wwPDB EM Validation Summary Report ⓘ

Nov 4, 2024 – 06:31 AM JST

PDB ID	:	7VY3
EMDB ID	:	EMD-32193
Title	:	STRUCTURE OF PHOTOSYNTHETIC LH1-RC SUPER-COMPLEX OF RHODOBACTER SPHAEROIDES LACKING PROTEIN-U
Authors	:	Tani, K.; Kanno, R.; Kawamura, S.; Kikuchi, R.; Nagashima, K.V.P.; Hall, M.; Takahashi, A.; Yu, L.-J.; Kimura, Y.; Madigan, M.T.; Mizoguchi, A.; Humbel, B.M.; Wang-Otomo, Z.-Y.
Deposited on	:	2021-11-13
Resolution	:	2.63 Å(reported)
Based on initial model	:	7F0L

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

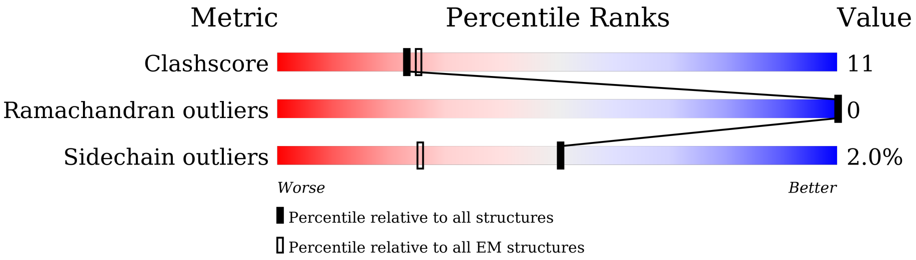
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

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

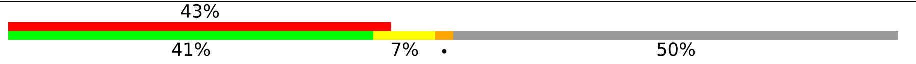
The reported resolution of this entry is 2.63 Å.

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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	L	281	
2	M	307	
3	H	260	
4	1	54	
4	A	54	
4	D	54	
4	F	54	

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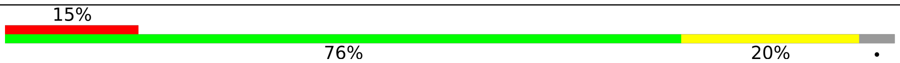
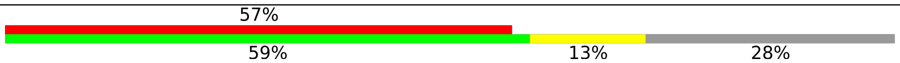
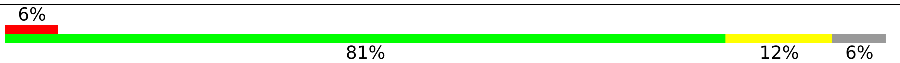
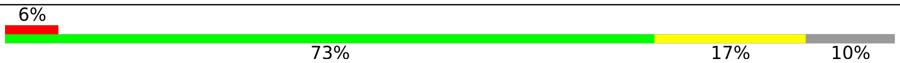
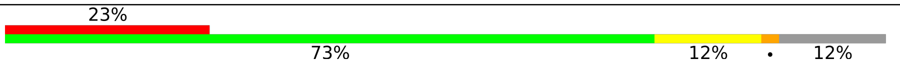
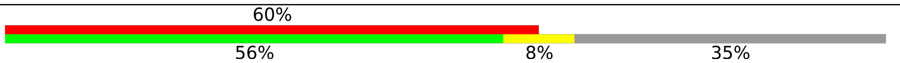
Mol	Chain	Length	Quality of chain
4	I	54	
4	K	54	
4	O	54	
4	Q	54	
4	S	54	
4	V	54	
4	Y	54	
5	B	48	
5	E	48	
5	G	48	
5	J	48	
5	N	48	
5	P	48	
5	R	48	
5	T	48	
5	W	48	
5	Z	48	
6	X	81	

2 Entry composition ⓘ

There are 16 unique types of molecules in this entry. The entry contains 18831 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 Photosynthetic reaction center L subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	0	0
			2233	1508	355	362	8		

- Molecule 2 is a protein called Reaction center protein M chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	306	Total	C	N	O	S	0	0
			2437	1627	398	401	11		

- Molecule 3 is a protein called Photosynthetic reaction center subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	246	Total	C	N	O	S	1	0
			1867	1199	314	344	10		

- Molecule 4 is a protein called Antenna pigment protein alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	45	Total	C	N	O	S	0	0
			386	266	59	58	3		
4	D	54	Total	C	N	O	S	0	0
			455	309	73	70	3		
4	F	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	I	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	K	54	Total	C	N	O	S	0	0
			457	311	73	70	3		
4	O	54	Total	C	N	O	S	0	0
			453	308	72	70	3		
4	Q	54	Total	C	N	O	S	0	0
			457	311	73	70	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	54	Total 454	C 309	N 73	O 70	S 2	0	0
4	V	52	Total 441	C 302	N 71	O 66	S 2	0	0
4	Y	39	Total 318	C 217	N 50	O 50	S 1	0	0
4	1	27	Total 216	C 147	N 36	O 32	S 1	0	0

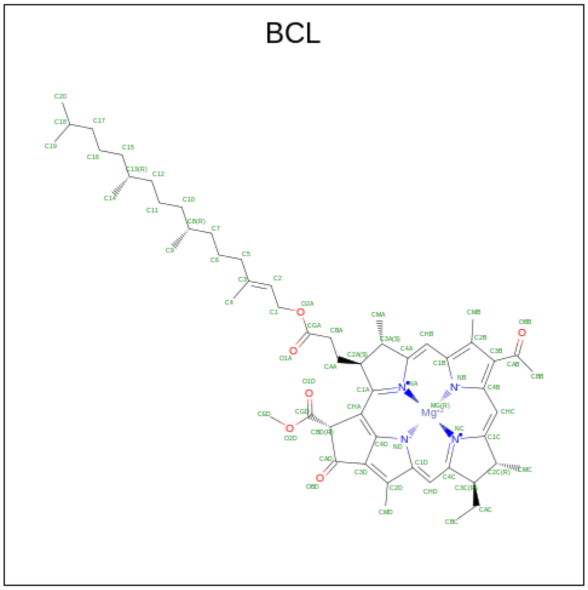
- Molecule 5 is a protein called Antenna pigment protein beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	44	Total 359	C 240	N 56	O 62	S 1	0	0
5	E	43	Total 351	C 236	N 55	O 59	S 1	0	0
5	G	45	Total 365	C 243	N 57	O 64	S 1	0	0
5	J	43	Total 351	C 236	N 55	O 59	S 1	0	0
5	N	43	Total 351	C 236	N 55	O 59	S 1	0	0
5	P	43	Total 351	C 236	N 55	O 59	S 1	0	0
5	R	43	Total 347	C 234	N 55	O 57	S 1	0	0
5	T	43	Total 351	C 236	N 55	O 59	S 1	0	0
5	W	42	Total 339	C 228	N 54	O 56	S 1	0	0
5	Z	31	Total 261	C 181	N 41	O 38	S 1	0	0

- Molecule 6 is a protein called PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	52	Total 401	C 267	N 68	O 63	S 3	0	0

- Molecule 7 is BACTERIOCHLOROPHYLL A (three-letter code: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
7	L	1	Total C Mg N O 66 55 1 4 6	0
7	L	1	Total C Mg N O 66 55 1 4 6	0
7	M	1	Total C Mg N O 66 55 1 4 6	0
7	M	1	Total C Mg N O 66 55 1 4 6	0
7	A	1	Total C Mg N O 61 50 1 4 6	0
7	B	1	Total C Mg N O 66 55 1 4 6	0
7	D	1	Total C Mg N O 66 55 1 4 6	0
7	E	1	Total C Mg N O 66 55 1 4 6	0
7	F	1	Total C Mg N O 66 55 1 4 6	0
7	G	1	Total C Mg N O 66 55 1 4 6	0
7	I	1	Total C Mg N O 66 55 1 4 6	0
7	J	1	Total C Mg N O 66 55 1 4 6	0
7	K	1	Total C Mg N O 66 55 1 4 6	0
7	N	1	Total C Mg N O 66 55 1 4 6	0

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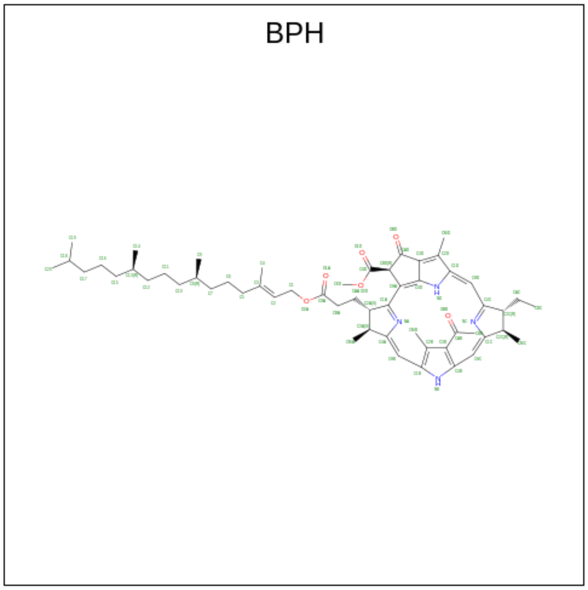
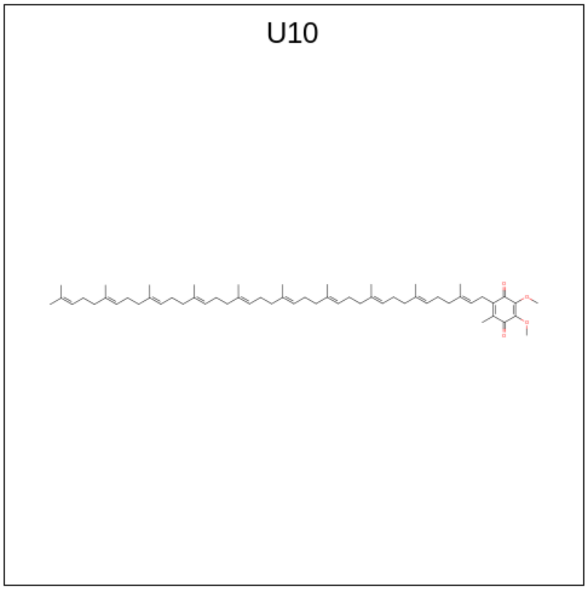
Mol	Chain	Residues	Atoms					AltConf
7	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	P	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Q	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	S	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	T	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	V	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
7	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 8 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$).



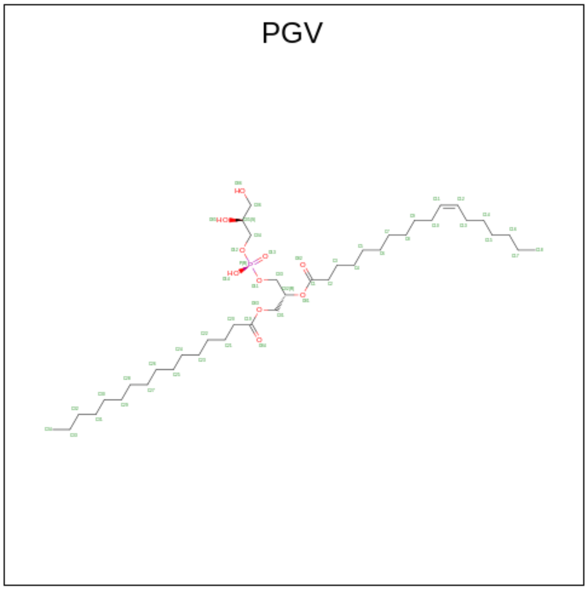
Mol	Chain	Residues	Atoms				AltConf
8	L	1	Total 65	C 55	N 4	O 6	0
8	M	1	Total 65	C 55	N 4	O 6	0

- Molecule 9 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



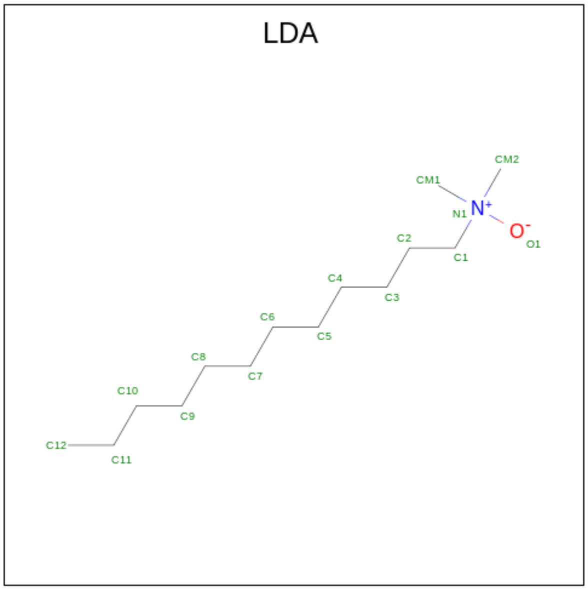
Mol	Chain	Residues	Atoms			AltConf
9	L	1	Total 35	C 31	O 4	0
9	L	1	Total 28	C 24	O 4	0
9	M	1	Total 63	C 59	O 4	0
9	D	1	Total 63	C 59	O 4	0

- Molecule 10 is (1R)-2-{[{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: $C_{40}H_{77}O_{10}P$).



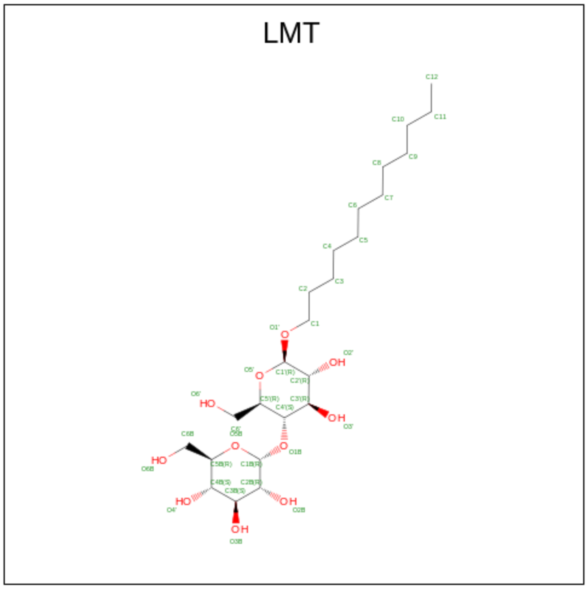
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
10	L	1	39	28	10	1	0
10	M	1	38	27	10	1	0
10	H	1	47	36	10	1	0
10	F	1	40	29	10	1	0
10	F	1	47	36	10	1	0
10	K	1	41	34	6	1	0
10	Q	1	39	28	10	1	0
10	Y	1	43	32	10	1	0

- Molecule 11 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms	AltConf
11	L	1	Total C N O 16 14 1 1	0
11	H	1	Total C N O 16 14 1 1	0
11	Y	1	Total C N O 12 10 1 1	0
11	X	1	Total C N O 13 11 1 1	0

- Molecule 12 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).

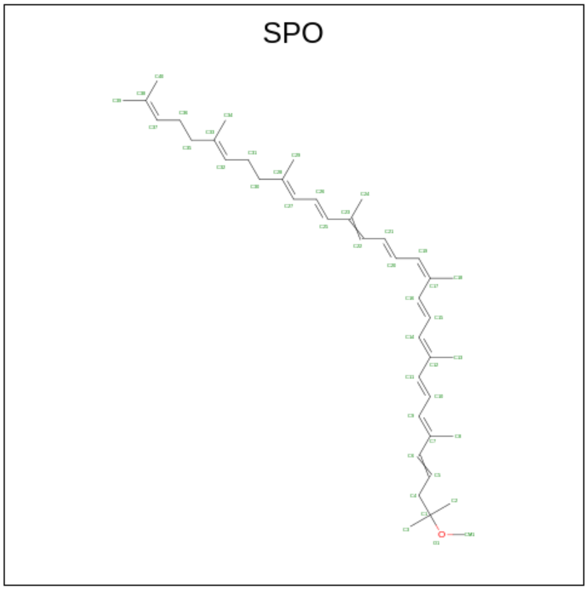


Mol	Chain	Residues	Atoms	AltConf
12	L	1	Total C O 35 24 11	0
12	L	1	Total C O 34 23 11	0
12	M	1	Total C O 27 20 7	0
12	M	1	Total C O 25 19 6	0
12	H	1	Total C O 35 24 11	0
12	H	1	Total C O 35 24 11	0
12	H	1	Total C O 30 19 11	0
12	A	1	Total C O 35 24 11	0
12	A	1	Total C O 35 24 11	0
12	B	1	Total C O 27 16 11	0
12	D	1	Total C O 27 16 11	0
12	F	1	Total C O 17 11 6	0
12	I	1	Total C O 26 16 10	0
12	I	1	Total C O 27 16 11	0
12	K	1	Total C O 35 24 11	0
12	Q	1	Total C O 24 18 6	0
12	Q	1	Total C O 19 13 6	0

- Molecule 13 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	AltConf
13	M	1	Total Fe 1 1	0

- Molecule 14 is SPHEROIDENE (three-letter code: SPO) (formula: $C_{41}H_{60}O$).



Mol	Chain	Residues	Atoms	AltConf
14	M	1	Total C O 42 41 1	0
14	B	1	Total C O 42 41 1	0
14	B	1	Total C O 42 41 1	0
14	D	1	Total C O 42 41 1	0
14	D	1	Total C O 42 41 1	0
14	F	1	Total C O 42 41 1	0
14	G	1	Total C O 42 41 1	0
14	G	1	Total C O 42 41 1	0
14	J	1	Total C O 42 41 1	0
14	K	1	Total C O 42 41 1	0
14	K	1	Total C O 42 41 1	0
14	O	1	Total C O 42 41 1	0
14	P	1	Total C O 42 41 1	0
14	Q	1	Total C O 42 41 1	0

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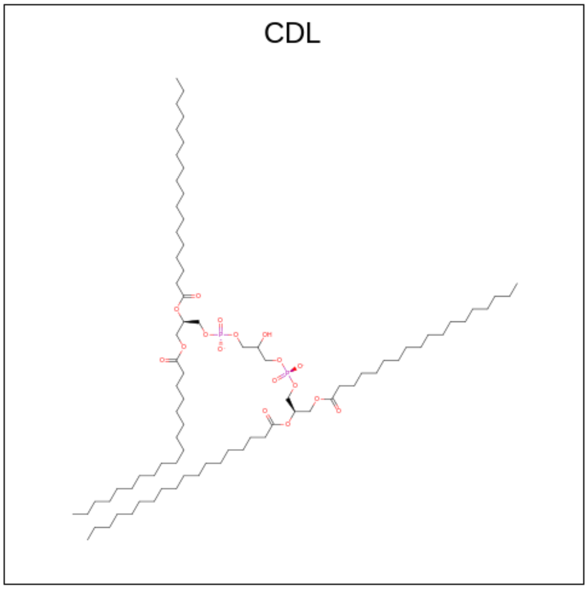
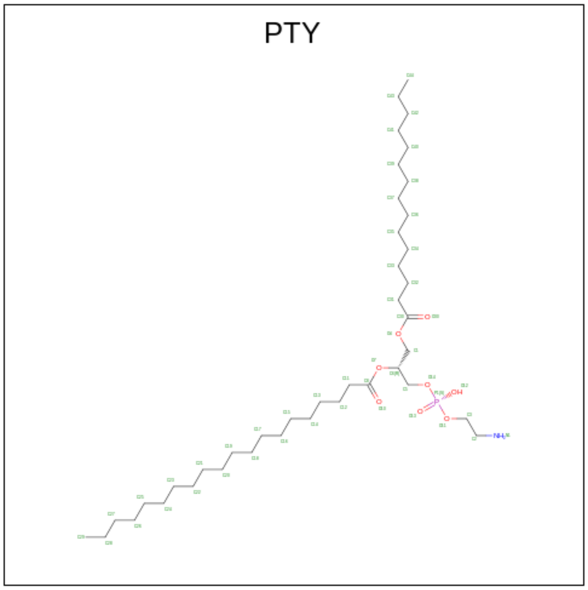
Mol	Chain	Residues	Atoms	AltConf
14	S	1	Total C O 42 41 1	0
14	S	1	Total C O 42 41 1	0
14	V	1	Total C O 42 41 1	0
14	V	1	Total C O 42 41 1	0
14	Z	1	Total C O 42 41 1	0

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms	AltConf
15	M	1	Total C O P 79 60 17 2	0
15	H	1	Total C O P 61 42 17 2	0
15	Y	1	Total C O P 35 19 14 2	0

- Molecule 16 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).

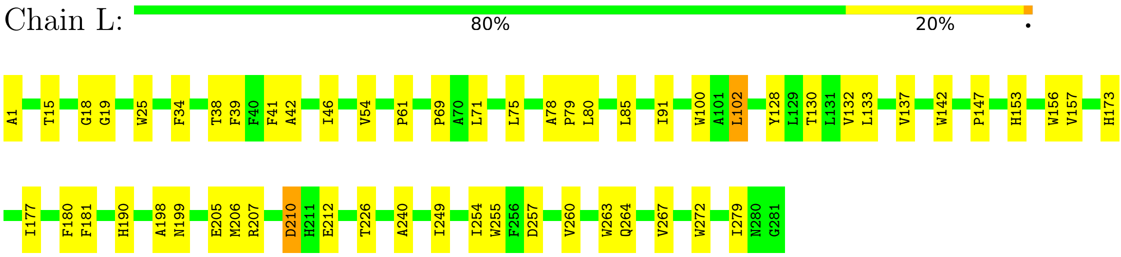


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
16	H	1	46	36	1	8	1	0
			Total	C	N	O	P	
16	F	1	48	38	1	8	1	0

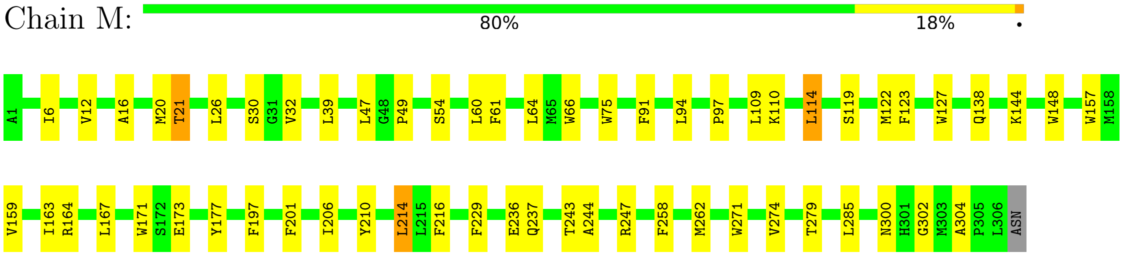
3 Residue-property plots ⓘ

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.

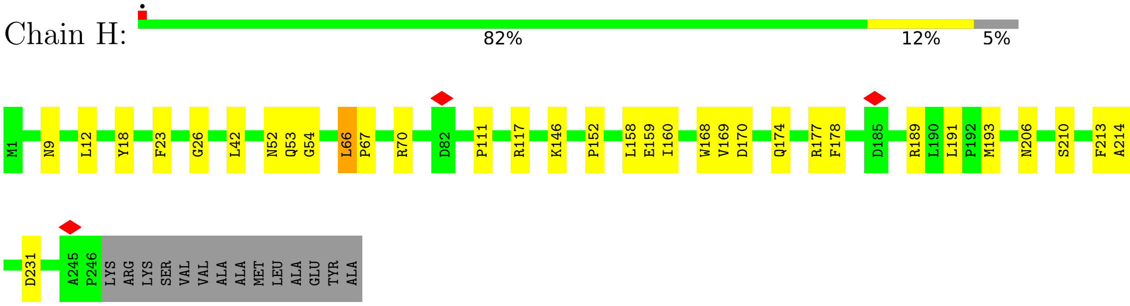
- Molecule 1: Photosynthetic reaction center L subunit



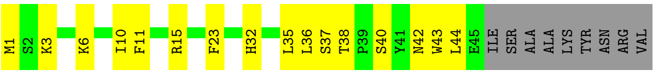
- Molecule 2: Reaction center protein M chain



- Molecule 3: Photosynthetic reaction center subunit H

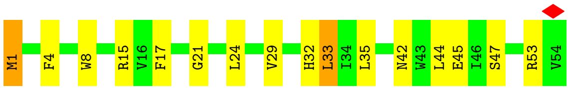


- Molecule 4: Antenna pigment protein alpha chain



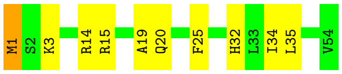
- Molecule 4: Antenna pigment protein alpha chain

Chain D:



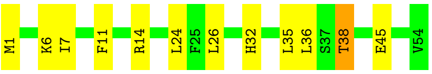
- Molecule 4: Antenna pigment protein alpha chain

Chain F:



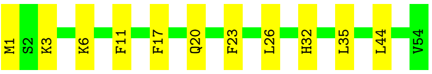
- Molecule 4: Antenna pigment protein alpha chain

Chain I:



- Molecule 4: Antenna pigment protein alpha chain

Chain K:

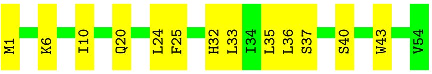


- Molecule 4: Antenna pigment protein alpha chain

Chain O:

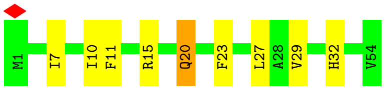
- Molecule 4: Antenna pigment protein alpha chain

Chain Q:



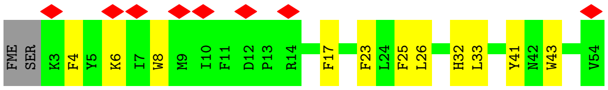
- Molecule 4: Antenna pigment protein alpha chain

Chain S:



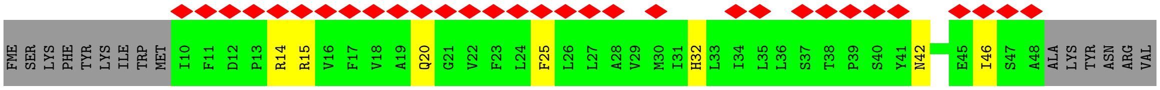
- Molecule 4: Antenna pigment protein alpha chain

Chain V:



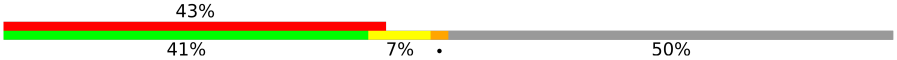
- Molecule 4: Antenna pigment protein alpha chain

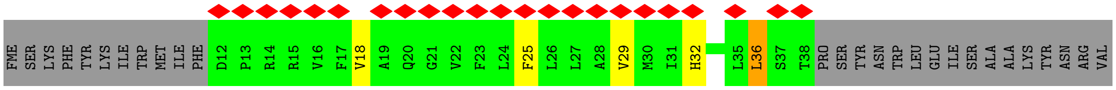
Chain Y:



- Molecule 4: Antenna pigment protein alpha chain

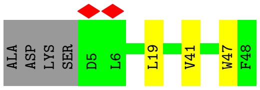
Chain 1:





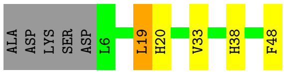
- Molecule 5: Antenna pigment protein beta chain

Chain B:



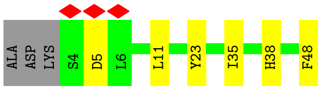
- Molecule 5: Antenna pigment protein beta chain

Chain E:



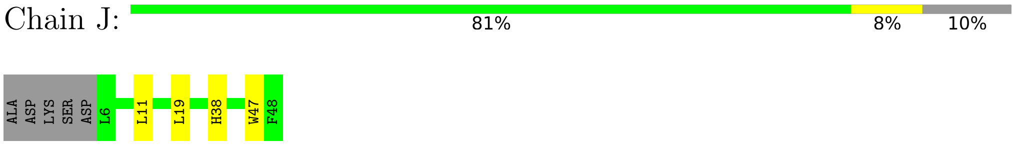
- Molecule 5: Antenna pigment protein beta chain

Chain G:



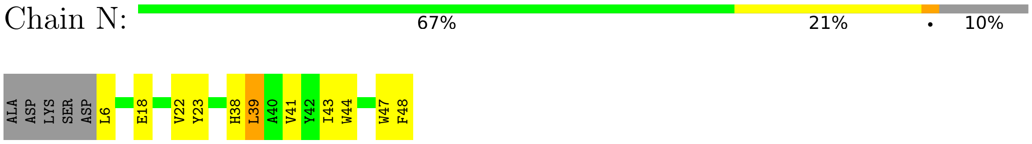
- Molecule 5: Antenna pigment protein beta chain

Chain J:



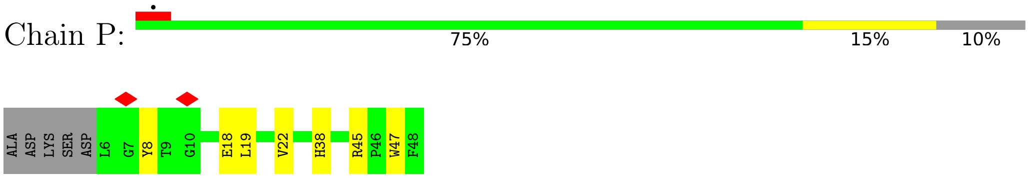
- Molecule 5: Antenna pigment protein beta chain

Chain N:



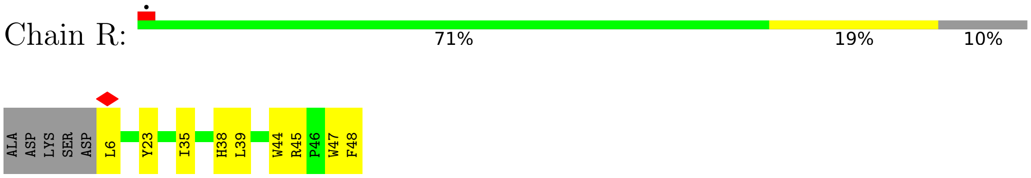
- Molecule 5: Antenna pigment protein beta chain

Chain P:



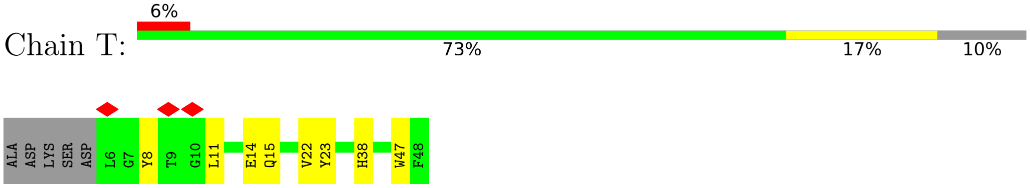
- Molecule 5: Antenna pigment protein beta chain

Chain R:



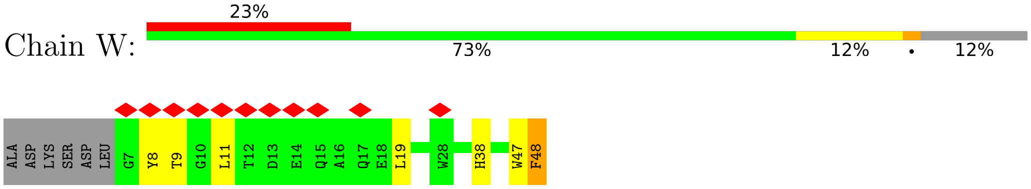
- Molecule 5: Antenna pigment protein beta chain

Chain T:



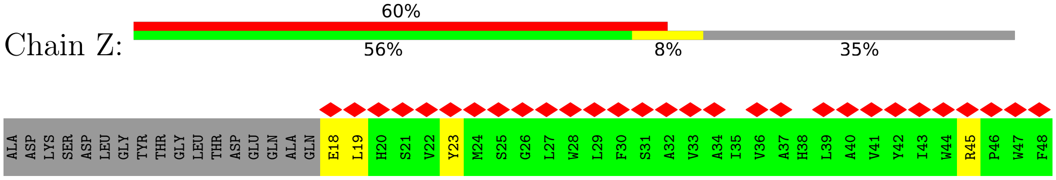
- Molecule 5: Antenna pigment protein beta chain

Chain W:

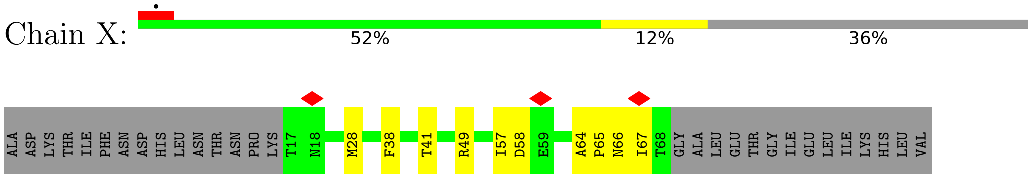


- Molecule 5: Antenna pigment protein beta chain

Chain Z:



- Molecule 6: PufX



4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	124589	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.265	Depositor
Minimum map value	-0.146	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82000005, 0.82000005, 0.82000005	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, SPO, BPH, LMT, CDL, PTY, U10, PGV, FME, BCL, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	L	0.27	0/2321	0.42	0/3177
2	M	0.26	0/2530	0.42	0/3455
3	H	0.26	0/1920	0.47	0/2615
4	1	0.24	0/220	0.43	0/298
4	A	0.27	0/389	0.40	0/528
4	D	0.28	0/459	0.41	0/622
4	F	0.26	0/461	0.41	0/625
4	I	0.28	0/461	0.39	0/625
4	K	0.27	0/461	0.42	0/625
4	O	0.27	0/457	0.40	0/621
4	Q	0.26	0/461	0.42	0/625
4	S	0.25	0/461	0.41	0/625
4	V	0.26	0/455	0.40	0/617
4	Y	0.24	0/327	0.40	0/446
5	B	0.26	0/372	0.37	0/510
5	E	0.25	0/364	0.40	0/499
5	G	0.27	0/378	0.37	0/518
5	J	0.25	0/364	0.39	0/499
5	N	0.25	0/364	0.38	0/499
5	P	0.24	0/364	0.38	0/499
5	R	0.25	0/360	0.37	0/494
5	T	0.24	0/364	0.37	0/499
5	W	0.23	0/352	0.37	0/483
5	Z	0.23	0/273	0.36	0/375
6	X	0.25	0/413	0.46	0/561
All	All	0.26	0/15351	0.41	0/20940

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	L	2233	0	2189	42	0
2	M	2437	0	2355	43	0
3	H	1867	0	1867	22	0
4	1	216	0	236	5	0
4	A	386	0	400	13	0
4	D	455	0	469	15	0
4	F	457	0	476	10	0
4	I	457	0	476	12	0
4	K	457	0	476	14	0
4	O	453	0	465	16	0
4	Q	457	0	476	11	0
4	S	454	0	469	9	0
4	V	441	0	460	11	0
4	Y	318	0	331	7	0
5	B	359	0	340	2	0
5	E	351	0	336	5	0
5	G	365	0	345	5	0
5	J	351	0	336	5	0
5	N	351	0	336	11	0
5	P	351	0	336	9	0
5	R	347	0	332	9	0
5	T	351	0	336	10	0
5	W	339	0	321	7	0
5	Z	261	0	254	6	0
6	X	401	0	409	8	0
7	1	66	0	74	9	0
7	A	61	0	61	5	0
7	B	66	0	74	4	0
7	D	66	0	74	12	0
7	E	66	0	74	2	0
7	F	66	0	74	9	0
7	G	66	0	74	3	0
7	I	66	0	74	4	0
7	J	66	0	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	K	66	0	74	7	0
7	L	132	0	148	5	0
7	M	132	0	148	8	0
7	N	66	0	74	7	0
7	O	66	0	74	5	0
7	P	66	0	74	6	0
7	Q	132	0	148	20	0
7	S	66	0	74	7	0
7	T	66	0	74	8	0
7	V	66	0	74	7	0
7	W	66	0	74	5	0
7	Y	66	0	74	7	0
7	Z	66	0	74	5	0
8	L	65	0	76	3	0
8	M	65	0	76	8	0
9	D	63	0	90	11	0
9	L	63	0	74	4	0
9	M	63	0	90	5	0
10	F	87	0	110	6	0
10	H	47	0	65	1	0
10	K	41	0	60	2	0
10	L	39	0	47	2	0
10	M	38	0	45	4	0
10	Q	39	0	48	2	0
10	Y	43	0	54	3	0
11	H	16	0	31	1	0
11	L	16	0	31	0	0
11	X	13	0	22	0	0
11	Y	12	0	20	2	0
12	A	70	0	92	4	0
12	B	27	0	27	0	0
12	D	27	0	27	1	0
12	F	17	0	16	0	0
12	H	100	0	125	10	0
12	I	53	0	51	3	0
12	K	35	0	46	4	0
12	L	69	0	87	2	0
12	M	52	0	71	1	0
12	Q	43	0	55	3	0
13	M	1	0	0	0	0
14	B	84	0	120	11	0
14	D	84	0	120	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	F	42	0	60	6	0
14	G	84	0	120	11	0
14	J	42	0	60	6	0
14	K	84	0	120	11	0
14	M	42	0	60	5	0
14	O	42	0	60	4	0
14	P	42	0	60	8	0
14	Q	42	0	60	5	0
14	S	84	0	120	10	0
14	V	84	0	120	10	0
14	Z	42	0	60	11	0
15	H	61	0	66	5	0
15	M	79	0	105	5	0
15	Y	35	0	32	2	0
16	F	48	0	72	4	0
16	H	46	0	68	6	0
All	All	18831	0	19682	418	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 11.

The worst 5 of 418 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)
14:D:104:SPO:H6	7:I:102:BCL:HMB2	1.60	0.83
14:B:104:SPO:H342	9:D:105:U10:H38	1.61	0.81
14:Q:105:SPO:H6	7:S:101:BCL:HMB2	1.61	0.81
4:F:1:FME:HCN	4:F:3:LYS:H	1.47	0.78
2:M:109:LEU:HB2	11:Y:101:LDA:H11	1.63	0.78

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	L	279/281 (99%)	271 (97%)	8 (3%)	0	100	100
2	M	304/307 (99%)	292 (96%)	12 (4%)	0	100	100
3	H	245/260 (94%)	238 (97%)	7 (3%)	0	100	100
4	1	25/54 (46%)	25 (100%)	0	0	100	100
4	A	43/54 (80%)	43 (100%)	0	0	100	100
4	D	52/54 (96%)	52 (100%)	0	0	100	100
4	F	52/54 (96%)	52 (100%)	0	0	100	100
4	I	52/54 (96%)	52 (100%)	0	0	100	100
4	K	52/54 (96%)	52 (100%)	0	0	100	100
4	O	52/54 (96%)	52 (100%)	0	0	100	100
4	Q	52/54 (96%)	52 (100%)	0	0	100	100
4	S	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
4	V	50/54 (93%)	49 (98%)	1 (2%)	0	100	100
4	Y	37/54 (68%)	37 (100%)	0	0	100	100
5	B	42/48 (88%)	41 (98%)	1 (2%)	0	100	100
5	E	41/48 (85%)	41 (100%)	0	0	100	100
5	G	43/48 (90%)	42 (98%)	1 (2%)	0	100	100
5	J	41/48 (85%)	41 (100%)	0	0	100	100
5	N	41/48 (85%)	41 (100%)	0	0	100	100
5	P	41/48 (85%)	39 (95%)	2 (5%)	0	100	100
5	R	41/48 (85%)	41 (100%)	0	0	100	100
5	T	41/48 (85%)	41 (100%)	0	0	100	100
5	W	40/48 (83%)	39 (98%)	1 (2%)	0	100	100
5	Z	29/48 (60%)	29 (100%)	0	0	100	100
6	X	50/81 (62%)	48 (96%)	2 (4%)	0	100	100
All	All	1797/2003 (90%)	1761 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	L	220/220 (100%)	215 (98%)	5 (2%)	45	65
2	M	239/240 (100%)	234 (98%)	5 (2%)	48	69
3	H	198/208 (95%)	192 (97%)	6 (3%)	36	55
4	1	24/48 (50%)	23 (96%)	1 (4%)	25	41
4	A	41/48 (85%)	41 (100%)	0	100	100
4	D	47/48 (98%)	46 (98%)	1 (2%)	48	69
4	F	48/48 (100%)	48 (100%)	0	100	100
4	I	48/48 (100%)	47 (98%)	1 (2%)	48	69
4	K	48/48 (100%)	48 (100%)	0	100	100
4	O	47/48 (98%)	46 (98%)	1 (2%)	48	69
4	Q	48/48 (100%)	48 (100%)	0	100	100
4	S	48/48 (100%)	46 (96%)	2 (4%)	25	41
4	V	47/48 (98%)	47 (100%)	0	100	100
4	Y	35/48 (73%)	35 (100%)	0	100	100
5	B	36/39 (92%)	35 (97%)	1 (3%)	38	58
5	E	35/39 (90%)	34 (97%)	1 (3%)	37	57
5	G	37/39 (95%)	36 (97%)	1 (3%)	40	60
5	J	35/39 (90%)	35 (100%)	0	100	100
5	N	35/39 (90%)	34 (97%)	1 (3%)	37	57
5	P	35/39 (90%)	35 (100%)	0	100	100
5	R	34/39 (87%)	33 (97%)	1 (3%)	37	57
5	T	35/39 (90%)	34 (97%)	1 (3%)	37	57
5	W	33/39 (85%)	32 (97%)	1 (3%)	36	55
5	Z	26/39 (67%)	26 (100%)	0	100	100
6	X	40/65 (62%)	39 (98%)	1 (2%)	42	63
All	All	1519/1651 (92%)	1489 (98%)	30 (2%)	50	70

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

Mol	Chain	Res	Type
3	H	206	ASN
5	W	48	PHE
4	D	33	LEU
6	X	67	ILE
4	S	20	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
6	X	66	ASN
4	1	20	GLN
5	N	17	GLN
5	G	17	GLN
4	Y	20	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
4	FME	Q	1	4	8,9,10	0.52	0	7,9,11	0.94	1 (14%)
4	FME	F	1	4	8,9,10	0.50	0	7,9,11	1.07	1 (14%)
4	FME	S	1	4	5,6,10	0.79	0	3,6,11	0.75	0
4	FME	D	1	4	8,9,10	0.50	0	7,9,11	1.07	1 (14%)
4	FME	K	1	4	8,9,10	0.52	0	7,9,11	1.05	1 (14%)
4	FME	A	1	4	8,9,10	0.53	0	7,9,11	0.92	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	FME	O	1	4	8,9,10	0.51	0	7,9,11	1.04	1 (14%)
4	FME	I	1	4	8,9,10	0.52	0	7,9,11	0.99	1 (14%)

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
4	FME	Q	1	4	-	0/7/9/11	-
4	FME	F	1	4	-	1/7/9/11	-
4	FME	S	1	4	-	1/2/5/11	-
4	FME	D	1	4	-	0/7/9/11	-
4	FME	K	1	4	-	0/7/9/11	-
4	FME	A	1	4	-	3/7/9/11	-
4	FME	O	1	4	-	1/7/9/11	-
4	FME	I	1	4	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1	FME	O-C-CA	-2.59	117.98	124.78
4	O	1	FME	O-C-CA	-2.56	118.06	124.78
4	K	1	FME	O-C-CA	-2.56	118.07	124.78
4	F	1	FME	O-C-CA	-2.51	118.20	124.78
4	I	1	FME	O-C-CA	-2.44	118.37	124.78

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	FME	O1-CN-N-CA
4	A	1	FME	N-CA-CB-CG
4	F	1	FME	O1-CN-N-CA
4	O	1	FME	O1-CN-N-CA
4	S	1	FME	O1-CN-N-CA

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1	FME	1	0
4	D	1	FME	1	0
4	O	1	FME	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 85 ligands modelled in this entry, 1 is monoatomic - leaving 84 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	$\#\|Z\| > 2$
7	BCL	Q	106	-	64,74,74	1.70	14 (21%)	78,115,115	2.19	20 (25%)
7	BCL	K	102	-	64,74,74	1.67	12 (18%)	78,115,115	2.28	20 (25%)
14	SPO	G	103	-	40,41,41	0.63	0	47,50,50	1.81	12 (25%)
12	LMT	M	407	-	25,25,36	0.41	0	30,30,47	0.64	0
14	SPO	K	105	-	40,41,41	0.64	0	47,50,50	1.67	12 (25%)
12	LMT	H	304	-	36,36,36	0.39	0	47,47,47	0.88	1 (2%)
7	BCL	O	101	-	64,74,74	1.69	14 (21%)	78,115,115	2.32	22 (28%)
10	PGV	L	305	-	38,38,50	1.06	2 (5%)	41,44,56	1.11	2 (4%)
12	LMT	H	305	-	31,31,36	0.48	0	42,42,47	0.93	1 (2%)
7	BCL	Y	103	-	64,74,74	1.73	14 (21%)	78,115,115	2.16	18 (23%)
7	BCL	N	101	-	64,74,74	1.70	13 (20%)	78,115,115	2.18	20 (25%)
14	SPO	S	103	-	40,41,41	0.62	0	47,50,50	1.85	13 (27%)
14	SPO	B	104	-	40,41,41	0.64	0	47,50,50	2.10	13 (27%)
14	SPO	F	105	-	40,41,41	0.63	0	47,50,50	1.92	16 (34%)
12	LMT	L	307	-	36,36,36	0.42	0	47,47,47	1.07	3 (6%)
10	PGV	K	104	-	38,40,50	1.03	2 (5%)	40,42,56	1.08	3 (7%)
7	BCL	J	101	-	64,74,74	1.68	14 (21%)	78,115,115	2.17	20 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
11	LDA	H	302	-	12,15,15	2.08	1 (8%)	14,17,17	0.51	0
14	SPO	D	104	-	40,41,41	0.62	0	47,50,50	1.70	11 (23%)
7	BCL	G	101	-	64,74,74	1.70	14 (21%)	78,115,115	2.19	20 (25%)
8	BPH	L	302	-	51,70,70	0.56	1 (1%)	52,101,101	0.65	1 (1%)
12	LMT	A	102	-	36,36,36	0.39	0	47,47,47	0.74	1 (2%)
14	SPO	M	405	-	40,41,41	0.63	0	47,50,50	1.64	12 (25%)
9	U10	L	303	-	35,35,63	0.83	2 (5%)	42,45,79	0.69	0
12	LMT	K	101	-	36,36,36	0.39	0	47,47,47	0.84	2 (4%)
12	LMT	Q	102	-	19,19,36	0.44	0	24,24,47	0.54	0
12	LMT	F	106	-	17,17,36	0.46	0	22,22,47	0.52	0
7	BCL	B	103	-	64,74,74	1.72	14 (21%)	78,115,115	2.16	20 (25%)
7	BCL	T	101	-	64,74,74	1.69	14 (21%)	78,115,115	2.22	19 (24%)
12	LMT	H	303	-	36,36,36	0.37	0	47,47,47	0.79	2 (4%)
14	SPO	O	102	-	40,41,41	0.63	0	47,50,50	1.76	13 (27%)
12	LMT	D	103	-	28,28,36	0.46	0	39,39,47	0.67	1 (2%)
14	SPO	V	103	-	40,41,41	0.64	0	47,50,50	1.81	13 (27%)
7	BCL	I	102	-	64,74,74	1.67	13 (20%)	78,115,115	2.28	21 (26%)
11	LDA	Y	101	-	8,11,15	2.53	1 (12%)	10,13,17	0.43	0
14	SPO	B	101	-	40,41,41	0.64	0	47,50,50	1.78	11 (23%)
12	LMT	I	103	-	28,28,36	0.44	0	39,39,47	0.57	1 (2%)
7	BCL	V	101	-	64,74,74	1.68	13 (20%)	78,115,115	2.33	22 (28%)
7	BCL	D	101	-	64,74,74	1.69	13 (20%)	78,115,115	2.30	20 (25%)
12	LMT	Q	101	-	24,24,36	0.40	0	29,29,47	0.71	0
15	CDL	Y	102	-	34,34,99	0.85	1 (2%)	37,43,111	0.74	1 (2%)
7	BCL	L	301	-	64,74,74	1.69	14 (21%)	78,115,115	2.29	21 (26%)
14	SPO	G	102	-	40,41,41	0.64	0	47,50,50	1.74	10 (21%)
14	SPO	K	103	-	40,41,41	0.64	0	47,50,50	1.71	11 (23%)
14	SPO	D	102	-	40,41,41	0.63	0	47,50,50	1.73	12 (25%)
9	U10	D	105	-	63,63,63	0.62	2 (3%)	76,79,79	0.62	0
7	BCL	M	401	-	64,74,74	1.69	13 (20%)	78,115,115	2.27	22 (28%)
10	PGV	F	103	-	46,46,50	0.96	2 (4%)	49,52,56	1.06	3 (6%)
12	LMT	B	102	-	28,28,36	0.44	0	39,39,47	0.69	1 (2%)
9	U10	M	410	-	63,63,63	0.62	2 (3%)	76,79,79	0.53	0
16	PTY	H	306	-	45,45,49	0.29	0	48,50,54	0.42	0
15	CDL	H	307	-	60,60,99	1.18	4 (6%)	66,72,111	1.12	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	U10	L	304	-	28,28,63	0.85	2 (7%)	34,37,79	0.78	2 (5%)
12	LMT	M	406	-	27,27,36	0.49	0	32,33,47	0.71	1 (3%)
7	BCL	1	101	-	64,74,74	1.79	14 (21%)	78,115,115	2.16	18 (23%)
7	BCL	F	101	-	64,74,74	1.68	13 (20%)	78,115,115	2.30	20 (25%)
7	BCL	L	309	-	64,74,74	1.76	14 (21%)	78,115,115	2.17	21 (26%)
7	BCL	Q	104	-	64,74,74	1.69	14 (21%)	78,115,115	2.23	20 (25%)
14	SPO	Q	105	-	40,41,41	0.65	0	47,50,50	1.76	14 (29%)
7	BCL	W	101	-	64,74,74	1.77	14 (21%)	78,115,115	2.13	20 (25%)
10	PGV	H	301	-	46,46,50	0.94	2 (4%)	49,52,56	1.05	4 (8%)
11	LDA	L	306	-	12,15,15	2.08	1 (8%)	14,17,17	0.49	0
11	LDA	X	101	-	9,12,15	2.41	1 (11%)	11,14,17	0.50	0
10	PGV	M	409	-	37,37,50	1.05	2 (5%)	40,43,56	1.14	3 (7%)
10	PGV	F	102	-	39,39,50	1.04	2 (5%)	42,45,56	1.26	5 (11%)
10	PGV	Y	104	-	42,42,50	1.01	2 (4%)	44,48,56	1.06	3 (6%)
14	SPO	V	102	-	40,41,41	0.63	0	47,50,50	1.83	13 (27%)
7	BCL	A	103	-	59,69,74	1.82	14 (23%)	72,109,115	2.30	21 (29%)
10	PGV	Q	103	-	38,38,50	1.04	2 (5%)	41,44,56	1.08	3 (7%)
7	BCL	P	101	-	64,74,74	1.72	13 (20%)	78,115,115	2.16	20 (25%)
7	BCL	M	402	-	64,74,74	1.71	14 (21%)	78,115,115	2.32	20 (25%)
12	LMT	L	308	-	35,35,36	0.42	0	46,46,47	0.78	1 (2%)
14	SPO	Z	101	-	40,41,41	0.64	0	47,50,50	1.74	12 (25%)
7	BCL	Z	102	-	64,74,74	1.83	14 (21%)	78,115,115	2.22	22 (28%)
12	LMT	A	101	-	36,36,36	0.37	0	47,47,47	0.69	0
7	BCL	E	101	-	64,74,74	1.70	14 (21%)	78,115,115	2.17	20 (25%)
15	CDL	M	408	-	78,78,99	1.05	4 (5%)	84,90,111	1.13	6 (7%)
7	BCL	S	101	-	64,74,74	1.68	13 (20%)	78,115,115	2.29	22 (28%)
14	SPO	P	102	-	40,41,41	0.65	0	47,50,50	3.67	16 (34%)
12	LMT	I	101	-	27,27,36	0.47	0	38,38,47	0.80	1 (2%)
14	SPO	J	102	-	40,41,41	0.65	0	47,50,50	1.89	13 (27%)
16	PTY	F	104	-	47,47,49	0.28	0	50,52,54	0.56	1 (2%)
14	SPO	S	102	-	40,41,41	0.64	0	47,50,50	1.72	12 (25%)
8	BPH	M	403	-	51,70,70	0.51	1 (1%)	52,101,101	0.73	0

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
7	BCL	Q	106	-	-	18/37/137/137	-
7	BCL	K	102	-	-	3/37/137/137	-
14	SPO	G	103	-	-	8/47/47/47	-
12	LMT	M	407	-	-	5/17/37/61	0/1/1/2
14	SPO	K	105	-	-	2/47/47/47	-
12	LMT	H	304	-	-	8/21/61/61	0/2/2/2
7	BCL	O	101	-	-	8/37/137/137	-
10	PGV	L	305	-	-	9/43/43/55	-
12	LMT	H	305	-	-	7/16/56/61	0/2/2/2
7	BCL	Y	103	-	-	20/37/137/137	-
7	BCL	N	101	-	-	17/37/137/137	-
14	SPO	S	103	-	-	7/47/47/47	-
14	SPO	B	104	-	-	11/47/47/47	-
14	SPO	F	105	-	-	6/47/47/47	-
12	LMT	L	307	-	-	6/21/61/61	0/2/2/2
10	PGV	K	104	-	-	12/40/42/55	-
7	BCL	J	101	-	-	17/37/137/137	-
11	LDA	H	302	-	-	1/13/13/13	-
14	SPO	D	104	-	-	4/47/47/47	-
7	BCL	G	101	-	-	12/37/137/137	-
8	BPH	L	302	-	-	5/37/105/105	0/5/6/6
12	LMT	A	102	-	-	4/21/61/61	0/2/2/2
14	SPO	M	405	-	-	2/47/47/47	-
9	U10	L	303	-	-	7/30/54/87	0/1/1/1
12	LMT	K	101	-	-	4/21/61/61	0/2/2/2
12	LMT	Q	102	-	-	2/11/31/61	0/1/1/2
12	LMT	F	106	-	-	0/9/29/61	0/1/1/2
7	BCL	B	103	-	-	12/37/137/137	-
7	BCL	T	101	-	-	16/37/137/137	-
12	LMT	H	303	-	-	6/21/61/61	0/2/2/2
14	SPO	O	102	-	-	5/47/47/47	-
12	LMT	D	103	-	-	4/13/53/61	0/2/2/2
14	SPO	V	103	-	-	5/47/47/47	-
7	BCL	I	102	-	-	13/37/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LDA	Y	101	-	-	1/9/9/13	-
14	SPO	B	101	-	-	1/47/47/47	-
12	LMT	I	103	-	-	4/13/53/61	0/2/2/2
7	BCL	V	101	-	-	12/37/137/137	-
7	BCL	D	101	-	-	10/37/137/137	-
12	LMT	Q	101	-	-	3/15/35/61	0/1/1/2
15	CDL	Y	102	-	-	15/40/40/110	-
7	BCL	L	301	-	-	10/37/137/137	-
14	SPO	G	102	-	-	3/47/47/47	-
14	SPO	K	103	-	-	6/47/47/47	-
14	SPO	D	102	-	-	2/47/47/47	-
9	U10	D	105	-	-	20/63/87/87	0/1/1/1
7	BCL	M	401	-	-	12/37/137/137	-
10	PGV	F	103	-	-	12/51/51/55	-
12	LMT	B	102	-	-	1/13/53/61	0/2/2/2
9	U10	M	410	-	-	6/63/87/87	0/1/1/1
16	PTY	H	306	-	-	8/49/49/53	-
15	CDL	H	307	-	-	19/71/71/110	-
9	U10	L	304	-	-	3/21/45/87	0/1/1/1
12	LMT	M	406	-	-	2/19/39/61	0/1/1/2
7	BCL	1	101	-	-	12/37/137/137	-
7	BCL	F	101	-	-	12/37/137/137	-
7	BCL	L	309	-	-	17/37/137/137	-
7	BCL	Q	104	-	-	14/37/137/137	-
14	SPO	Q	105	-	-	2/47/47/47	-
7	BCL	W	101	-	-	12/37/137/137	-
10	PGV	H	301	-	-	12/51/51/55	-
11	LDA	L	306	-	-	2/13/13/13	-
11	LDA	X	101	-	-	0/10/10/13	-
10	PGV	M	409	-	-	20/42/42/55	-
10	PGV	F	102	-	-	11/44/44/55	-
10	PGV	Y	104	-	-	8/47/47/55	-
14	SPO	V	102	-	-	5/47/47/47	-
7	BCL	A	103	-	-	13/31/131/137	-
10	PGV	Q	103	-	-	10/43/43/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BCL	P	101	-	-	15/37/137/137	-
7	BCL	M	402	-	-	3/37/137/137	-
12	LMT	L	308	-	-	6/20/60/61	0/2/2/2
14	SPO	Z	101	-	-	5/47/47/47	-
7	BCL	Z	102	-	-	14/37/137/137	-
12	LMT	A	101	-	-	6/21/61/61	0/2/2/2
7	BCL	E	101	-	-	14/37/137/137	-
15	CDL	M	408	-	-	26/89/89/110	-
7	BCL	S	101	-	-	12/37/137/137	-
14	SPO	P	102	-	-	14/47/47/47	-
12	LMT	I	101	-	-	3/11/51/61	0/2/2/2
14	SPO	J	102	-	-	9/47/47/47	-
16	PTY	F	104	-	-	10/51/51/53	-
14	SPO	S	102	-	-	2/47/47/47	-
8	BPH	M	403	-	-	7/37/105/105	0/5/6/6

The worst 5 of 379 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	X	101	LDA	O1-N1	-7.19	1.25	1.42
11	L	306	LDA	O1-N1	-7.18	1.25	1.42
11	H	302	LDA	O1-N1	-7.16	1.25	1.42
11	Y	101	LDA	O1-N1	-7.12	1.25	1.42
7	Z	102	BCL	C3B-C2B	5.38	1.49	1.39

The worst 5 of 806 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	P	102	SPO	C2-C1-C4	-16.52	85.50	110.86
14	P	102	SPO	C3-C1-C4	-13.75	89.74	110.86
7	Z	102	BCL	CHD-C1D-ND	-8.71	116.45	124.45
7	Y	103	BCL	CHD-C1D-ND	-8.68	116.48	124.45
7	1	101	BCL	CHD-C1D-ND	-8.52	116.62	124.45

There are no chirality outliers.

5 of 712 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	L	301	BCL	C2-C3-C5-C6
7	A	103	BCL	C1A-C2A-CAA-CBA
7	A	103	BCL	C3A-C2A-CAA-CBA
7	A	103	BCL	C2C-C3C-CAC-CBC
7	A	103	BCL	C4C-C3C-CAC-CBC

There are no ring outliers.

76 monomers are involved in 305 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Q	106	BCL	10	0
7	K	102	BCL	7	0
14	G	103	SPO	3	0
12	M	407	LMT	1	0
14	K	105	SPO	7	0
12	H	304	LMT	4	0
7	O	101	BCL	5	0
10	L	305	PGV	2	0
12	H	305	LMT	4	0
7	Y	103	BCL	7	0
7	N	101	BCL	7	0
14	S	103	SPO	3	0
14	B	104	SPO	7	0
14	F	105	SPO	6	0
10	K	104	PGV	2	0
7	J	101	BCL	5	0
11	H	302	LDA	1	0
14	D	104	SPO	4	0
7	G	101	BCL	3	0
8	L	302	BPH	3	0
12	A	102	LMT	3	0
14	M	405	SPO	5	0
9	L	303	U10	3	0
12	K	101	LMT	4	0
12	Q	102	LMT	3	0
7	B	103	BCL	4	0
7	T	101	BCL	8	0
12	H	303	LMT	2	0
14	O	102	SPO	4	0
12	D	103	LMT	1	0
14	V	103	SPO	2	0
7	I	102	BCL	4	0
11	Y	101	LDA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	101	SPO	4	0
7	V	101	BCL	7	0
7	D	101	BCL	12	0
15	Y	102	CDL	2	0
7	L	301	BCL	2	0
14	G	102	SPO	8	0
14	K	103	SPO	4	0
14	D	102	SPO	4	0
9	D	105	U10	11	0
7	M	401	BCL	4	0
10	F	103	PGV	4	0
9	M	410	U10	5	0
16	H	306	PTY	6	0
15	H	307	CDL	5	0
9	L	304	U10	1	0
7	1	101	BCL	9	0
7	F	101	BCL	9	0
7	L	309	BCL	3	0
7	Q	104	BCL	10	0
14	Q	105	SPO	5	0
7	W	101	BCL	5	0
10	H	301	PGV	1	0
10	M	409	PGV	4	0
10	F	102	PGV	2	0
10	Y	104	PGV	3	0
14	V	102	SPO	8	0
7	A	103	BCL	5	0
10	Q	103	PGV	2	0
7	P	101	BCL	6	0
7	M	402	BCL	4	0
12	L	308	LMT	2	0
14	Z	101	SPO	11	0
7	Z	102	BCL	5	0
12	A	101	LMT	1	0
7	E	101	BCL	2	0
15	M	408	CDL	5	0
7	S	101	BCL	7	0
14	P	102	SPO	8	0
12	I	101	LMT	3	0
14	J	102	SPO	6	0
16	F	104	PTY	4	0
14	S	102	SPO	7	0

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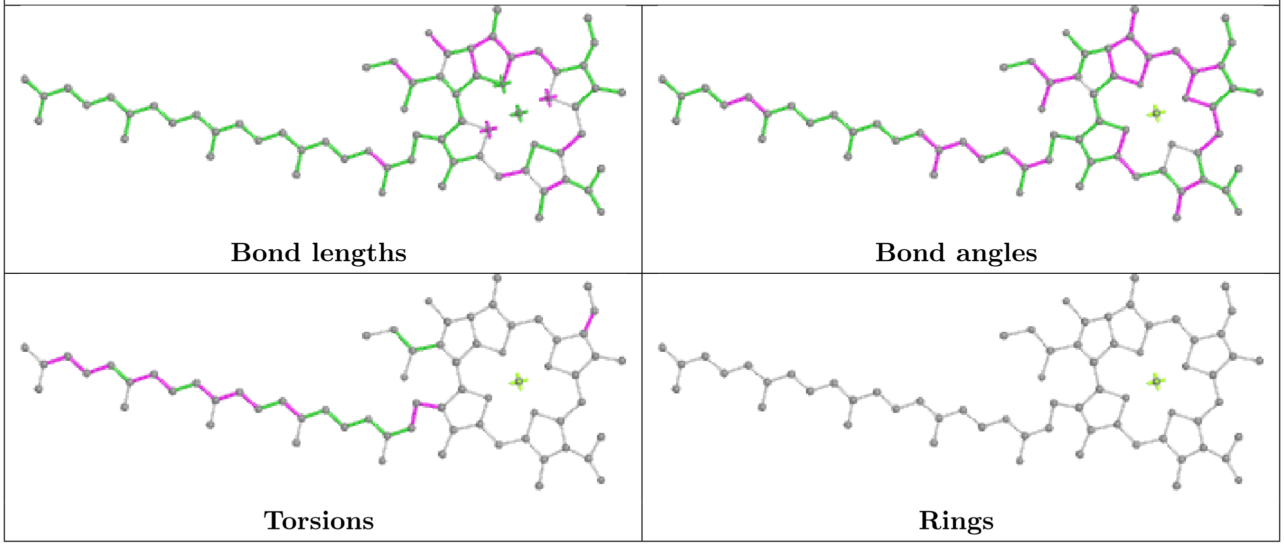
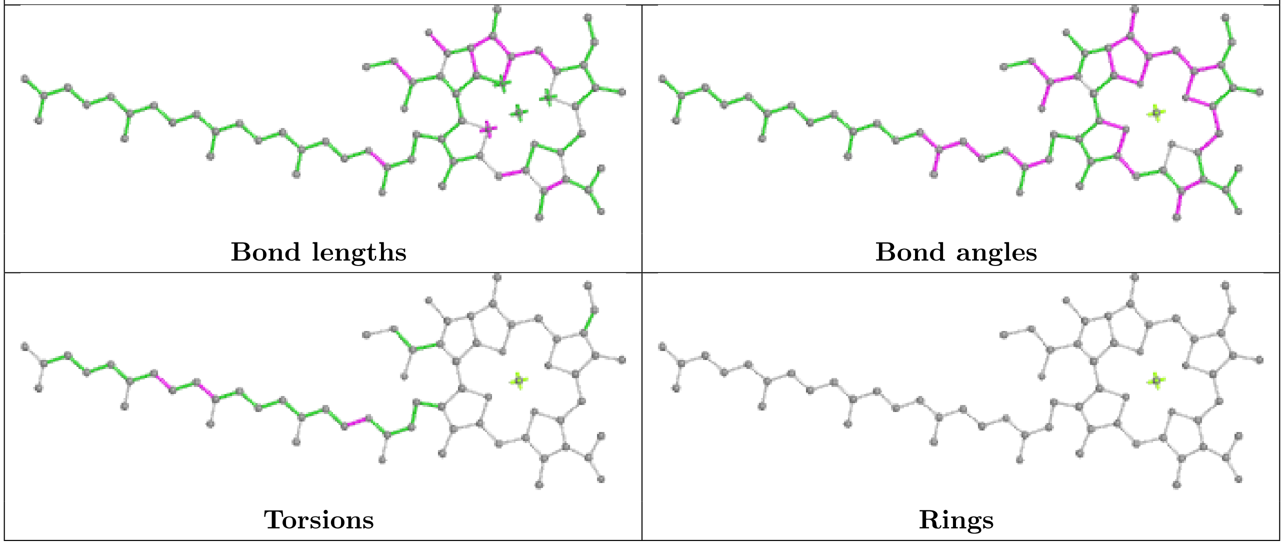
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	M	403	BPH	8	0

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 BCL Q 106



Ligand BCL K 102



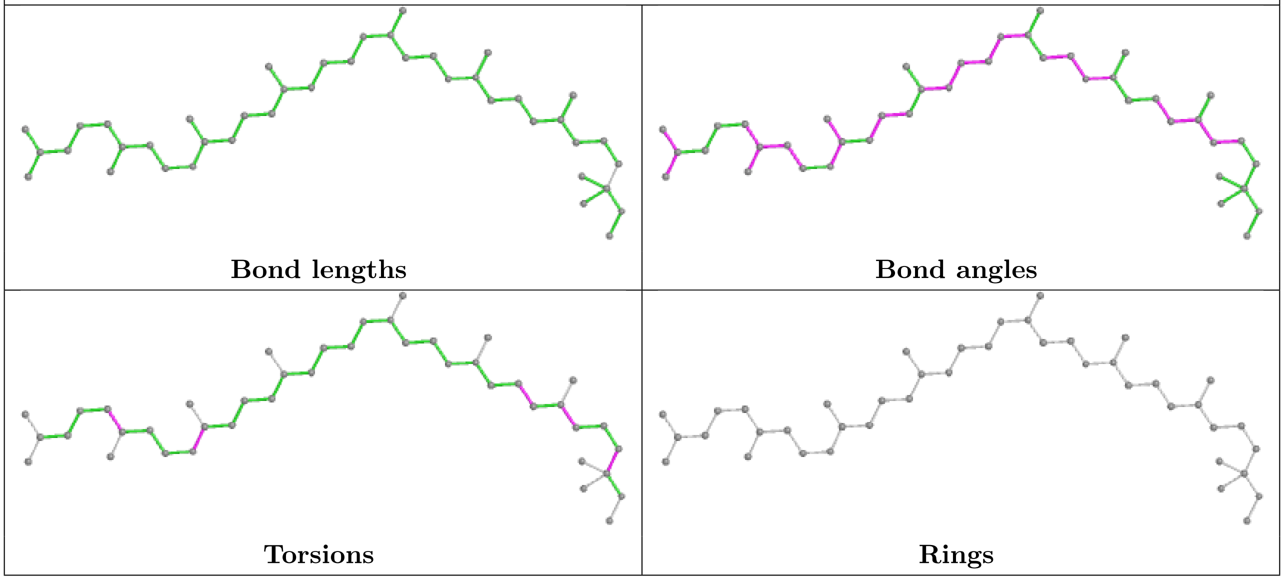
Bond lengths

Bond angles

Torsions

Rings

Ligand SPO G 103



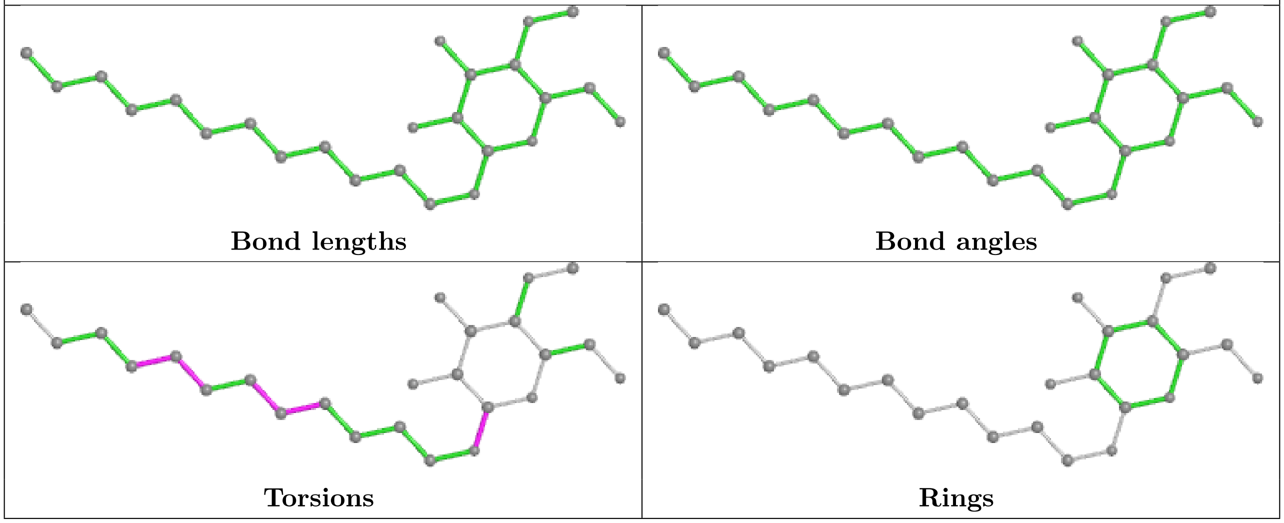
Bond lengths

Bond angles

Torsions

Rings

Ligand LMT M 407



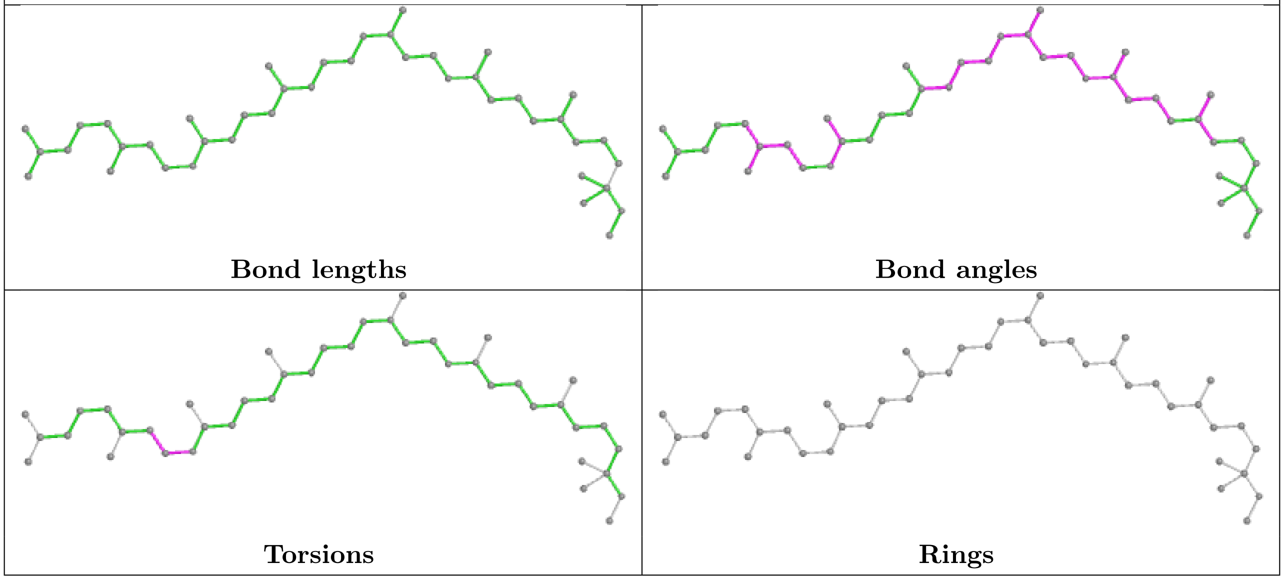
Bond lengths

Bond angles

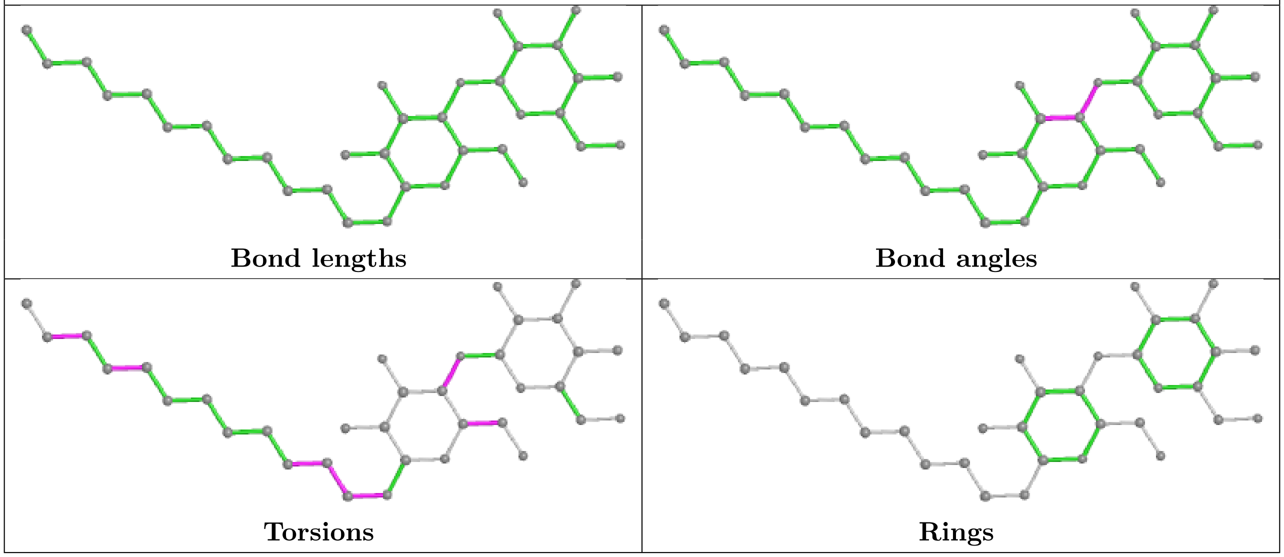
Torsions

Rings

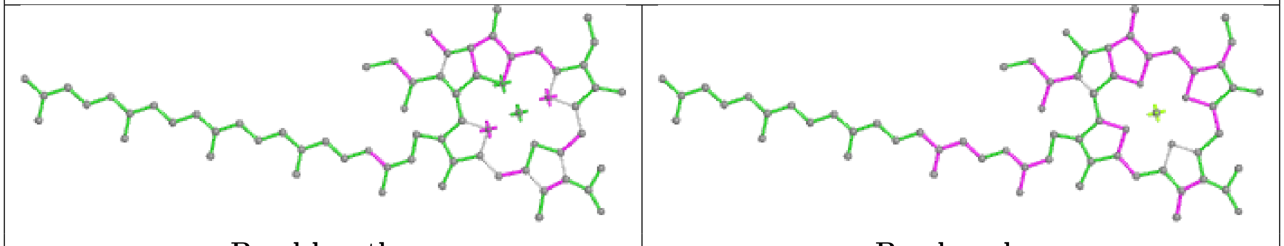
Ligand SPO K 105



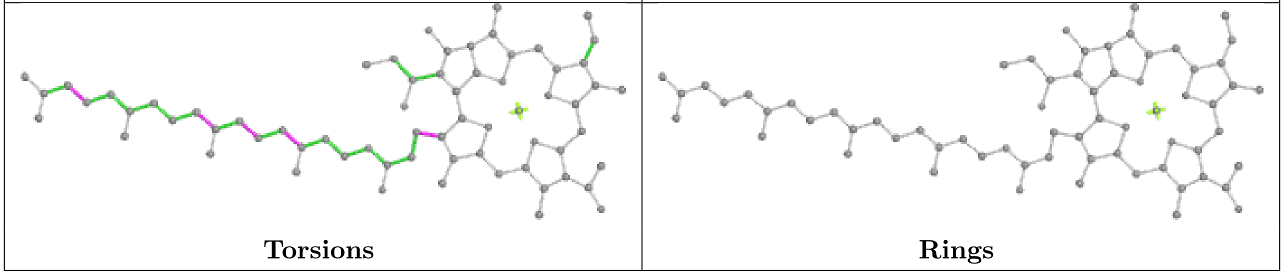
Ligand LMT H 304



Ligand BCL O 101

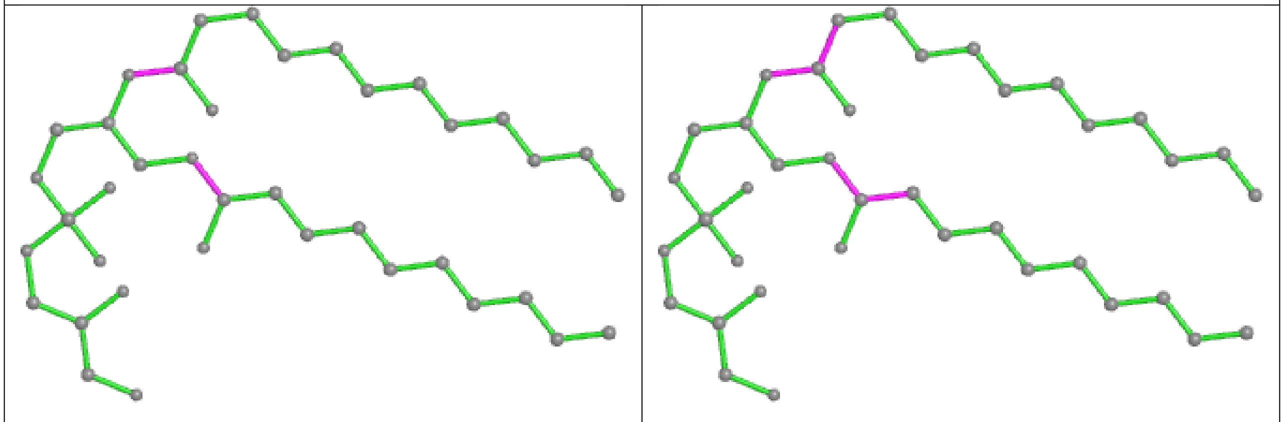

Bond lengths

Bond angles

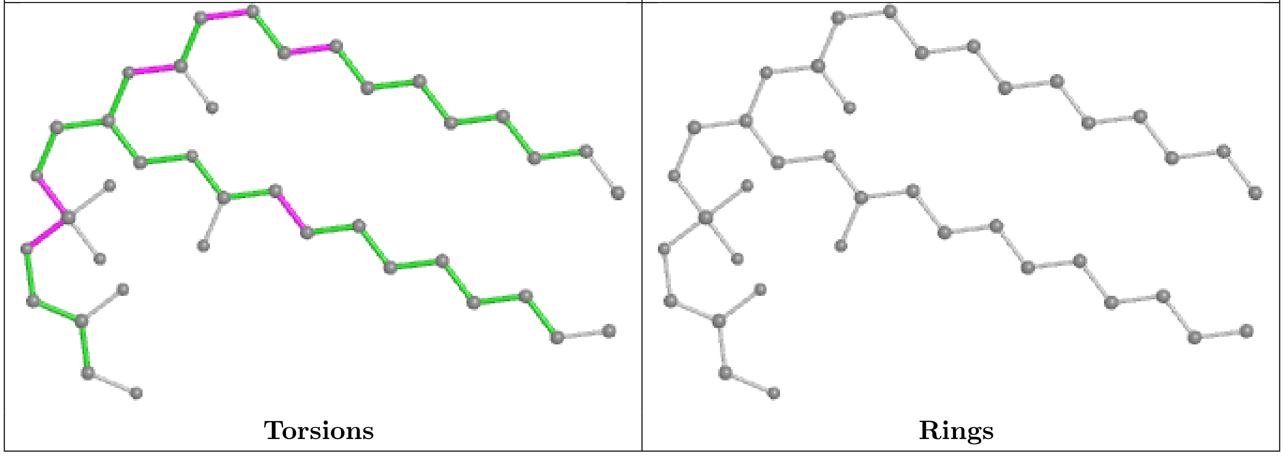

Torsions

Rings

Ligand PGV L 305

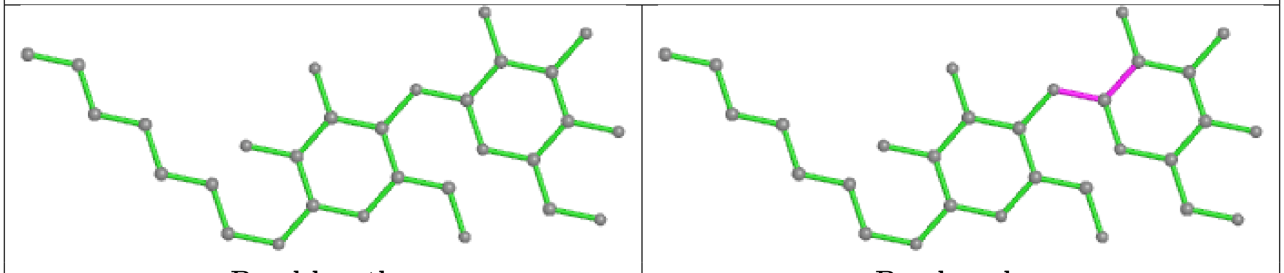

Bond lengths

Bond angles


Torsions

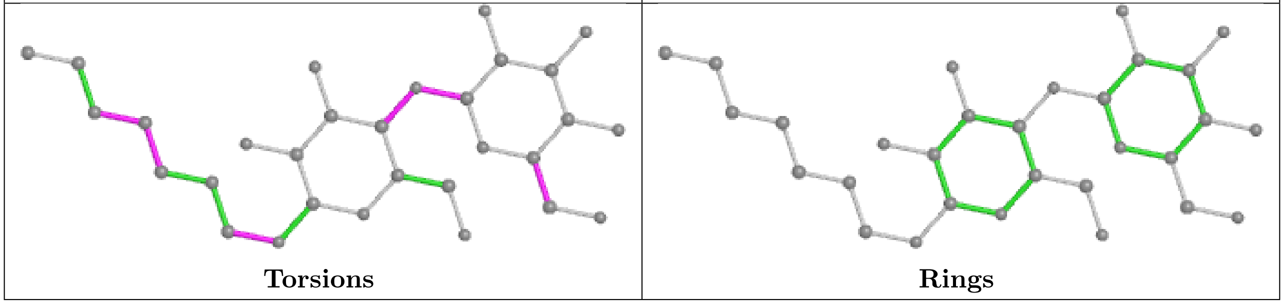
Rings

Ligand LMT H 305



Bond lengths

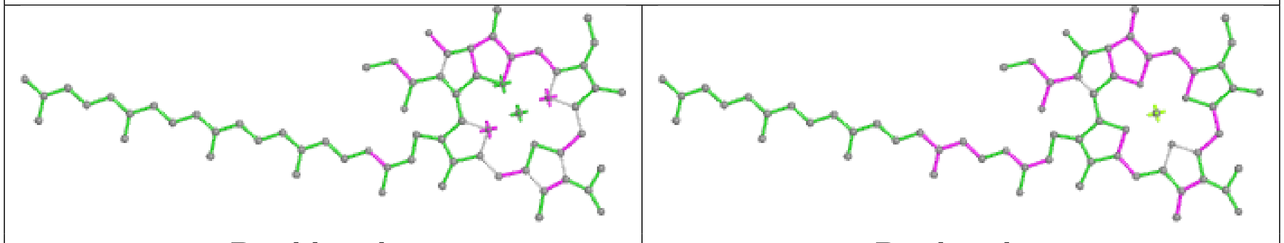
Bond angles



Torsions

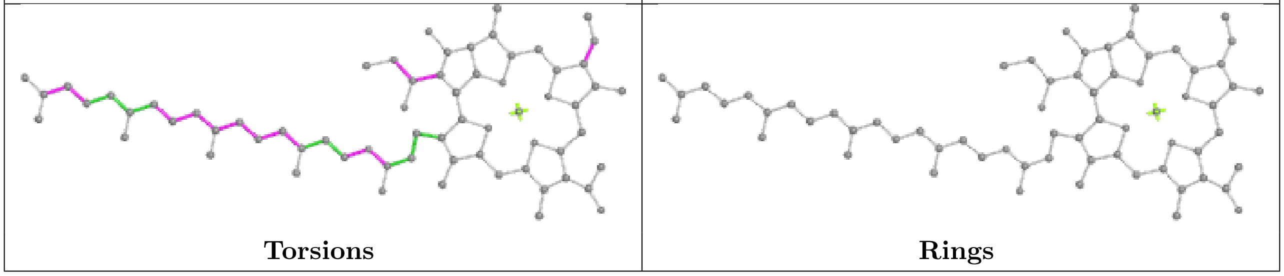
Rings

Ligand BCL Y 103



Bond lengths

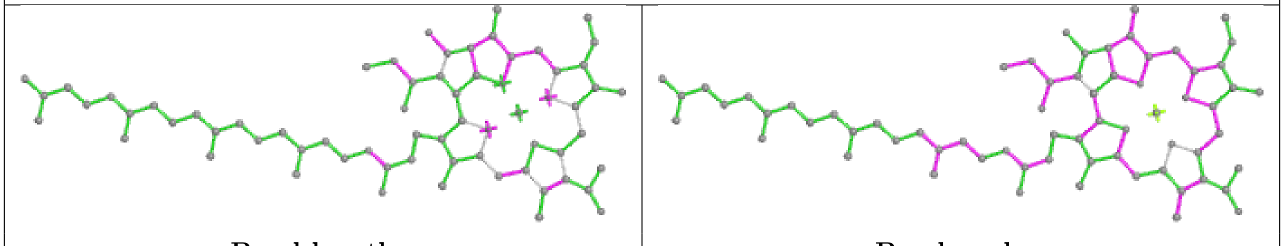
Bond angles



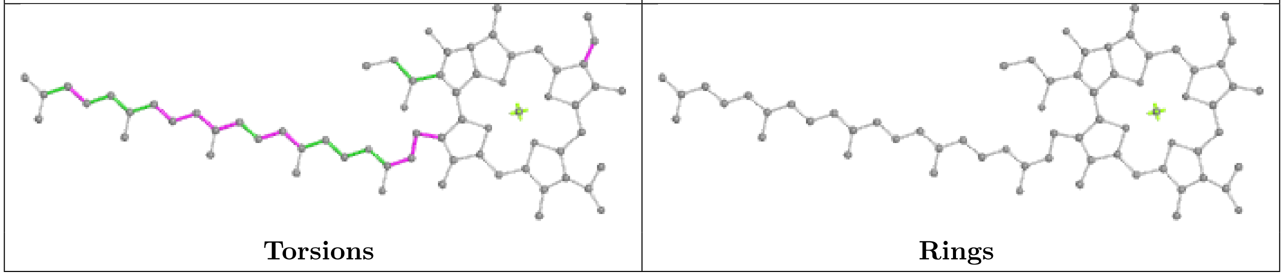
Torsions

Rings

Ligand BCL N 101



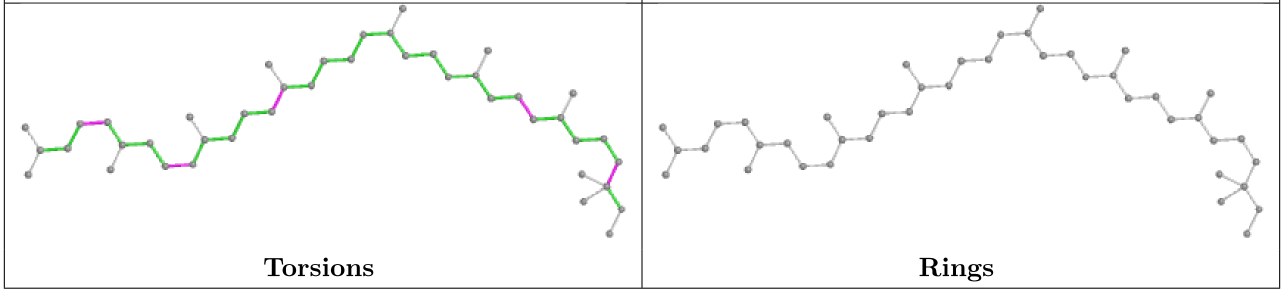
Bond lengths Bond angles



Torsions Rings

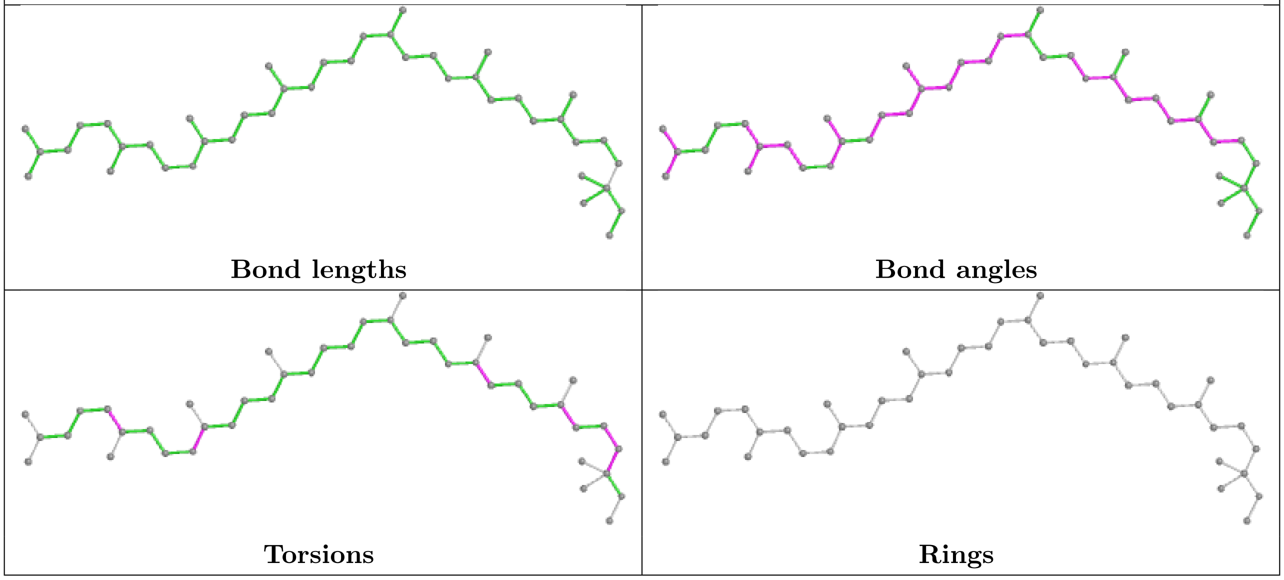
Ligand SPO S 103

Bond lengths Bond angles



Torsions Rings

Ligand SPO B 104



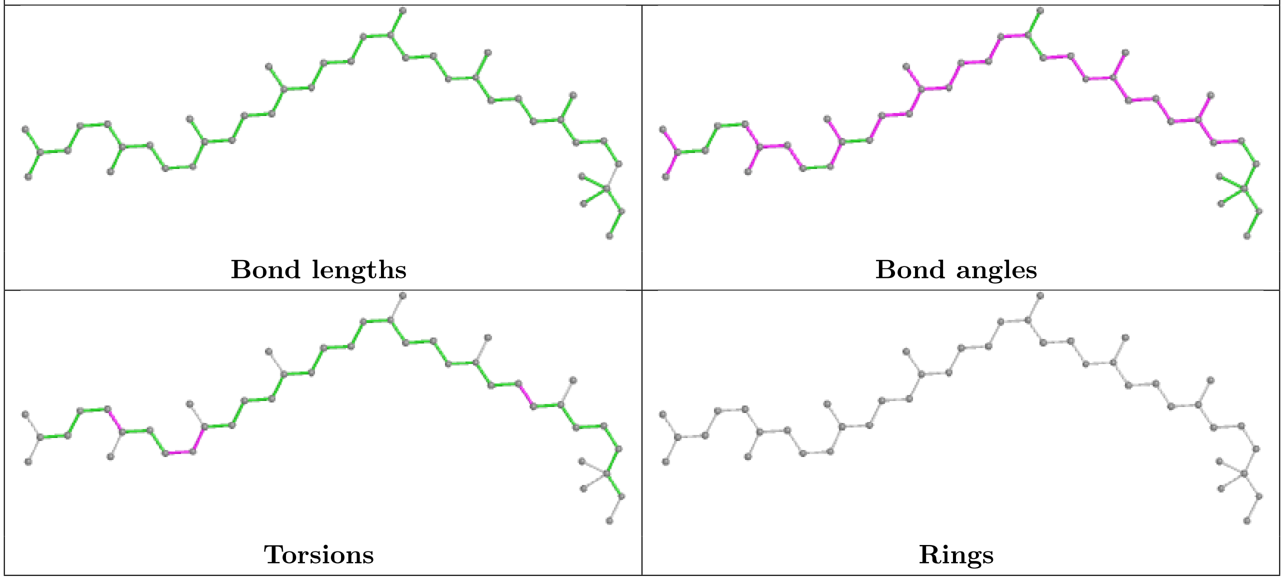
Bond lengths

Bond angles

Torsions

Rings

Ligand SPO F 105



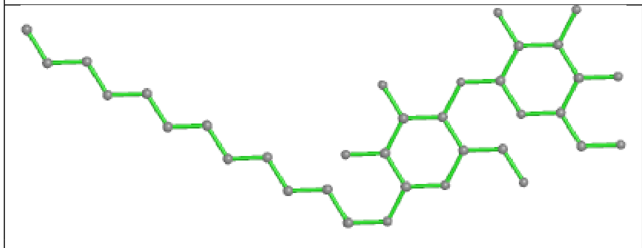
Bond lengths

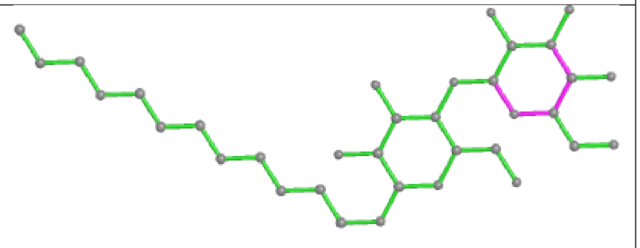
Bond angles

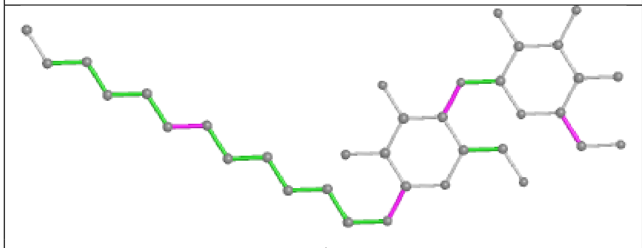
Torsions

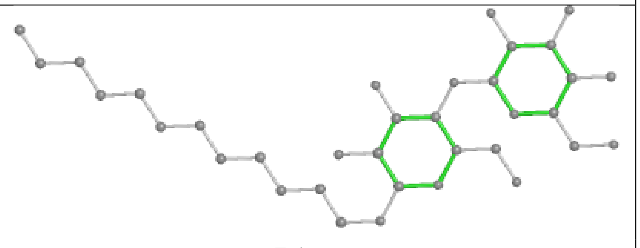
Rings

Ligand LMT L 307

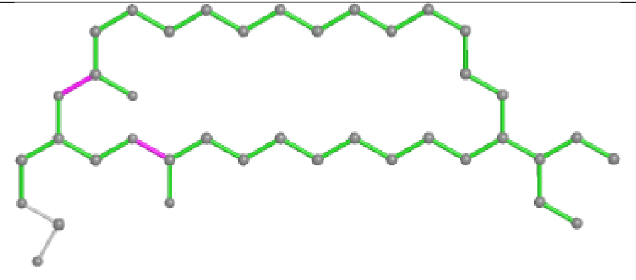

Bond lengths

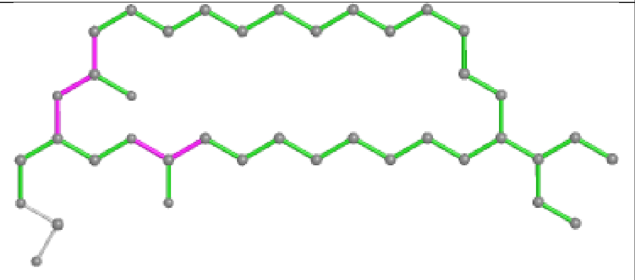

Bond angles

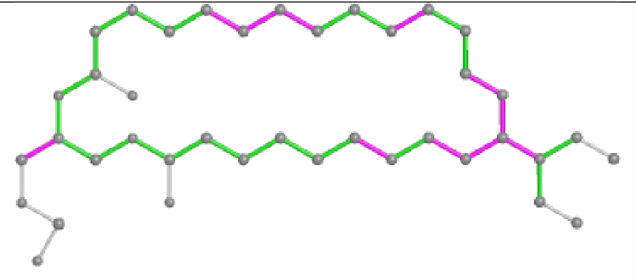

Torsions

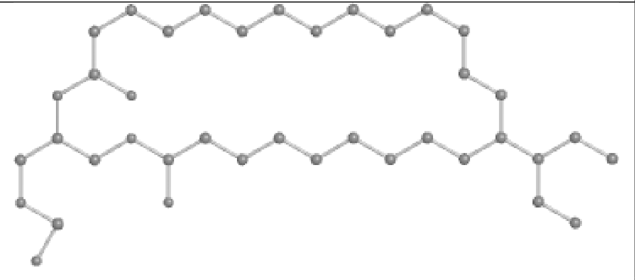

Rings

Ligand PGV K 104

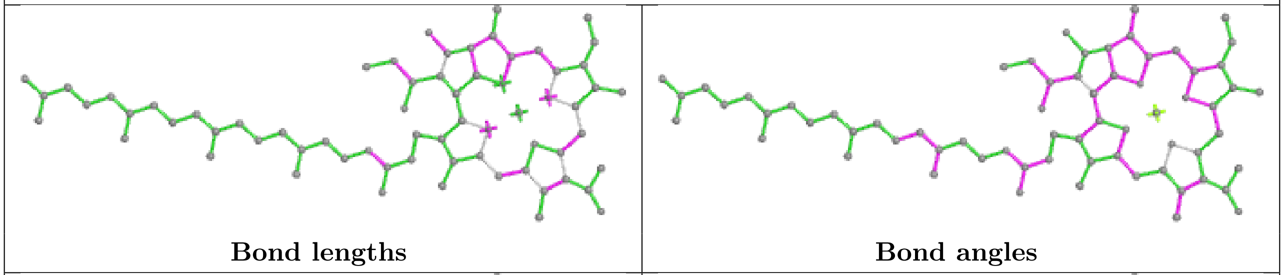

Bond lengths


Bond angles

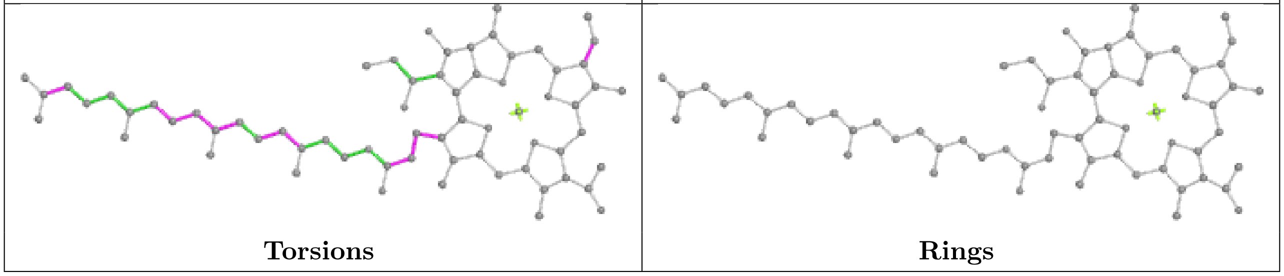

Torsions


Rings

Ligand BCL J 101

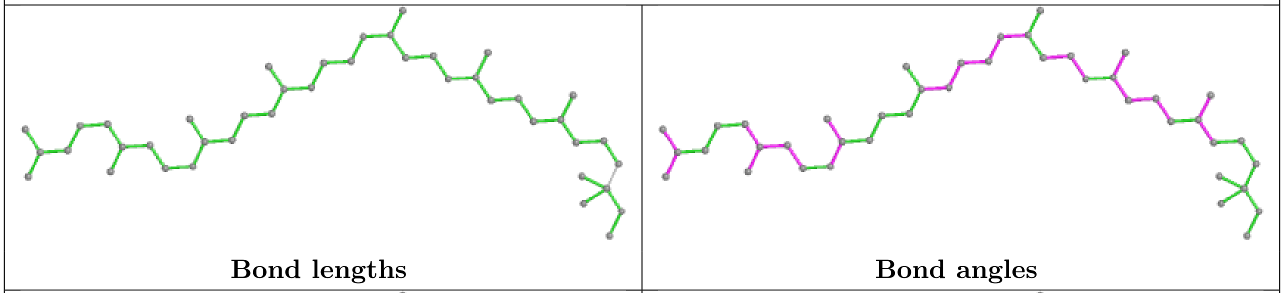


Bond lengths Bond angles

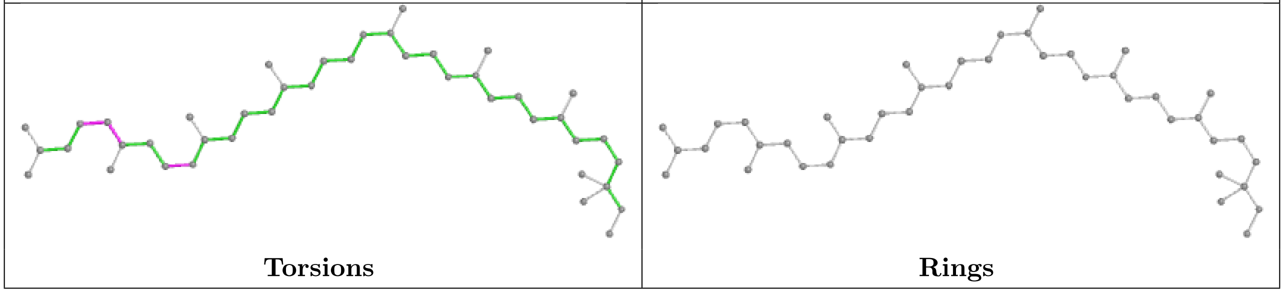


Torsions Rings

Ligand SPO D 104

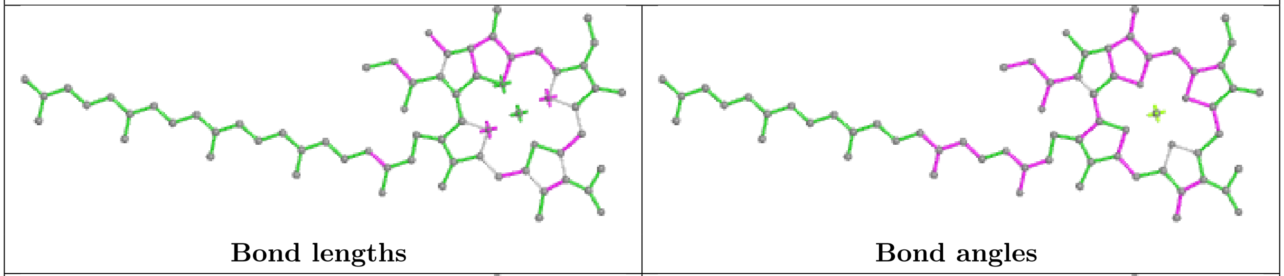


Bond lengths Bond angles

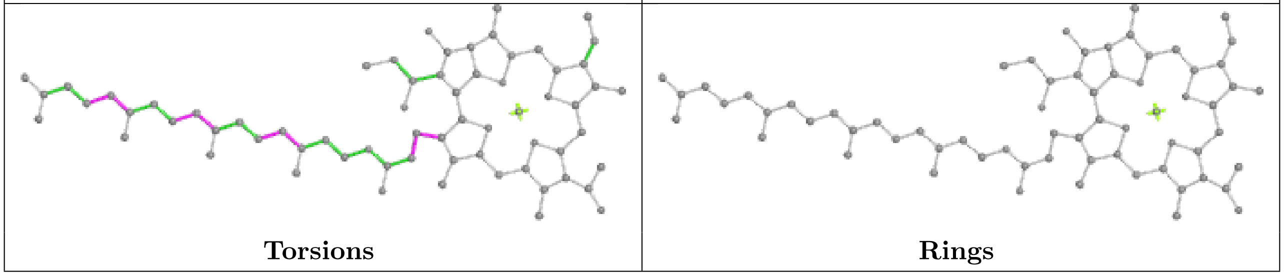


Torsions Rings

Ligand BCL G 101

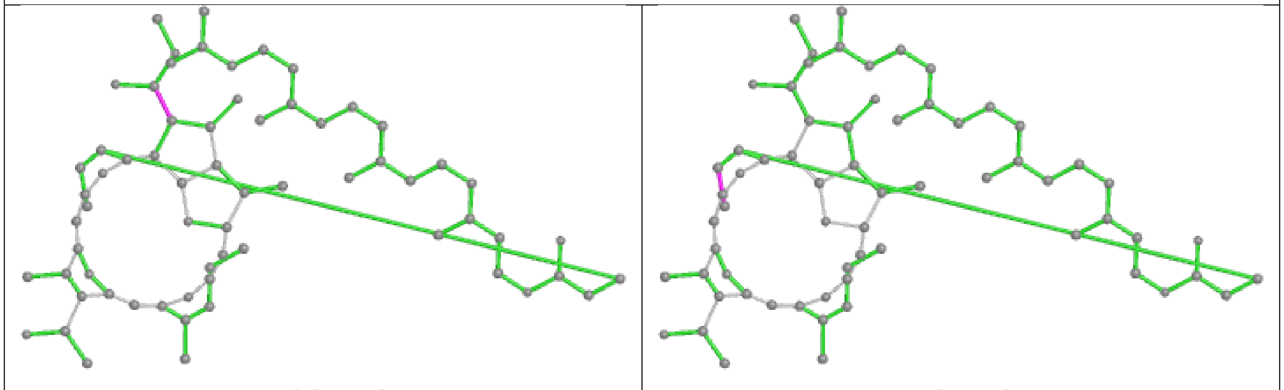


Bond lengths Bond angles



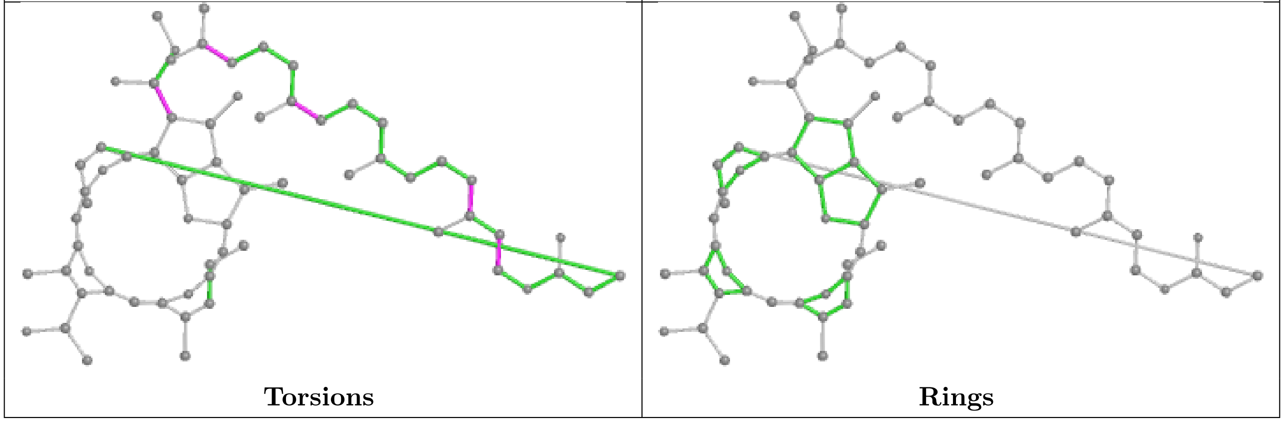
Torsions Rings

Ligand BPH L 302



Bond lengths

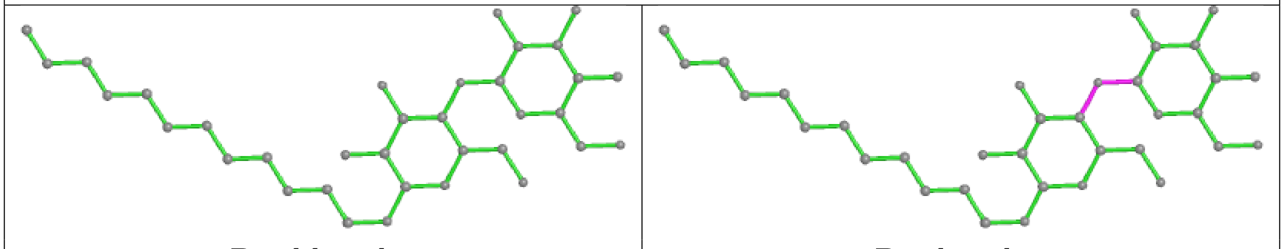
Bond angles



Torsions

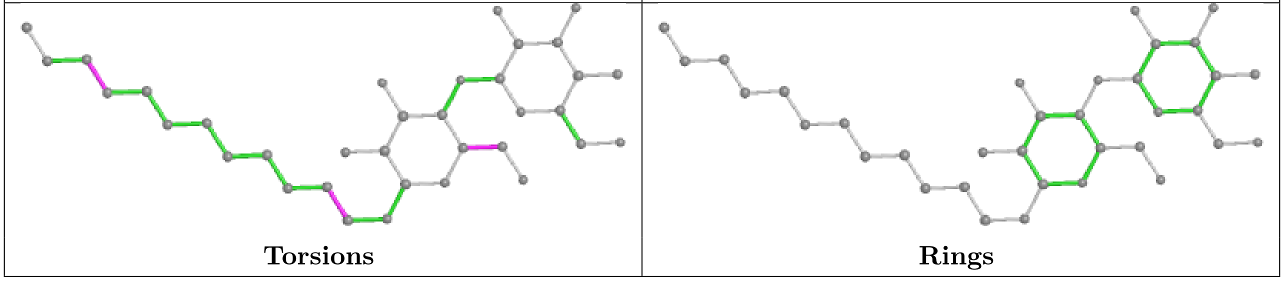
Rings

Ligand LMT A 102



Bond lengths

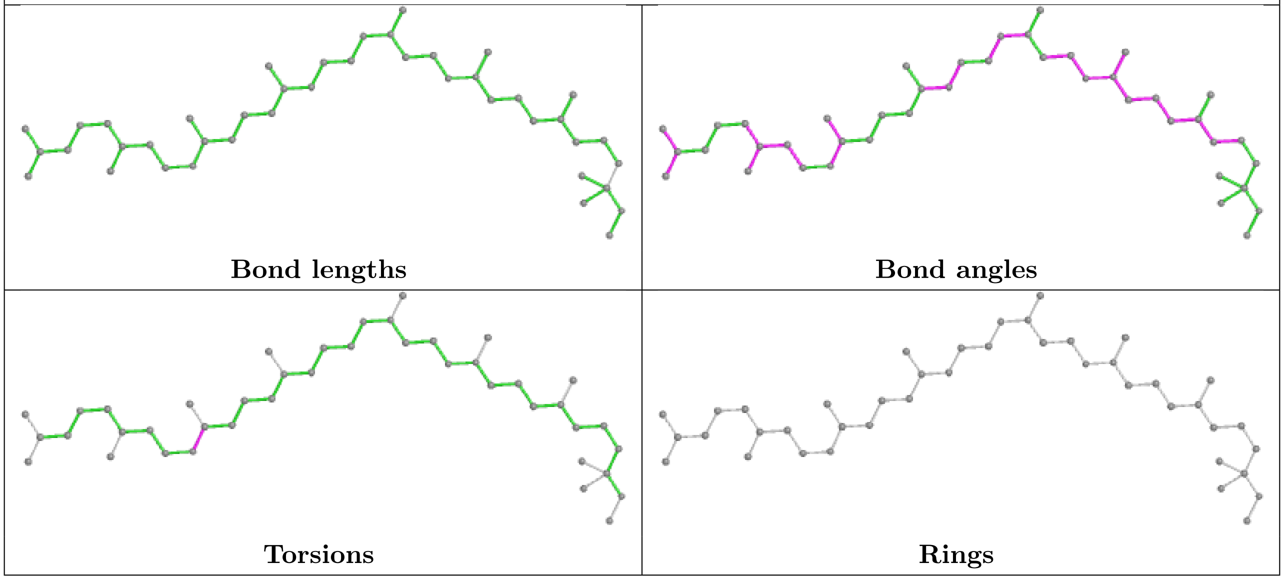
Bond angles



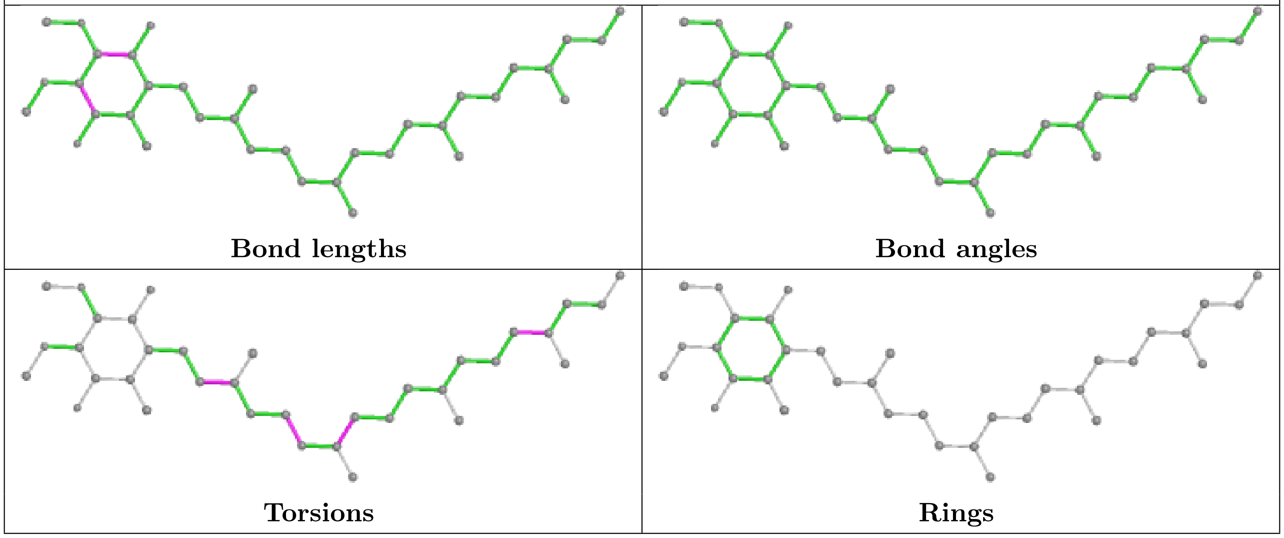
Torsions

Rings

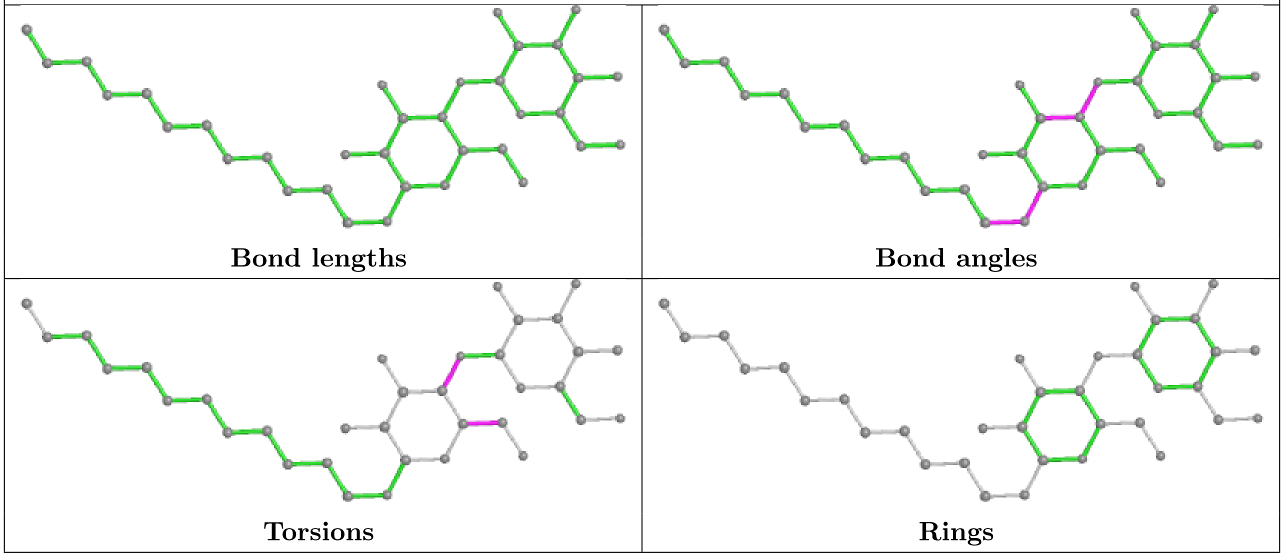
Ligand SPO M 405



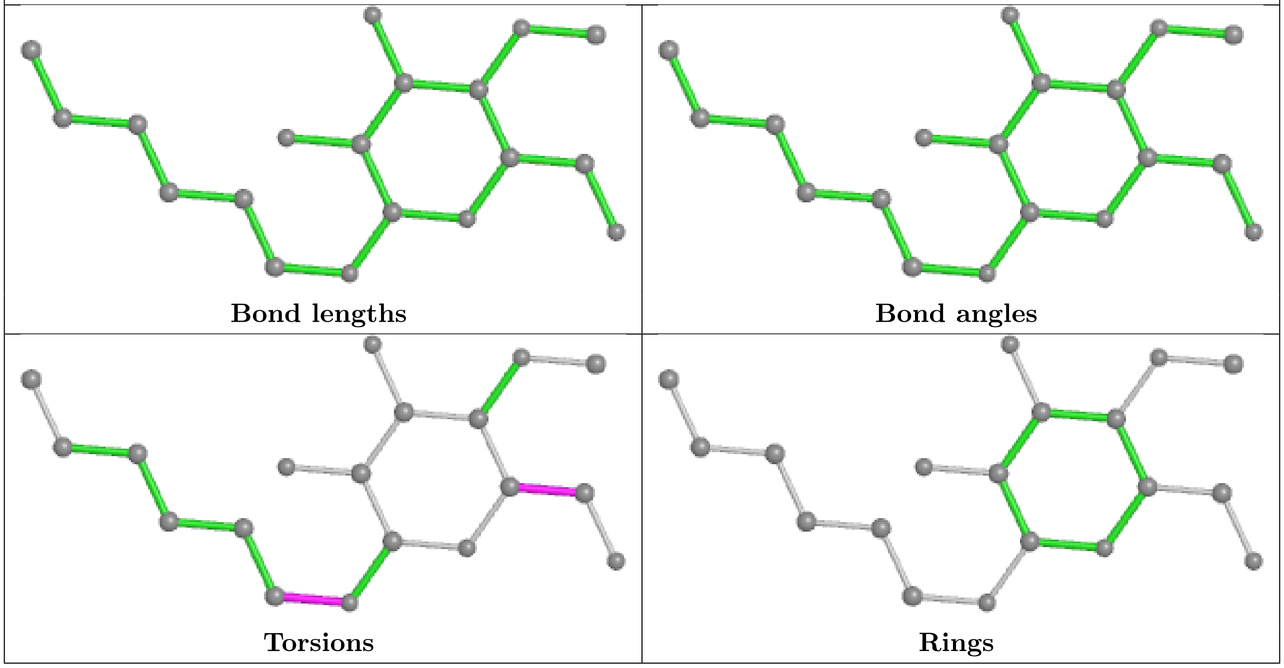
Ligand U10 L 303



Ligand LMT K 101



Ligand LMT Q 102



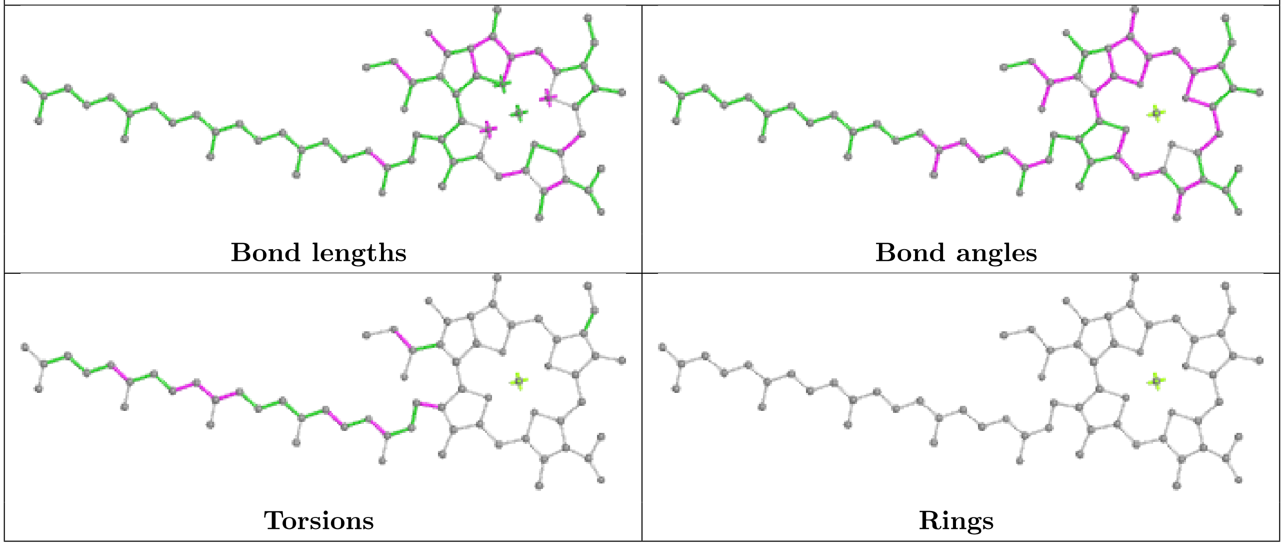
Bond lengths

Bond angles

Torsions

Rings

Ligand BCL B 103



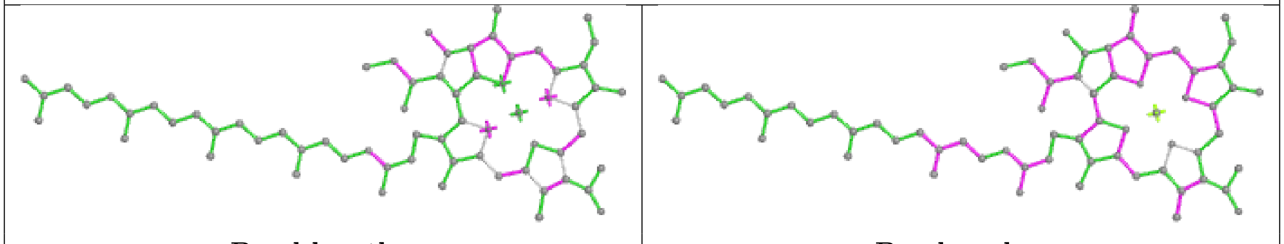
Bond lengths

Bond angles

Torsions

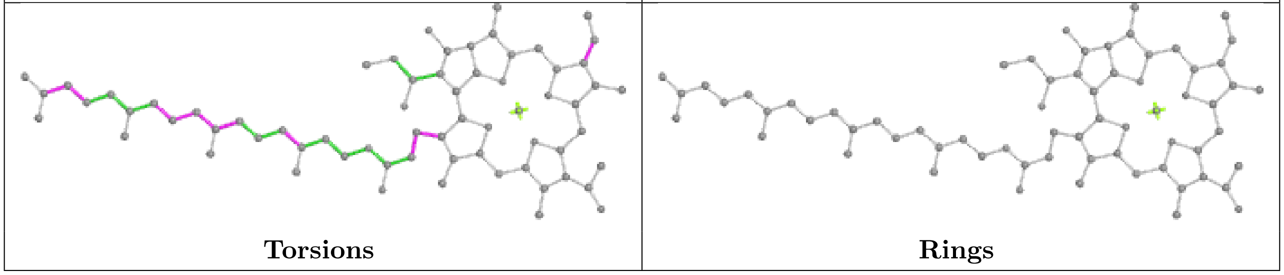
Rings

Ligand BCL T 101



Bond lengths

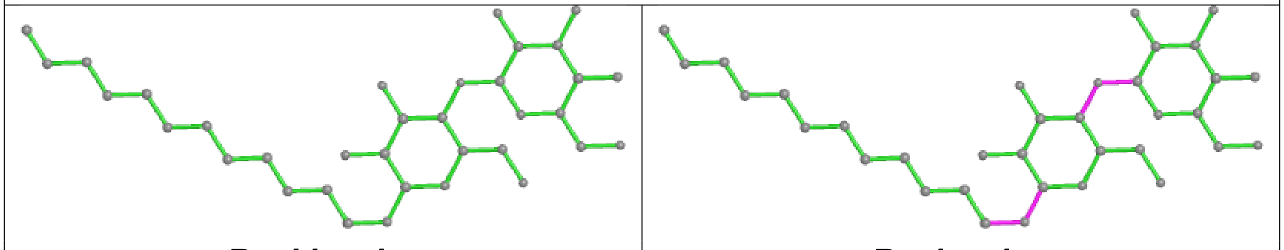
Bond angles



Torsions

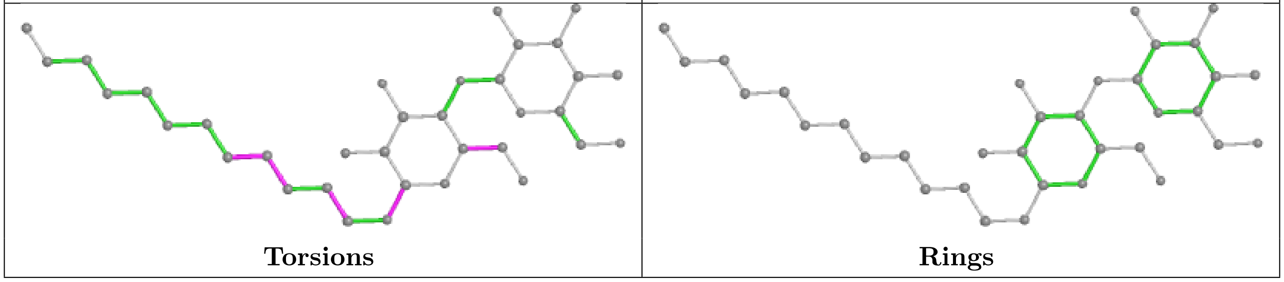
Rings

Ligand LMT H 303



Bond lengths

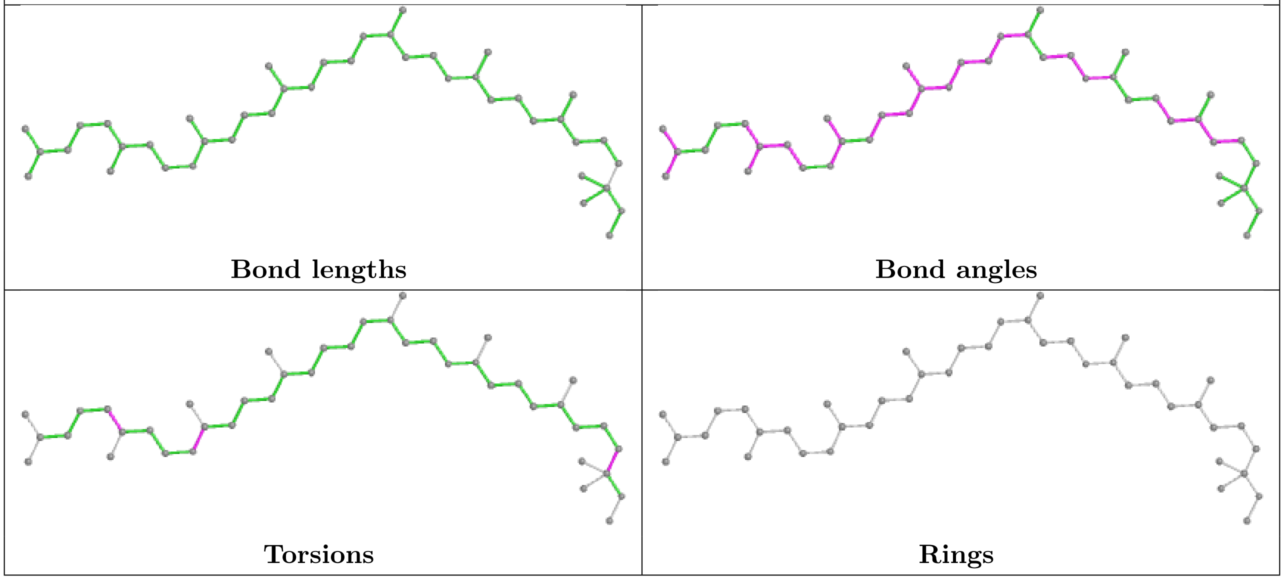
Bond angles



Torsions

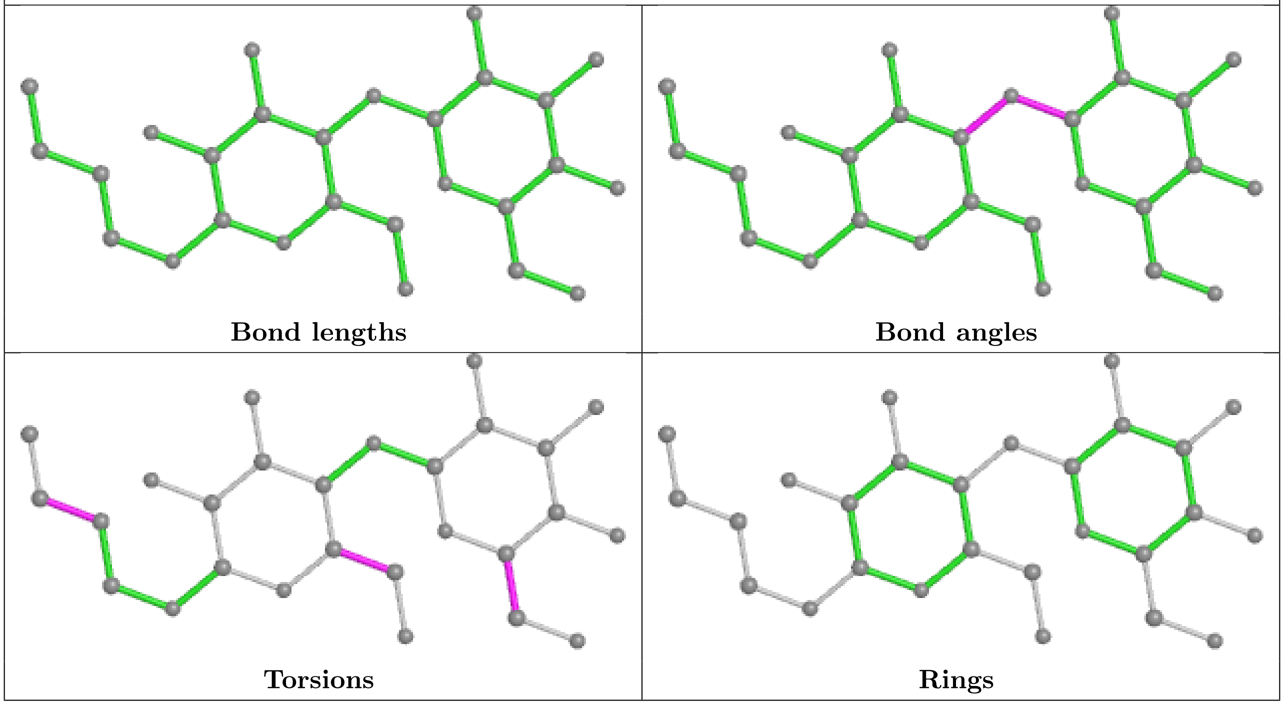
Rings

Ligand SPO O 102


Bond lengths Bond angles

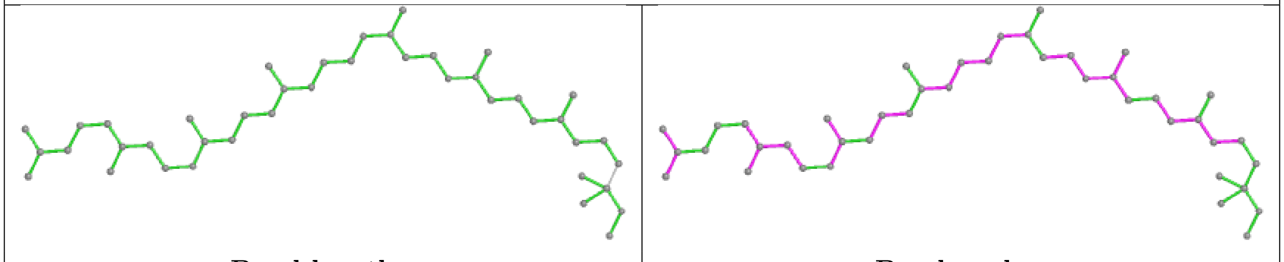
Torsions Rings

Ligand LMT D 103


Bond lengths Bond angles

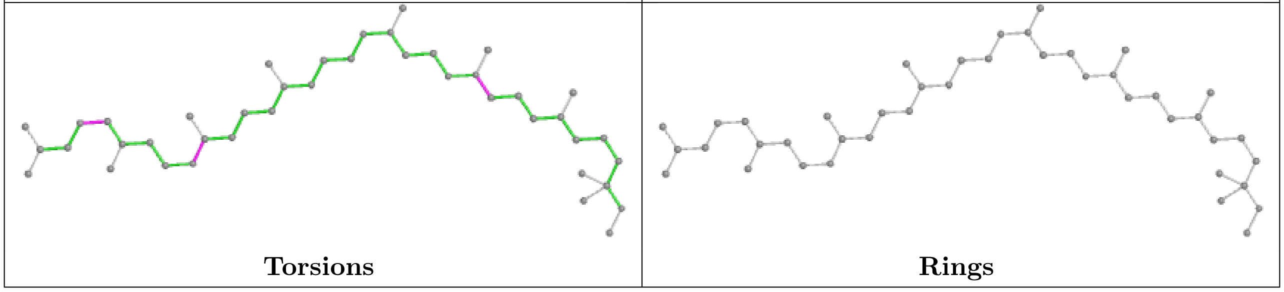
Torsions Rings

Ligand SPO V 103



Bond lengths

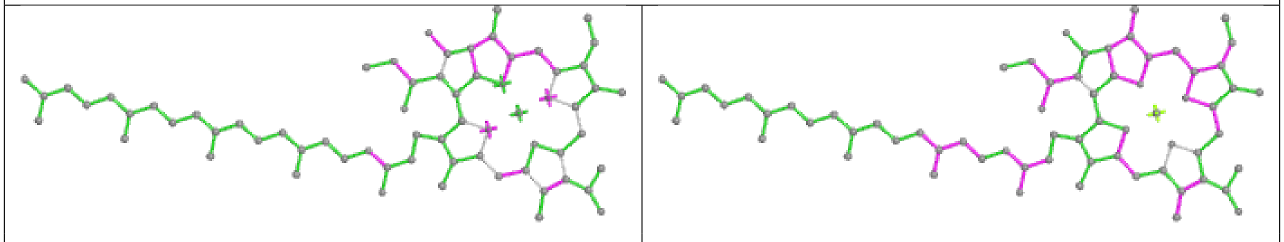
Bond angles



Torsions

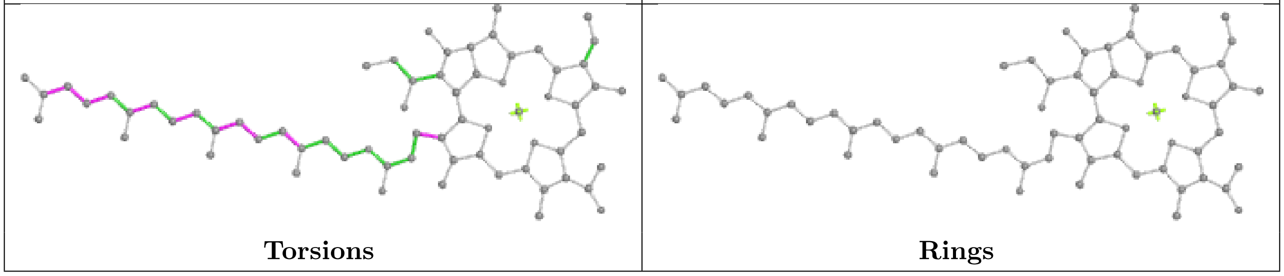
Rings

Ligand BCL I 102



Bond lengths

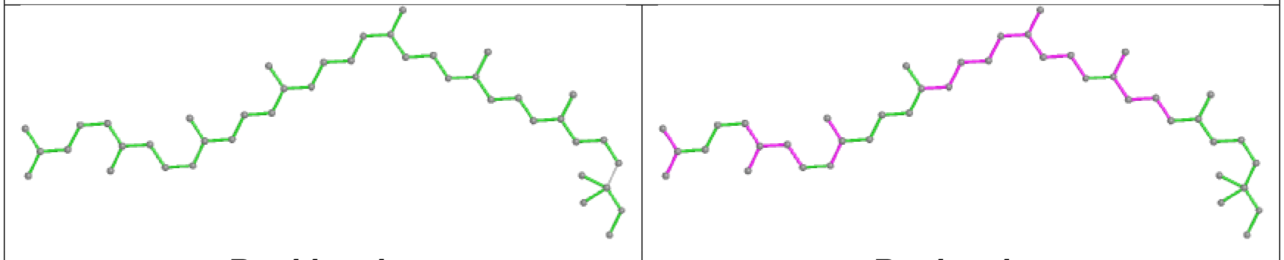
Bond angles



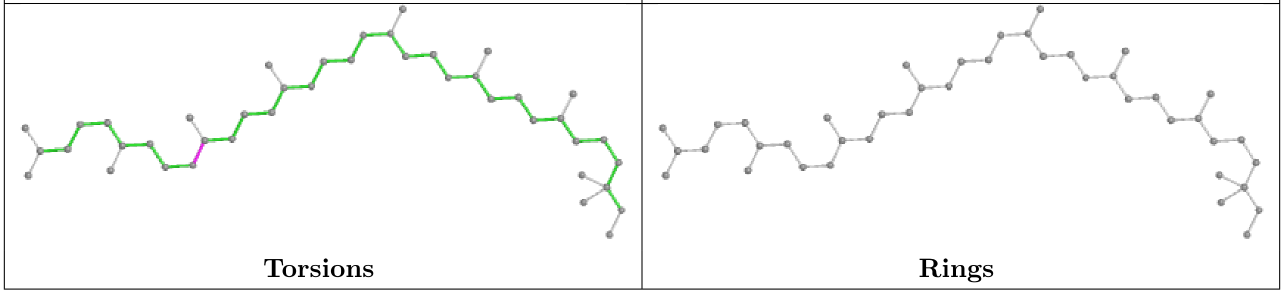
Torsions

Rings

Ligand SPO B 101

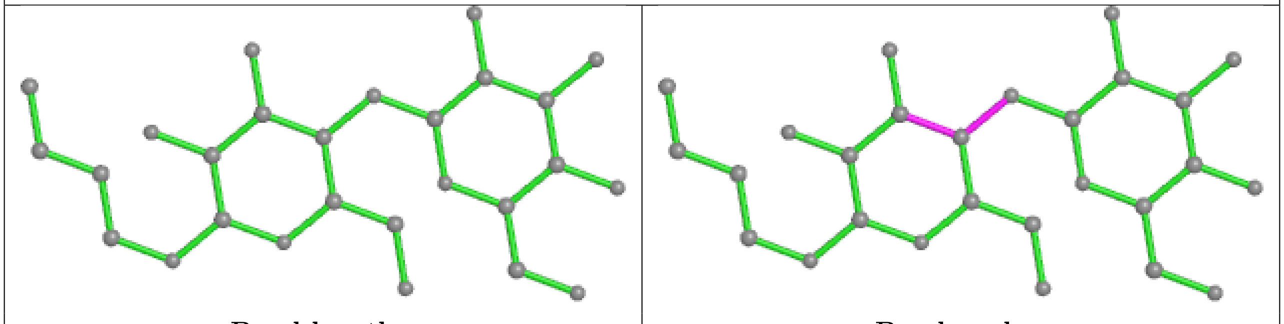


Bond lengths Bond angles

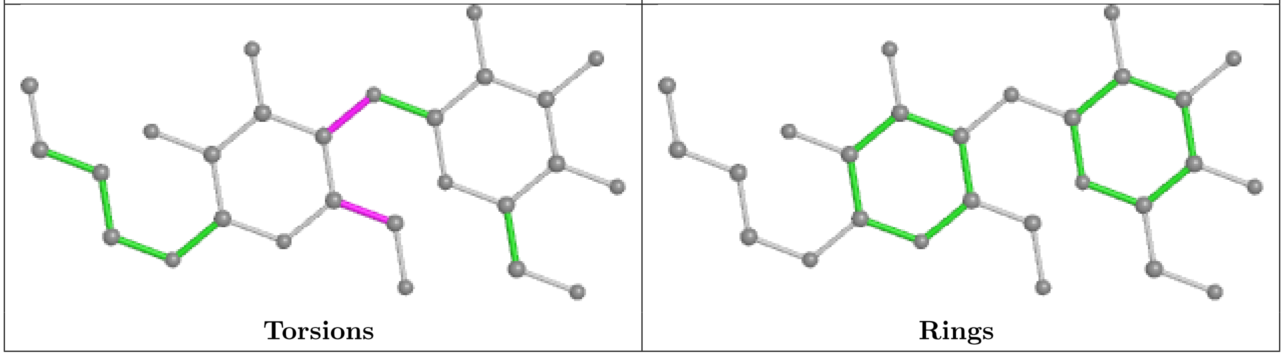


Torsions Rings

Ligand LMT I 103

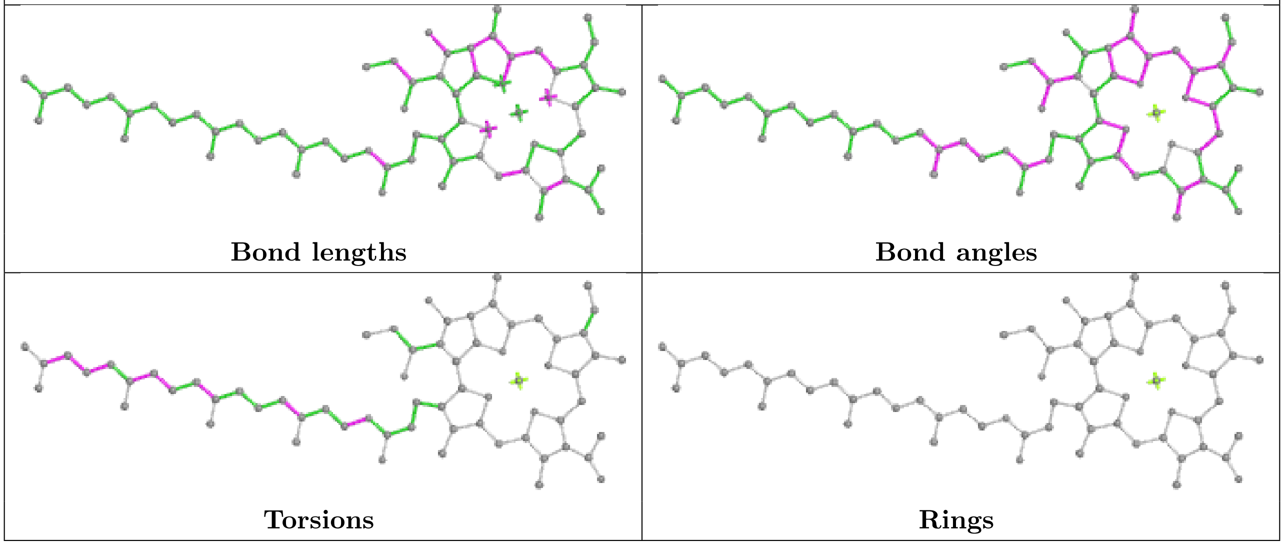


Bond lengths Bond angles

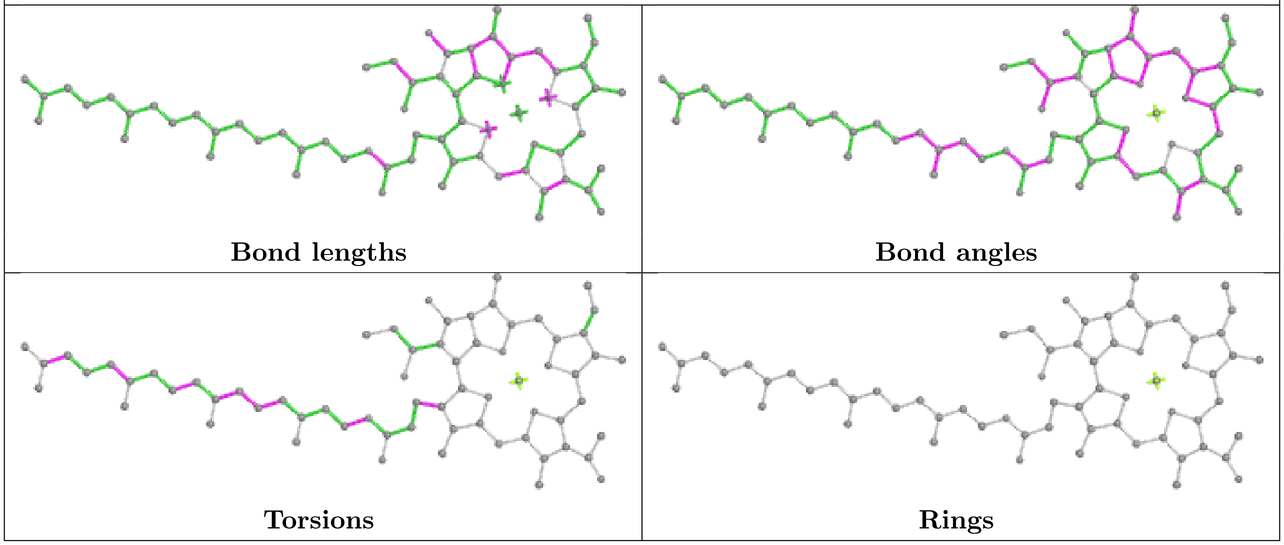


Torsions Rings

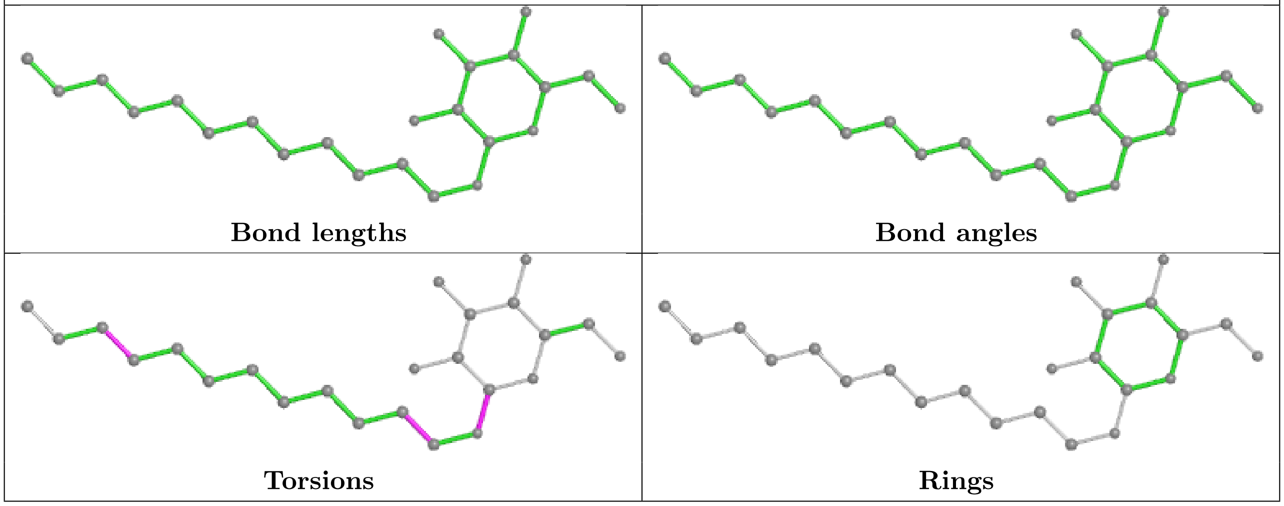
Ligand BCL V 101



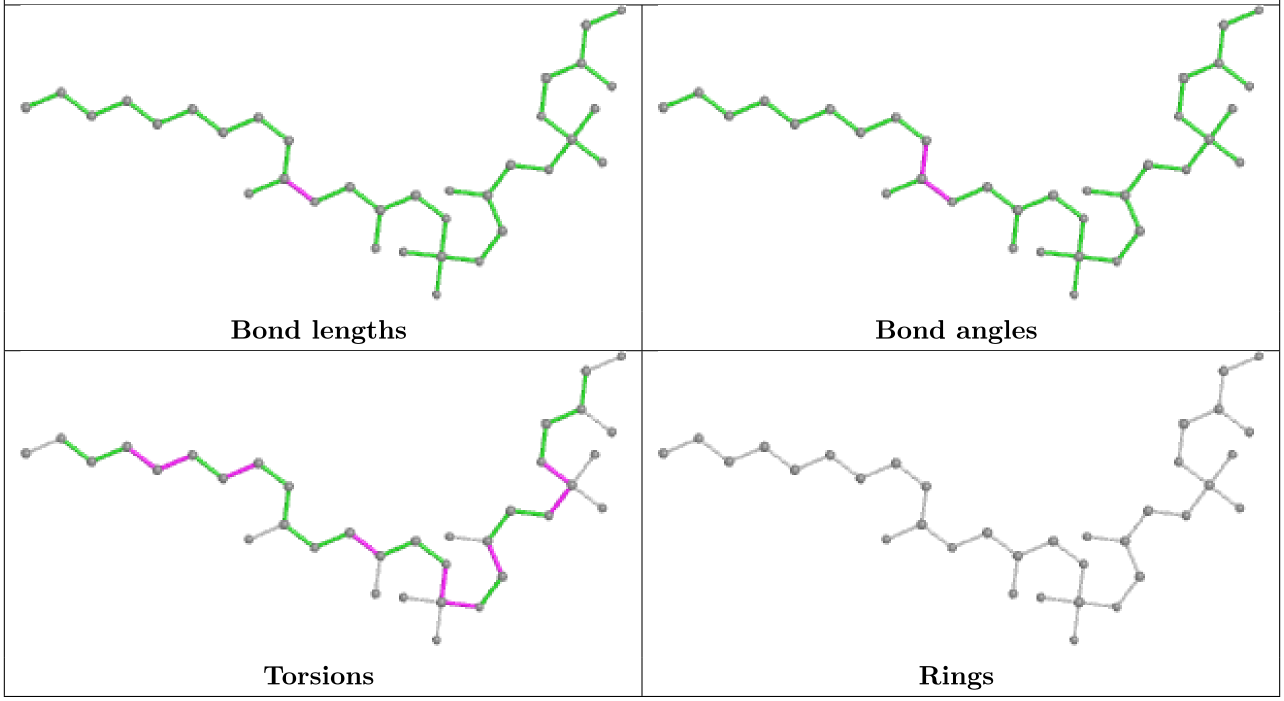
Ligand BCL D 101



Ligand LMT Q 101



Ligand CDL Y 102



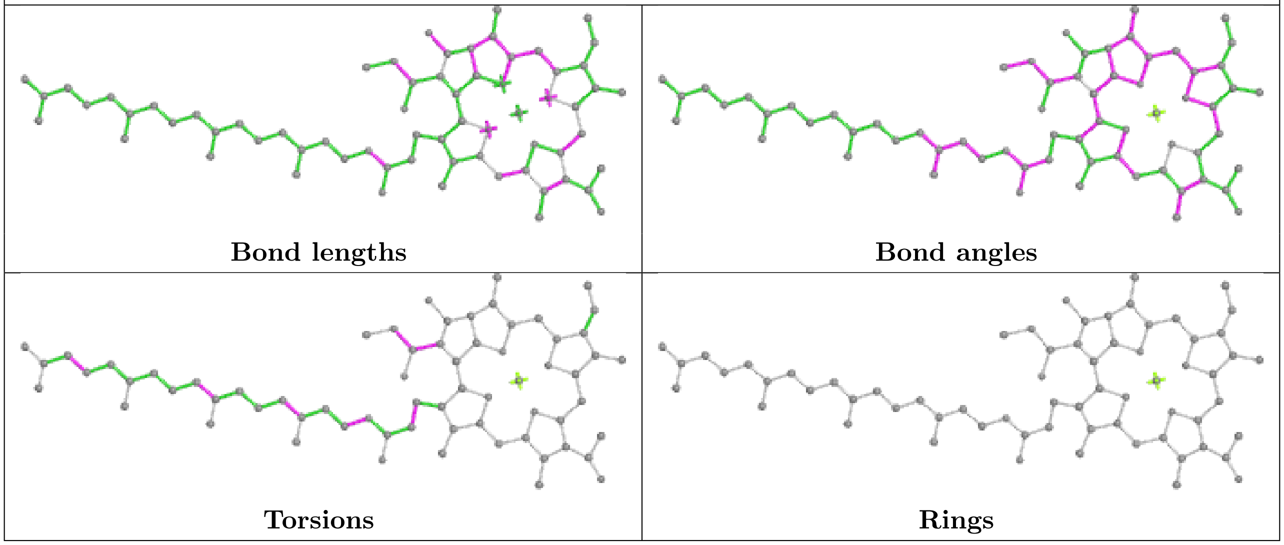
Bond lengths

Bond angles

Torsions

Rings

Ligand BCL L 301



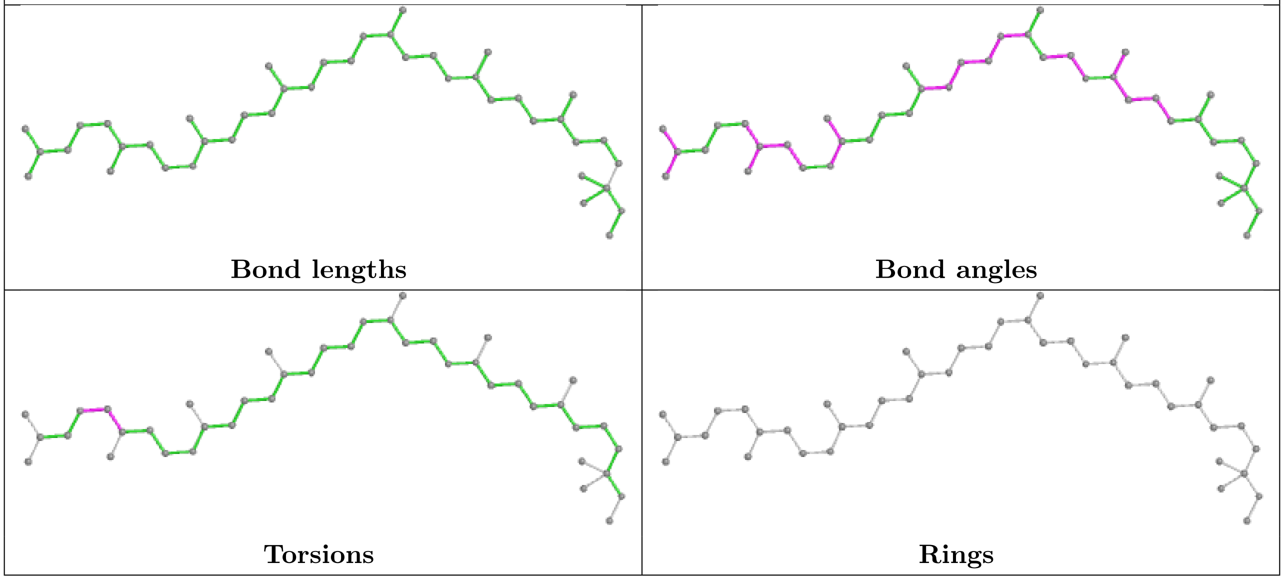
Bond lengths

Bond angles

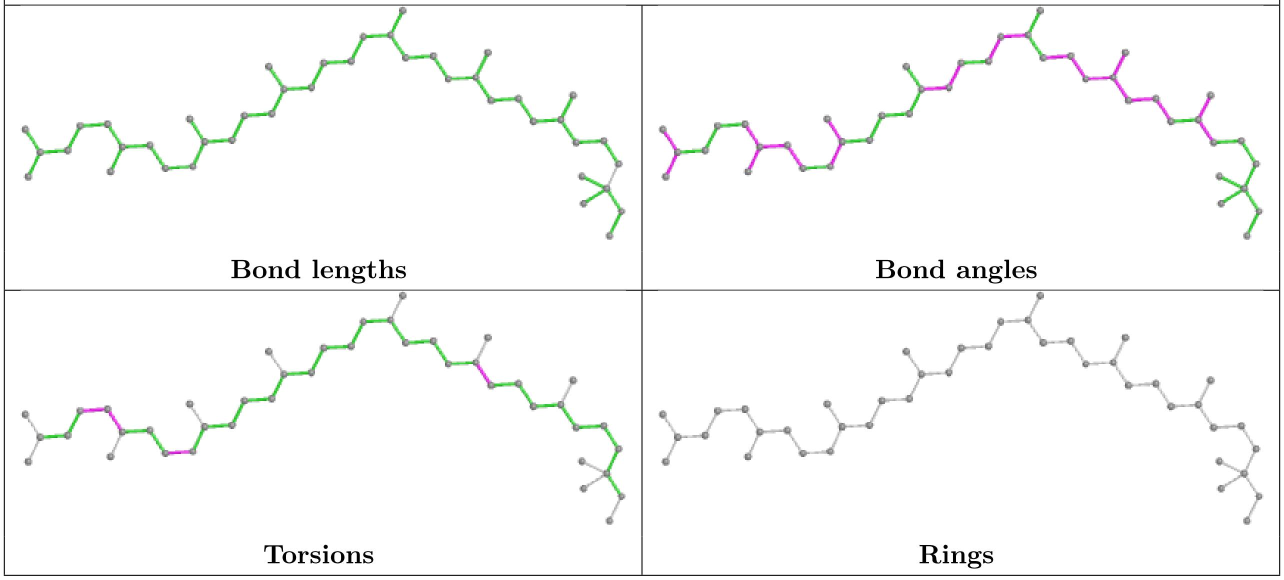
Torsions

Rings

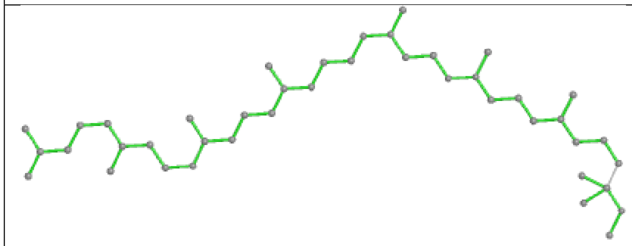
Ligand SPO G 102



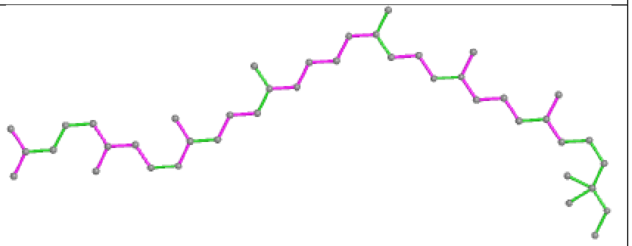
Ligand SPO K 103



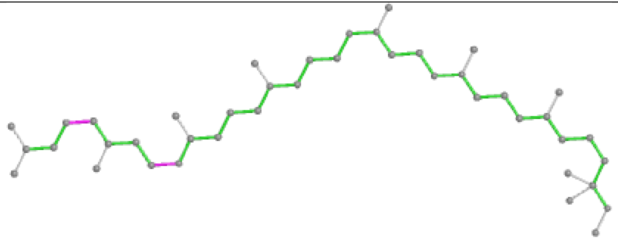
Ligand SPO D 102



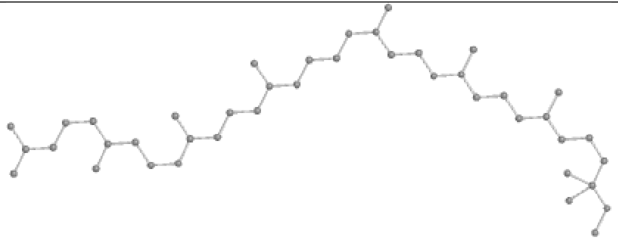
Bond lengths



Bond angles

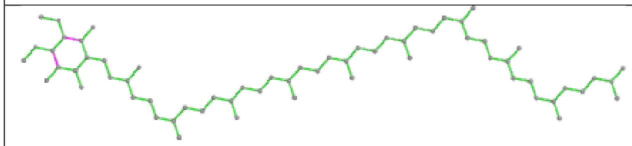


Torsions

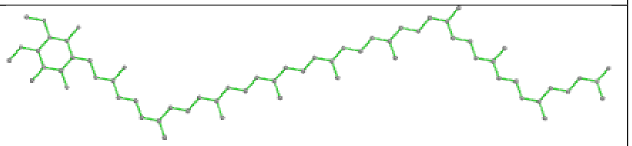


Rings

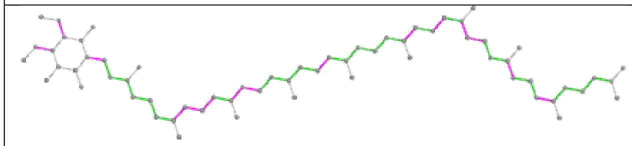
Ligand U10 D 105



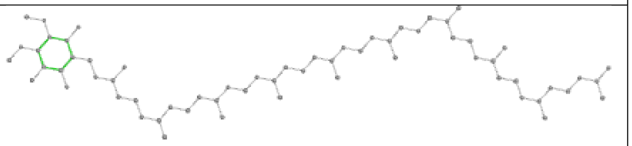
Bond lengths



Bond angles

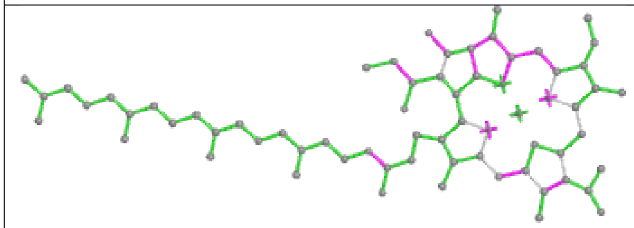


Torsions

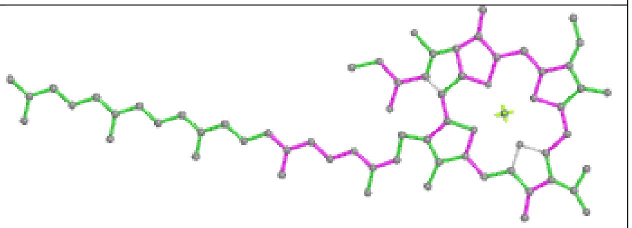


Rings

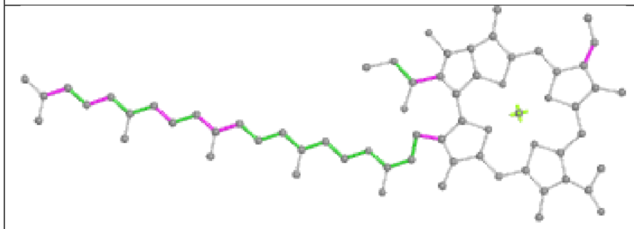
Ligand BCL M 401



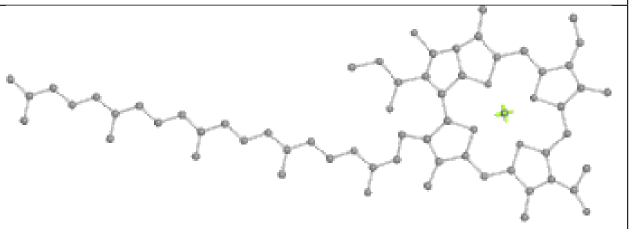
Bond lengths



Bond angles

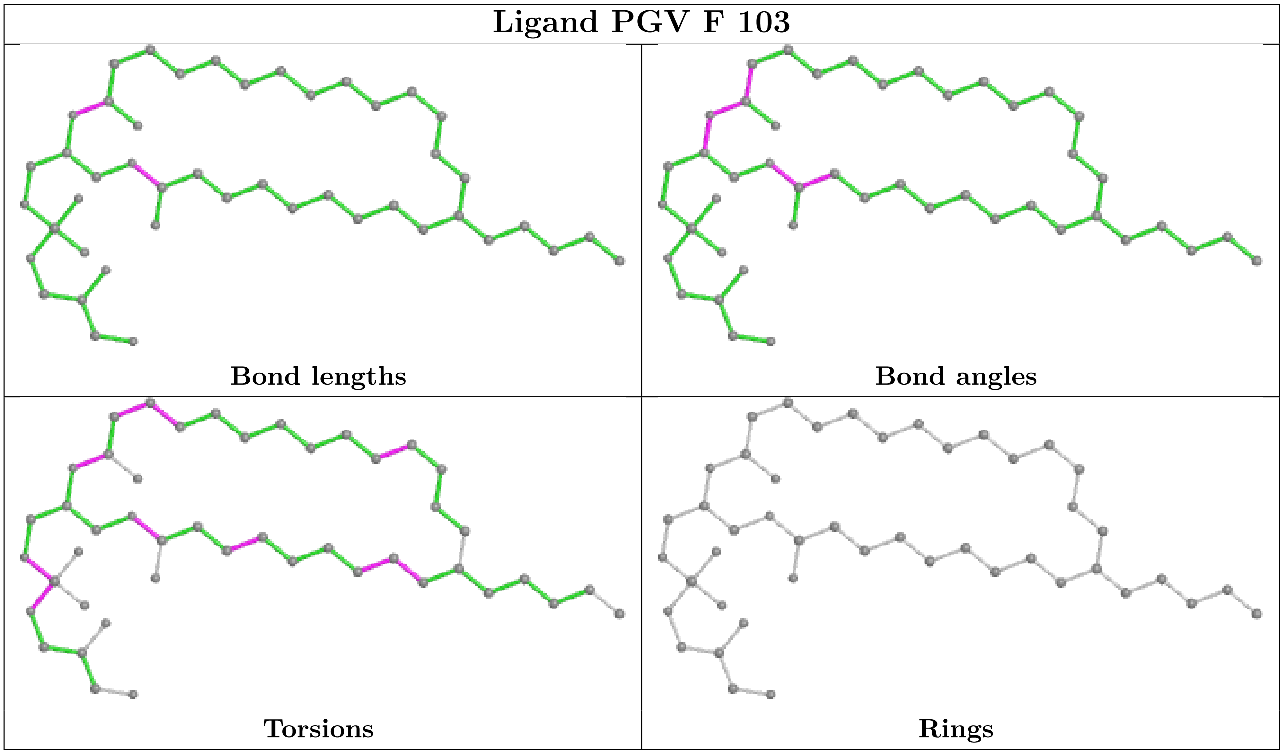


Torsions

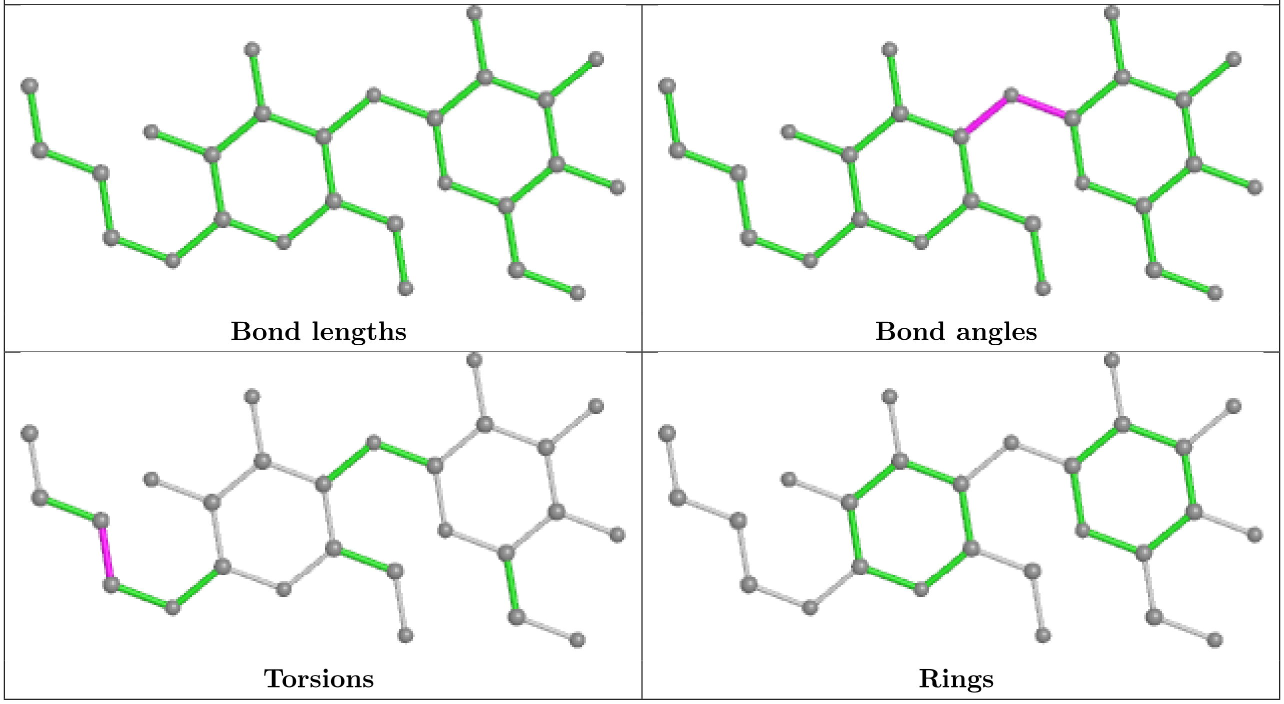


Rings

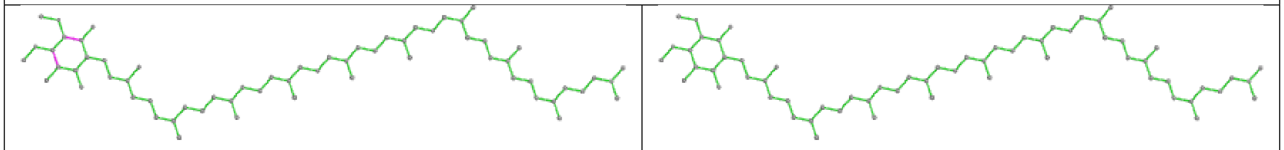
Ligand PGV F 103



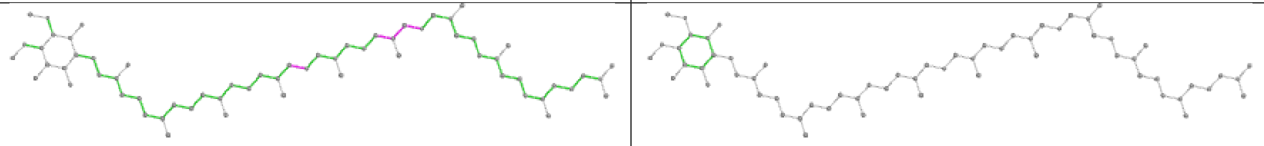
Ligand LMT B 102



Ligand U10 M 410

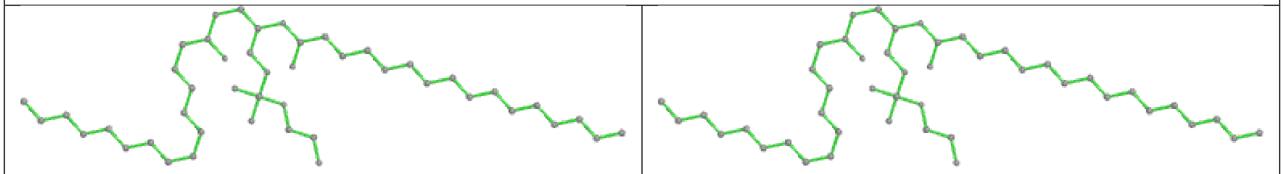


Bond lengths Bond angles

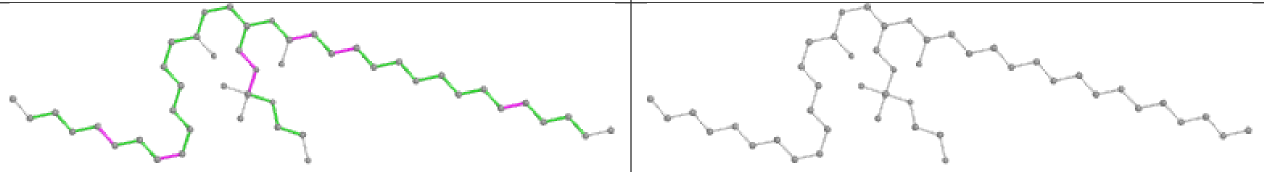


Torsions Rings

Ligand PTY H 306

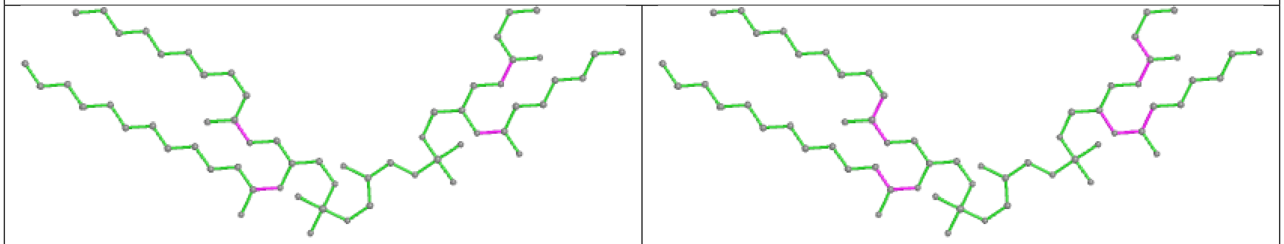


Bond lengths Bond angles

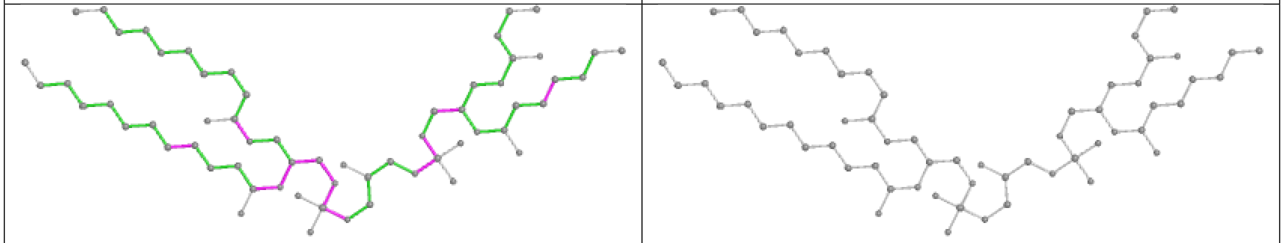


Torsions Rings

Ligand CDL H 307

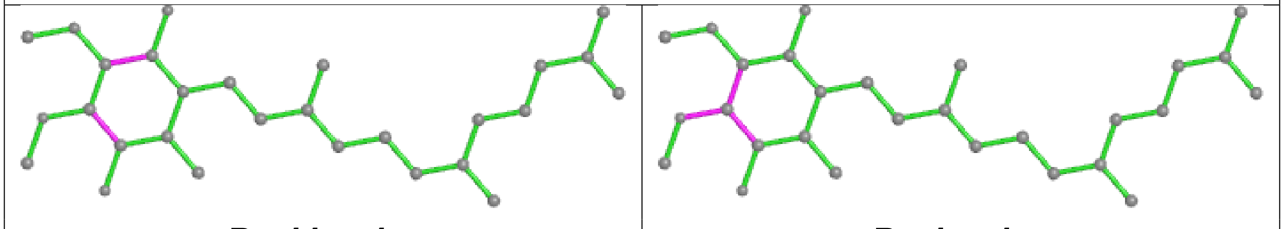


Bond lengths Bond angles

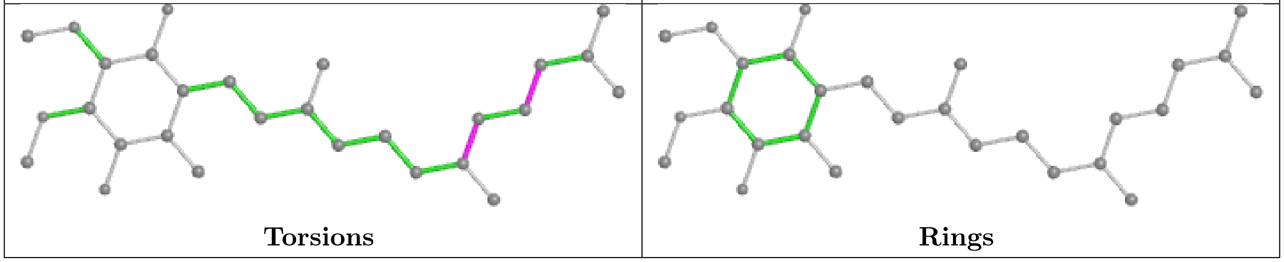


Torsions Rings

Ligand U10 L 304

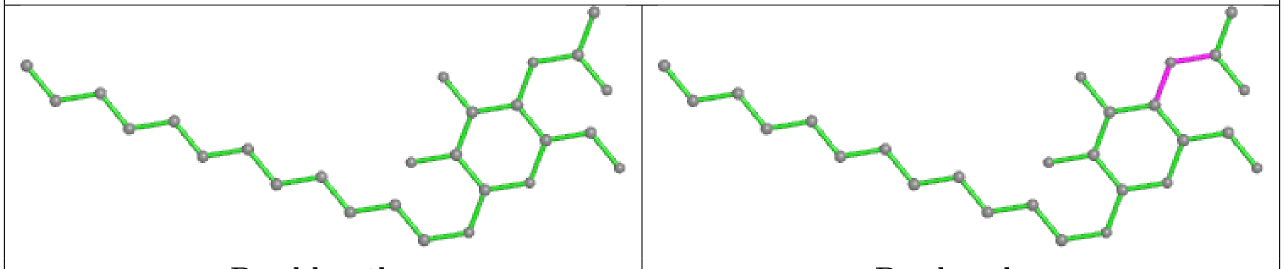


Bond lengths **Bond angles**

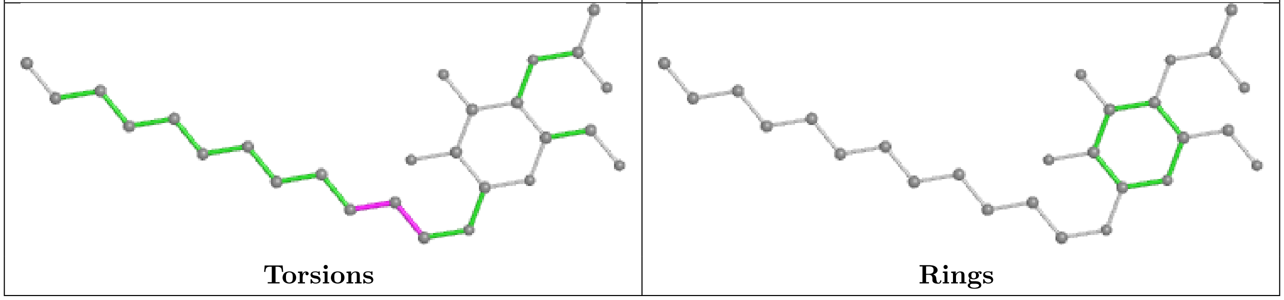


Torsions **Rings**

Ligand LMT M 406

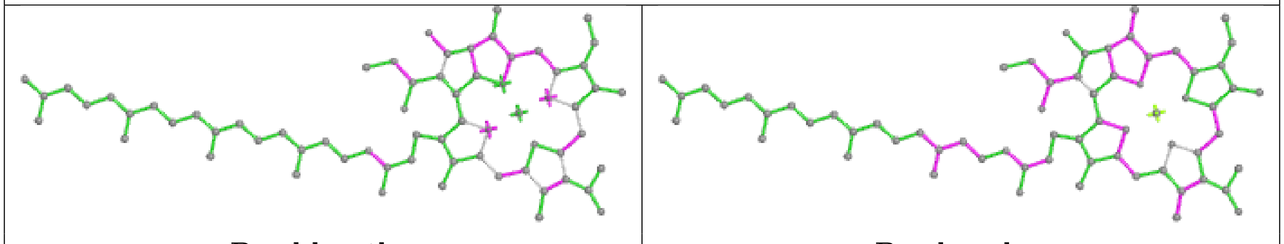


Bond lengths **Bond angles**

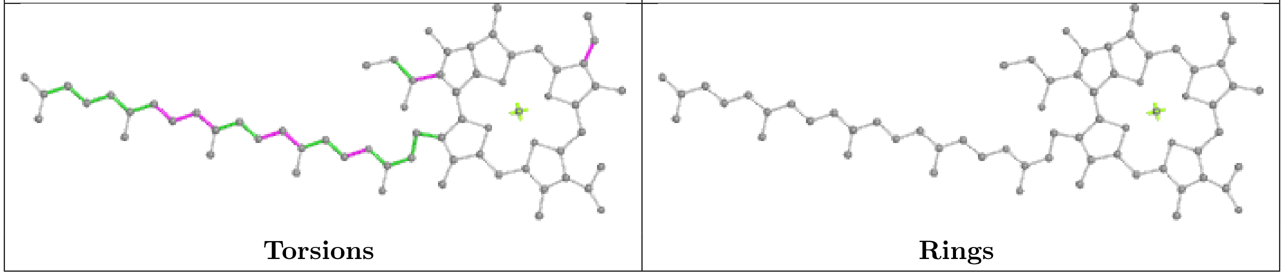


Torsions **Rings**

Ligand BCL 1 101

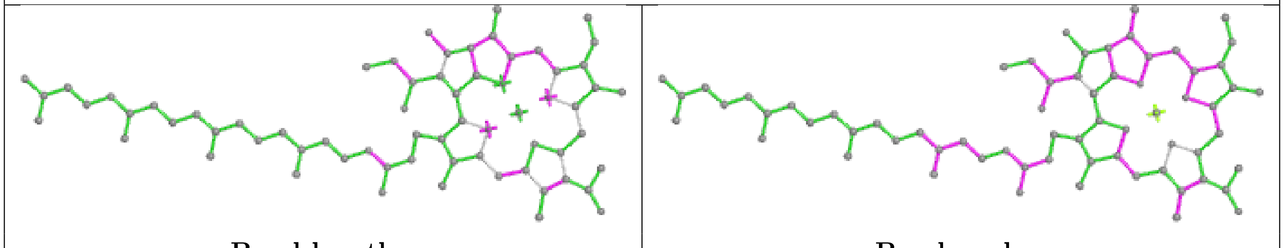


Bond lengths **Bond angles**

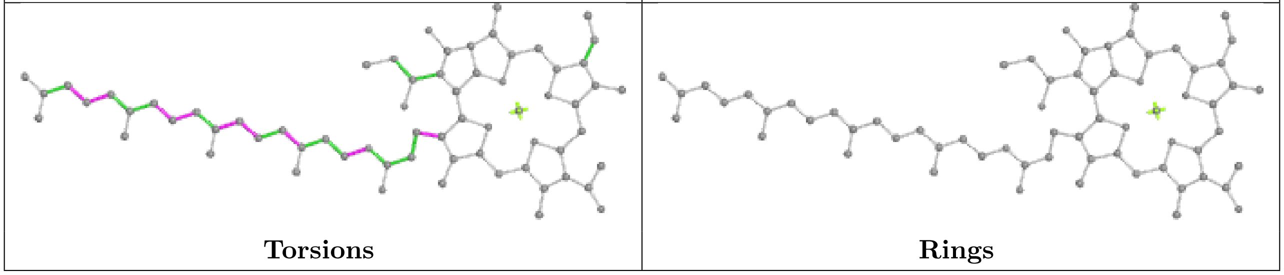


Torsions **Rings**

Ligand BCL F 101

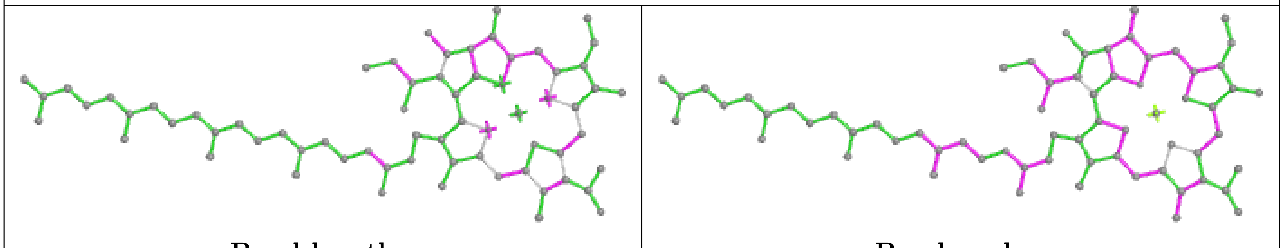


Bond lengths Bond angles

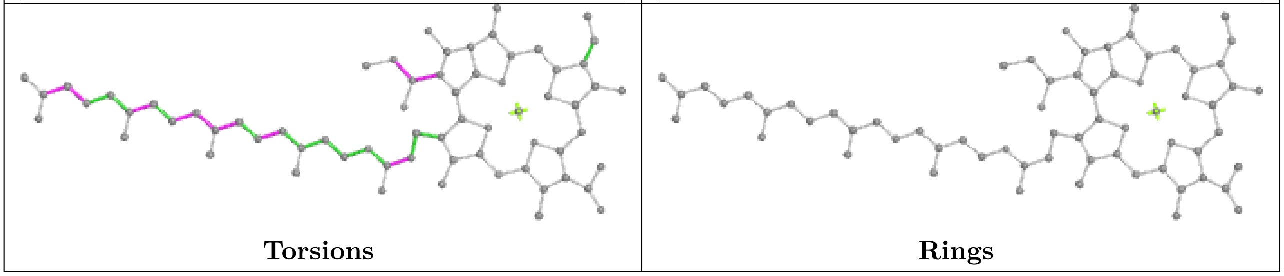


Torsions Rings

Ligand BCL L 309

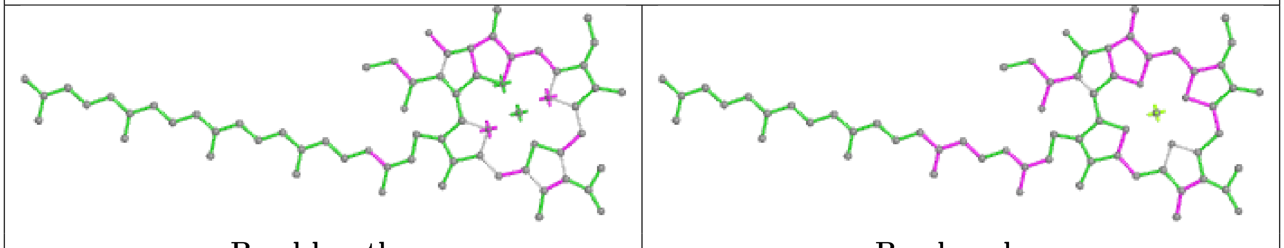


Bond lengths Bond angles

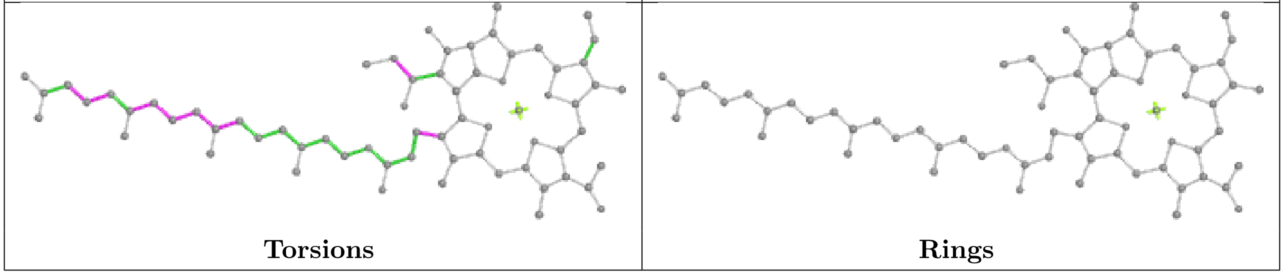


Torsions Rings

Ligand BCL Q 104

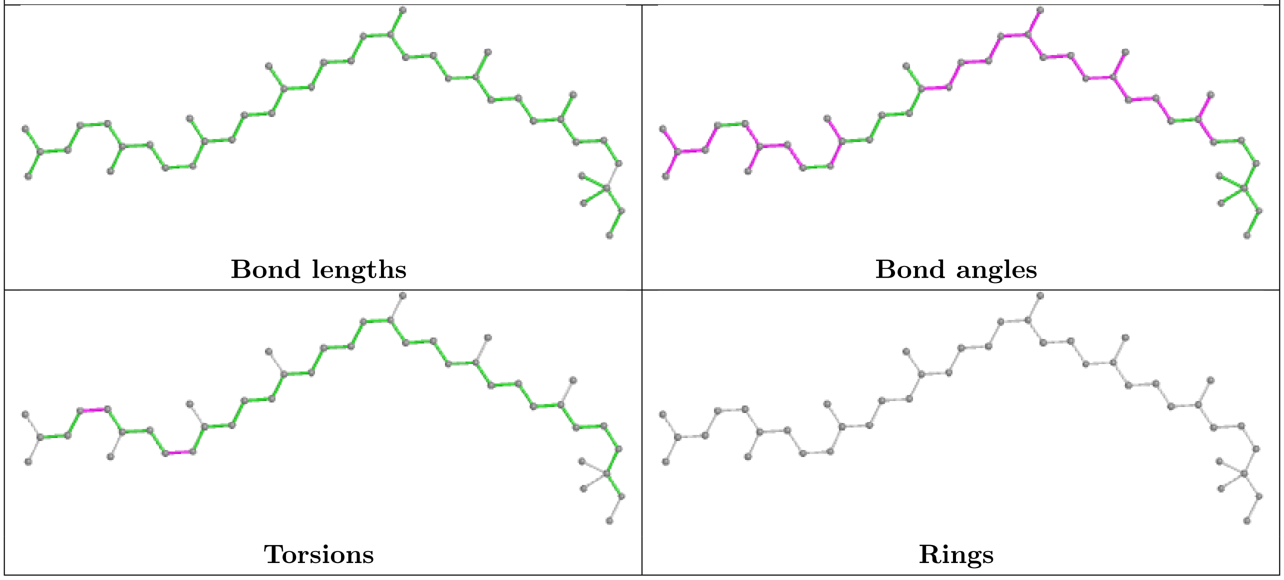


Bond lengths Bond angles

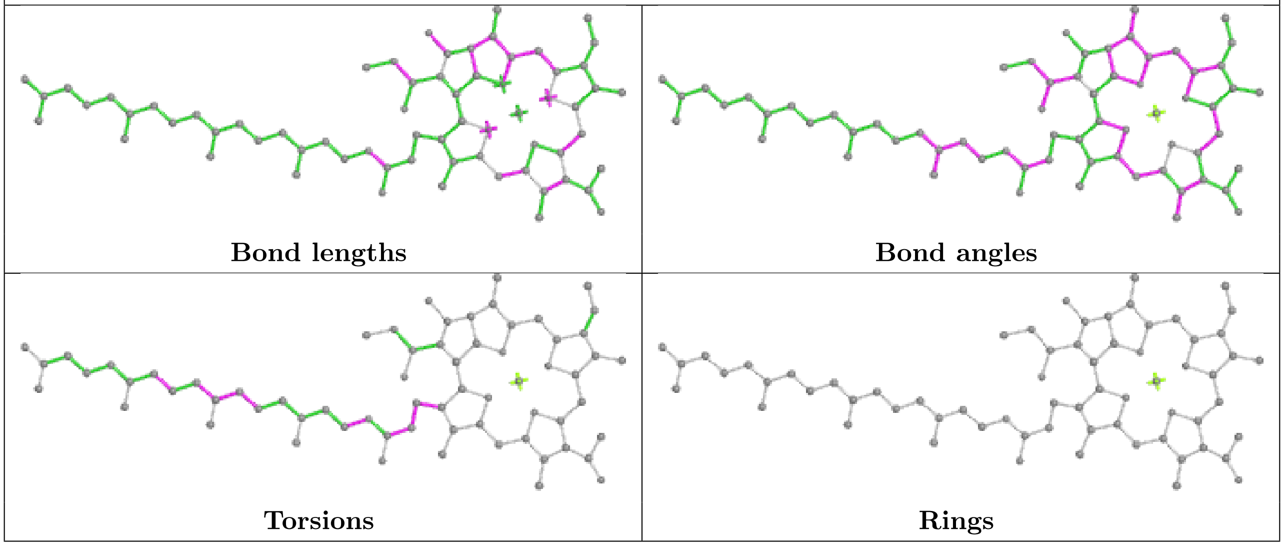


Torsions Rings

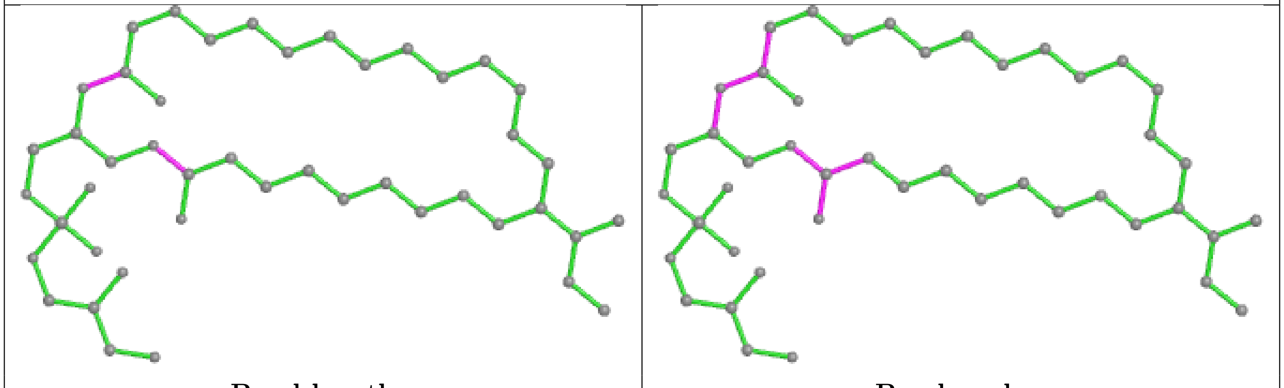
Ligand SPO Q 105



Ligand BCL W 101

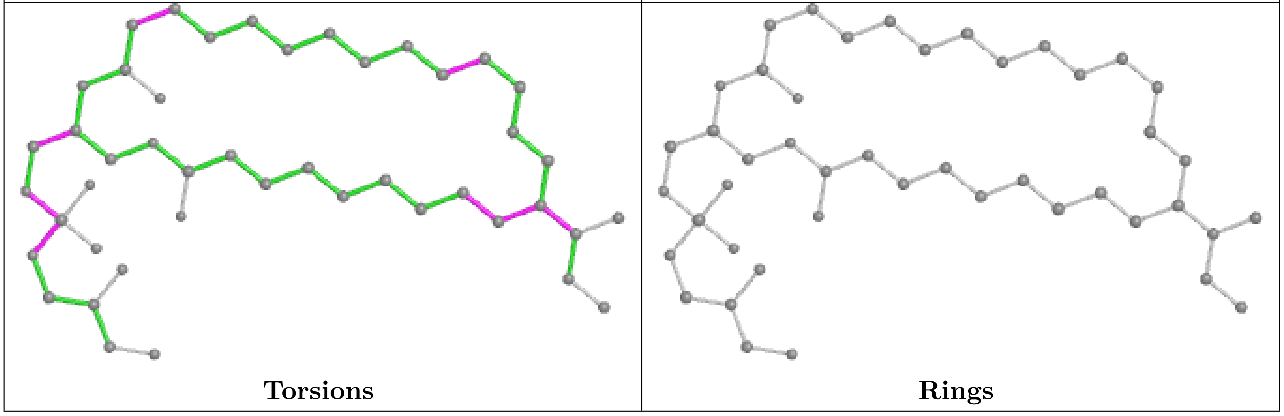


Ligand PGV H 301



Bond lengths

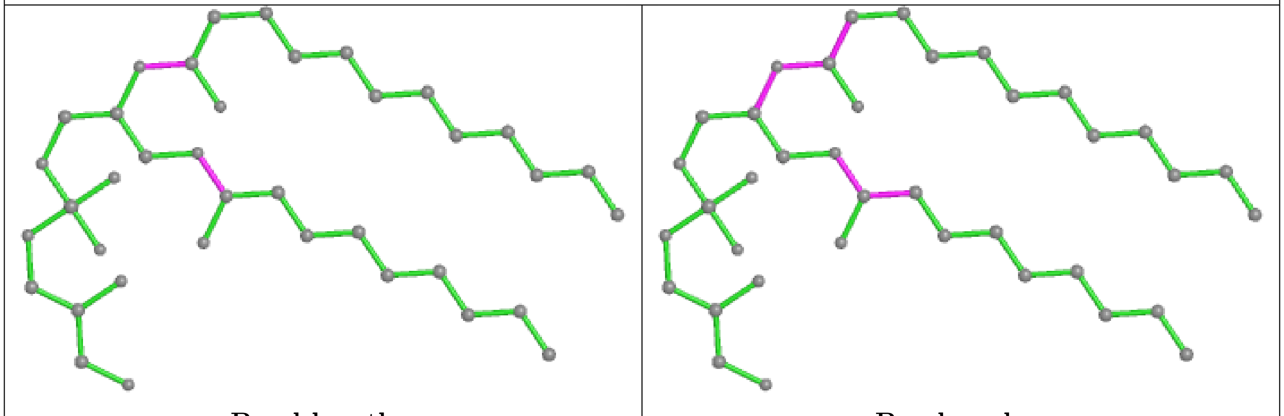
Bond angles



Torsions

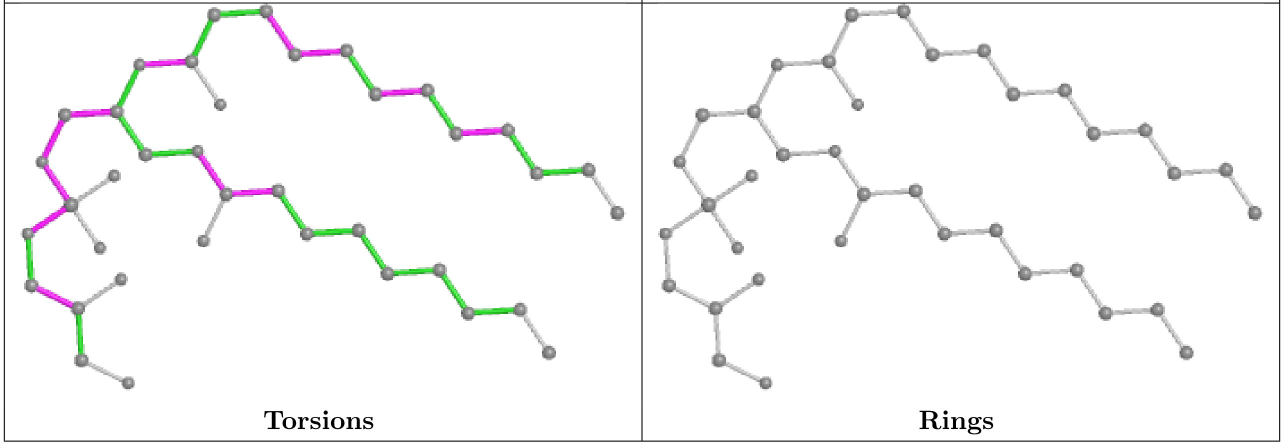
Rings

Ligand PGV M 409



Bond lengths

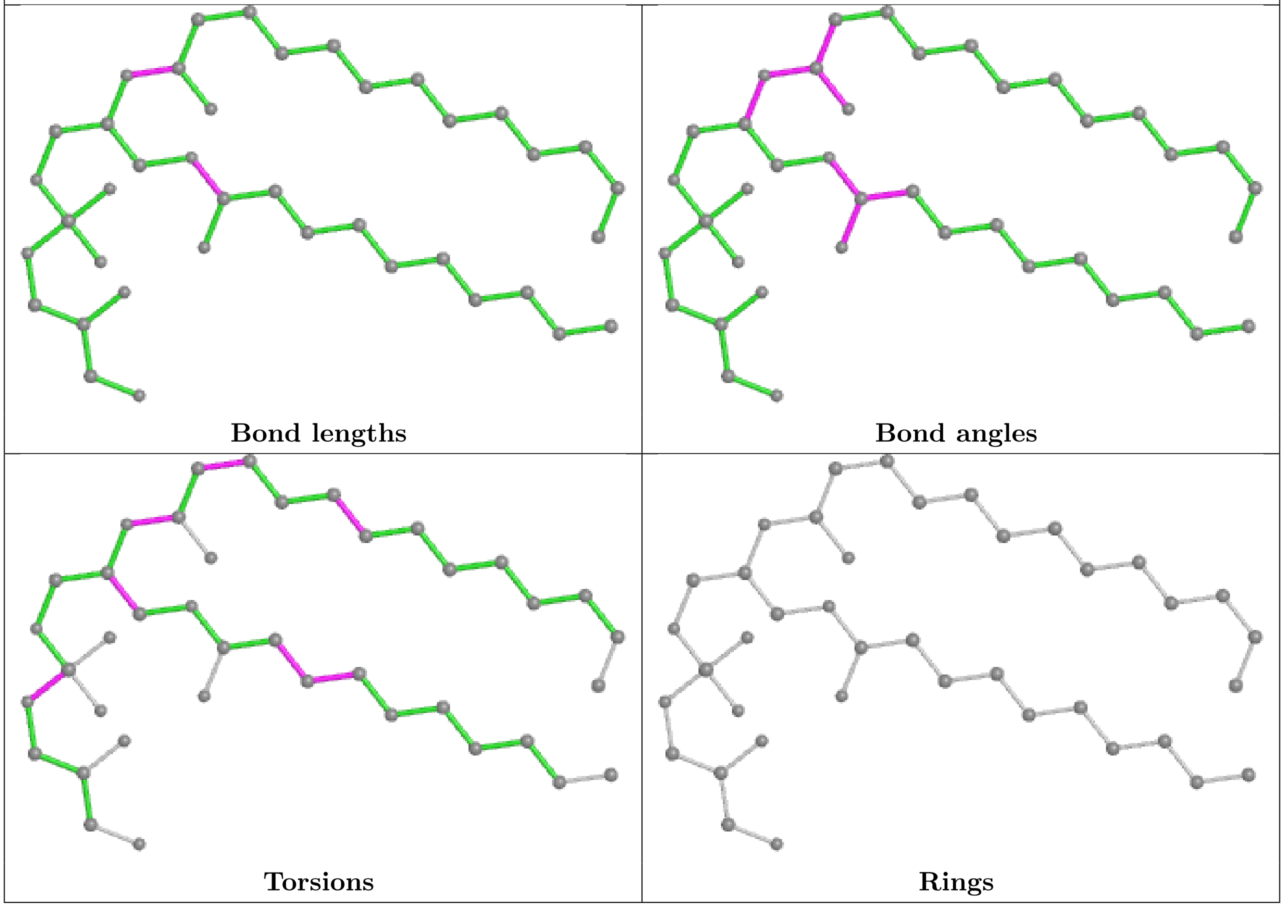
Bond angles



Torsions

Rings

Ligand PGV F 102



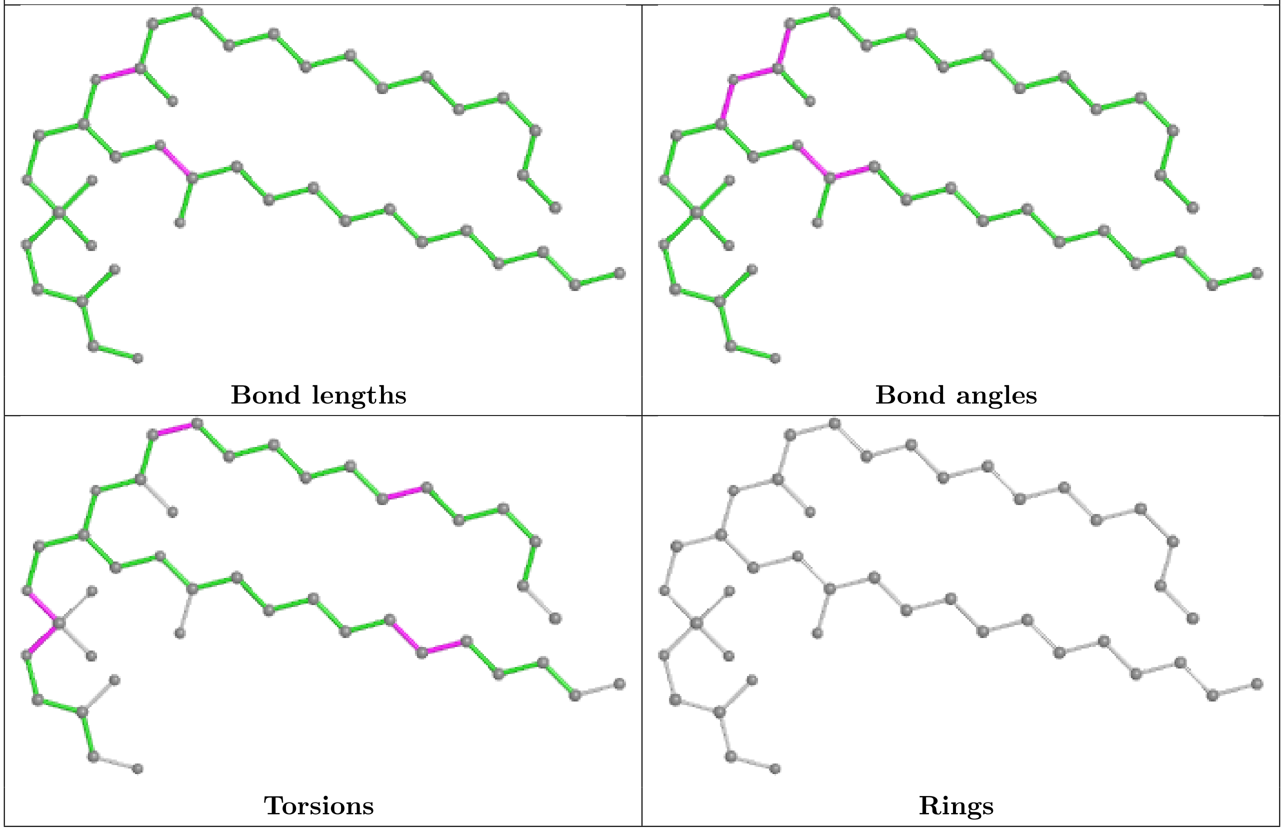
Bond lengths

Bond angles

Torsions

Rings

Ligand PGV Y 104



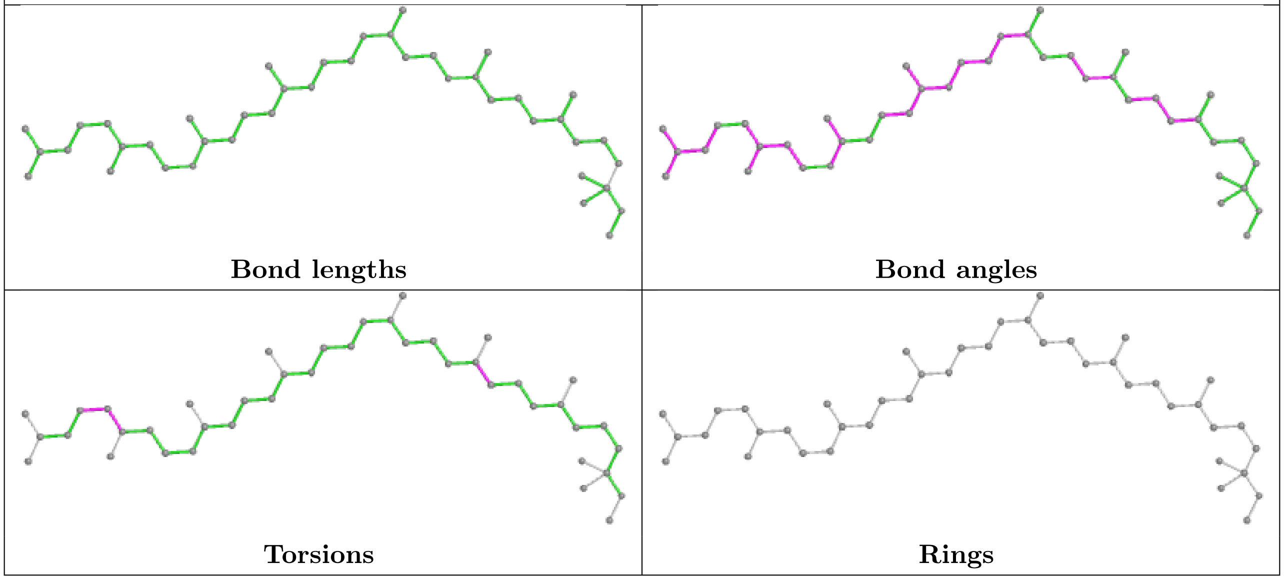
Bond lengths

Bond angles

Torsions

Rings

Ligand SPO V 102



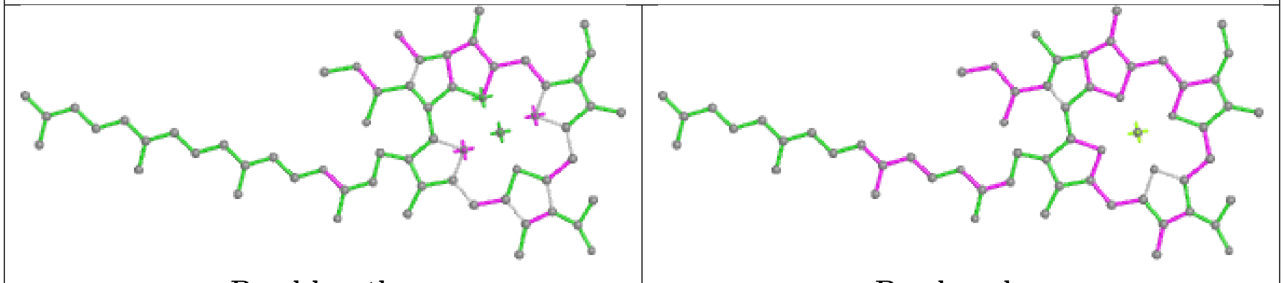
Bond lengths

Bond angles

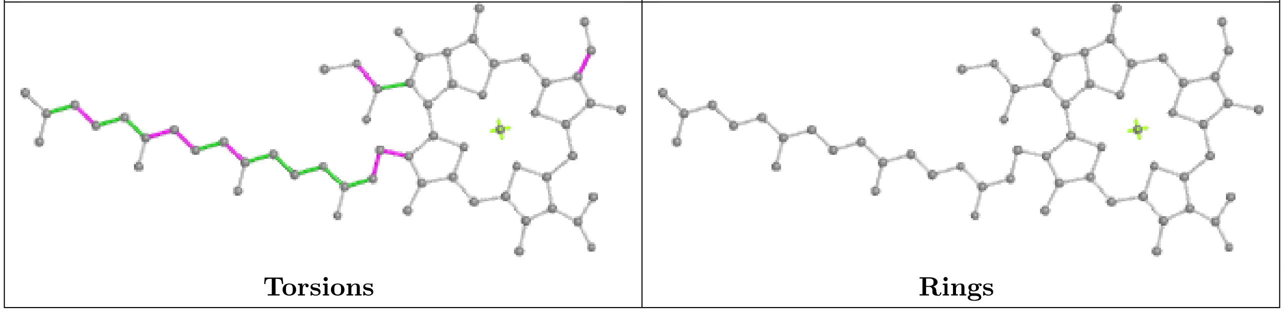
Torsions

Rings

Ligand BCL A 103

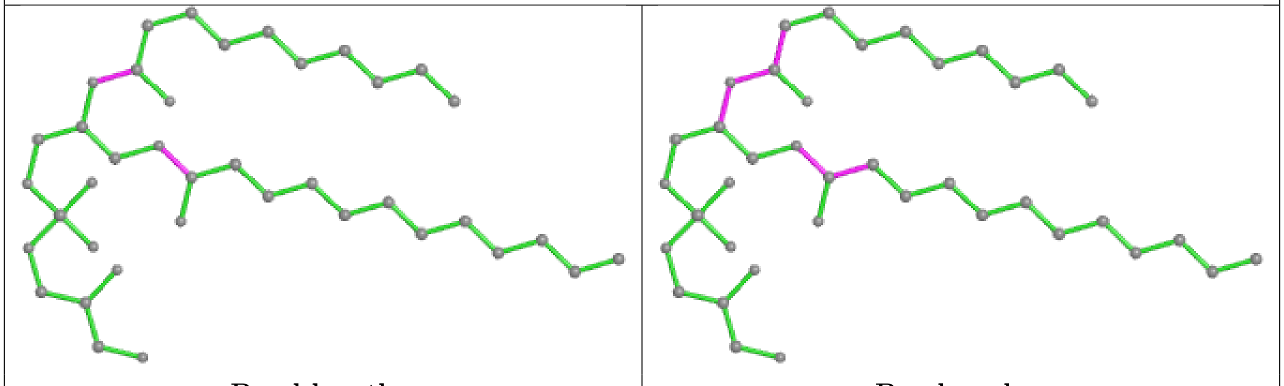


Bond lengths Bond angles

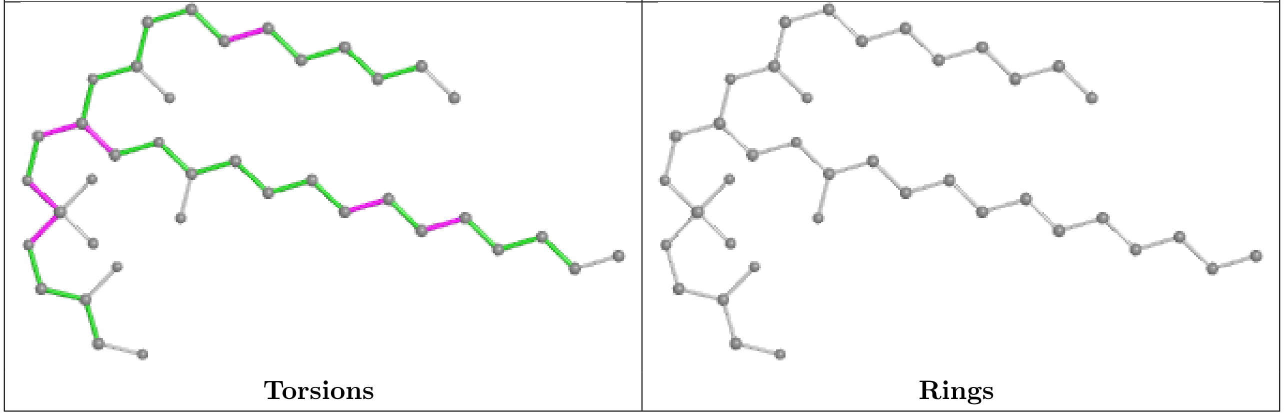


Torsions Rings

Ligand PGV Q 103

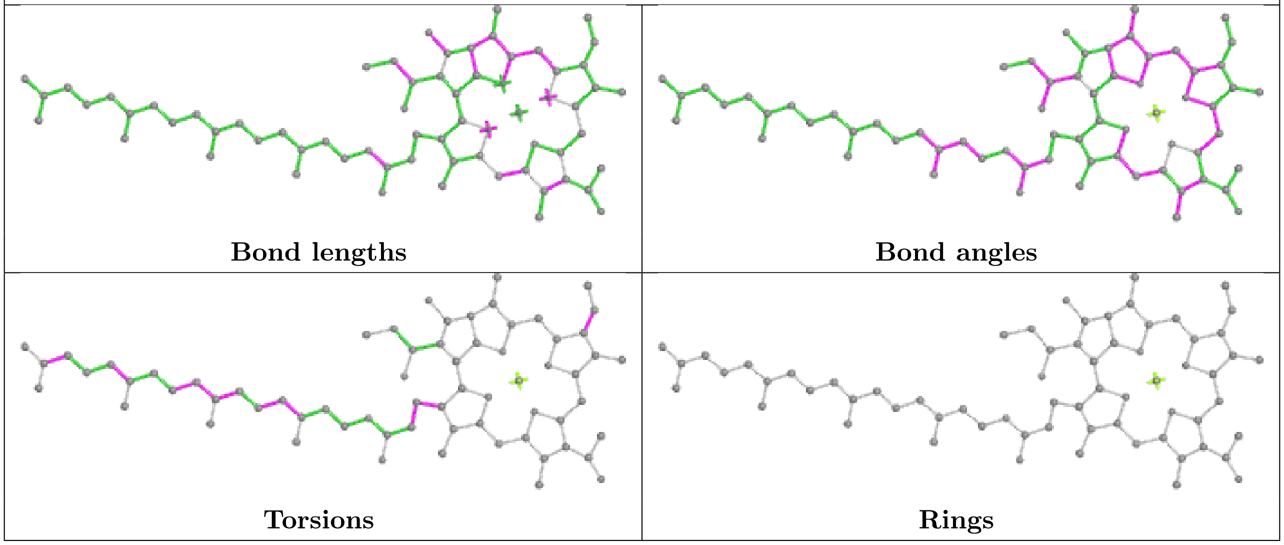


Bond lengths Bond angles

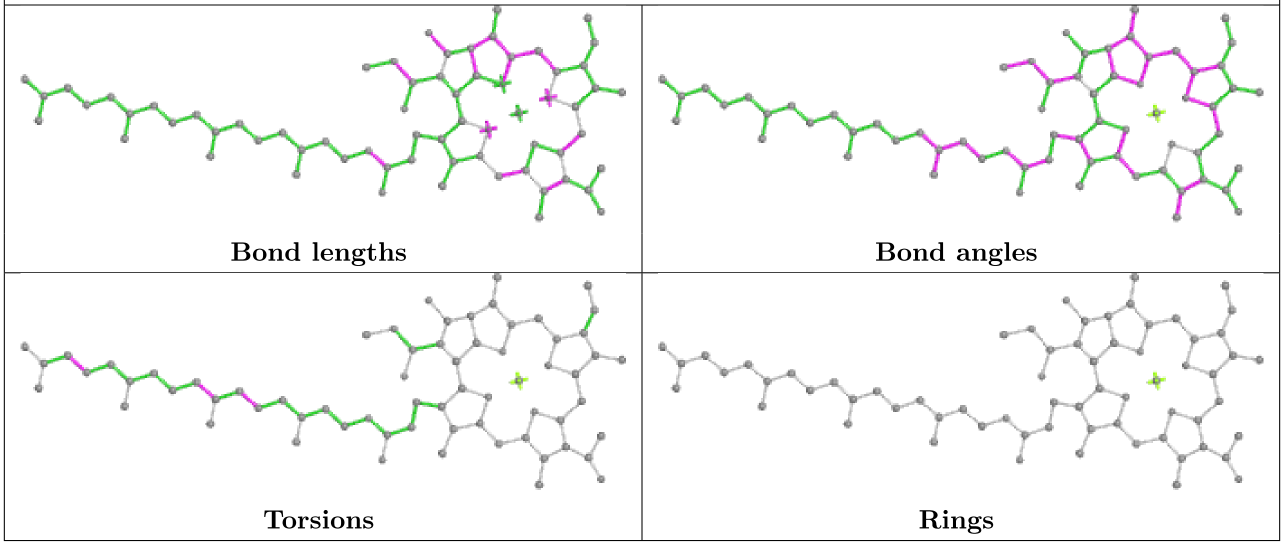


Torsions Rings

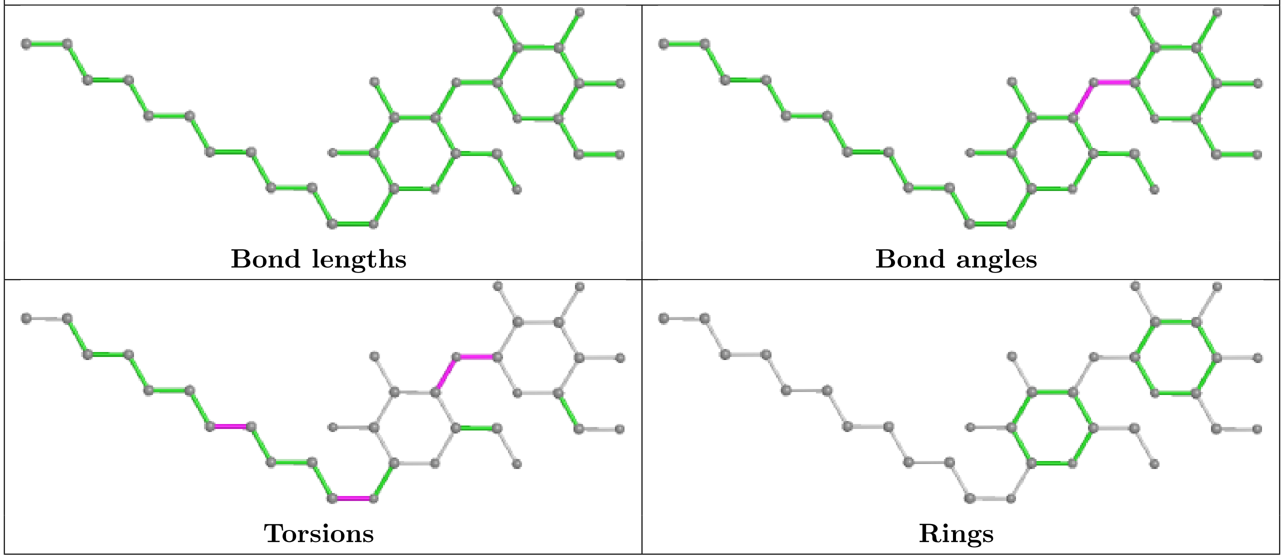
Ligand BCL P 101



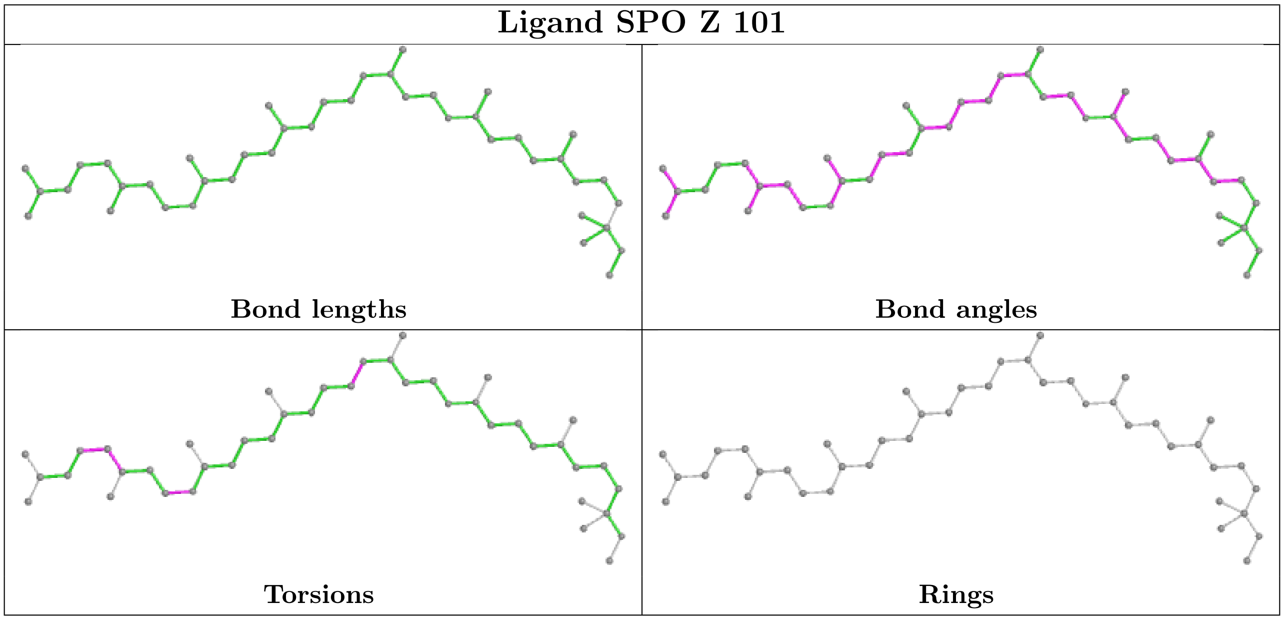
Ligand BCL M 402



Ligand LMT L 308



Ligand SPO Z 101



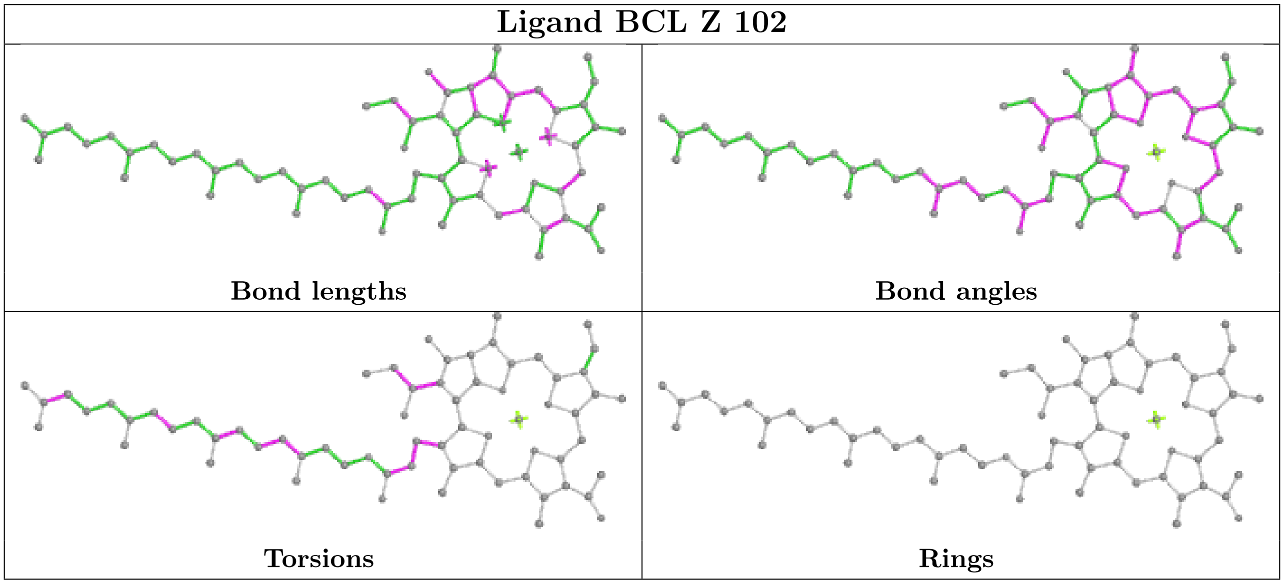
Bond lengths

Bond angles

Torsions

Rings

Ligand BCL Z 102



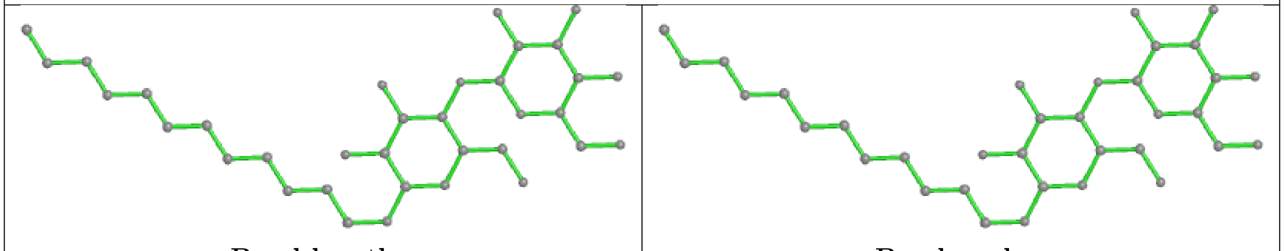
Bond lengths

Bond angles

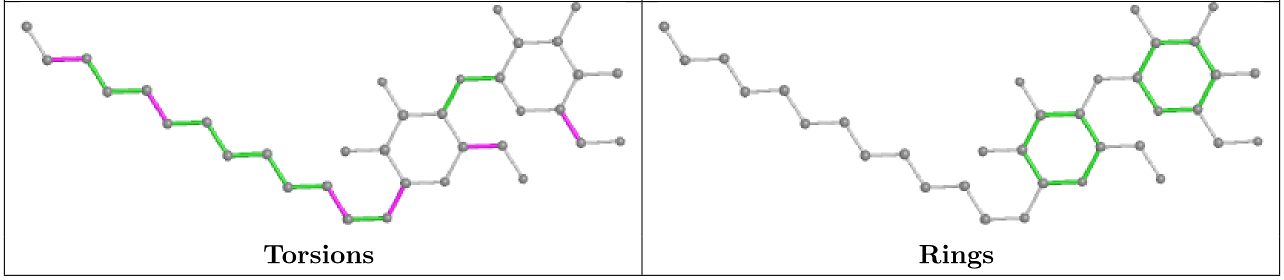
Torsions

Rings

Ligand LMT A 101

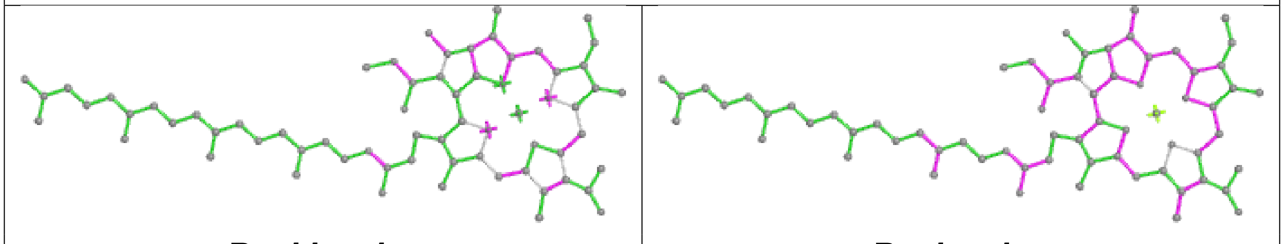


Bond lengths Bond angles

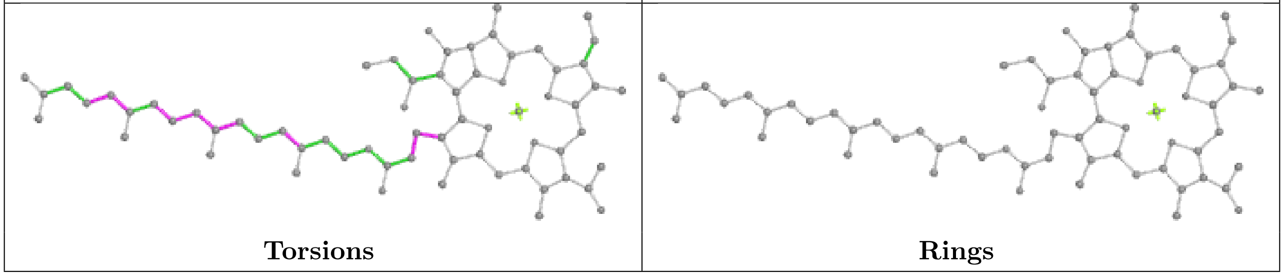


Torsions Rings

Ligand BCL E 101

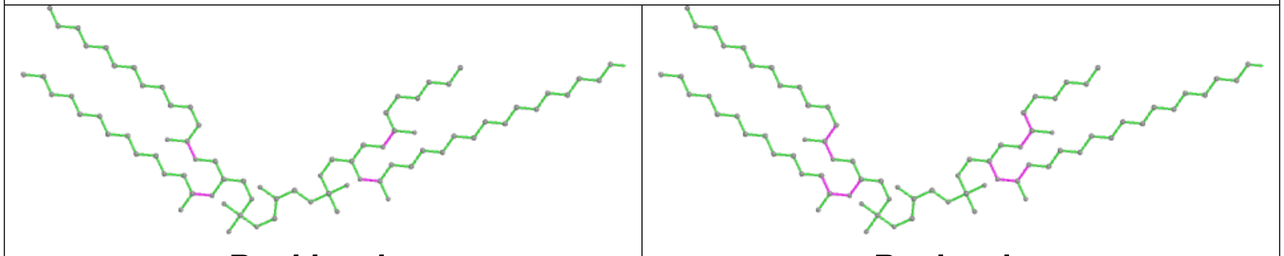


Bond lengths Bond angles

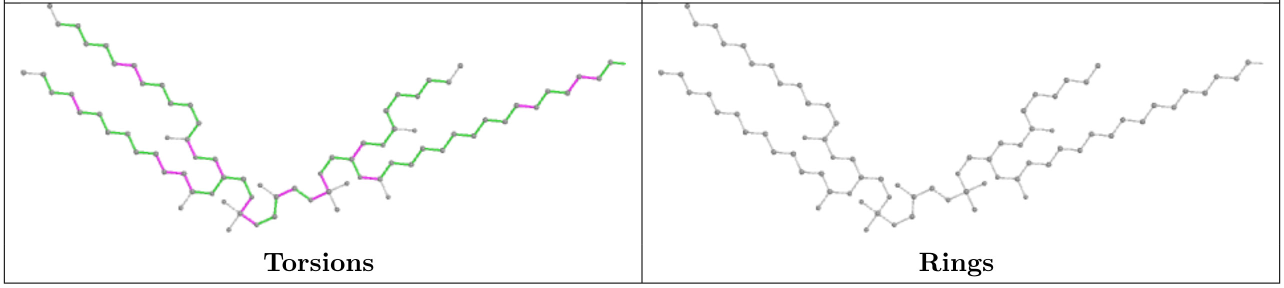


Torsions Rings

Ligand CDL M 408

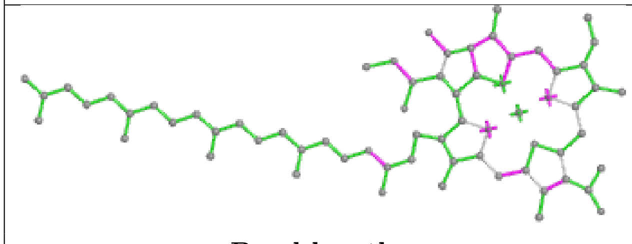


Bond lengths Bond angles

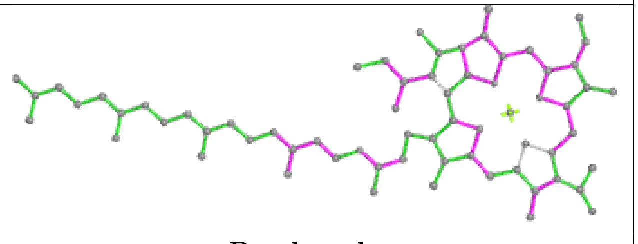


Torsions Rings

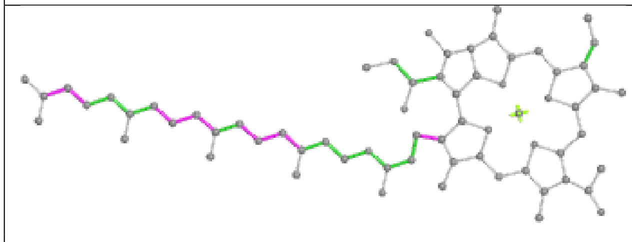
Ligand BCL S 101



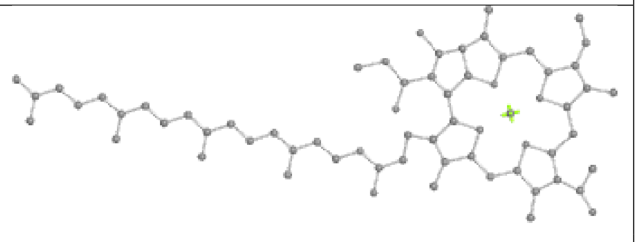
Bond lengths



Bond angles

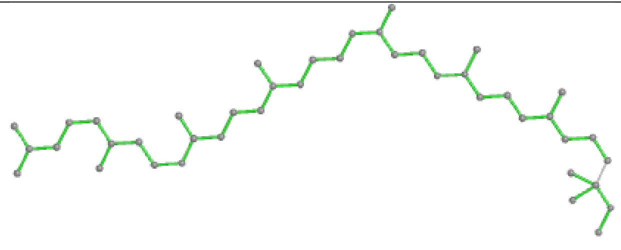


Torsions

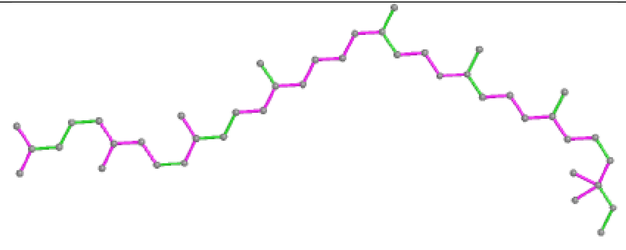


Rings

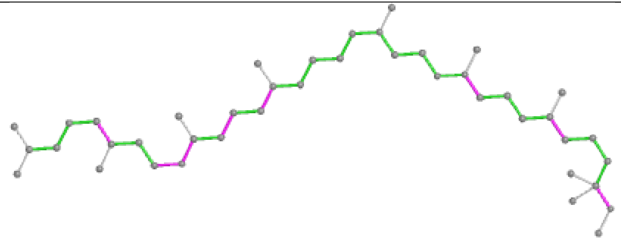
Ligand SPO P 102



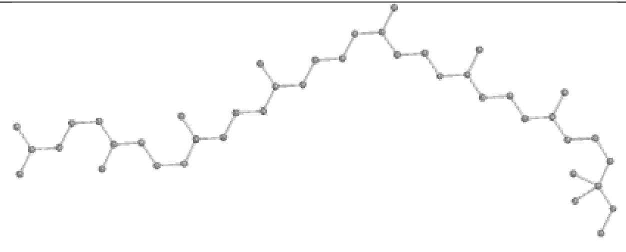
Bond lengths



Bond angles

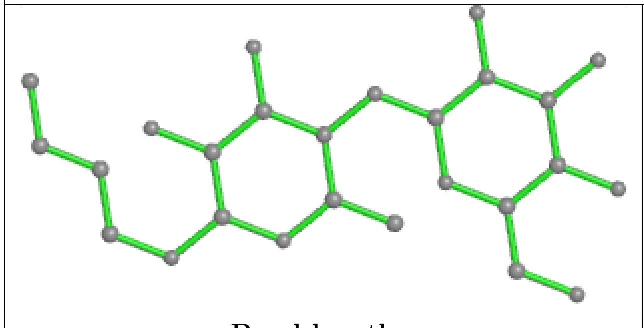


Torsions

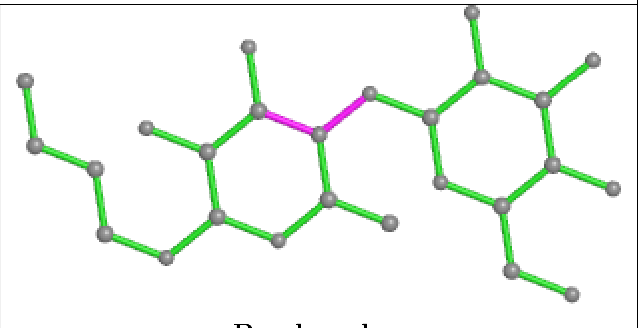


Rings

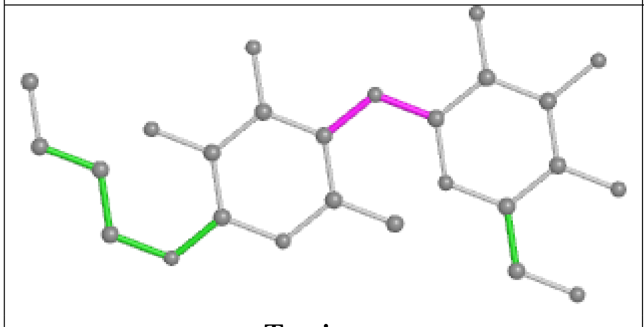
Ligand LMT I 101



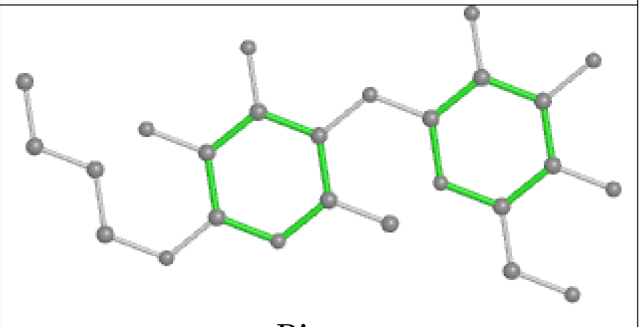
Bond lengths



Bond angles

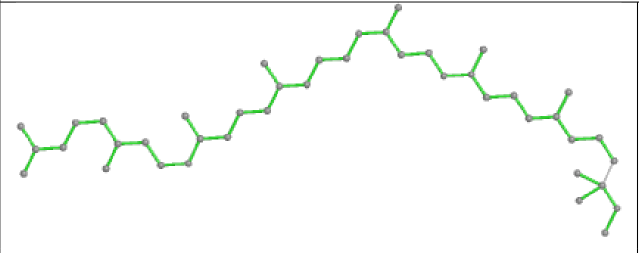


Torsions

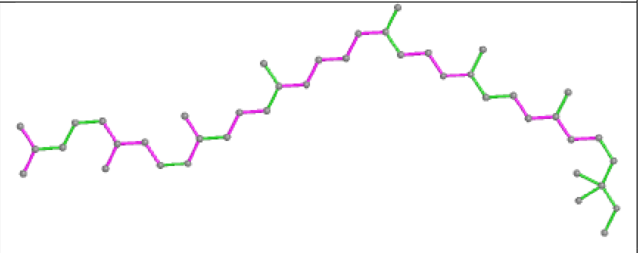


Rings

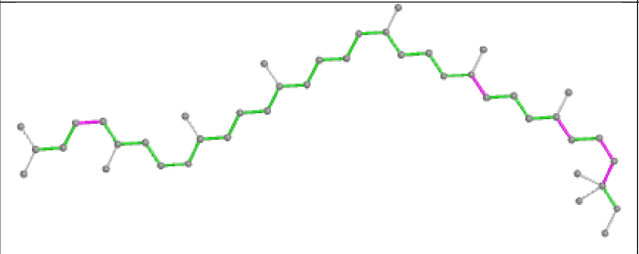
Ligand SPO J 102



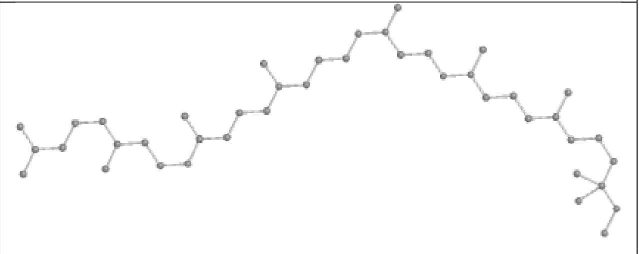
Bond lengths



Bond angles

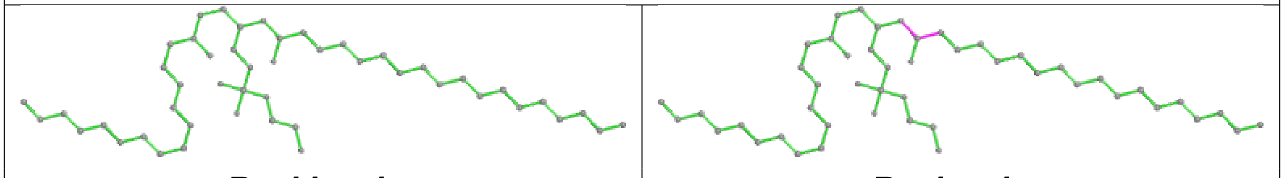


Torsions



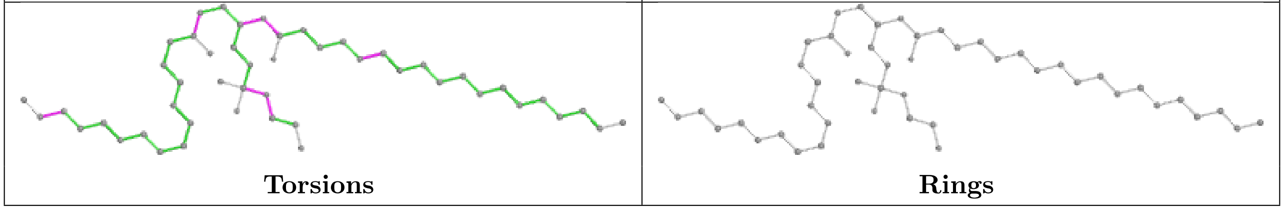
Rings

Ligand PTY F 104



Bond lengths

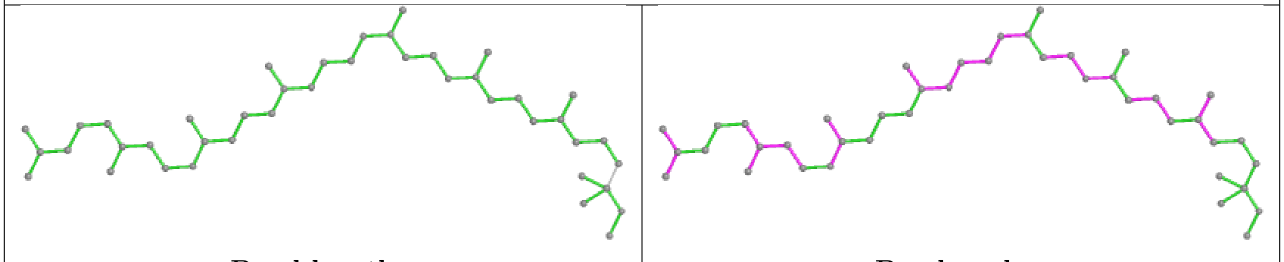
Bond angles



Torsions

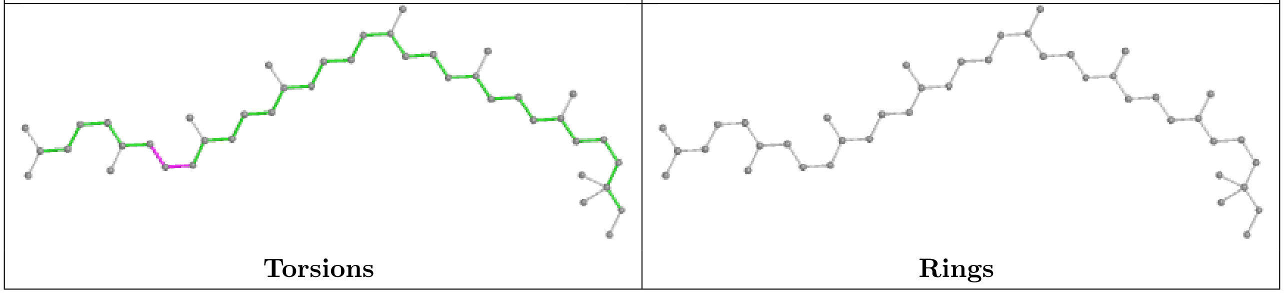
Rings

Ligand SPO S 102



Bond lengths

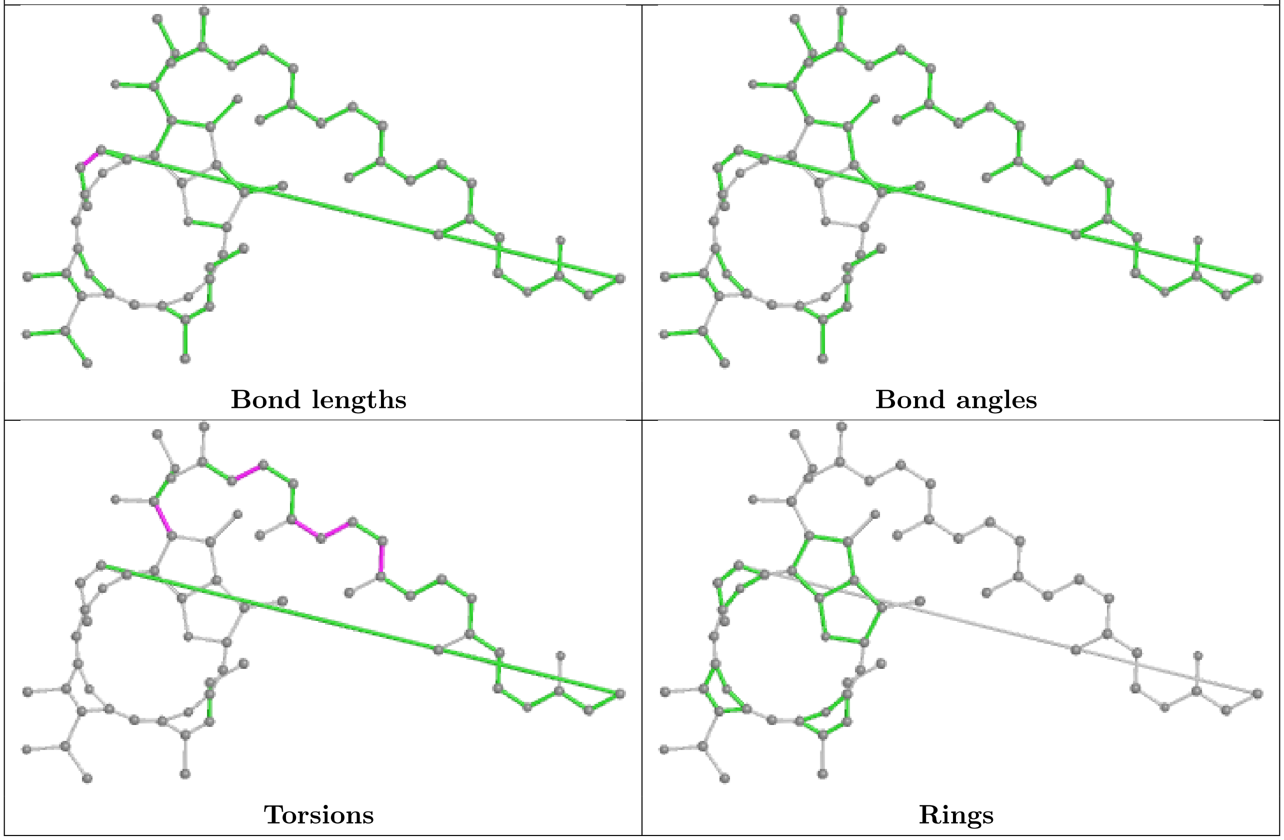
Bond angles



Torsions

Rings

Ligand BPH M 403



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.

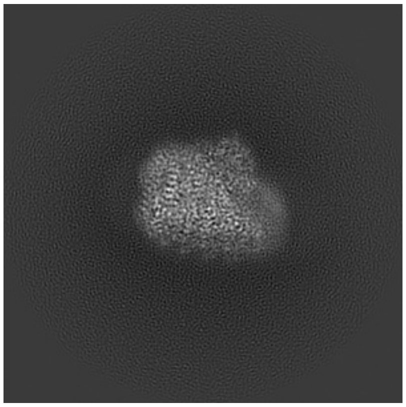
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-32193. These allow visual inspection of the internal detail of the map and identification of artifacts.

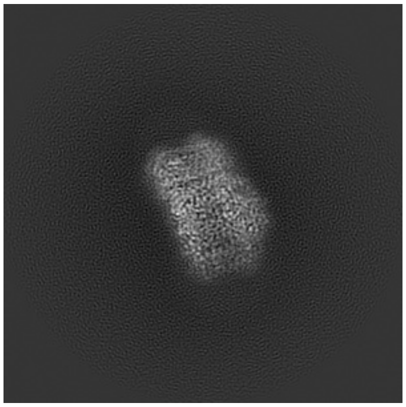
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

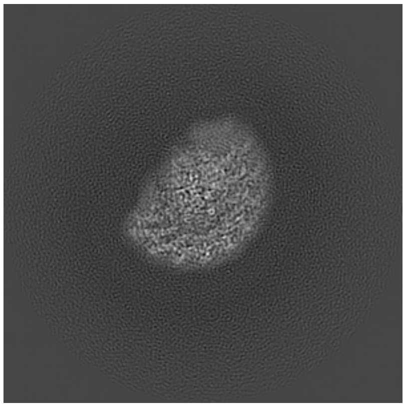
6.1.1 Primary map



X



Y

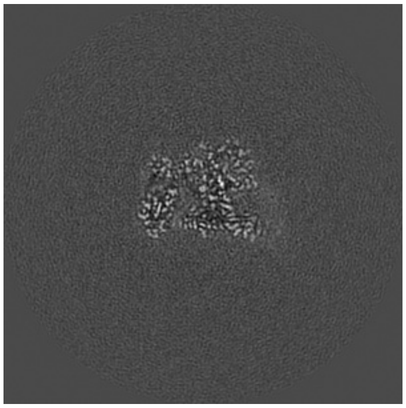


Z

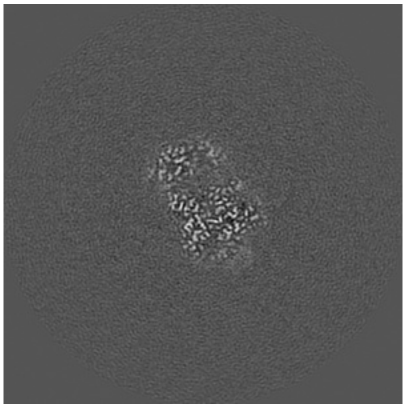
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

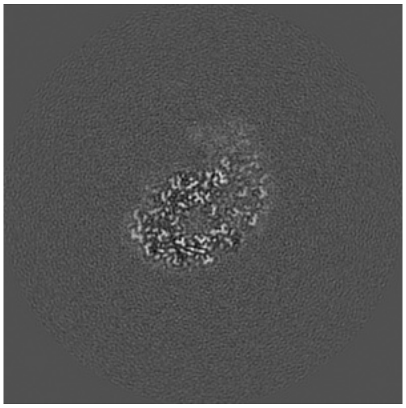
6.2.1 Primary map



X Index: 180



Y Index: 180

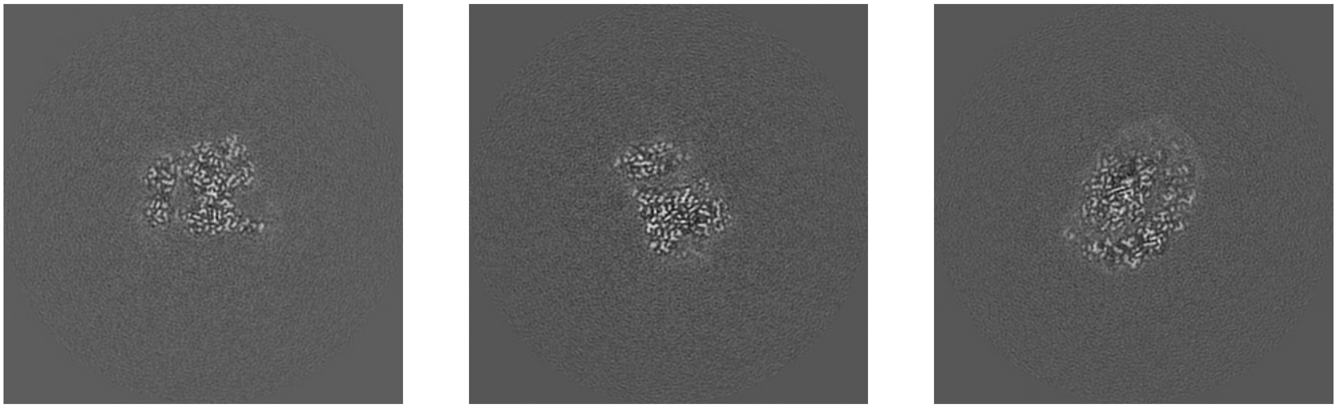


Z Index: 180

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

6.3 Largest variance slices

6.3.1 Primary map

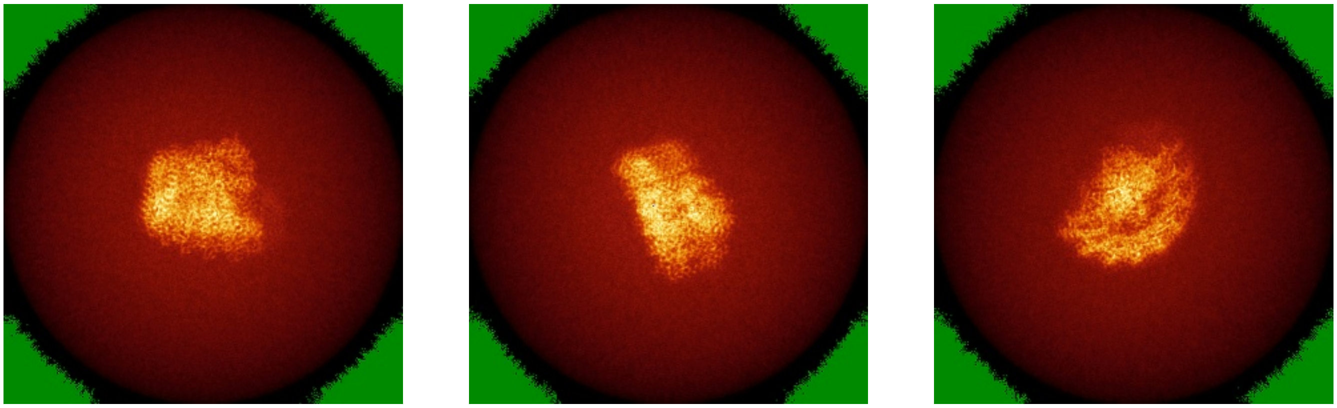


X Index: 169 Y Index: 185 Z Index: 168

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

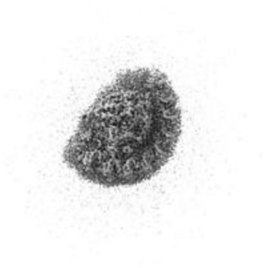
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

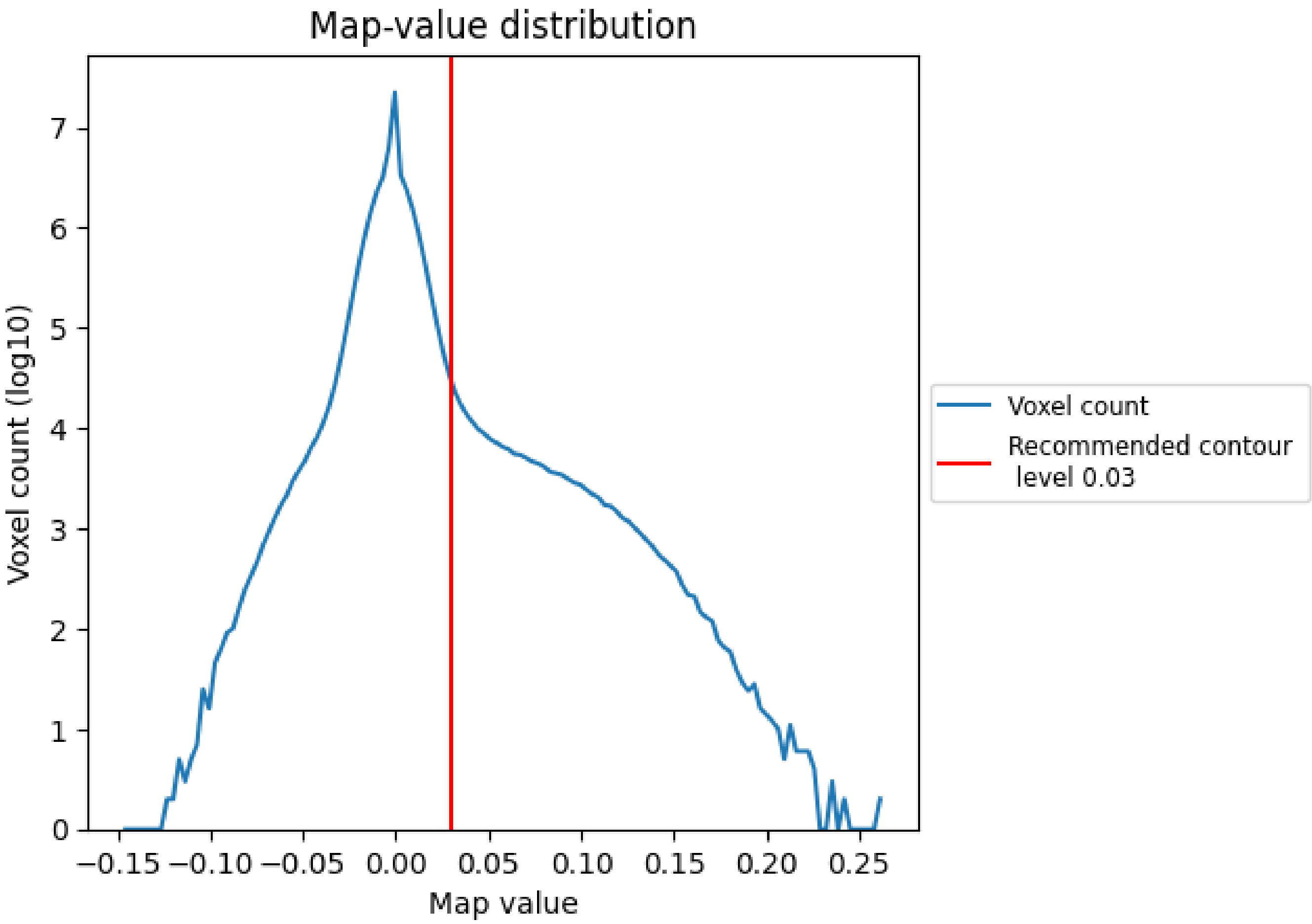
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

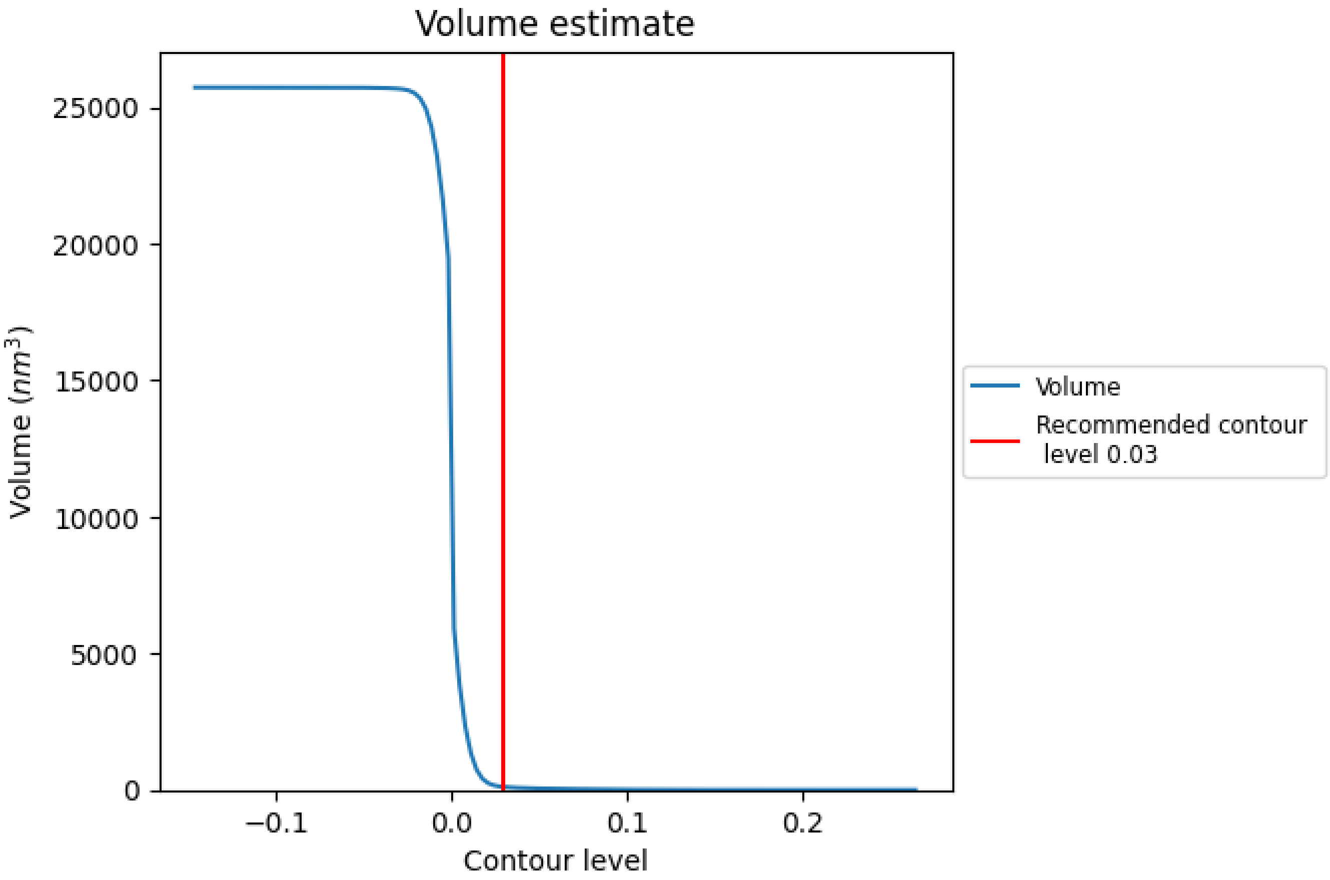
This section contains the results of statistical analysis of the map.

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.

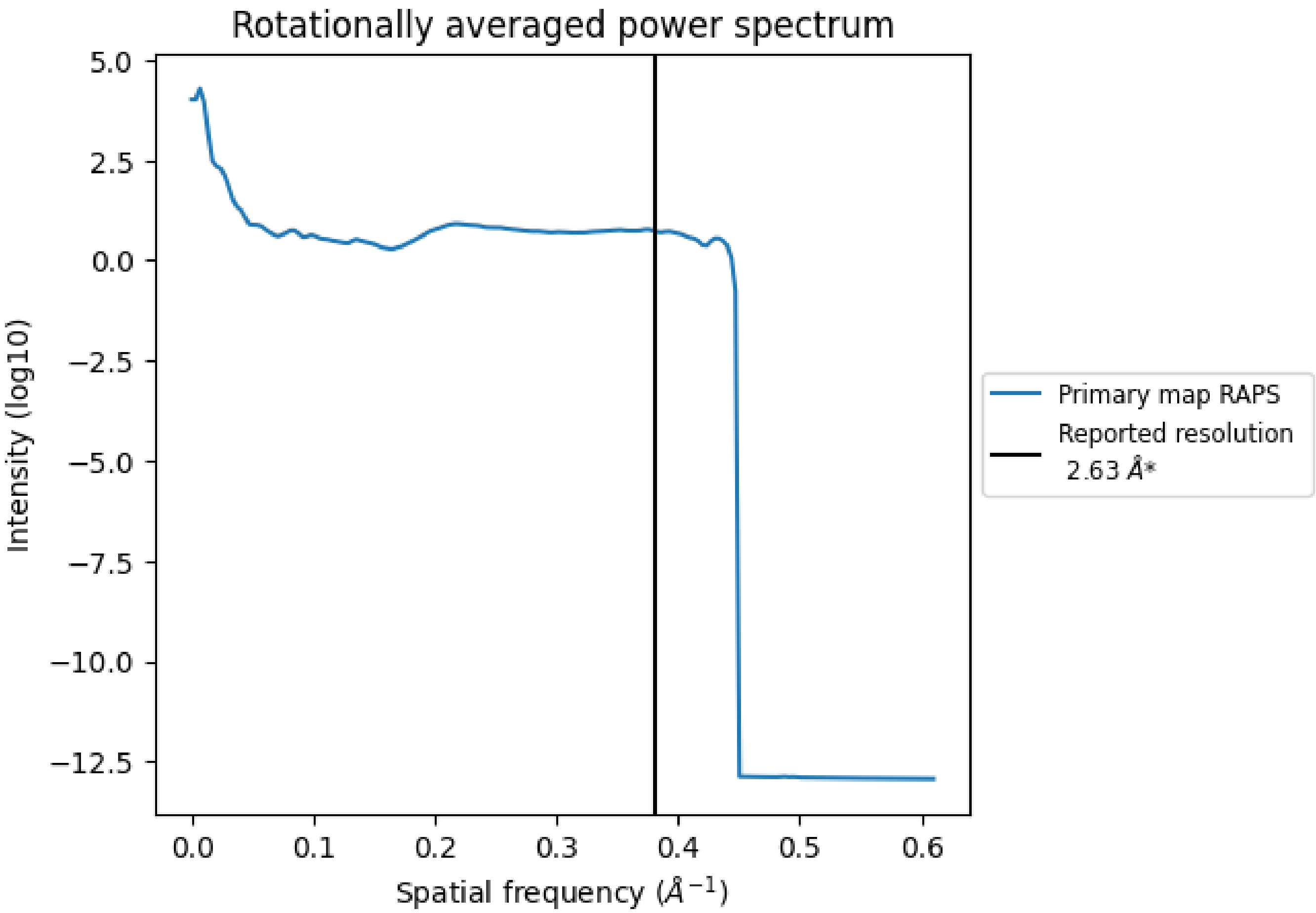
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 110 nm^3; this corresponds to an approximate mass of 100 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 ⓘ

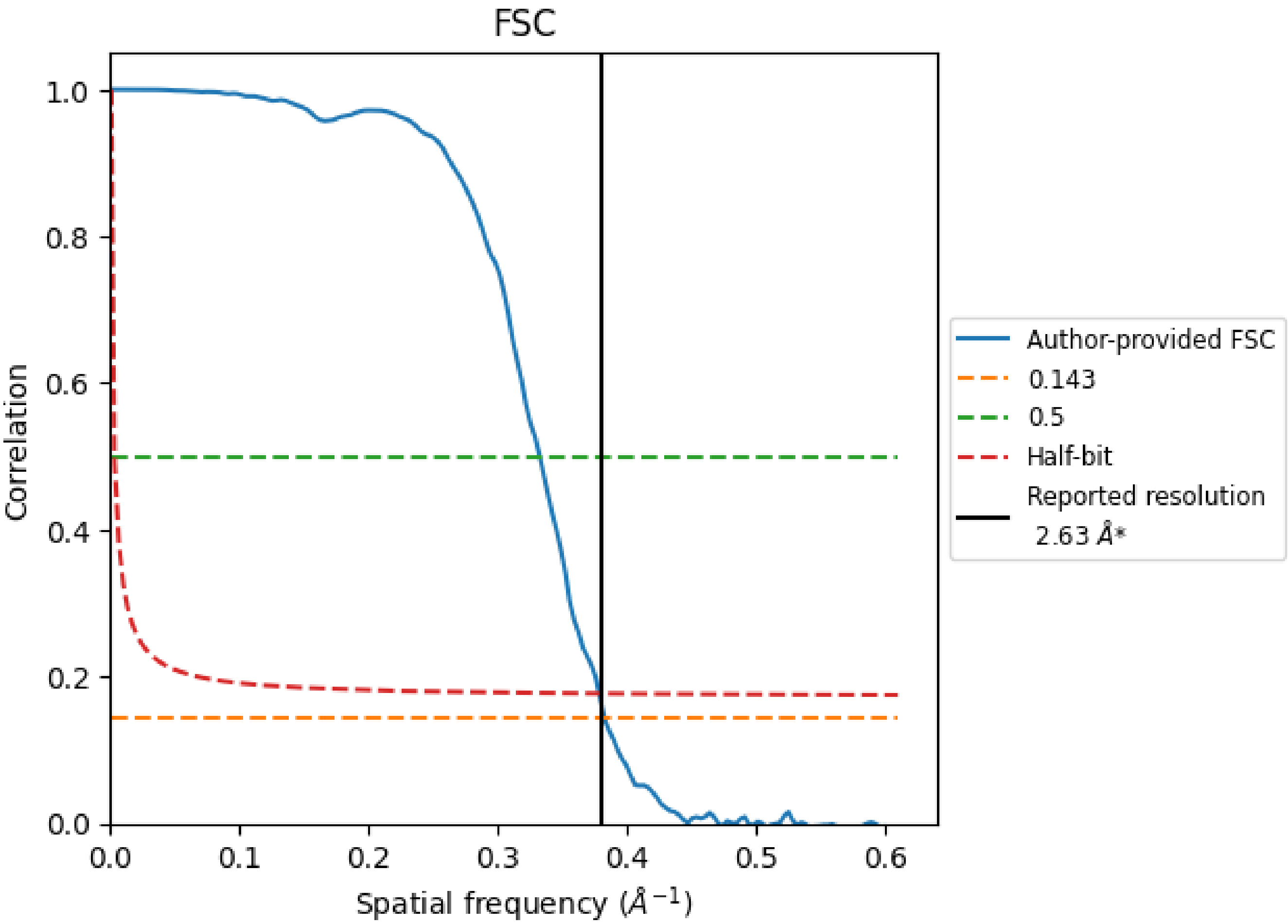


*Reported resolution corresponds to spatial frequency of 0.380 $Å^{-1}$

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.380 $Å^{-1}$

8.2 Resolution estimates

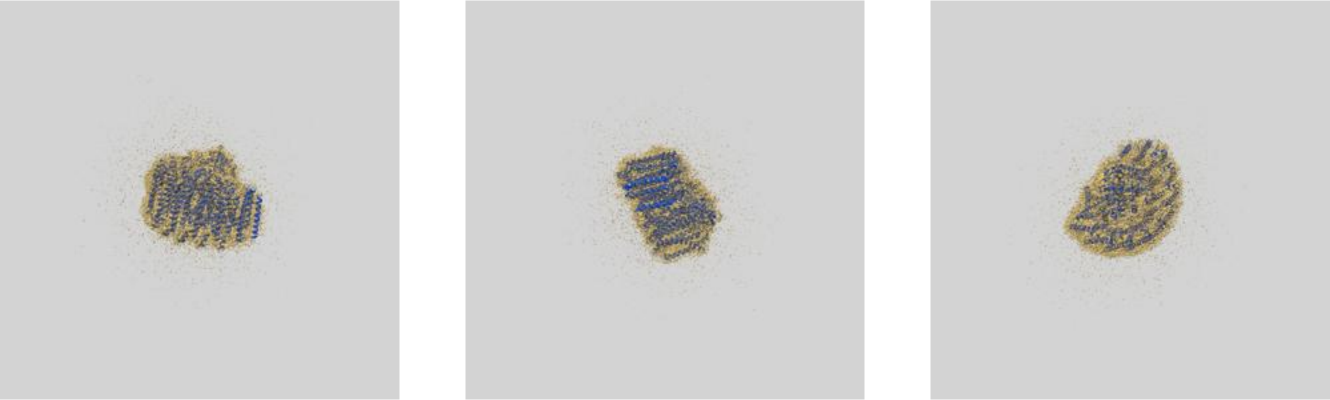
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.63	-	-
Author-provided FSC curve	2.61	3.01	2.64
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-32193 and PDB model 7VY3. Per-residue inclusion information can be found in section 3 on page 15.

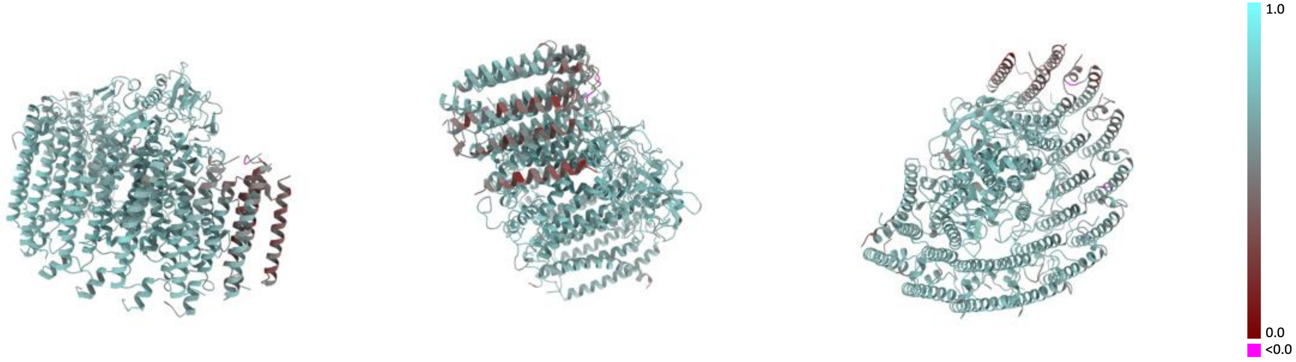
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

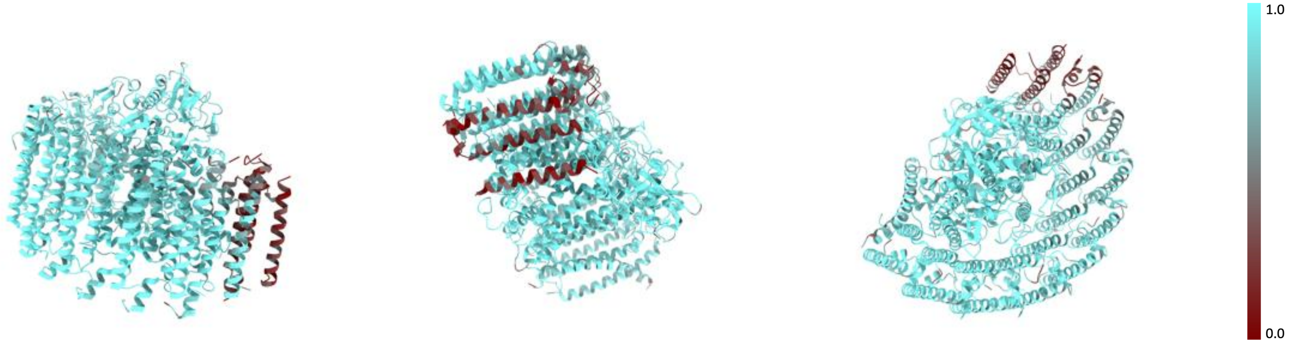
9.2 Q-score mapped to coordinate model ⓘ



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.

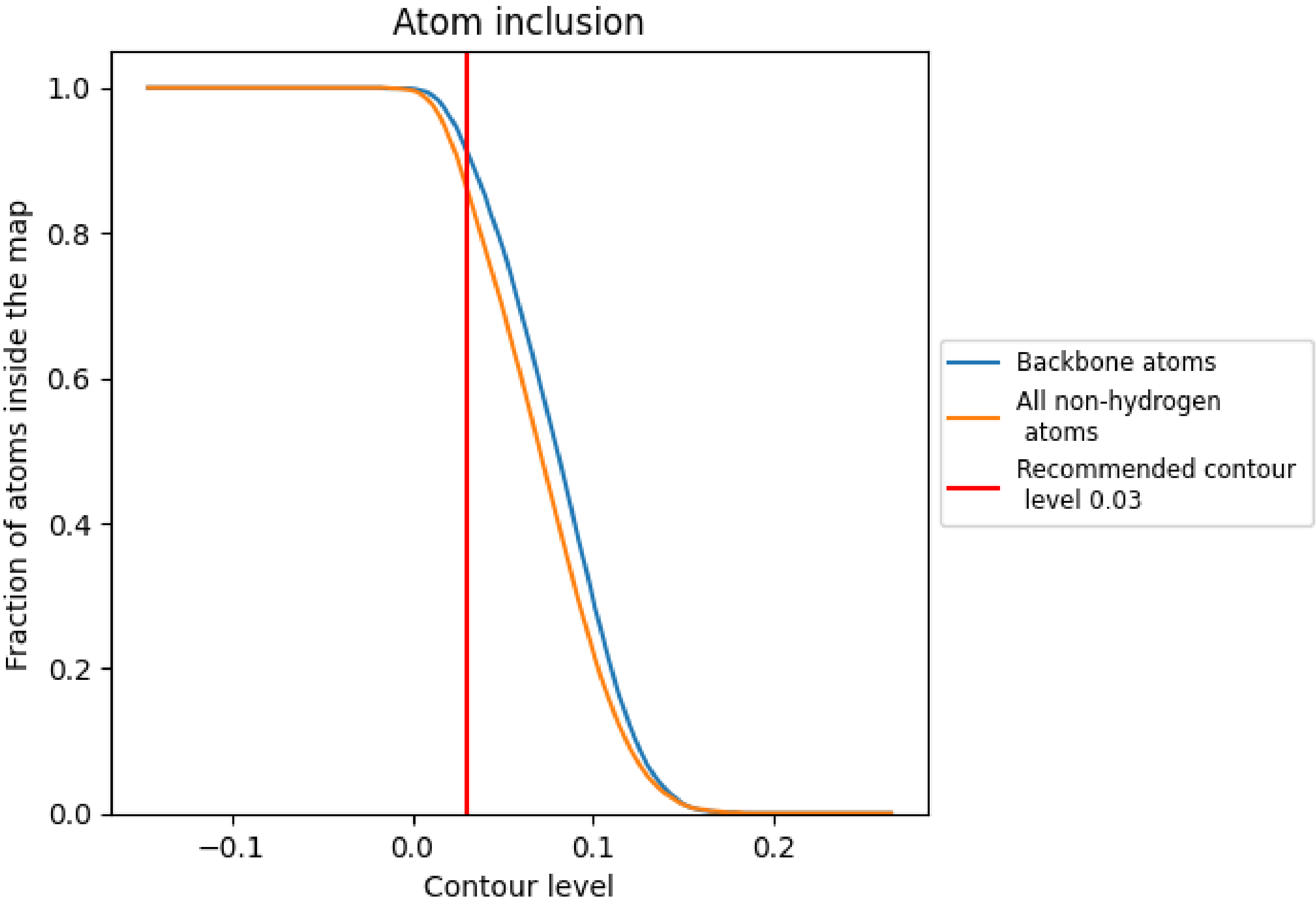
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.03).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8620	0.6280
1	0.2040	0.3620
A	0.9210	0.6360
B	0.8550	0.6120
D	0.9070	0.6430
E	0.9330	0.6520
F	0.9070	0.6460
G	0.9140	0.6500
H	0.9030	0.6430
I	0.9270	0.6470
J	0.9280	0.6550
K	0.9070	0.6410
L	0.9560	0.6780
M	0.9550	0.6760
N	0.9260	0.6500
O	0.9190	0.6440
P	0.8730	0.6150
Q	0.8430	0.6100
R	0.8790	0.6260
S	0.8460	0.6120
T	0.8020	0.5860
V	0.6940	0.5490
W	0.6740	0.5360
X	0.7780	0.6000
Y	0.3450	0.4390
Z	0.2350	0.3920