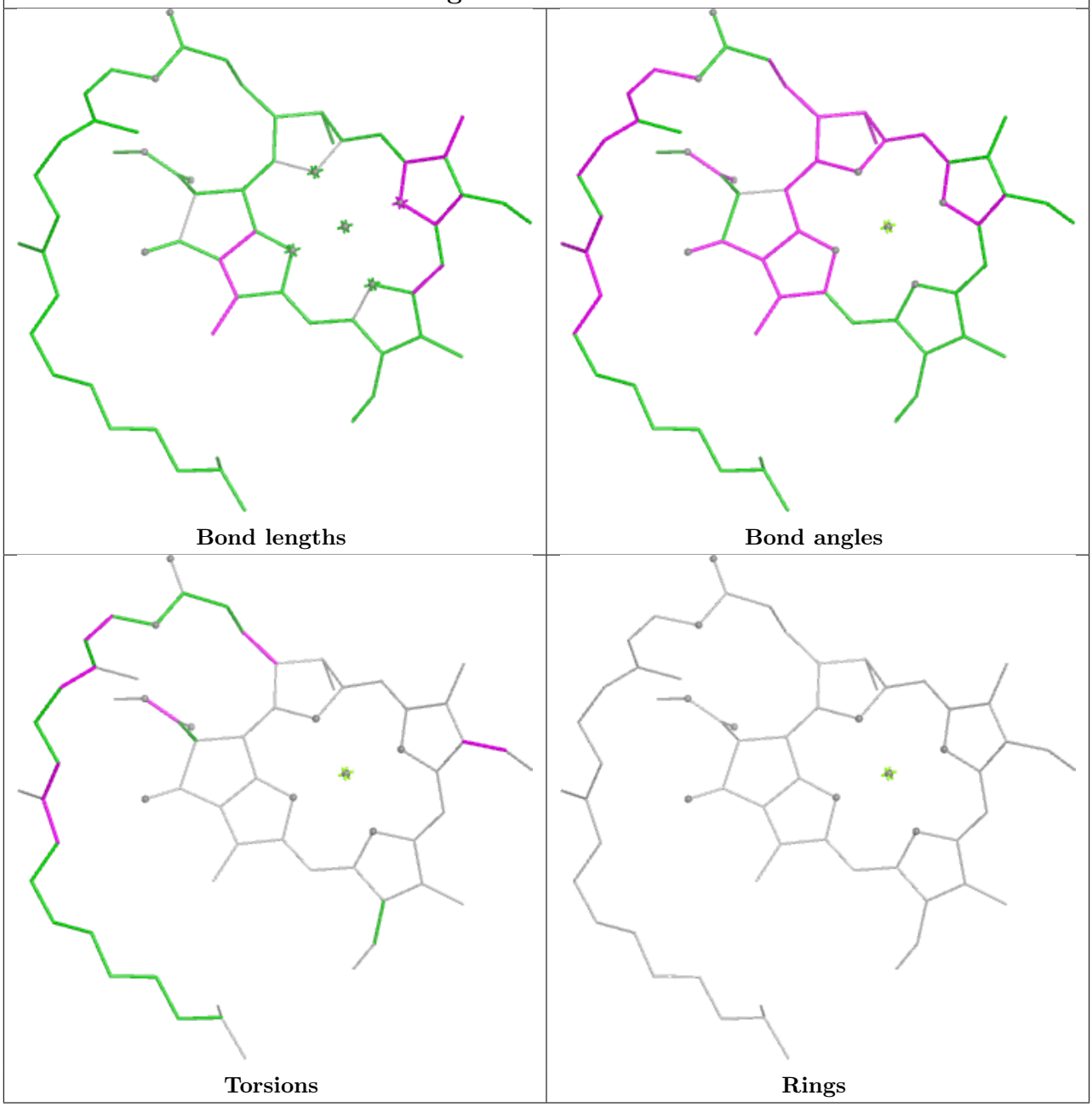
Ligand LMG C 502

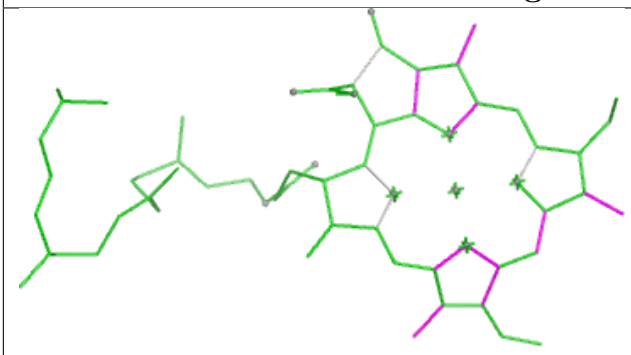
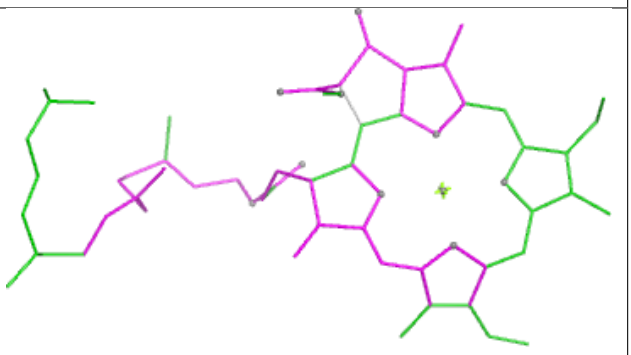
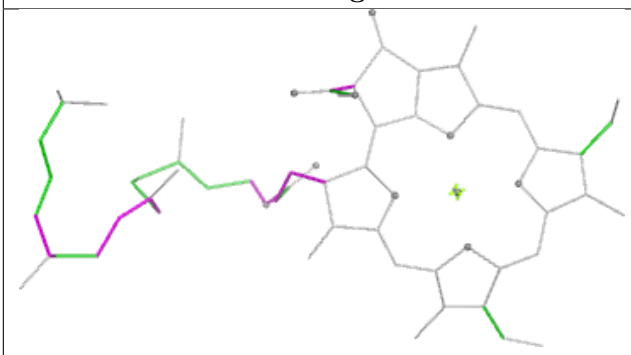
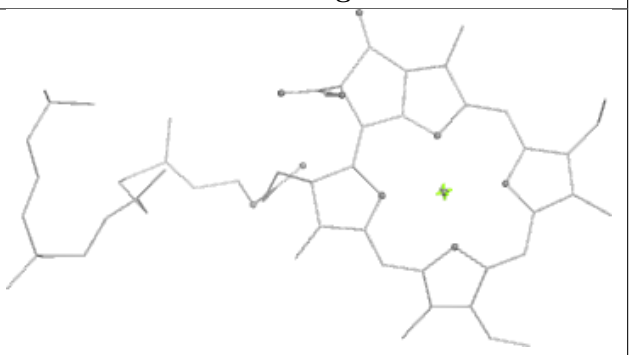


Ligand CLA B 607

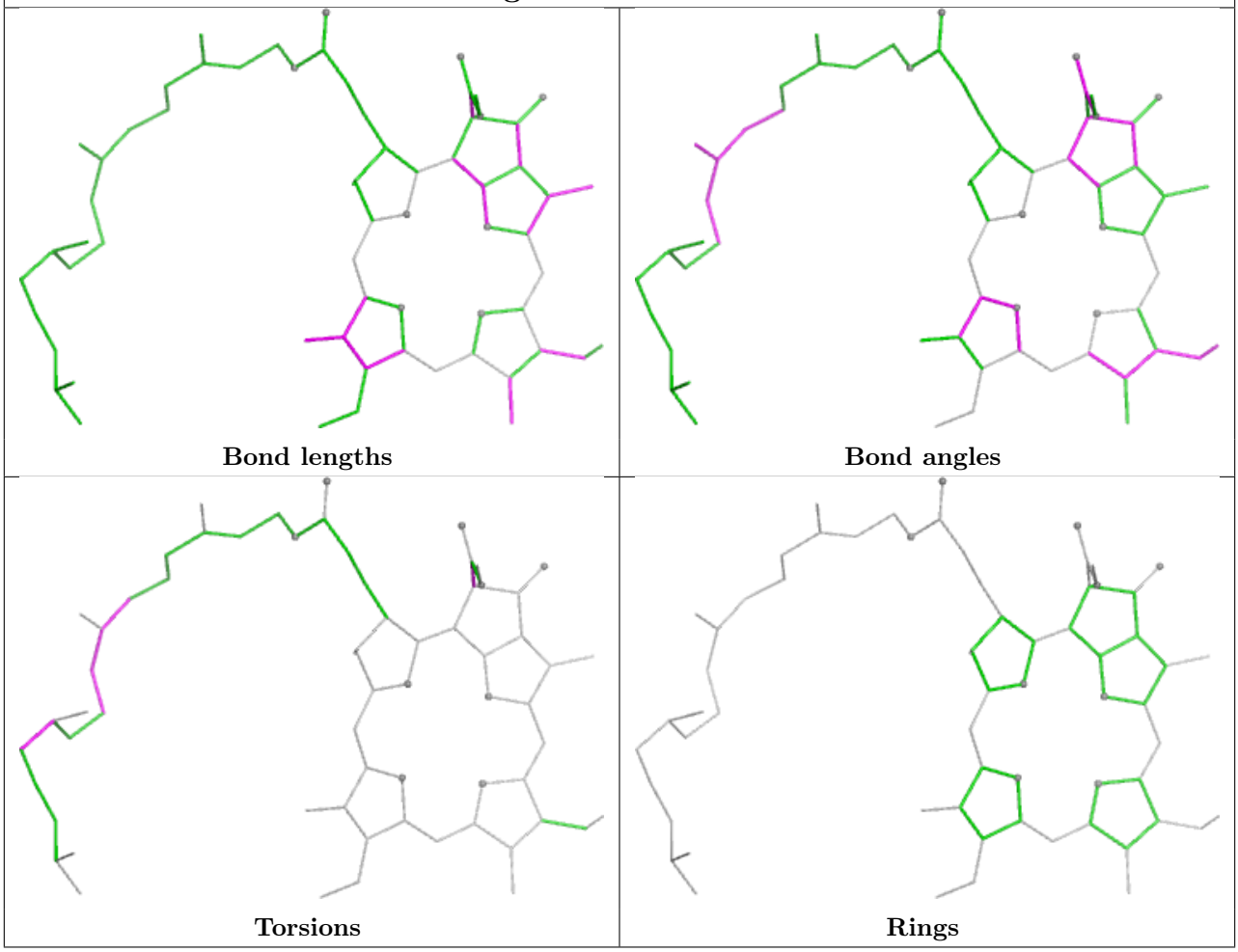


Ligand CLA B 601

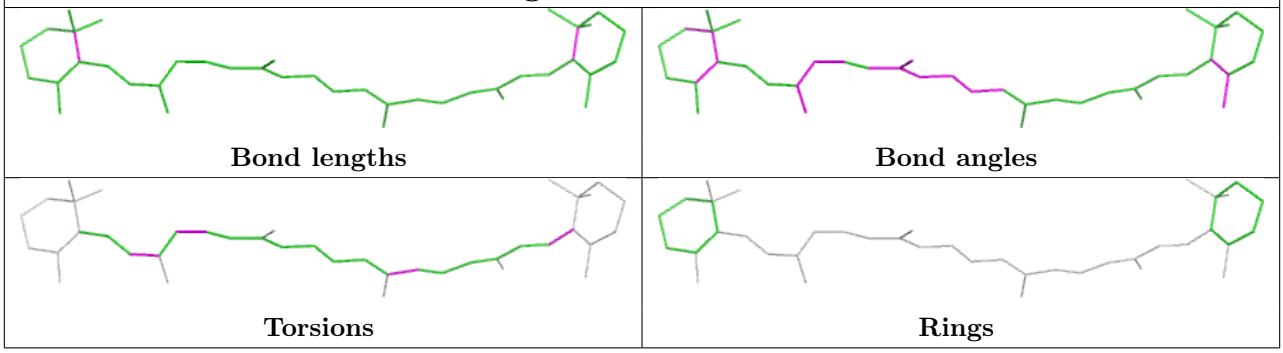


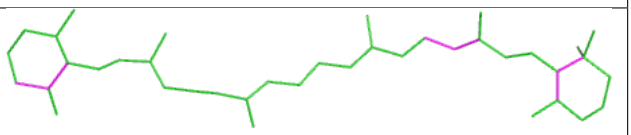
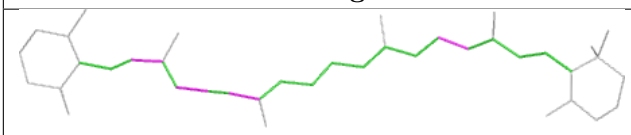
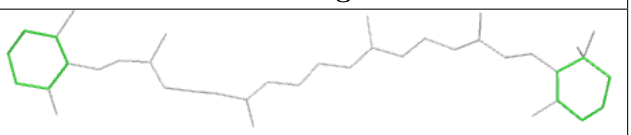
Ligand CLA B 612	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PHO D 407



Ligand BCR C 515



Ligand BCR B 617	
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.

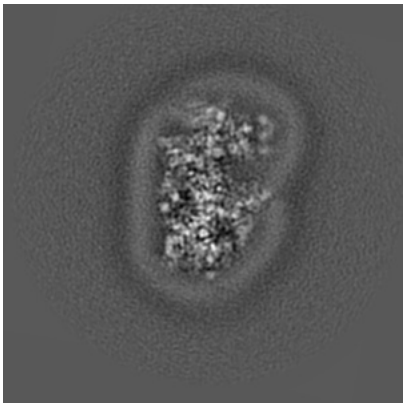
6 Map visualisation (i)

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.

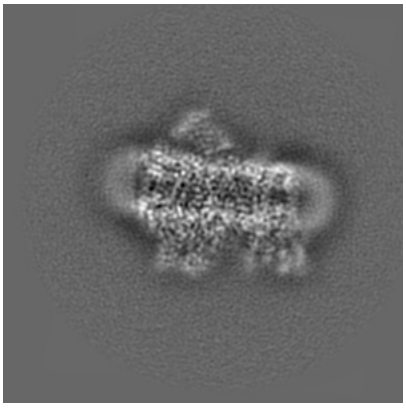
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

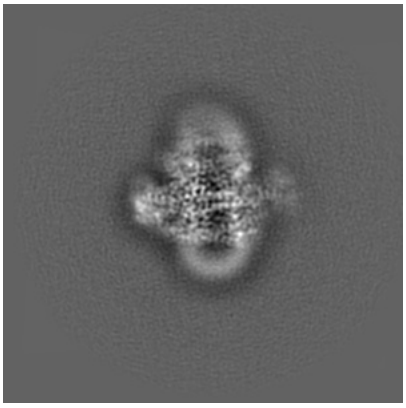
6.1.1 Primary map



X



Y

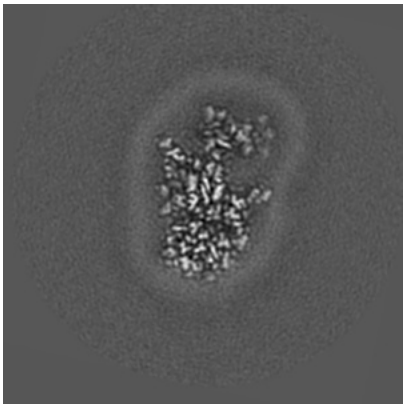


Z

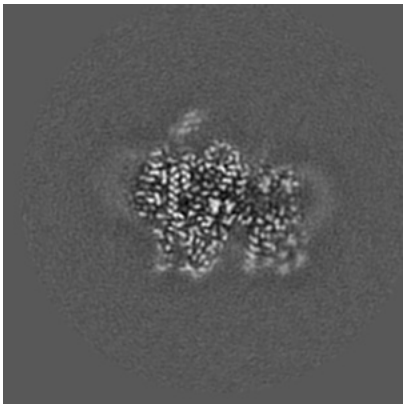
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

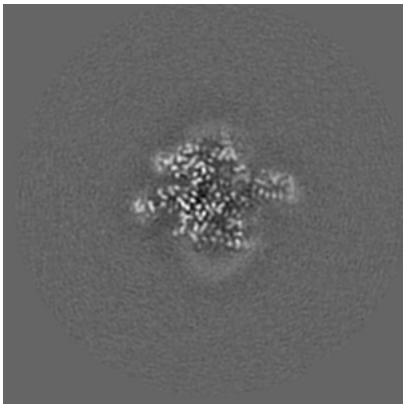
6.2.1 Primary map



X Index: 130



Y Index: 130

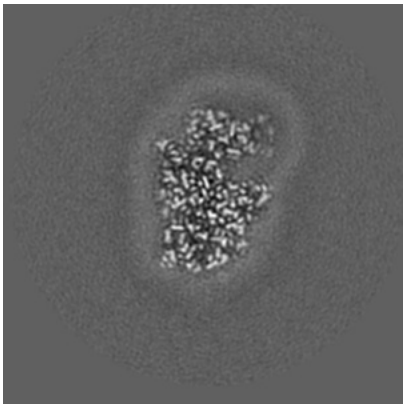


Z Index: 130

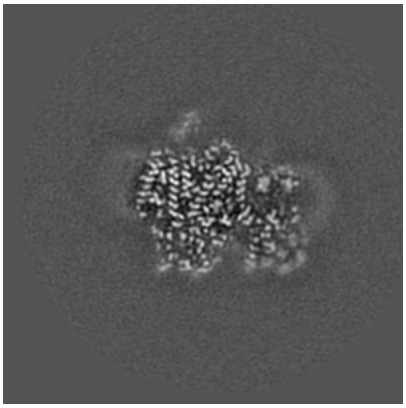
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

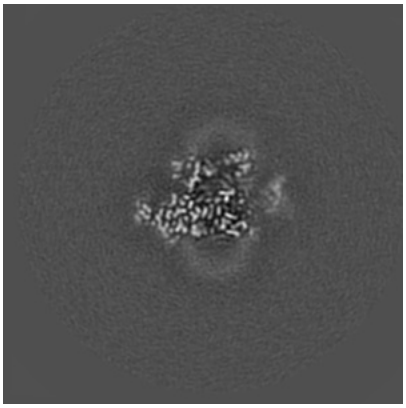
6.3.1 Primary map



X Index: 125



Y Index: 129

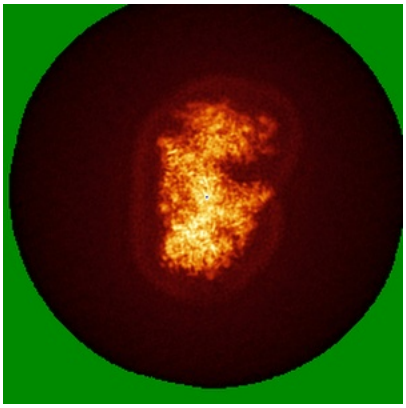


Z Index: 115

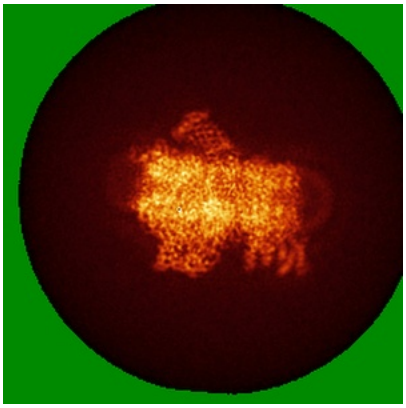
The images above show the largest variance slices of the map in three orthogonal directions.

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

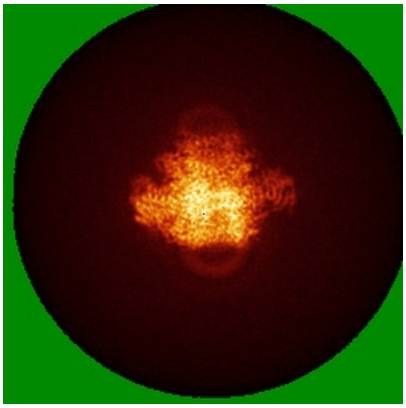
6.4.1 Primary map



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.

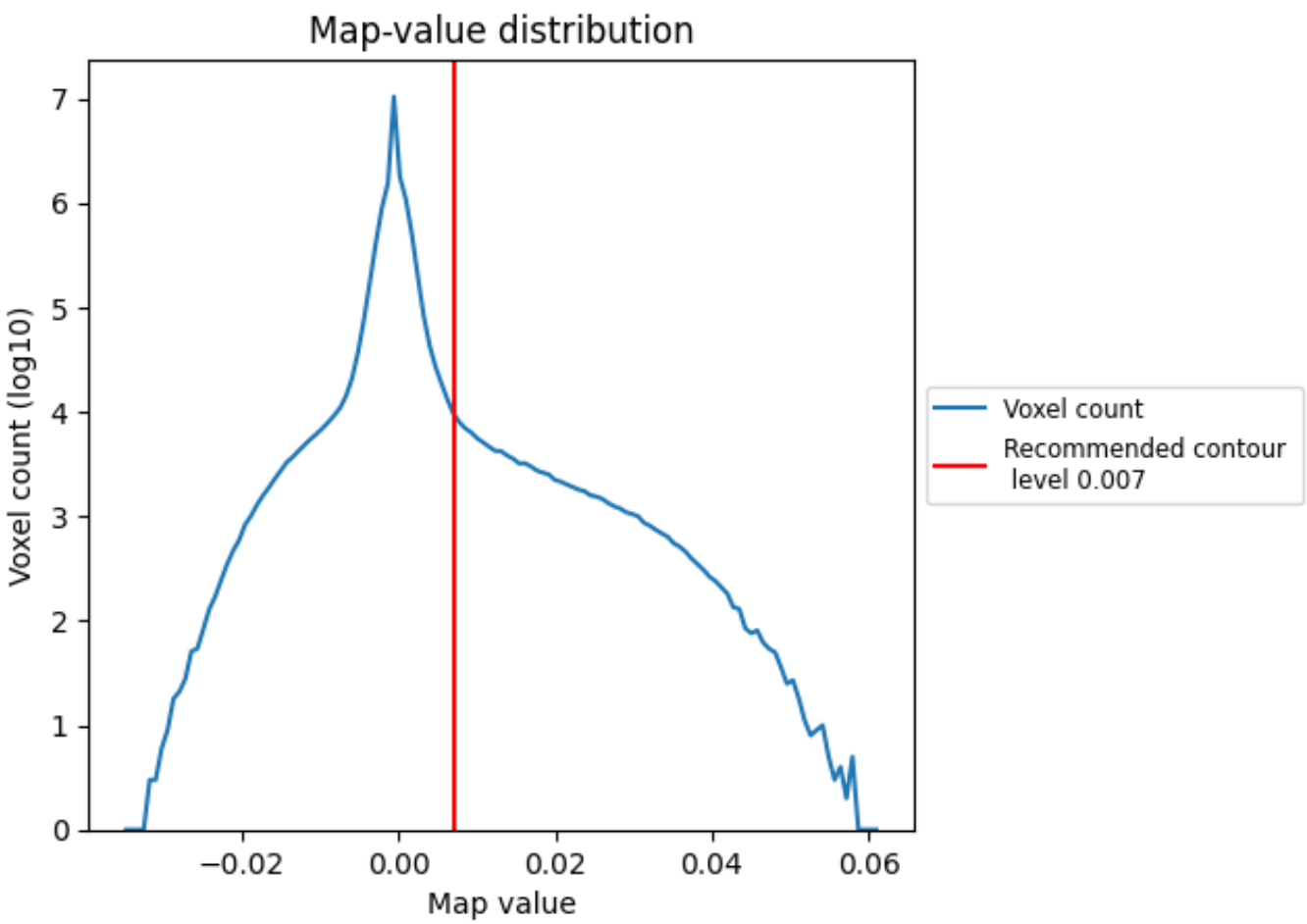
6.6 Mask visualisation (i)

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

7 Map analysis (i)

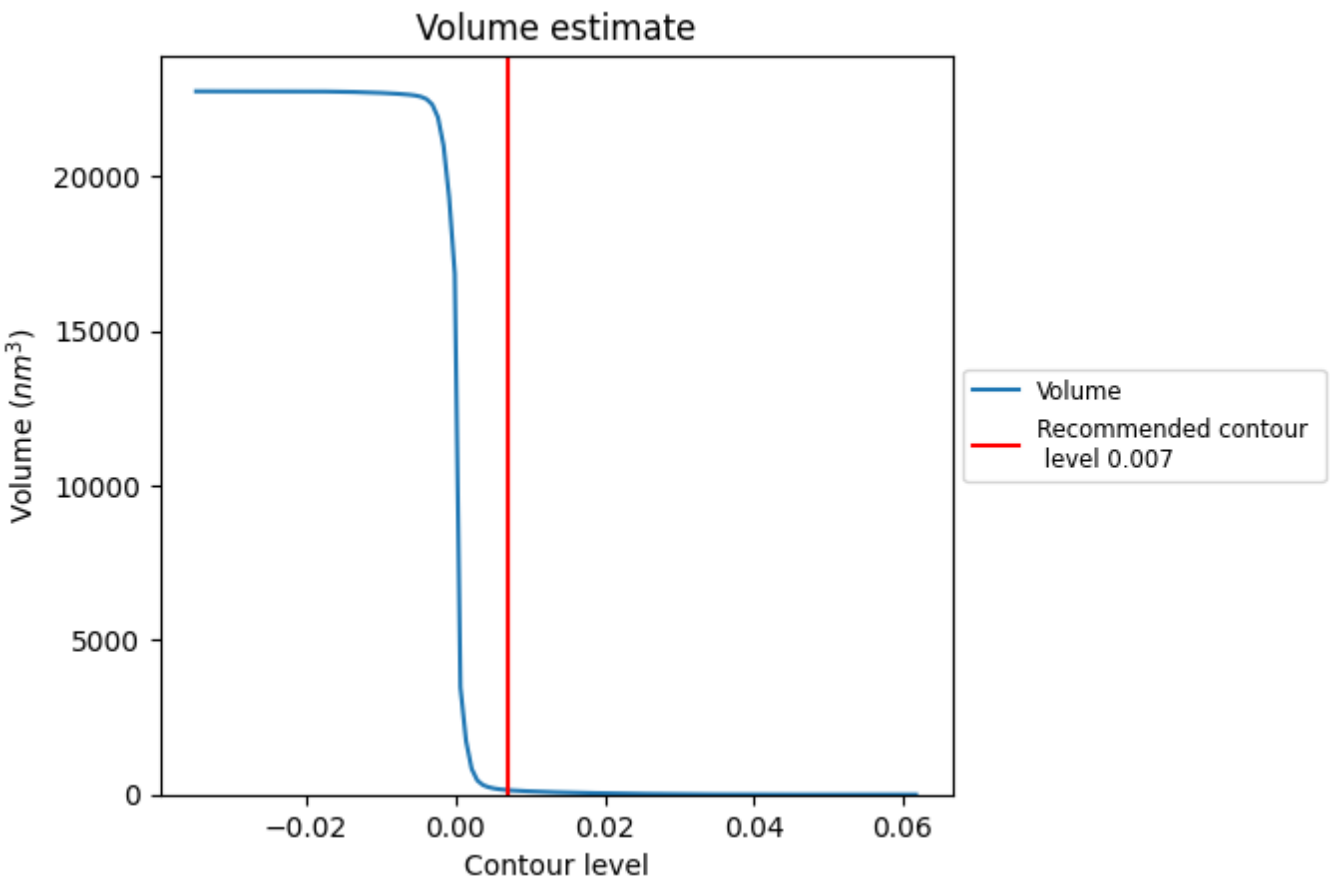
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

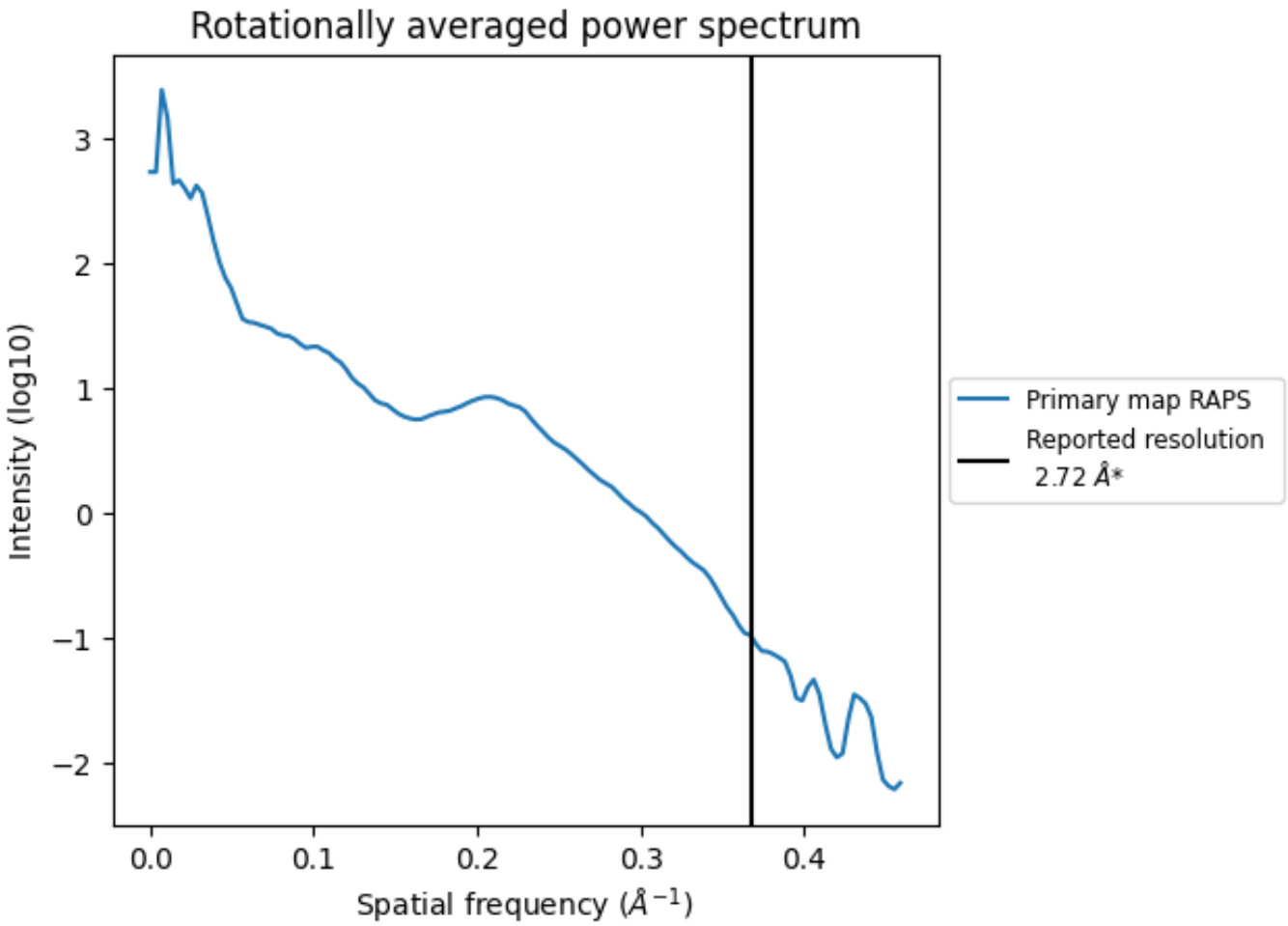
7.2 Volume estimate (i)



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}

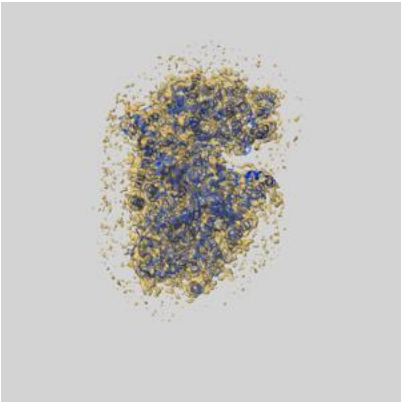
8 Fourier-Shell correlation (i)

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

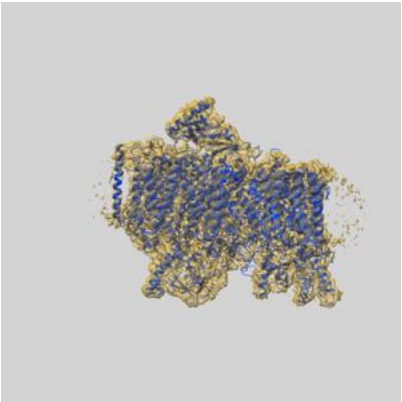
9 Map-model fit (i)

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.

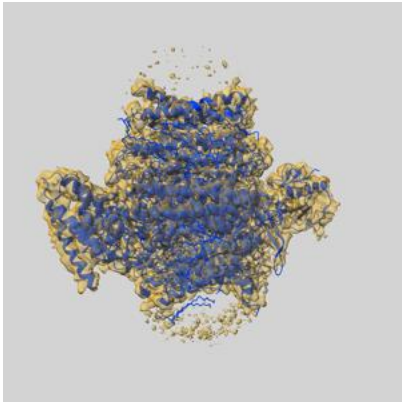
9.1 Map-model overlay (i)



X



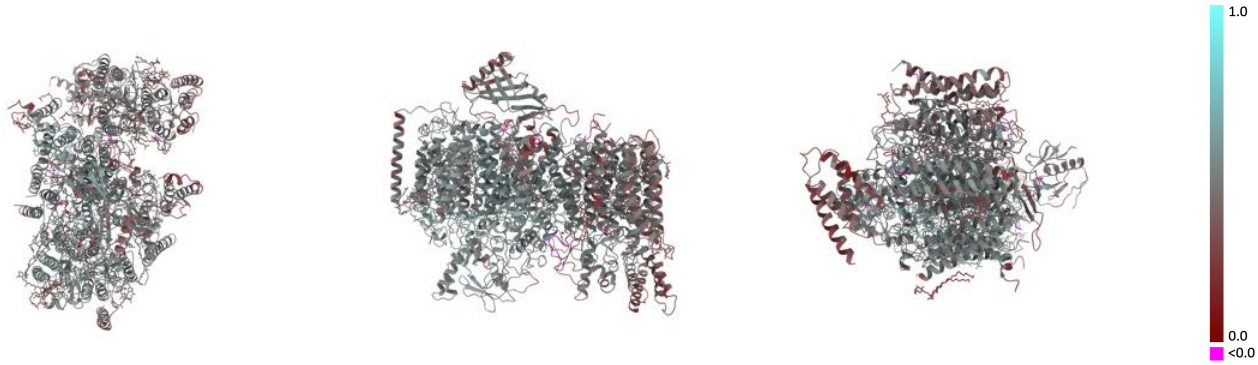
Y



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.

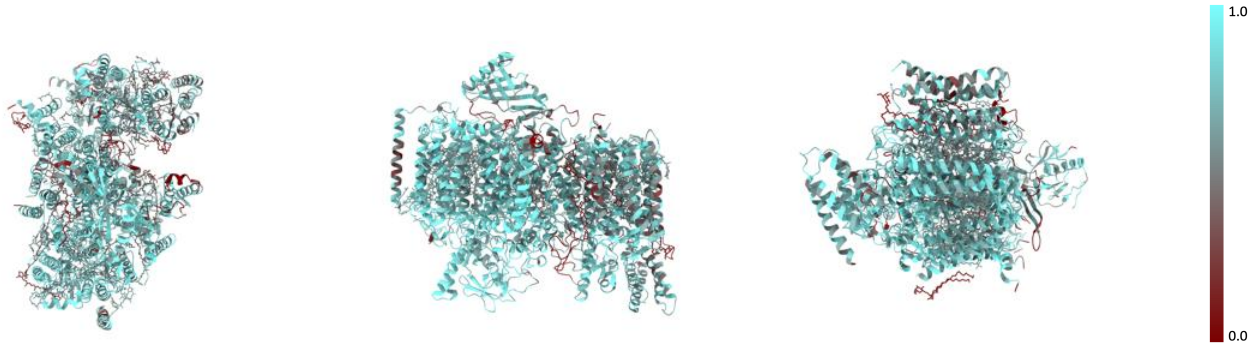
9.2 Q-score mapped to coordinate model (i)



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.

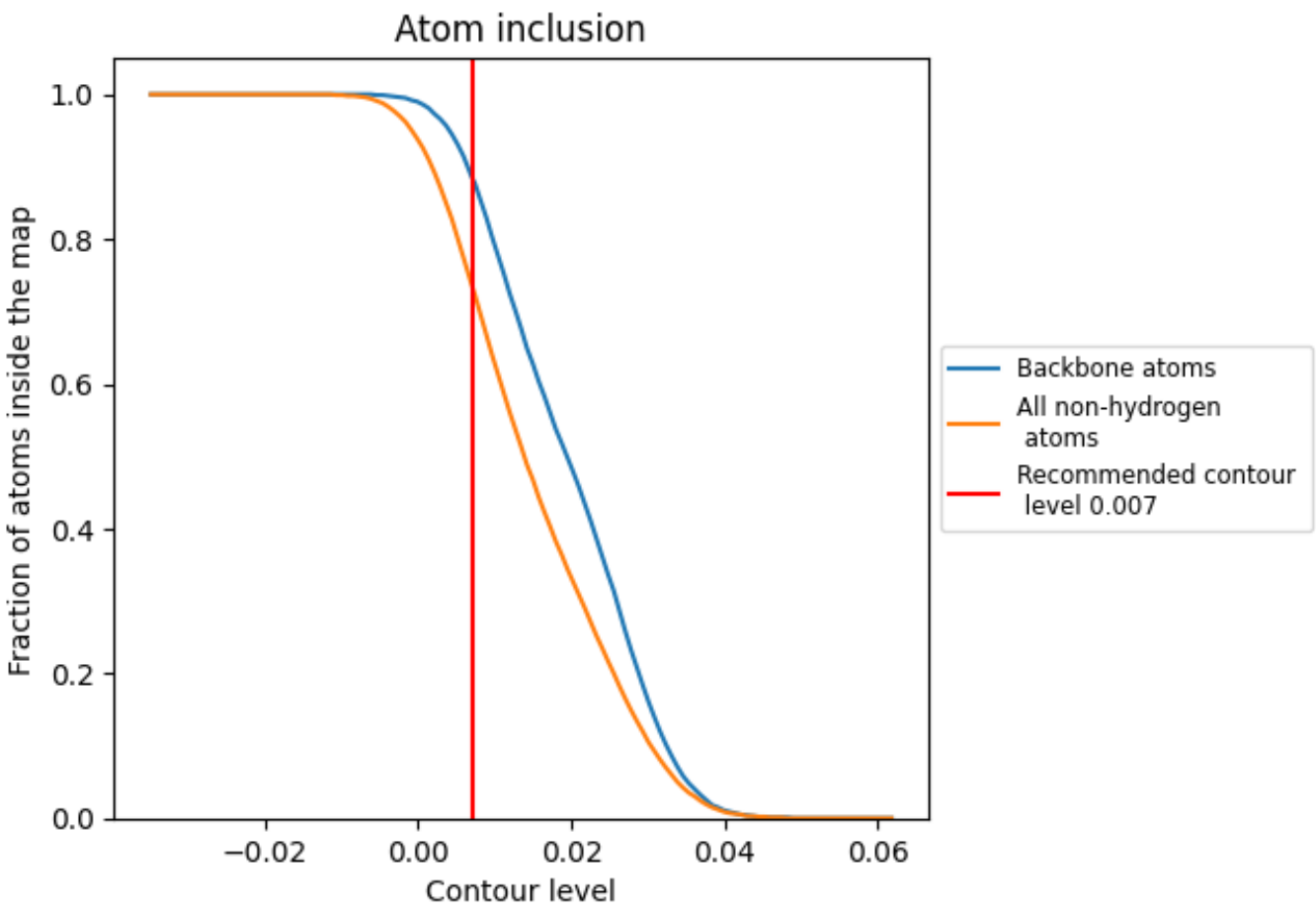
9.3 Atom inclusion mapped to coordinate model (i)



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 (i)

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