wwPDB EM Validation Summary Report ⓘ

Apr 23, 2024 – 12:24 am BST

PDB ID	:	7NHO
EMDB ID	:	EMD-12335
Title	:	Structure of PSII-M
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	:	2.66 Å(reported)

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

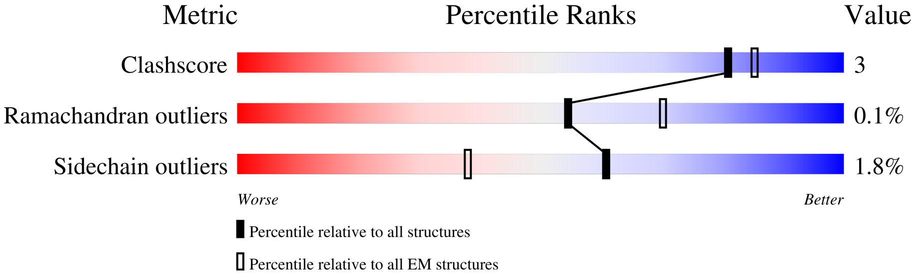
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance ⓘ

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

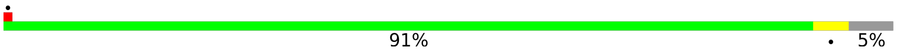
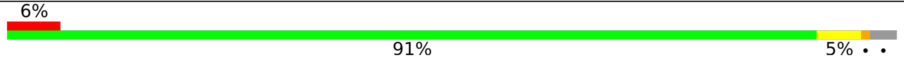
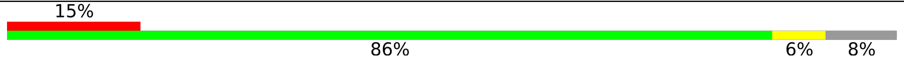
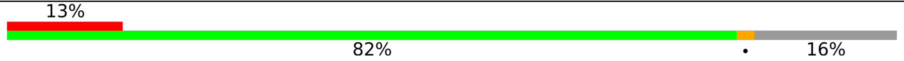
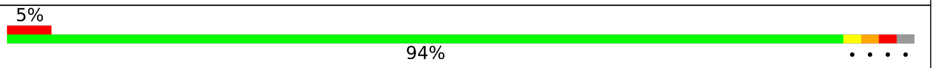
The reported resolution of this entry is 2.66 Å.

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	
2	B	510	
3	C	461	
4	D	352	
5	E	84	
6	F	45	
7	H	66	
8	I	38	

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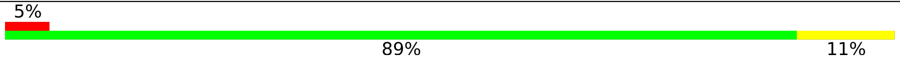
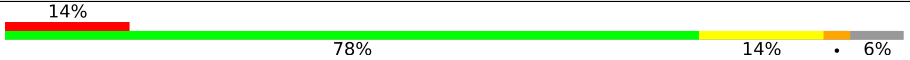
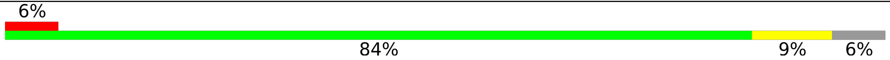
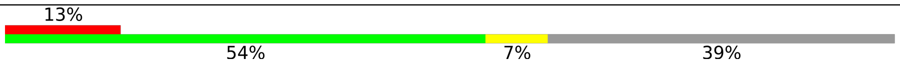
Mol	Chain	Length	Quality of chain
9	K	46	
10	L	37	
11	M	36	
12	T	32	
13	X	41	
14	y	46	
15	Z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	PHO	A	404	X	-	-	-
19	PHO	D	405	X	-	-	-
20	CLA	A	405	X	-	-	-
20	CLA	A	406	X	-	-	-
20	CLA	A	407	X	-	-	-
20	CLA	A	408	X	-	-	-
20	CLA	B	602	X	-	-	-
20	CLA	B	603	X	-	-	-
20	CLA	B	604	X	-	-	-
20	CLA	B	605	X	-	-	-
20	CLA	B	606	X	-	-	-
20	CLA	B	607	X	-	-	-
20	CLA	B	608	X	-	-	-
20	CLA	B	609	X	-	-	-
20	CLA	B	610	X	-	-	-
20	CLA	B	611	X	-	-	-
20	CLA	B	612	X	-	-	-
20	CLA	B	613	X	-	-	-
20	CLA	B	614	X	-	-	-
20	CLA	B	615	X	-	-	-
20	CLA	B	616	X	-	-	-
20	CLA	B	617	X	-	-	-
20	CLA	C	502	X	-	-	-
20	CLA	C	503	X	-	-	-
20	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	C	505	X	-	-	-
20	CLA	C	506	X	-	-	-
20	CLA	C	507	X	-	-	-
20	CLA	C	508	X	-	-	-
20	CLA	C	509	X	-	-	-
20	CLA	C	510	X	-	-	-
20	CLA	C	511	X	-	-	-
20	CLA	C	512	X	-	-	-
20	CLA	C	513	X	-	-	-
20	CLA	C	515	X	-	-	-
20	CLA	D	406	X	-	-	-
20	CLA	D	407	X	-	-	-

2 Entry composition (i)

There are 26 unique types of molecules in this entry. The entry contains 19800 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	485	3812	2505	635	659	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	448	3465	2270	580	602	13	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	340	2705	1794	440	459	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	35	286	195	45	45	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	30	256	180	36	38	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	62	479	328	72	77	2	0	0

- Molecule 16 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

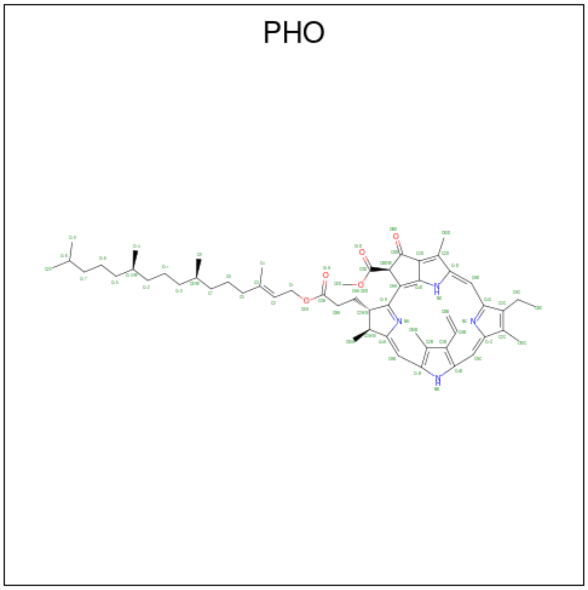
- Molecule 17 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

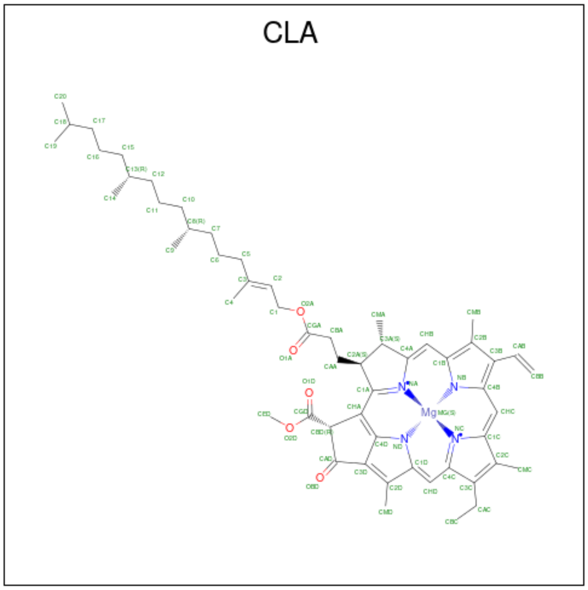
Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
18	A	1	1	1	0

- Molecule 19 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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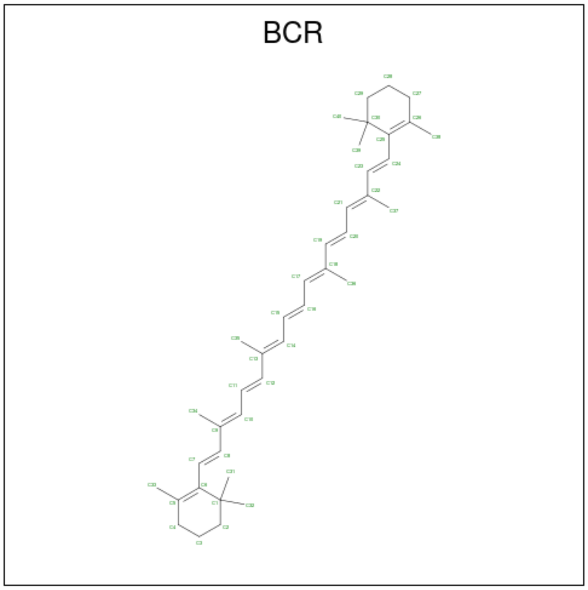
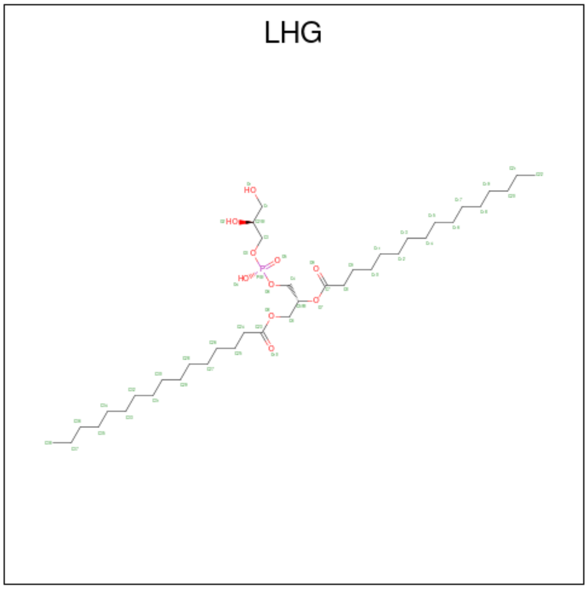
Mol	Chain	Residues	Atoms	AltConf
20	C	1	Total C Mg N O 65 55 1 4 5	0
20	C	1	Total C Mg N O 65 55 1 4 5	0
20	C	1	Total C Mg N O 65 55 1 4 5	0
20	C	1	Total C Mg N O 65 55 1 4 5	0
20	C	1	Total C Mg N O 65 55 1 4 5	0
20	C	1	Total C Mg N O 65 55 1 4 5	0
20	C	1	Total C Mg N O 65 55 1 4 5	0
20	C	1	Total C Mg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

- Molecule 21 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

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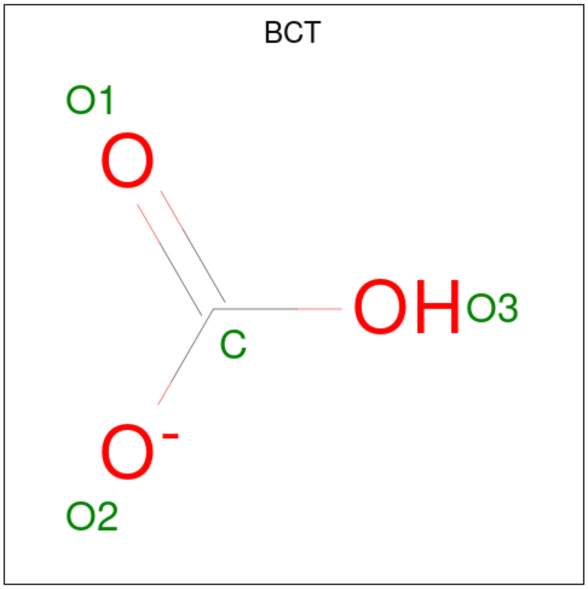
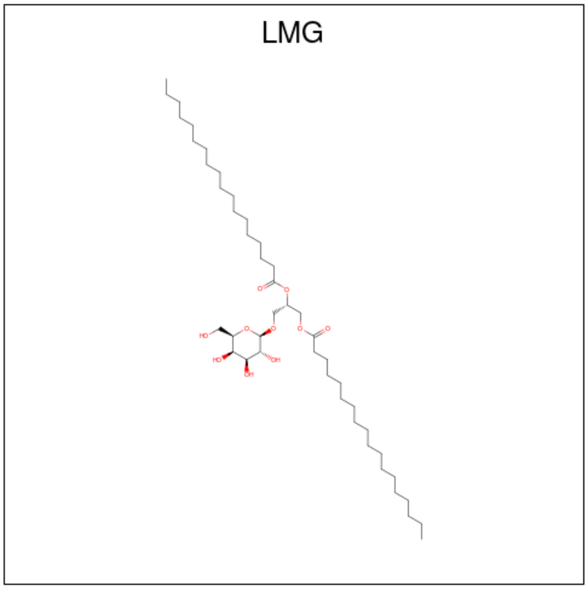
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
22	A	1	49	38	10	1	0

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



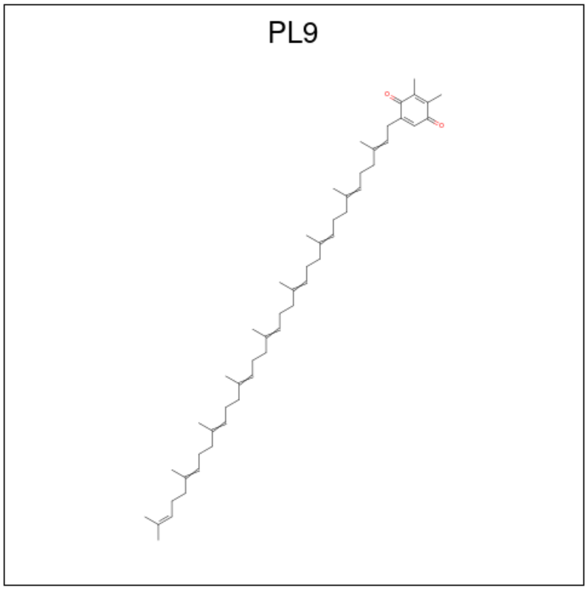
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	A	1	4	1	3	0

- Molecule 24 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



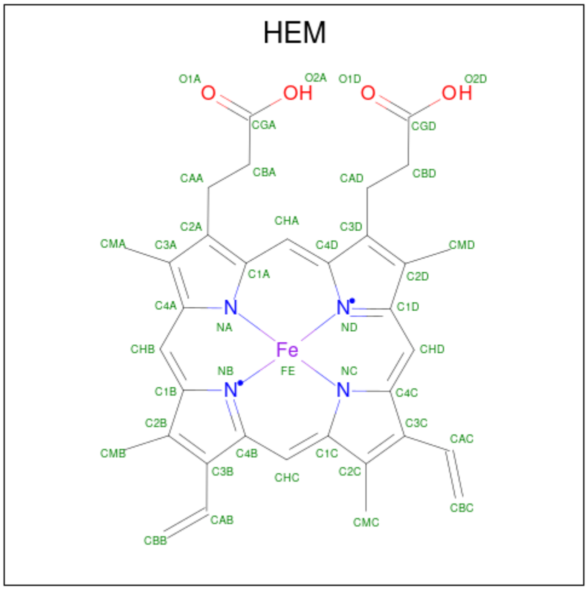
Mol	Chain	Residues	Atoms			AltConf
24	B	1	Total 55	C 45	O 10	0
24	C	1	Total 55	C 45	O 10	0
24	D	1	Total 55	C 45	O 10	0
24	D	1	Total 55	C 45	O 10	0
24	D	1	Total 55	C 45	O 10	0
24	I	1	Total 55	C 45	O 10	0
24	M	1	Total 55	C 45	O 10	0

- Molecule 25 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
25	D	1	Total 55	C 53	O 2	0

- Molecule 26 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_{4}O_{4}$).



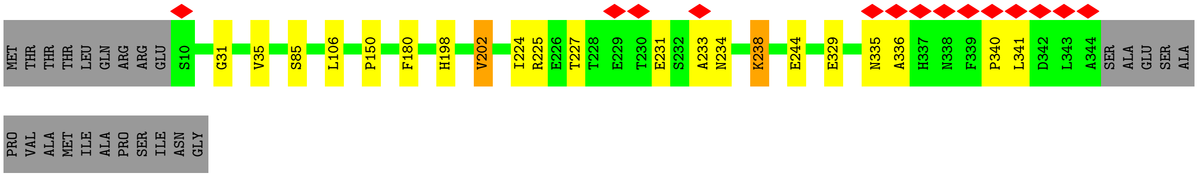
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
26	E	1	43	34	1	4	4	0

3 Residue-property plots ⓘ

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.

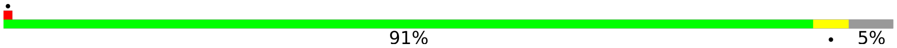
- Molecule 1: Photosystem II protein D1 1

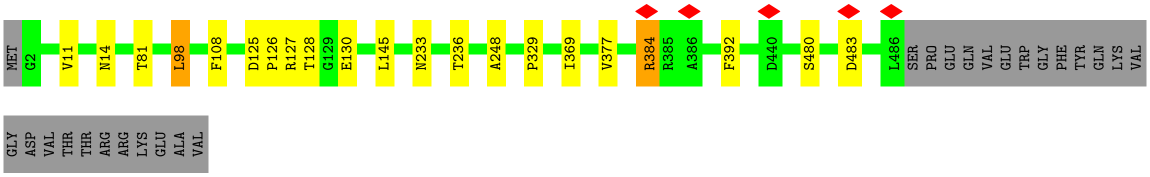
Chain A:



- Molecule 2: Photosystem II CP47 reaction center protein

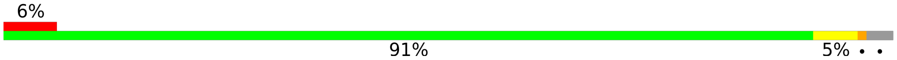
Chain B:

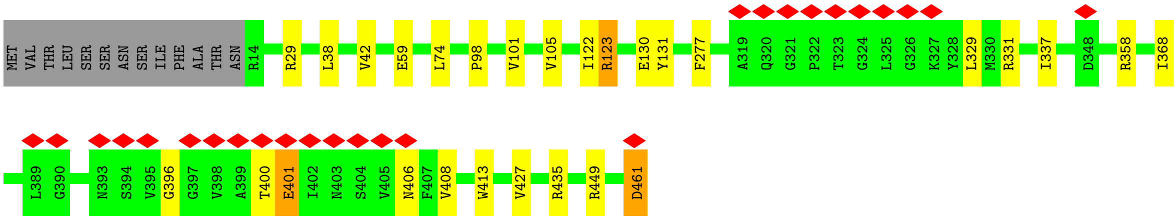




- Molecule 3: Photosystem II CP43 reaction center protein

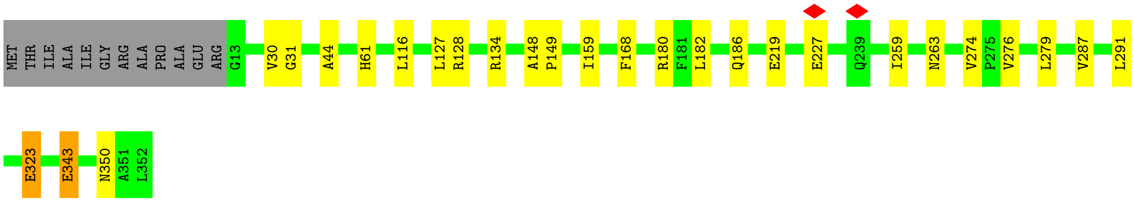
Chain C:





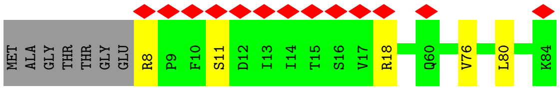
- Molecule 4: Photosystem II D2 protein

Chain D:



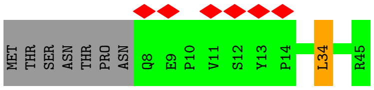
- Molecule 5: Cytochrome b559 subunit alpha

Chain E:



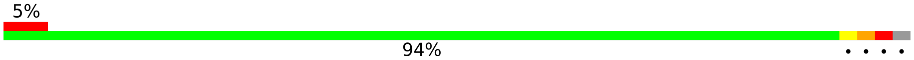
- Molecule 6: Cytochrome b559 subunit beta

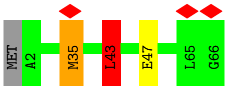
Chain F:



- Molecule 7: Photosystem II reaction center protein H

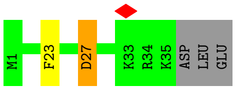
Chain H:





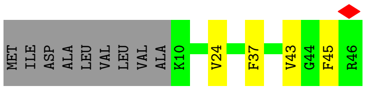
- Molecule 8: Photosystem II reaction center protein I

Chain I:



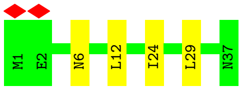
- Molecule 9: Photosystem II reaction center protein K

Chain K:



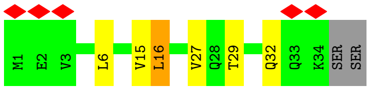
- Molecule 10: Photosystem II reaction center protein L

Chain L:



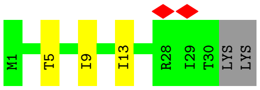
- Molecule 11: Photosystem II reaction center protein M

Chain M:



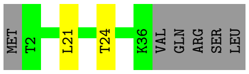
- Molecule 12: Photosystem II reaction center protein T

Chain T:



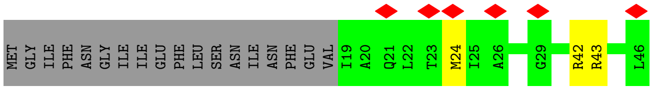
- Molecule 13: Photosystem II reaction center X protein

Chain X:



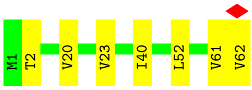
- Molecule 14: Photosystem II reaction center protein Ycf12

Chain y:



- Molecule 15: Photosystem II reaction center protein Z

Chain Z:



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	166411	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 $(e^-/\text{Å}^2)$	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	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	283.4, 283.4, 283.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.54	0/2712	0.86	2/3700 (0.1%)
2	B	0.54	0/3947	0.89	5/5379 (0.1%)
3	C	0.55	0/3578	0.92	8/4872 (0.2%)
4	D	0.53	0/2800	0.90	5/3818 (0.1%)
5	E	0.59	0/654	1.00	3/891 (0.3%)
6	F	0.57	0/317	1.05	2/433 (0.5%)
7	H	0.60	0/524	0.99	1/713 (0.1%)
8	I	0.64	0/293	0.95	0/395
9	K	0.58	0/303	0.96	0/416
10	L	0.59	0/311	0.85	0/422
11	M	0.59	0/270	1.05	0/367
12	T	0.56	0/265	0.83	0/359
13	X	0.53	0/257	0.88	0/348
14	y	0.54	0/209	1.01	1/279 (0.4%)
15	Z	0.57	0/490	0.93	0/669
All	All	0.55	0/16930	0.91	27/23061 (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	2
3	C	0	1
4	D	0	2
7	H	0	1
8	I	0	1
11	M	0	1
14	y	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	13

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	GLU	CA-CB-CG	9.59	134.49	113.40
14	y	43	ARG	NE-CZ-NH2	8.60	124.60	120.30
4	D	323	GLU	OE1-CD-OE2	-6.74	115.21	123.30
3	C	123	ARG	NE-CZ-NH2	6.48	123.54	120.30
2	B	98	LEU	CA-CB-CG	6.41	130.03	115.30

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	GLU	Sidechain
1	A	238	LYS	Peptide
1	A	244	GLU	Sidechain
1	A	341	LEU	Peptide
2	B	384	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	9	0
2	B	3812	0	3683	10	0
3	C	3465	0	3389	12	0
4	D	2705	0	2608	15	0
5	E	635	0	625	1	0
6	F	307	0	312	0	0
7	H	511	0	532	1	0
8	I	286	0	308	1	0
9	K	293	0	305	3	0
10	L	304	0	316	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	M	267	0	289	2	0
12	T	256	0	262	2	0
13	X	254	0	282	1	0
14	y	208	0	237	0	0
15	Z	479	0	516	3	0
16	A	1	0	0	0	0
17	A	1	0	0	0	0
18	A	1	0	0	0	0
19	A	64	0	74	1	0
19	D	64	0	74	3	0
20	A	260	0	284	8	0
20	B	1040	0	1142	14	0
20	C	845	0	928	13	0
20	D	130	0	143	5	0
21	A	40	0	56	1	0
21	B	120	0	168	6	0
21	C	80	0	112	3	0
21	F	40	0	56	0	0
21	H	40	0	56	1	0
21	K	40	0	56	1	0
21	Z	40	0	56	0	0
22	A	98	0	148	1	0
23	A	4	0	1	0	0
24	B	55	0	86	1	0
24	C	55	0	86	1	0
24	D	165	0	258	2	0
24	I	55	0	86	0	0
24	M	55	0	86	0	0
25	D	55	0	80	2	0
26	E	43	0	30	1	0
All	All	19800	0	20254	97	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 3.

The worst 5 of 97 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)
20:A:408:CLA:HMB1	20:A:408:CLA:HBB1	1.66	0.78
20:C:509:CLA:H93	9:K:37:PHE:CZ	2.31	0.65
20:C:515:CLA:HMB1	20:C:515:CLA:HBB1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:511:CLA:HMB1	20:C:511:CLA:HBB1	1.80	0.64
20:B:609:CLA:H42	4:D:127:LEU:HD11	1.81	0.62

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	309 (93%)	23 (7%)	1 (0%)	41	56
2	B	483/510 (95%)	459 (95%)	24 (5%)	0	100	100
3	C	446/461 (97%)	420 (94%)	26 (6%)	0	100	100
4	D	338/352 (96%)	326 (96%)	12 (4%)	0	100	100
5	E	75/84 (89%)	68 (91%)	7 (9%)	0	100	100
6	F	36/45 (80%)	33 (92%)	3 (8%)	0	100	100
7	H	63/66 (96%)	56 (89%)	6 (10%)	1 (2%)	9	14
8	I	33/38 (87%)	31 (94%)	2 (6%)	0	100	100
9	K	35/46 (76%)	34 (97%)	0	1 (3%)	4	6
10	L	35/37 (95%)	35 (100%)	0	0	100	100
11	M	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
12	T	28/32 (88%)	28 (100%)	0	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	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
All	All	2056/2216 (93%)	1941 (94%)	112 (5%)	3 (0%)	54	69

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	H	35	MET
1	A	340	PRO
9	K	45	PHE

5.3.2 Protein sidechains ⓘ

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%)	84	91
2	B	385/407 (95%)	379 (98%)	6 (2%)	62	78
3	C	350/362 (97%)	345 (99%)	5 (1%)	67	81
4	D	275/283 (97%)	270 (98%)	5 (2%)	59	75
5	E	69/73 (94%)	67 (97%)	2 (3%)	42	60
6	F	32/39 (82%)	31 (97%)	1 (3%)	40	57
7	H	54/55 (98%)	53 (98%)	1 (2%)	57	74
8	I	32/35 (91%)	32 (100%)	0	100	100
9	K	30/37 (81%)	29 (97%)	1 (3%)	38	54
10	L	35/35 (100%)	34 (97%)	1 (3%)	42	60
11	M	31/33 (94%)	28 (90%)	3 (10%)	8	11
12	T	27/29 (93%)	27 (100%)	0	100	100
13	X	28/34 (82%)	28 (100%)	0	100	100
14	y	21/37 (57%)	20 (95%)	1 (5%)	25	39
15	Z	52/52 (100%)	50 (96%)	2 (4%)	33	49
All	All	1692/1802 (94%)	1662 (98%)	30 (2%)	61	75

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	186	GLN
14	y	24	MET
4	D	350	ASN
15	Z	52	LEU

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Mol	Chain	Res	Type
11	M	6	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	263	ASN
4	D	336	HIS
7	H	15	ASN
4	D	350	ASN
4	D	186	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 62 ligands modelled in this entry, 3 are monoatomic - leaving 59 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	$\#\|Z\| > 2$
20	CLA	B	603	-	65,73,73	1.53	10 (15%)	76,113,113	2.10	18 (23%)
19	PHO	D	405	-	51,69,69	1.09	6 (11%)	47,99,99	1.21	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	PL9	D	404	-	55,55,55	1.07	5 (9%)	68,69,69	1.40	10 (14%)
20	CLA	C	509	-	65,73,73	1.74	13 (20%)	76,113,113	1.74	13 (17%)
21	BCR	C	516	-	41,41,41	0.69	0	56,56,56	1.26	4 (7%)
21	BCR	Z	101	-	41,41,41	0.81	1 (2%)	56,56,56	1.14	4 (7%)
20	CLA	B	608	-	65,73,73	1.66	11 (16%)	76,113,113	1.84	18 (23%)
20	CLA	B	615	-	65,73,73	1.66	11 (16%)	76,113,113	1.94	12 (15%)
24	LMG	D	401	-	55,55,55	1.01	3 (5%)	63,63,63	0.85	0
21	BCR	K	101	-	41,41,41	0.77	1 (2%)	56,56,56	1.41	10 (17%)
24	LMG	M	101	-	55,55,55	1.12	3 (5%)	63,63,63	0.91	1 (1%)
20	CLA	B	614	-	65,73,73	1.87	11 (16%)	76,113,113	1.84	16 (21%)
20	CLA	B	609	-	65,73,73	1.79	8 (12%)	76,113,113	1.57	10 (13%)
20	CLA	C	506	-	65,73,73	1.77	11 (16%)	76,113,113	2.46	24 (31%)
22	LHG	A	411	-	48,48,48	0.82	1 (2%)	51,54,54	0.81	1 (1%)
20	CLA	B	602	-	65,73,73	1.69	8 (12%)	76,113,113	2.30	19 (25%)
21	BCR	C	514	-	41,41,41	0.94	0	56,56,56	1.35	9 (16%)
24	LMG	D	403	-	55,55,55	1.17	4 (7%)	63,63,63	0.99	3 (4%)
24	LMG	D	402	-	55,55,55	1.01	2 (3%)	63,63,63	1.04	4 (6%)
20	CLA	C	504	-	65,73,73	1.74	10 (15%)	76,113,113	1.80	16 (21%)
20	CLA	C	511	3	65,73,73	1.74	13 (20%)	76,113,113	2.11	18 (23%)
20	CLA	B	616	-	65,73,73	1.61	10 (15%)	76,113,113	1.78	15 (19%)
21	BCR	B	618	-	41,41,41	0.79	1 (2%)	56,56,56	1.10	4 (7%)
22	LHG	A	410	-	48,48,48	0.85	2 (4%)	51,54,54	0.73	1 (1%)
24	LMG	C	501	-	55,55,55	0.95	2 (3%)	63,63,63	0.97	3 (4%)
20	CLA	A	405	-	65,73,73	1.71	12 (18%)	76,113,113	1.66	18 (23%)
19	PHO	A	404	-	51,69,69	1.07	4 (7%)	47,99,99	1.23	5 (10%)
20	CLA	B	610	-	65,73,73	1.71	12 (18%)	76,113,113	2.25	21 (27%)
20	CLA	C	507	-	65,73,73	1.72	11 (16%)	76,113,113	1.88	15 (19%)
21	BCR	A	409	-	41,41,41	0.72	0	56,56,56	0.97	2 (3%)
24	LMG	I	101	-	55,55,55	0.91	1 (1%)	63,63,63	0.99	3 (4%)
20	CLA	A	406	-	65,73,73	1.48	10 (15%)	76,113,113	1.68	20 (26%)
23	BCT	A	412	16	2,3,3	1.29	0	2,3,3	3.38	1 (50%)
20	CLA	B	607	-	65,73,73	1.59	8 (12%)	76,113,113	1.62	10 (13%)
20	CLA	A	407	-	65,73,73	1.60	7 (10%)	76,113,113	1.89	22 (28%)
20	CLA	B	617	-	65,73,73	1.68	14 (21%)	76,113,113	2.06	15 (19%)
21	BCR	H	101	-	41,41,41	0.91	1 (2%)	56,56,56	1.21	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
20	CLA	D	406	-	65,73,73	1.63	10 (15%)	76,113,113	1.75	19 (25%)
24	LMG	B	601	-	55,55,55	0.98	1 (1%)	63,63,63	1.13	4 (6%)
20	CLA	C	505	-	65,73,73	1.64	13 (20%)	76,113,113	1.89	23 (30%)
20	CLA	C	503	-	65,73,73	1.49	10 (15%)	76,113,113	1.90	14 (18%)
20	CLA	B	612	-	65,73,73	1.64	9 (13%)	76,113,113	2.11	16 (21%)
20	CLA	B	606	-	65,73,73	1.67	10 (15%)	76,113,113	1.86	16 (21%)
21	BCR	B	619	-	41,41,41	0.85	1 (2%)	56,56,56	1.00	5 (8%)
21	BCR	B	620	-	41,41,41	0.91	0	56,56,56	1.30	10 (17%)
26	HEM	E	101	5	41,50,50	1.47	6 (14%)	45,82,82	1.32	4 (8%)
20	CLA	B	613	-	65,73,73	1.59	8 (12%)	76,113,113	1.87	20 (26%)
21	BCR	F	101	-	41,41,41	0.72	0	56,56,56	1.25	6 (10%)
20	CLA	B	604	-	65,73,73	1.62	9 (13%)	76,113,113	1.96	16 (21%)
20	CLA	B	605	-	65,73,73	1.65	11 (16%)	76,113,113	1.65	15 (19%)
20	CLA	A	408	-	65,73,73	1.62	11 (16%)	76,113,113	1.46	11 (14%)
20	CLA	C	510	-	65,73,73	1.72	12 (18%)	76,113,113	1.68	18 (23%)
20	CLA	C	515	-	65,73,73	1.58	8 (12%)	76,113,113	2.05	18 (23%)
20	CLA	C	512	-	65,73,73	1.74	13 (20%)	76,113,113	1.94	15 (19%)
20	CLA	D	407	-	65,73,73	1.74	10 (15%)	76,113,113	1.64	13 (17%)
20	CLA	C	513	-	65,73,73	1.69	15 (23%)	76,113,113	1.82	18 (23%)
20	CLA	C	508	-	65,73,73	1.55	9 (13%)	76,113,113	1.78	14 (18%)
20	CLA	B	611	-	65,73,73	1.64	13 (20%)	76,113,113	1.96	15 (19%)
20	CLA	C	502	-	65,73,73	1.60	11 (16%)	76,113,113	1.73	14 (18%)

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
20	CLA	B	603	-	2/2/15/20	3/37/115/115	-
19	PHO	D	405	-	1/1/17/22	8/37/103/103	0/5/6/6
25	PL9	D	404	-	-	7/53/73/73	0/1/1/1
20	CLA	C	509	-	2/2/15/20	4/37/115/115	-
21	BCR	C	516	-	-	13/29/63/63	0/2/2/2
21	BCR	Z	101	-	-	5/29/63/63	0/2/2/2
20	CLA	B	608	-	2/2/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	615	-	2/2/15/20	5/37/115/115	-
24	LMG	D	401	-	-	18/50/70/70	0/1/1/1
21	BCR	K	101	-	-	13/29/63/63	0/2/2/2
24	LMG	M	101	-	-	6/50/70/70	0/1/1/1
20	CLA	B	614	-	2/2/15/20	5/37/115/115	-
20	CLA	B	609	-	1/1/15/20	5/37/115/115	-
20	CLA	C	506	-	2/2/15/20	8/37/115/115	-
22	LHG	A	411	-	-	19/53/53/53	-
20	CLA	B	602	-	1/1/15/20	10/37/115/115	-
21	BCR	C	514	-	-	7/29/63/63	0/2/2/2
24	LMG	D	403	-	-	8/50/70/70	0/1/1/1
24	LMG	D	402	-	-	9/50/70/70	0/1/1/1
20	CLA	C	504	-	1/1/15/20	8/37/115/115	-
20	CLA	C	511	3	2/2/15/20	8/37/115/115	-
20	CLA	B	616	-	1/1/15/20	8/37/115/115	-
21	BCR	B	618	-	-	5/29/63/63	0/2/2/2
22	LHG	A	410	-	-	13/53/53/53	-
24	LMG	C	501	-	-	14/50/70/70	0/1/1/1
20	CLA	A	405	-	2/2/15/20	7/37/115/115	-
19	PHO	A	404	-	1/1/17/22	7/37/103/103	0/5/6/6
20	CLA	B	610	-	2/2/15/20	8/37/115/115	-
20	CLA	C	507	-	2/2/15/20	7/37/115/115	-
21	BCR	A	409	-	-	6/29/63/63	0/2/2/2
24	LMG	I	101	-	-	3/50/70/70	0/1/1/1
20	CLA	A	406	-	2/2/15/20	11/37/115/115	-
20	CLA	B	607	-	2/2/15/20	7/37/115/115	-
20	CLA	A	407	-	1/1/15/20	2/37/115/115	-
20	CLA	B	617	-	1/1/15/20	3/37/115/115	-
21	BCR	H	101	-	-	8/29/63/63	0/2/2/2
20	CLA	D	406	-	2/2/15/20	11/37/115/115	-
24	LMG	B	601	-	-	9/50/70/70	0/1/1/1
20	CLA	C	505	-	1/1/15/20	5/37/115/115	-
20	CLA	C	503	-	2/2/15/20	12/37/115/115	-
20	CLA	B	612	-	2/2/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	606	-	2/2/15/20	2/37/115/115	-
21	BCR	B	619	-	-	7/29/63/63	0/2/2/2
21	BCR	B	620	-	-	6/29/63/63	0/2/2/2
26	HEM	E	101	5	-	4/12/54/54	-
20	CLA	B	613	-	1/1/15/20	8/37/115/115	-
21	BCR	F	101	-	-	5/29/63/63	0/2/2/2
20	CLA	B	604	-	2/2/15/20	9/37/115/115	-
20	CLA	B	605	-	2/2/15/20	4/37/115/115	-
20	CLA	A	408	-	1/1/15/20	12/37/115/115	-
20	CLA	C	510	-	1/1/15/20	7/37/115/115	-
20	CLA	C	515	-	1/1/15/20	5/37/115/115	-
20	CLA	C	512	-	1/1/15/20	10/37/115/115	-
20	CLA	D	407	-	1/1/15/20	5/37/115/115	-
20	CLA	C	513	-	1/1/15/20	7/37/115/115	-
20	CLA	C	508	-	1/1/15/20	4/37/115/115	-
20	CLA	B	611	-	2/2/15/20	11/37/115/115	-
20	CLA	C	502	-	2/2/15/20	3/37/115/115	-

The worst 5 of 417 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	614	CLA	C4B-NB	10.88	1.44	1.35
20	B	609	CLA	C4B-NB	9.63	1.43	1.35
20	B	602	CLA	C4B-NB	9.54	1.43	1.35
20	A	407	CLA	C4B-NB	9.16	1.43	1.35
20	C	512	CLA	C4B-NB	9.15	1.43	1.35

The worst 5 of 678 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	503	CLA	C4A-NA-C1A	10.38	111.37	106.71
20	B	612	CLA	C4A-NA-C1A	9.87	111.14	106.71
20	B	602	CLA	C4D-C3D-CAD	9.79	119.64	108.10
20	B	617	CLA	C4D-C3D-CAD	9.50	119.29	108.10
20	C	506	CLA	C4A-NA-C1A	9.20	110.84	106.71

5 of 57 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	404	PHO	C8
19	D	405	PHO	C8
20	A	405	CLA	ND
20	A	405	CLA	C8
20	A	406	CLA	ND

5 of 442 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	404	PHO	O2A-C1-C2-C3
20	A	405	CLA	C11-C10-C8-C7
20	A	406	CLA	C1A-C2A-CAA-CBA
20	A	406	CLA	C3A-C2A-CAA-CBA
20	B	602	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

41 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	603	CLA	1	0
19	D	405	PHO	3	0
25	D	404	PL9	2	0
20	C	509	CLA	2	0
20	B	608	CLA	2	0
21	K	101	BCR	1	0
20	B	614	CLA	1	0
20	B	609	CLA	2	0
22	A	411	LHG	1	0
21	C	514	BCR	3	0
24	D	403	LMG	1	0
24	D	402	LMG	1	0
20	C	504	CLA	1	0
20	C	511	CLA	2	0
20	B	616	CLA	2	0
21	B	618	BCR	2	0
24	C	501	LMG	1	0
20	A	405	CLA	5	0
19	A	404	PHO	1	0
20	B	610	CLA	1	0
20	C	507	CLA	1	0
21	A	409	BCR	1	0
20	A	406	CLA	4	0
21	H	101	BCR	1	0

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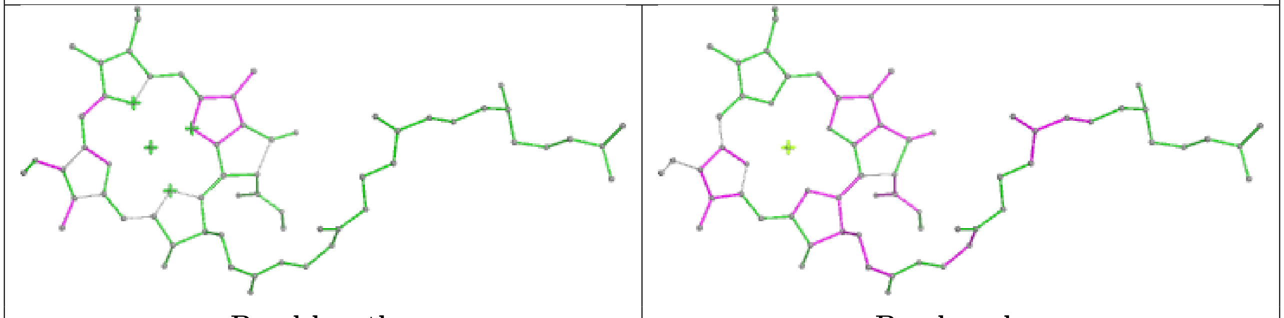
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	406	CLA	3	0
24	B	601	LMG	1	0
20	C	505	CLA	1	0
20	C	503	CLA	3	0
20	B	612	CLA	1	0
20	B	606	CLA	1	0
21	B	619	BCR	2	0
21	B	620	BCR	2	0
26	E	101	HEM	1	0
20	B	613	CLA	2	0
20	B	604	CLA	1	0
20	B	605	CLA	2	0
20	A	408	CLA	1	0
20	C	515	CLA	2	0
20	D	407	CLA	2	0
20	C	513	CLA	1	0
20	C	502	CLA	1	0

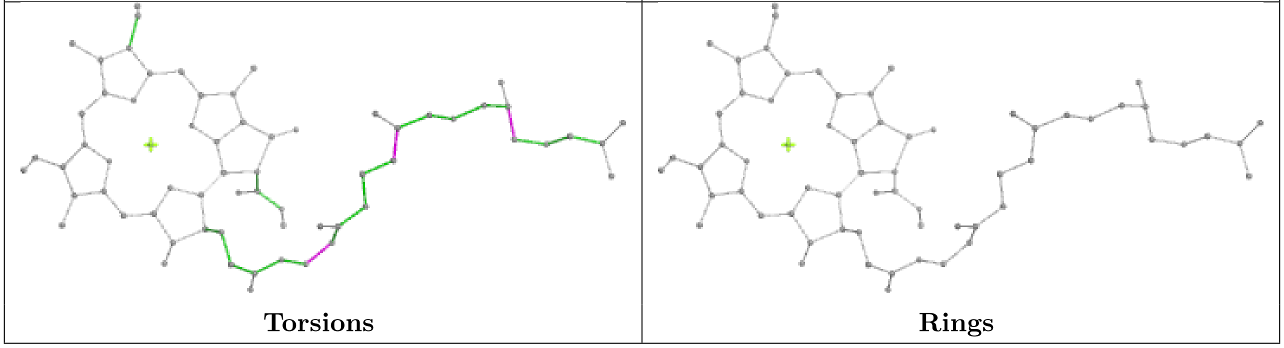
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand CLA B 603



Bond lengths

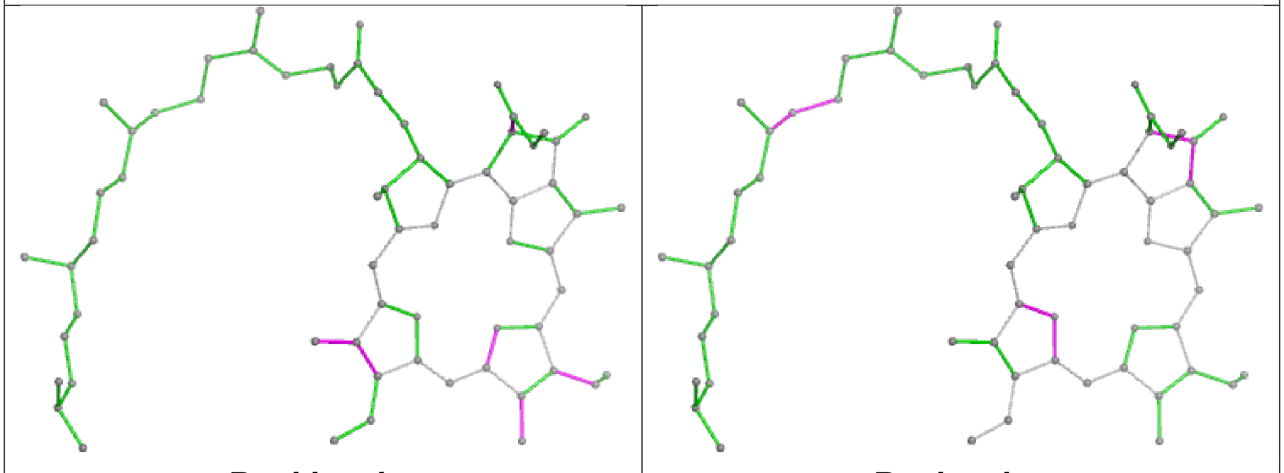
Bond angles



Torsions

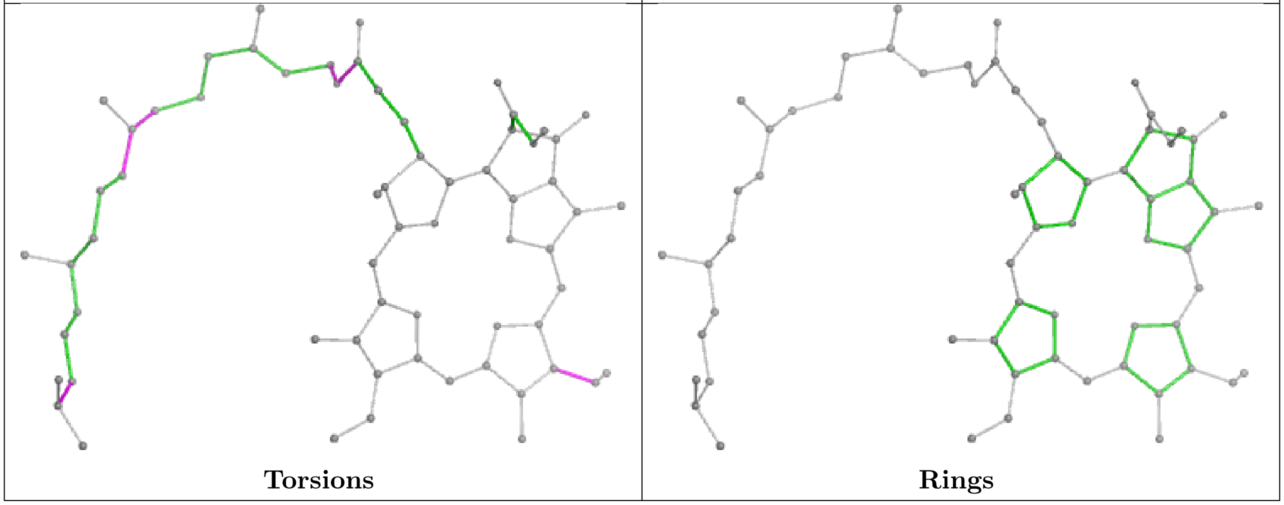
Rings

Ligand PHO D 405



Bond lengths

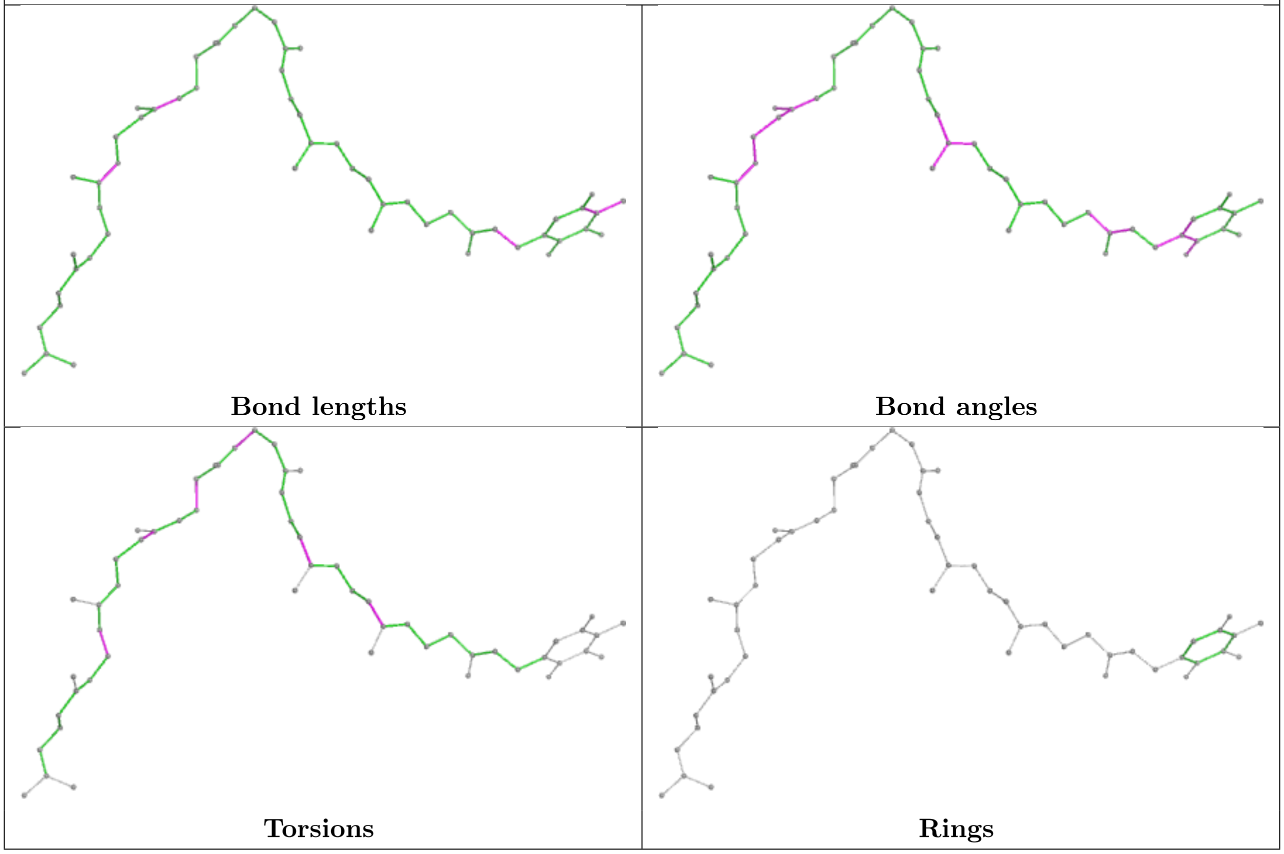
Bond angles



Torsions

Rings

Ligand PL9 D 404



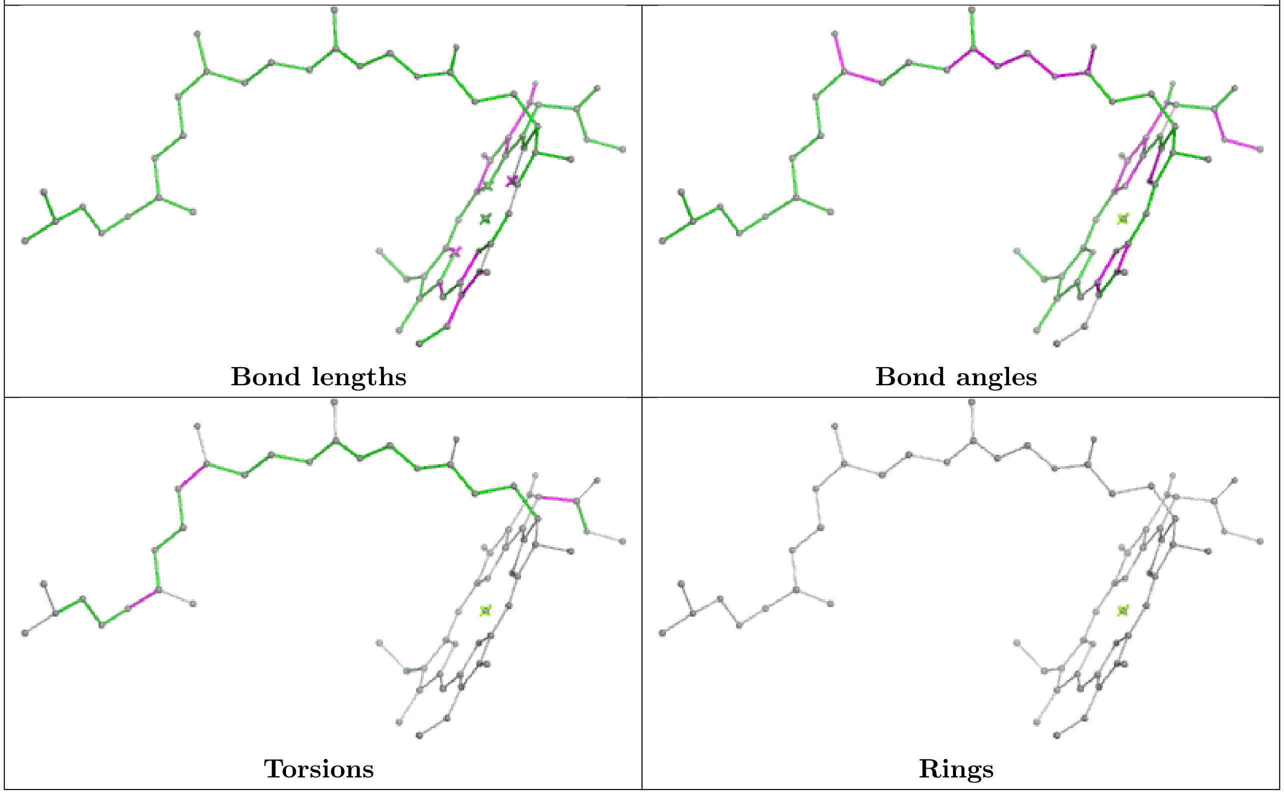
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA C 509



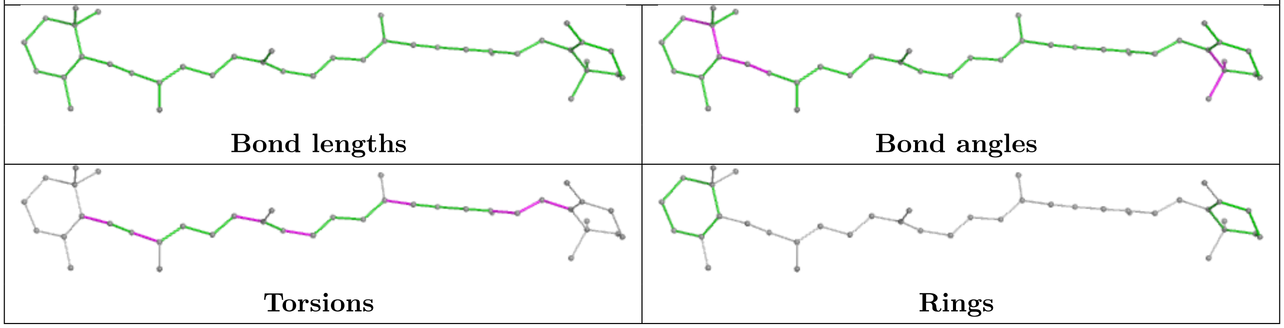
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR C 516



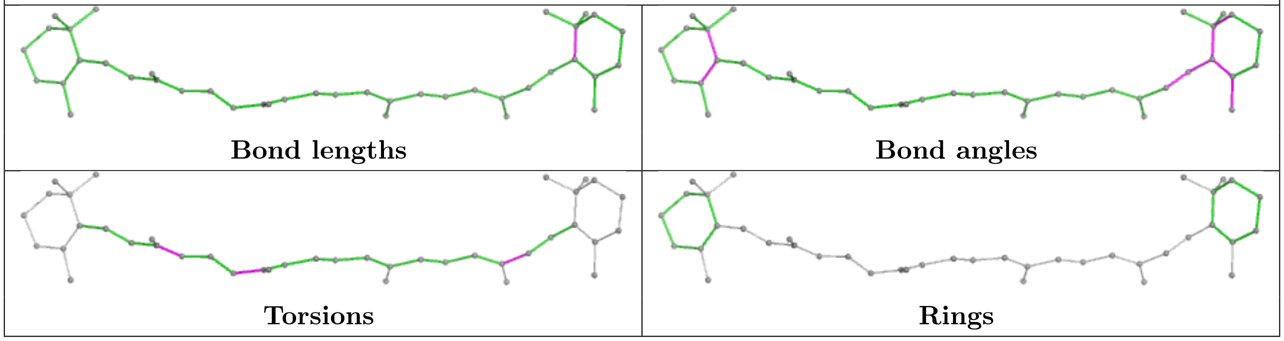
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR Z 101



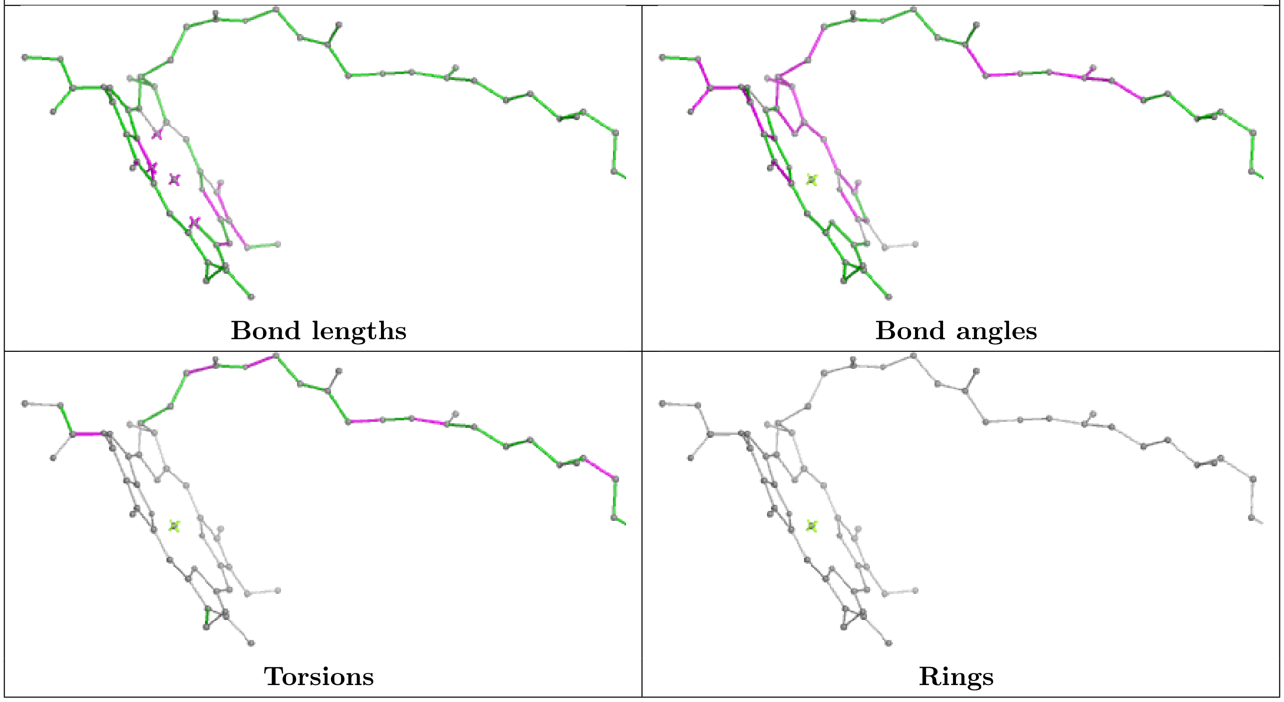
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 608



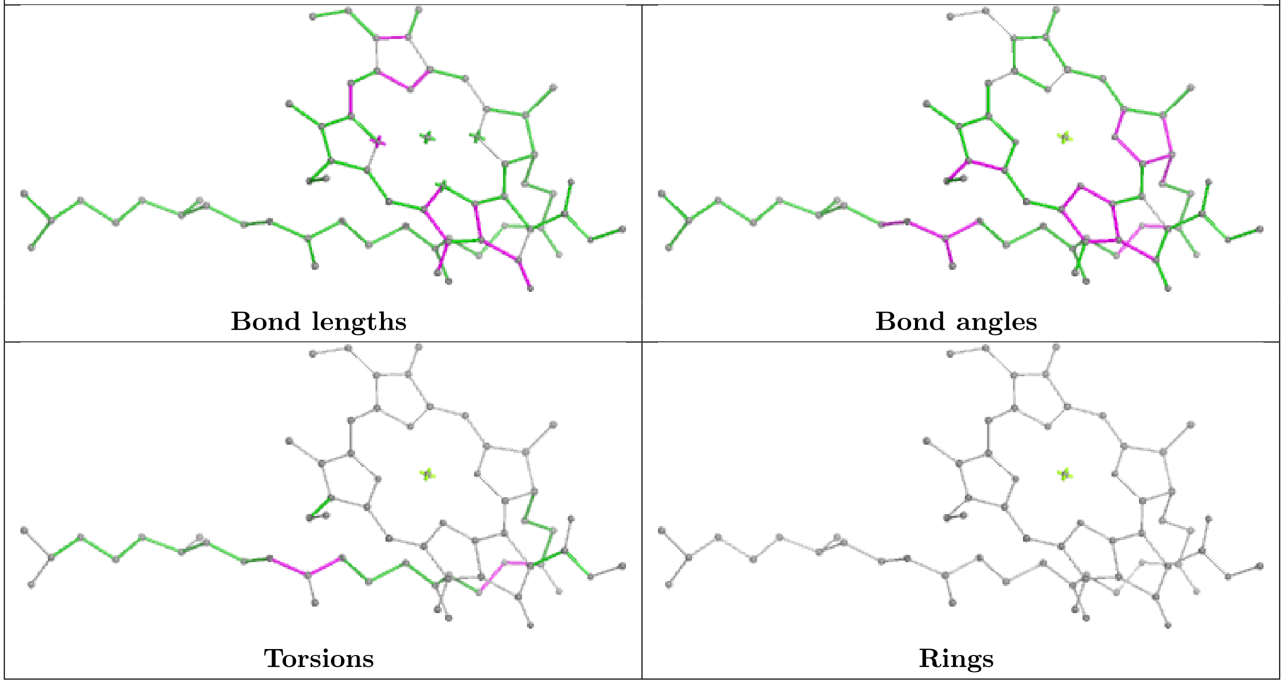
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 615



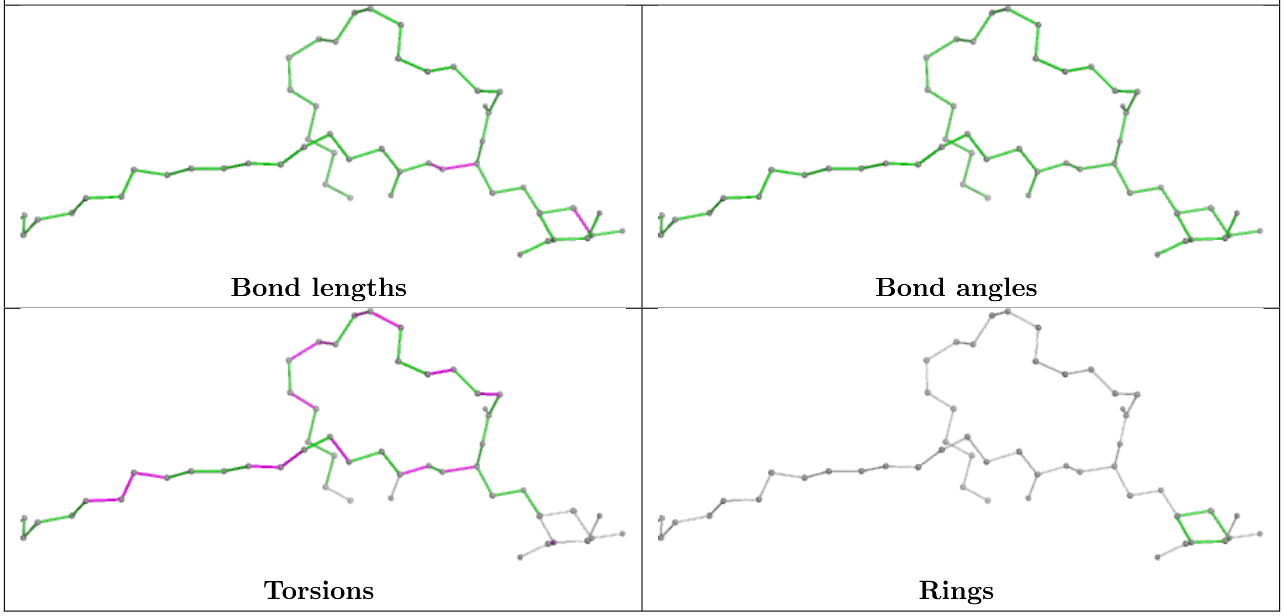
Bond lengths

Bond angles

Torsions

Rings

Ligand LMG D 401



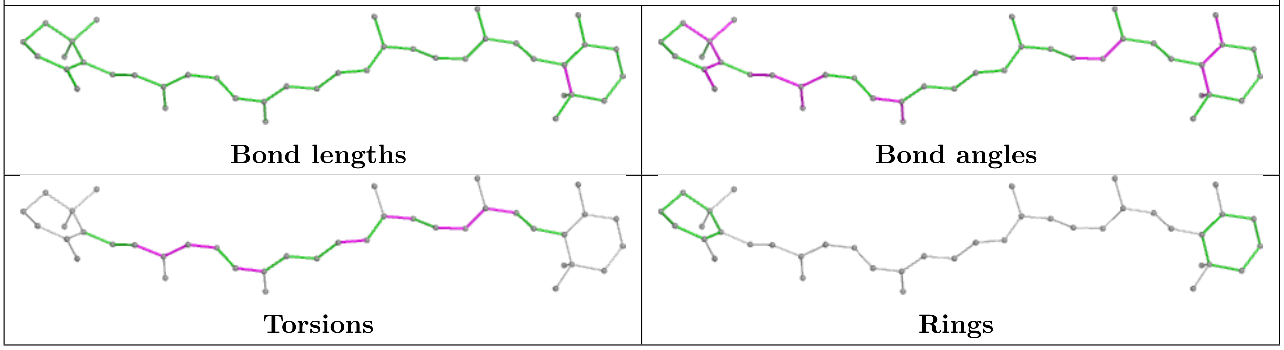
Bond lengths

Bond angles

Torsions

Rings

Ligand BCR K 101



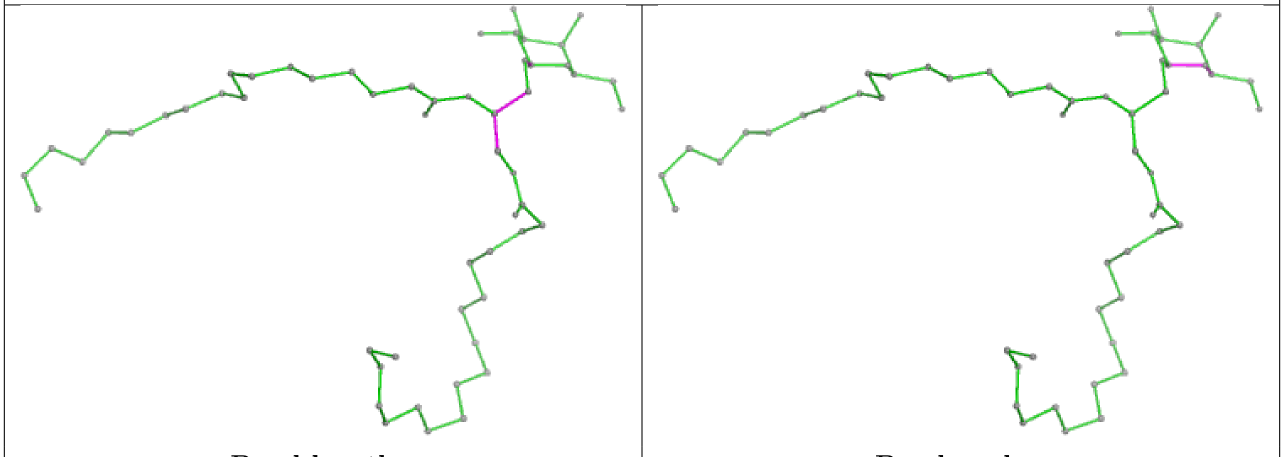
Bond lengths

Bond angles

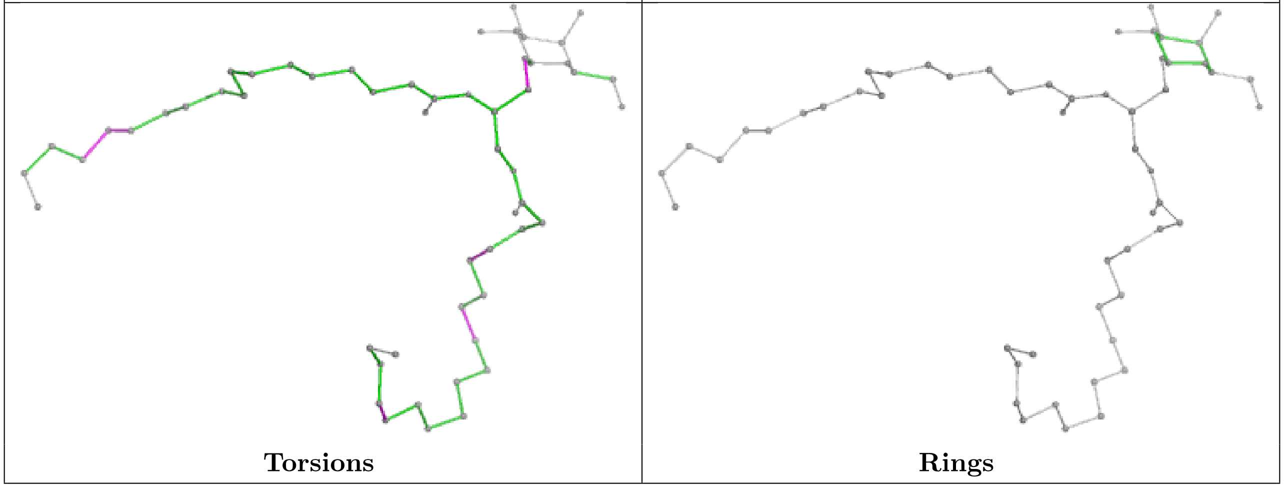
Torsions

Rings

Ligand LMG M 101

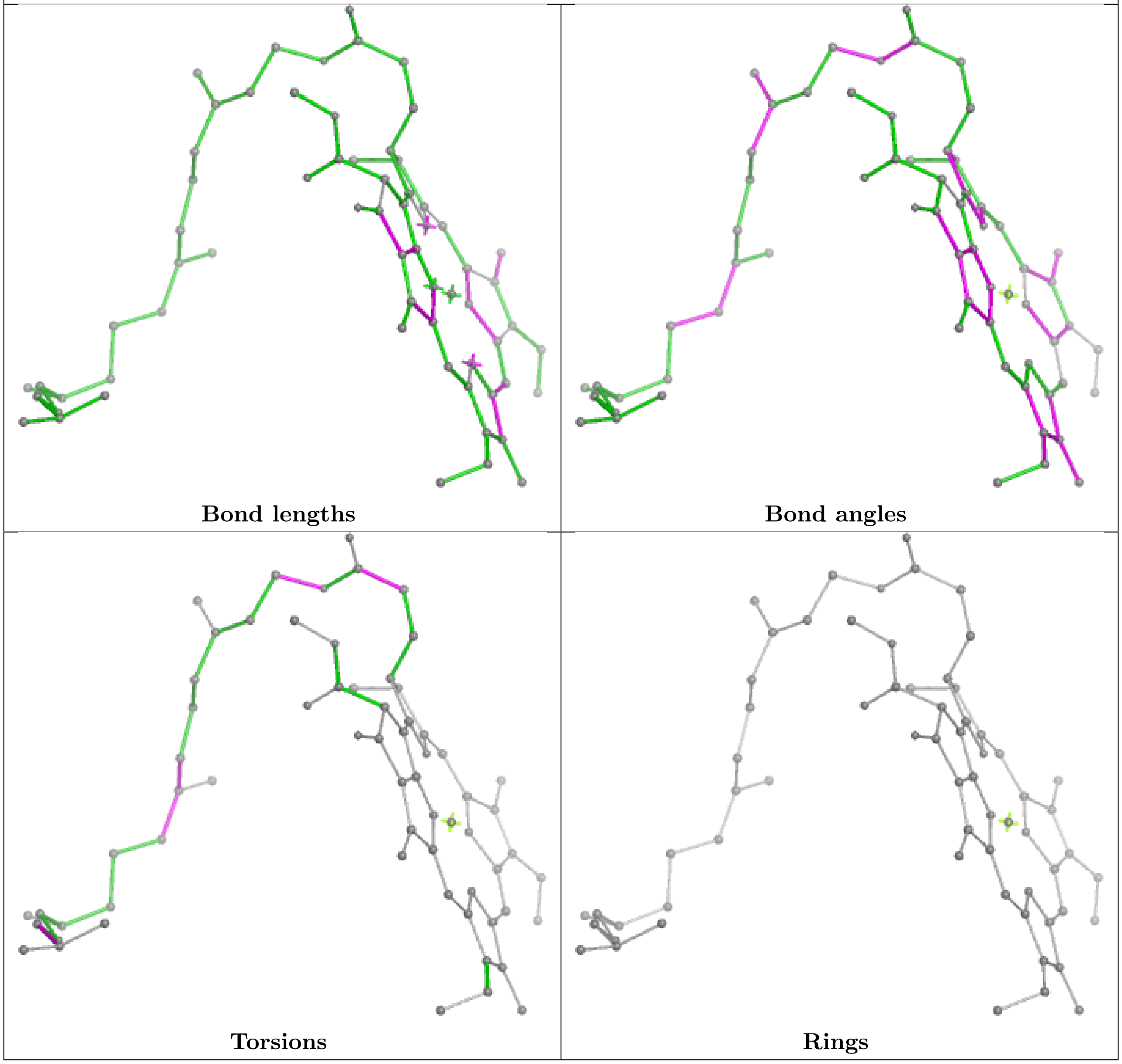


Bond lengths **Bond angles**



Torsions **Rings**

Ligand CLA B 614



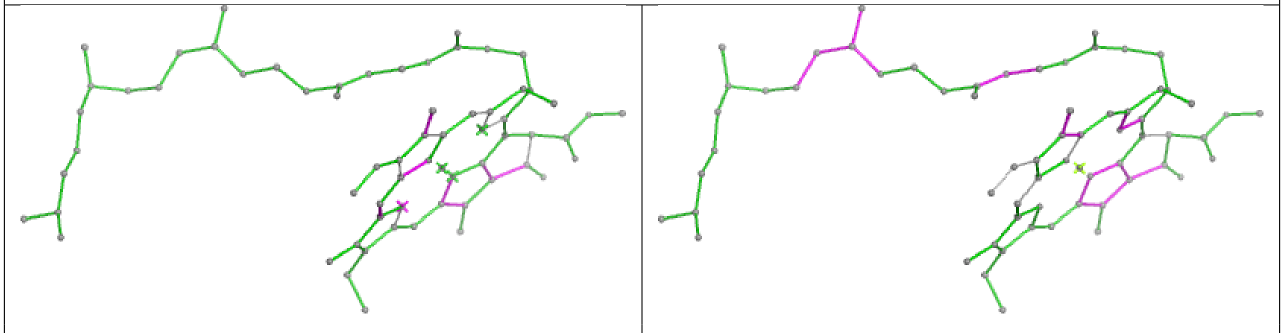
Bond lengths

Bond angles

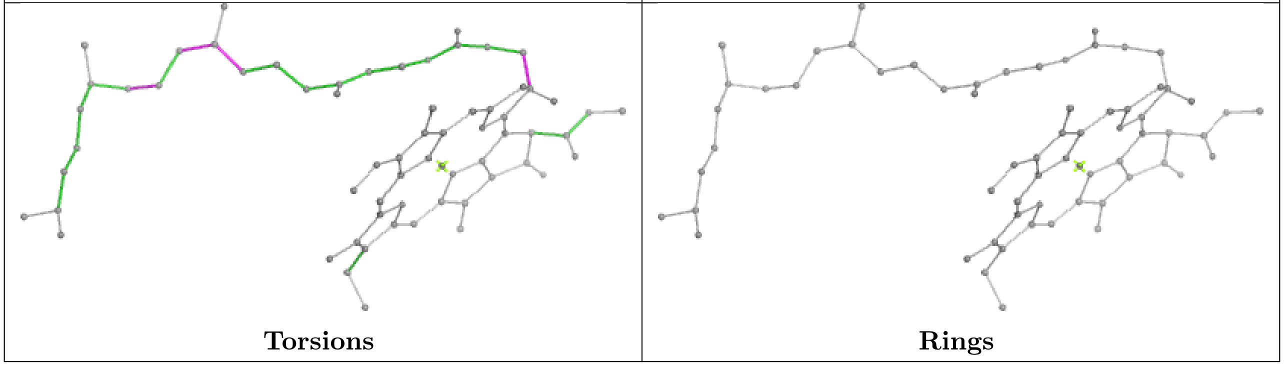
Torsions

Rings

Ligand CLA B 609

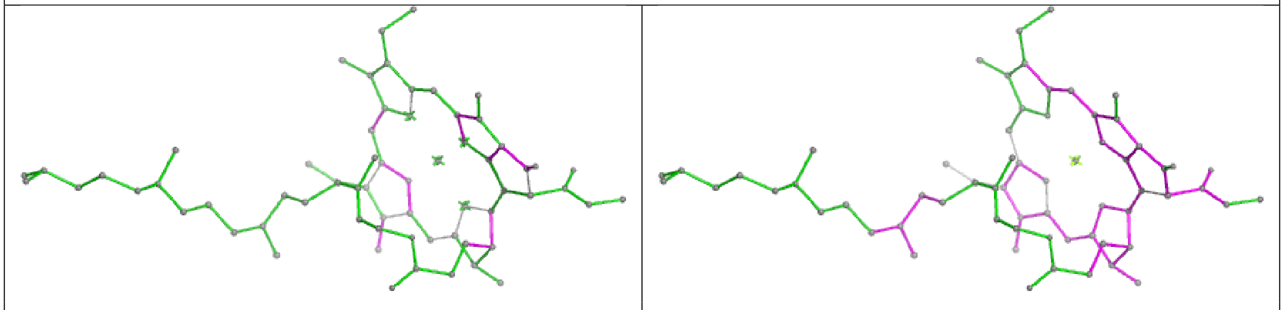


Bond lengths Bond angles

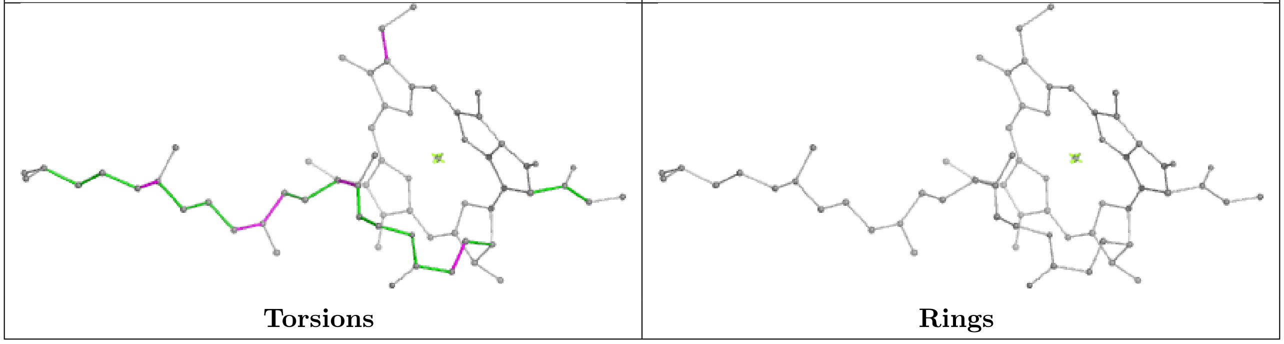


Torsions Rings

Ligand CLA C 506

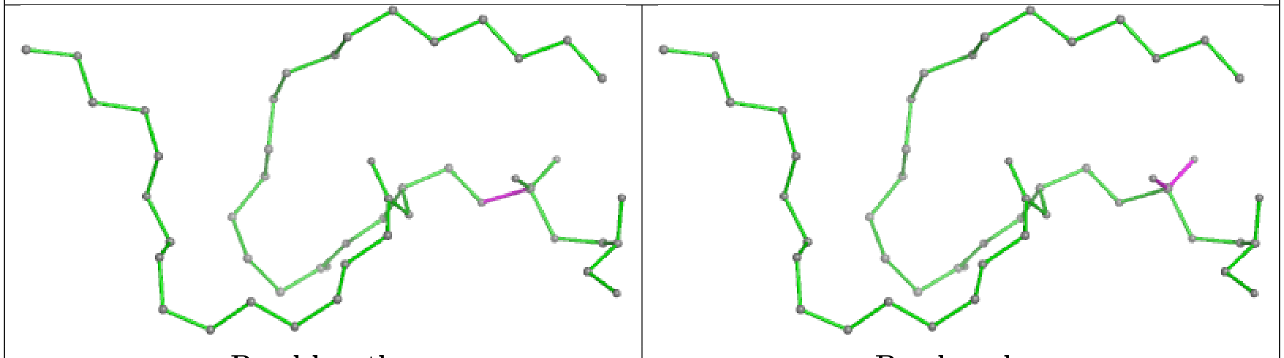


Bond lengths Bond angles

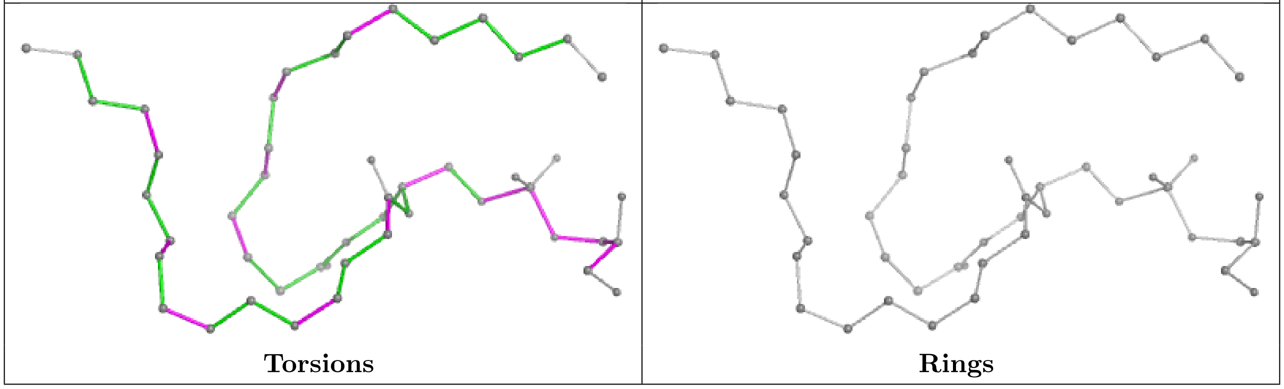


Torsions Rings

Ligand LHG A 411

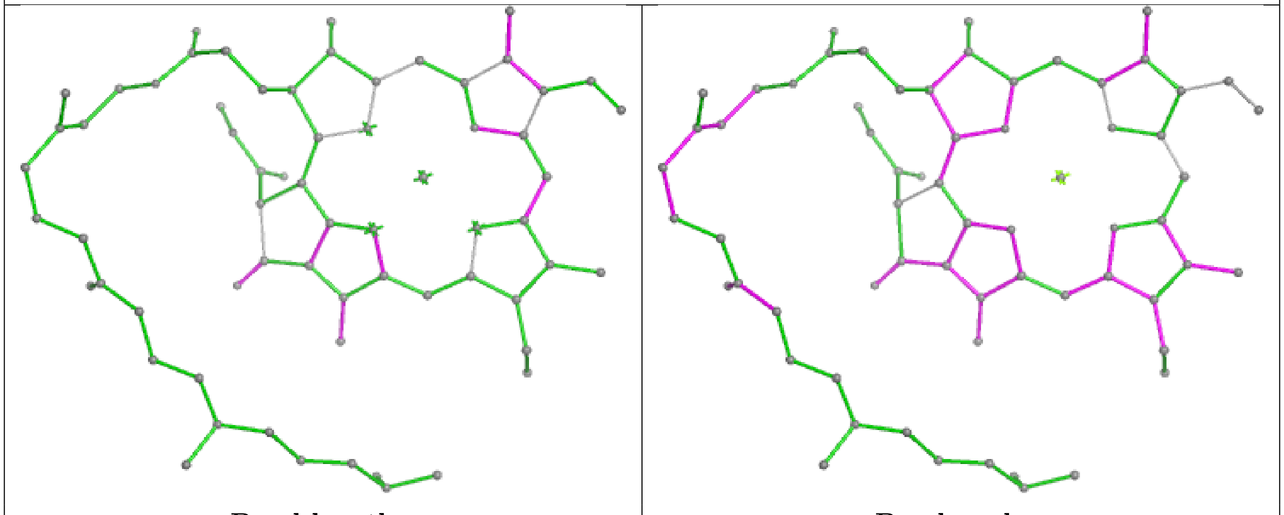


Bond lengths **Bond angles**



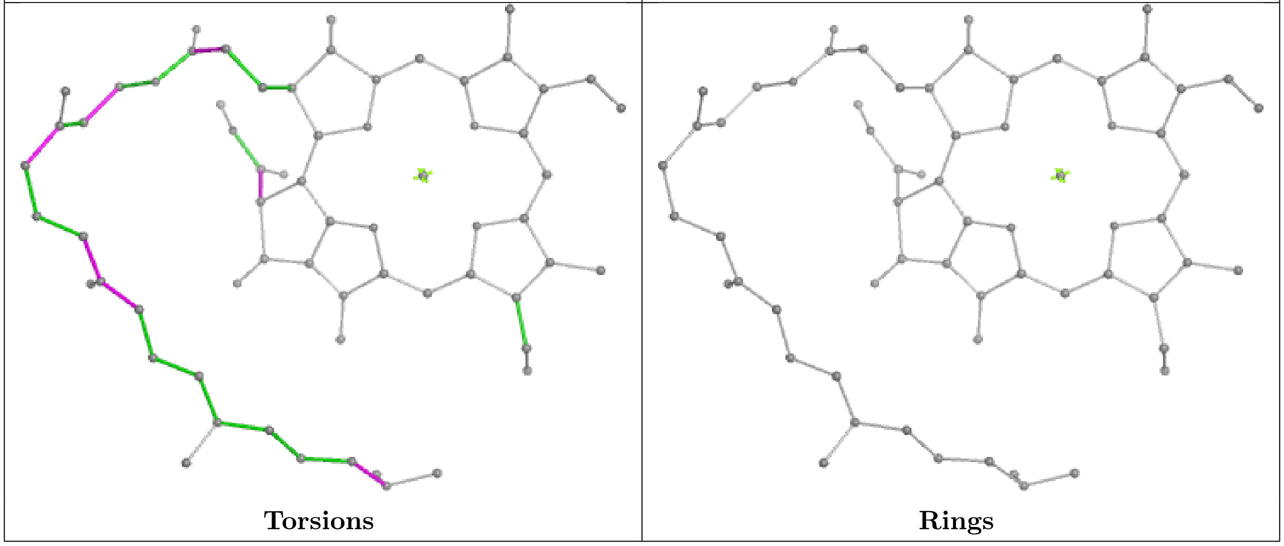
Torsions **Rings**

Ligand CLA B 602



Bond lengths

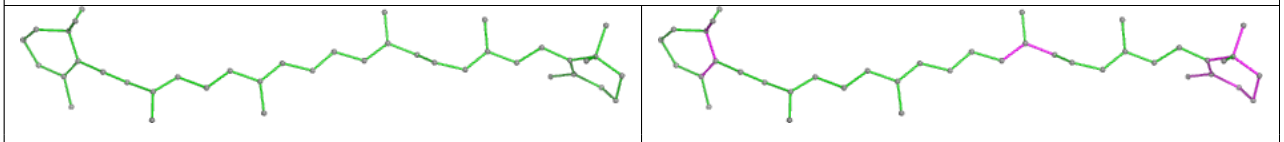
Bond angles



Torsions

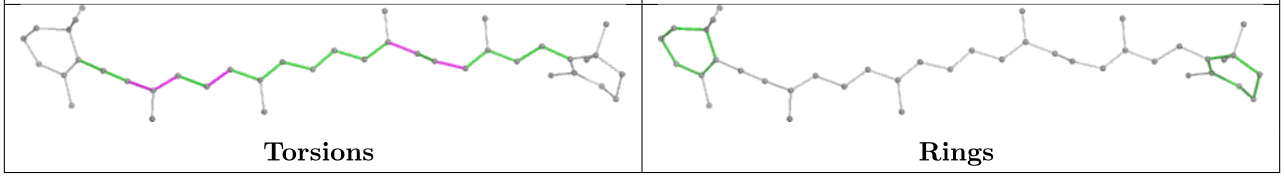
Rings

Ligand BCR C 514



Bond lengths

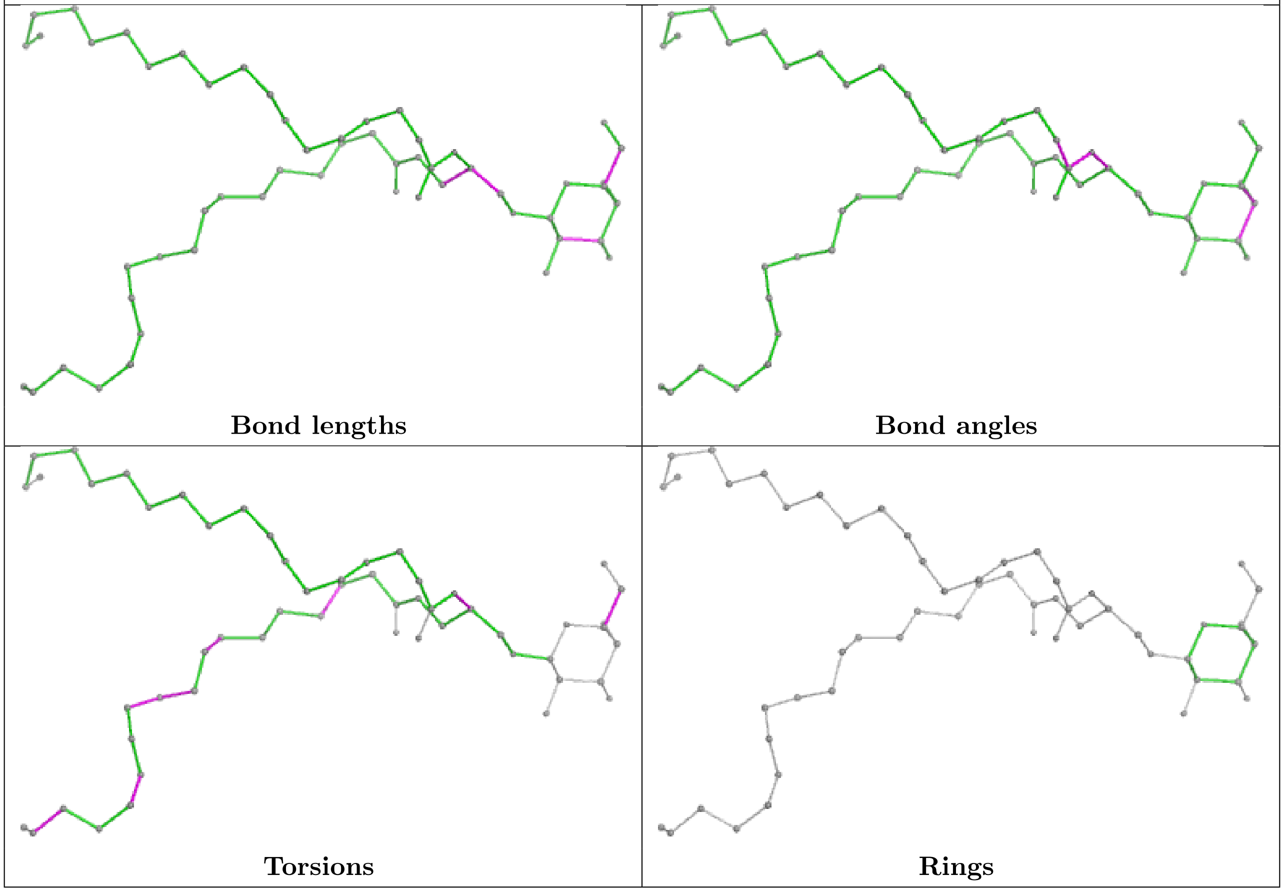
Bond angles



Torsions

Rings

Ligand LMG D 403



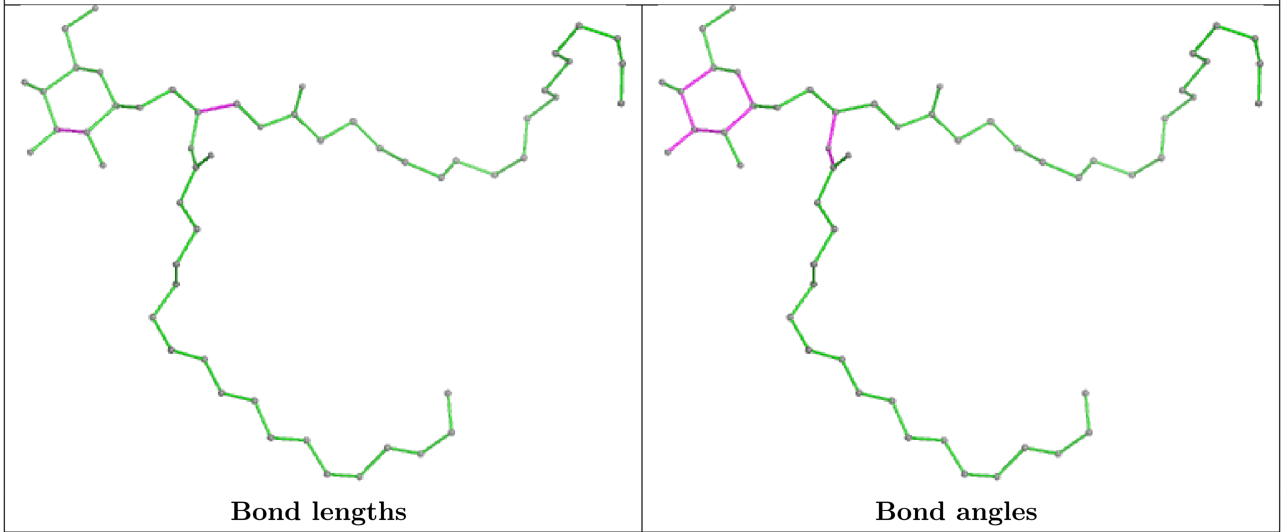
Bond lengths

Bond angles

Torsions

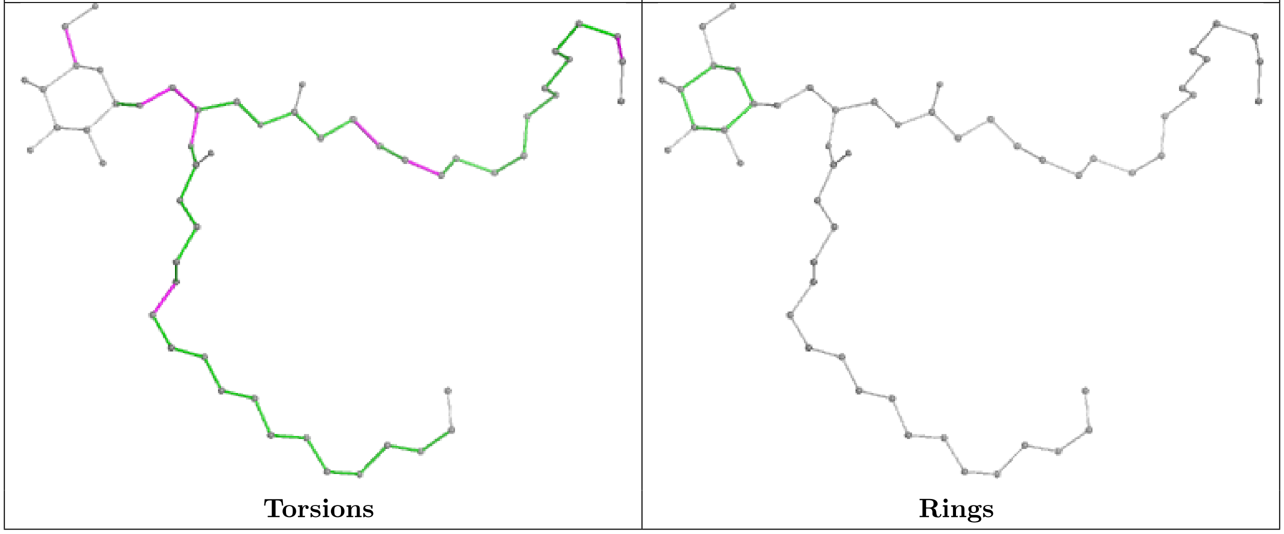
Rings

Ligand LMG D 402



Bond lengths

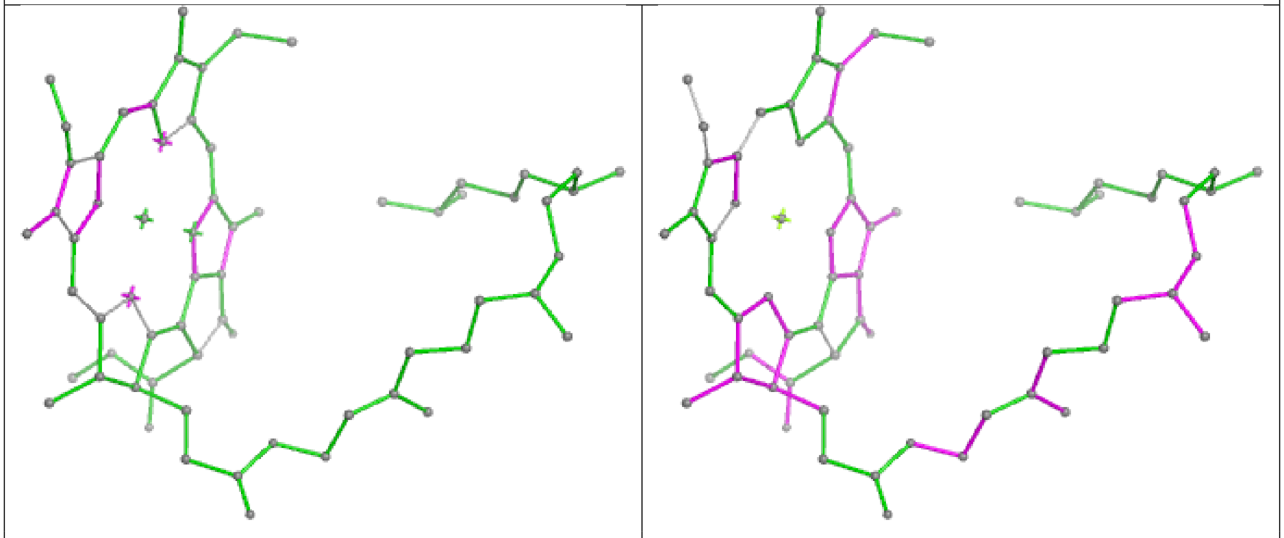
Bond angles



Torsions

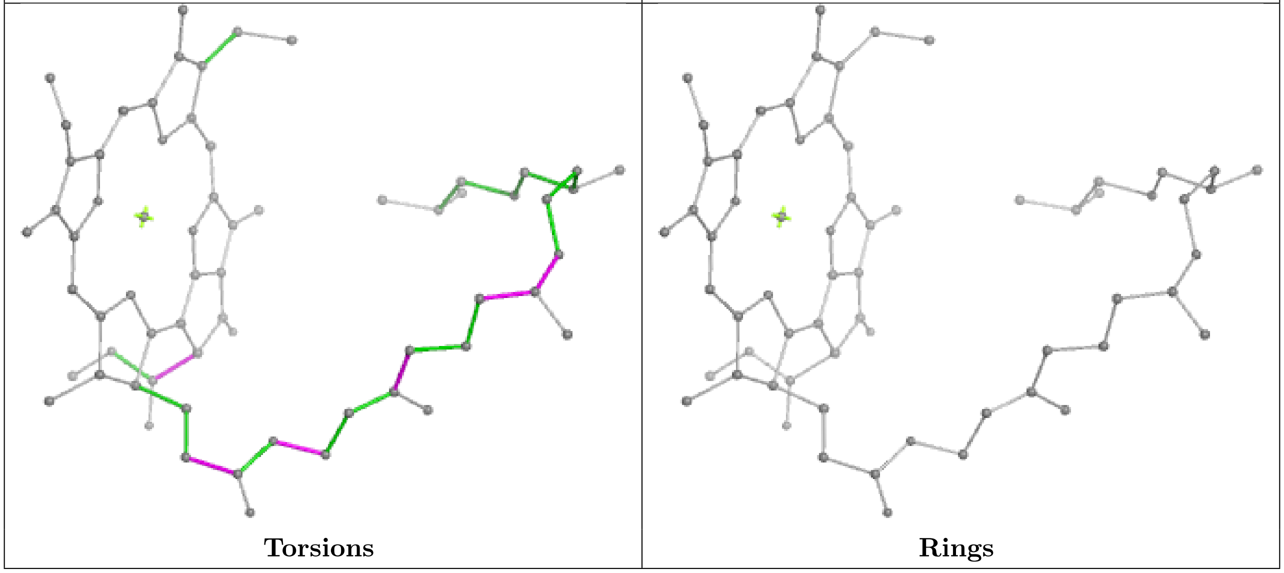
Rings

Ligand CLA C 504



Bond lengths

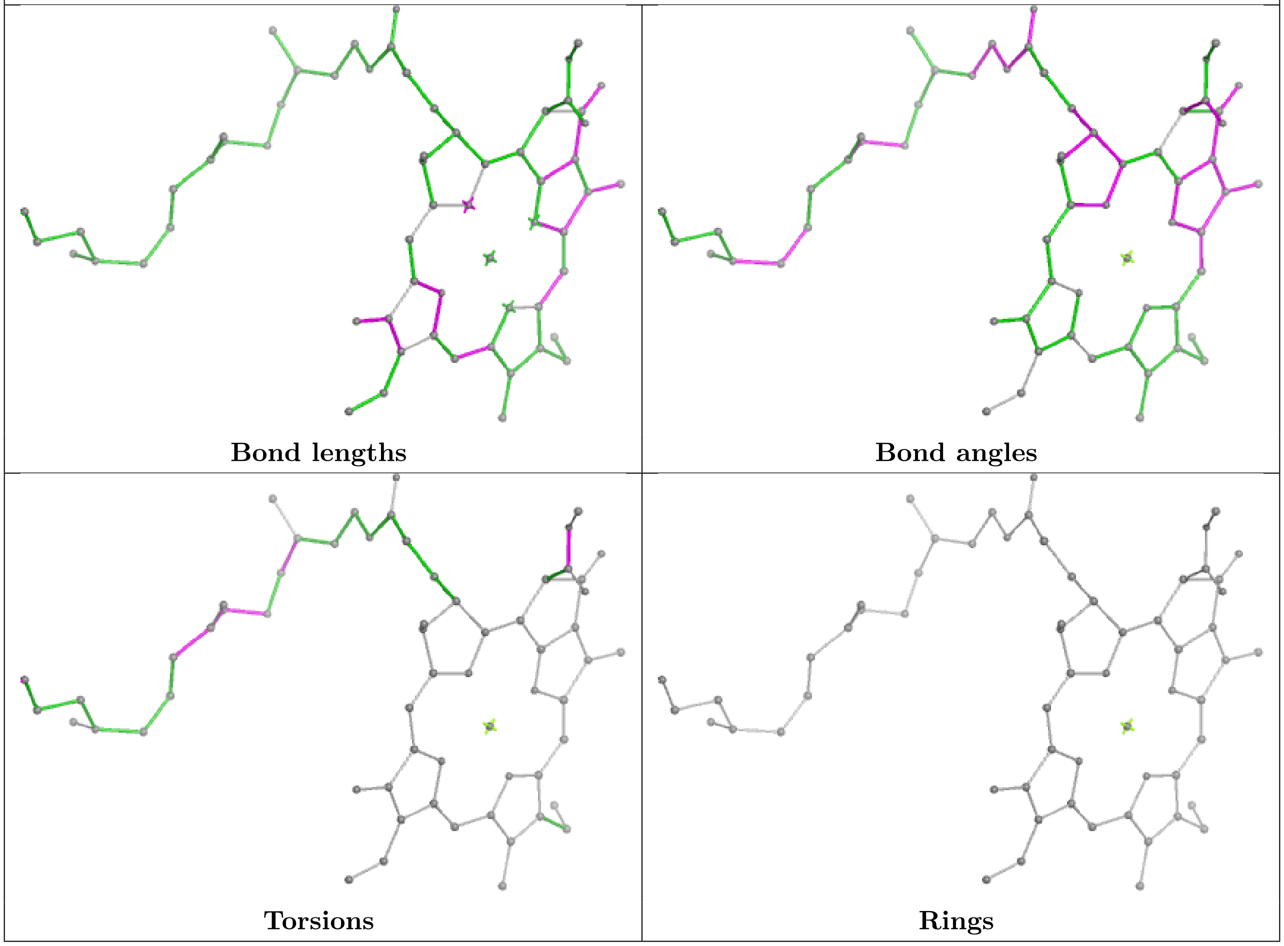
Bond angles



Torsions

Rings

Ligand CLA C 511



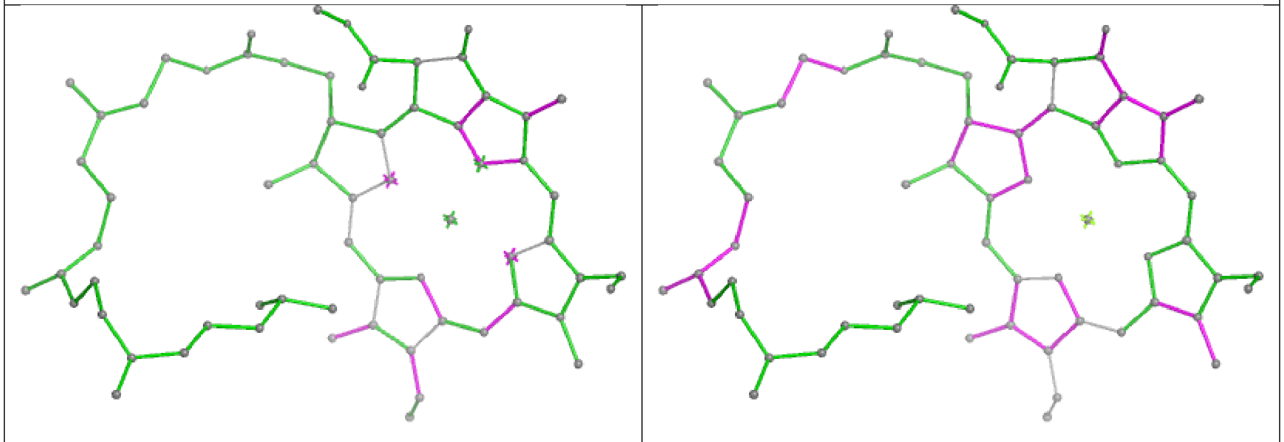
Bond lengths

Bond angles

Torsions

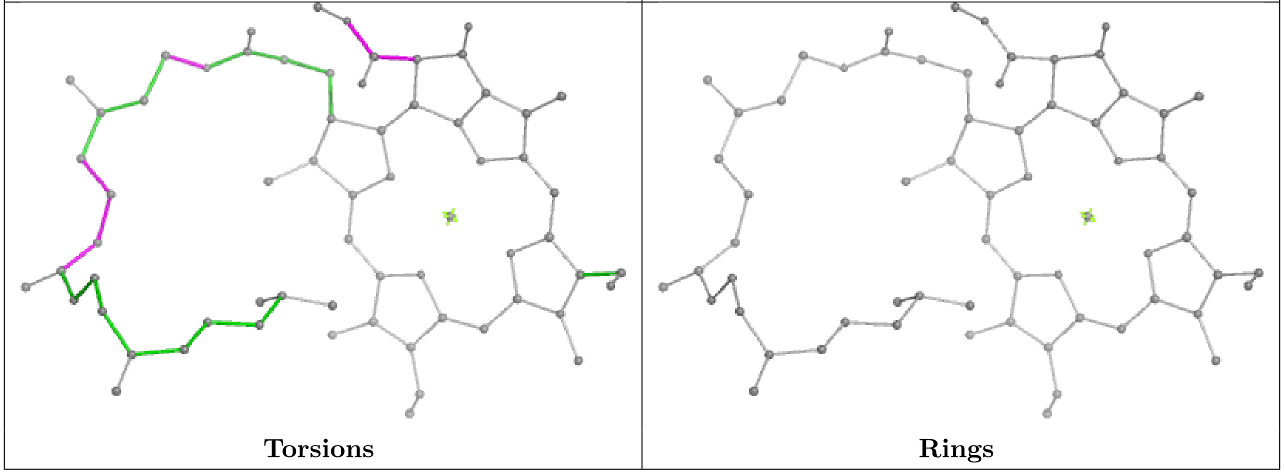
Rings

Ligand CLA B 616



Bond lengths

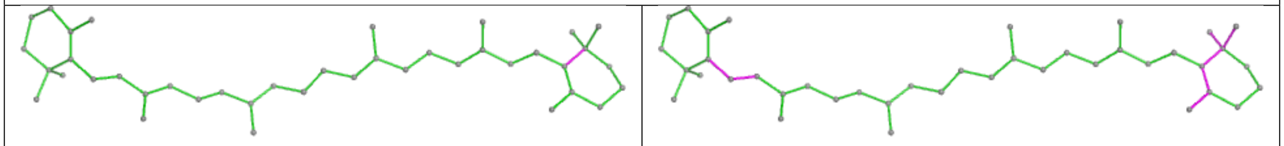
Bond angles



Torsions

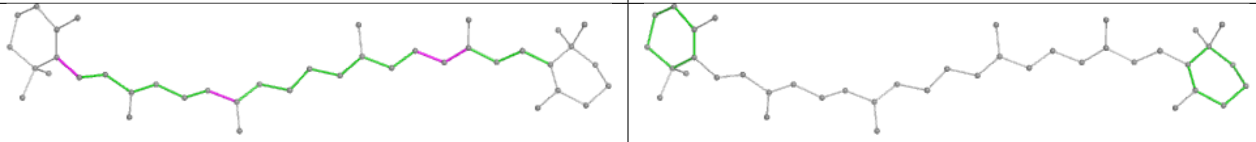
Rings

Ligand BCR B 618



Bond lengths

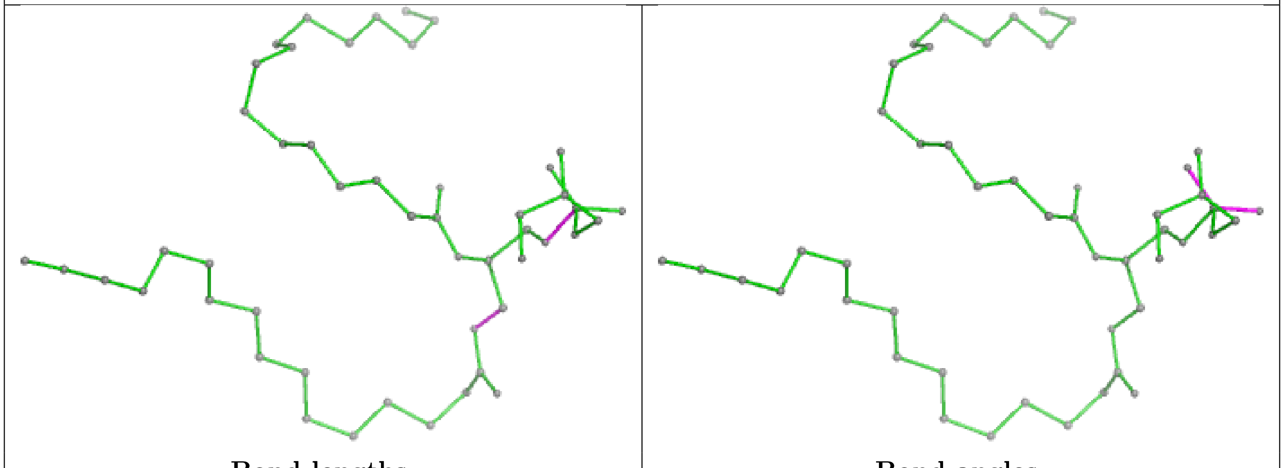
Bond angles



Torsions

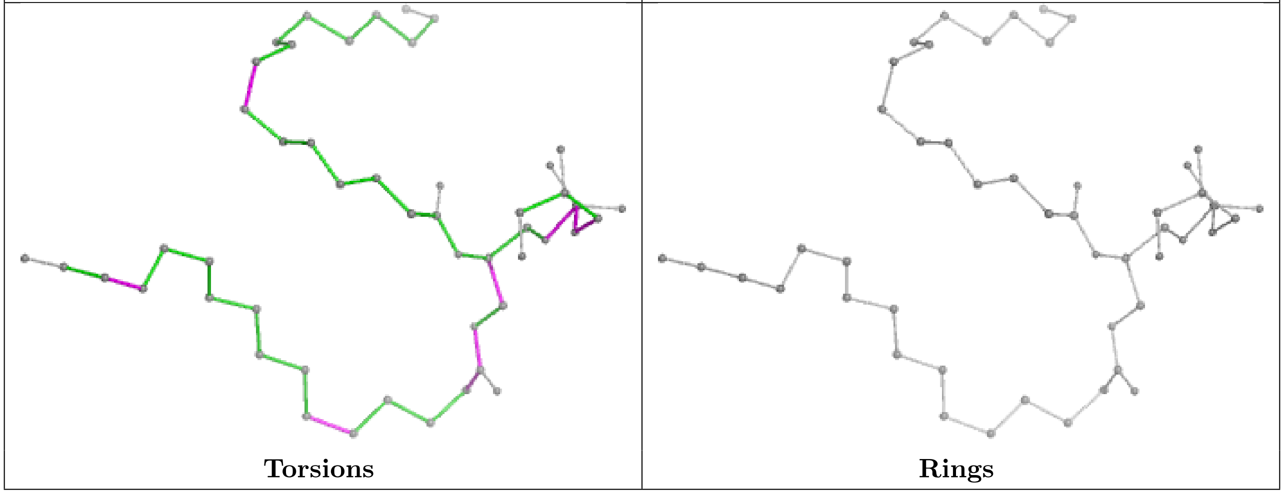
Rings

Ligand LHG A 410



Bond lengths

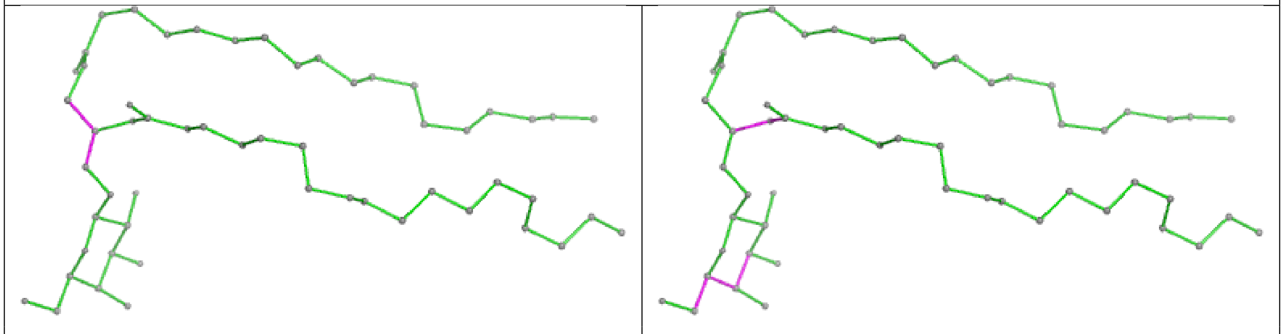
Bond angles



Torsions

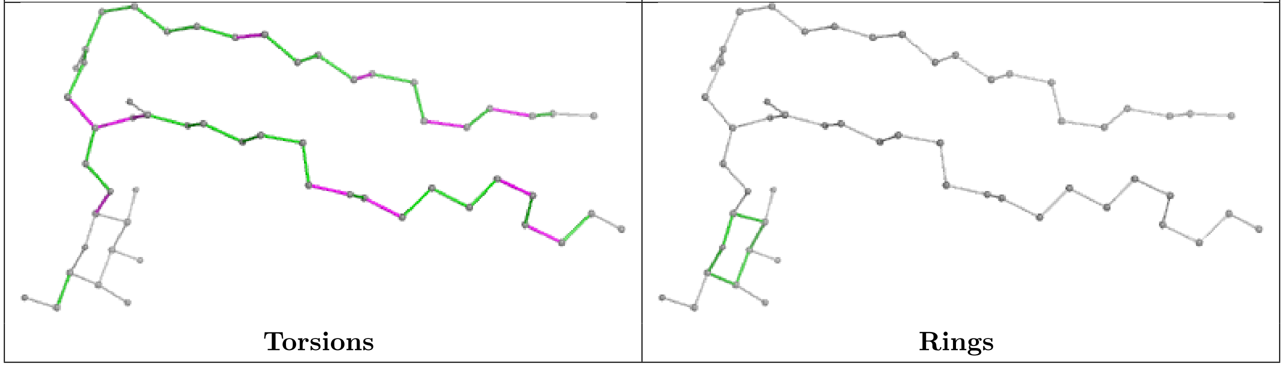
Rings

Ligand LMG C 501



Bond lengths

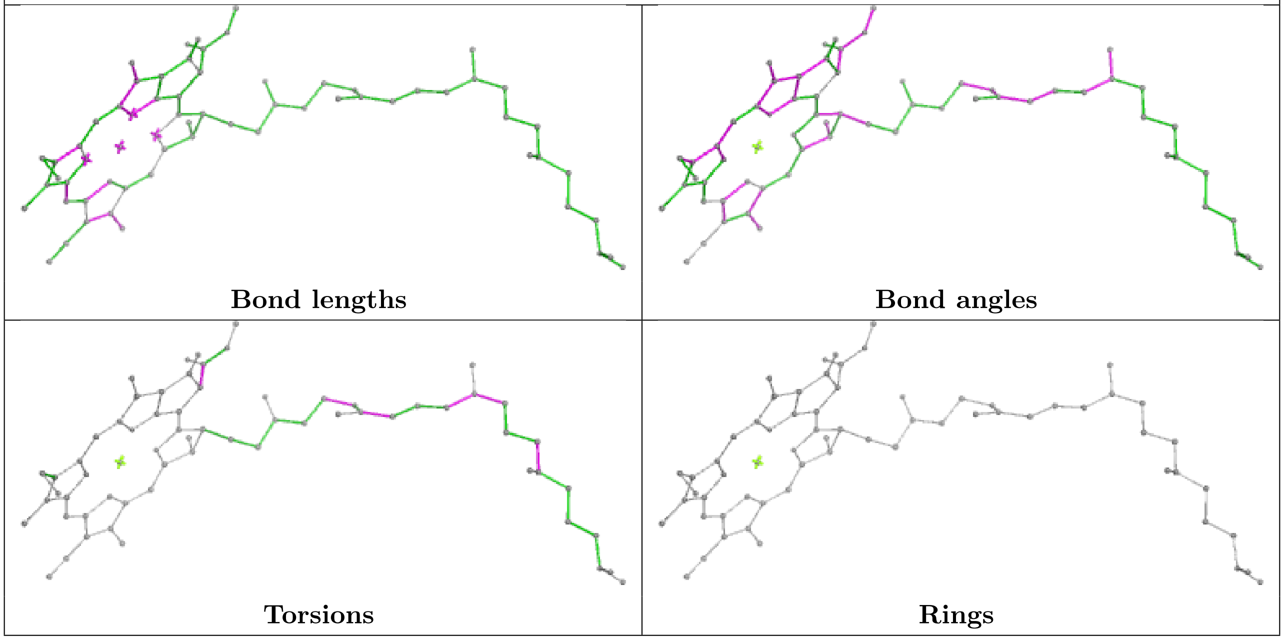
Bond angles



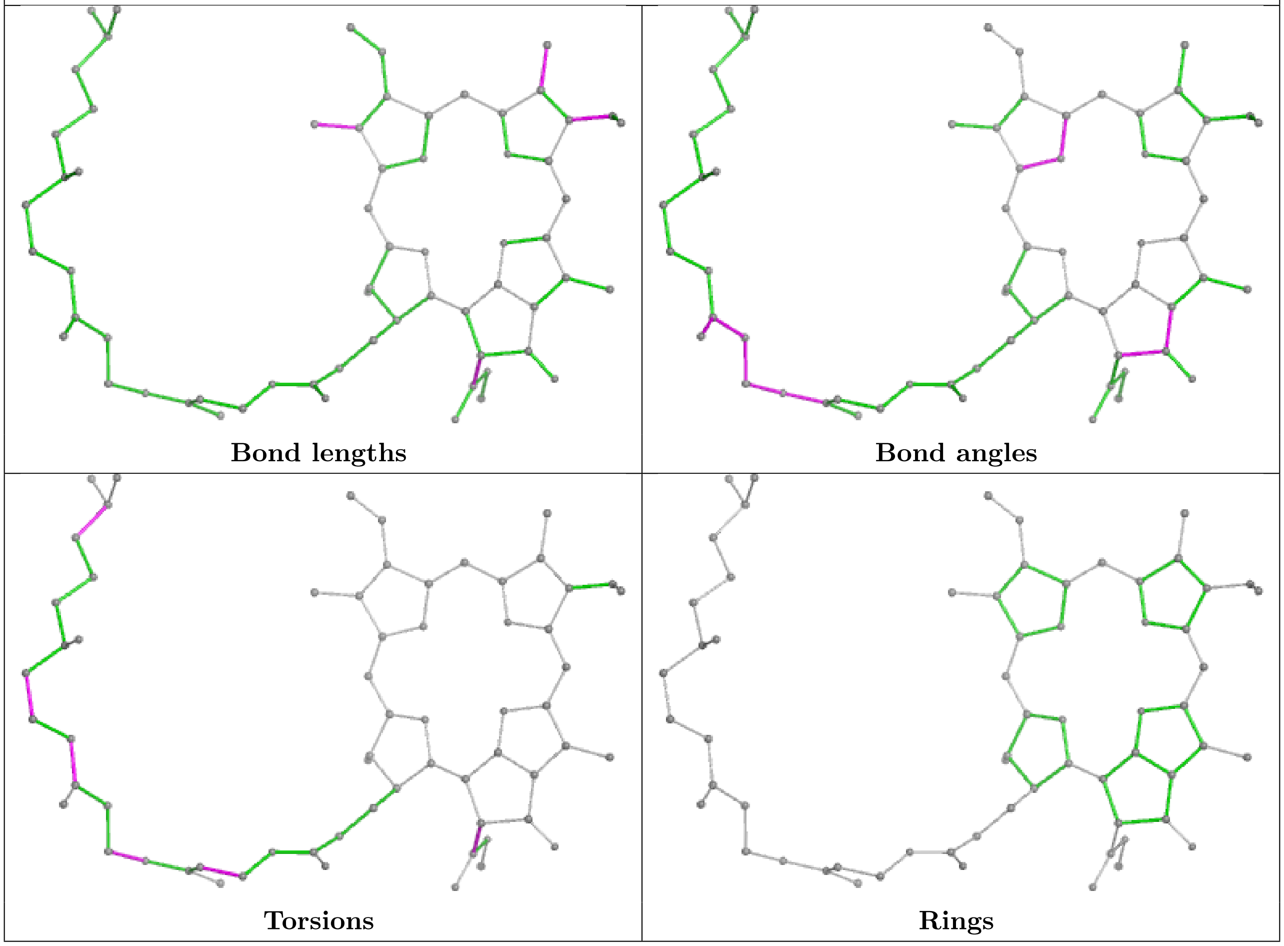
Torsions

Rings

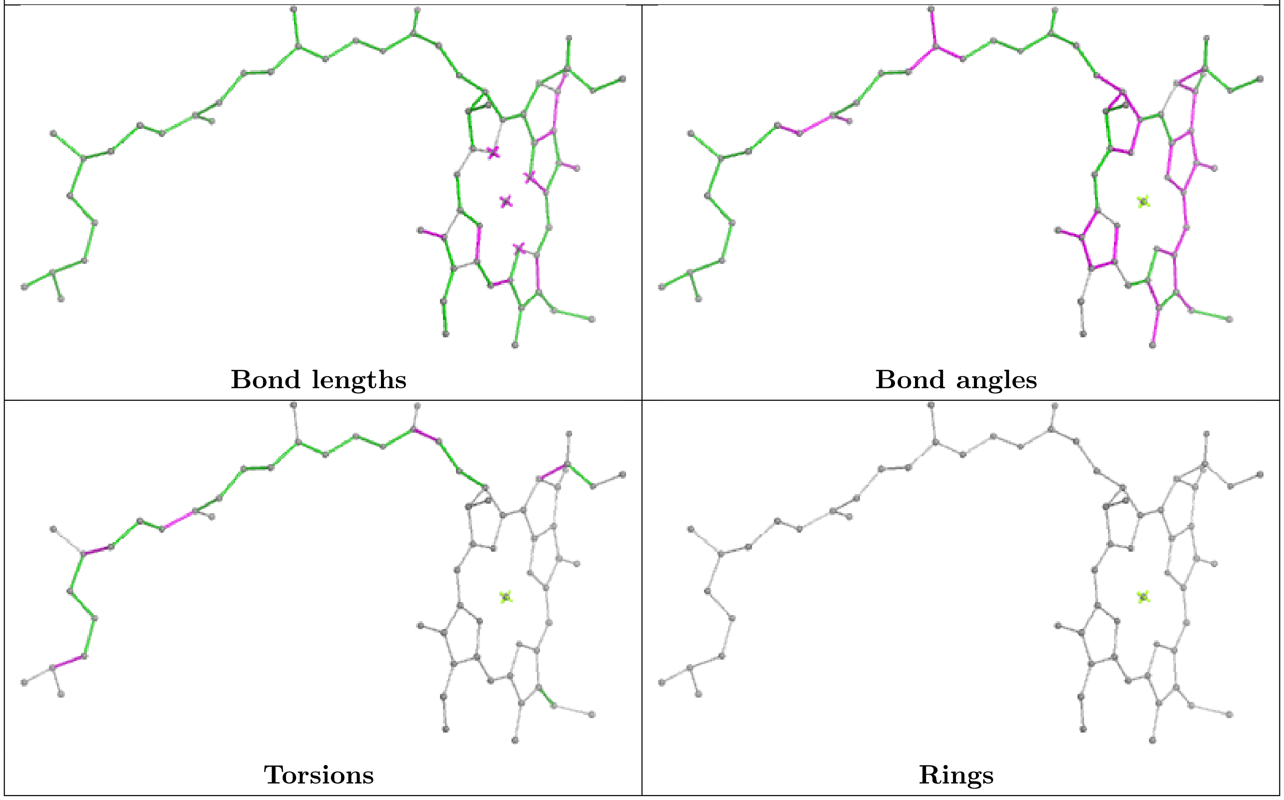
Ligand CLA A 405



Ligand PHO A 404



Ligand CLA B 610



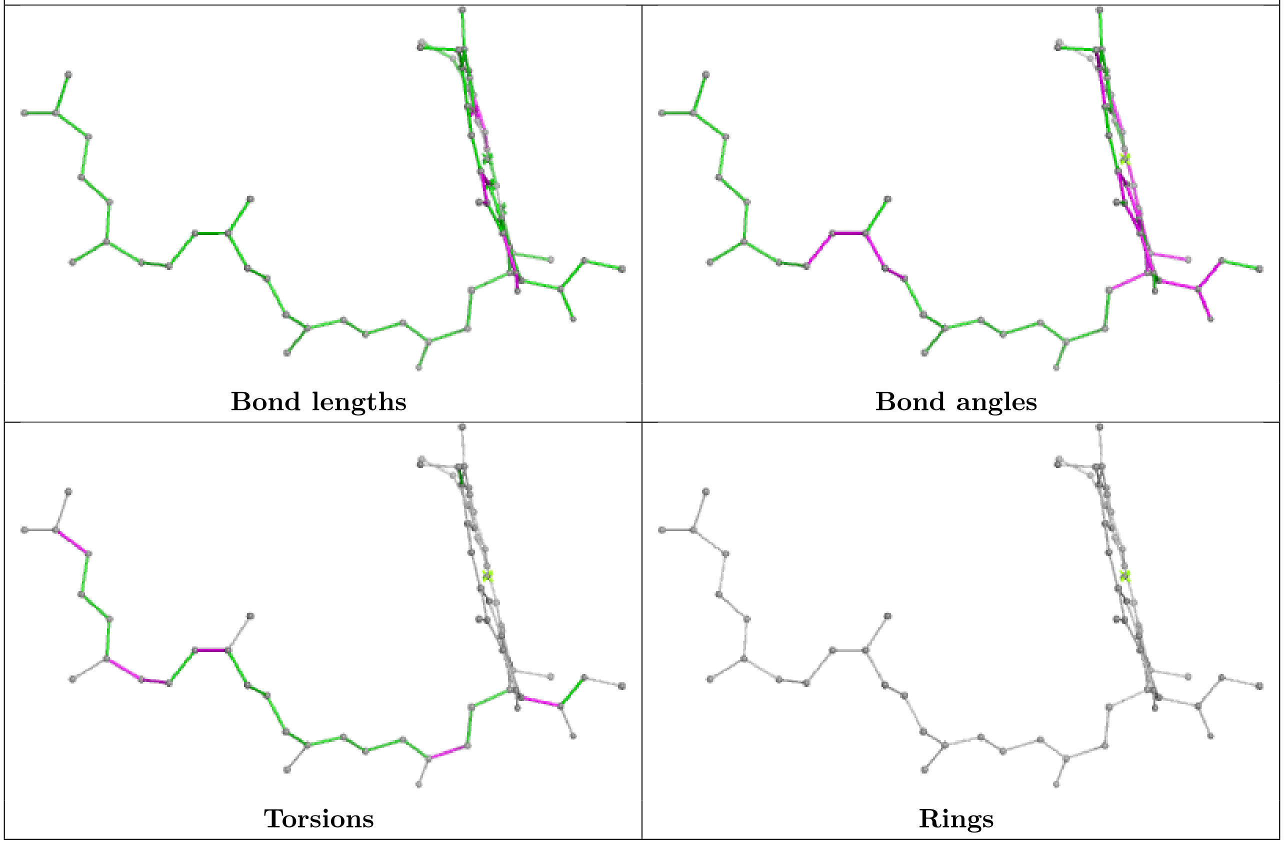
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA C 507



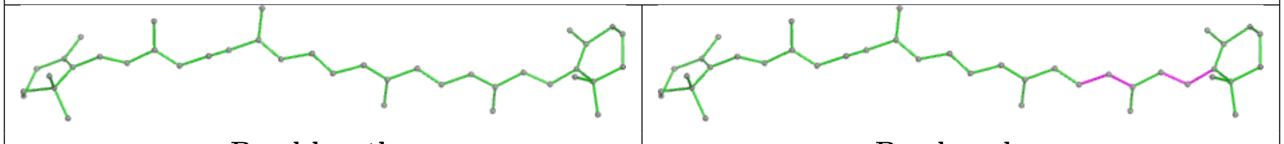
Bond lengths

Bond angles

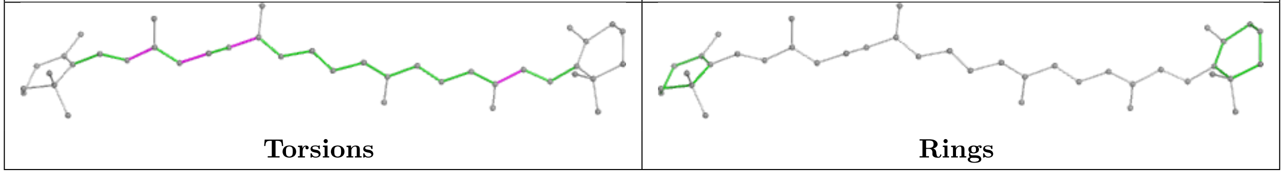
Torsions

Rings

Ligand BCR A 409

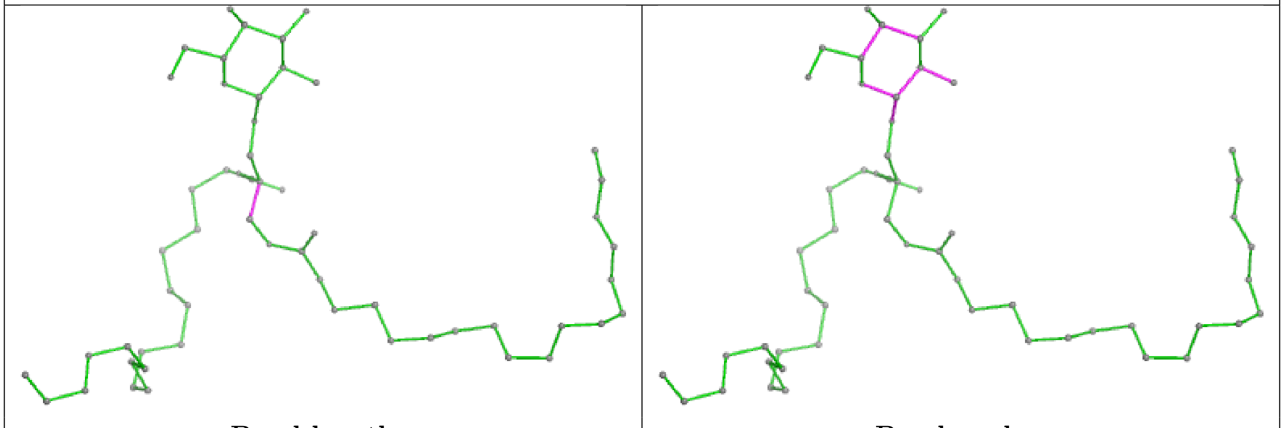


Bond lengths Bond angles

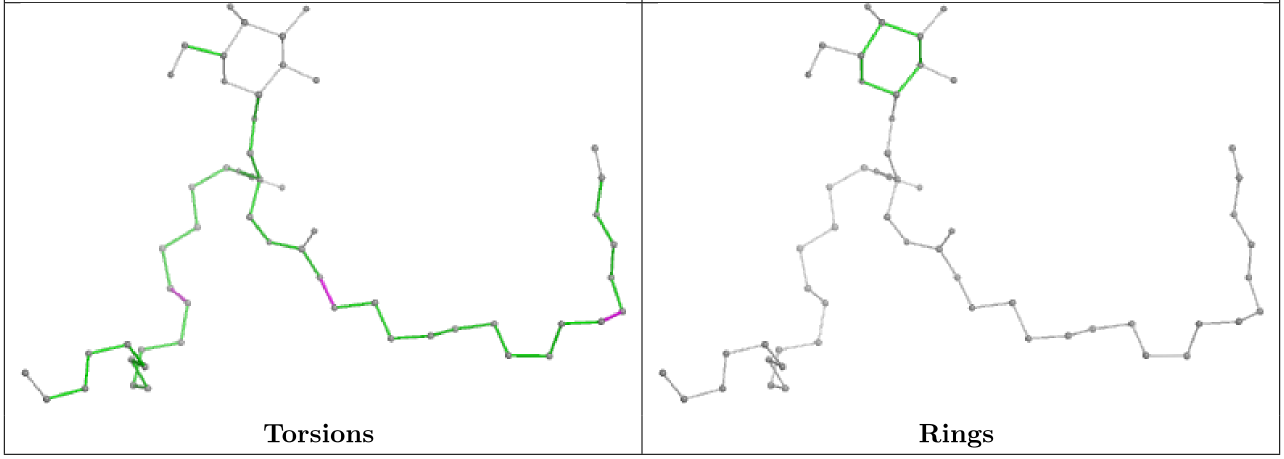


Torsions Rings

Ligand LMG I 101

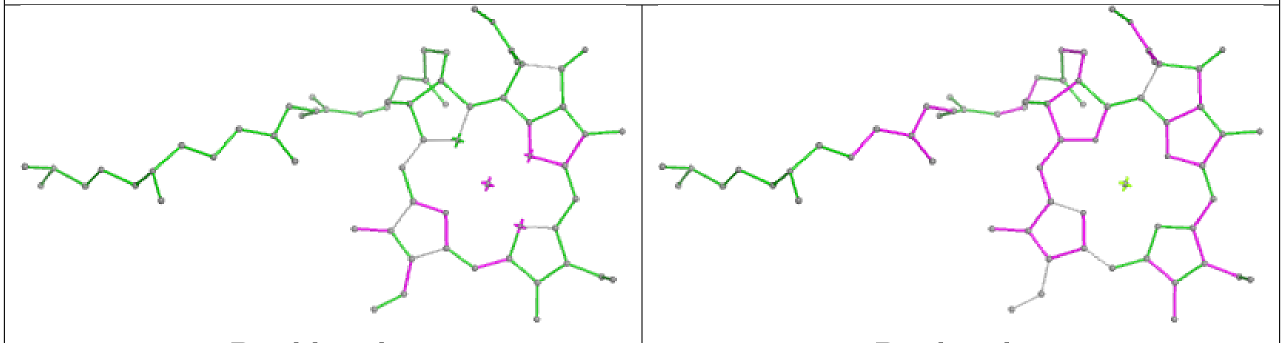


Bond lengths Bond angles

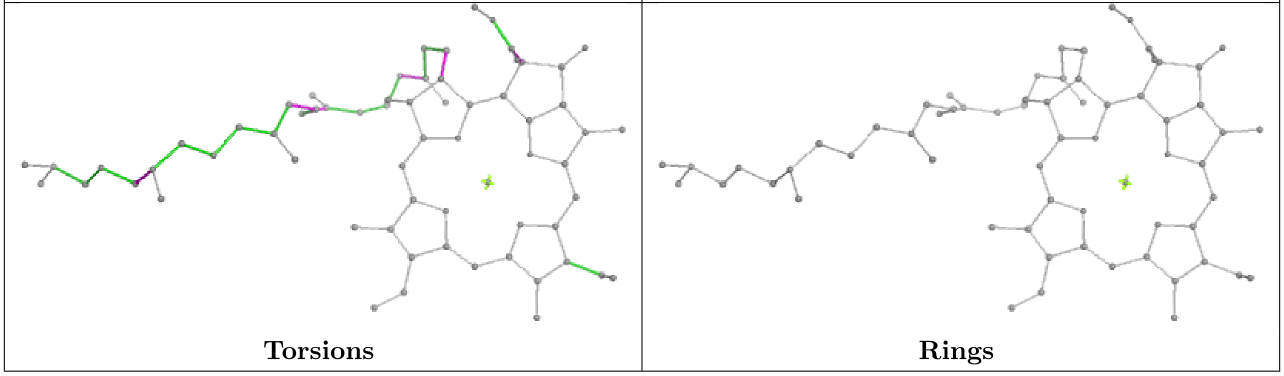


Torsions Rings

Ligand CLA A 406

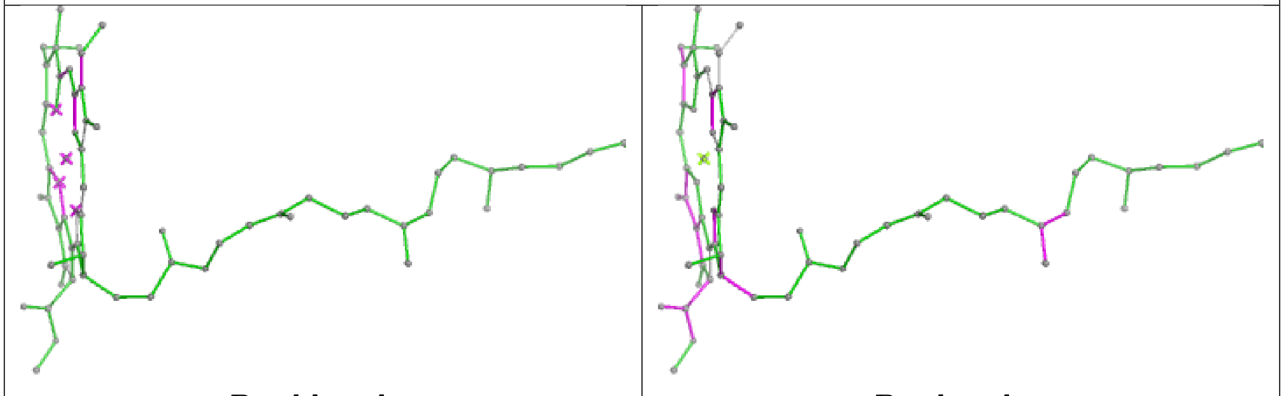


Bond lengths Bond angles

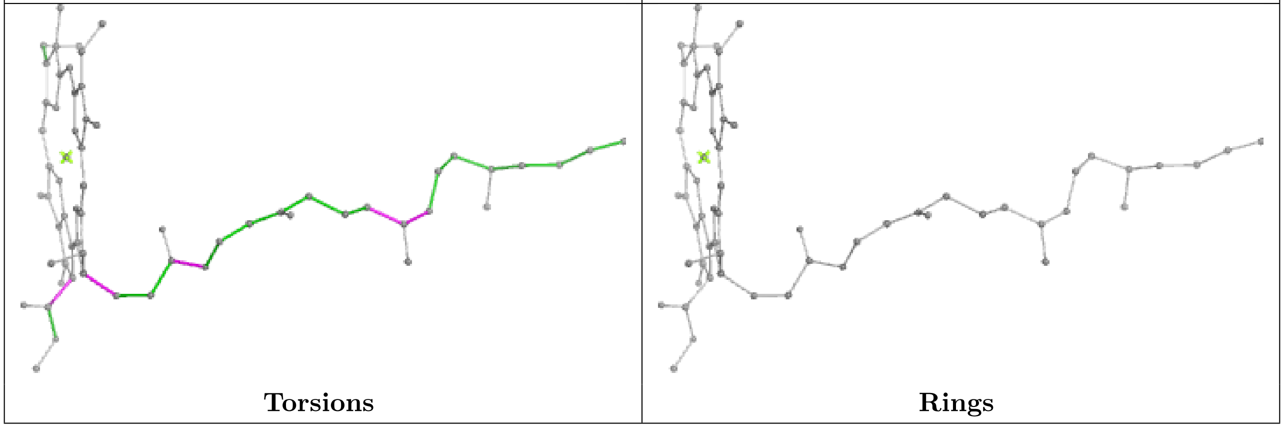


Torsions Rings

Ligand CLA B 607

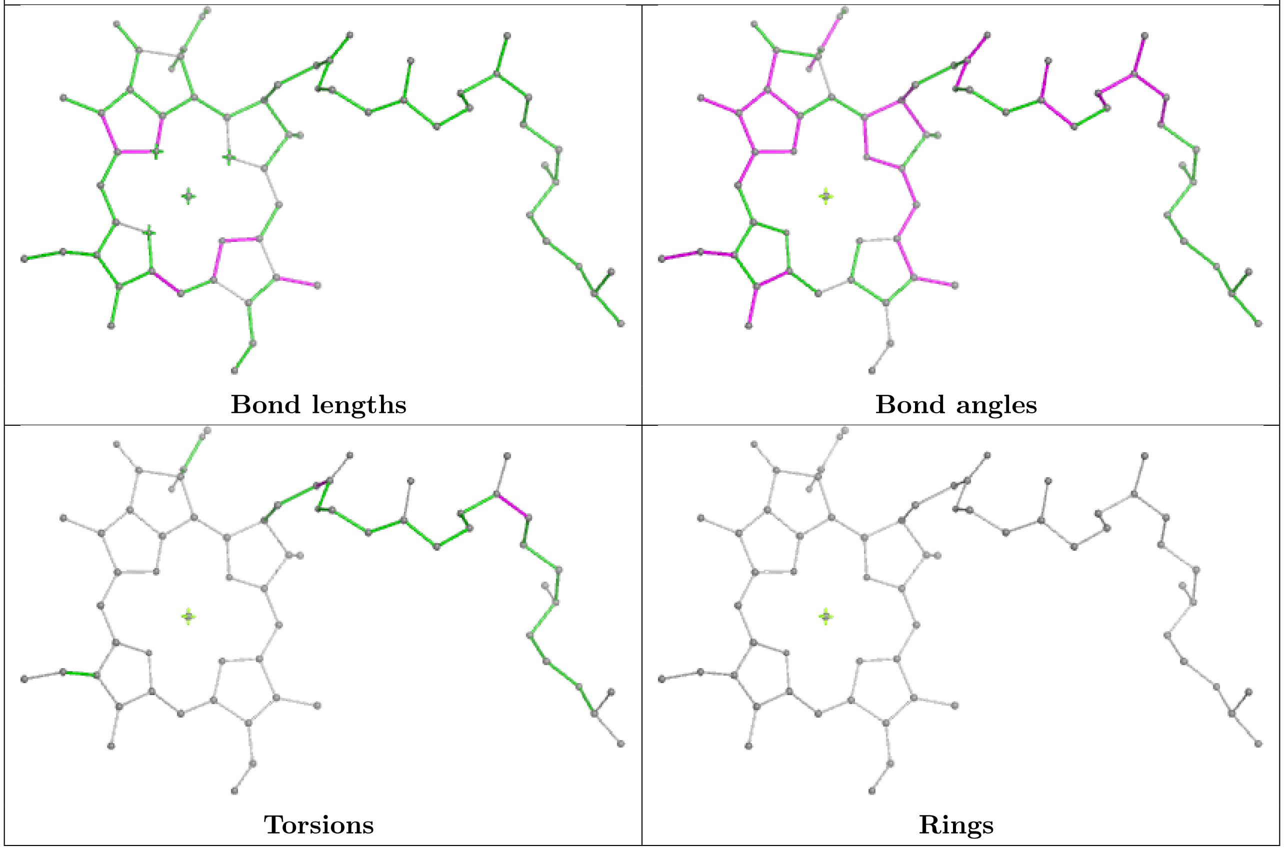


Bond lengths Bond angles



Torsions Rings

Ligand CLA A 407



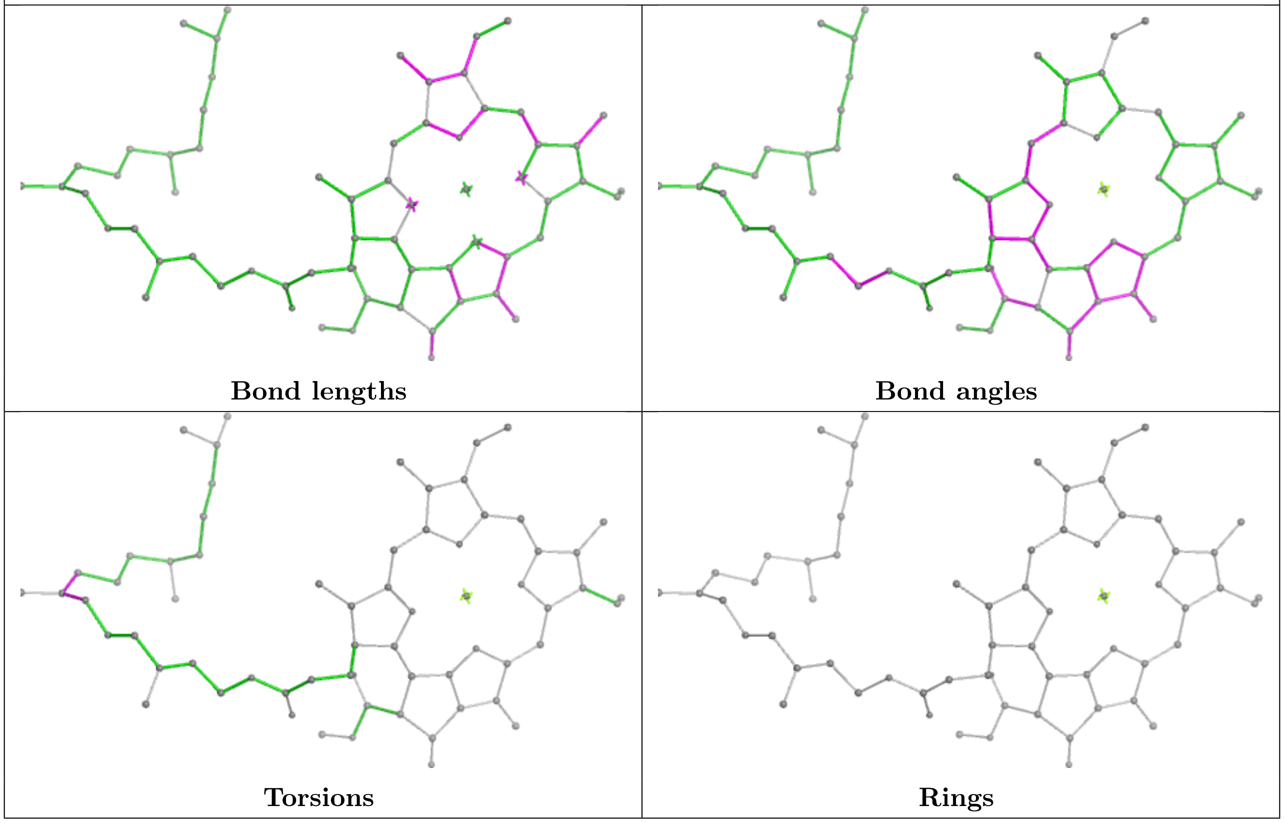
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 617



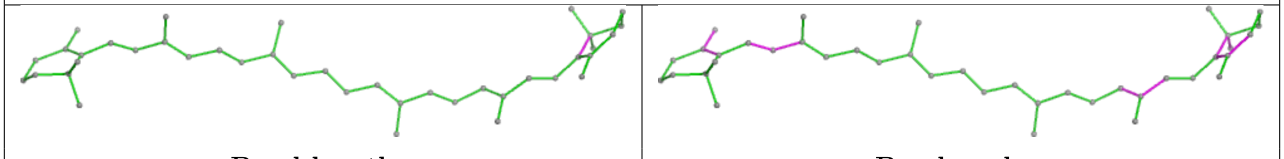
Bond lengths

Bond angles

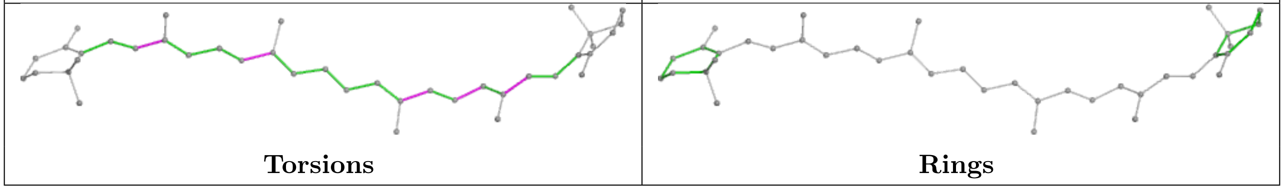
Torsions

Rings

Ligand BCR H 101

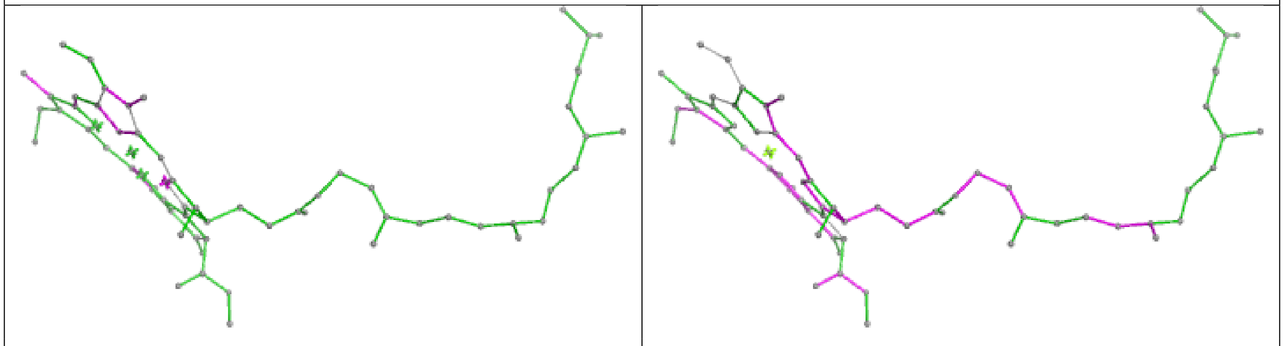


Bond lengths Bond angles

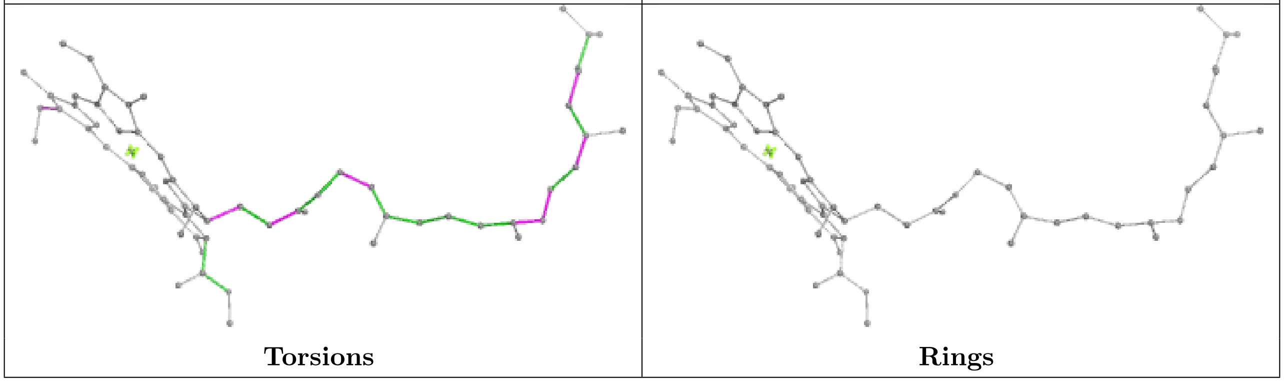


Torsions Rings

Ligand CLA D 406

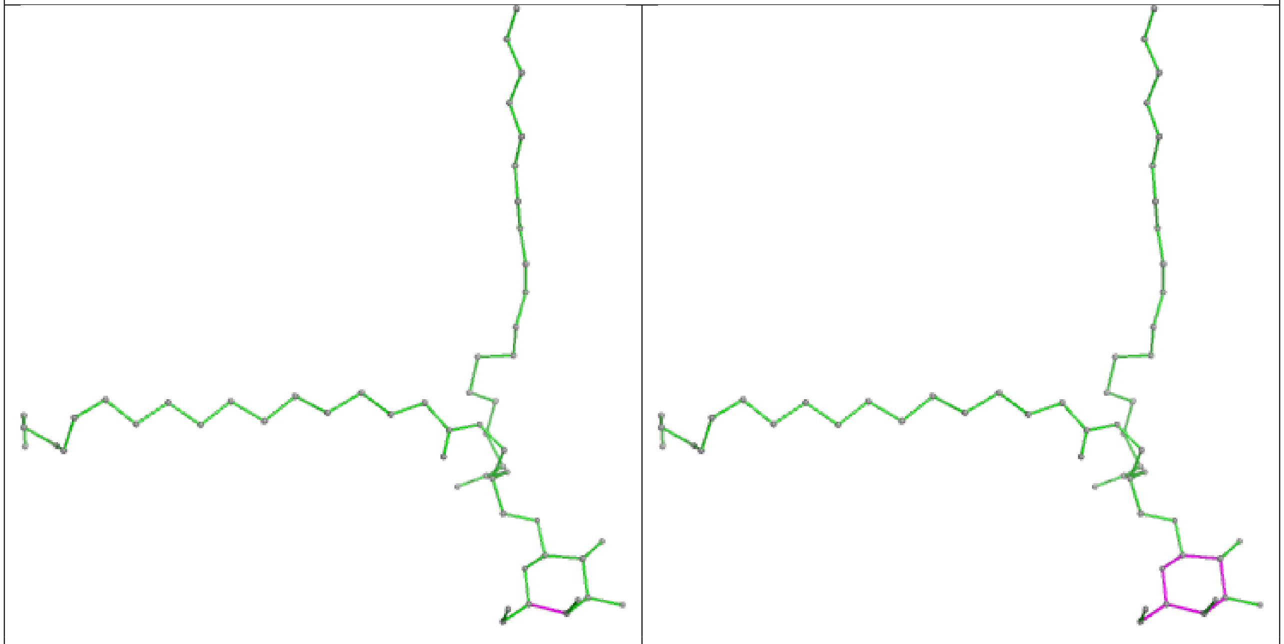


Bond lengths Bond angles

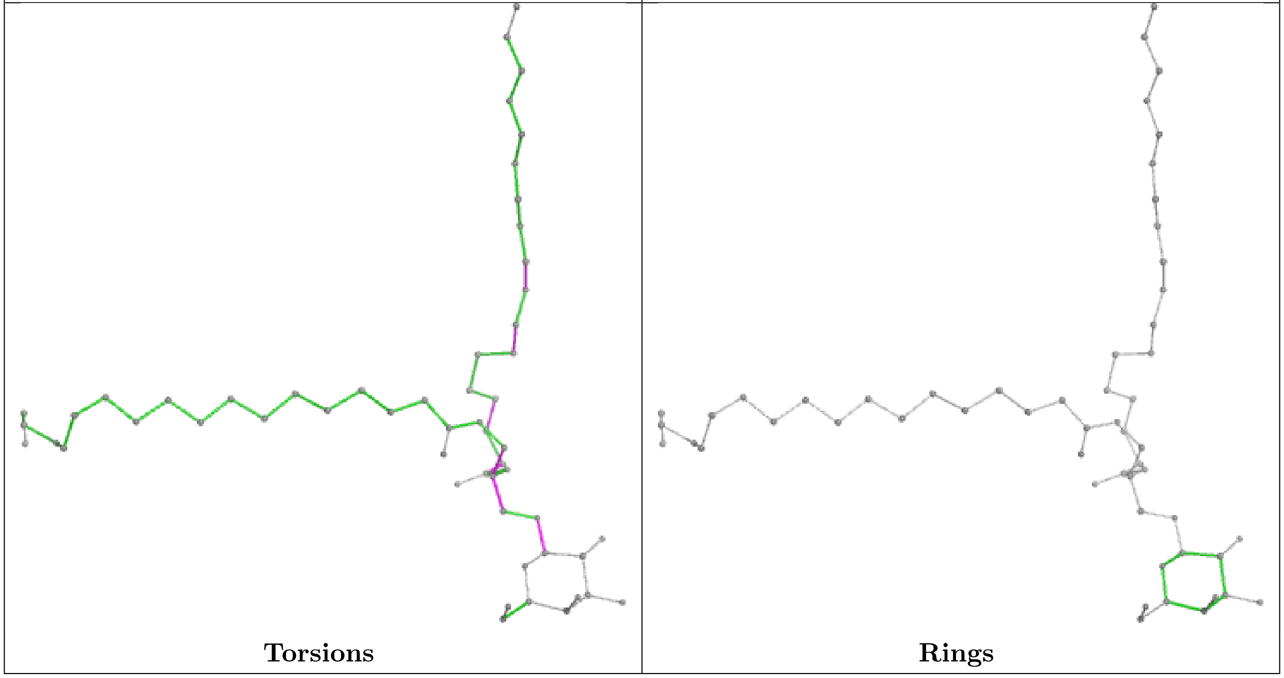


Torsions Rings

Ligand LMG B 601

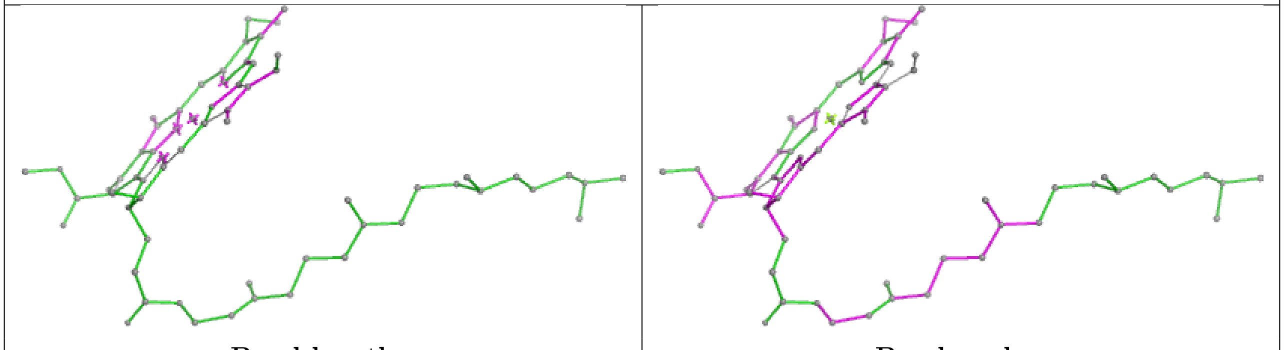


Bond lengths **Bond angles**



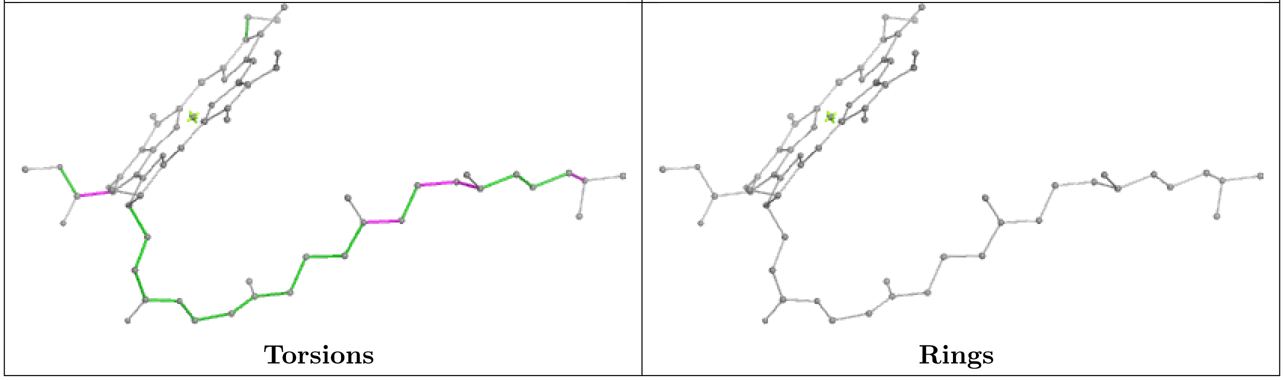
Torsions **Rings**

Ligand CLA C 505



Bond lengths

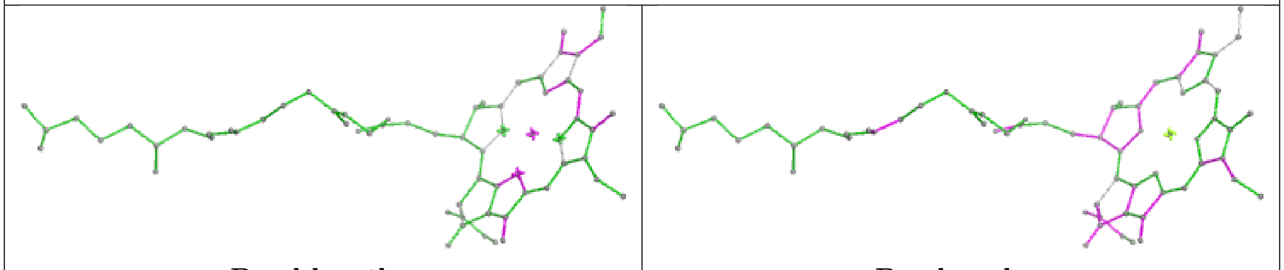
Bond angles



Torsions

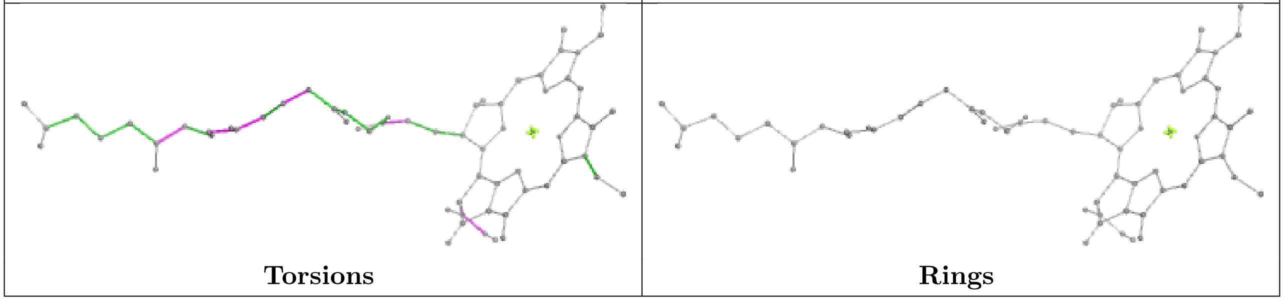
Rings

Ligand CLA C 503



Bond lengths

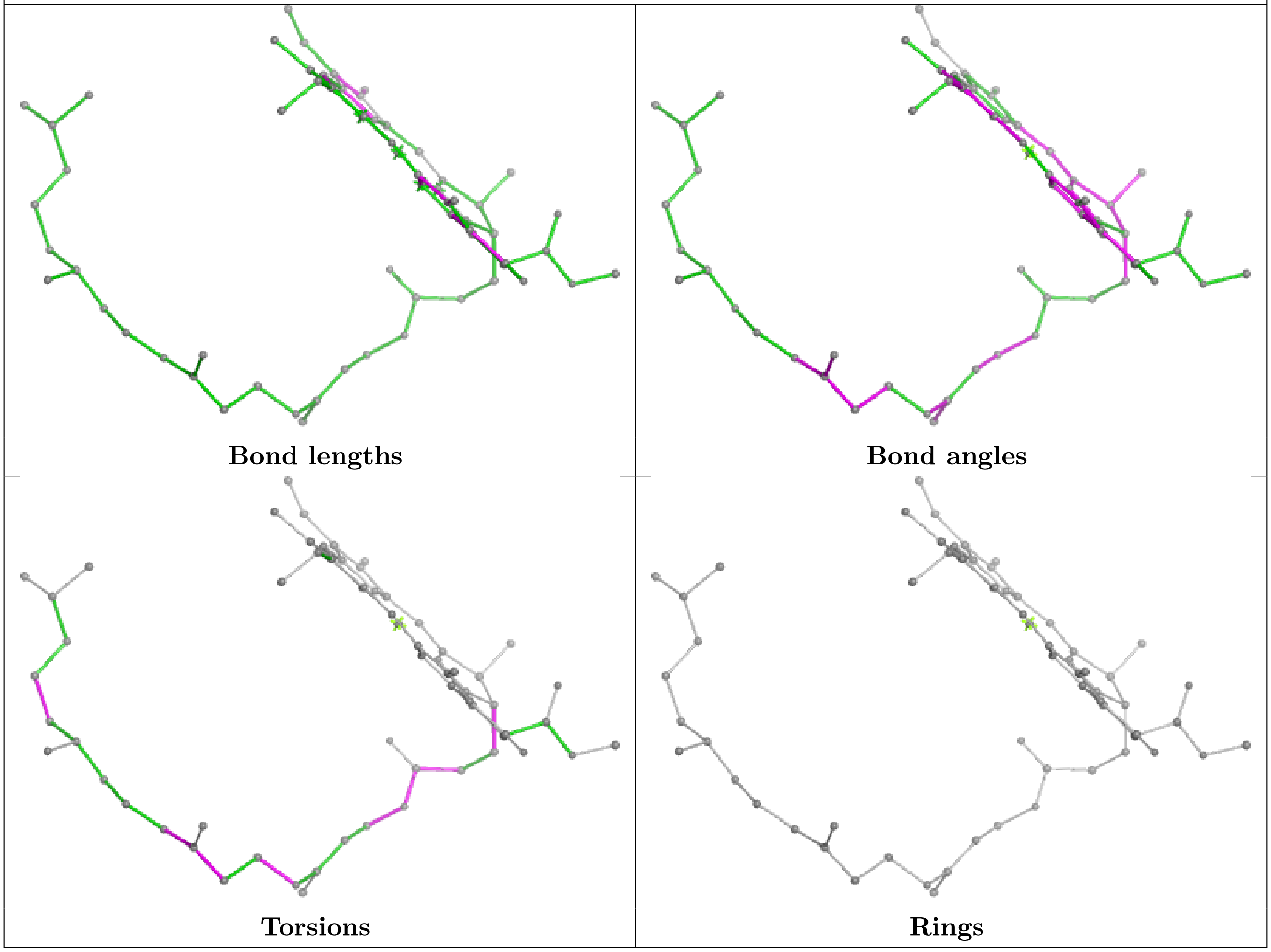
Bond angles



Torsions

Rings

Ligand CLA B 612



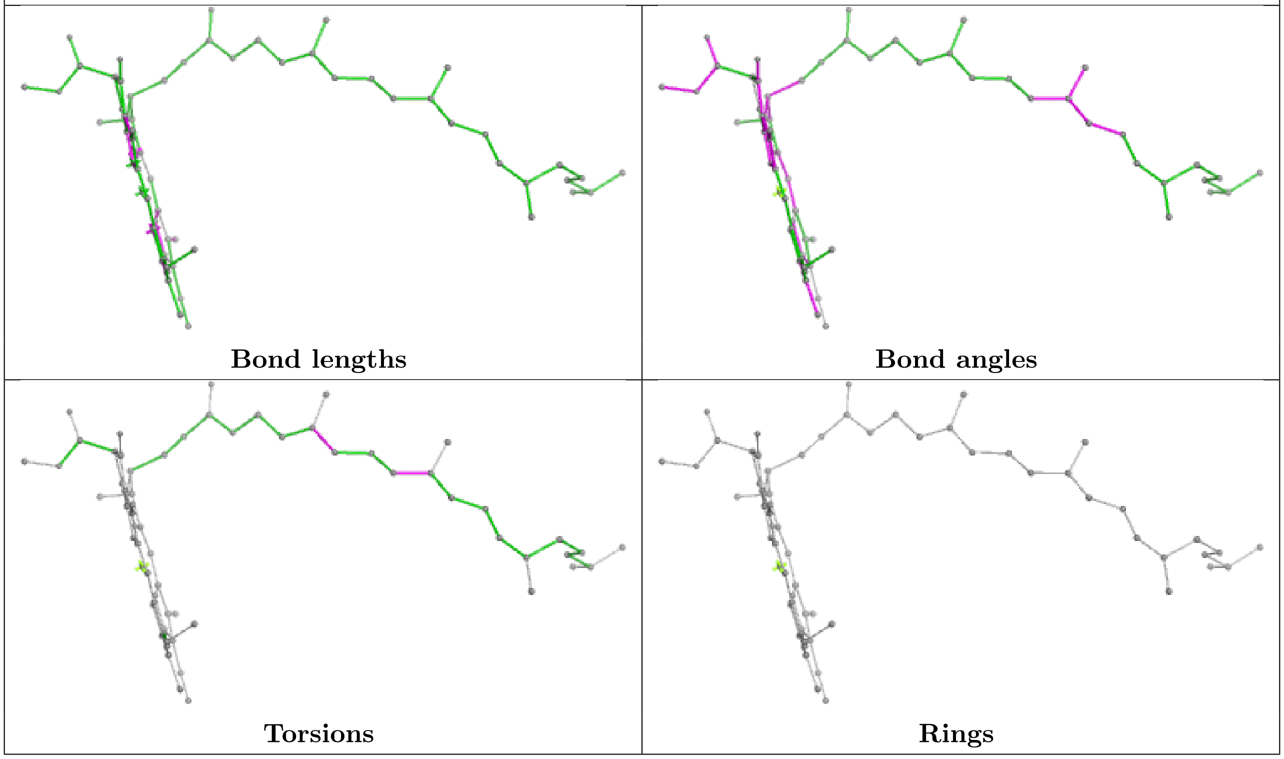
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 606



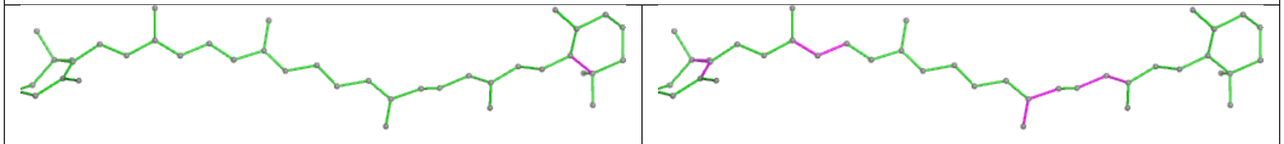
Bond lengths

Bond angles

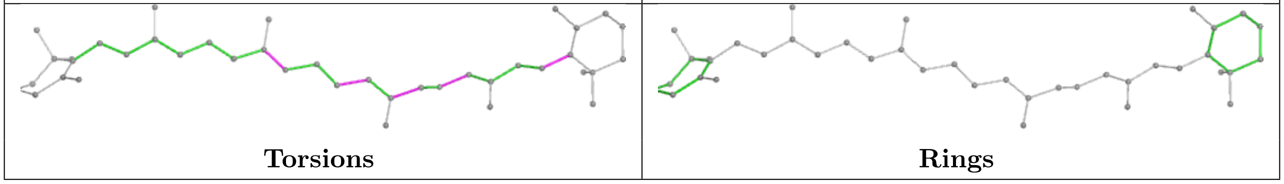
Torsions

Rings

Ligand BCR B 619

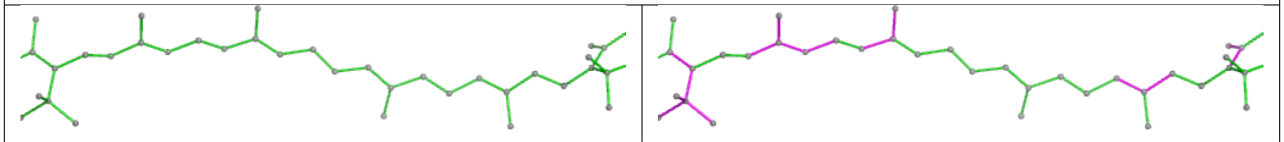


Bond lengths **Bond angles**

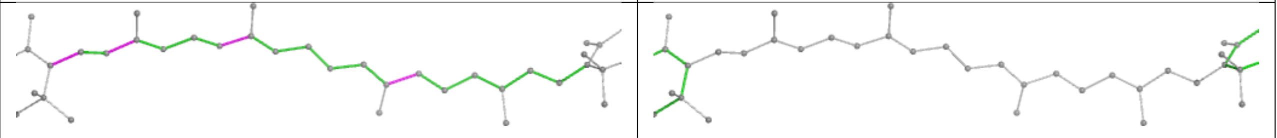


Torsions **Rings**

Ligand BCR B 620

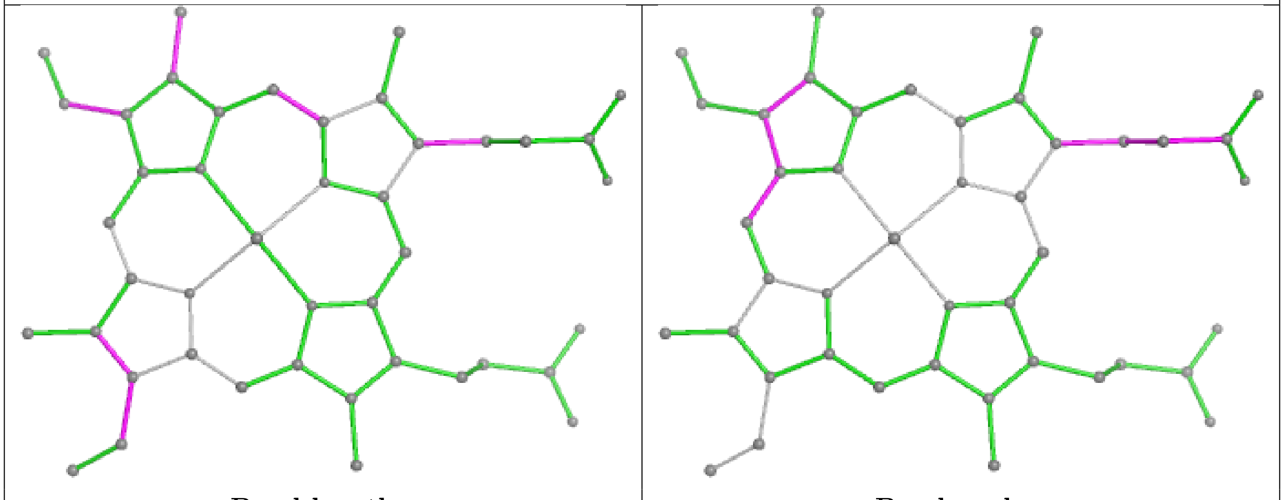


Bond lengths **Bond angles**



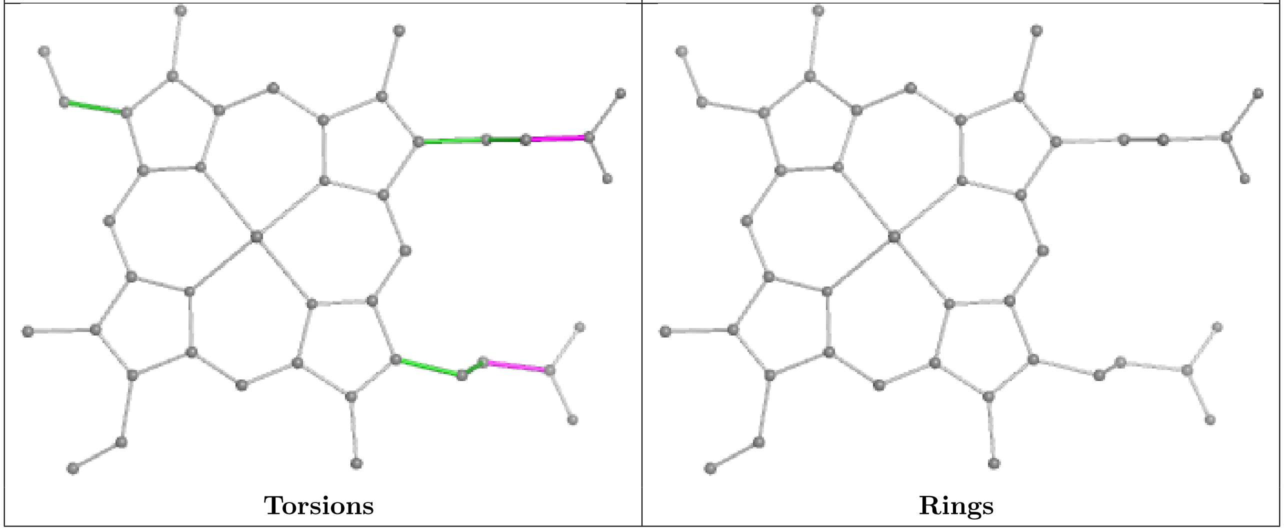
Torsions **Rings**

Ligand HEM E 101



Bond lengths

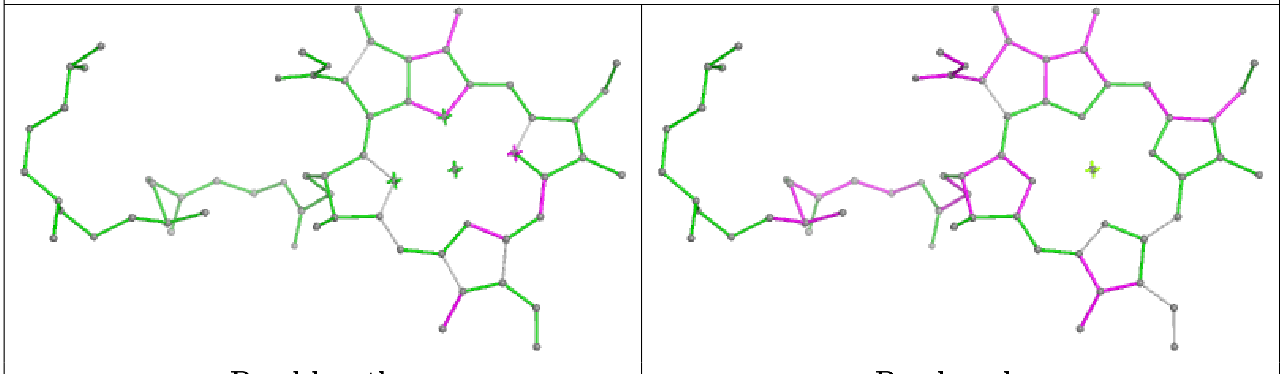
Bond angles



Torsions

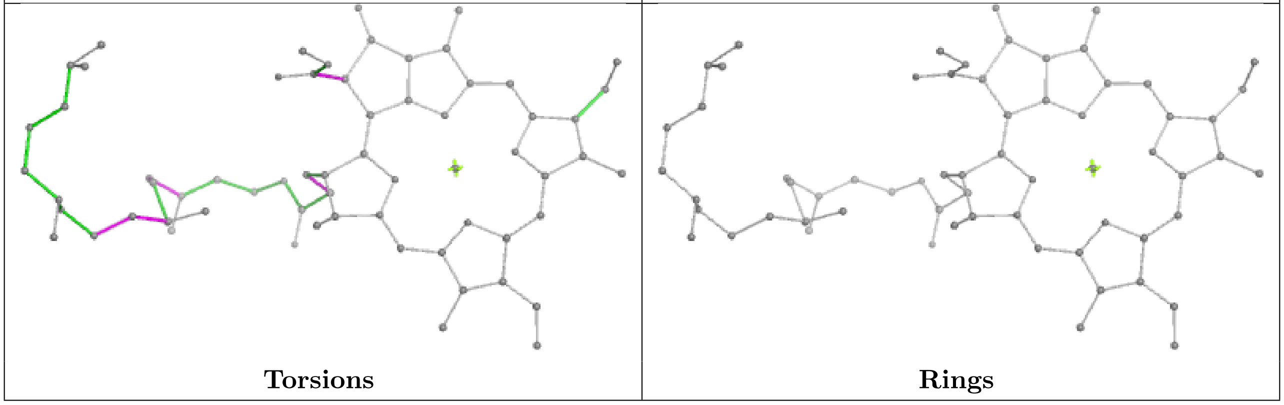
Rings

Ligand CLA B 613



Bond lengths

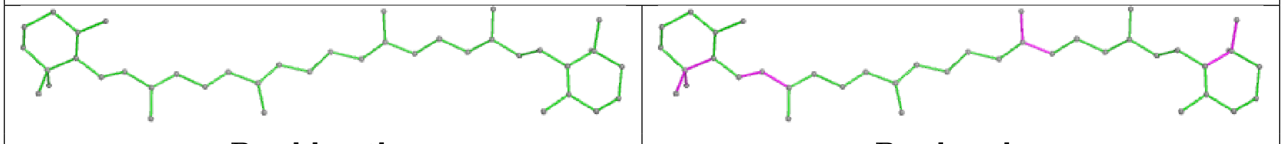
Bond angles



Torsions

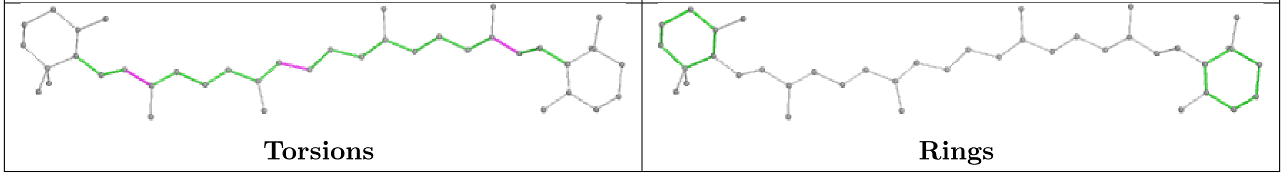
Rings

Ligand BCR F 101



Bond lengths

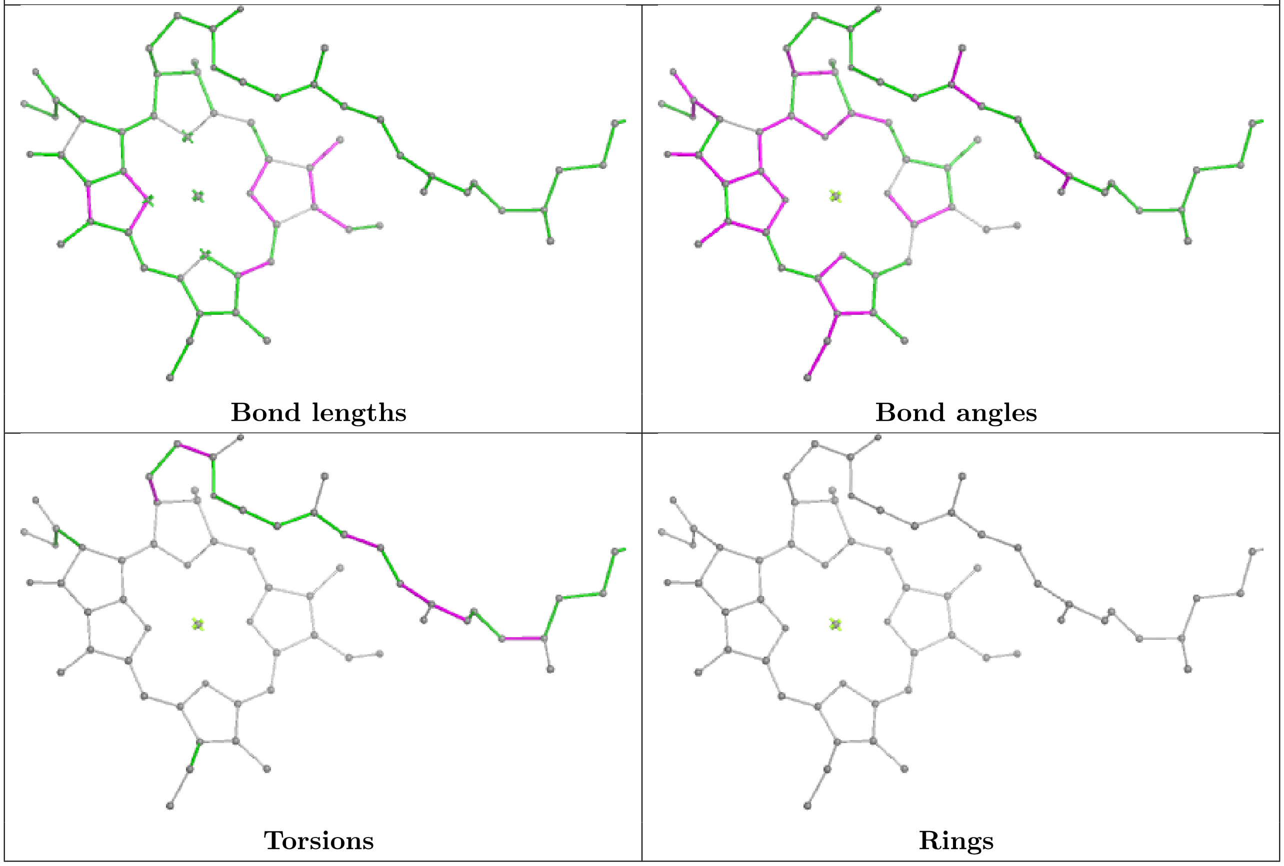
Bond angles



Torsions

Rings

Ligand CLA B 604



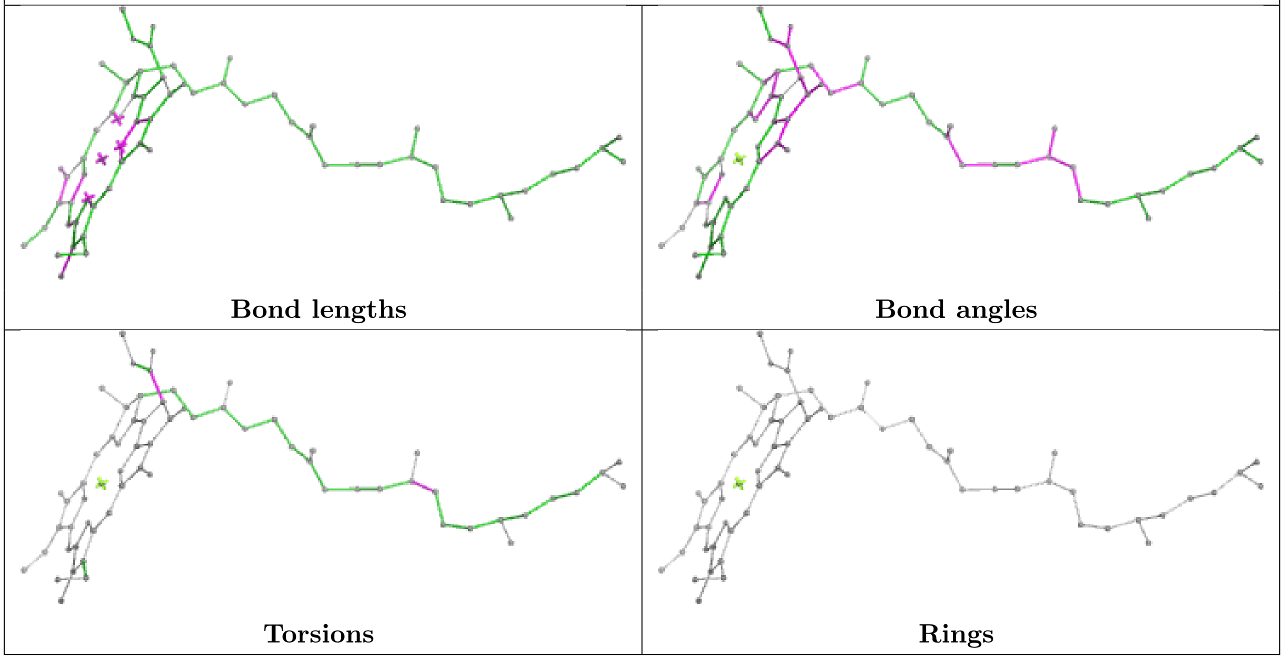
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA B 605



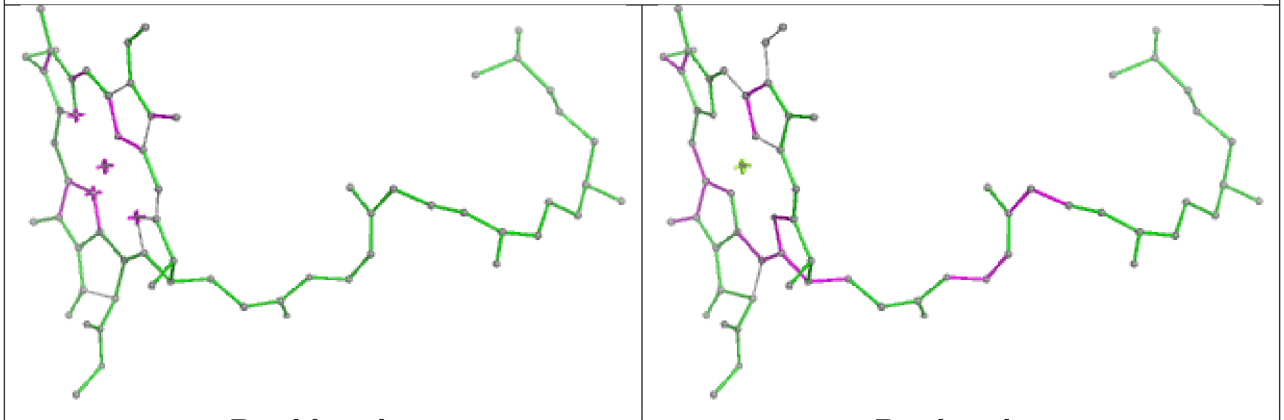
Bond lengths

Bond angles

Torsions

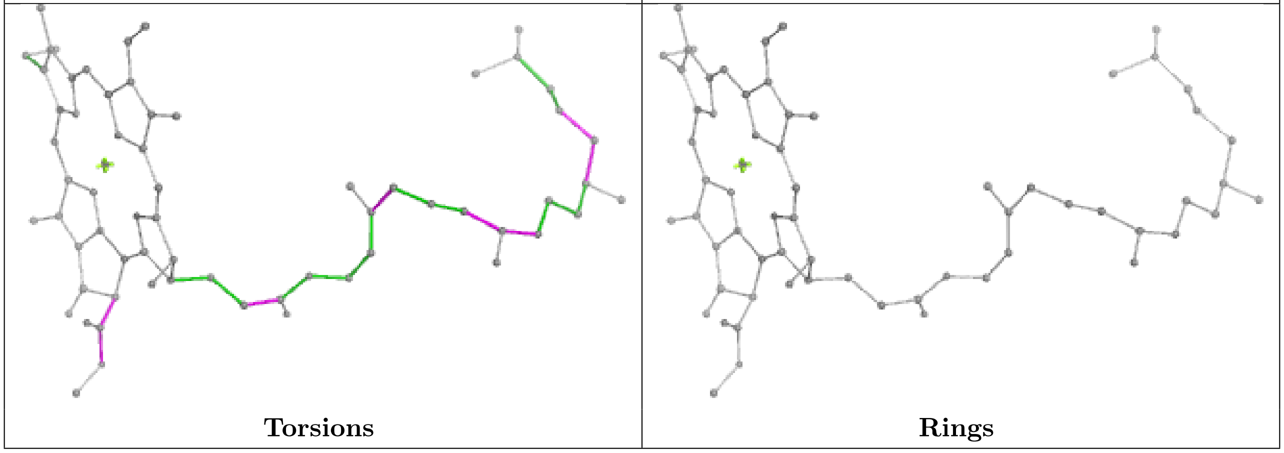
Rings

Ligand CLA A 408



Bond lengths

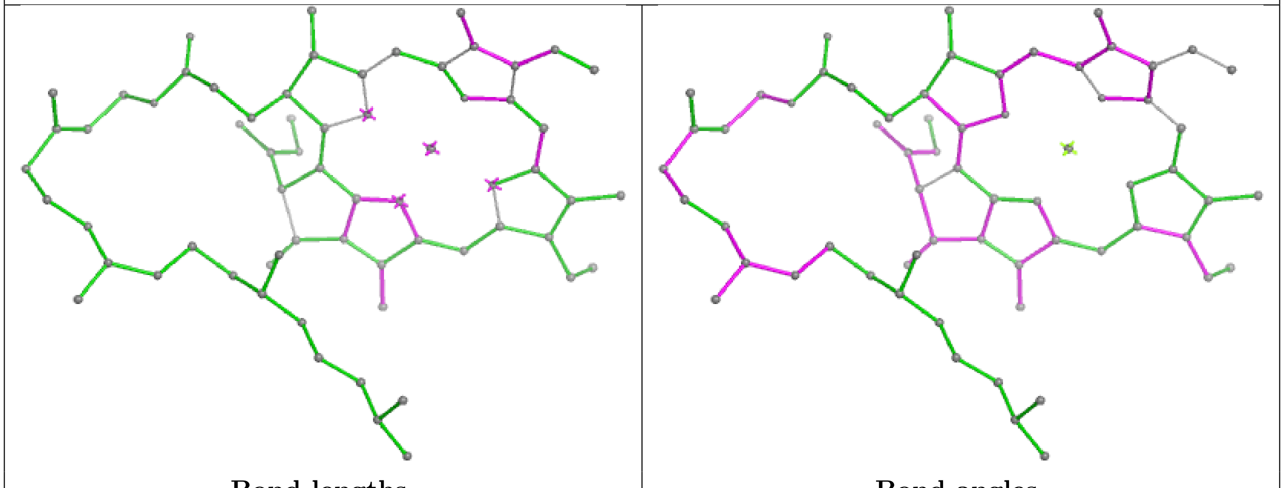
Bond angles



Torsions

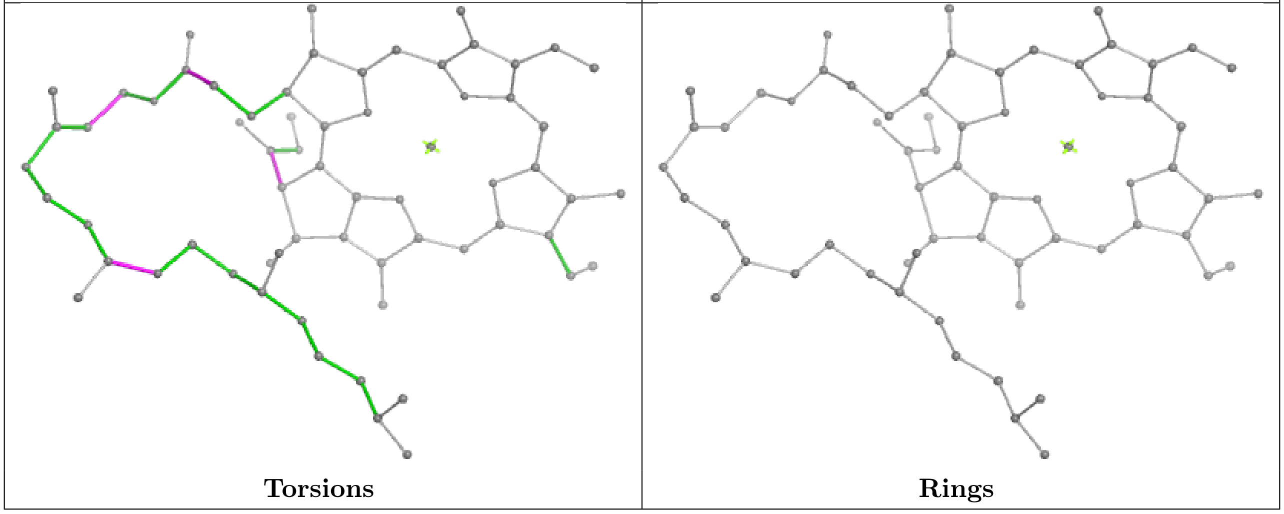
Rings

Ligand CLA C 510



Bond lengths

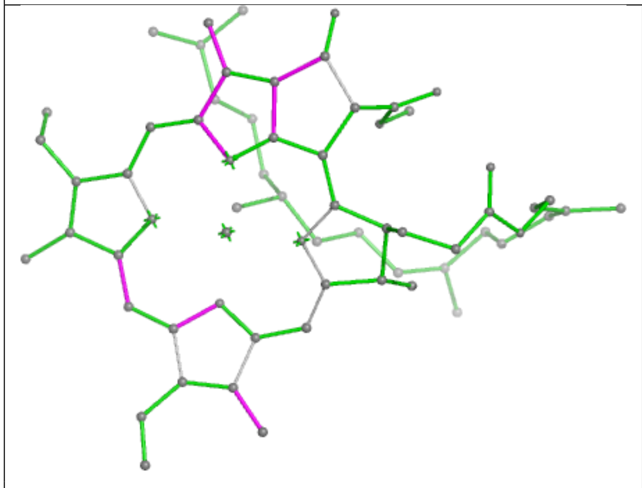
Bond angles



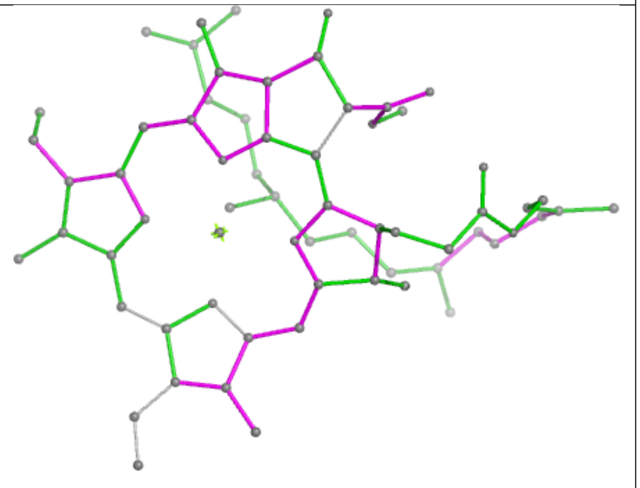
Torsions

Rings

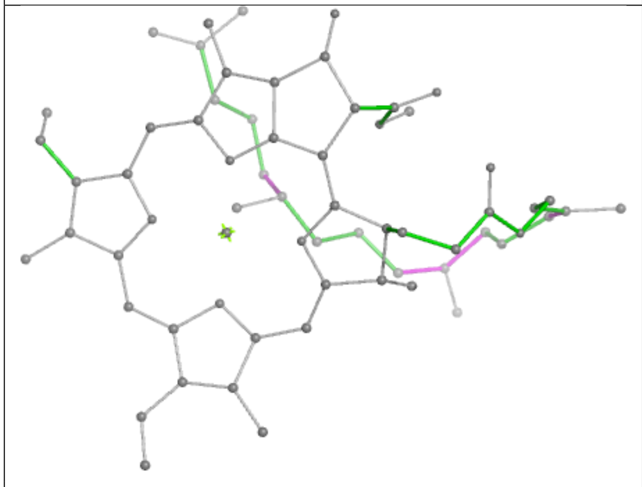
Ligand CLA C 515



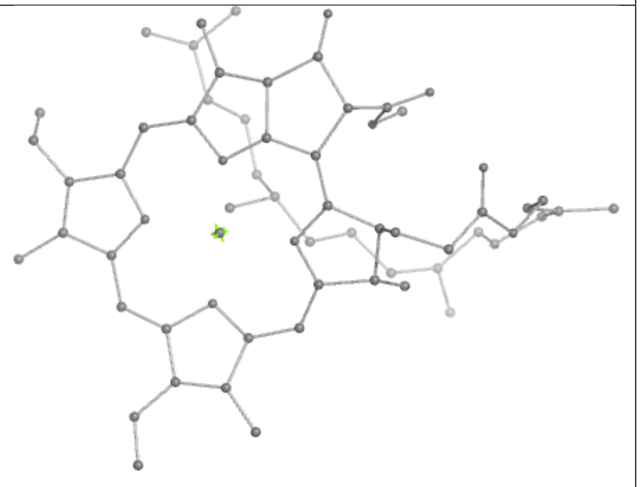
Bond lengths



Bond angles

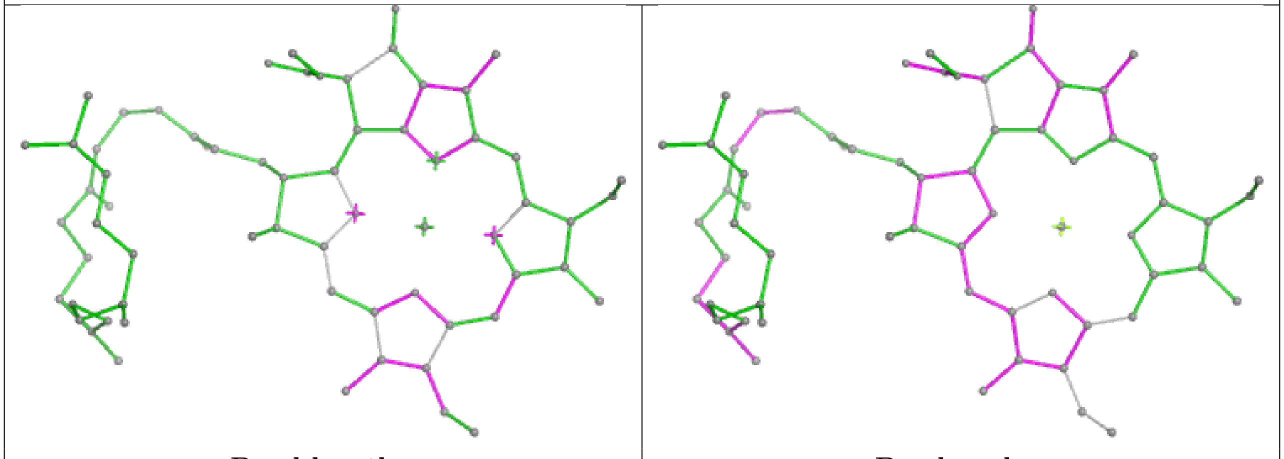


Torsions



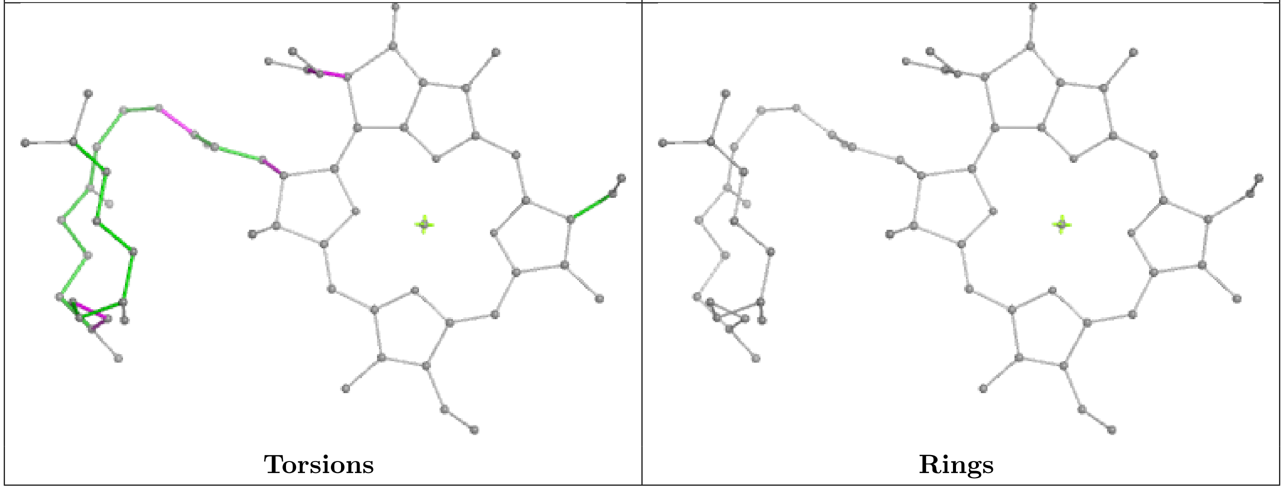
Rings

Ligand CLA C 512



Bond lengths

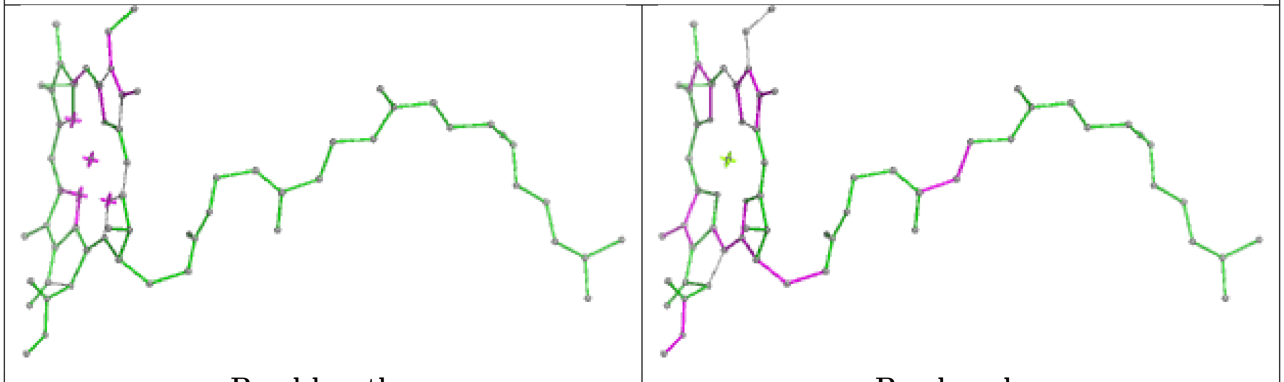
Bond angles



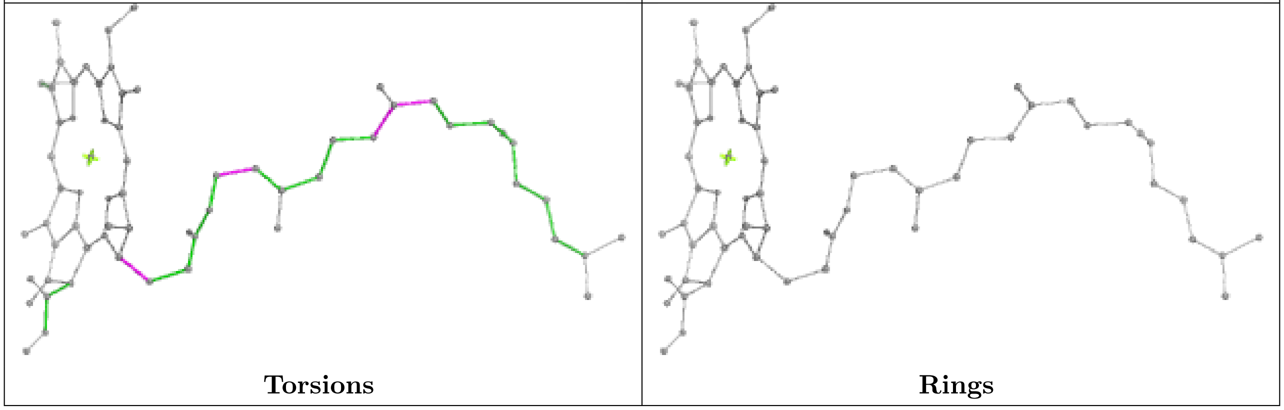
Torsions

Rings

Ligand CLA D 407

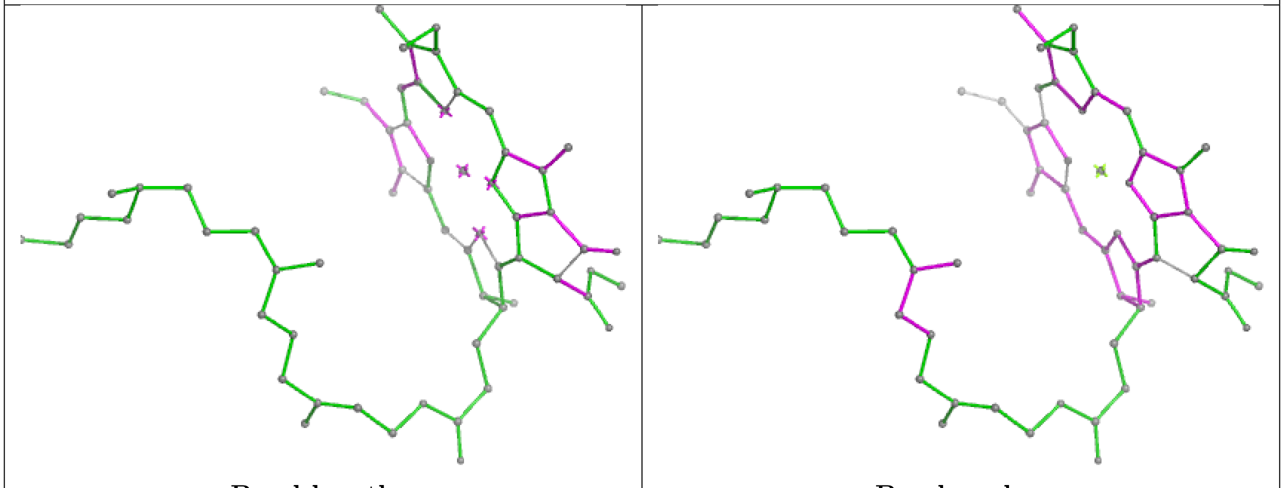


Bond lengths **Bond angles**



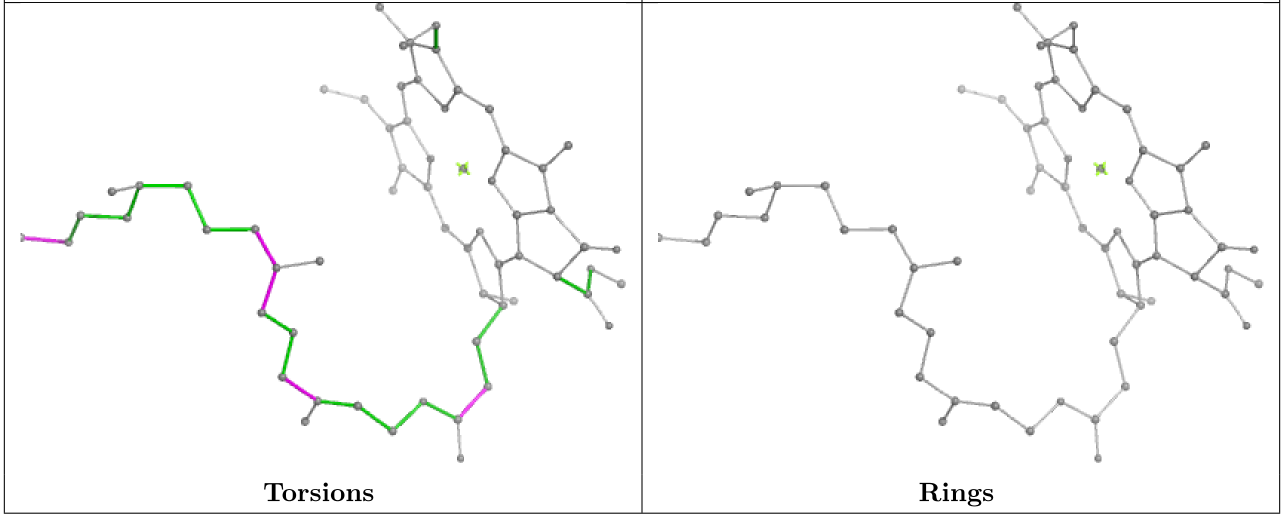
Torsions **Rings**

Ligand CLA C 513



Bond lengths

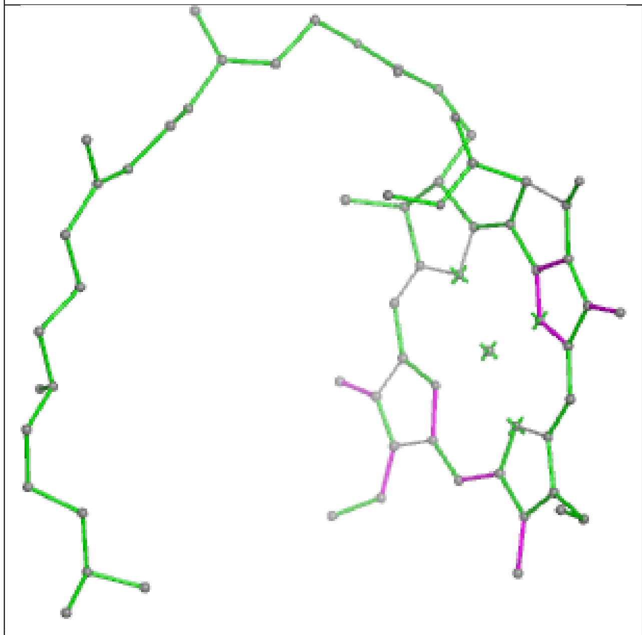
Bond angles



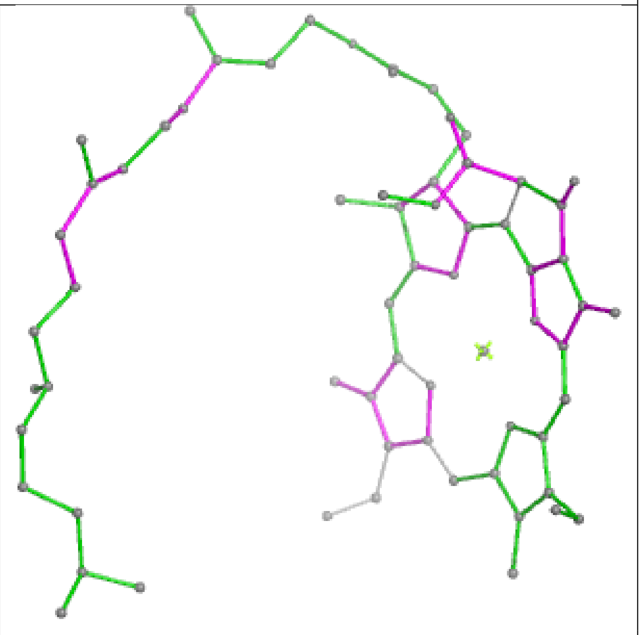
Torsions

Rings

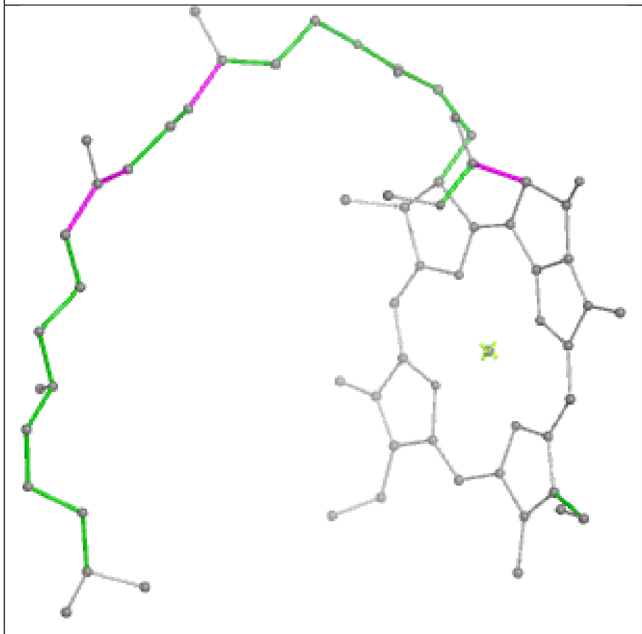
Ligand CLA C 508



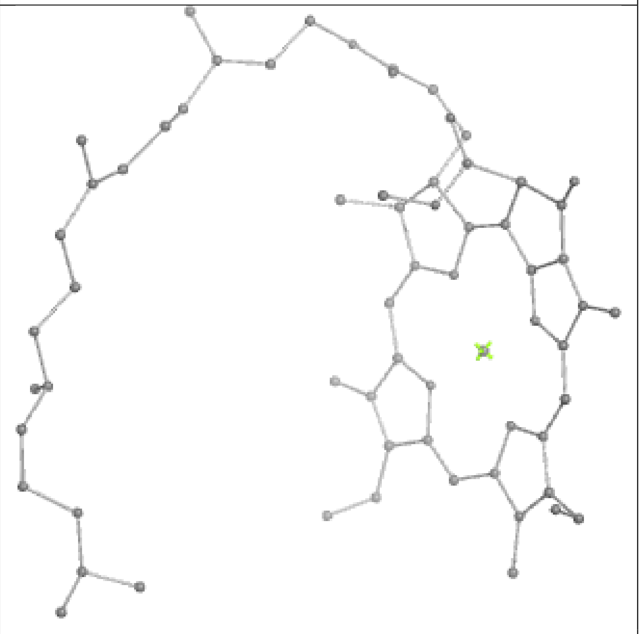
Bond lengths



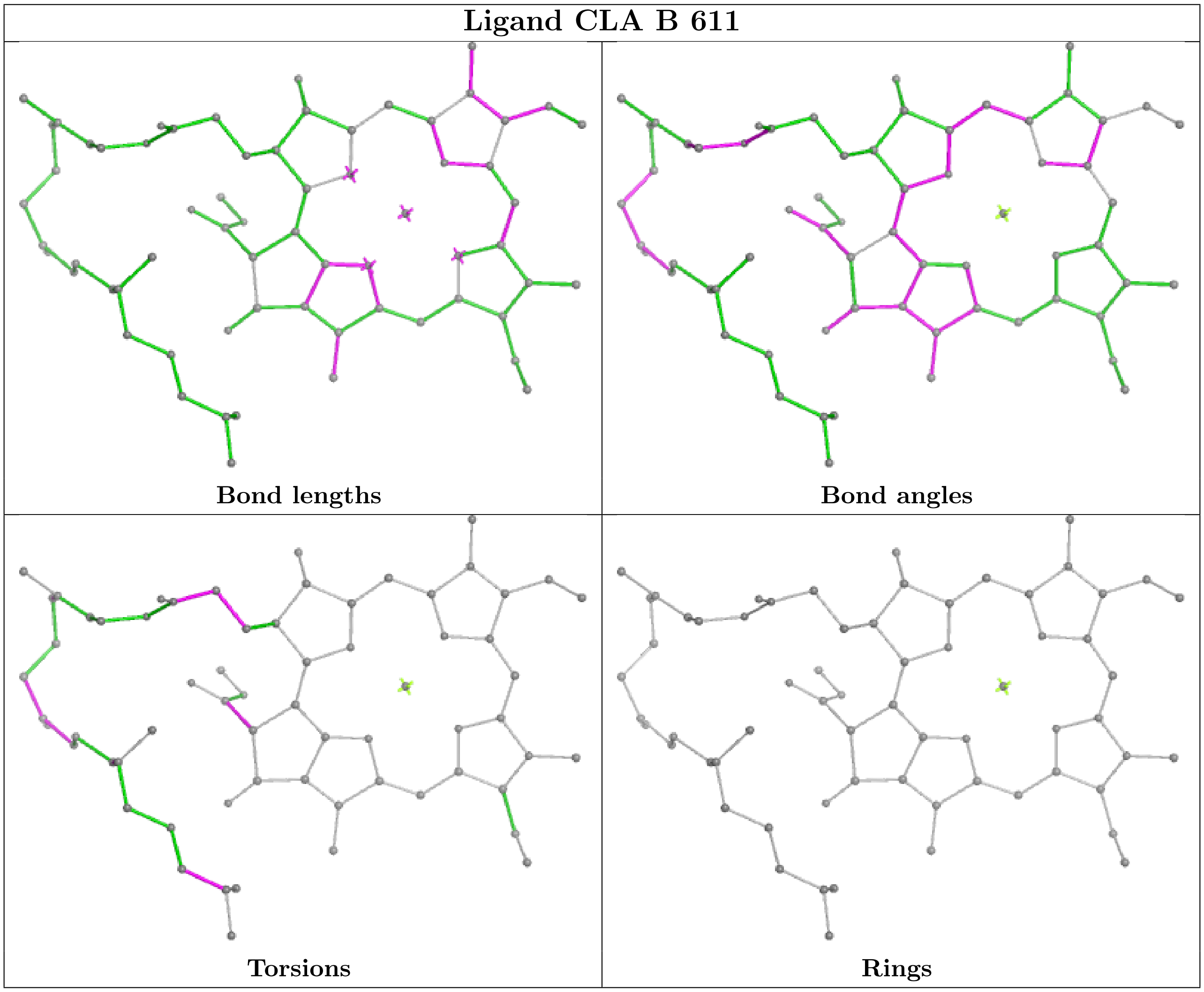
Bond angles



Torsions



Rings


Ligand CLA B 611

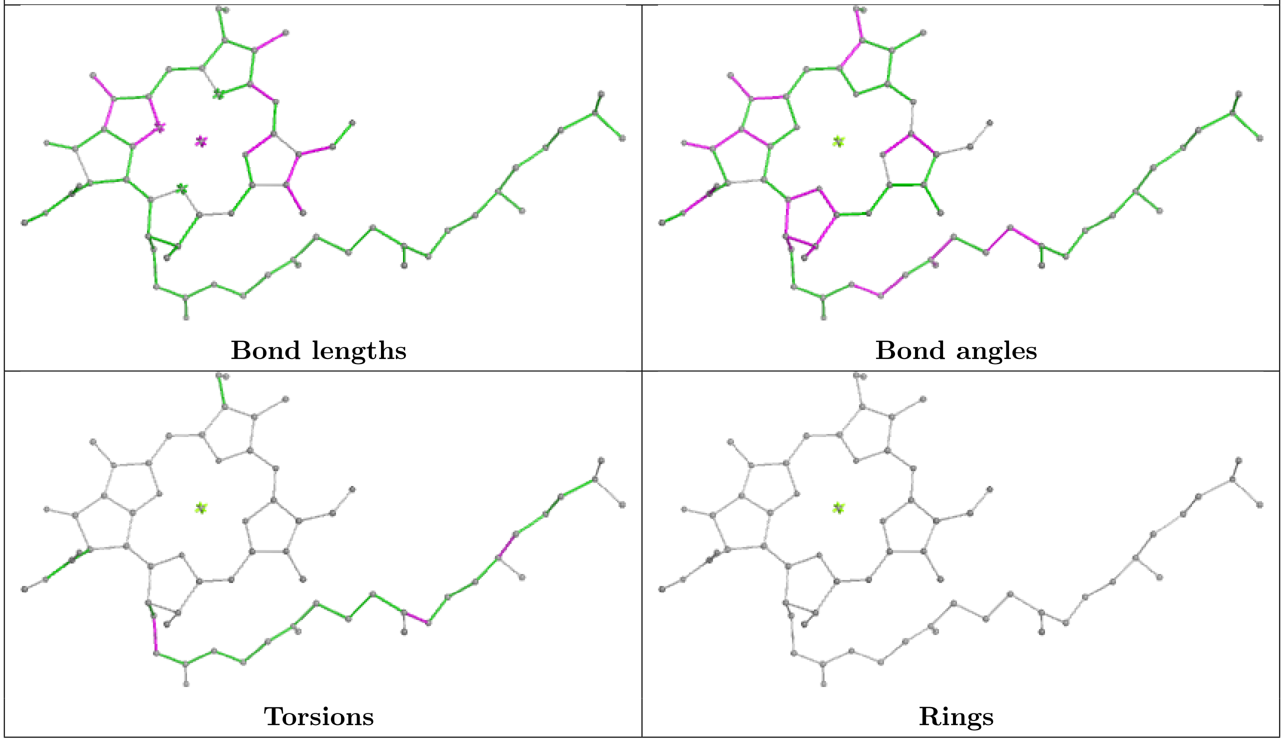
Bond lengths

Bond angles

Torsions

Rings

Ligand CLA C 502



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

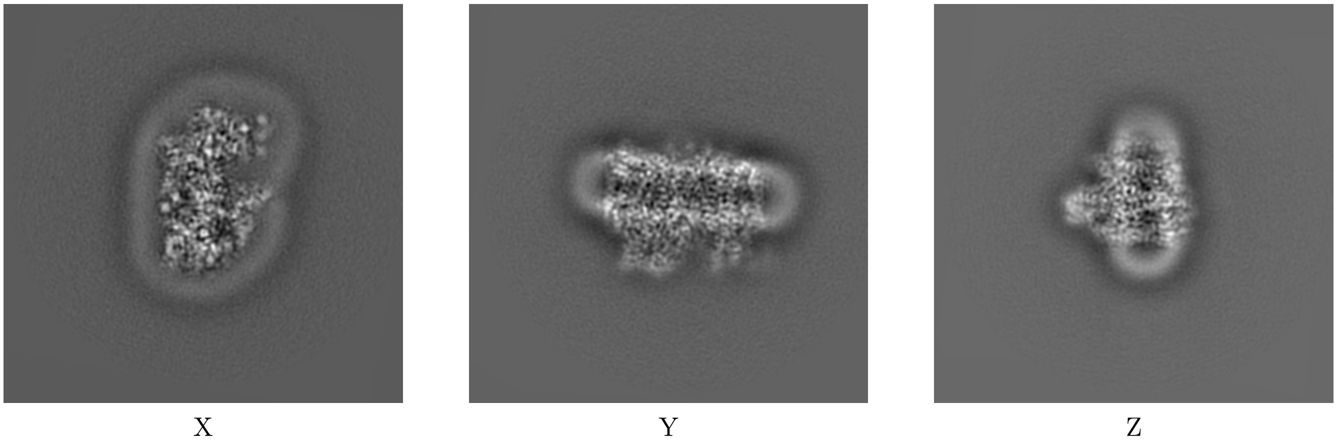
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-12335. 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 ⓘ

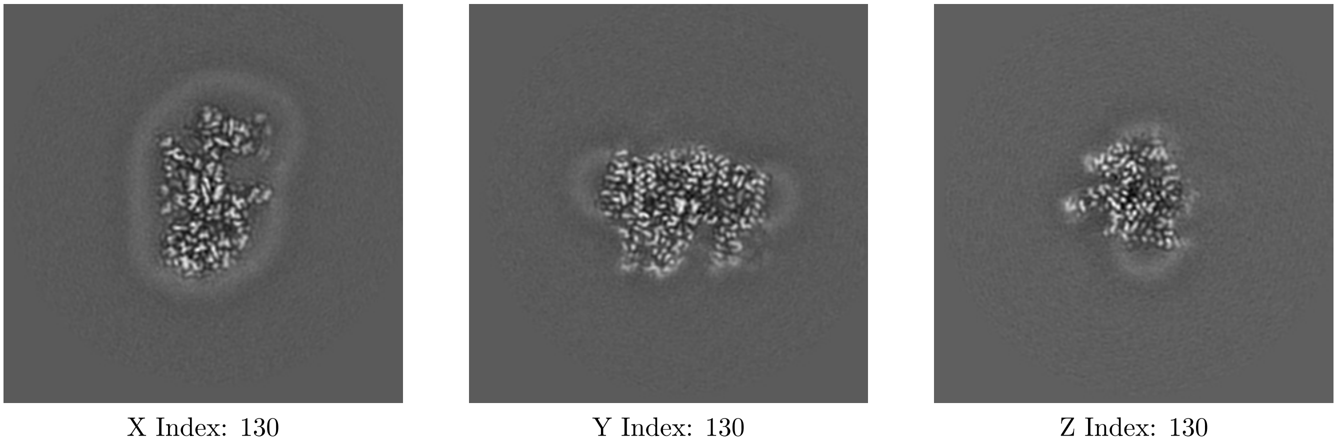
6.1.1 Primary map


X Y Z

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

6.2 Central slices ⓘ

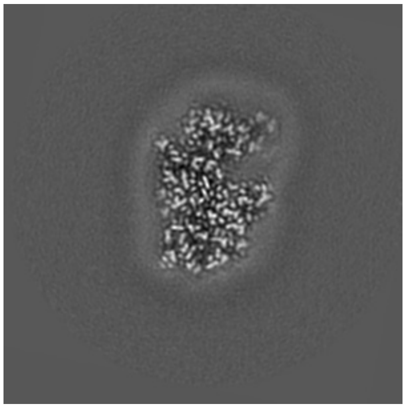
6.2.1 Primary map


X Index: 130 Y Index: 130 Z Index: 130

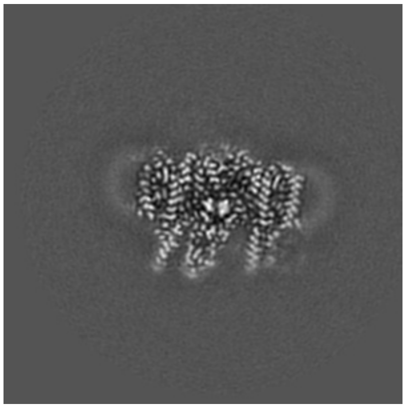
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

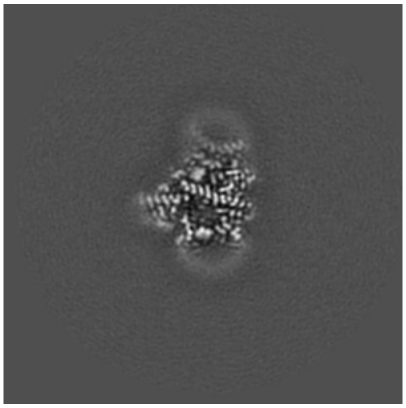
6.3.1 Primary map



X Index: 125



Y Index: 132

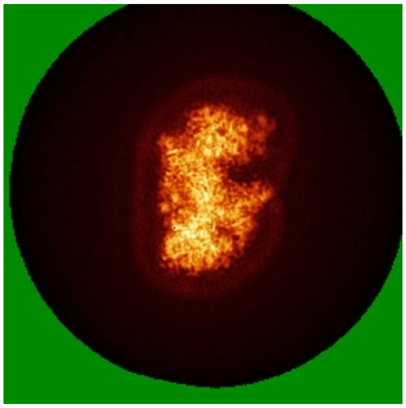


Z Index: 164

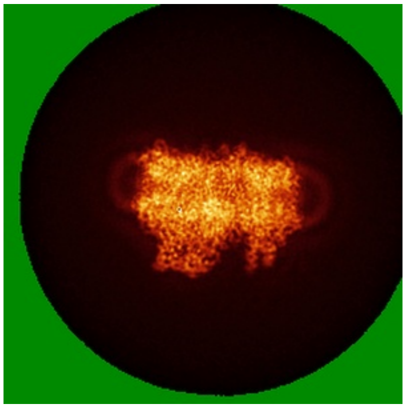
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

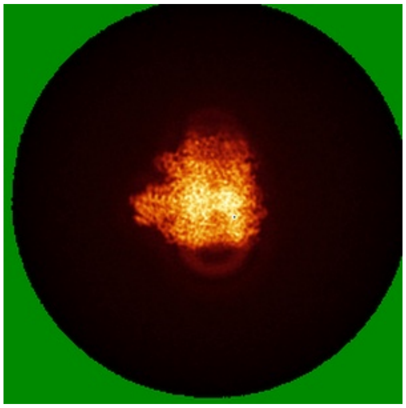
6.4.1 Primary map



X



Y

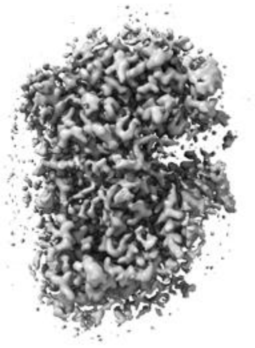


Z

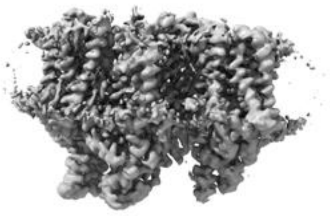
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

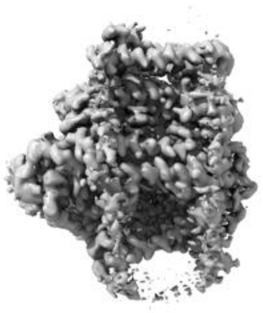
6.5.1 Primary map



X



Y



Z

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

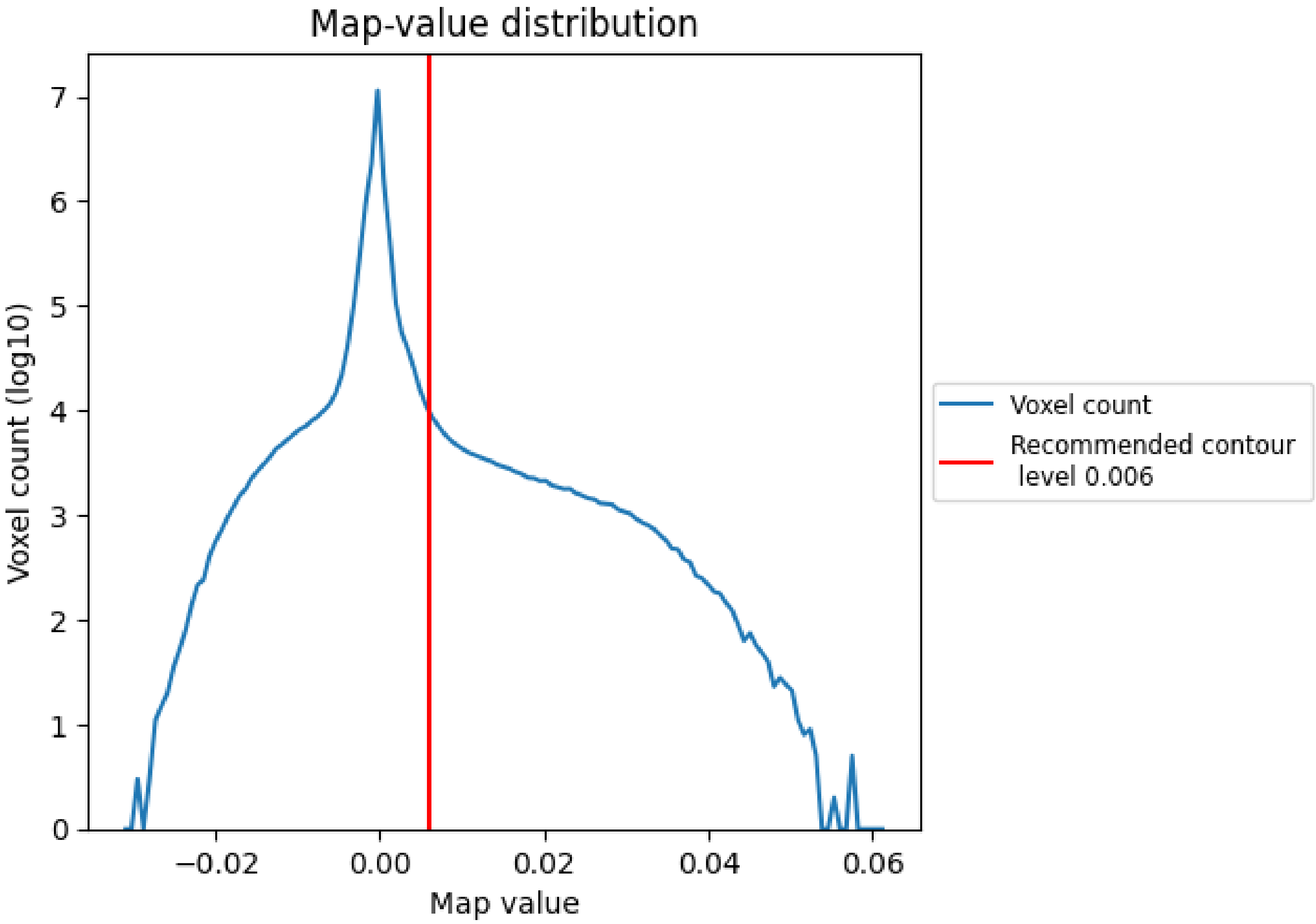
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

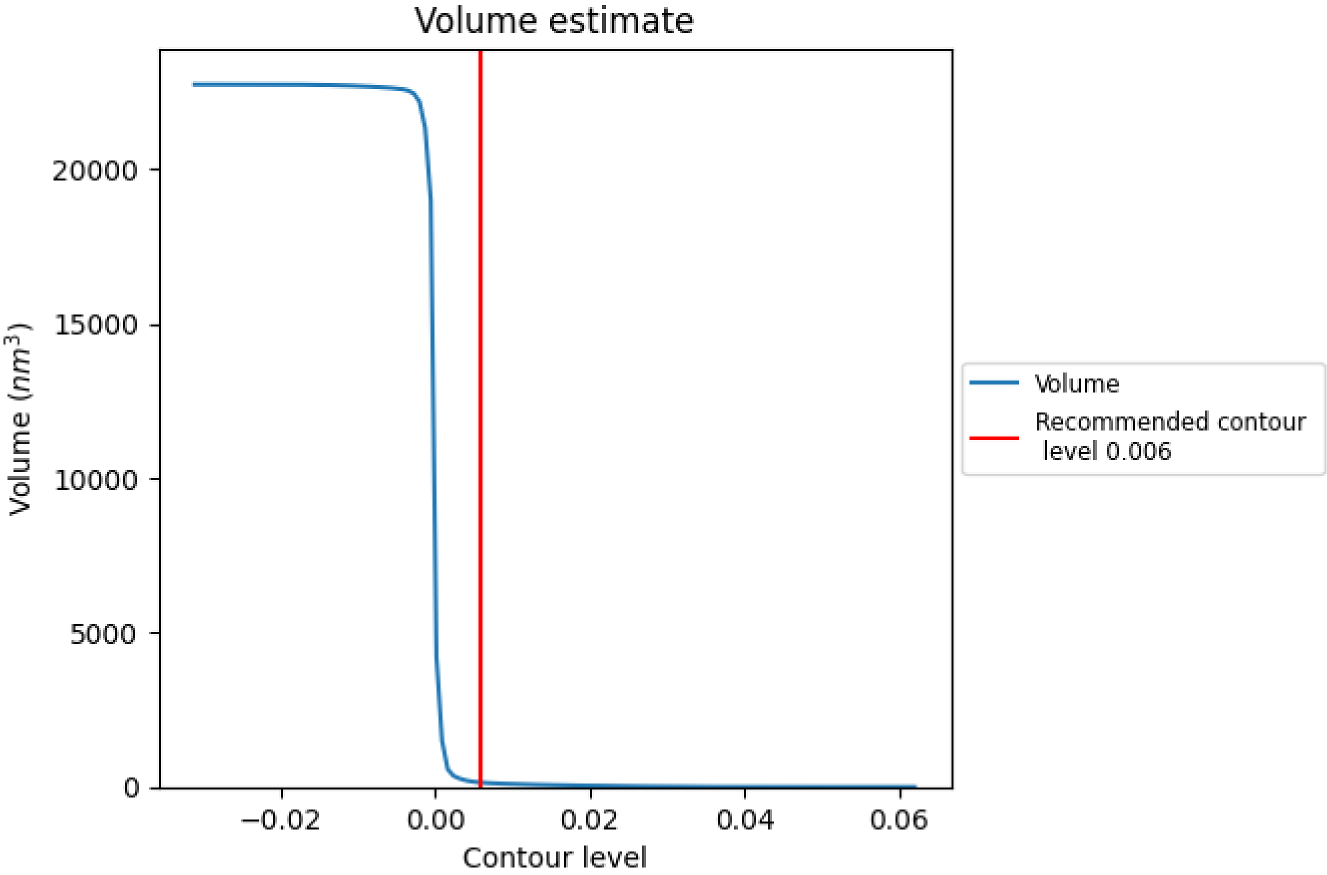
This section contains the results of statistical analysis of the map.

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.

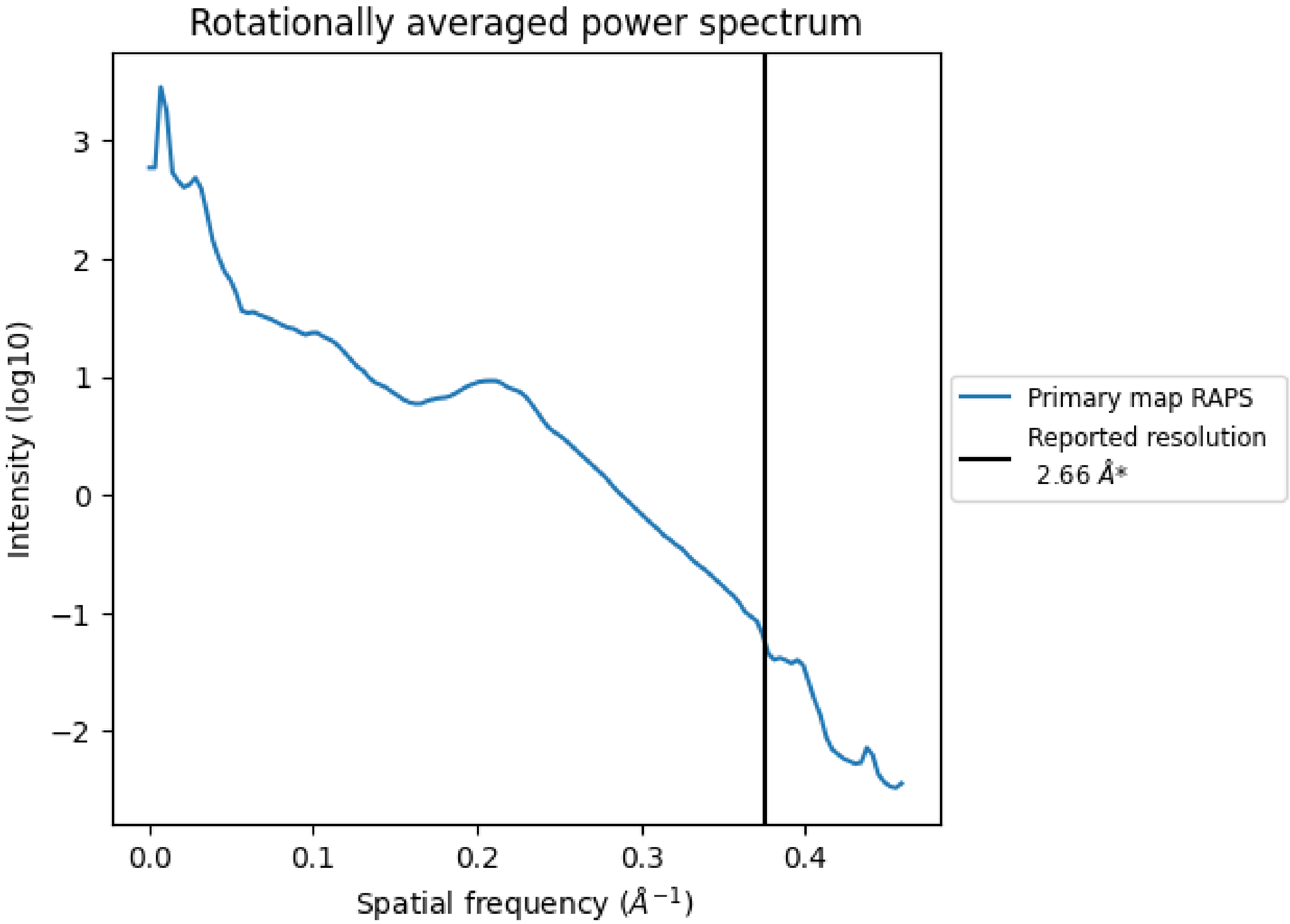
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 142 nm^3; this corresponds to an approximate mass of 129 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.376 Å^{-1}

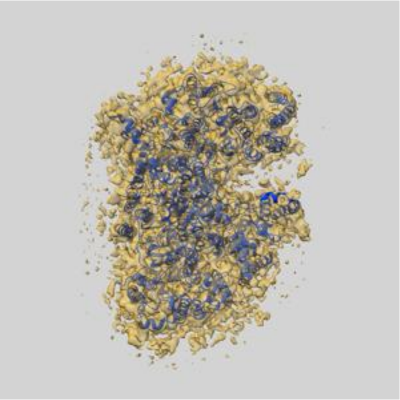
8 Fourier-Shell correlation

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

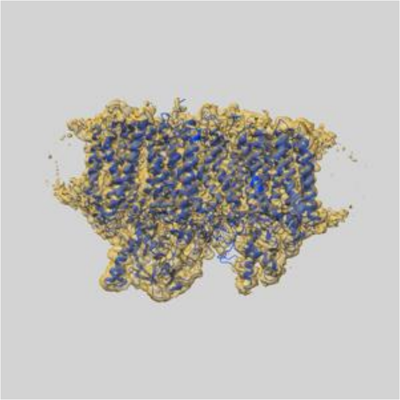
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-12335 and PDB model 7NHO. Per-residue inclusion information can be found in section 3 on page 15.

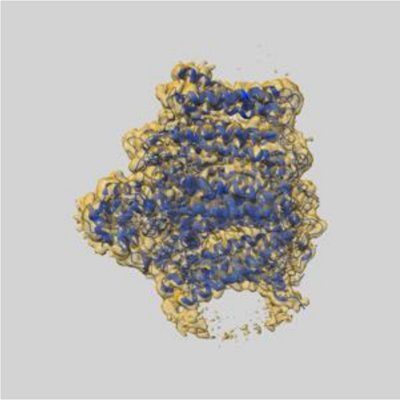
9.1 Map-model overlay



X



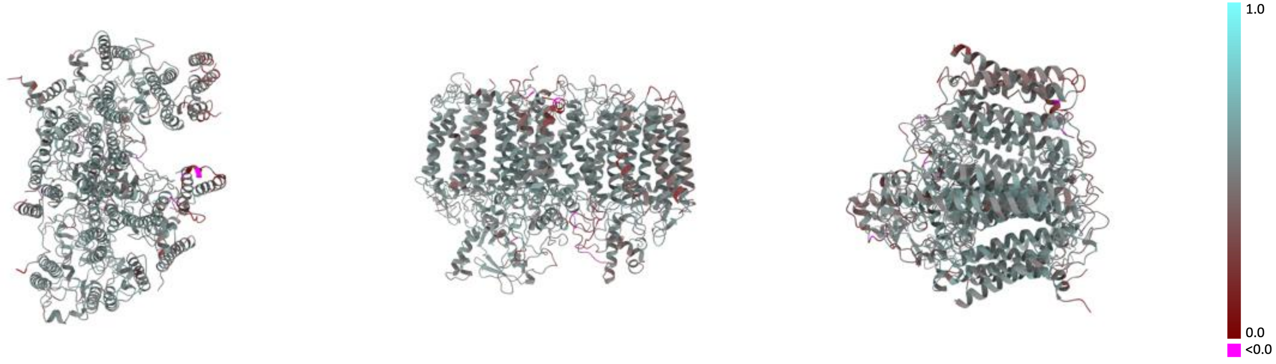
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

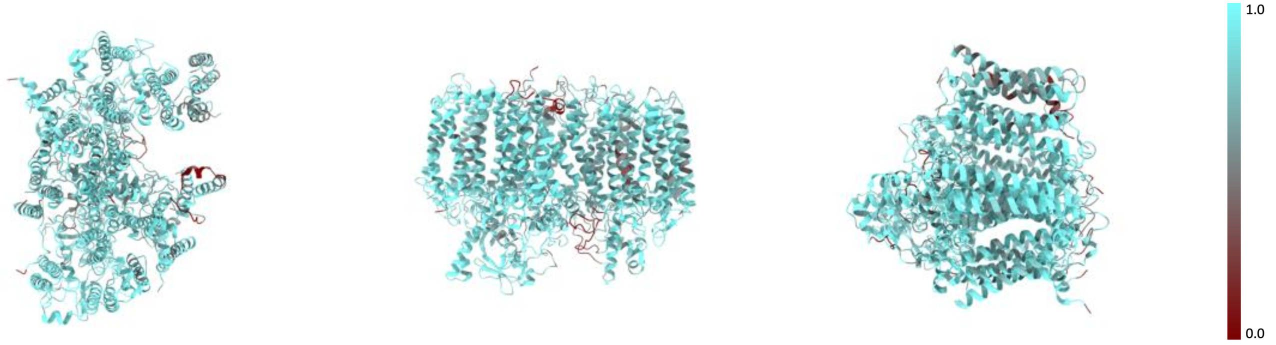
9.2 Q-score mapped to coordinate model ⓘ



X Y Z

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

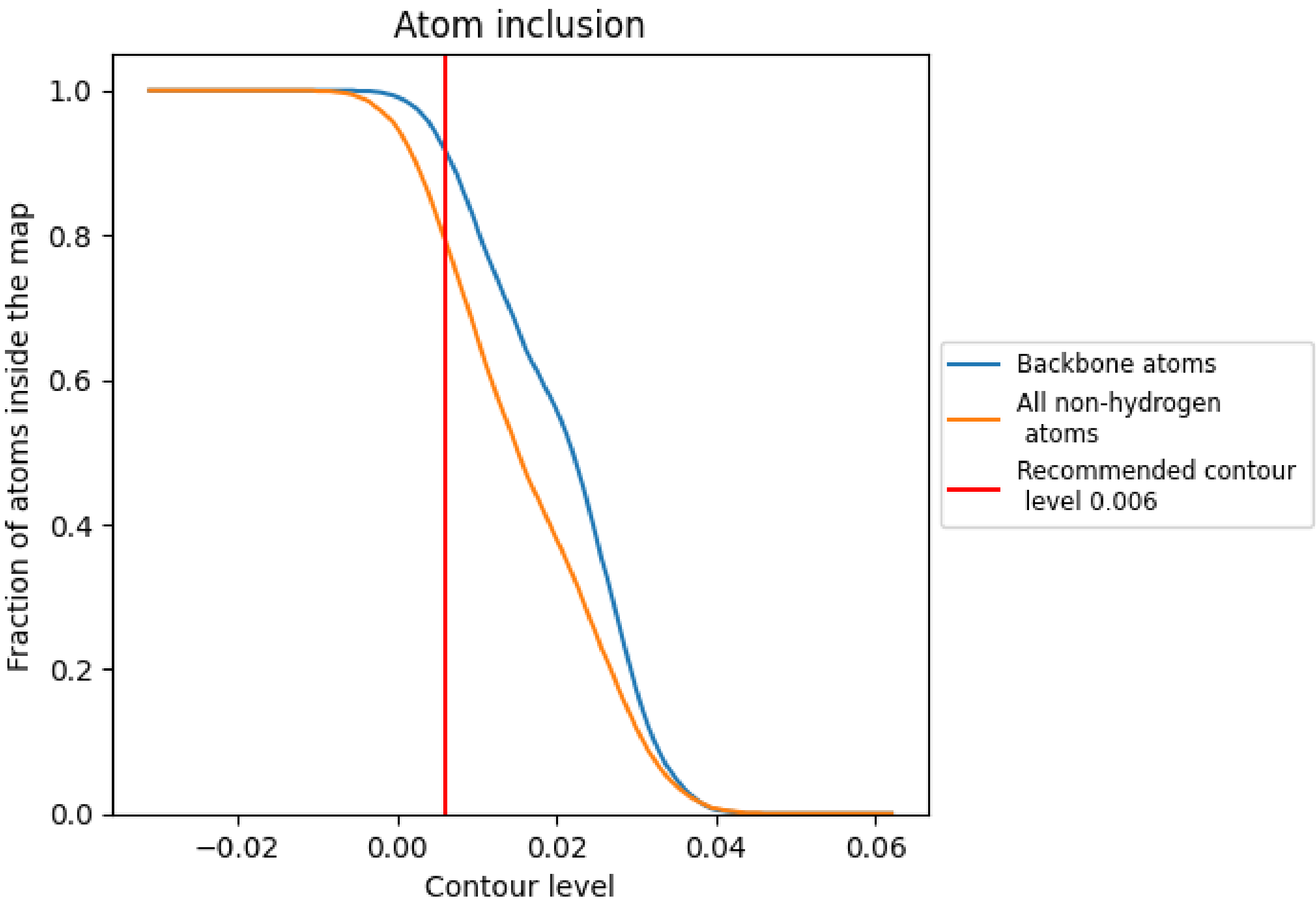
9.3 Atom inclusion mapped to coordinate model ⓘ



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 79% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7940	0.5010
A	0.7880	0.5100
B	0.8390	0.5250
C	0.7820	0.4940
D	0.8430	0.5380
E	0.7260	0.4090
F	0.6480	0.3980
H	0.8590	0.5020
I	0.7200	0.4590
K	0.7050	0.4700
L	0.8020	0.5040
M	0.5920	0.3780
T	0.7650	0.4940
X	0.7760	0.4730
Z	0.6750	0.4130
y	0.5740	0.3790