



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 09:21 AM JST

PDB ID : 7VNY / pdb_00007vny
EMDB ID : EMD-32047
Title : Rba sphaeroides WT RC-LH1 monomer
Authors : Bracun, L.; Yamagata, A.; Liu, L.N.; Shirouzu, M.
Deposited on : 2021-10-12
Resolution : 2.79 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

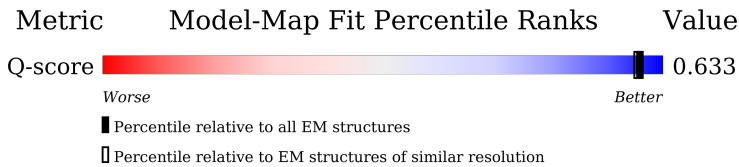
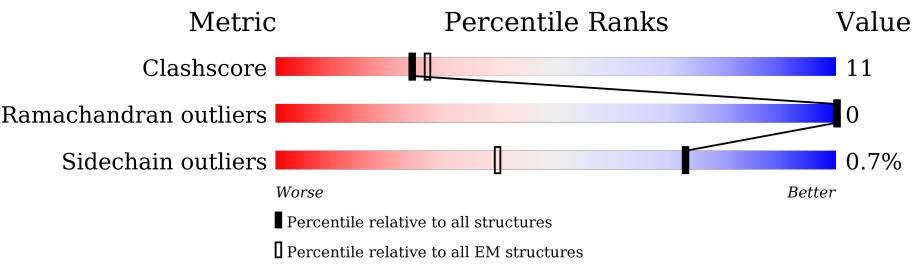
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.79 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10811 (2.29 - 3.29)

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 $\leq 5\%$. 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	282	83%17%
2	M	308	81%18%
3	H	260	7% 80%15%5%
4	1	58	38% 74%17%9%

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Mol	Chain	Length	Quality of chain
4	3	58	
4	7	58	
4	9	58	
4	A	58	
4	D	58	
4	F	58	
4	I	58	
4	K	58	
4	O	58	
4	Q	58	
4	S	58	
4	U	58	
4	W	58	
5	0	49	
5	2	49	
5	8	49	
5	B	49	
5	C	49	
5	E	49	
5	G	49	
5	J	49	
5	N	49	
5	P	49	
5	R	49	
5	T	49	

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Mol	Chain	Length	Quality of chain
5	V	49	
5	Z	49	
6	X	82	
7	Y	53	

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
13	SPO	0	101	-	X	-	-
13	SPO	3	102	-	X	-	-
13	SPO	3	104	-	X	-	-
13	SPO	8	102	-	X	-	-
13	SPO	9	102	-	X	-	-
13	SPO	B	101	-	X	-	-
13	SPO	D	102	-	X	-	-
13	SPO	D	103	-	X	-	-
13	SPO	E	102	-	X	-	-
13	SPO	F	102	-	X	-	-
13	SPO	G	101	-	X	-	-
13	SPO	I	102	-	X	-	-
13	SPO	J	101	-	X	-	-
13	SPO	J	103	-	X	-	-
13	SPO	M	405	-	X	-	-
13	SPO	N	102	-	X	-	-
13	SPO	O	102	-	X	-	-
13	SPO	O	104	-	X	-	-
13	SPO	P	101	-	X	-	-
13	SPO	T	101	-	X	-	-
13	SPO	T	102	-	X	-	-
13	SPO	U	102	-	X	-	-
13	SPO	U	104	-	X	-	-
13	SPO	V	101	-	X	-	-
13	SPO	W	103	-	X	-	-
13	SPO	X	101	-	X	-	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 22472 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 Reaction center protein L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L	281	Total	C	N	O	S	0	0
			2232	1507	355	362	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	M	305	Total	C	N	O	S	0	0
			2431	1623	397	400	11		

- Molecule 3 is a protein called Reaction center protein H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	247	Total	C	N	O	S	0	0
			1875	1202	318	345	10		

- Molecule 4 is a protein called Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	D	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	F	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	I	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	K	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	O	54	Total	C	N	O	S	0	0
			455	310	73	69	3		
4	Q	54	Total	C	N	O	S	0	0
			455	310	73	69	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	S	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	U	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	W	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	3	54	Total 455	C 310	N 73	O 69	S 3	0	0
4	1	53	Total 447	C 305	N 72	O 68	S 2	0	0
4	7	46	Total 392	C 271	N 60	O 58	S 3	0	0
4	9	54	Total 455	C 310	N 73	O 69	S 3	0	0

- Molecule 5 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	45	Total 365	C 243	N 57	O 64	S 1	0	0
5	E	43	Total 351	C 236	N 55	O 59	S 1	0	0
5	G	43	Total 351	C 236	N 55	O 59	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 351	C 236	N 55	O 59	S 1	0	0
5	T	43	Total 351	C 236	N 55	O 59	S 1	0	0
5	V	43	Total 351	C 236	N 55	O 59	S 1	0	0
5	C	43	Total 351	C 236	N 55	O 59	S 1	0	0
5	Z	42	Total 343	C 230	N 54	O 58	S 1	0	0
5	2	39	Total 316	C 210	N 51	O 54	S 1	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
5	0	44	Total	C	N	O	S	0	0
			359	240	56	62	1		

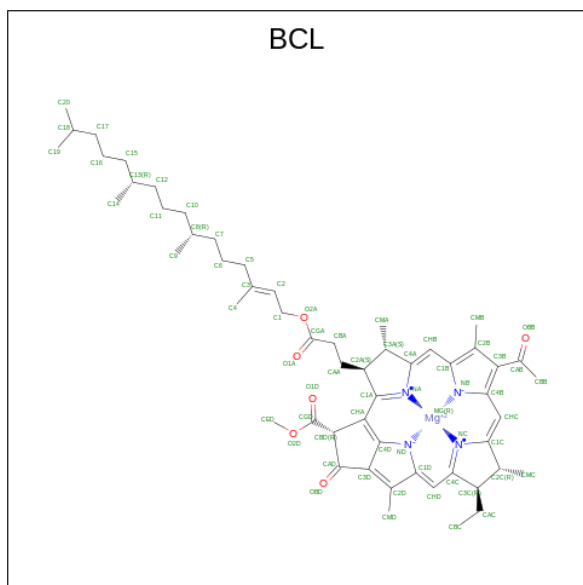
- Molecule 6 is a protein called Intrinsic membrane protein PufX.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	52	Total	C	N	O	S	0	0
			406	270	71	62	3		

- Molecule 7 is a protein called Rsp_7571 Protein-Y PufY.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	50	Total	C	N	O	S	0	0
			368	250	57	58	3		

- Molecule 8 is BACTERIOCHLOROPHYLL A (CCD ID: BCL) (formula: $C_{55}H_{74}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	L	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	L	1	Total	C	Mg	N	O	0
			63	52	1	4	6	

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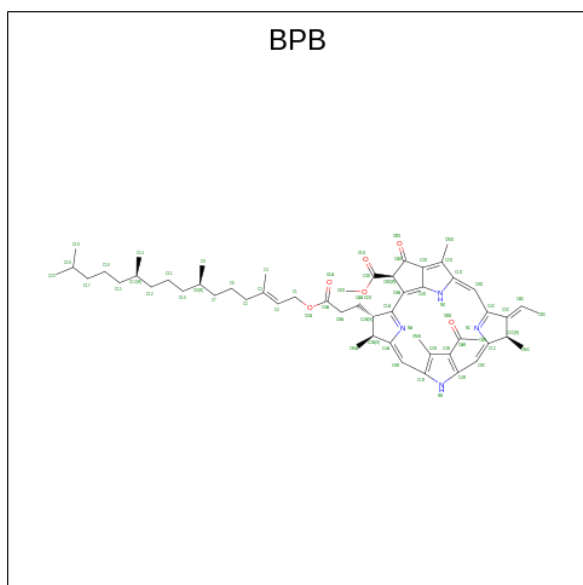
Mol	Chain	Residues	Atoms					AltConf
8	L	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	M	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	A	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	D	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	E	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	F	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	I	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	J	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	K	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	O	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	Q	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	R	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	S	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	U	1	Total 66	C 55	Mg 1	N 4	O 6	0
8	W	1	Total 66	C 55	Mg 1	N 4	O 6	0

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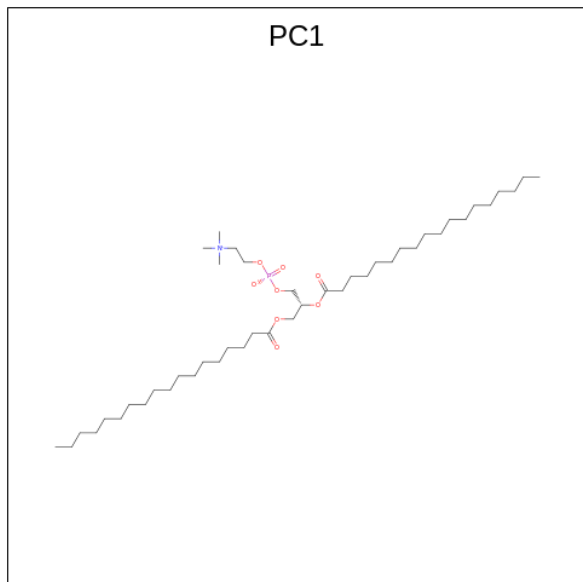
Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
8	1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
8	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	8	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
8	9	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
8	0	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 9 is BACTERIOPHEOPHYTIN B (CCD ID: BPB) (formula: $C_{55}H_{74}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



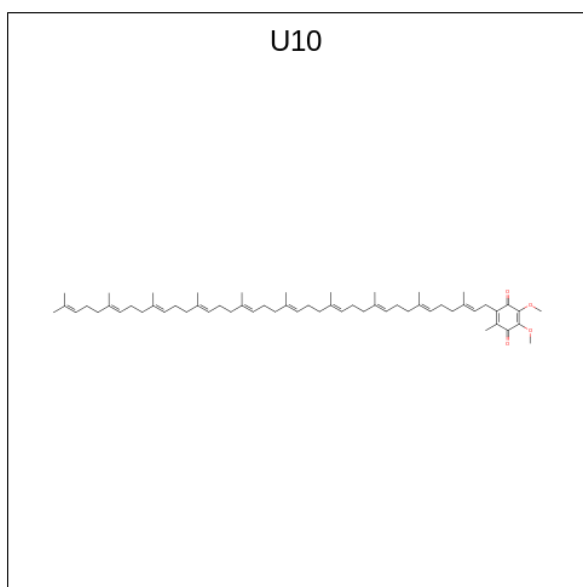
Mol	Chain	Residues	Atoms				AltConf
9	L	1	Total	C	N	O	0
			62	52	4	6	
9	M	1	Total	C	N	O	0
			55	45	4	6	

- Molecule 10 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
10	L	1	Total	C	N	O	P	0
			36	26	1	8	1	
10	H	1	Total	C	N	O	P	0
			40	30	1	8	1	
10	H	1	Total	C	N	O	P	0
			42	32	1	8	1	
10	H	1	Total	C	N	O	P	0
			20	10	1	8	1	
10	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
10	A	1	Total	C	N	O	P	0
			32	22	1	8	1	
10	D	1	Total	C	N	O	P	0
			37	27	1	8	1	
10	W	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 11 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

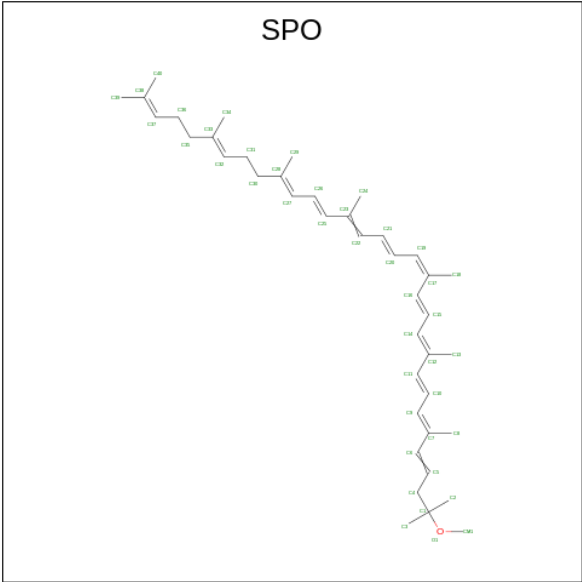


Mol	Chain	Residues	Atoms			AltConf
11	L	1	Total	C	O	0
			43	39	4	
11	L	1	Total	C	O	0
			38	34	4	
11	M	1	Total	C	O	0
			48	44	4	
11	Y	1	Total	C	O	0
			38	34	4	

- Molecule 12 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 13 is SPHEROIDENE (CCD ID: SPO) (formula: C₄₁H₆₀O) (labeled as "Ligand of Interest" by depositor).



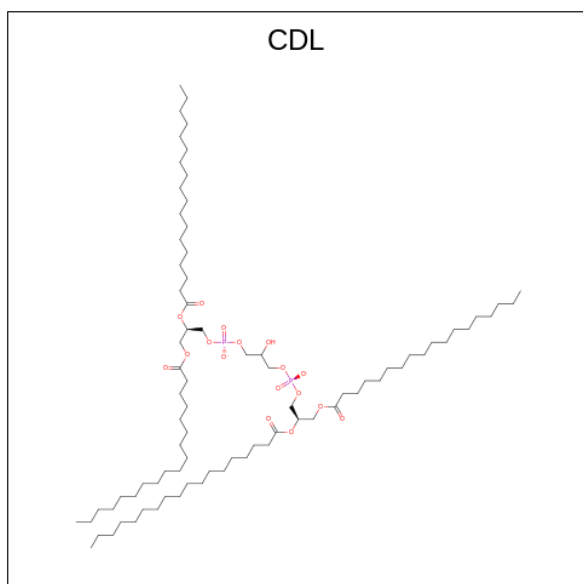
Mol	Chain	Residues	Atoms			AltConf
13	M	1	Total	C	O	0
			42	41	1	
13	B	1	Total	C	O	0
			42	41	1	
13	D	1	Total	C	O	0
			42	41	1	
13	D	1	Total	C	O	0
			42	41	1	
13	E	1	Total	C	O	0
			42	41	1	
13	F	1	Total	C	O	0
			42	41	1	
13	G	1	Total	C	O	0
			42	41	1	
13	I	1	Total	C	O	0
			42	41	1	
13	J	1	Total	C	O	0
			42	41	1	
13	J	1	Total	C	O	0
			42	41	1	
13	N	1	Total	C	O	0
			42	41	1	
13	O	1	Total	C	O	0
			42	41	1	
13	O	1	Total	C	O	0
			42	41	1	
13	P	1	Total	C	O	0
			42	41	1	

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Mol	Chain	Residues	Atoms			AltConf
13	T	1	Total	C	O	0
			42	41	1	
13	T	1	Total	C	O	0
			42	41	1	
13	U	1	Total	C	O	0
			42	41	1	
13	U	1	Total	C	O	0
			42	41	1	
13	V	1	Total	C	O	0
			42	41	1	
13	W	1	Total	C	O	0
			42	41	1	
13	3	1	Total	C	O	0
			42	41	1	
13	3	1	Total	C	O	0
			42	41	1	
13	8	1	Total	C	O	0
			42	41	1	
13	9	1	Total	C	O	0
			42	41	1	
13	0	1	Total	C	O	0
			42	41	1	
13	X	1	Total	C	O	0
			39	38	1	

- Molecule 14 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

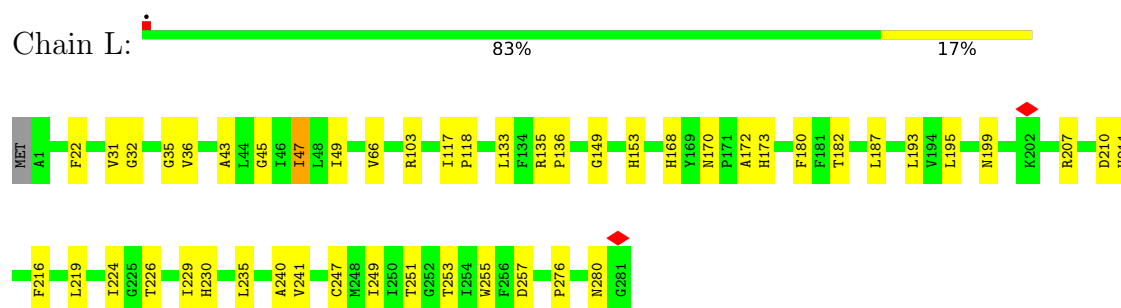


Mol	Chain	Residues	Atoms				AltConf
14	M	1	Total	C	O	P	0
			100	81	17	2	
14	H	1	Total	C	O	P	0
			78	59	17	2	

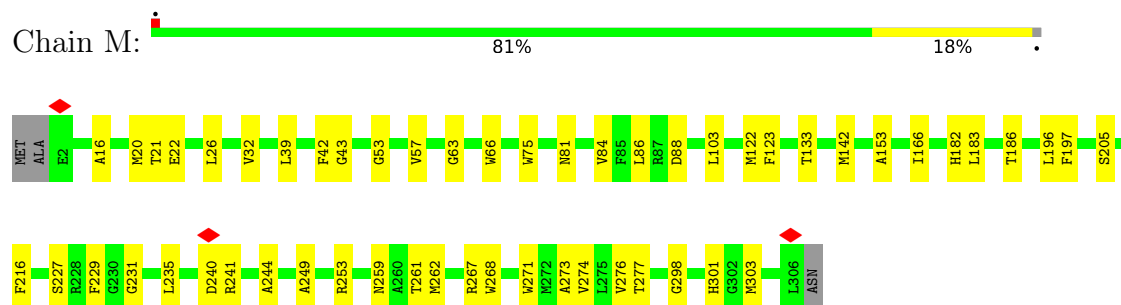
3 Residue-property plots

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.

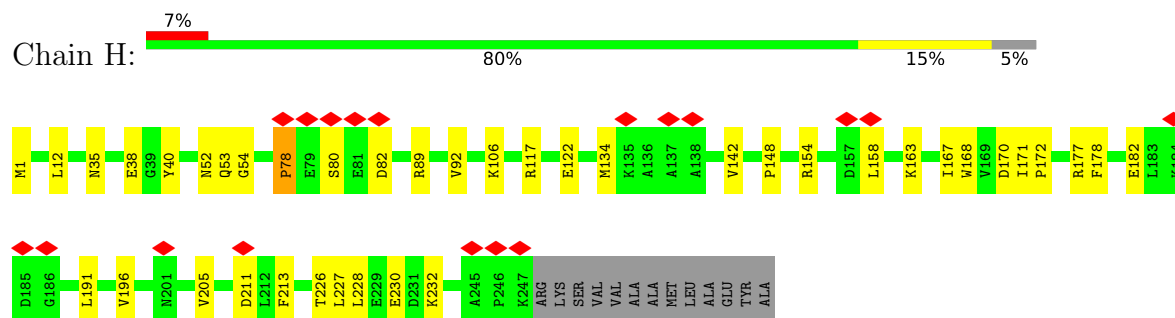
- Molecule 1: Reaction center protein L chain



- Molecule 2: Reaction center protein M chain



- Molecule 3: Reaction center protein H chain

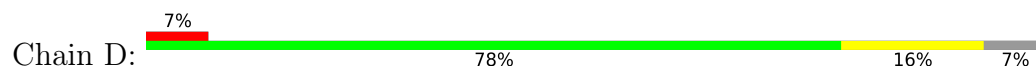


- Molecule 4: Light-harvesting protein B-875 alpha chain

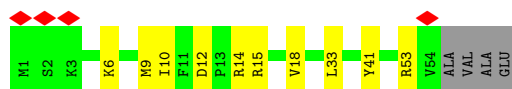
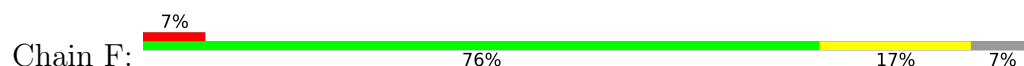




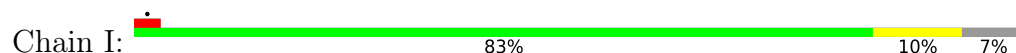
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- Molecule 4: Light-harvesting protein B-875 alpha chain



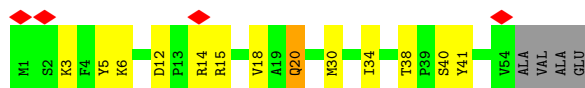
- Molecule 4: Light-harvesting protein B-875 alpha chain



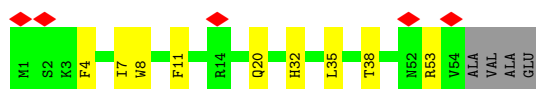
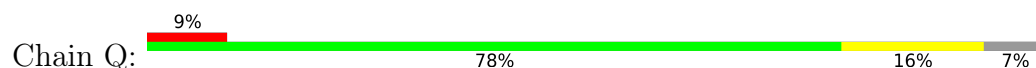
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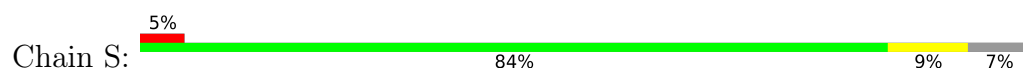
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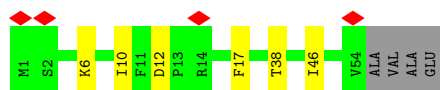
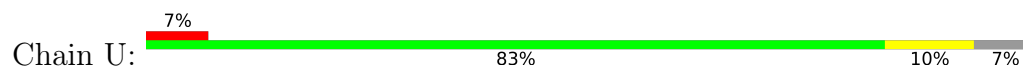
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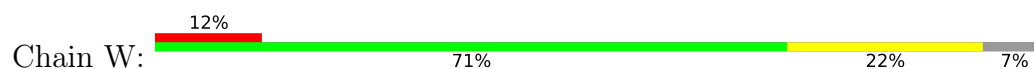
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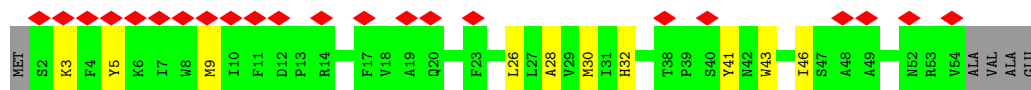
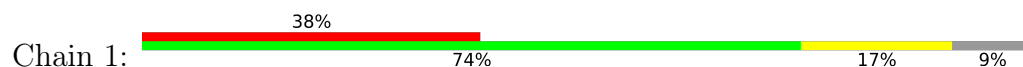
- Molecule 4: Light-harvesting protein B-875 alpha chain



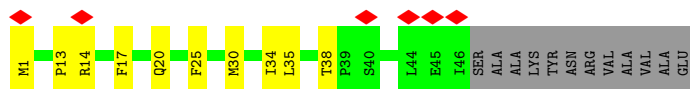
- Molecule 4: Light-harvesting protein B-875 alpha chain



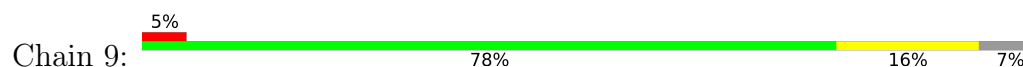
- Molecule 4: Light-harvesting protein B-875 alpha chain



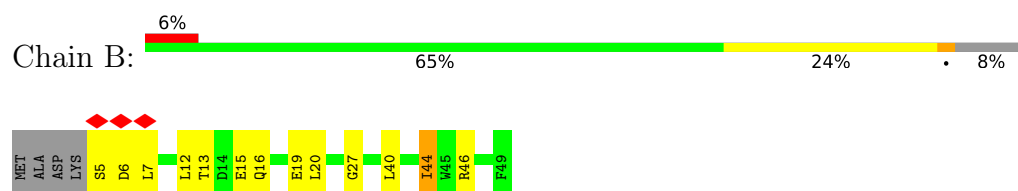
- Molecule 4: Light-harvesting protein B-875 alpha chain



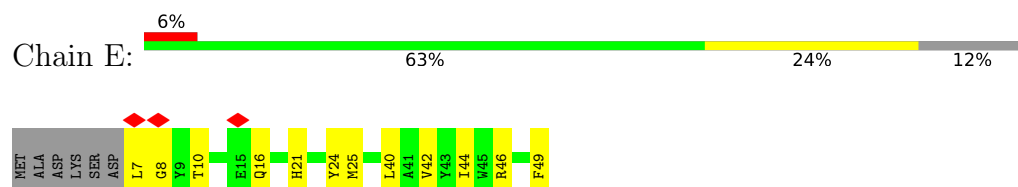
- Molecule 4: Light-harvesting protein B-875 alpha chain



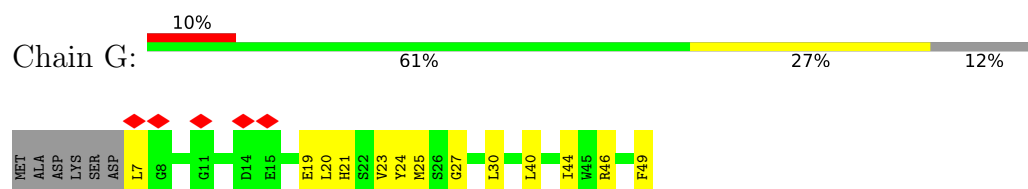
- Molecule 5: Light-harvesting protein B-875 beta chain



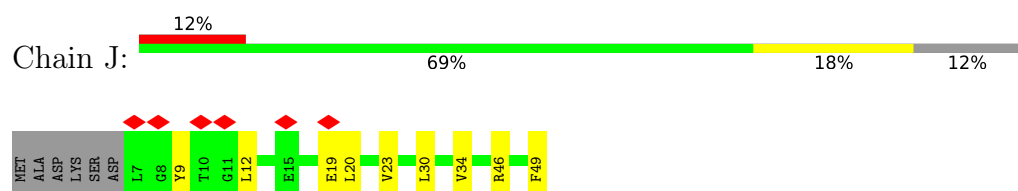
- Molecule 5: Light-harvesting protein B-875 beta chain



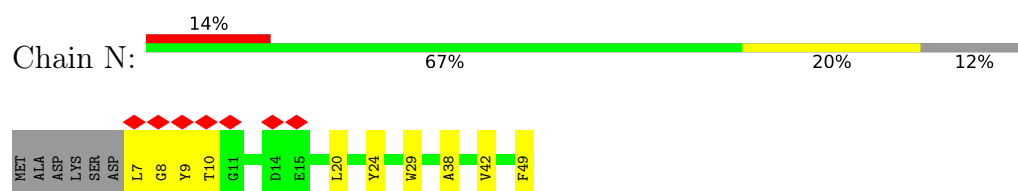
- Molecule 5: Light-harvesting protein B-875 beta chain



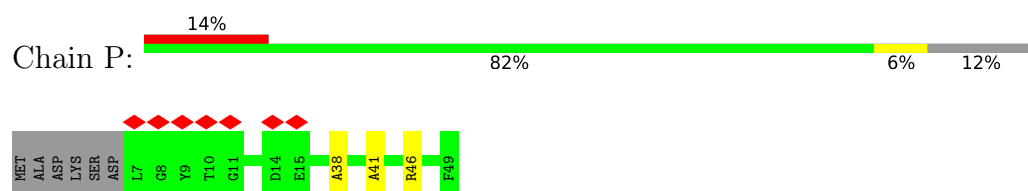
- Molecule 5: Light-harvesting protein B-875 beta chain



- Molecule 5: Light-harvesting protein B-875 beta chain

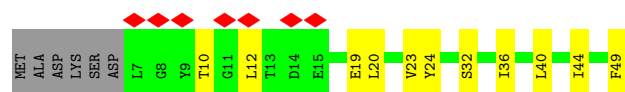


- Molecule 5: Light-harvesting protein B-875 beta chain

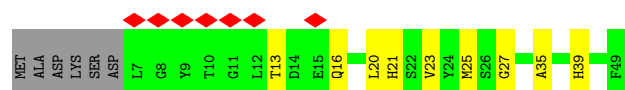
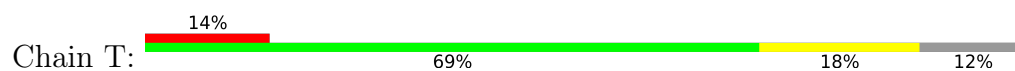


- Molecule 5: Light-harvesting protein B-875 beta chain

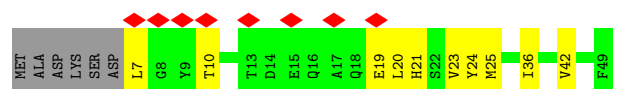




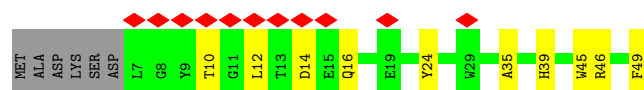
- Molecule 5: Light-harvesting protein B-875 beta chain



- Molecule 5: Light-harvesting protein B-875 beta chain



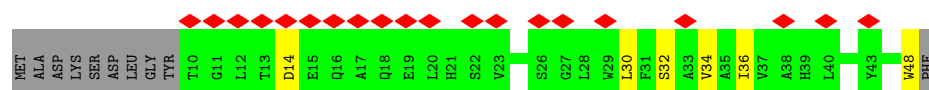
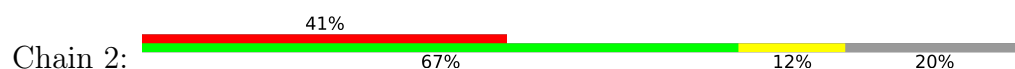
- Molecule 5: Light-harvesting protein B-875 beta chain



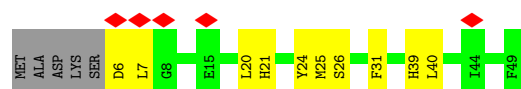
- Molecule 5: Light-harvesting protein B-875 beta chain



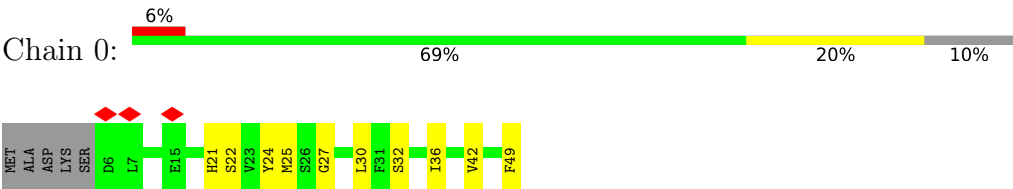
- Molecule 5: Light-harvesting protein B-875 beta chain



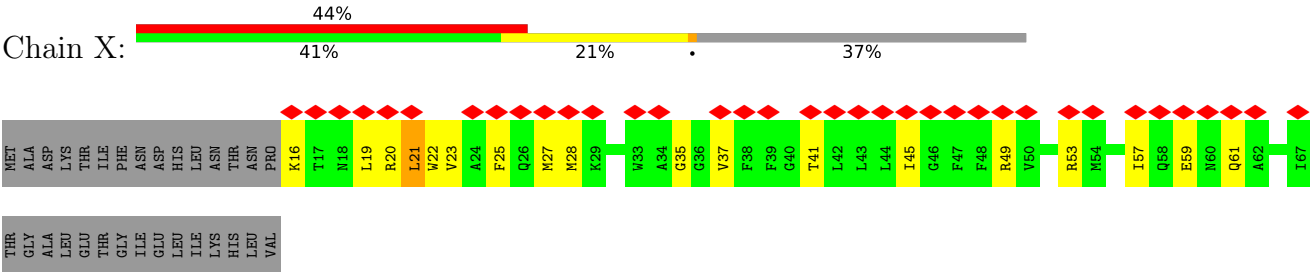
- Molecule 5: Light-harvesting protein B-875 beta chain



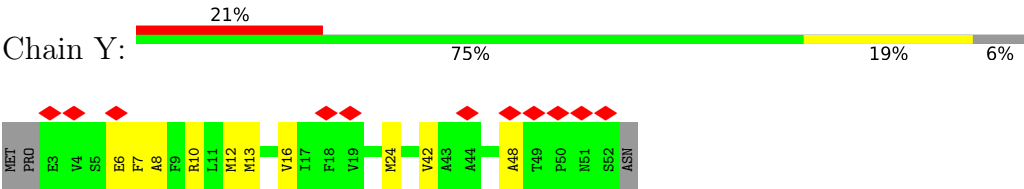
- Molecule 5: Light-harvesting protein B-875 beta chain



• Molecule 6: Intrinsic membrane protein PufX



• Molecule 7: Rsp_7571 Protein-Y PufY



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68554	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 ($e^-/\text{\AA}^2$)	45.026	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.295	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	265.0, 265.0, 265.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, PC1, SPO, BCL, U10, CDL, BPB

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	0.21	0/2320	0.37	0/3175
2	M	0.23	0/2524	0.40	0/3446
3	H	0.23	0/1925	0.44	2/2620 (0.1%)
4	1	0.15	0/461	0.33	0/625
4	3	0.20	0/469	0.40	0/635
4	7	0.17	0/405	0.32	0/549
4	9	0.21	0/469	0.34	0/635
4	A	0.18	0/469	0.31	0/635
4	D	0.19	0/469	0.30	0/635
4	F	0.20	0/469	0.35	0/635
4	I	0.18	0/469	0.29	0/635
4	K	0.19	0/469	0.40	0/635
4	O	0.20	0/469	0.34	0/635
4	Q	0.20	0/469	0.37	0/635
4	S	0.23	0/469	0.43	1/635 (0.2%)
4	U	0.20	0/469	0.35	0/635
4	W	0.24	0/469	0.43	0/635
5	0	0.20	0/372	0.32	0/510
5	2	0.24	0/327	0.43	0/449
5	8	0.21	0/372	0.33	0/510
5	B	0.20	0/378	0.34	0/518
5	C	0.17	0/364	0.29	0/499
5	E	0.19	0/364	0.38	0/499
5	G	0.20	0/364	0.31	0/499
5	J	0.20	0/364	0.35	0/499
5	N	0.19	0/364	0.30	0/499
5	P	0.17	0/364	0.29	0/499
5	R	0.19	0/364	0.30	0/499
5	T	0.19	0/364	0.31	0/499
5	V	0.19	0/364	0.37	0/499
5	Z	0.16	0/356	0.31	0/488
6	X	0.18	0/417	0.35	0/563

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	Y	0.18	0/379	0.37	0/513
All	All	0.21	0/19140	0.37	3/26077 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	78	PRO	CA-N-CD	-11.90	95.34	112.00
3	H	78	PRO	N-CD-CG	-5.86	94.41	103.20
4	S	39	PRO	CA-N-CD	-5.52	104.27	112.00

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	2232	0	2187	37	0
2	M	2431	0	2345	46	0
3	H	1875	0	1877	31	0
4	1	447	0	465	7	0
4	3	455	0	477	9	0
4	7	392	0	412	11	0
4	9	455	0	477	7	0
4	A	455	0	477	12	0
4	D	455	0	477	8	0
4	F	455	0	477	9	0
4	I	455	0	477	5	0
4	K	455	0	477	12	0
4	O	455	0	477	10	0
4	Q	455	0	477	8	0
4	S	455	0	477	6	0
4	U	455	0	477	6	0
4	W	455	0	477	15	0
5	0	359	0	340	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	2	316	0	304	4	0
5	8	359	0	340	13	0
5	B	365	0	345	9	0
5	C	351	0	336	10	0
5	E	351	0	336	13	0
5	G	351	0	336	10	0
5	J	351	0	336	7	0
5	N	351	0	336	14	0
5	P	351	0	336	4	0
5	R	351	0	336	9	0
5	T	351	0	336	7	0
5	V	351	0	336	9	0
5	Z	343	0	325	5	0
6	X	406	0	420	17	0
7	Y	368	0	363	7	0
8	0	61	0	61	3	0
8	1	117	0	112	3	0
8	3	132	0	148	2	0
8	7	66	0	74	8	0
8	8	61	0	61	4	0
8	9	66	0	74	3	0
8	A	132	0	148	9	0
8	C	66	0	74	2	0
8	D	66	0	74	2	0
8	E	66	0	74	1	0
8	F	132	0	148	5	0
8	I	66	0	74	1	0
8	J	66	0	74	5	0
8	K	66	0	74	0	0
8	L	195	0	213	5	0
8	M	66	0	74	1	0
8	N	66	0	74	4	0
8	O	132	0	148	4	0
8	Q	66	0	74	1	0
8	R	66	0	74	6	0
8	S	132	0	148	6	0
8	U	132	0	148	8	0
8	W	66	0	74	4	0
9	L	62	0	65	3	0
9	M	55	0	51	4	0
10	A	77	0	105	13	0
10	D	37	0	48	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	H	102	0	130	11	0
10	L	71	0	90	3	0
10	W	37	0	48	5	0
11	L	81	0	102	6	0
11	M	48	0	63	3	0
11	Y	38	0	47	2	0
12	M	1	0	0	0	0
13	0	42	0	59	8	0
13	3	84	0	117	16	0
13	8	42	0	59	5	0
13	9	42	0	60	5	0
13	B	42	0	60	10	0
13	D	84	0	119	12	0
13	E	42	0	60	4	0
13	F	42	0	59	8	0
13	G	42	0	58	6	0
13	I	42	0	59	7	0
13	J	84	0	117	11	0
13	M	42	0	60	7	0
13	N	42	0	60	9	0
13	O	84	0	120	10	0
13	P	42	0	58	5	0
13	T	84	0	120	17	0
13	U	84	0	119	12	0
13	V	42	0	59	8	0
13	W	42	0	60	8	0
13	X	39	0	53	6	0
14	H	78	0	106	6	0
14	M	100	0	156	4	0
All	All	22472	0	23315	490	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 490 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)
5:V:7:LEU:HD23	5:C:16:GLN:HE22	1.44	0.82
4:S:6:LYS:NZ	5:V:19:GLU:OE2	2.13	0.81
4:W:9:MET:HE1	5:C:14:ASP:HA	1.61	0.80
4:3:40:SER:O	5:Z:46:ARG:NH1	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:153:ALA:HA	2:M:277:THR:HG21	1.65	0.79

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	279/282 (99%)	267 (96%)	12 (4%)	0	100	100
2	M	303/308 (98%)	296 (98%)	7 (2%)	0	100	100
3	H	245/260 (94%)	240 (98%)	5 (2%)	0	100	100
4	1	51/58 (88%)	48 (94%)	3 (6%)	0	100	100
4	3	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	7	44/58 (76%)	43 (98%)	1 (2%)	0	100	100
4	9	52/58 (90%)	52 (100%)	0	0	100	100
4	A	52/58 (90%)	52 (100%)	0	0	100	100
4	D	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	F	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	I	52/58 (90%)	52 (100%)	0	0	100	100
4	K	52/58 (90%)	52 (100%)	0	0	100	100
4	O	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	Q	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
4	S	52/58 (90%)	52 (100%)	0	0	100	100
4	U	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
4	W	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
5	0	42/49 (86%)	42 (100%)	0	0	100	100
5	2	37/49 (76%)	37 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	8	42/49 (86%)	42 (100%)	0	0	100	100
5	B	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
5	C	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	E	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
5	G	41/49 (84%)	41 (100%)	0	0	100	100
5	J	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
5	N	41/49 (84%)	41 (100%)	0	0	100	100
5	P	41/49 (84%)	41 (100%)	0	0	100	100
5	R	41/49 (84%)	41 (100%)	0	0	100	100
5	T	41/49 (84%)	41 (100%)	0	0	100	100
5	V	41/49 (84%)	41 (100%)	0	0	100	100
5	Z	40/49 (82%)	40 (100%)	0	0	100	100
6	X	50/82 (61%)	50 (100%)	0	0	100	100
7	Y	48/53 (91%)	48 (100%)	0	0	100	100
All	All	2217/2483 (89%)	2173 (98%)	44 (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	220/221 (100%)	219 (100%)	1 (0%)	81	93
2	M	239/241 (99%)	239 (100%)	0	100	100
3	H	199/208 (96%)	199 (100%)	0	100	100
4	1	48/51 (94%)	48 (100%)	0	100	100
4	3	49/51 (96%)	48 (98%)	1 (2%)	48	80
4	7	43/51 (84%)	43 (100%)	0	100	100
4	9	49/51 (96%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	49/51 (96%)	48 (98%)	1 (2%)	48	80
4	D	49/51 (96%)	49 (100%)	0	100	100
4	F	49/51 (96%)	49 (100%)	0	100	100
4	I	49/51 (96%)	48 (98%)	1 (2%)	48	80
4	K	49/51 (96%)	49 (100%)	0	100	100
4	O	49/51 (96%)	48 (98%)	1 (2%)	48	80
4	Q	49/51 (96%)	49 (100%)	0	100	100
4	S	49/51 (96%)	49 (100%)	0	100	100
4	U	49/51 (96%)	48 (98%)	1 (2%)	48	80
4	W	49/51 (96%)	49 (100%)	0	100	100
5	0	36/40 (90%)	35 (97%)	1 (3%)	38	73
5	2	32/40 (80%)	32 (100%)	0	100	100
5	8	36/40 (90%)	36 (100%)	0	100	100
5	B	37/40 (92%)	35 (95%)	2 (5%)	20	51
5	C	35/40 (88%)	35 (100%)	0	100	100
5	E	35/40 (88%)	35 (100%)	0	100	100
5	G	35/40 (88%)	34 (97%)	1 (3%)	37	73
5	J	35/40 (88%)	35 (100%)	0	100	100
5	N	35/40 (88%)	35 (100%)	0	100	100
5	P	35/40 (88%)	35 (100%)	0	100	100
5	R	35/40 (88%)	35 (100%)	0	100	100
5	T	35/40 (88%)	35 (100%)	0	100	100
5	V	35/40 (88%)	34 (97%)	1 (3%)	37	73
5	Z	34/40 (85%)	34 (100%)	0	100	100
6	X	40/66 (61%)	38 (95%)	2 (5%)	22	54
7	Y	34/37 (92%)	34 (100%)	0	100	100
All	All	1901/2047 (93%)	1888 (99%)	13 (1%)	73	91

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	U	46	ILE
5	V	36	ILE

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Mol	Chain	Res	Type
6	X	27	MET
5	0	22	SER
6	X	21	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
5	V	16	GLN
4	W	42	ASN
6	X	60	ASN
5	C	16	GLN
3	H	68	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 76 ligands modelled in this entry, 1 is monoatomic - leaving 75 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	$\# Z > 2$
13	SPO	V	101	-	40,41,41	3.32	21 (52%)	47,50,50	12.23	32 (68%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	I	101	4	69,74,74	1.17	7 (10%)	83,115,115	1.49	13 (15%)
8	BCL	Q	101	4	69,74,74	1.17	6 (8%)	83,115,115	1.52	12 (14%)
13	SPO	P	101	-	40,41,41	3.65	23 (57%)	47,50,50	10.39	29 (61%)
8	BCL	7	101	5	69,74,74	1.12	6 (8%)	83,115,115	1.56	11 (13%)
8	BCL	3	103	5	69,74,74	1.10	4 (5%)	83,115,115	1.41	10 (12%)
13	SPO	T	102	-	40,41,41	3.57	21 (52%)	47,50,50	10.06	31 (65%)
11	U10	L	305	-	43,43,63	2.69	13 (30%)	52,55,79	1.68	13 (25%)
13	SPO	O	102	-	40,41,41	3.45	20 (50%)	47,50,50	10.05	32 (68%)
8	BCL	C	101	5	69,74,74	1.10	5 (7%)	83,115,115	1.50	12 (14%)
8	BCL	J	102	5	69,74,74	1.14	5 (7%)	83,115,115	1.46	11 (13%)
8	BCL	A	103	5	69,74,74	1.09	5 (7%)	83,115,115	1.49	12 (14%)
14	CDL	H	304	-	77,77,99	1.27	6 (7%)	83,89,111	1.45	6 (7%)
8	BCL	R	101	5	69,74,74	1.12	5 (7%)	83,115,115	1.56	11 (13%)
8	BCL	9	101	4	69,74,74	1.13	7 (10%)	83,115,115	1.58	13 (15%)
8	BCL	1	101	4	59,64,74	1.25	6 (10%)	71,103,115	1.63	15 (21%)
8	BCL	O	101	4	69,74,74	1.16	7 (10%)	83,115,115	1.50	12 (14%)
11	U10	M	404	-	48,48,63	2.68	14 (29%)	58,61,79	1.62	14 (24%)
11	U10	Y	501	-	38,38,63	2.69	12 (31%)	46,49,79	1.58	10 (21%)
13	SPO	B	101	-	40,41,41	3.37	21 (52%)	47,50,50	10.36	31 (65%)
10	PC1	H	303	-	19,19,53	2.14	6 (31%)	21,25,61	1.03	1 (4%)
8	BCL	L	307	2	69,74,74	1.14	7 (10%)	83,115,115	1.66	16 (19%)
13	SPO	0	101	-	40,41,41	3.50	22 (55%)	47,50,50	11.31	30 (63%)
8	BCL	A	101	4	69,74,74	1.16	7 (10%)	83,115,115	1.47	12 (14%)
10	PC1	H	302	-	41,41,53	1.35	6 (14%)	47,49,61	1.20	4 (8%)
8	BCL	8	101	4	64,69,74	1.17	5 (7%)	77,109,115	1.48	10 (12%)
10	PC1	A	104	-	31,31,53	1.51	6 (19%)	37,39,61	1.17	3 (8%)
8	BCL	K	101	4	69,74,74	1.11	6 (8%)	83,115,115	1.46	11 (13%)
8	BCL	F	103	5	69,74,74	1.10	4 (5%)	83,115,115	1.50	12 (14%)
10	PC1	W	101	-	36,36,53	1.45	6 (16%)	42,44,61	1.13	2 (4%)
13	SPO	D	102	-	40,41,41	3.40	21 (52%)	47,50,50	10.07	28 (59%)
13	SPO	E	102	-	40,41,41	3.64	20 (50%)	47,50,50	10.47	32 (68%)
13	SPO	N	102	-	40,41,41	3.48	22 (55%)	47,50,50	10.55	32 (68%)
13	SPO	M	405	-	40,41,41	3.42	21 (52%)	47,50,50	10.10	32 (68%)
8	BCL	E	101	5	69,74,74	1.13	5 (7%)	83,115,115	1.62	13 (15%)
13	SPO	U	104	-	40,41,41	3.48	21 (52%)	47,50,50	10.14	33 (70%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	BCL	N	101	5	69,74,74	1.16	6 (8%)	83,115,115	1.57	15 (18%)
13	SPO	U	102	-	40,41,41	3.35	21 (52%)	47,50,50	10.13	29 (61%)
8	BCL	U	101	4	69,74,74	1.15	7 (10%)	83,115,115	1.51	11 (13%)
8	BCL	F	101	4	69,74,74	1.15	6 (8%)	83,115,115	1.51	12 (14%)
13	SPO	3	104	-	40,41,41	3.79	21 (52%)	47,50,50	10.29	30 (63%)
8	BCL	3	101	4	69,74,74	1.16	6 (8%)	83,115,115	1.46	12 (14%)
8	BCL	S	102	5	69,74,74	1.15	5 (7%)	83,115,115	1.56	13 (15%)
8	BCL	O	103	5	69,74,74	1.14	6 (8%)	83,115,115	1.50	14 (16%)
8	BCL	S	101	4	69,74,74	1.17	6 (8%)	83,115,115	1.47	12 (14%)
13	SPO	F	102	-	40,41,41	3.47	21 (52%)	47,50,50	10.27	28 (59%)
8	BCL	1	102	5	64,69,74	1.15	5 (7%)	77,109,115	1.42	8 (10%)
13	SPO	J	103	-	40,41,41	3.59	21 (52%)	47,50,50	10.79	30 (63%)
13	SPO	9	102	-	40,41,41	3.43	20 (50%)	47,50,50	10.20	28 (59%)
8	BCL	0	102	5	64,69,74	1.15	5 (7%)	77,109,115	1.60	13 (16%)
13	SPO	3	102	-	40,41,41	3.52	23 (57%)	47,50,50	10.25	28 (59%)
8	BCL	L	302	1	66,71,74	1.15	7 (10%)	79,111,115	1.50	11 (13%)
8	BCL	W	102	4	69,74,74	1.14	7 (10%)	83,115,115	1.48	13 (15%)
13	SPO	T	101	-	40,41,41	3.36	20 (50%)	47,50,50	10.29	29 (61%)
13	SPO	W	103	-	40,41,41	3.50	22 (55%)	47,50,50	10.01	31 (65%)
9	BPB	M	403	-	47,60,70	1.69	5 (10%)	44,89,101	2.39	10 (22%)
9	BPB	L	303	-	54,67,70	1.61	5 (9%)	52,97,101	2.22	10 (19%)
13	SPO	O	104	-	40,41,41	3.41	21 (52%)	47,50,50	9.99	29 (61%)
13	SPO	G	101	-	40,41,41	3.59	24 (60%)	47,50,50	11.59	32 (68%)
8	BCL	L	301	1	69,74,74	1.17	7 (10%)	83,115,115	1.49	13 (15%)
10	PC1	L	304	-	34,34,53	1.44	6 (17%)	40,42,61	1.16	3 (7%)
10	PC1	L	306	-	35,35,53	1.45	7 (20%)	41,43,61	1.18	3 (7%)
8	BCL	D	101	4	69,74,74	1.16	7 (10%)	83,115,115	1.49	12 (14%)
8	BCL	U	103	5	69,74,74	1.16	5 (7%)	83,115,115	1.65	16 (19%)
13	SPO	D	103	-	40,41,41	3.55	21 (52%)	47,50,50	10.76	32 (68%)
13	SPO	J	101	-	40,41,41	3.33	19 (47%)	47,50,50	10.62	34 (72%)
10	PC1	A	102	-	44,44,53	1.34	6 (13%)	50,52,61	1.14	3 (6%)
10	PC1	D	104	-	36,36,53	1.41	6 (16%)	42,44,61	1.08	2 (4%)
13	SPO	8	102	-	40,41,41	3.57	21 (52%)	47,50,50	11.36	34 (72%)
13	SPO	I	102	-	40,41,41	3.47	21 (52%)	47,50,50	9.90	30 (63%)
11	U10	L	308	-	38,38,63	2.69	12 (31%)	46,49,79	1.58	10 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	PC1	H	301	-	39,39,53	1.39	6 (15%)	45,47,61	1.09	2 (4%)
8	BCL	M	402	2	69,74,74	1.18	7 (10%)	83,115,115	1.56	15 (18%)
14	CDL	M	406	-	99,99,99	1.15	6 (6%)	105,111,111	1.44	7 (6%)
13	SPO	X	101	-	37,38,41	3.43	21 (56%)	43,46,50	10.84	29 (67%)

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
13	SPO	V	101	-	-	14/47/47/47	-
8	BCL	I	101	4	-	0/41/137/137	-
8	BCL	Q	101	4	-	0/41/137/137	-
13	SPO	P	101	-	-	13/47/47/47	-
8	BCL	7	101	5	-	10/41/137/137	-
8	BCL	3	103	5	-	4/41/137/137	-
13	SPO	T	102	-	-	18/47/47/47	-
11	U10	L	305	-	-	16/39/63/87	0/1/1/1
13	SPO	O	102	-	-	16/47/47/47	-
8	BCL	C	101	5	-	9/41/137/137	-
8	BCL	J	102	5	-	6/41/137/137	-
8	BCL	A	103	5	-	4/41/137/137	-
14	CDL	H	304	-	-	37/88/88/110	-
8	BCL	R	101	5	-	5/41/137/137	-
8	BCL	9	101	4	-	5/41/137/137	-
8	BCL	1	101	4	-	3/29/125/137	-
8	BCL	O	101	4	-	5/41/137/137	-
11	U10	M	404	-	-	7/45/69/87	0/1/1/1
11	U10	Y	501	-	-	10/33/57/87	0/1/1/1
13	SPO	B	101	-	-	13/47/47/47	-
10	PC1	H	303	-	-	6/21/21/57	-
8	BCL	L	307	2	-	5/41/137/137	-
13	SPO	0	101	-	-	14/47/47/47	-
8	BCL	A	101	4	-	0/41/137/137	-
10	PC1	H	302	-	-	14/45/45/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BCL	8	101	4	-	7/35/131/137	-
10	PC1	A	104	-	-	15/35/35/57	-
8	BCL	K	101	4	-	0/41/137/137	-
8	BCL	F	103	5	-	5/41/137/137	-
10	PC1	W	101	-	-	12/40/40/57	-
13	SPO	D	102	-	-	7/47/47/47	-
13	SPO	E	102	-	-	13/47/47/47	-
13	SPO	N	102	-	-	22/47/47/47	-
13	SPO	M	405	-	-	14/47/47/47	-
8	BCL	E	101	5	-	6/41/137/137	-
13	SPO	U	104	-	-	20/47/47/47	-
8	BCL	N	101	5	-	10/41/137/137	-
13	SPO	U	102	-	-	17/47/47/47	-
8	BCL	U	101	4	-	4/41/137/137	-
8	BCL	F	101	4	-	4/41/137/137	-
13	SPO	3	104	-	-	19/47/47/47	-
8	BCL	3	101	4	-	0/41/137/137	-
8	BCL	S	102	5	-	7/41/137/137	-
8	BCL	O	103	5	-	7/41/137/137	-
8	BCL	S	101	4	-	4/41/137/137	-
13	SPO	F	102	-	-	12/47/47/47	-
8	BCL	1	102	5	-	6/35/131/137	-
13	SPO	J	103	-	-	18/47/47/47	-
13	SPO	9	102	-	-	19/47/47/47	-
8	BCL	0	102	5	-	4/35/131/137	-
13	SPO	3	102	-	-	7/47/47/47	-
8	BCL	L	302	1	-	2/38/134/137	-
8	BCL	W	102	4	-	2/41/137/137	-
13	SPO	T	101	-	-	7/47/47/47	-
13	SPO	W	103	-	-	20/47/47/47	-
9	BPB	M	403	-	-	6/25/93/105	0/5/6/6
9	BPB	L	303	-	-	6/34/102/105	0/5/6/6
13	SPO	O	104	-	-	16/47/47/47	-
13	SPO	G	101	-	-	15/47/47/47	-
8	BCL	L	301	1	-	1/41/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	PC1	L	304	-	-	12/38/38/57	-
10	PC1	L	306	-	-	13/39/39/57	-
8	BCL	D	101	4	-	0/41/137/137	-
8	BCL	U	103	5	-	11/41/137/137	-
13	SPO	D	103	-	-	13/47/47/47	-
13	SPO	J	101	-	-	16/47/47/47	-
10	PC1	A	102	-	-	17/48/48/57	-
10	PC1	D	104	-	-	13/40/40/57	-
13	SPO	8	102	-	-	23/47/47/47	-
13	SPO	I	102	-	-	16/47/47/47	-
11	U10	L	308	-	-	6/33/57/87	0/1/1/1
10	PC1	H	301	-	-	15/43/43/57	-
8	BCL	M	402	2	-	2/41/137/137	-
14	CDL	M	406	-	-	53/110/110/110	-
13	SPO	X	101	-	-	16/44/44/47	-

The worst 5 of 867 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	102	SPO	C25-C23	9.18	1.65	1.45
13	T	102	SPO	C16-C17	9.06	1.65	1.45
13	3	104	SPO	C16-C17	8.99	1.65	1.45
9	L	303	BPB	CAC-C3C	8.97	1.56	1.33
13	J	103	SPO	C25-C23	8.88	1.65	1.45

The worst 5 of 1294 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	V	101	SPO	C29-C28-C30	-49.64	31.77	115.27
13	J	103	SPO	C34-C33-C35	-32.50	60.59	115.27
13	N	102	SPO	C24-C23-C22	31.82	167.50	122.92
13	3	104	SPO	C34-C33-C35	-31.75	61.87	115.27
13	O	104	SPO	C24-C23-C22	31.71	167.35	122.92

There are no chirality outliers.

5 of 794 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	L	307	BCL	O2A-C1-C2-C3
8	A	103	BCL	C1A-C2A-CAA-CBA
8	E	101	BCL	C1A-C2A-CAA-CBA
8	F	103	BCL	C1A-C2A-CAA-CBA
8	J	102	BCL	C1A-C2A-CAA-CBA

There are no ring outliers.

73 monomers are involved in 276 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	V	101	SPO	8	0
8	I	101	BCL	1	0
8	Q	101	BCL	1	0
13	P	101	SPO	5	0
8	7	101	BCL	8	0
8	3	103	BCL	1	0
13	T	102	SPO	10	0
11	L	305	U10	5	0
13	O	102	SPO	5	0
8	C	101	BCL	2	0
8	J	102	BCL	5	0
8	A	103	BCL	8	0
14	H	304	CDL	6	0
8	R	101	BCL	6	0
8	9	101	BCL	3	0
8	1	101	BCL	1	0
8	O	101	BCL	1	0
11	M	404	U10	3	0
11	Y	501	U10	2	0
13	B	101	SPO	10	0
8	L	307	BCL	1	0
13	0	101	SPO	8	0
8	A	101	BCL	1	0
10	H	302	PC1	5	0
8	8	101	BCL	4	0
10	A	104	PC1	6	0
8	F	103	BCL	2	0
10	W	101	PC1	5	0
13	D	102	SPO	4	0
13	E	102	SPO	4	0
13	N	102	SPO	9	0
13	M	405	SPO	7	0
8	E	101	BCL	1	0

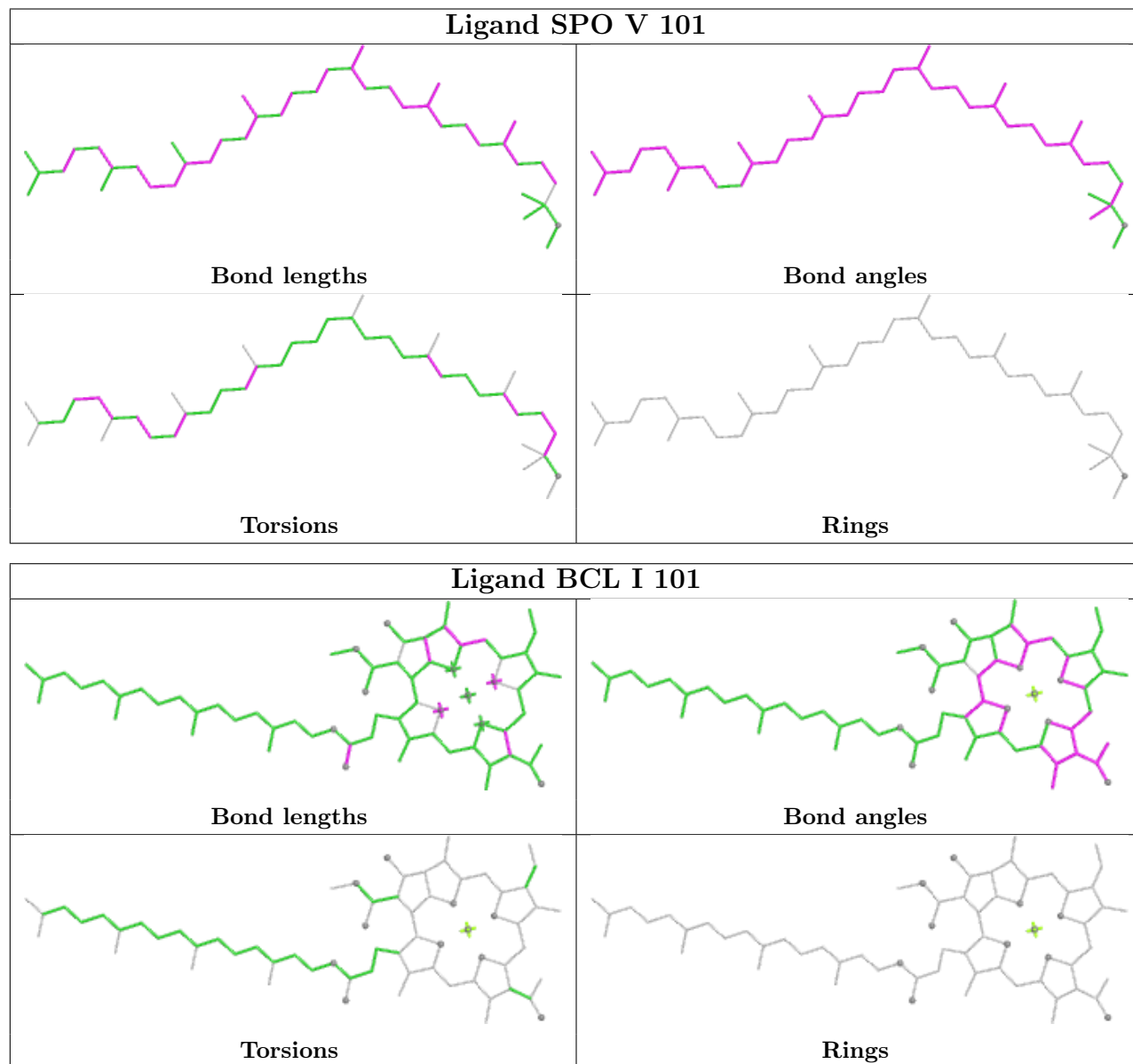
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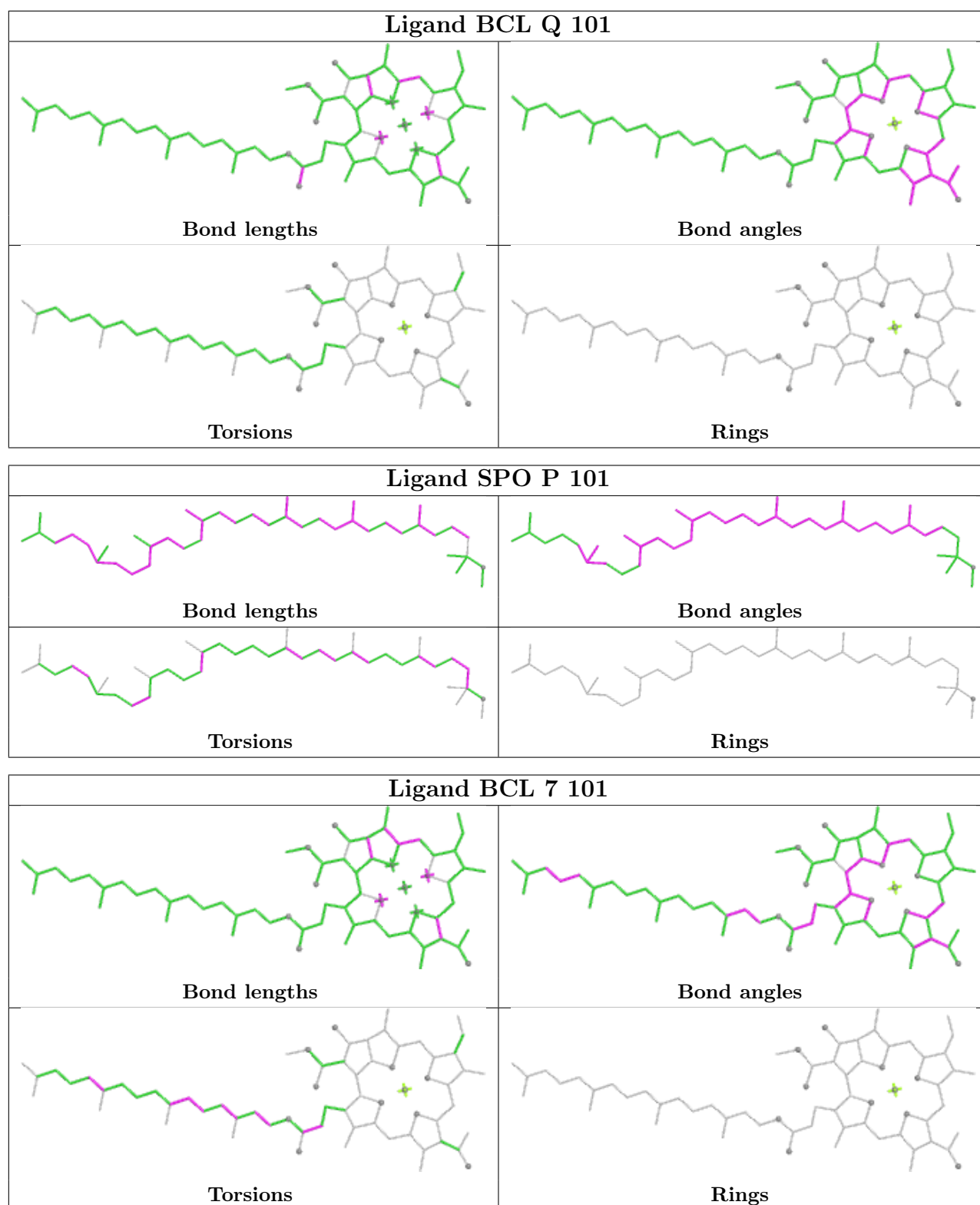
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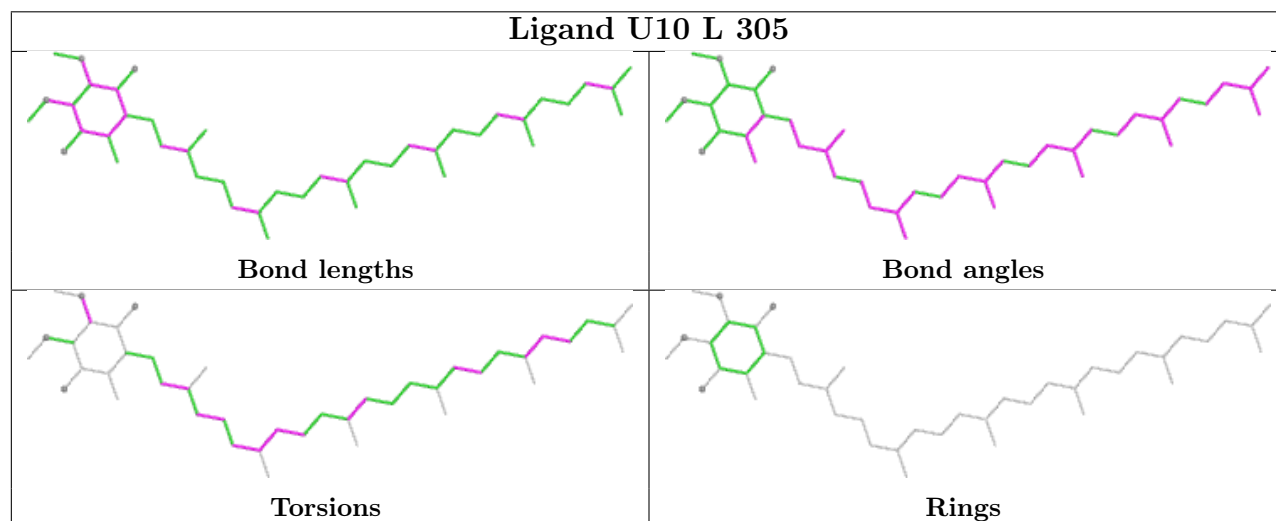
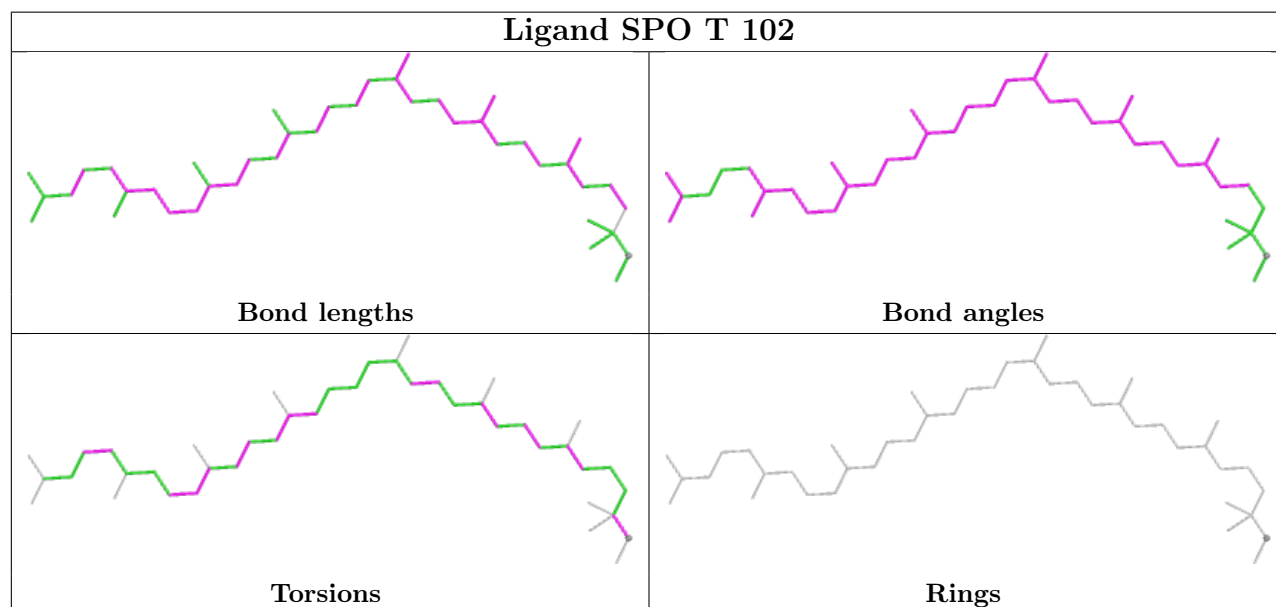
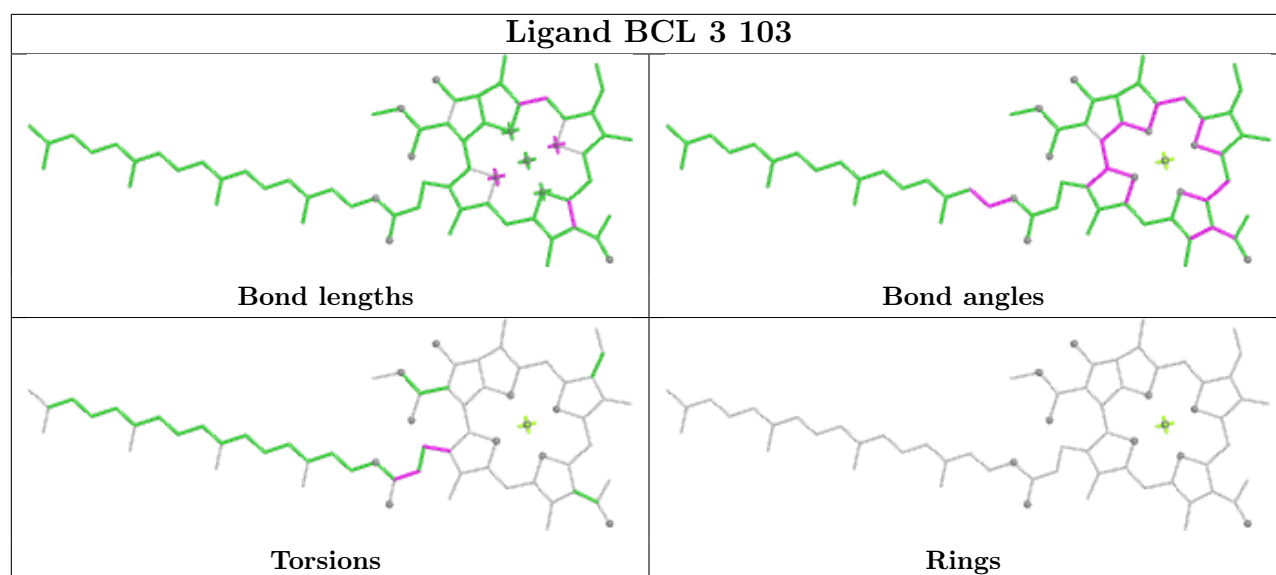
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	U	104	SPO	4	0
8	N	101	BCL	4	0
13	U	102	SPO	8	0
8	U	101	BCL	5	0
8	F	101	BCL	3	0
13	3	104	SPO	7	0
8	3	101	BCL	1	0
8	S	102	BCL	4	0
8	O	103	BCL	3	0
8	S	101	BCL	2	0
13	F	102	SPO	8	0
8	1	102	BCL	2	0
13	J	103	SPO	8	0
13	9	102	SPO	5	0
8	0	102	BCL	3	0
13	3	102	SPO	9	0
8	L	302	BCL	2	0
8	W	102	BCL	4	0
13	T	101	SPO	7	0
13	W	103	SPO	8	0
9	M	403	BPB	4	0
9	L	303	BPB	3	0
13	O	104	SPO	5	0
13	G	101	SPO	6	0
8	L	301	BCL	2	0
10	L	304	PC1	1	0
10	L	306	PC1	2	0
8	D	101	BCL	2	0
8	U	103	BCL	3	0
13	D	103	SPO	9	0
13	J	101	SPO	3	0
10	A	102	PC1	7	0
10	D	104	PC1	5	0
13	8	102	SPO	5	0
13	I	102	SPO	7	0
11	L	308	U10	1	0
10	H	301	PC1	6	0
8	M	402	BCL	1	0
14	M	406	CDL	4	0
13	X	101	SPO	6	0

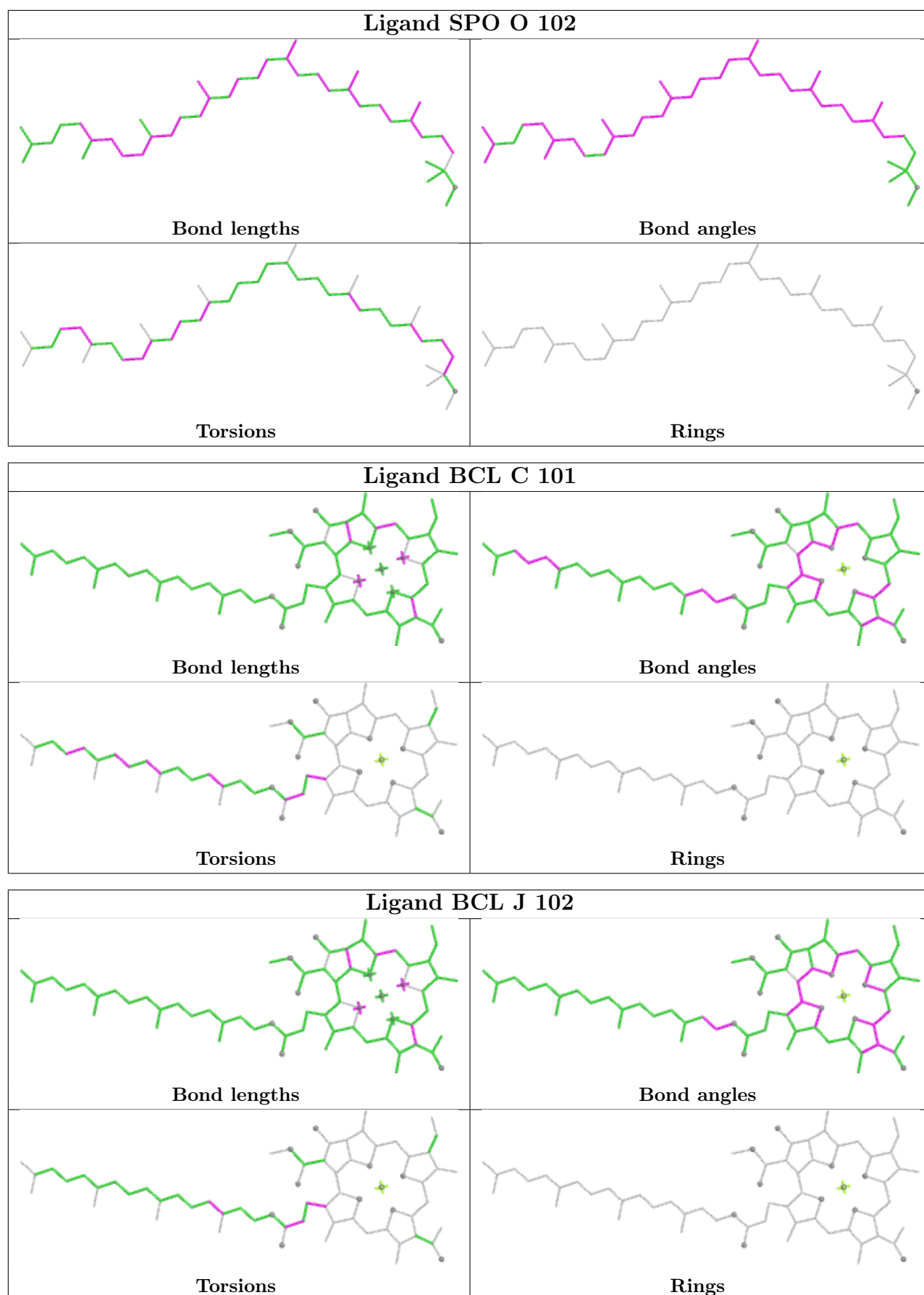
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

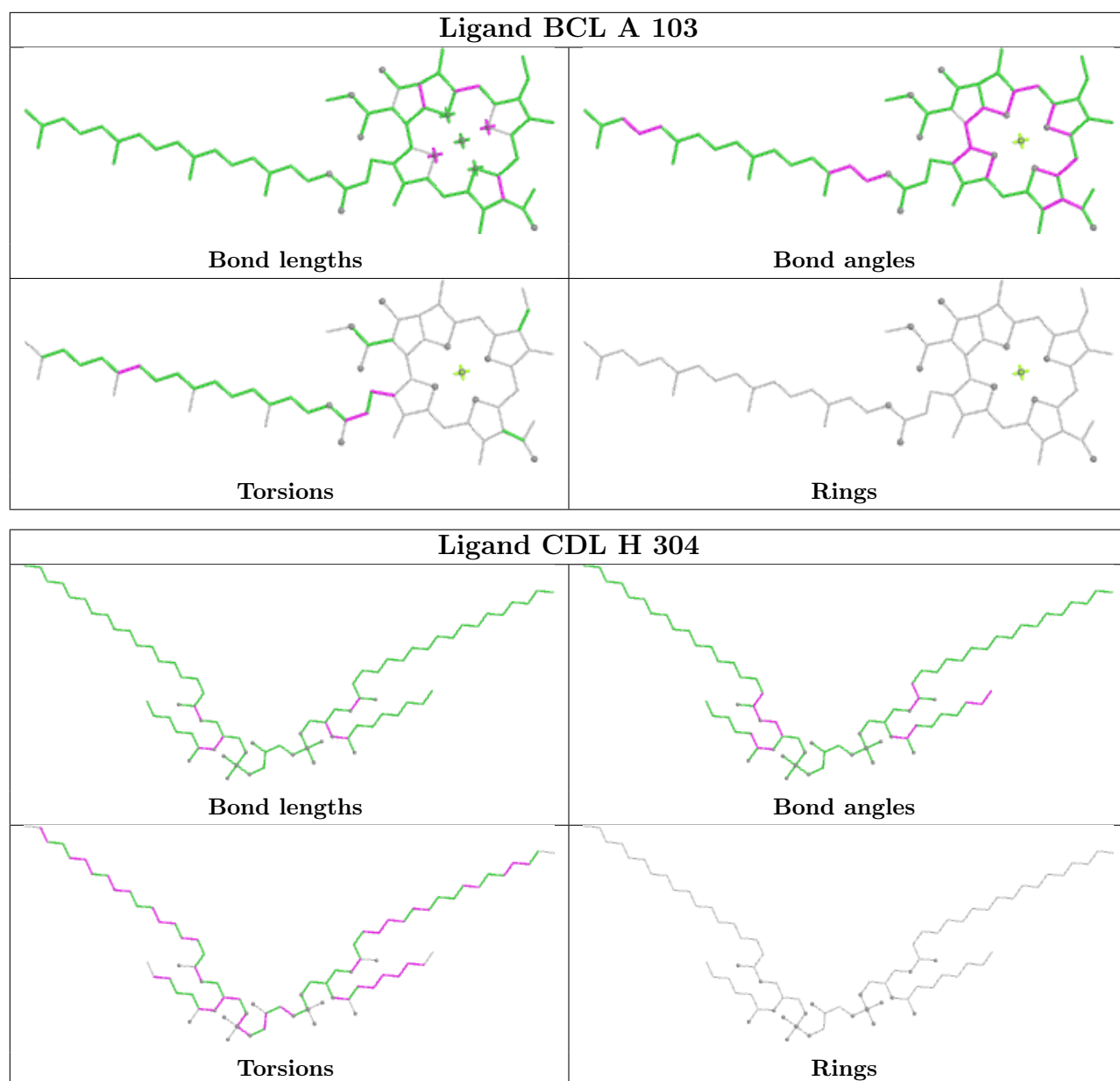
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

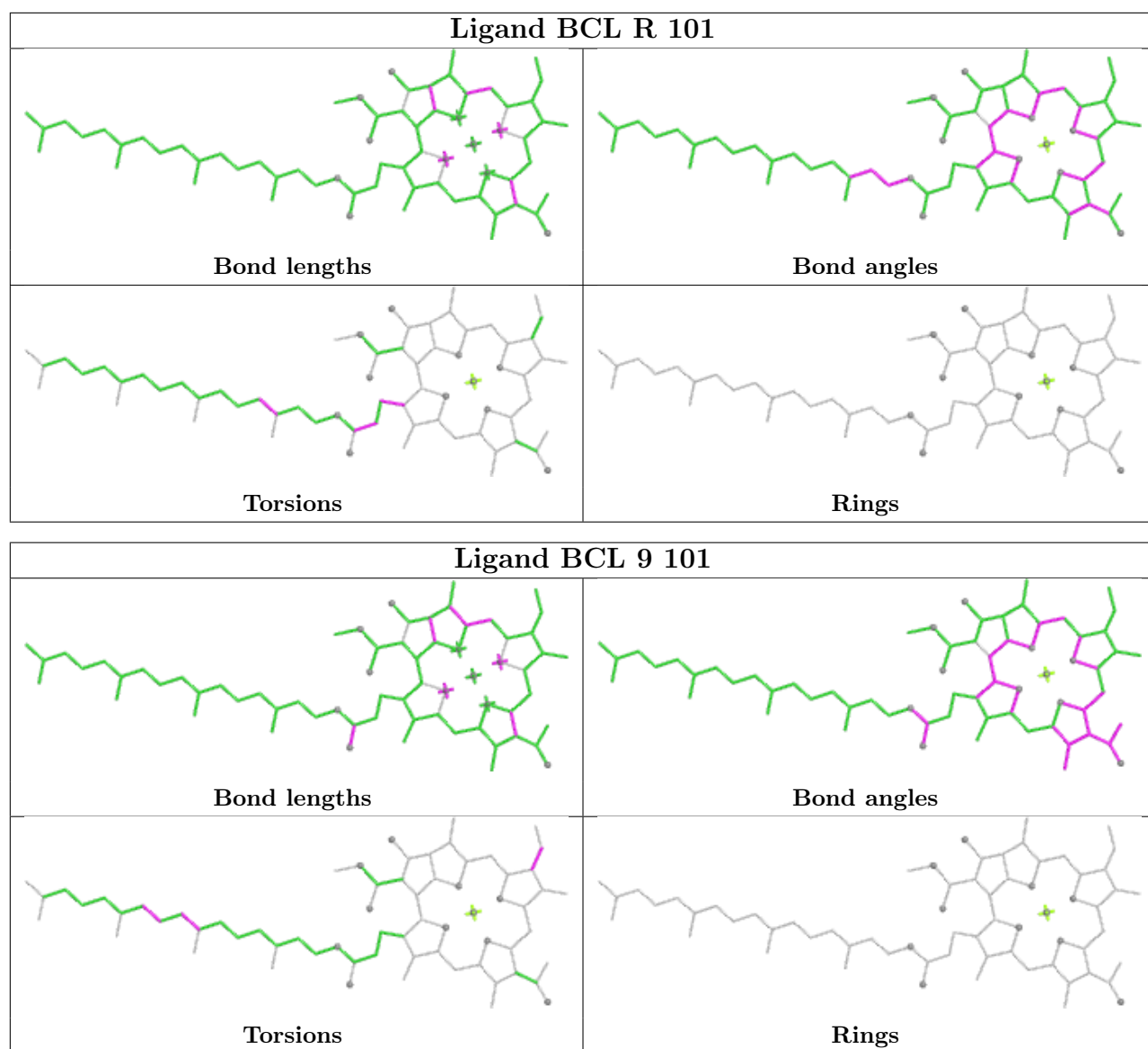


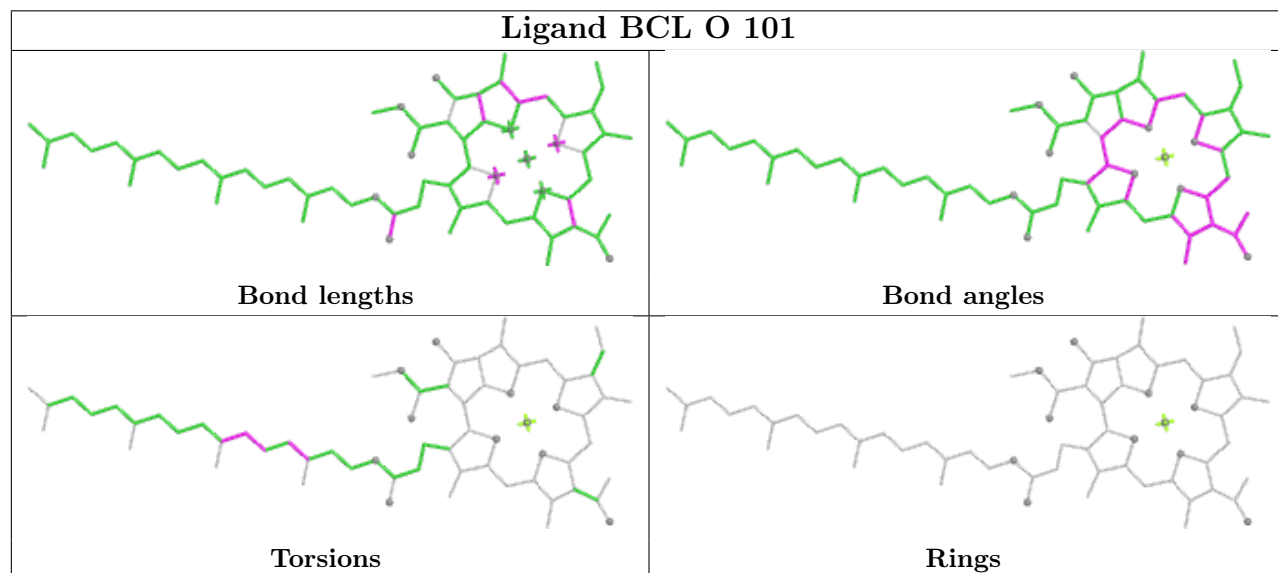
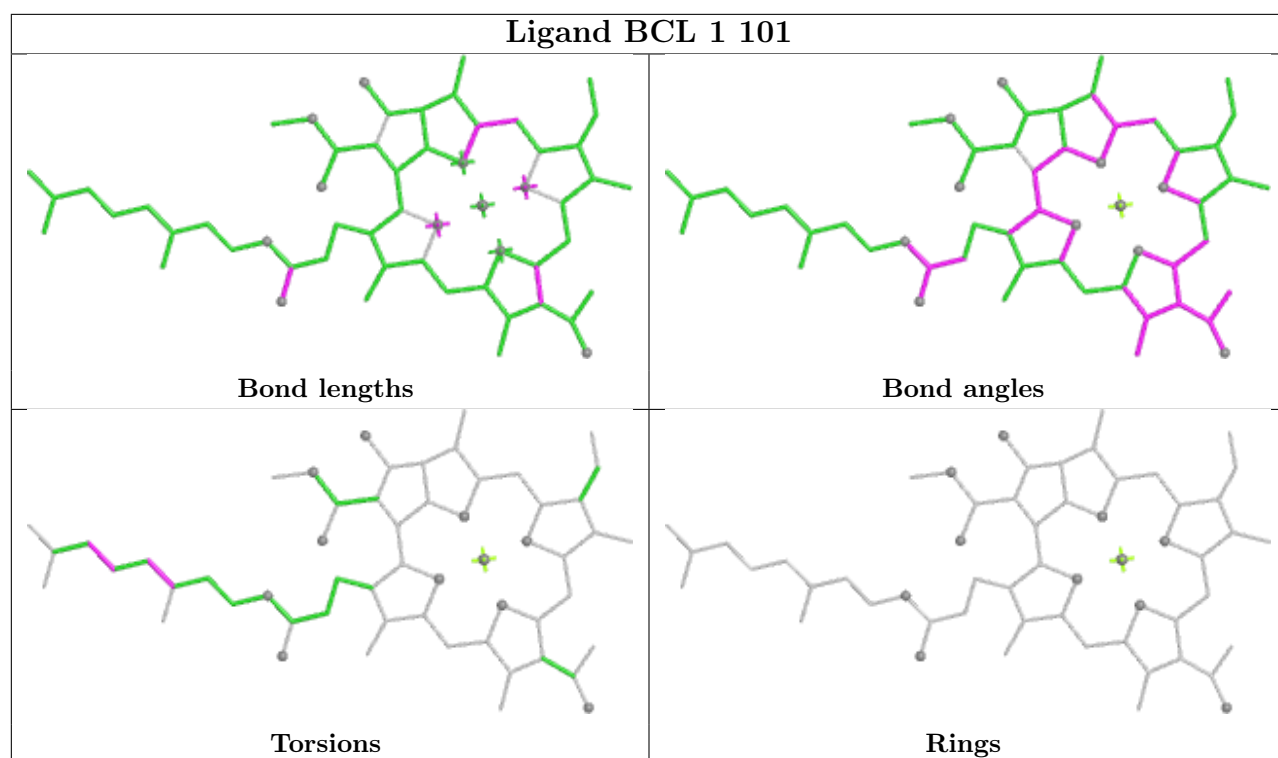


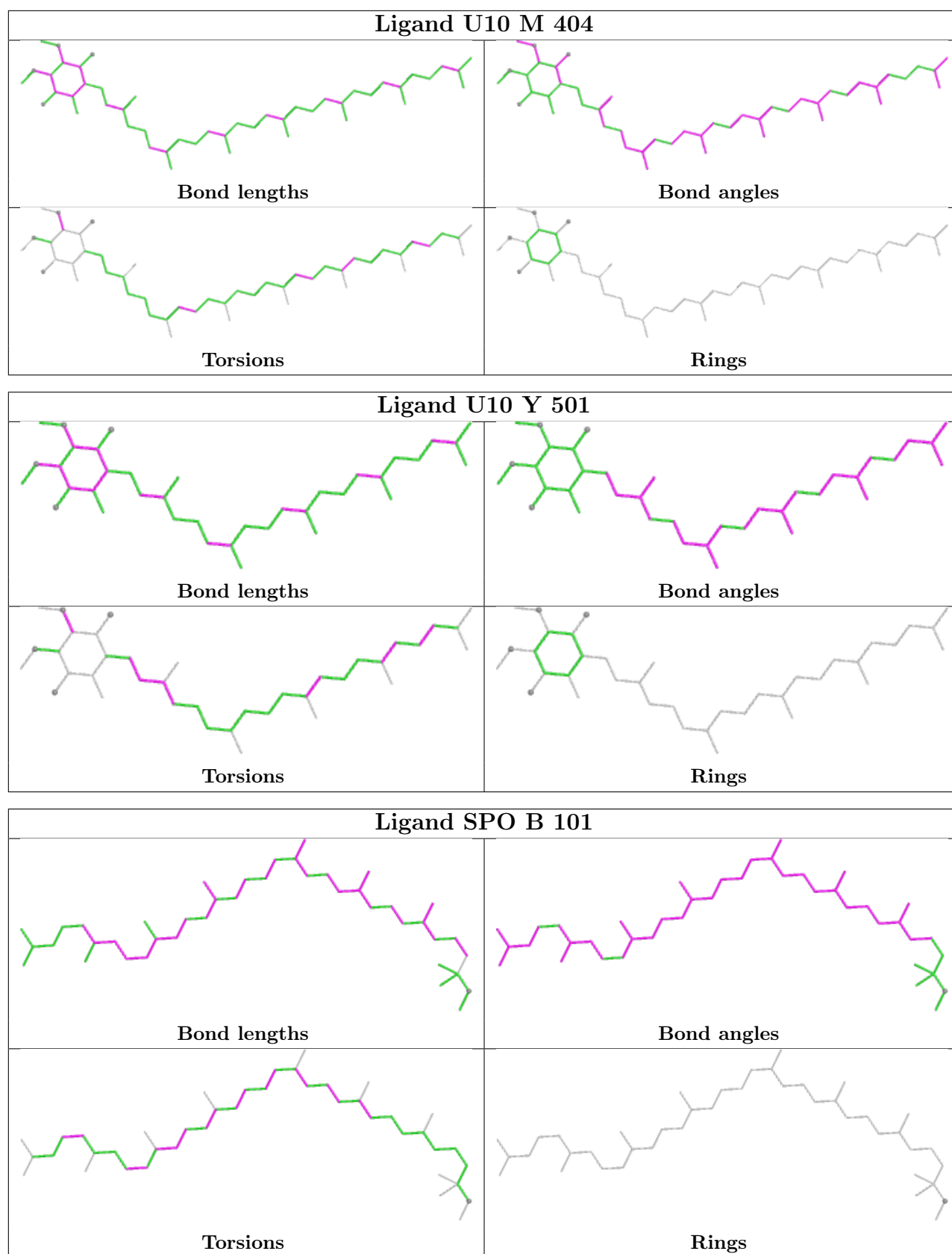


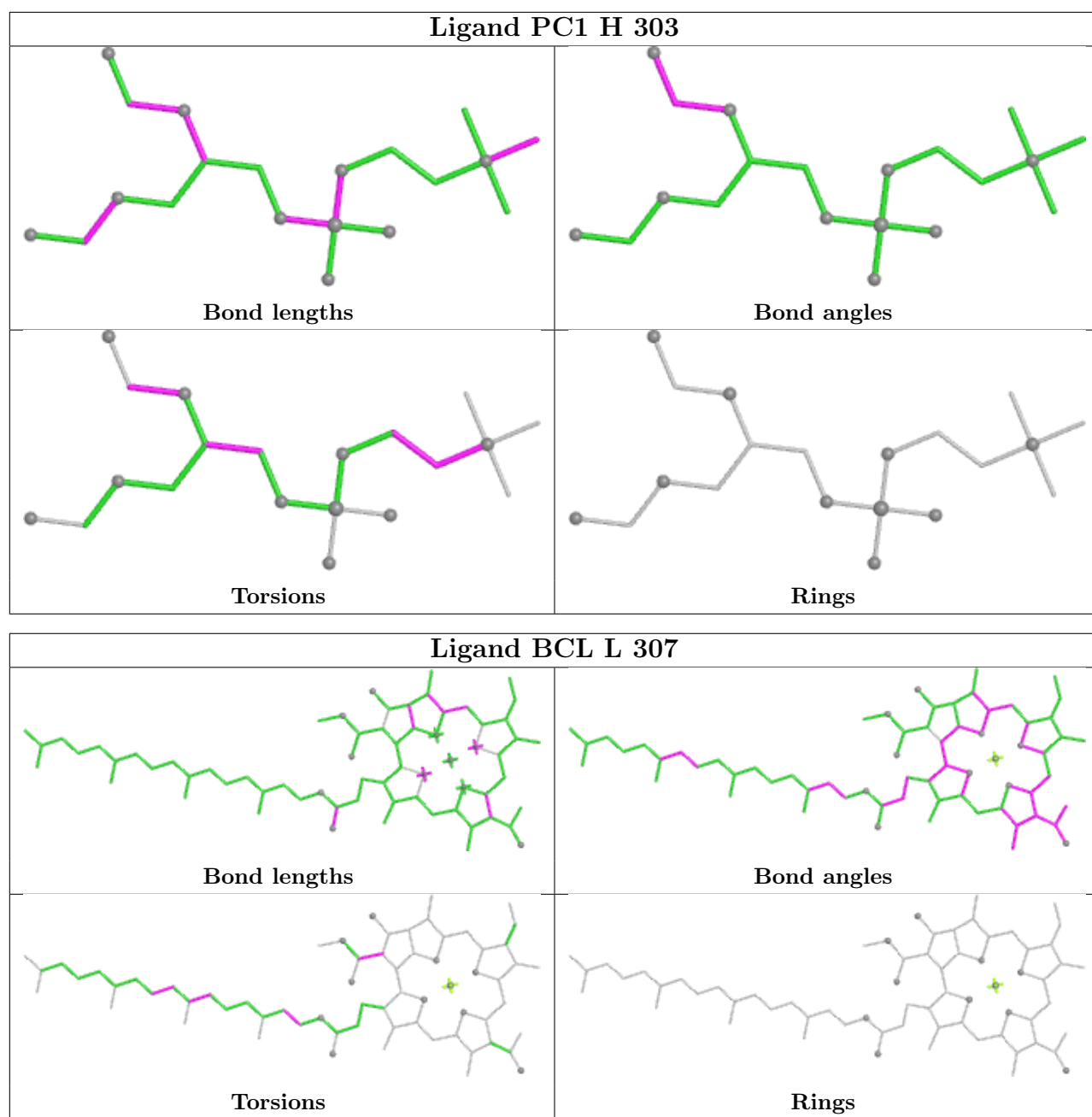


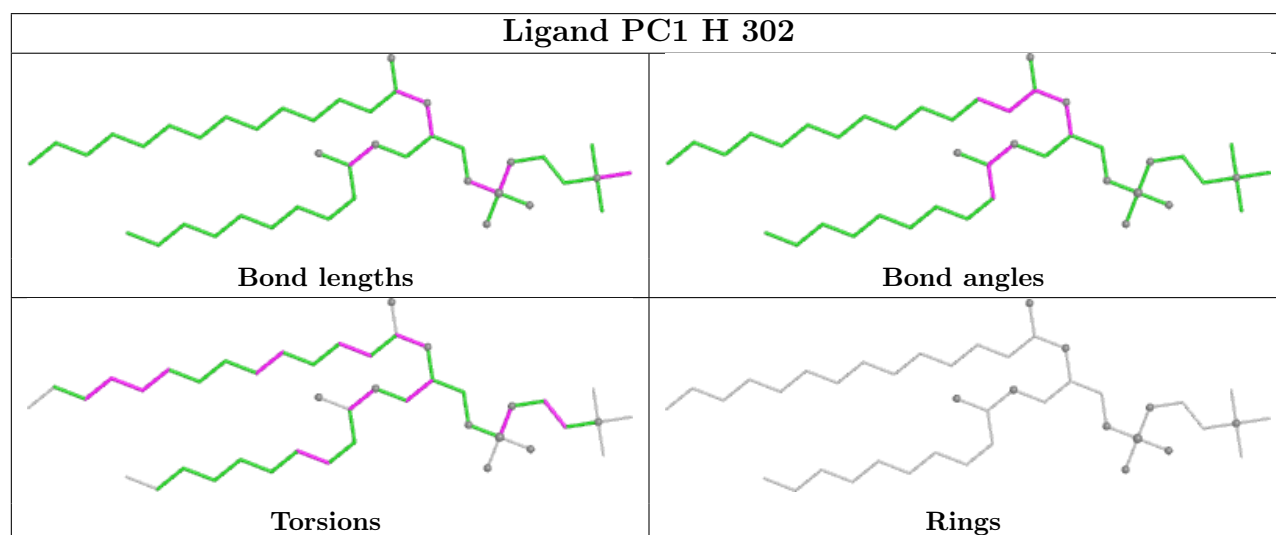
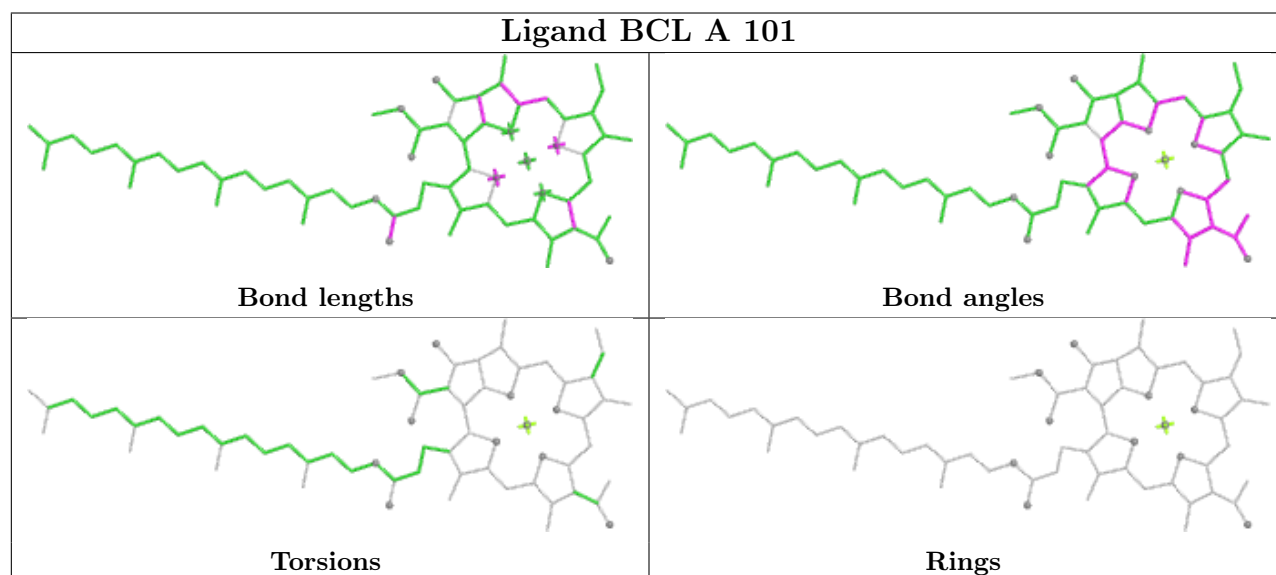
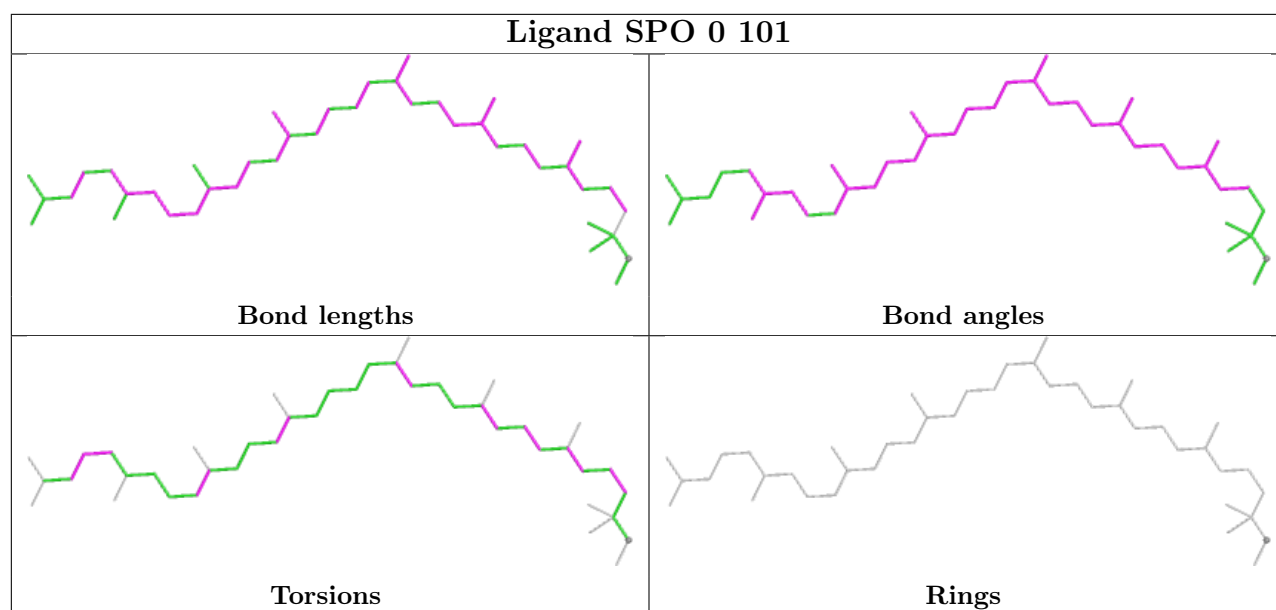


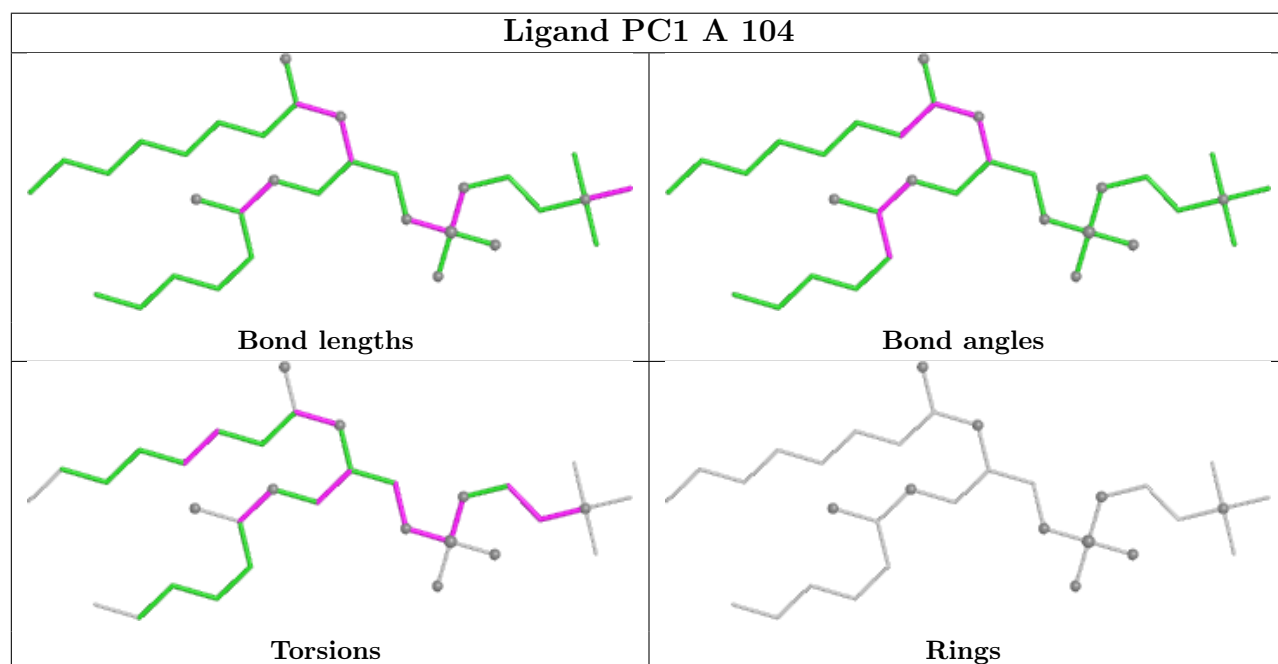
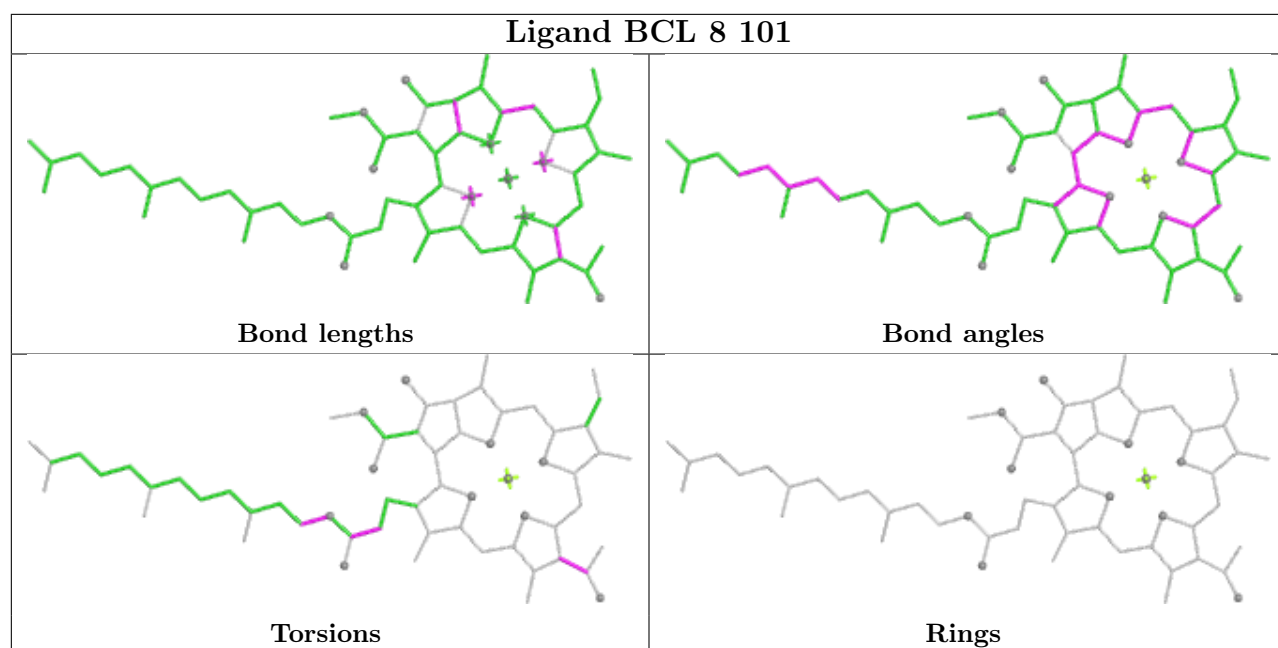


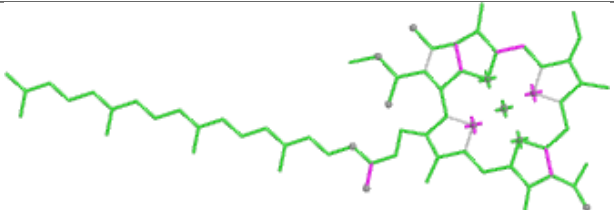
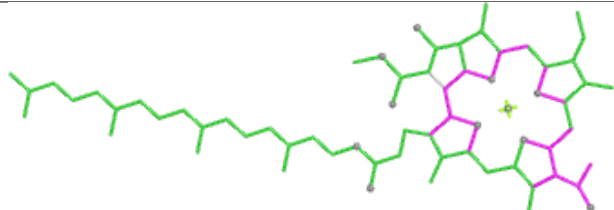
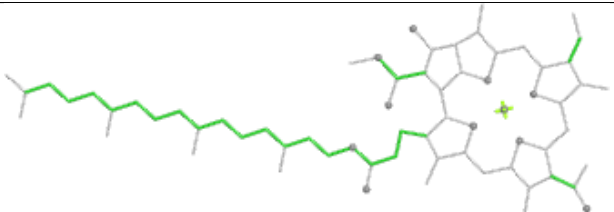
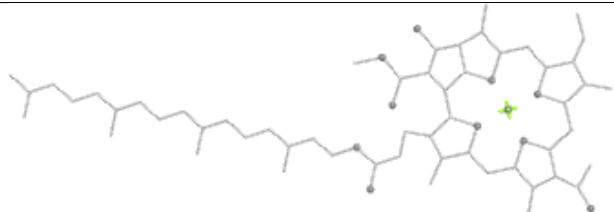


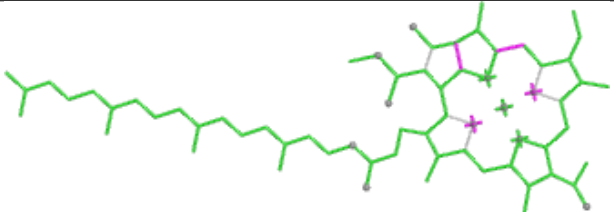
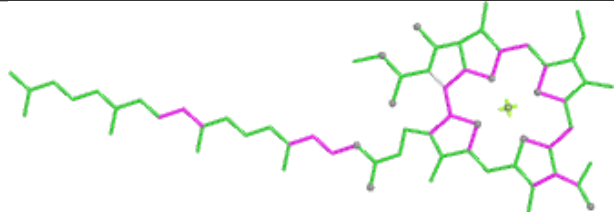
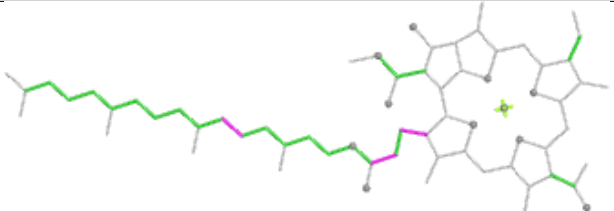
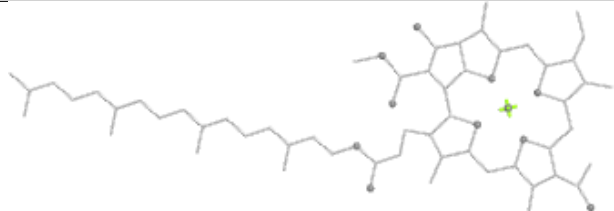


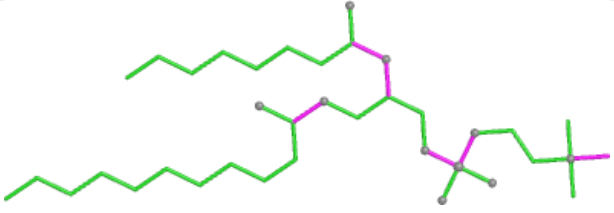
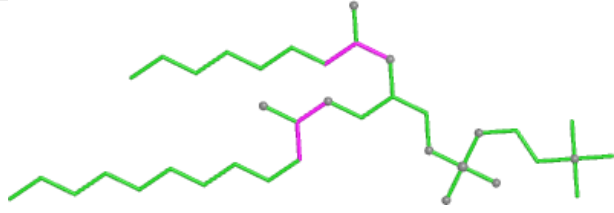
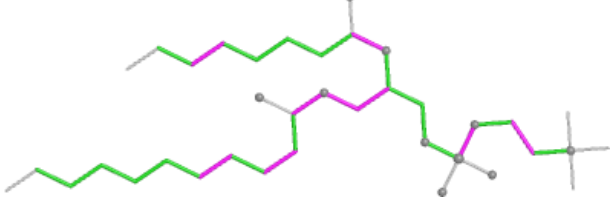
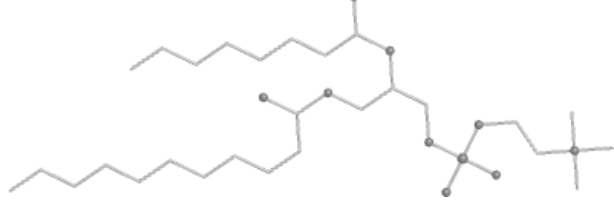


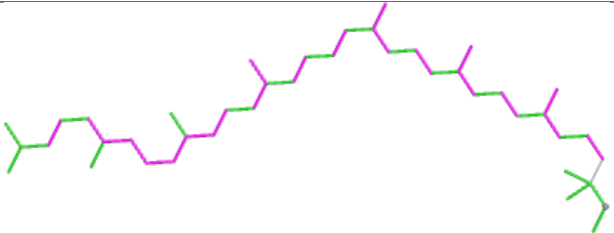
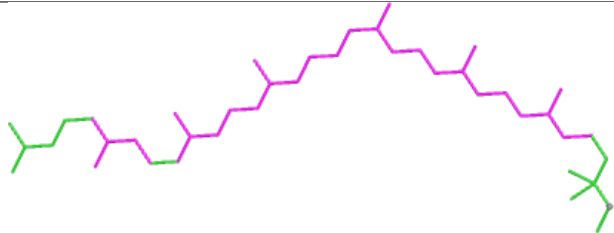
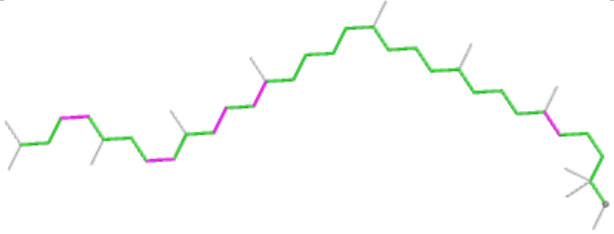
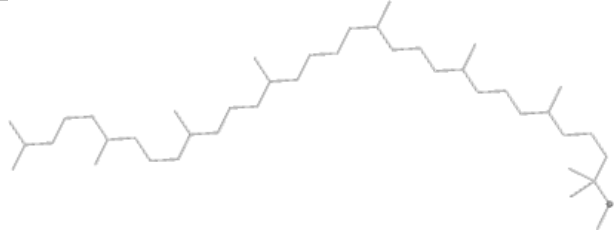


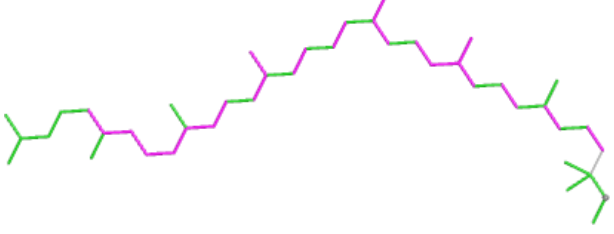
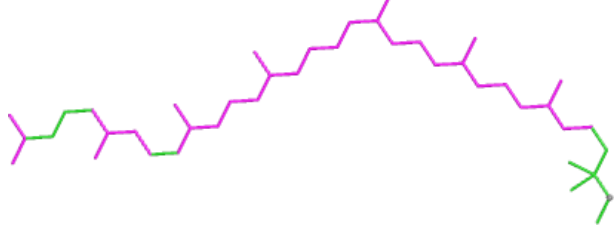
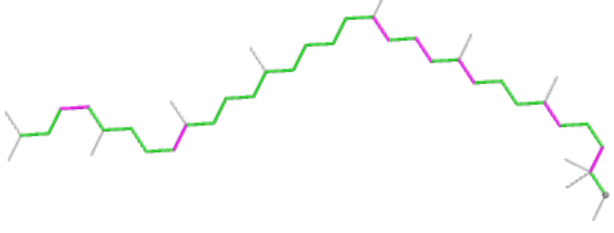


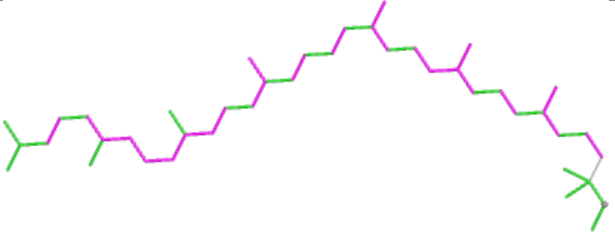
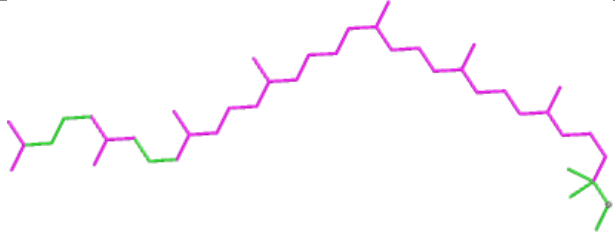
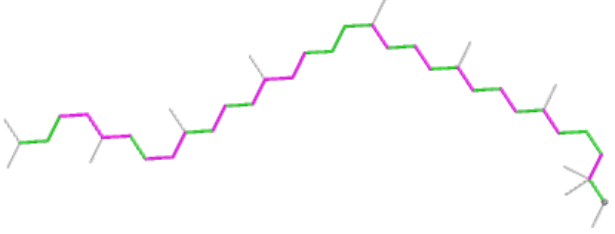
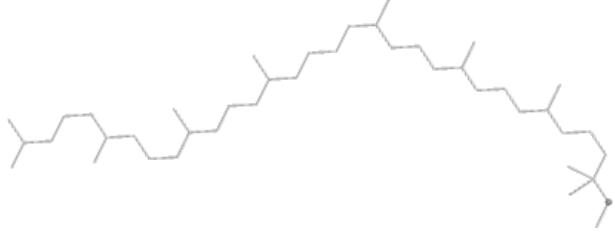
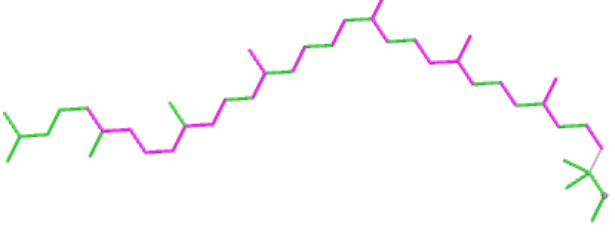
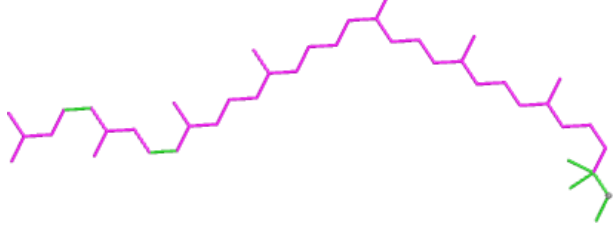
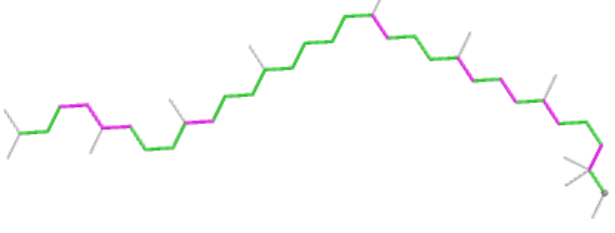
Ligand BCL K 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

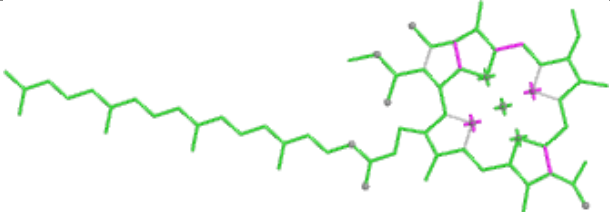
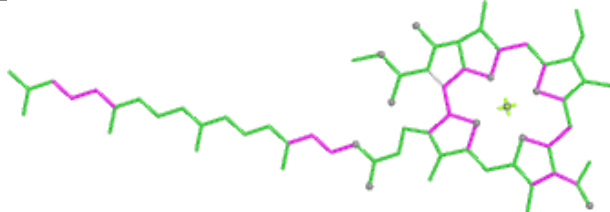
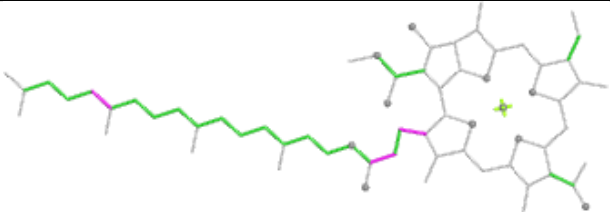
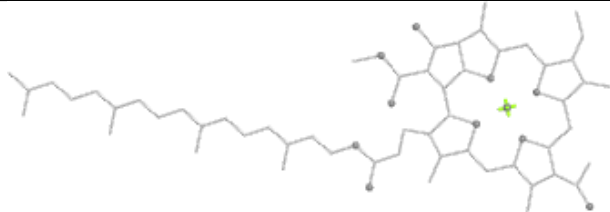
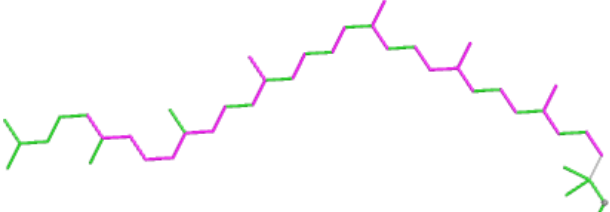
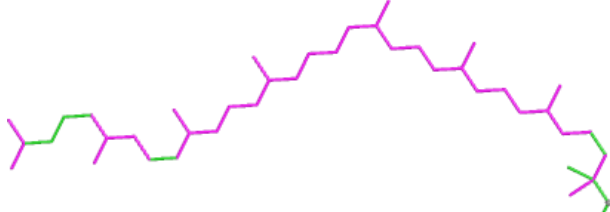
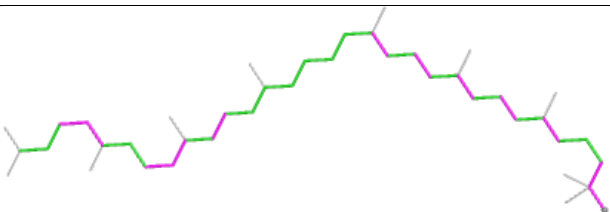
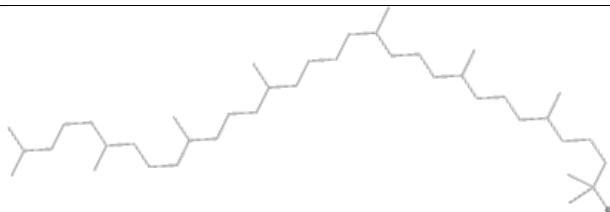
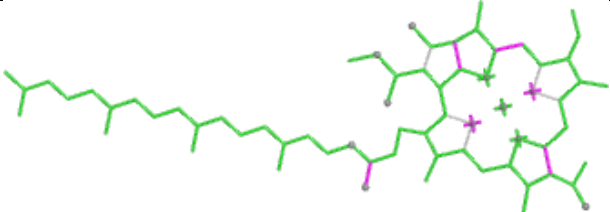
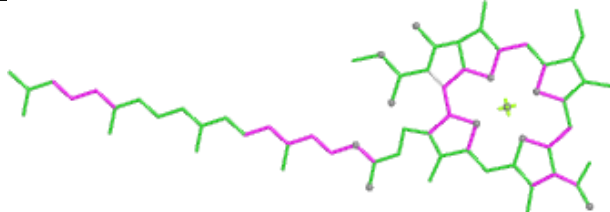
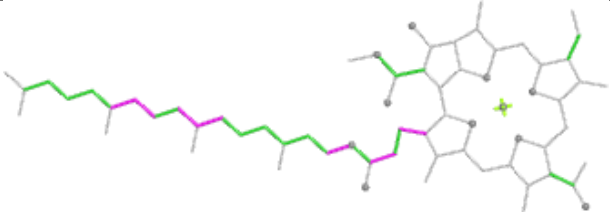
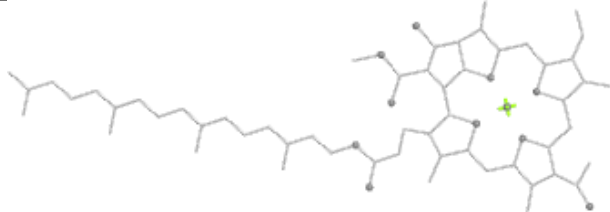
Ligand BCL F 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

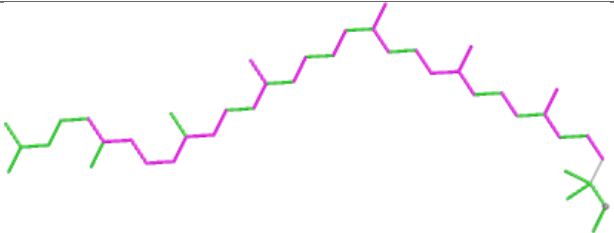
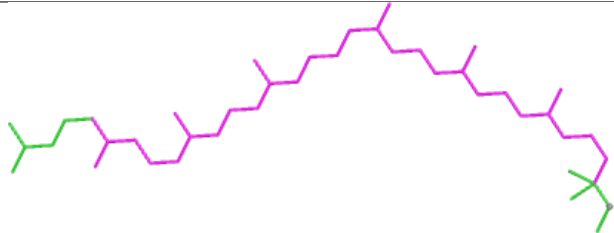
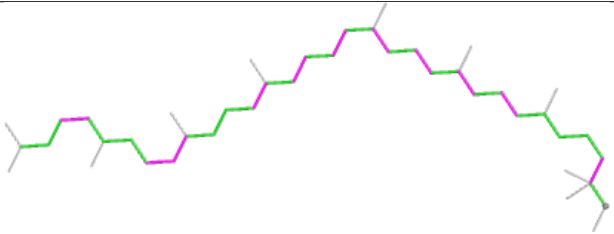
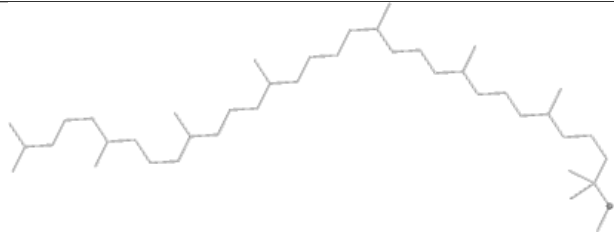
Ligand PC1 W 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

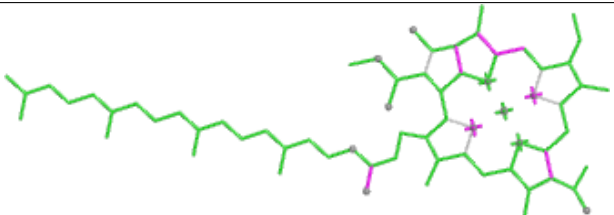
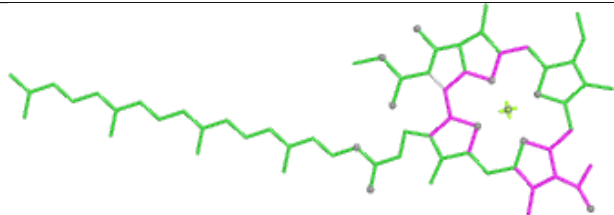
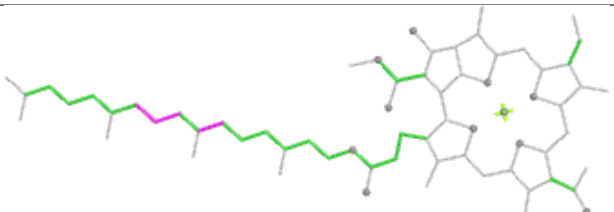
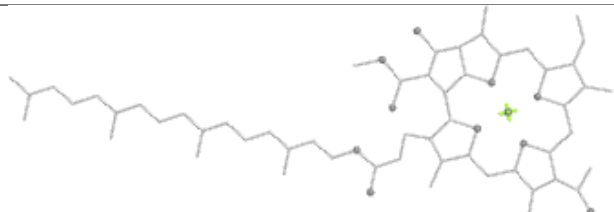
Ligand SPO D 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

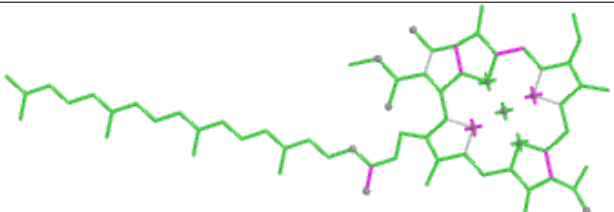
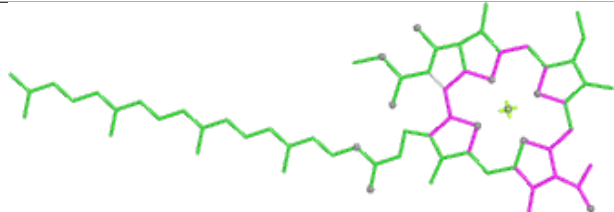
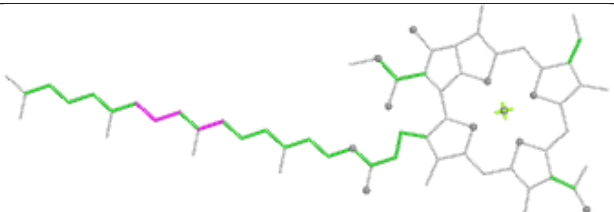
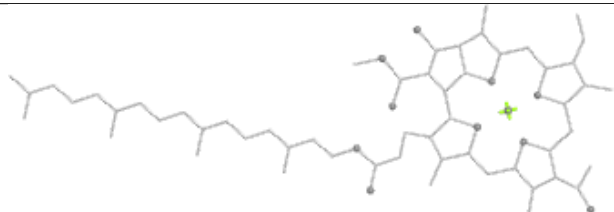
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Bond lengths	Bond angles
	
Torsions	Rings

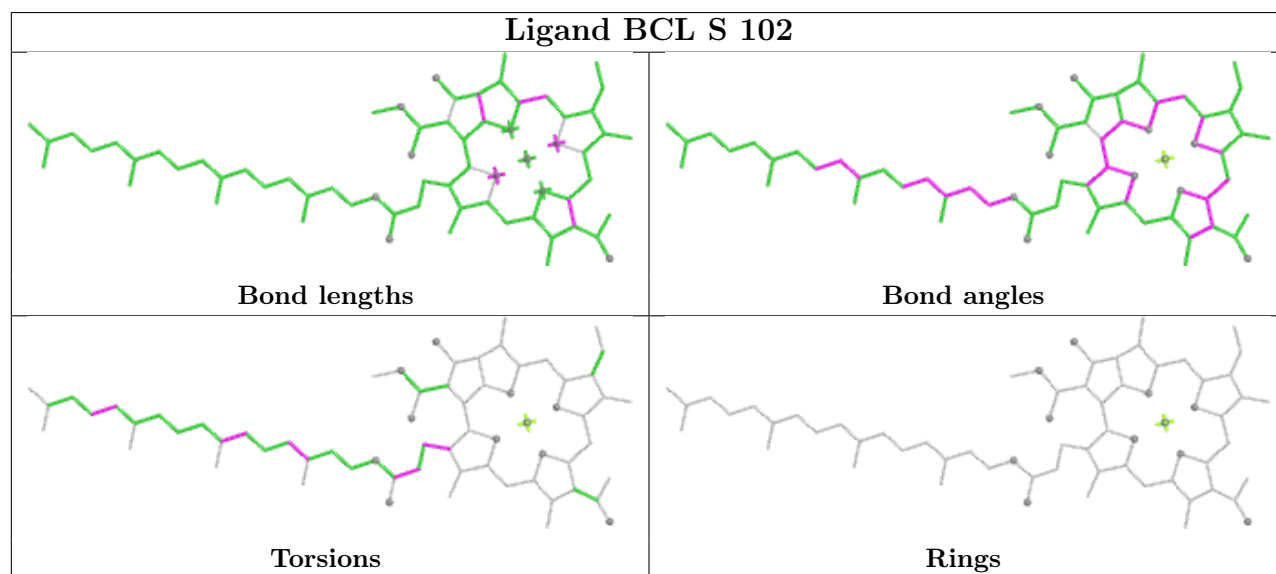
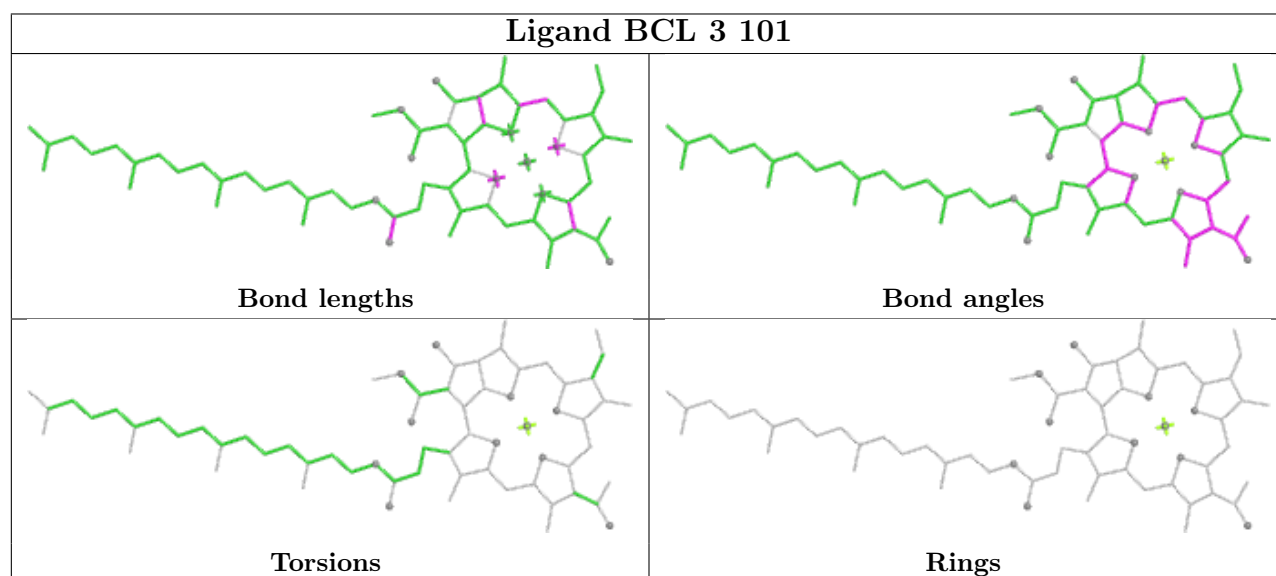
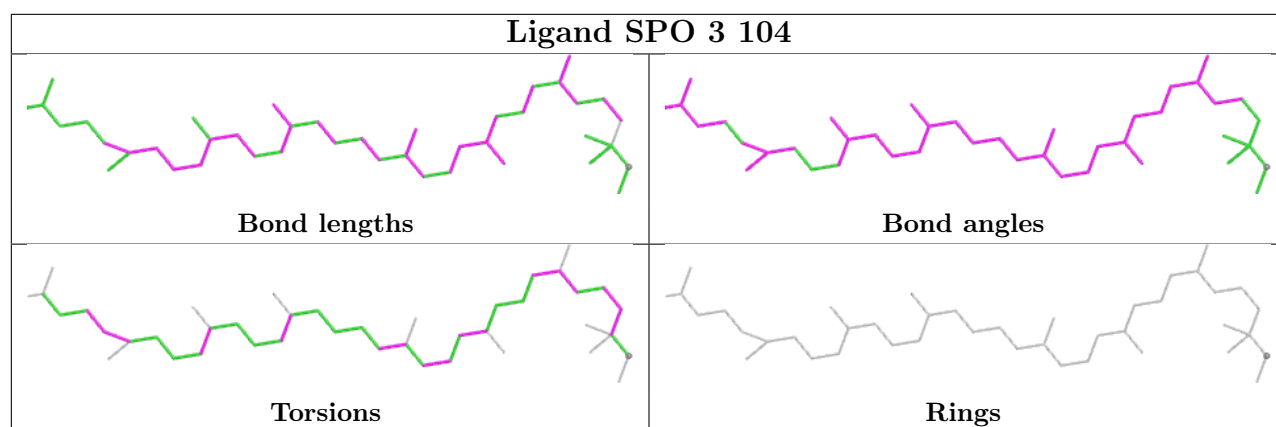
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Bond lengths			
		Bond angles	
			
Torsions			
		Rings	
Ligand SPO M 405			
			
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		Bond angles	
			
Torsions			
		Rings	

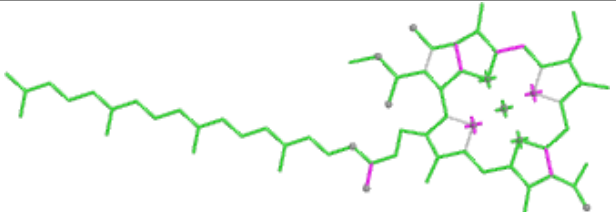
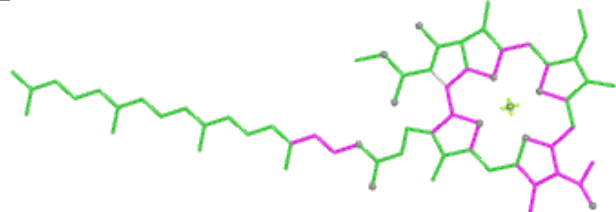
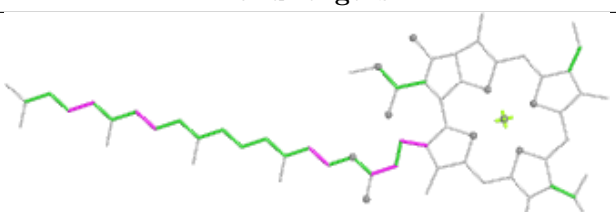
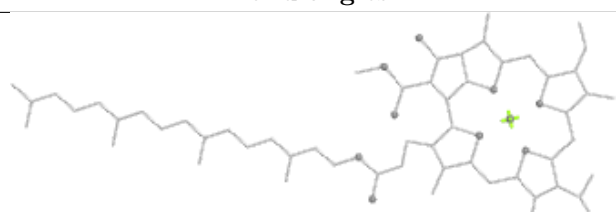
Ligand BCL E 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand SPO U 104	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL N 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

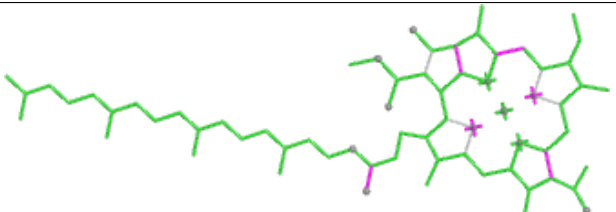
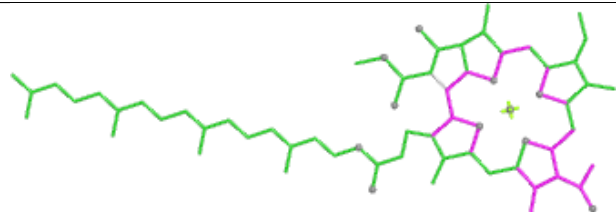
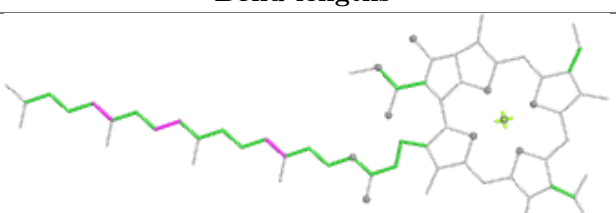
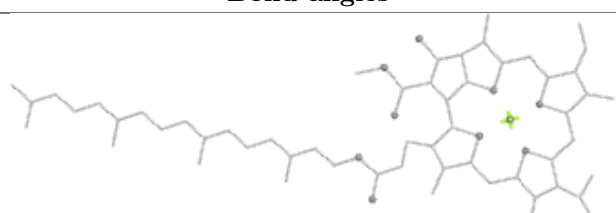
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Bond lengths	Bond angles
	
Torsions	Rings

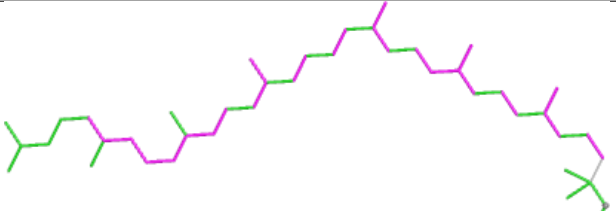
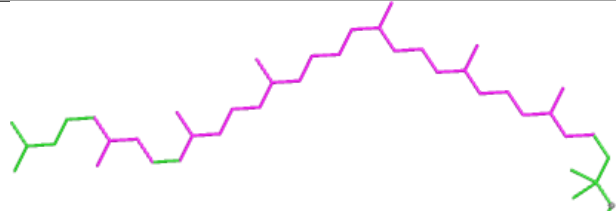
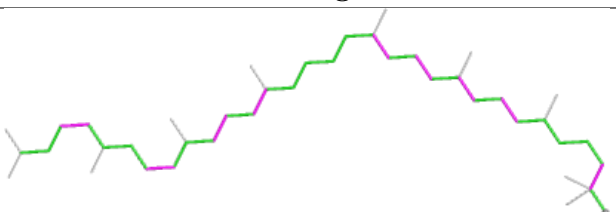
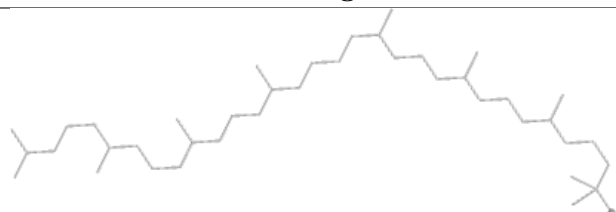
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Bond lengths	Bond angles
	
Torsions	Rings

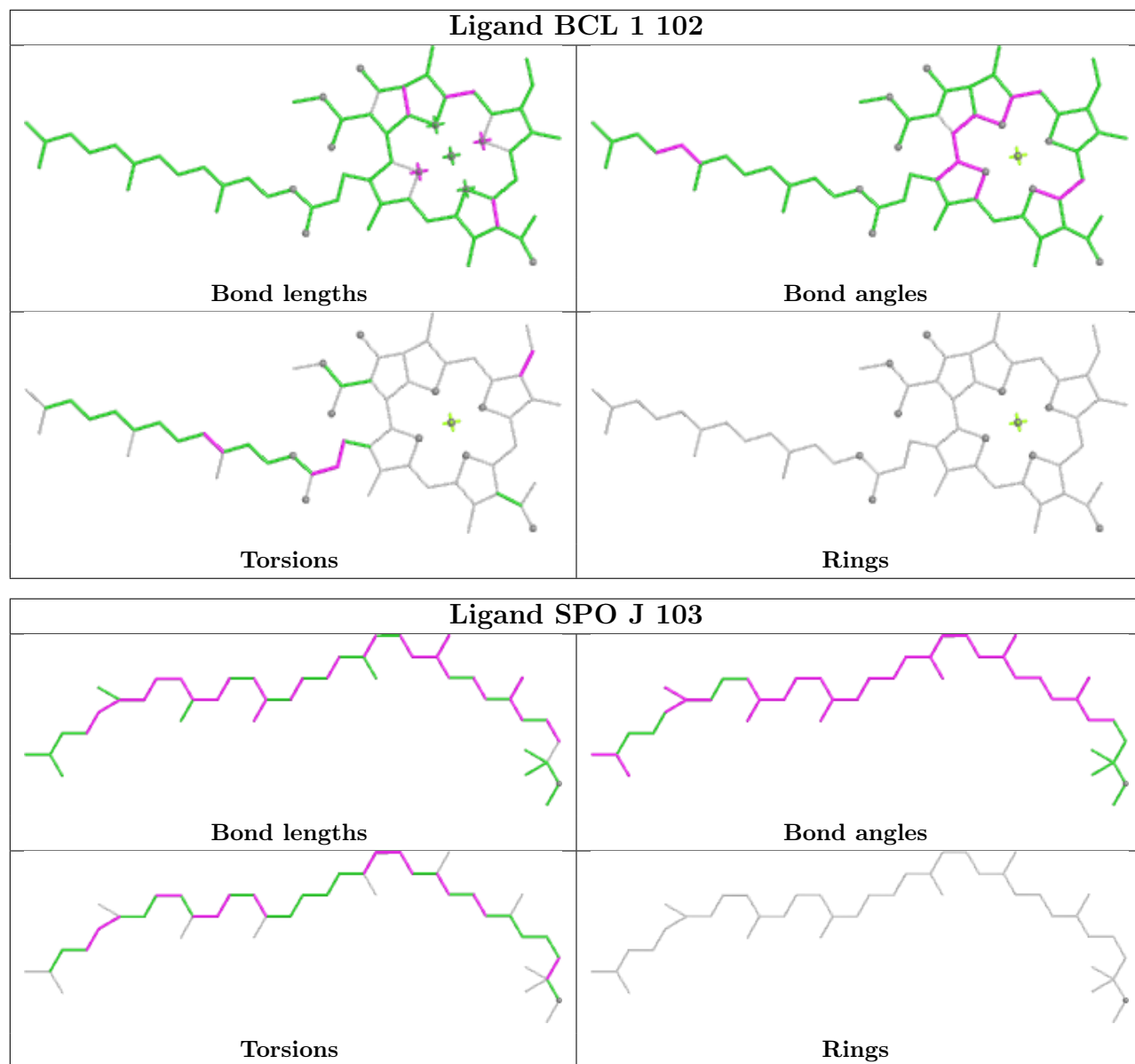
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Bond lengths	Bond angles
	
Torsions	Rings

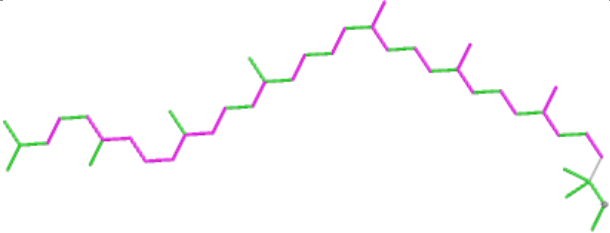
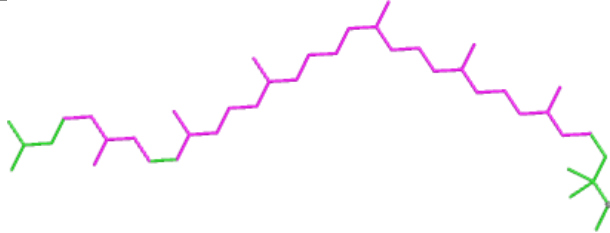
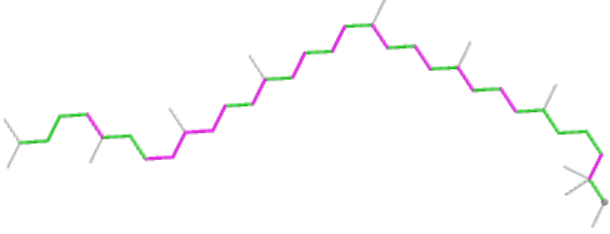
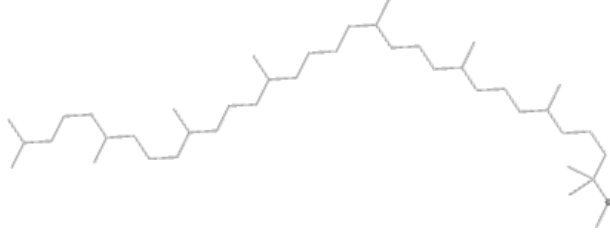
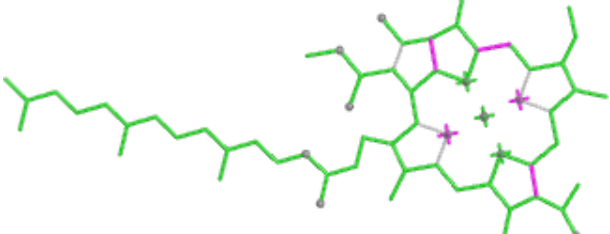
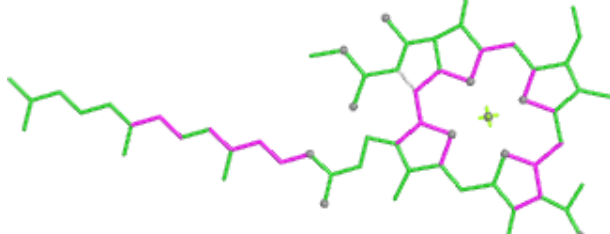
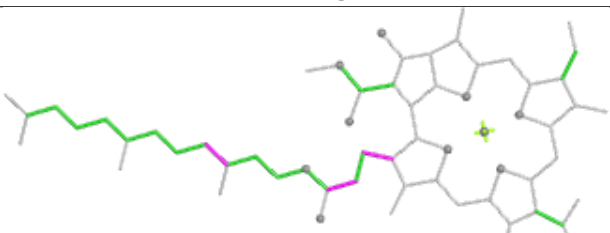
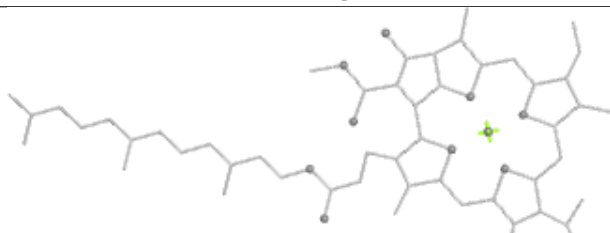


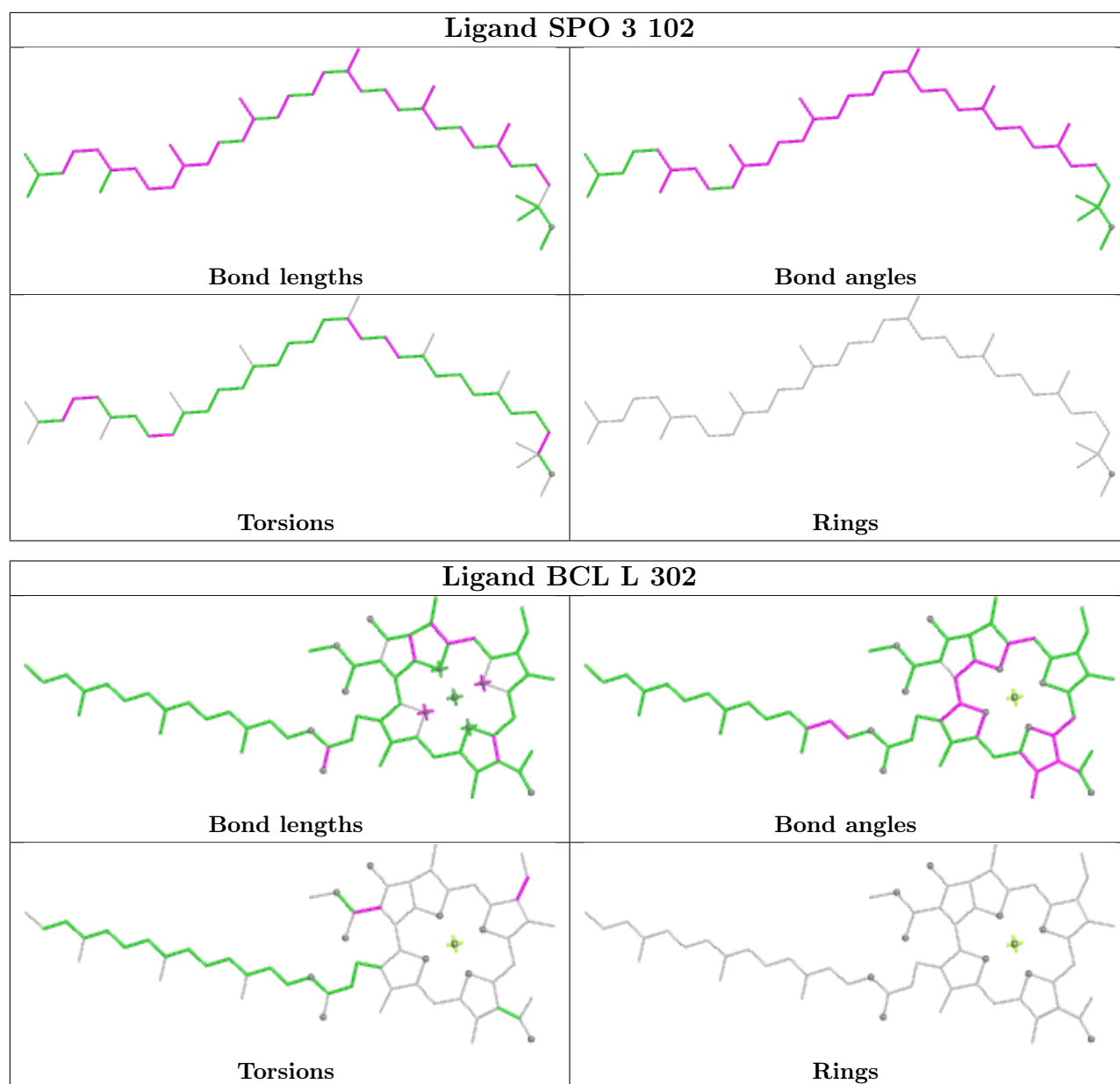
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Bond lengths	Bond angles
	
Torsions	Rings

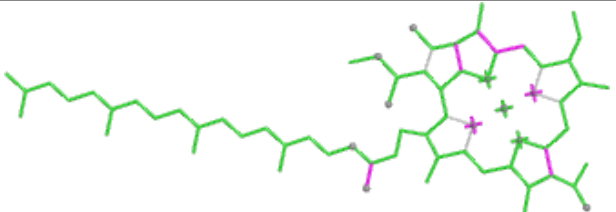
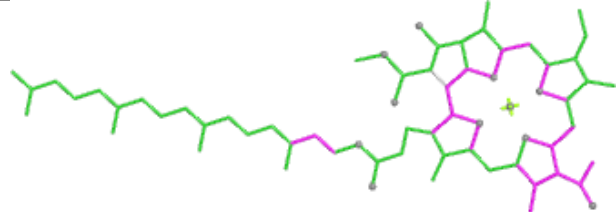
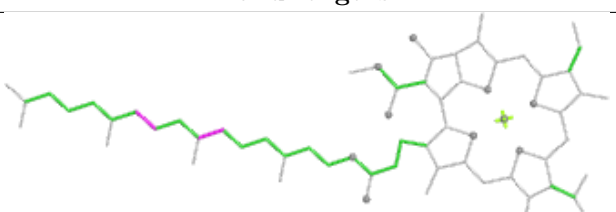
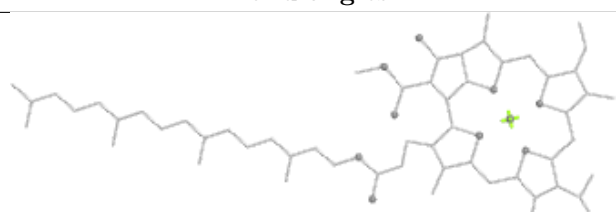
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Bond lengths	Bond angles
	
Torsions	Rings

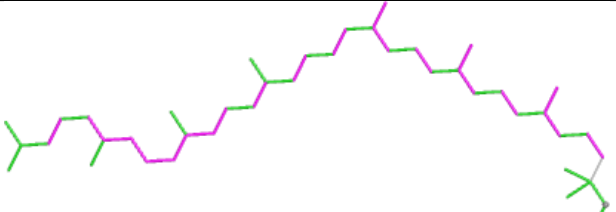
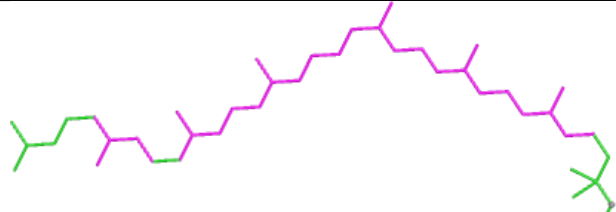
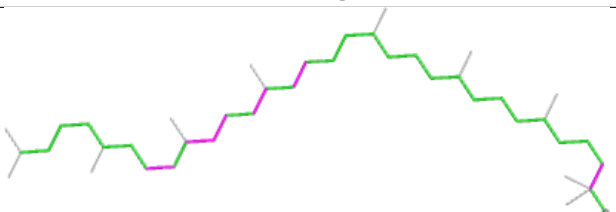
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Bond lengths	Bond angles
	
Torsions	Rings

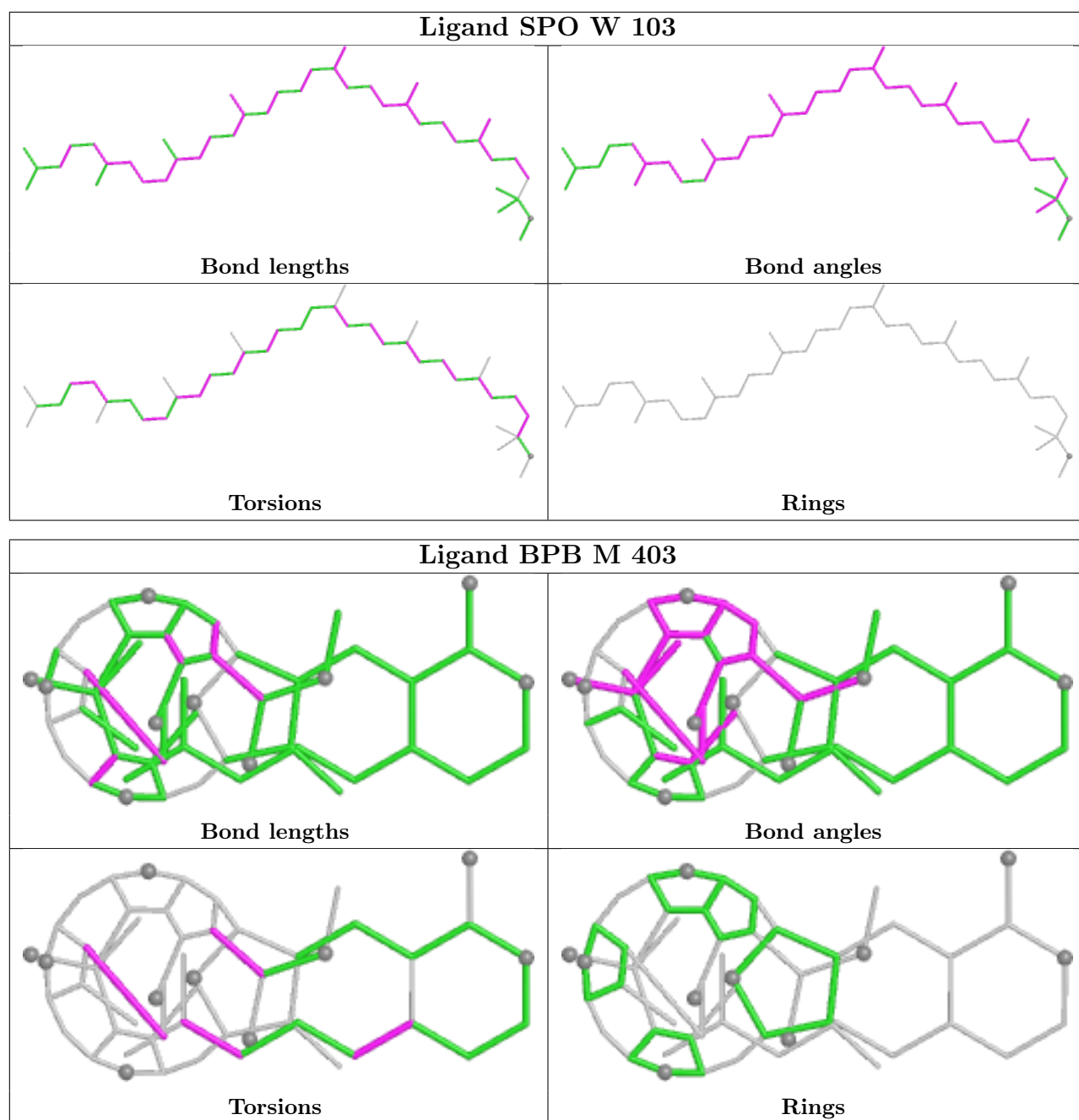


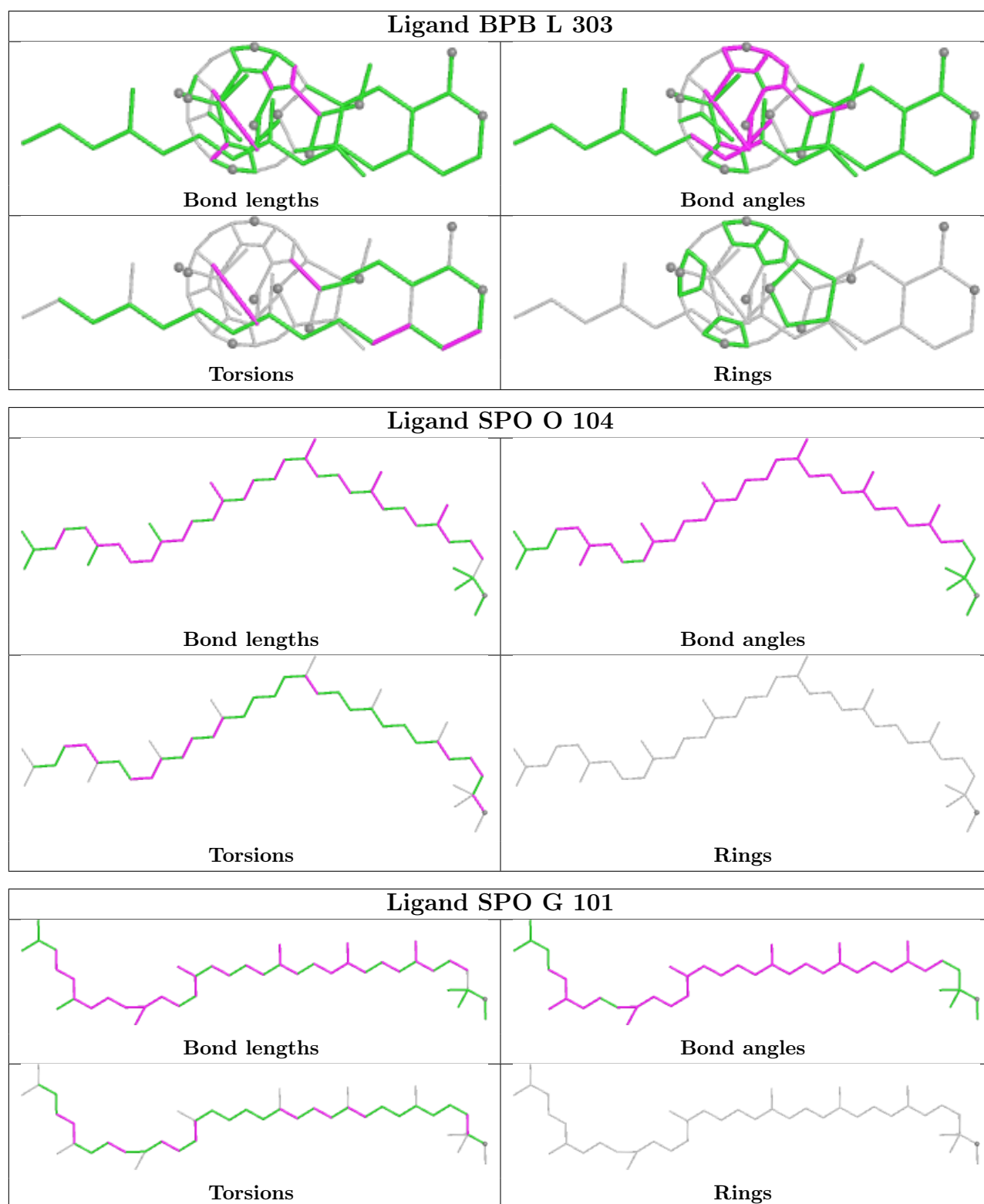
Ligand SPO 9 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCL 0 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

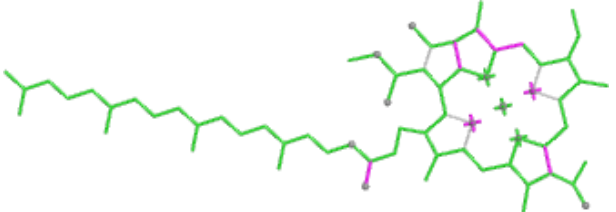
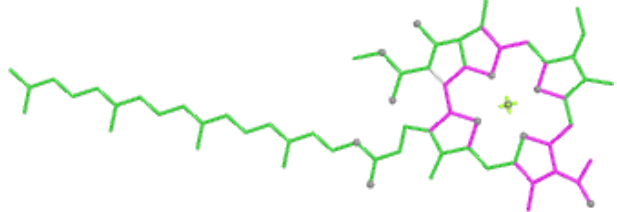
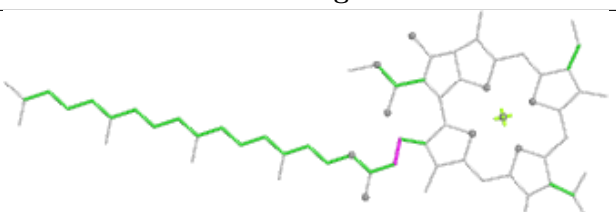
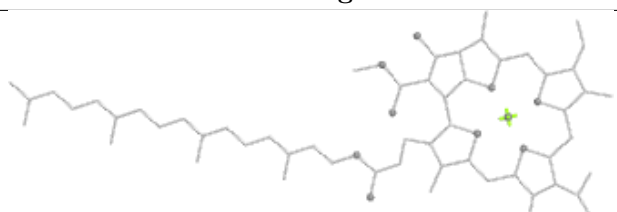
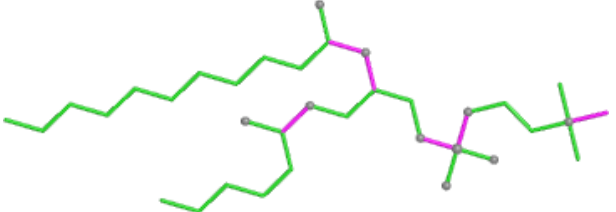
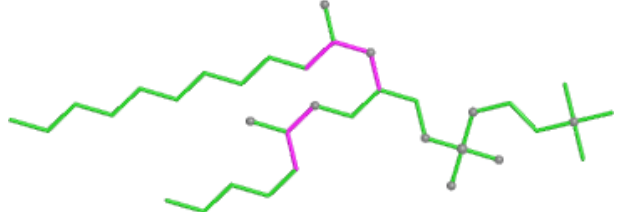
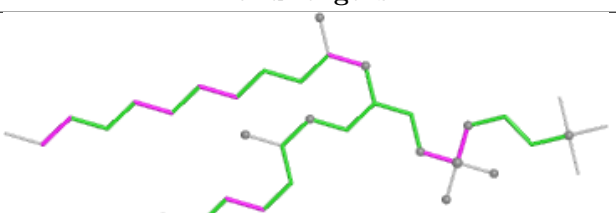
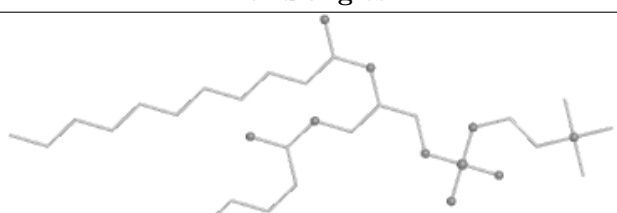
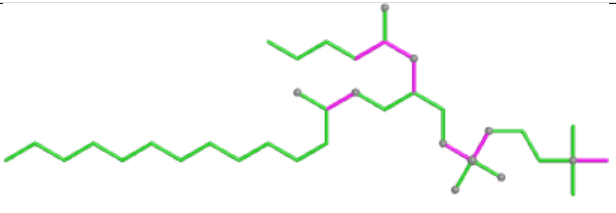
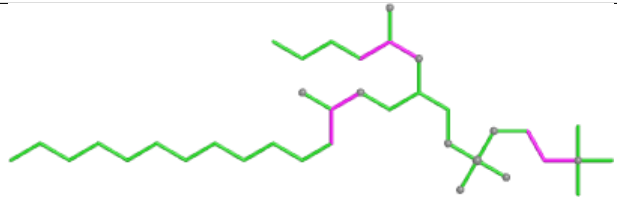
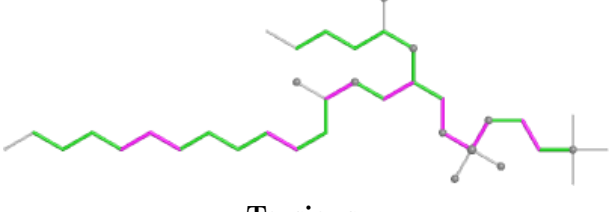
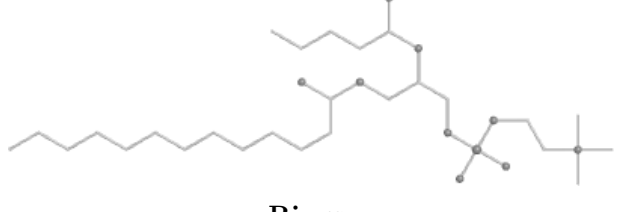


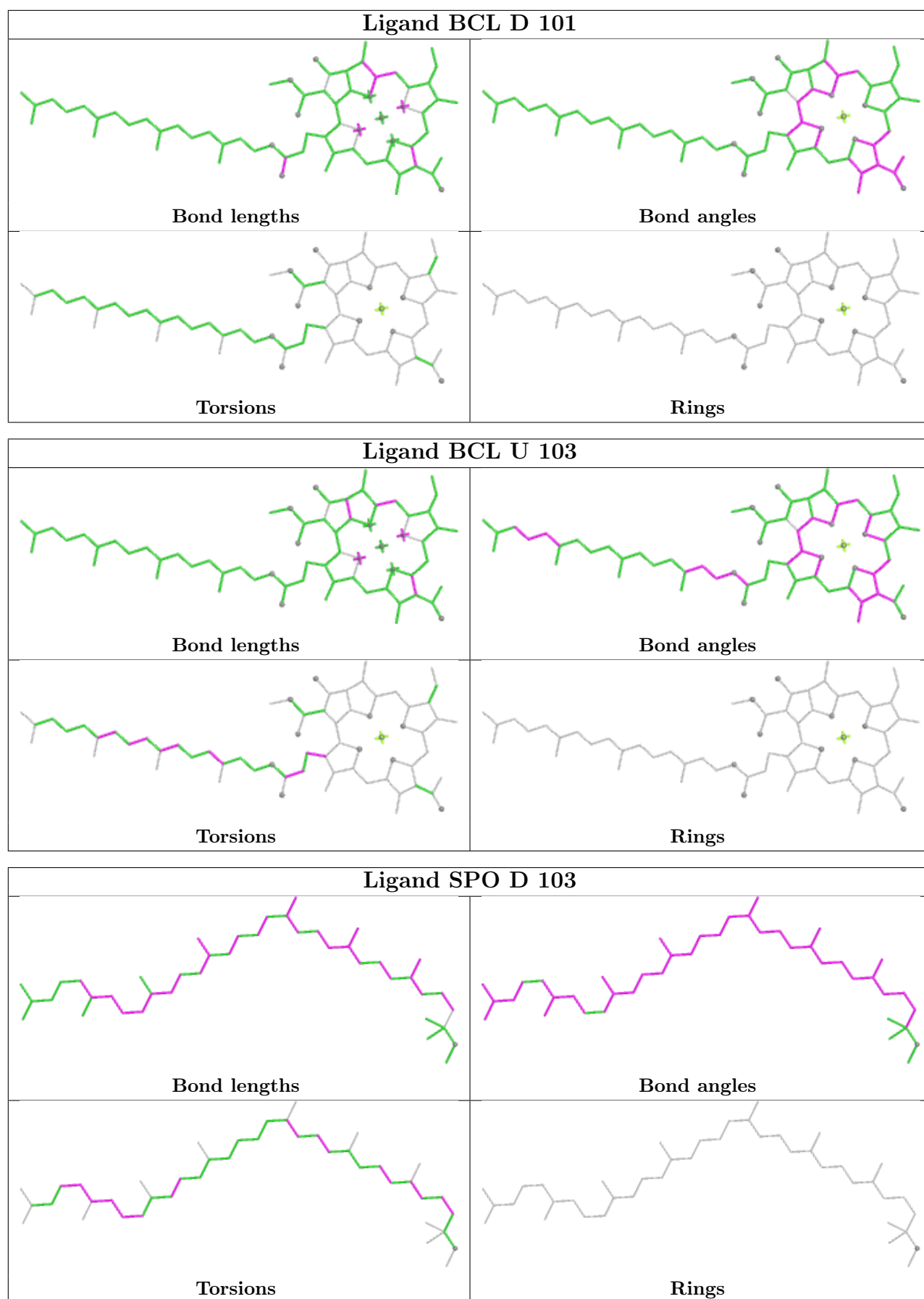
Ligand BCL W 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

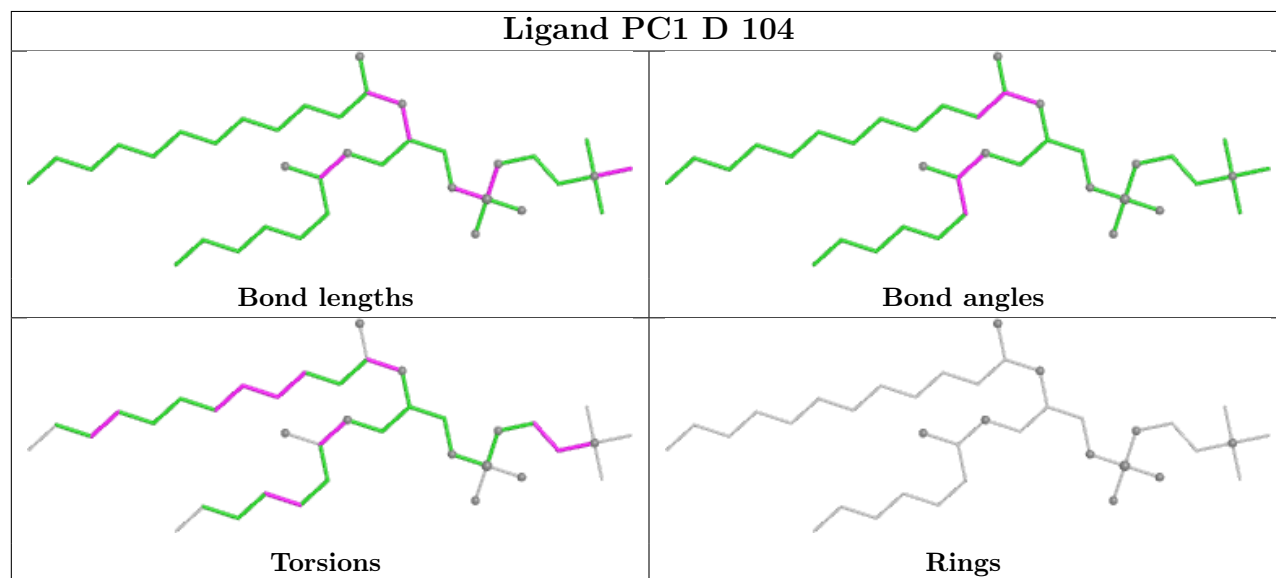
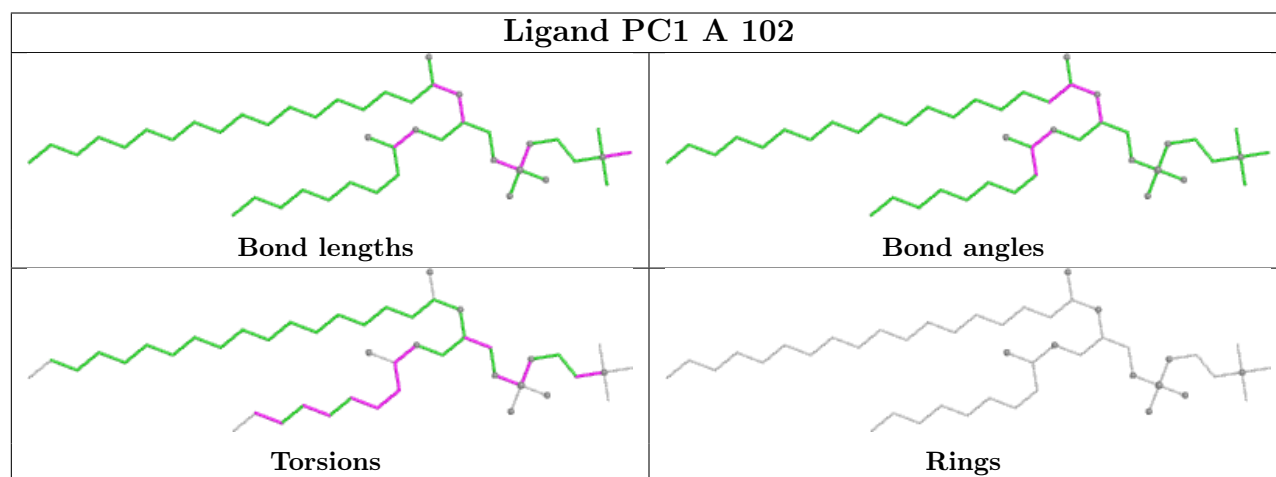
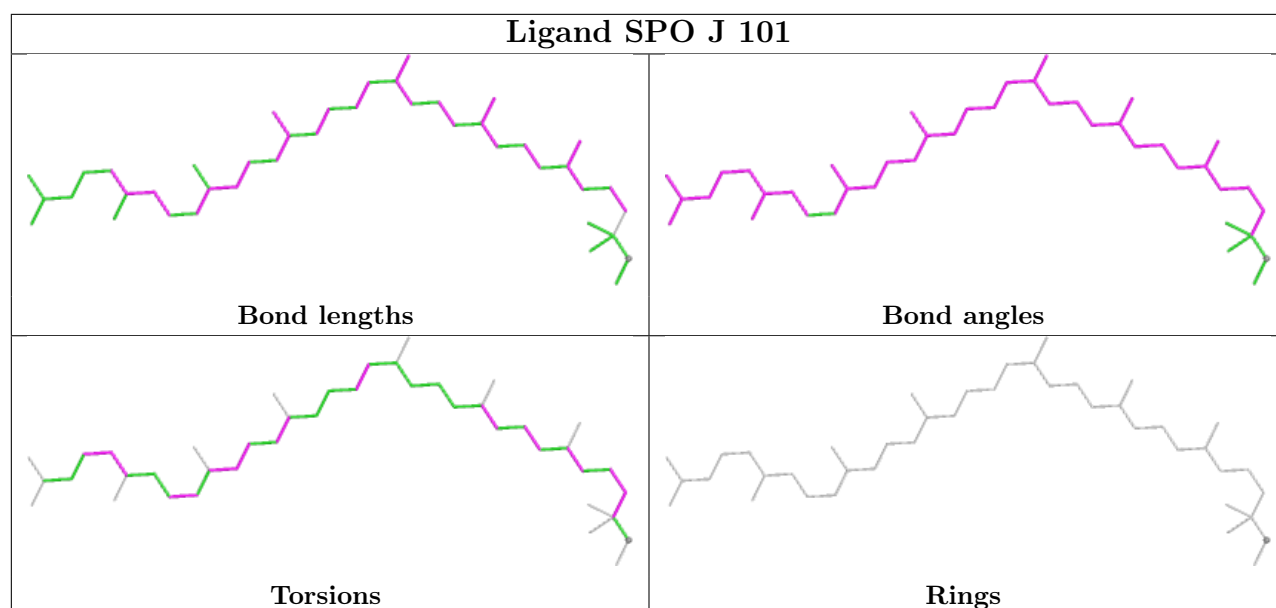
Ligand SPO T 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

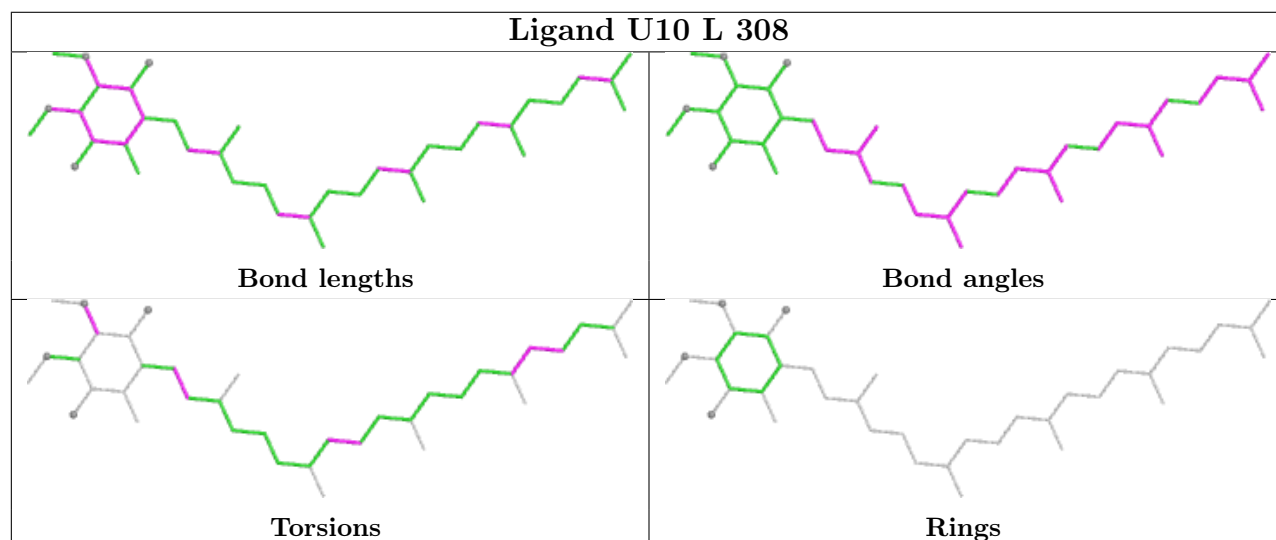
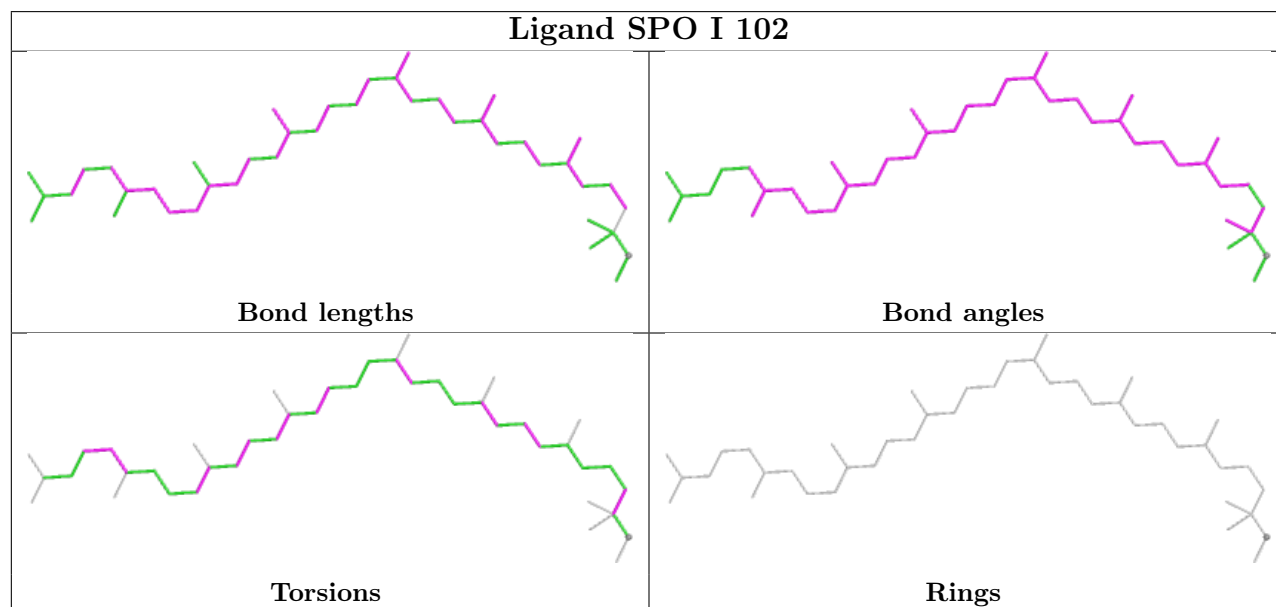
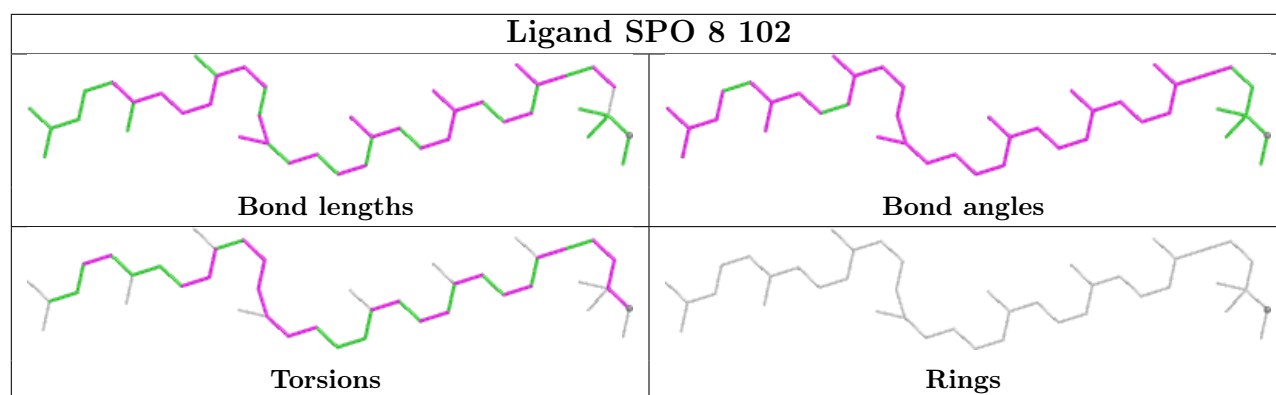


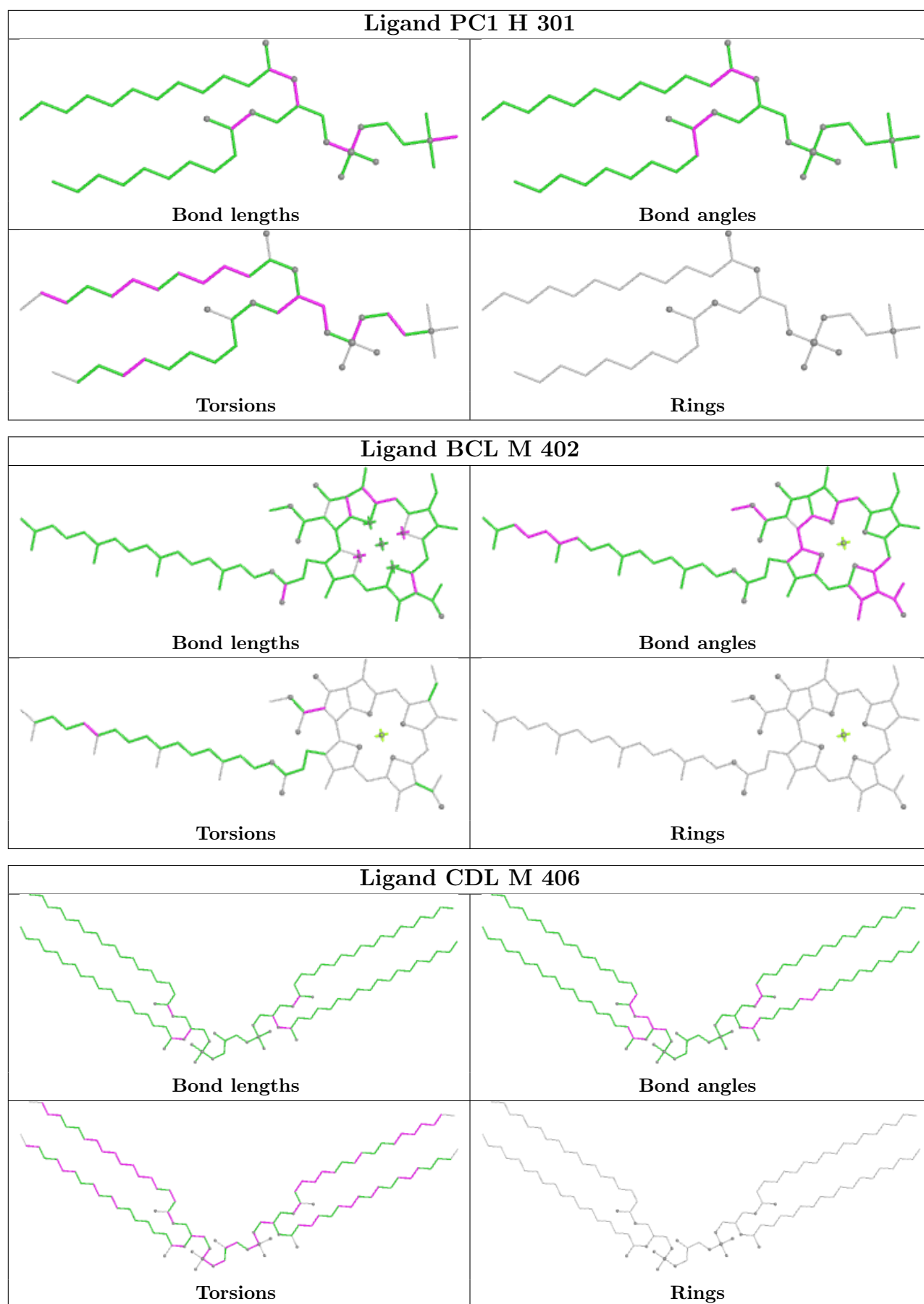


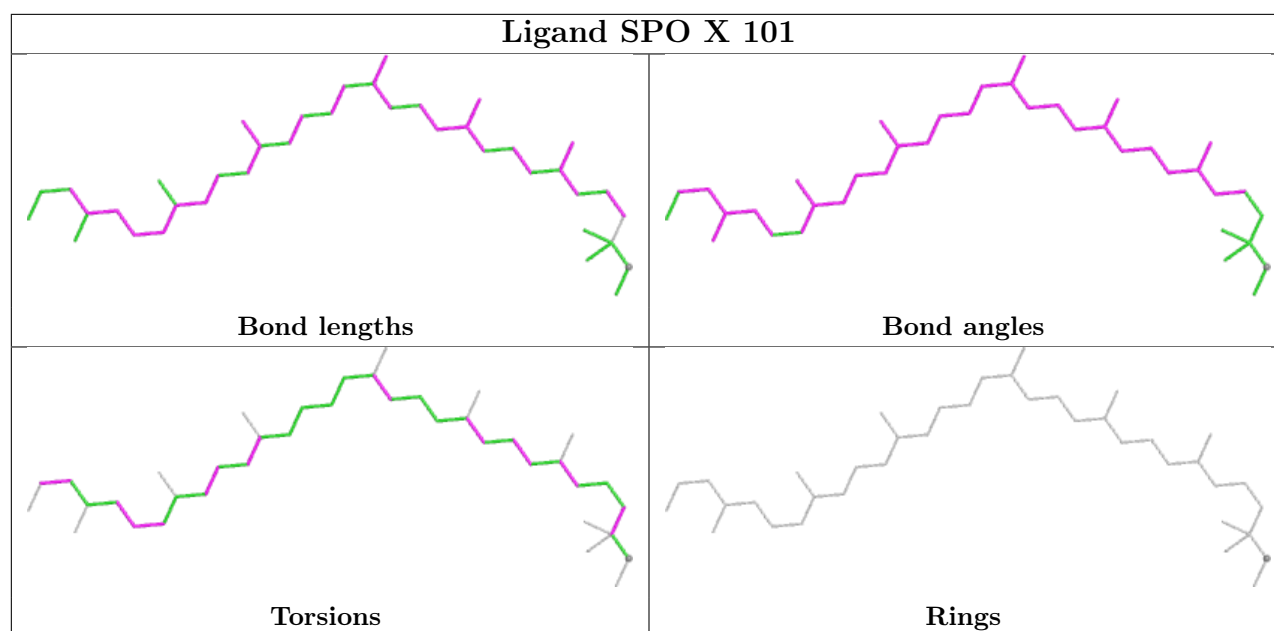
Ligand BCL L 301	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 L 304	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 L 306	
 Bond lengths	 Bond angles
 Torsions	 Rings











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

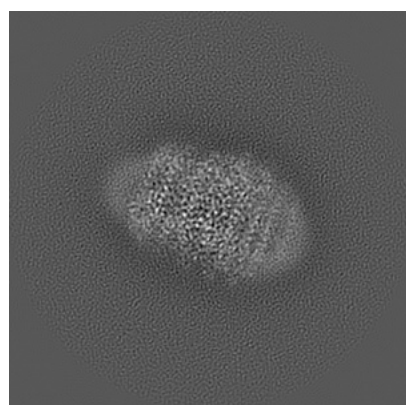
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32047. These allow visual inspection of the internal detail of the map and identification of artifacts.

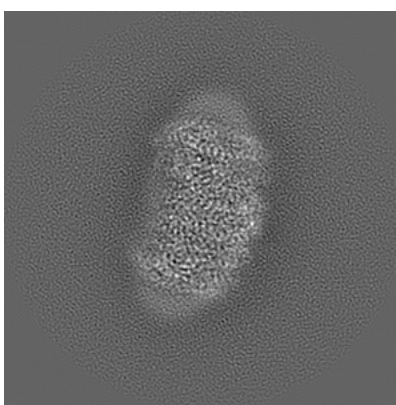
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

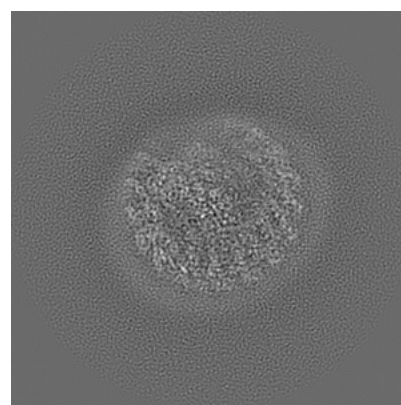
6.1.1 Primary map



X



Y

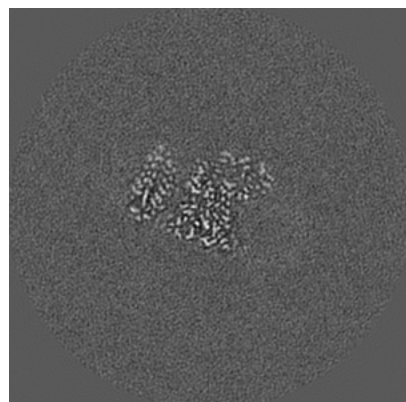


Z

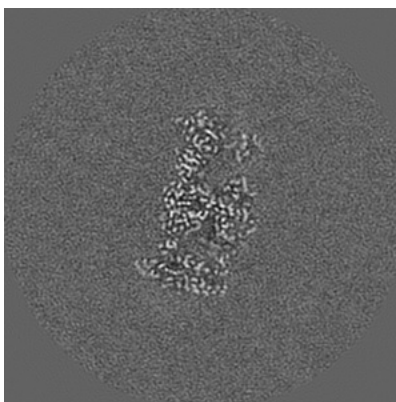
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

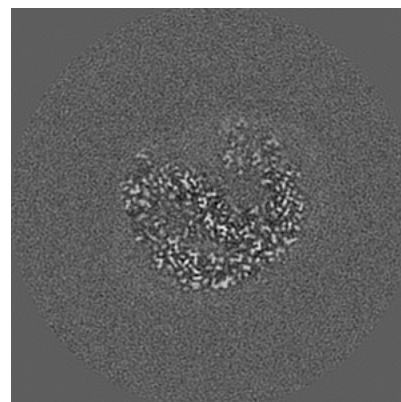
6.2.1 Primary map



X Index: 125



Y Index: 125

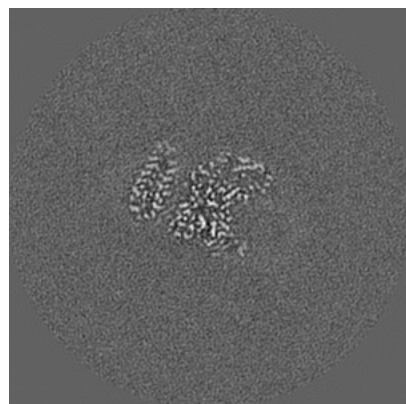


Z Index: 125

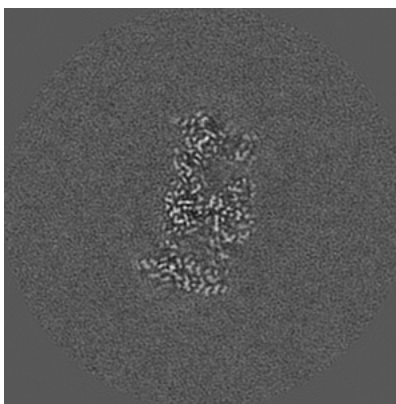
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

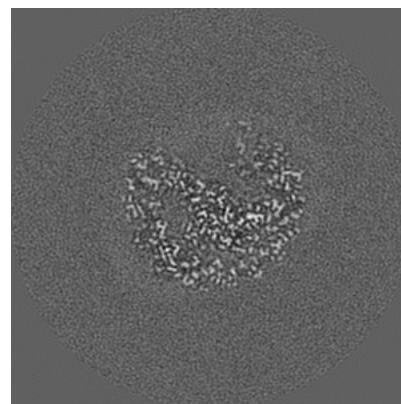
6.3.1 Primary map



X Index: 126



Y Index: 124

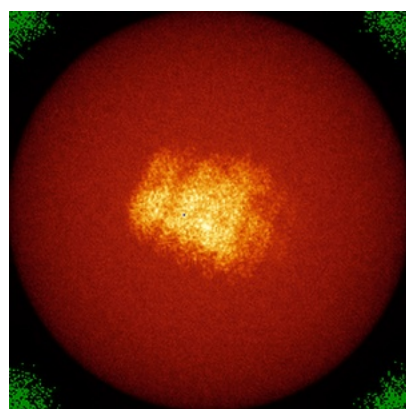


Z Index: 119

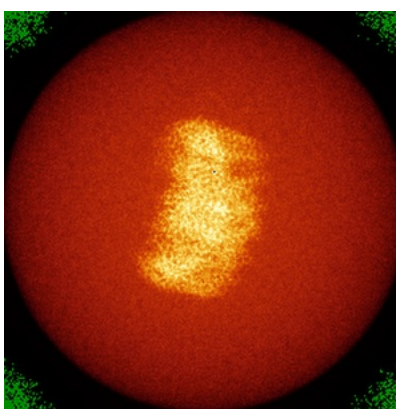
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

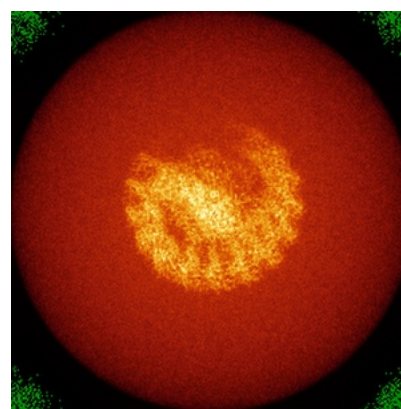
6.4.1 Primary map



X



Y

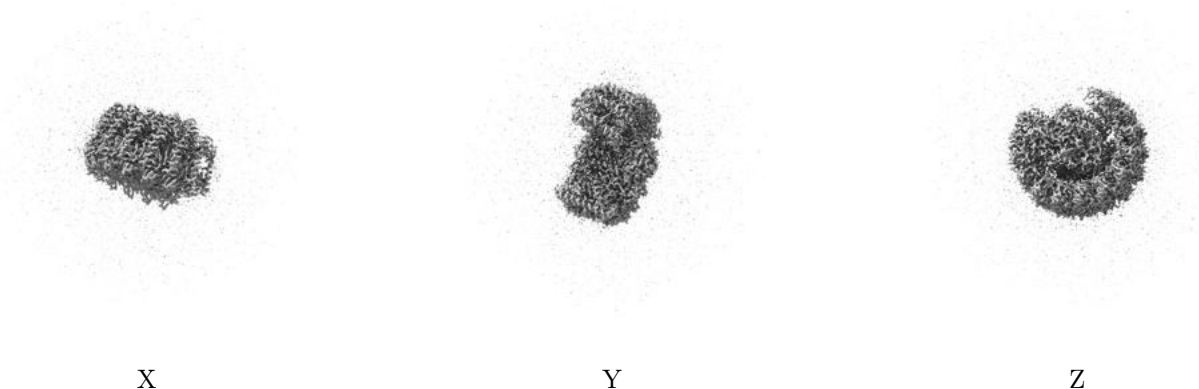


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

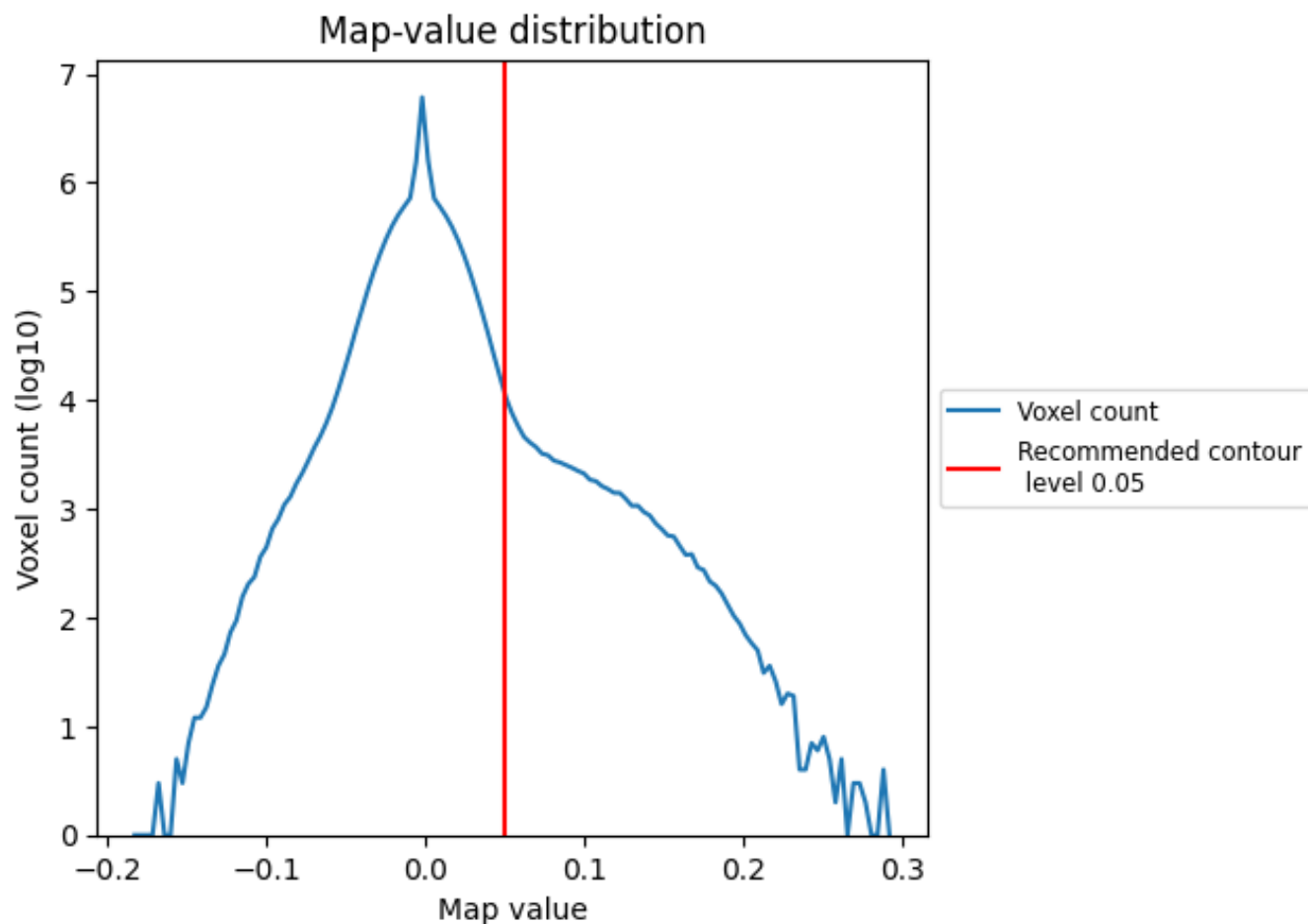
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

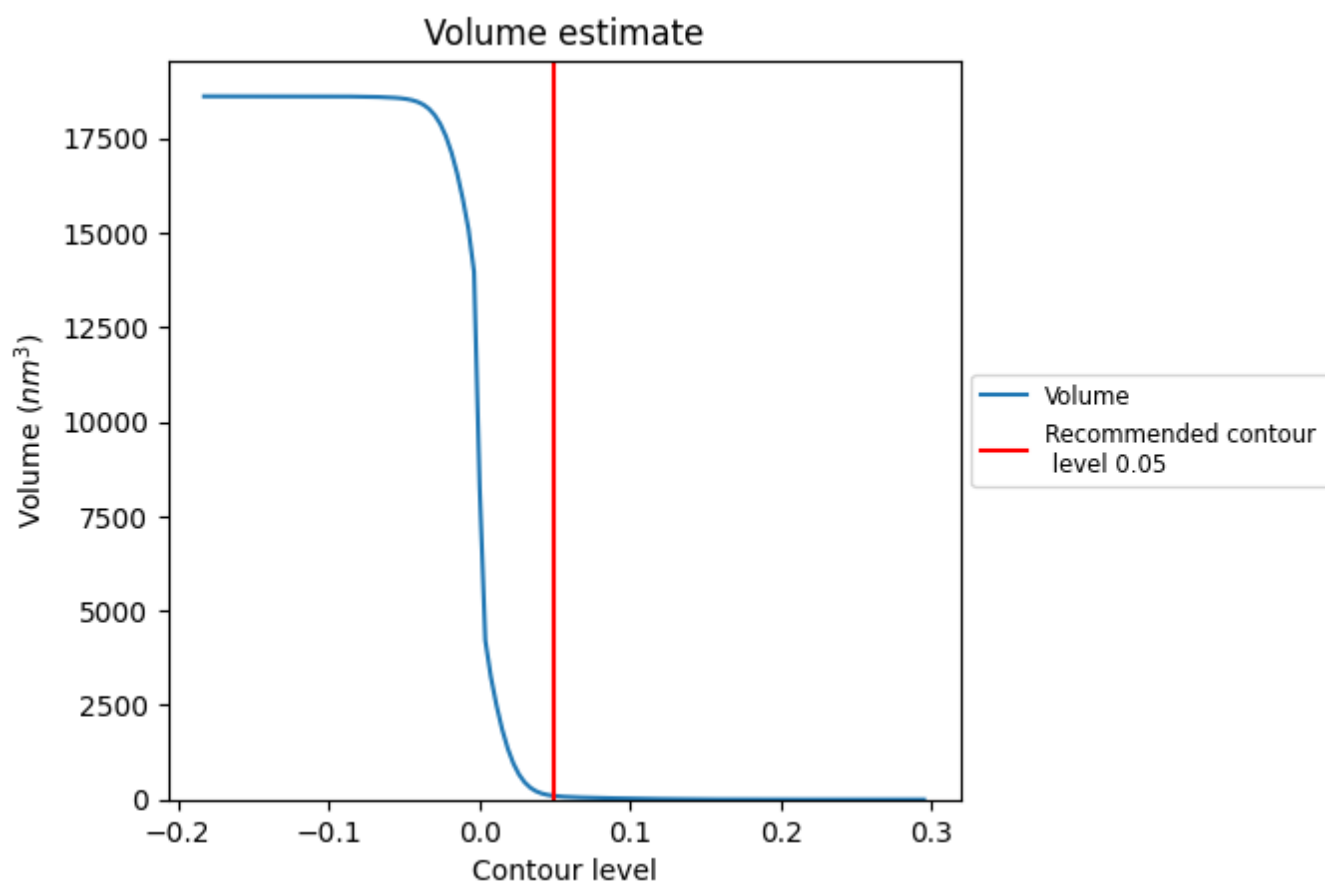
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

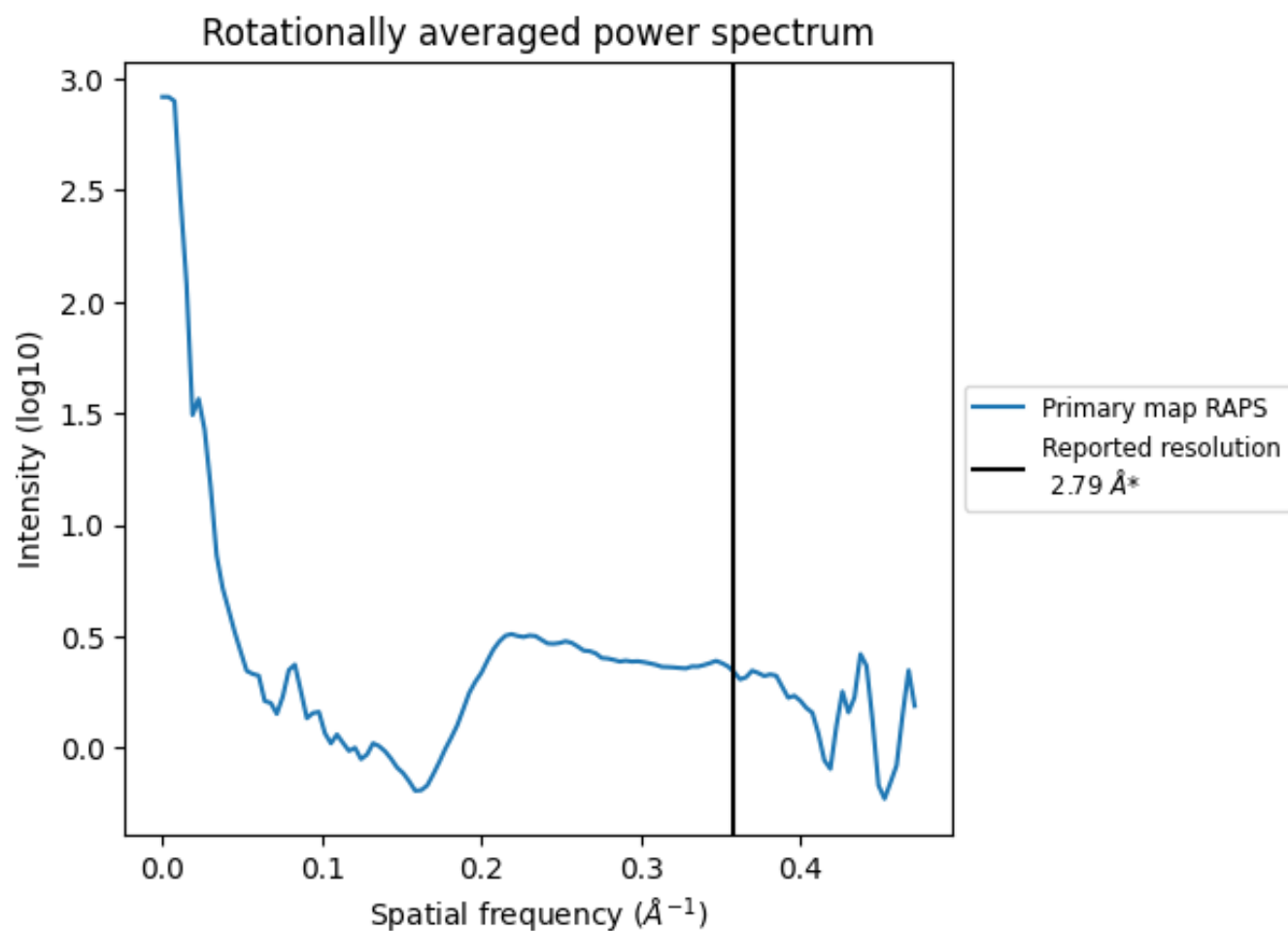
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 96 nm³; this corresponds to an approximate mass of 87 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 ⓘ

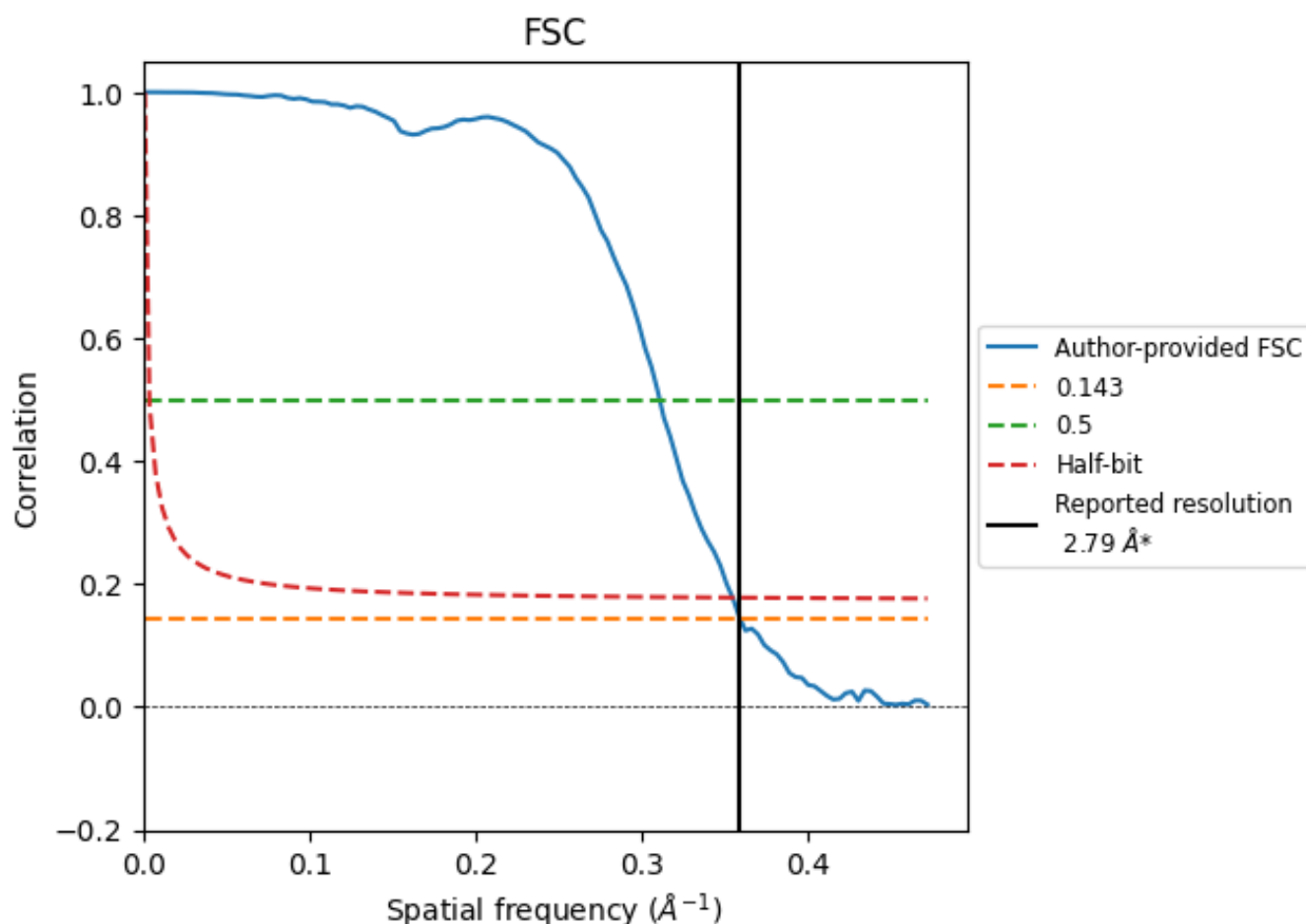


*Reported resolution corresponds to spatial frequency of 0.358 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.358 Å⁻¹

8.2 Resolution estimates [i](#)

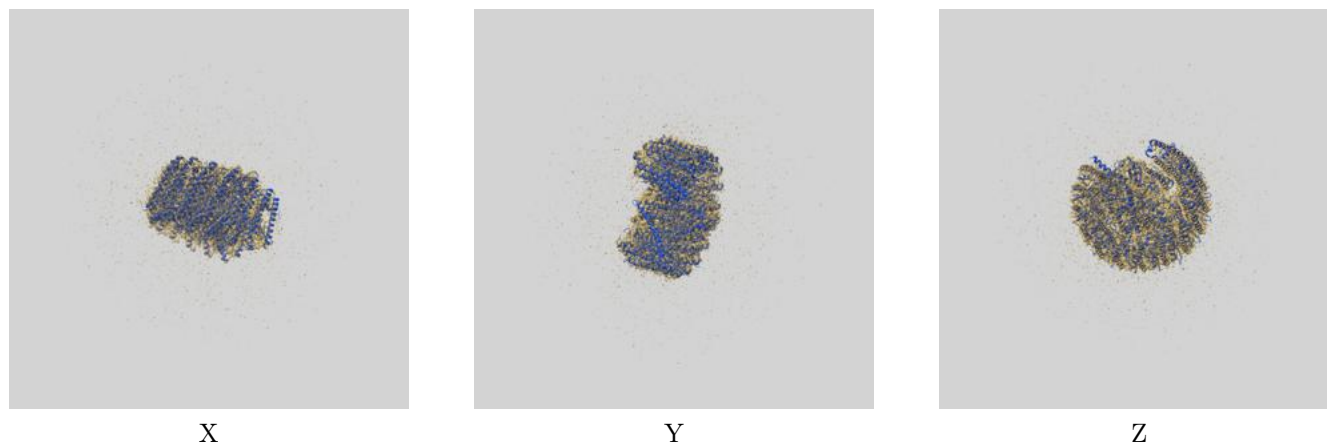
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.78	3.22	2.82
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

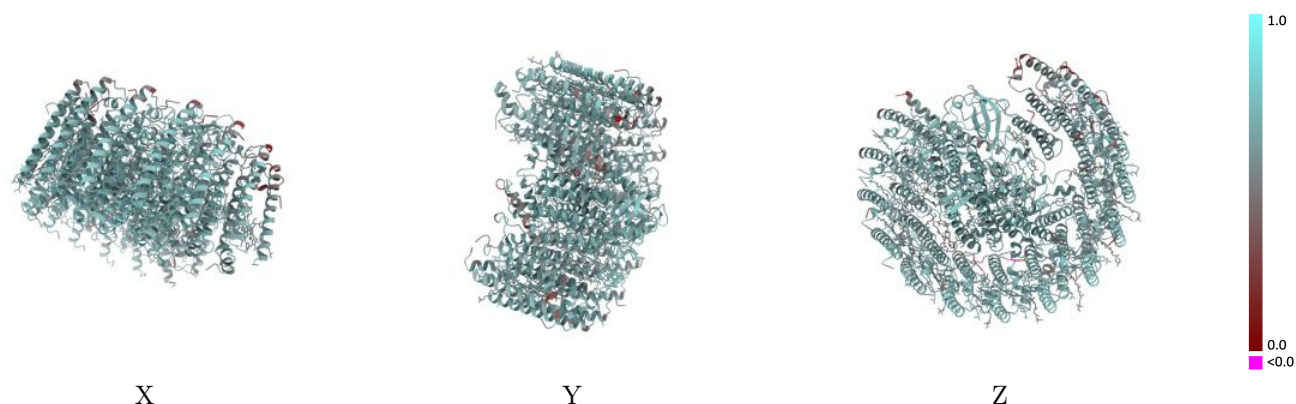
This section contains information regarding the fit between EMDB map EMD-32047 and PDB model 7VNY. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



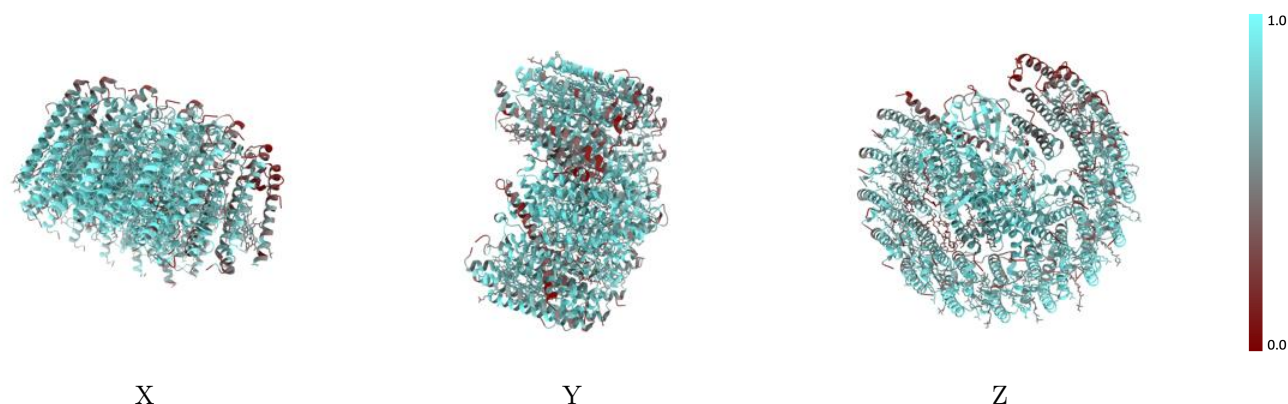
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



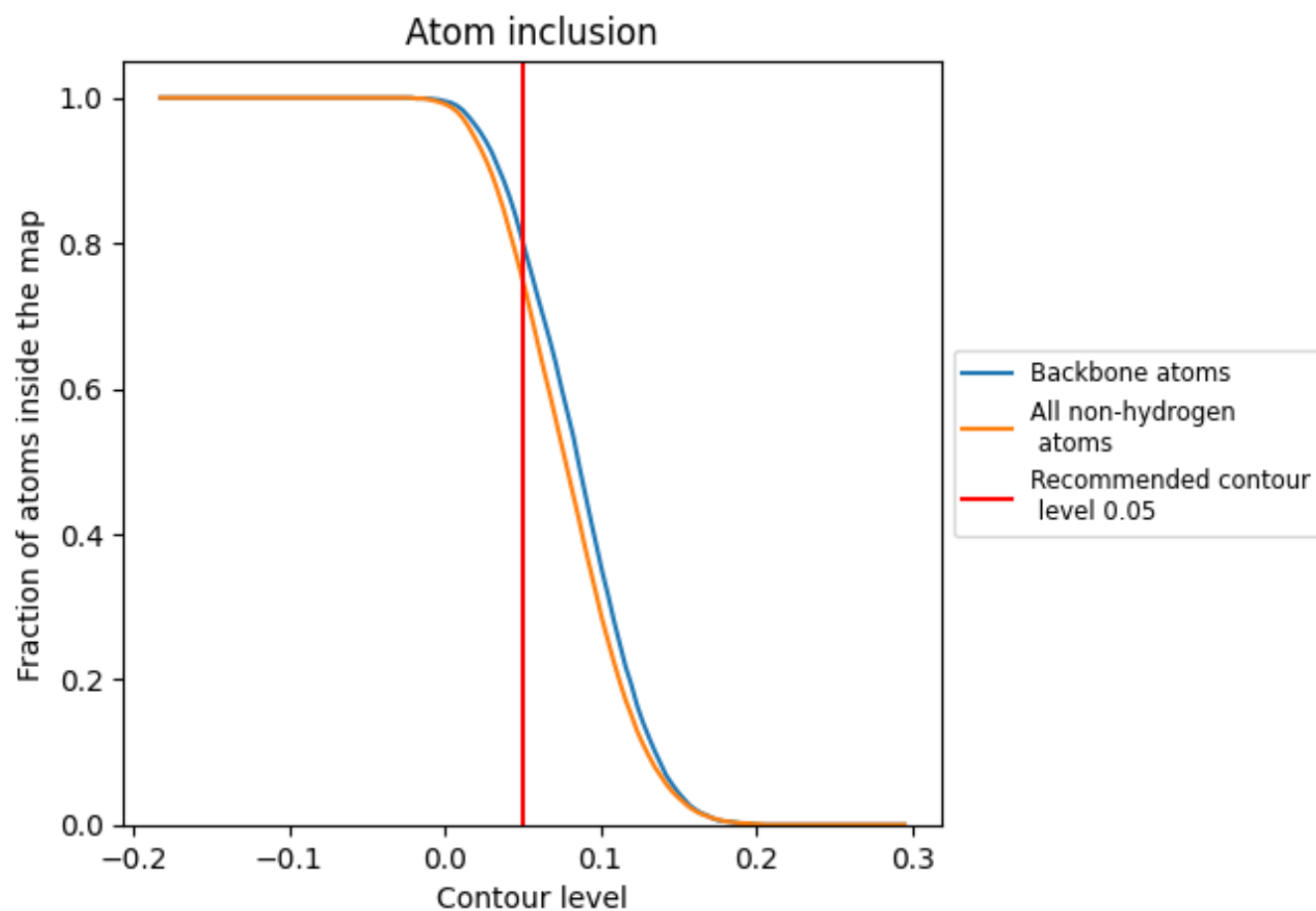
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7490	 0.6330
0	 0.7710	 0.6240
1	 0.4770	 0.5590
2	 0.3950	 0.5260
3	 0.6430	 0.6080
7	 0.6970	 0.6110
8	 0.6130	 0.5870
9	 0.8010	 0.6460
A	 0.7780	 0.6500
B	 0.7820	 0.6390
C	 0.6570	 0.5890
D	 0.7620	 0.6440
E	 0.7410	 0.6150
F	 0.8100	 0.6530
G	 0.7330	 0.6280
H	 0.7060	 0.6330
I	 0.8100	 0.6510
J	 0.7340	 0.6160
K	 0.7940	 0.6440
L	 0.8700	 0.6720
M	 0.8940	 0.6800
N	 0.7070	 0.6110
O	 0.7870	 0.6380
P	 0.6940	 0.6020
Q	 0.7870	 0.6380
R	 0.7380	 0.6240
S	 0.8190	 0.6460
T	 0.7000	 0.6100
U	 0.7970	 0.6340
V	 0.7010	 0.6010
W	 0.6990	 0.6220
X	 0.3360	 0.5130
Y	 0.5530	 0.5940
Z	 0.5730	 0.5580

