



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 02:55 AM JST

PDB ID : 7VOY
EMDB ID : EMD-32062
Title : Rba sphaeroides PufX-KO RC-LH1
Authors : Bracun, L.; Yamagata, A.; Liu, L.N.; Shirouzu, M.
Deposited on : 2021-10-15
Resolution : 4.20 Å (reported)

This is a Full wwPDB EM Validation 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:

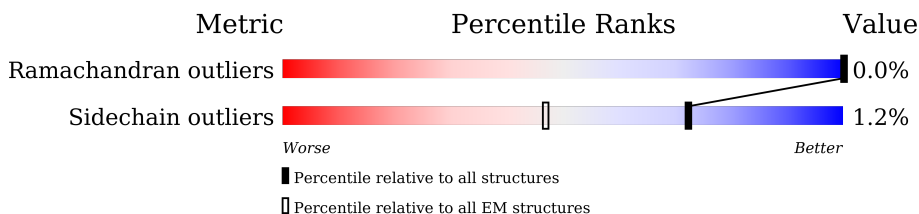
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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 4.20 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1	58	
1	4	58	
1	6	58	
1	7	58	
1	9	58	
1	A	58	
1	C	58	
1	D	58	
1	F	58	

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Mol	Chain	Length	Quality of chain
1	I	58	31% 91% 7%
1	K	58	16% 91% 7%
1	O	58	9% 93% 7%
1	Q	58	10% 93% 7%
1	S	58	16% 93% 7%
1	U	58	10% 93% 7%
1	W	58	21% 93% 7%
1	Y	58	16% 91% 7%
2	0	49	41% 86% 10%
2	2	49	16% 80% 18%
2	3	49	35% 88% 8%
2	5	49	41% 90% 8%
2	8	49	39% 86% 10%
2	B	49	49% 90% 8%
2	E	49	45% 86% 12%
2	G	49	41% 86% 12%
2	J	49	22% 86% 12%
2	N	49	16% 86% 12%
2	P	49	20% 84% 12%
2	R	49	18% 86% 12%
2	T	49	20% 86% 12%
2	V	49	18% 82% 6% 12%
2	X	49	18% 86% 12%
2	Z	49	16% 84% 14%
2	t	49	39% 90% 8%

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Mol	Chain	Length	Quality of chain
3	L	282	96%
			99%
4	M	308	94%
			99%
5	H	260	93%
			95%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 22119 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 Light-harvesting protein B-875 alpha chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	54	455	310	73	69	3	0	0
1	D	54	455	310	73	69	3	0	0
1	F	54	455	310	73	69	3	0	0
1	I	54	455	310	73	69	3	0	0
1	K	54	455	310	73	69	3	0	0
1	O	54	455	310	73	69	3	0	0
1	Q	54	455	310	73	69	3	0	0
1	S	54	455	310	73	69	3	0	0
1	U	54	455	310	73	69	3	0	0
1	W	54	455	310	73	69	3	0	0
1	Y	54	455	310	73	69	3	0	0
1	1	53	447	305	72	68	2	0	0
1	7	46	392	271	60	58	3	0	0
1	9	54	455	310	73	69	3	0	0
1	4	54	455	310	73	69	3	0	0
1	6	54	455	310	73	69	3	0	0
1	C	54	455	310	73	69	3	0	0

- Molecule 2 is a protein called Light-harvesting protein B-875 beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	45	Total	C	N	O	S	0	0
			365	243	57	64	1		
2	E	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	G	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	J	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	N	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	P	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	R	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	T	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	V	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	X	43	Total	C	N	O	S	0	0
			351	236	55	59	1		
2	Z	42	Total	C	N	O	S	0	0
			343	230	54	58	1		
2	2	40	Total	C	N	O	S	0	0
			327	219	52	55	1		
2	8	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
2	0	44	Total	C	N	O	S	0	0
			359	240	56	62	1		
2	t	45	Total	C	N	O	S	0	0
			365	243	57	64	1		
2	5	45	Total	C	N	O	S	0	0
			365	243	57	64	1		
2	3	45	Total	C	N	O	S	0	0
			365	243	57	64	1		

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

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

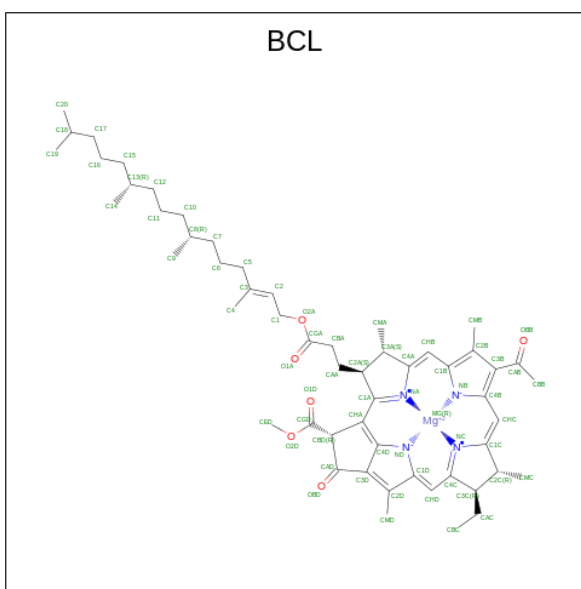
- Molecule 4 is a protein called Reaction center protein M chain.

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

- Molecule 5 is a protein called Reaction center protein H chain.

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

- Molecule 6 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
			Total	C	Mg	N	O	
6	A	1	46	35	1	4	6	0
6	B	1	46	35	1	4	6	0
6	E	1	92	70	2	8	12	0
6	E	1	92	70	2	8	12	0
6	F	1	46	35	1	4	6	0
6	G	1	46	35	1	4	6	0
6	I	1	46	35	1	4	6	0

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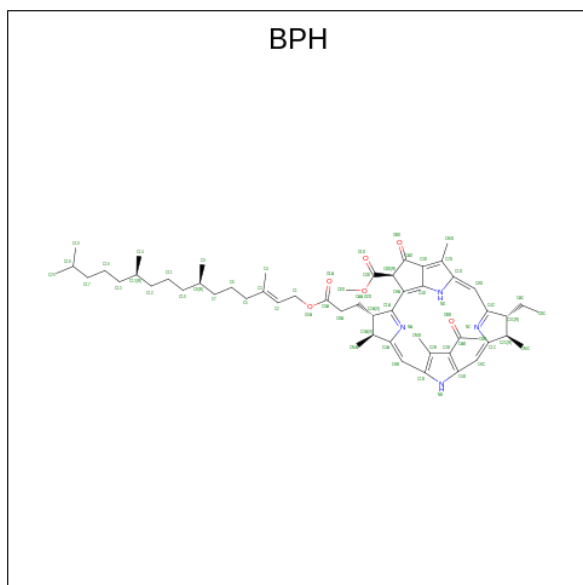
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
6	J	1	46	35	1	4	6	0
6	K	1	46	35	1	4	6	0
6	N	1	46	35	1	4	6	0
6	O	1	46	35	1	4	6	0
6	P	1	46	35	1	4	6	0
6	Q	1	46	35	1	4	6	0
6	R	1	46	35	1	4	6	0
6	S	1	46	35	1	4	6	0
6	T	1	46	35	1	4	6	0
6	U	1	46	35	1	4	6	0
6	V	1	46	35	1	4	6	0
6	W	1	46	35	1	4	6	0
6	X	1	46	35	1	4	6	0
6	Y	1	46	35	1	4	6	0
6	Z	1	46	35	1	4	6	0
6	1	1	46	35	1	4	6	0
6	2	1	46	35	1	4	6	0
6	7	1	46	35	1	4	6	0
6	8	1	46	35	1	4	6	0
6	9	1	46	35	1	4	6	0
6	0	1	46	35	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
6	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
6	t	1	Total 46	C 35	Mg 1	N 4	O 6	0
6	5	1	Total 92	C 70	Mg 2	N 8	O 12	0
6	5	1	Total 92	C 70	Mg 2	N 8	O 12	0
6	C	1	Total 46	C 35	Mg 1	N 4	O 6	0
6	3	1	Total 46	C 35	Mg 1	N 4	O 6	0
6	L	1	Total 46	C 35	Mg 1	N 4	O 6	0
6	M	1	Total 138	C 105	Mg 3	N 12	O 18	0
6	M	1	Total 138	C 105	Mg 3	N 12	O 18	0
6	M	1	Total 138	C 105	Mg 3	N 12	O 18	0

- Molecule 7 is BACTERIOPHEOPHYTIN A (three-letter code: BPH) (formula: $C_{55}H_{76}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



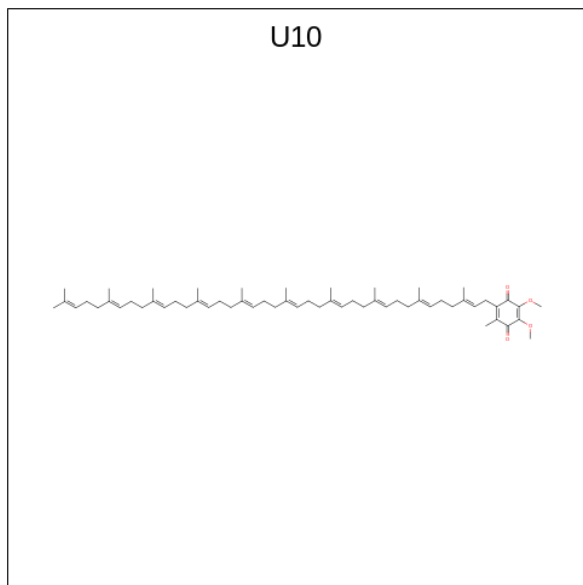
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	L	1	Total 45	C 35	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	M	1	45	35	4	6	0

- Molecule 8 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).

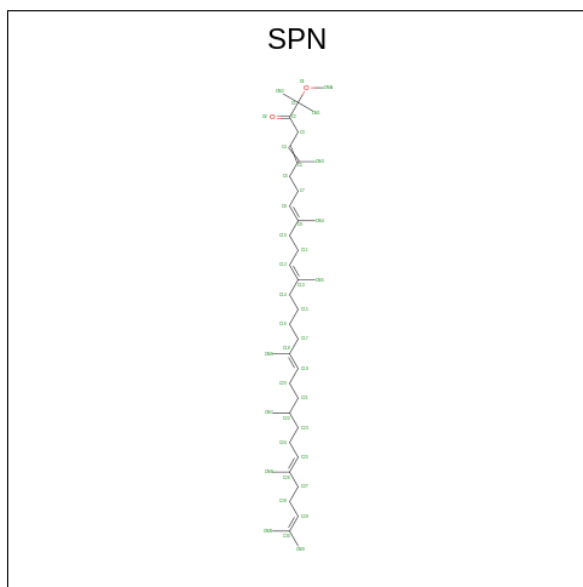


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	L	1	14	10	4	0
8	M	1	14	10	4	0

- Molecule 9 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 10 is SPEROIDENONE (three-letter code: SPN) (formula: $C_{41}H_{70}O_2$) (labeled as "Ligand of Interest" by depositor).

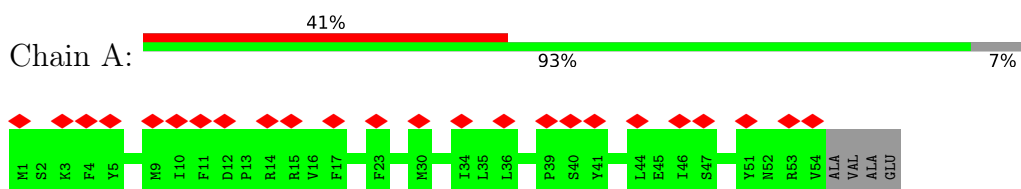


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	M	1	43	41	2	0

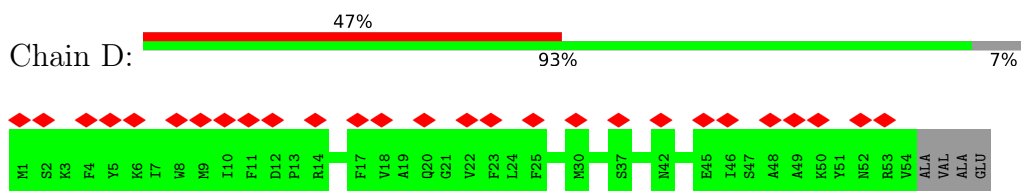
3 Residue-property plots [i](#)

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

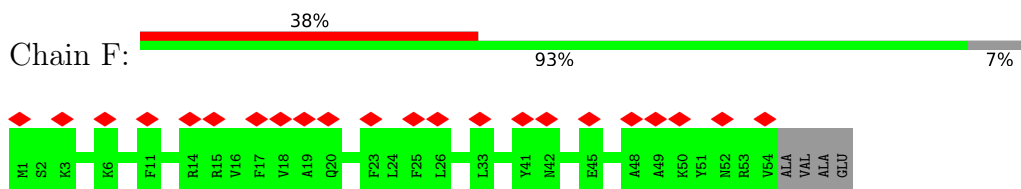
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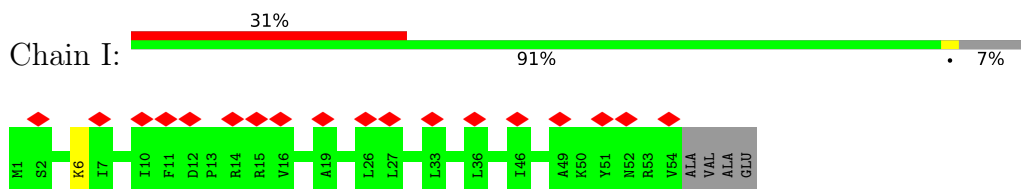
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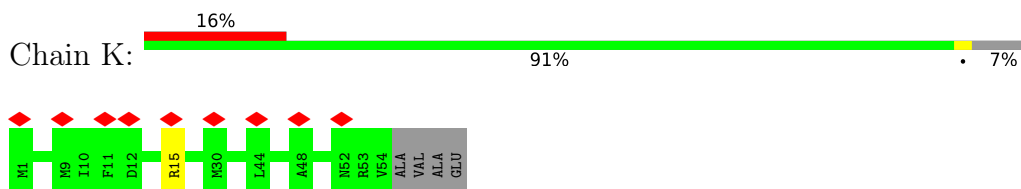
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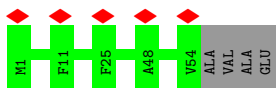
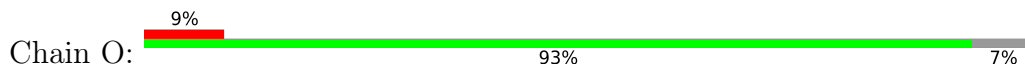
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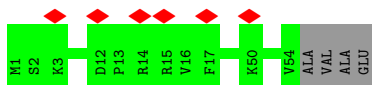
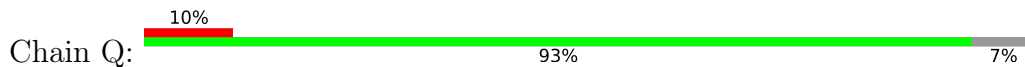
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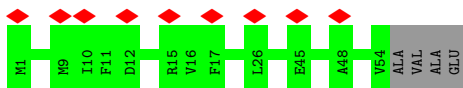
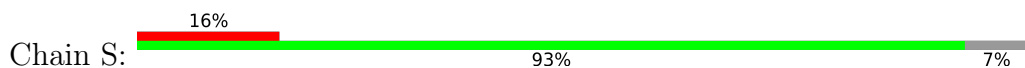
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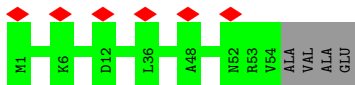
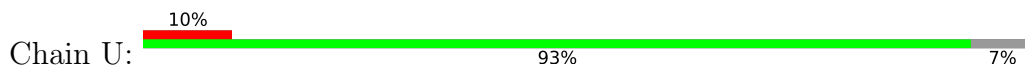
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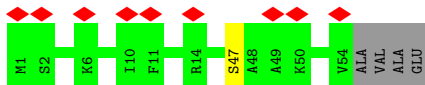
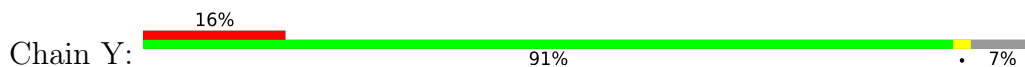
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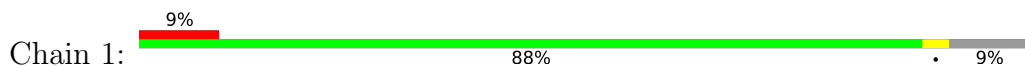
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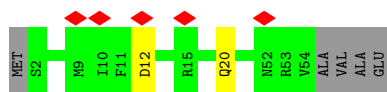


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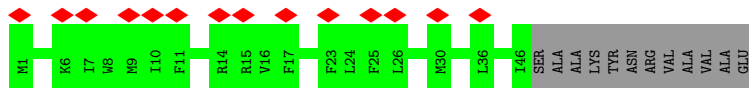
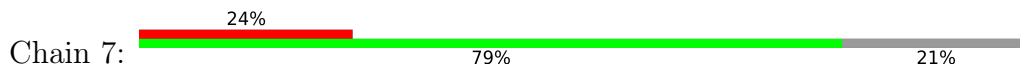


- Molecule 1: Light-harvesting protein B-875 alpha chain

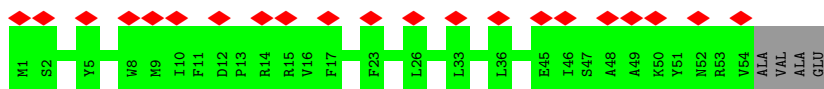




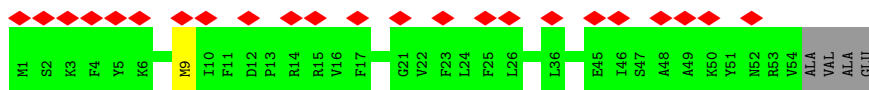
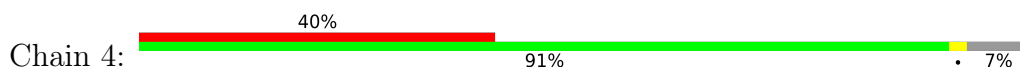
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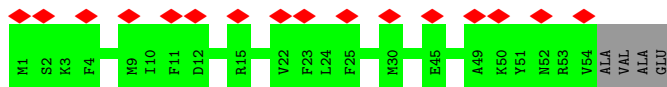
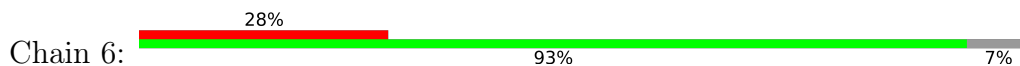
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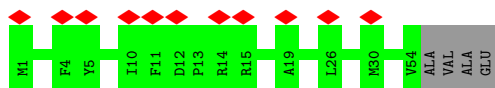
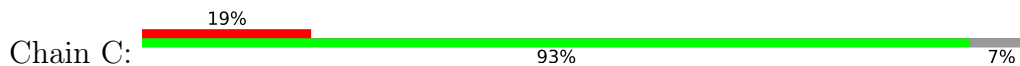
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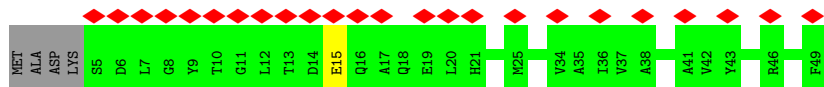
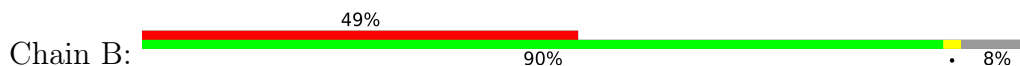
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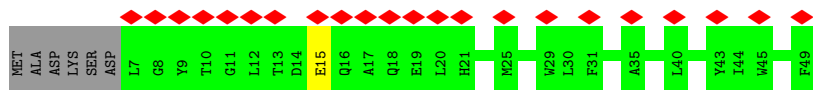
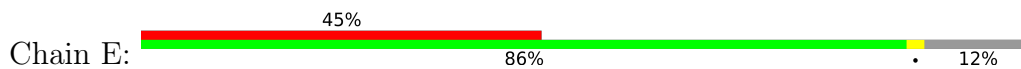
- Molecule 1: Light-harvesting protein B-875 alpha chain



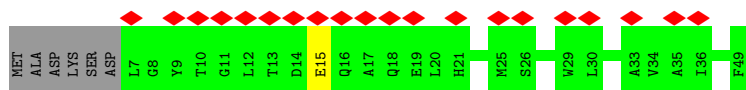
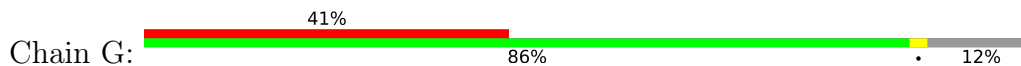
- Molecule 2: Light-harvesting protein B-875 beta chain



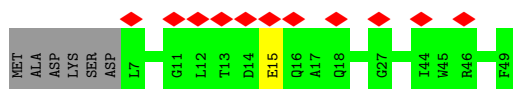
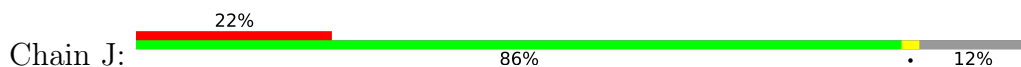
- Molecule 2: Light-harvesting protein B-875 beta chain



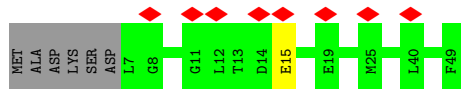
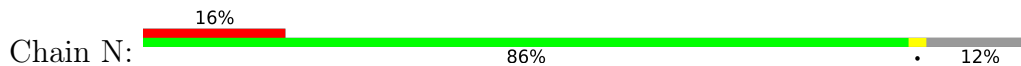
• Molecule 2: Light-harvesting protein B-875 beta chain



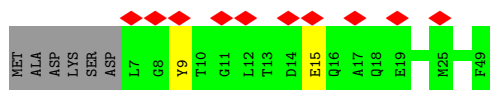
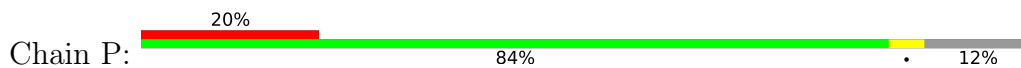
• Molecule 2: Light-harvesting protein B-875 beta chain



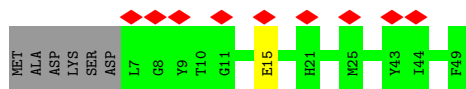
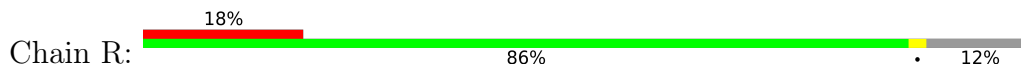
• Molecule 2: Light-harvesting protein B-875 beta chain



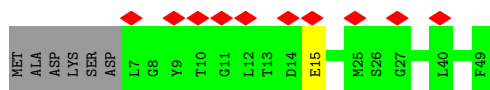
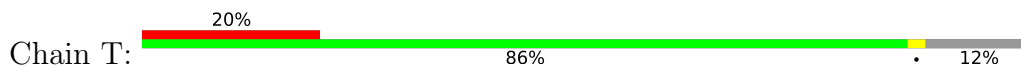
• Molecule 2: Light-harvesting protein B-875 beta chain



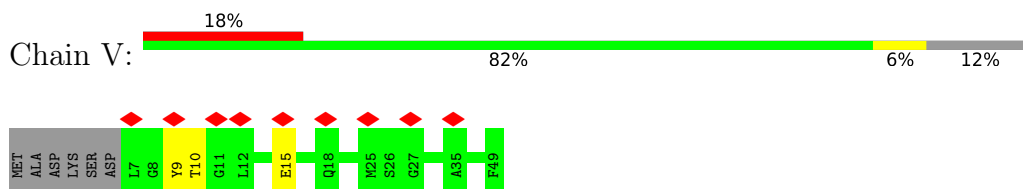
• Molecule 2: Light-harvesting protein B-875 beta chain



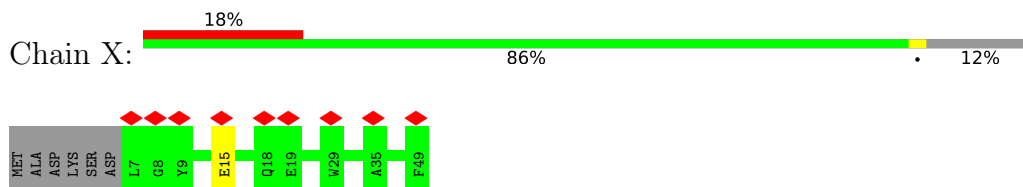
• Molecule 2: Light-harvesting protein B-875 beta chain



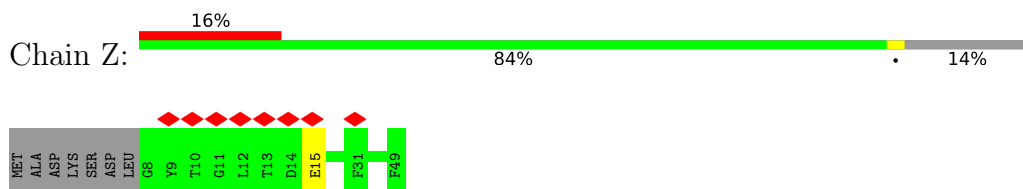
- Molecule 2: Light-harvesting protein B-875 beta chain



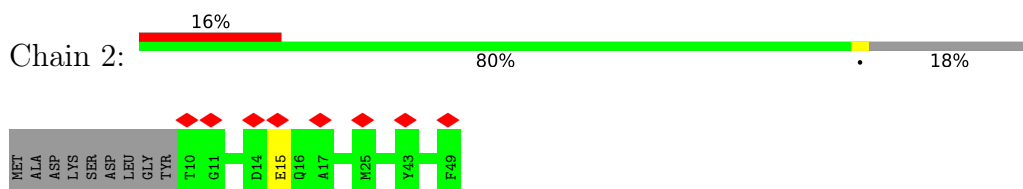
- Molecule 2: Light-harvesting protein B-875 beta chain



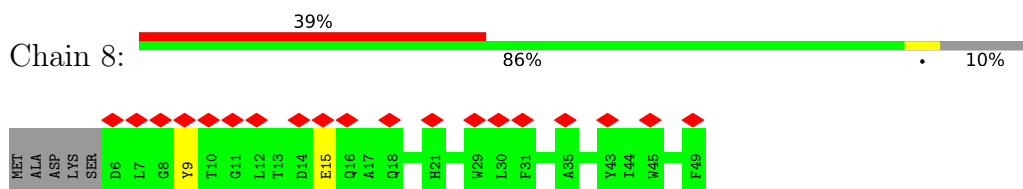
- Molecule 2: Light-harvesting protein B-875 beta chain



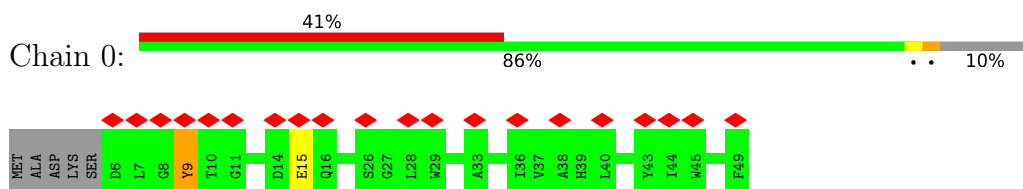
- Molecule 2: Light-harvesting protein B-875 beta chain



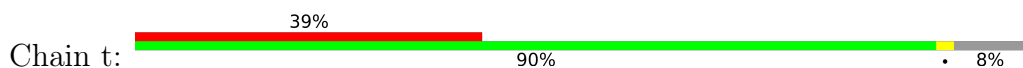
- Molecule 2: Light-harvesting protein B-875 beta chain



- Molecule 2: Light-harvesting protein B-875 beta chain

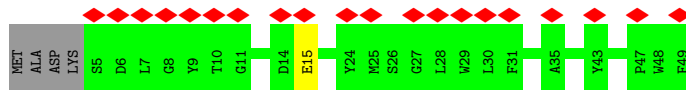
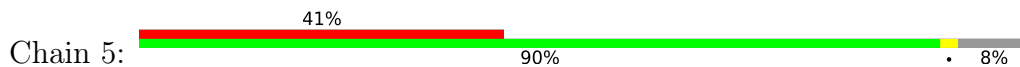


- Molecule 2: Light-harvesting protein B-875 beta chain

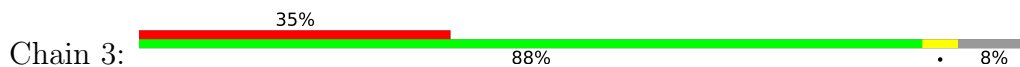




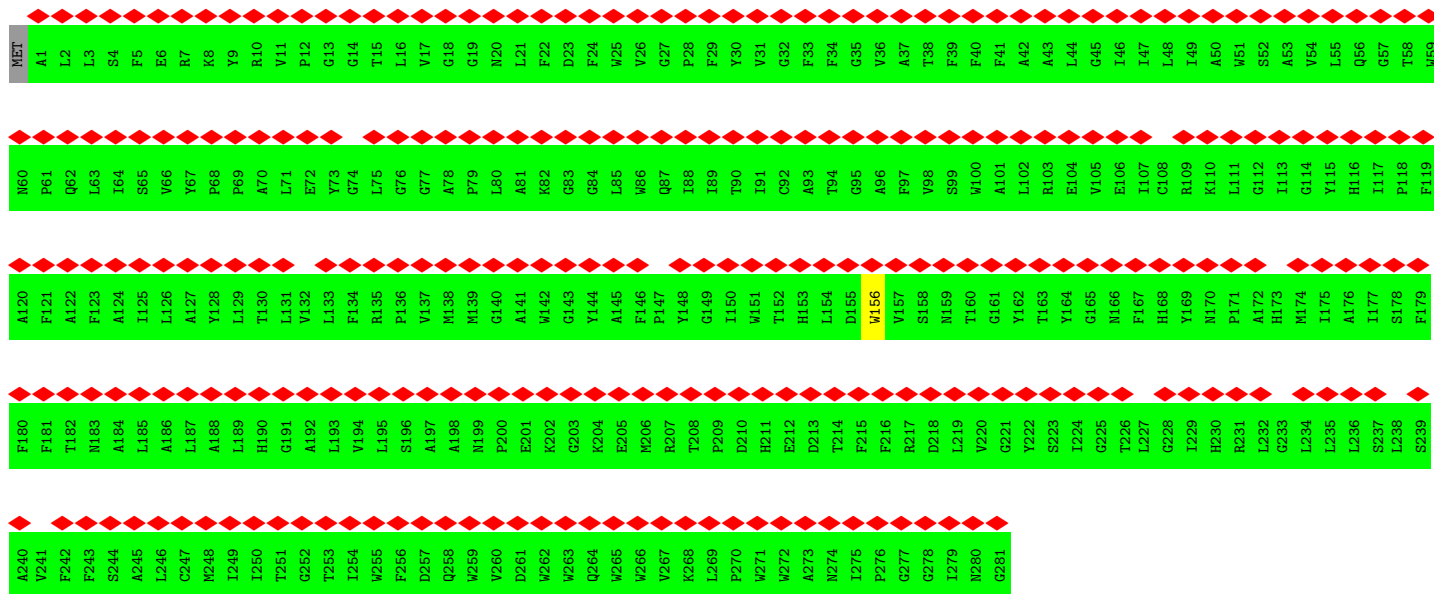
• Molecule 2: Light-harvesting protein B-875 beta chain



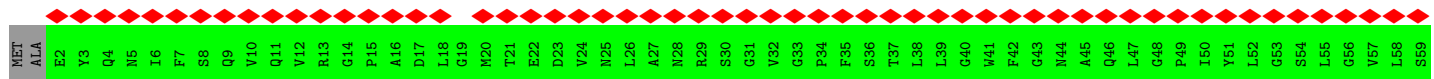
• Molecule 2: Light-harvesting protein B-875 beta chain



• Molecule 3: Reaction center protein L chain

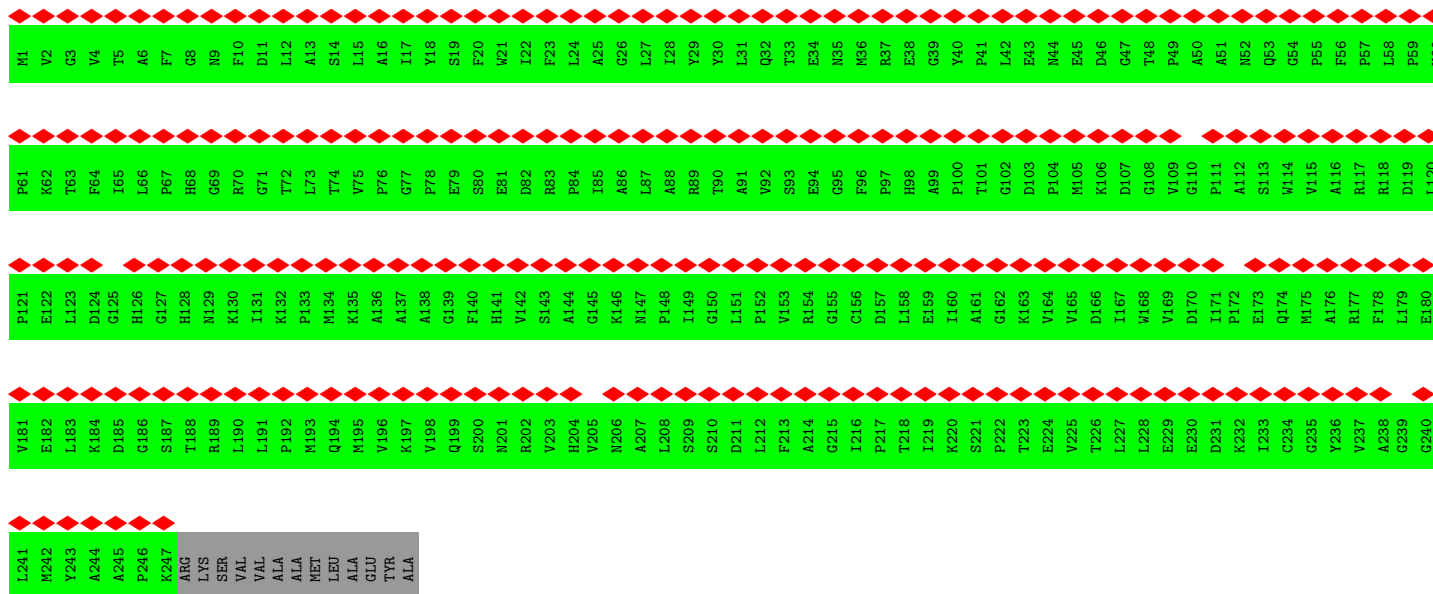


• Molecule 4: Reaction center protein M chain





• Molecule 5: Reaction center protein H chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66058	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 ($e^-/\text{\AA}^2$)	46.549	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.108	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0254	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCL, BPH, FE2, SPN, U10

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	1	0.42	0/461	0.47	0/625
1	4	0.43	0/469	0.46	0/635
1	6	0.38	0/469	0.45	0/635
1	7	0.40	0/405	0.48	0/549
1	9	0.38	0/469	0.47	0/635
1	A	0.48	0/469	0.45	0/635
1	C	0.43	0/469	0.44	0/635
1	D	0.40	0/469	0.45	0/635
1	F	0.41	0/469	0.46	0/635
1	I	0.40	0/469	0.45	0/635
1	K	0.41	0/469	0.48	0/635
1	O	0.40	0/469	0.51	0/635
1	Q	0.46	0/469	0.49	0/635
1	S	0.44	0/469	0.48	0/635
1	U	0.48	0/469	0.49	0/635
1	W	0.42	0/469	0.47	0/635
1	Y	0.43	0/469	0.49	0/635
2	0	0.38	0/372	0.52	1/510 (0.2%)
2	2	0.36	0/339	0.36	0/465
2	3	0.37	0/378	0.48	0/518
2	5	0.41	0/378	0.45	0/518
2	8	0.36	0/372	0.45	1/510 (0.2%)
2	B	0.37	0/378	0.39	0/518
2	E	0.38	0/364	0.38	0/499
2	G	0.37	0/364	0.38	0/499
2	J	0.36	0/364	0.42	0/499
2	N	0.38	0/364	0.45	0/499
2	P	0.36	0/364	0.44	0/499
2	R	0.36	0/364	0.40	0/499
2	T	0.35	0/364	0.40	0/499
2	V	0.38	0/364	0.40	0/499
2	X	0.36	0/364	0.38	0/499

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	Z	0.40	0/356	0.42	0/488
2	t	0.39	0/378	0.50	0/518
3	L	0.30	0/2320	0.47	0/3175
4	M	0.30	0/2524	0.46	0/3446
5	H	0.28	0/1925	0.49	0/2620
All	All	0.37	0/20897	0.46	2/28476 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	0	0	1
2	3	0	1
2	P	0	1
2	V	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	0	9	TYR	C-N-CA	-6.27	106.03	121.70
2	8	9	TYR	C-N-CA	5.10	134.44	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	0	9	TYR	Peptide
2	3	9	TYR	Peptide
2	P	9	TYR	Peptide
2	V	9	TYR	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	1	51/58 (88%)	48 (94%)	3 (6%)	0	100	100
1	4	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
1	6	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
1	7	44/58 (76%)	43 (98%)	1 (2%)	0	100	100
1	9	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
1	A	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
1	C	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
1	D	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
1	F	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
1	I	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
1	K	52/58 (90%)	52 (100%)	0	0	100	100
1	O	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
1	Q	52/58 (90%)	52 (100%)	0	0	100	100
1	S	52/58 (90%)	52 (100%)	0	0	100	100
1	U	52/58 (90%)	50 (96%)	2 (4%)	0	100	100
1	W	52/58 (90%)	51 (98%)	1 (2%)	0	100	100
1	Y	52/58 (90%)	49 (94%)	3 (6%)	0	100	100
2	0	42/49 (86%)	40 (95%)	2 (5%)	0	100	100
2	2	38/49 (78%)	37 (97%)	1 (3%)	0	100	100
2	3	43/49 (88%)	42 (98%)	1 (2%)	0	100	100
2	5	43/49 (88%)	40 (93%)	3 (7%)	0	100	100
2	8	42/49 (86%)	39 (93%)	3 (7%)	0	100	100
2	B	43/49 (88%)	40 (93%)	3 (7%)	0	100	100
2	E	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	G	41/49 (84%)	39 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	N	41/49 (84%)	37 (90%)	4 (10%)	0	100	100
2	P	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	R	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	T	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
2	V	41/49 (84%)	39 (95%)	1 (2%)	1 (2%)	6	36
2	X	41/49 (84%)	39 (95%)	2 (5%)	0	100	100
2	Z	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
2	t	43/49 (88%)	41 (95%)	2 (5%)	0	100	100
3	L	279/282 (99%)	257 (92%)	22 (8%)	0	100	100
4	M	303/308 (98%)	285 (94%)	18 (6%)	0	100	100
5	H	245/260 (94%)	229 (94%)	16 (6%)	0	100	100
All	All	2405/2669 (90%)	2294 (95%)	110 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	10	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	48/51 (94%)	46 (96%)	2 (4%)	30	55
1	4	49/51 (96%)	48 (98%)	1 (2%)	55	73
1	6	49/51 (96%)	49 (100%)	0	100	100
1	7	43/51 (84%)	43 (100%)	0	100	100
1	9	49/51 (96%)	49 (100%)	0	100	100
1	A	49/51 (96%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	49/51 (96%)	49 (100%)	0	100	100
1	D	49/51 (96%)	49 (100%)	0	100	100
1	F	49/51 (96%)	49 (100%)	0	100	100
1	I	49/51 (96%)	48 (98%)	1 (2%)	55	73
1	K	49/51 (96%)	48 (98%)	1 (2%)	55	73
1	O	49/51 (96%)	49 (100%)	0	100	100
1	Q	49/51 (96%)	49 (100%)	0	100	100
1	S	49/51 (96%)	49 (100%)	0	100	100
1	U	49/51 (96%)	49 (100%)	0	100	100
1	W	49/51 (96%)	49 (100%)	0	100	100
1	Y	49/51 (96%)	48 (98%)	1 (2%)	55	73
2	0	36/40 (90%)	35 (97%)	1 (3%)	43	65
2	2	33/40 (82%)	32 (97%)	1 (3%)	41	63
2	3	37/40 (92%)	36 (97%)	1 (3%)	44	66
2	5	37/40 (92%)	36 (97%)	1 (3%)	44	66
2	8	36/40 (90%)	35 (97%)	1 (3%)	43	65
2	B	37/40 (92%)	36 (97%)	1 (3%)	44	66
2	E	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	G	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	J	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	N	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	P	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	R	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	T	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	V	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	X	35/40 (88%)	34 (97%)	1 (3%)	42	64
2	Z	34/40 (85%)	33 (97%)	1 (3%)	42	64
2	t	37/40 (92%)	36 (97%)	1 (3%)	44	66
3	L	220/221 (100%)	219 (100%)	1 (0%)	88	93
4	M	239/241 (99%)	238 (100%)	1 (0%)	91	94
5	H	199/208 (96%)	199 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2086/2217 (94%)	2061 (99%)	25 (1%)	72 83

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	15	GLU
2	E	15	GLU
2	G	15	GLU
1	I	6	LYS
2	J	15	GLU
1	K	15	ARG
2	N	15	GLU
2	P	15	GLU
2	R	15	GLU
2	T	15	GLU
2	V	15	GLU
2	X	15	GLU
1	Y	47	SER
2	Z	15	GLU
1	1	12	ASP
1	1	20	GLN
2	2	15	GLU
2	8	15	GLU
2	0	15	GLU
1	4	9	MET
2	t	15	GLU
2	5	15	GLU
2	3	15	GLU
3	L	156	TRP
4	M	195	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	M	46	GLN
4	M	182	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 44 ligands modelled in this entry, 1 is monoatomic - leaving 43 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	BPH	L	302	-	31,50,70	1.04	2 (6%)	28,77,101	1.59	7 (25%)
6	BCL	X	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	7	101	-	38,54,74	1.45	5 (13%)	45,91,115	1.88	12 (26%)
7	BPH	M	405	-	31,50,70	1.12	3 (9%)	28,77,101	1.44	6 (21%)
6	BCL	4	101	-	38,54,74	1.46	6 (15%)	45,91,115	1.87	12 (26%)
6	BCL	9	101	-	38,54,74	1.45	7 (18%)	45,91,115	1.85	11 (24%)
6	BCL	3	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	A	101	-	38,54,74	1.46	6 (15%)	45,91,115	1.84	12 (26%)
6	BCL	Q	101	-	38,54,74	1.54	9 (23%)	45,91,115	1.78	11 (24%)
6	BCL	5	101	-	38,54,74	1.52	6 (15%)	45,91,115	1.84	14 (31%)
10	SPN	M	407	-	40,42,42	3.37	12 (30%)	50,52,52	2.37	18 (36%)
6	BCL	T	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	K	101	-	38,54,74	1.46	5 (13%)	45,91,115	1.80	10 (22%)
6	BCL	W	101	-	38,54,74	1.47	7 (18%)	45,91,115	1.66	9 (20%)
6	BCL	J	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	I	101	-	38,54,74	1.42	5 (13%)	45,91,115	1.84	13 (28%)
6	BCL	N	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
8	U10	M	406	-	14,14,63	2.63	6 (42%)	18,20,79	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	BCL	t	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	B	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	0	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	F	101	-	38,54,74	1.45	6 (15%)	45,91,115	1.75	10 (22%)
6	BCL	5	102	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	R	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	S	101	-	38,54,74	1.46	6 (15%)	45,91,115	1.79	10 (22%)
6	BCL	1	101	-	38,54,74	1.52	7 (18%)	45,91,115	1.90	10 (22%)
6	BCL	2	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	E	102	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	V	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	M	401	-	38,54,74	1.46	3 (7%)	45,91,115	1.85	12 (26%)
6	BCL	P	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	U	101	-	38,54,74	1.46	6 (15%)	45,91,115	1.89	12 (26%)
8	U10	L	303	-	14,14,63	2.64	6 (42%)	18,20,79	1.01	1 (5%)
6	BCL	L	301	-	38,54,74	1.34	4 (10%)	45,91,115	1.91	10 (22%)
6	BCL	Y	101	-	38,54,74	1.59	6 (15%)	45,91,115	1.68	11 (24%)
6	BCL	O	101	-	38,54,74	1.40	5 (13%)	45,91,115	1.86	12 (26%)
6	BCL	E	101	-	38,54,74	1.35	5 (13%)	45,91,115	5.26	12 (26%)
6	BCL	C	101	-	38,54,74	1.53	8 (21%)	45,91,115	1.81	12 (26%)
6	BCL	M	403	-	38,54,74	1.47	4 (10%)	45,91,115	1.79	12 (26%)
6	BCL	M	404	-	38,54,74	1.38	3 (7%)	45,91,115	1.72	8 (17%)
6	BCL	Z	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	8	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)
6	BCL	G	101	-	38,54,74	1.48	5 (13%)	45,91,115	1.51	9 (20%)

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	BPH	L	302	-	-	3/13/81/105	0/5/6/6
6	BCL	X	101	-	-	5/13/113/137	-
6	BCL	7	101	-	-	6/13/113/137	-
7	BPH	M	405	-	-	5/13/81/105	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCL	4	101	-	-	4/13/113/137	-
6	BCL	9	101	-	-	8/13/113/137	-
6	BCL	3	101	-	-	5/13/113/137	-
6	BCL	A	101	-	-	1/13/113/137	-
6	BCL	Q	101	-	-	2/13/113/137	-
6	BCL	5	101	-	-	7/13/113/137	-
10	SPN	M	407	-	-	25/50/51/51	-
6	BCL	T	101	-	-	5/13/113/137	-
6	BCL	K	101	-	-	2/13/113/137	-
6	BCL	W	101	-	-	5/13/113/137	-
6	BCL	J	101	-	-	5/13/113/137	-
6	BCL	I	101	-	-	6/13/113/137	-
6	BCL	N	101	-	-	5/13/113/137	-
8	U10	M	406	-	-	3/4/28/87	0/1/1/1
6	BCL	t	101	-	-	5/13/113/137	-
6	BCL	B	101	-	-	5/13/113/137	-
6	BCL	0	101	-	-	5/13/113/137	-
6	BCL	F	101	-	-	4/13/113/137	-
6	BCL	5	102	-	-	5/13/113/137	-
6	BCL	R	101	-	-	5/13/113/137	-
6	BCL	S	101	-	-	2/13/113/137	-
6	BCL	1	101	-	-	4/13/113/137	-
6	BCL	2	101	-	-	5/13/113/137	-
6	BCL	E	102	-	-	5/13/113/137	-
6	BCL	V	101	-	-	5/13/113/137	-
6	BCL	M	401	-	-	4/13/113/137	-
6	BCL	P	101	-	-	5/13/113/137	-
6	BCL	U	101	-	-	2/13/113/137	-
8	U10	L	303	-	-	1/4/28/87	0/1/1/1
6	BCL	L	301	-	-	2/13/113/137	-
6	BCL	Y	101	-	-	5/13/113/137	-
6	BCL	O	101	-	-	4/13/113/137	-
6	BCL	E	101	-	-	2/13/113/137	-
6	BCL	C	101	-	-	5/13/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	BCL	M	403	-	-	2/13/113/137	-
6	BCL	M	404	-	-	6/13/113/137	-
6	BCL	Z	101	-	-	5/13/113/137	-
6	BCL	8	101	-	-	5/13/113/137	-
6	BCL	G	101	-	-	5/13/113/137	-

All (233) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	407	SPN	C8-C9	8.69	1.53	1.33
10	M	407	SPN	C29-C30	7.85	1.54	1.32
10	M	407	SPN	CM8-C26	-7.20	1.32	1.50
10	M	407	SPN	CM5-C13	-6.49	1.34	1.50
10	M	407	SPN	CM3-C5	-6.15	1.34	1.50
10	M	407	SPN	CM6-C18	-6.02	1.35	1.50
10	M	407	SPN	C3-C4	6.00	1.59	1.50
8	L	303	U10	O3-C3	-5.50	1.23	1.36
8	L	303	U10	O4-C4	-5.43	1.23	1.36
8	M	406	U10	O4-C4	-5.40	1.23	1.36
8	M	406	U10	O3-C3	-5.38	1.23	1.36
6	M	401	BCL	C1B-NB	4.97	1.39	1.35
10	M	407	SPN	C15-C14	-4.92	1.34	1.52
6	M	403	BCL	C1B-NB	4.79	1.39	1.35
10	M	407	SPN	C16-C17	-4.71	1.34	1.52
6	M	403	BCL	MG-NA	4.69	2.17	2.06
6	t	101	BCL	C1B-NB	4.60	1.39	1.35
6	E	102	BCL	C1B-NB	4.60	1.39	1.35
6	P	101	BCL	C1B-NB	4.59	1.39	1.35
6	0	101	BCL	C1B-NB	4.59	1.39	1.35
6	5	102	BCL	C1B-NB	4.59	1.39	1.35
6	T	101	BCL	C1B-NB	4.59	1.39	1.35
6	X	101	BCL	C1B-NB	4.59	1.39	1.35
6	R	101	BCL	C1B-NB	4.59	1.39	1.35
6	2	101	BCL	C1B-NB	4.59	1.39	1.35
6	8	101	BCL	C1B-NB	4.59	1.39	1.35
6	3	101	BCL	C1B-NB	4.59	1.39	1.35
6	B	101	BCL	C1B-NB	4.59	1.39	1.35
6	G	101	BCL	C1B-NB	4.59	1.39	1.35
6	J	101	BCL	C1B-NB	4.59	1.39	1.35
6	V	101	BCL	C1B-NB	4.58	1.39	1.35
6	Z	101	BCL	C1B-NB	4.58	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	101	BCL	C1B-NB	4.58	1.39	1.35
6	M	404	BCL	C1B-NB	4.57	1.39	1.35
6	Y	101	BCL	MG-NA	4.56	2.17	2.06
6	L	301	BCL	MG-NA	4.45	2.16	2.06
6	T	101	BCL	MG-NA	4.44	2.16	2.06
6	5	102	BCL	MG-NA	4.44	2.16	2.06
6	Z	101	BCL	MG-NA	4.44	2.16	2.06
6	3	101	BCL	MG-NA	4.44	2.16	2.06
6	P	101	BCL	MG-NA	4.44	2.16	2.06
6	B	101	BCL	MG-NA	4.44	2.16	2.06
6	G	101	BCL	MG-NA	4.44	2.16	2.06
6	8	101	BCL	MG-NA	4.44	2.16	2.06
6	0	101	BCL	MG-NA	4.44	2.16	2.06
6	X	101	BCL	MG-NA	4.44	2.16	2.06
6	2	101	BCL	MG-NA	4.44	2.16	2.06
6	J	101	BCL	MG-NA	4.44	2.16	2.06
6	R	101	BCL	MG-NA	4.44	2.16	2.06
6	E	102	BCL	MG-NA	4.44	2.16	2.06
6	t	101	BCL	MG-NA	4.44	2.16	2.06
6	N	101	BCL	MG-NA	4.44	2.16	2.06
6	V	101	BCL	MG-NA	4.44	2.16	2.06
6	M	404	BCL	MG-NA	4.43	2.16	2.06
6	L	301	BCL	C1B-NB	4.41	1.39	1.35
6	M	401	BCL	MG-NA	4.33	2.16	2.06
6	5	101	BCL	MG-NA	4.29	2.16	2.06
6	1	101	BCL	MG-NA	4.13	2.16	2.06
6	Q	101	BCL	MG-NA	4.01	2.15	2.06
6	F	101	BCL	MG-NA	3.99	2.15	2.06
6	U	101	BCL	MG-NA	3.94	2.15	2.06
6	A	101	BCL	MG-NA	3.92	2.15	2.06
6	I	101	BCL	MG-NA	3.91	2.15	2.06
6	K	101	BCL	MG-NA	3.83	2.15	2.06
6	C	101	BCL	MG-NA	3.83	2.15	2.06
6	S	101	BCL	MG-NA	3.82	2.15	2.06
6	E	101	BCL	MG-NA	3.82	2.15	2.06
10	M	407	SPN	C1-C2	3.80	1.57	1.53
6	4	101	BCL	MG-NA	3.78	2.15	2.06
6	A	101	BCL	C1B-NB	3.75	1.38	1.35
6	Y	101	BCL	MG-NC	3.73	2.15	2.06
7	M	405	BPH	CBD-CGD	-3.72	1.47	1.52
6	O	101	BCL	MG-NA	3.71	2.15	2.06
6	7	101	BCL	MG-NA	3.70	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	9	101	BCL	MG-NA	3.69	2.15	2.06
6	5	101	BCL	C1B-NB	3.69	1.38	1.35
7	L	302	BPH	C2C-C3C	-3.59	1.51	1.54
6	W	101	BCL	MG-NA	3.54	2.14	2.06
6	5	101	BCL	MG-NC	3.44	2.14	2.06
6	Y	101	BCL	C1B-NB	3.44	1.38	1.35
8	M	406	U10	C4-C5	-3.42	1.39	1.48
6	F	101	BCL	C1B-NB	3.41	1.38	1.35
6	I	101	BCL	C1B-NB	3.38	1.38	1.35
6	M	403	BCL	MG-NC	3.38	2.14	2.06
6	Y	101	BCL	C3B-CAB	-3.31	1.40	1.49
6	M	401	BCL	MG-NC	3.27	2.14	2.06
6	A	101	BCL	MG-NC	3.25	2.14	2.06
8	L	303	U10	C3-C2	-3.23	1.39	1.48
6	E	101	BCL	C1B-NB	3.23	1.38	1.35
6	7	101	BCL	C1B-NB	3.23	1.38	1.35
8	M	406	U10	C3-C2	-3.22	1.39	1.48
6	C	101	BCL	C1B-NB	3.22	1.38	1.35
8	L	303	U10	C4-C5	-3.21	1.39	1.48
6	K	101	BCL	C1B-NB	3.15	1.38	1.35
6	9	101	BCL	MG-NC	3.11	2.13	2.06
6	9	101	BCL	C1B-NB	3.10	1.38	1.35
6	Q	101	BCL	C1B-NB	3.09	1.38	1.35
6	C	101	BCL	MG-NC	3.09	2.13	2.06
6	4	101	BCL	C1B-NB	3.09	1.38	1.35
6	E	101	BCL	MG-NC	3.09	2.13	2.06
6	S	101	BCL	C1B-NB	3.07	1.37	1.35
6	4	101	BCL	CBD-CGD	-3.04	1.42	1.52
6	O	101	BCL	C1B-NB	3.03	1.37	1.35
7	L	302	BPH	CBD-CGD	-3.01	1.48	1.52
6	F	101	BCL	MG-NC	3.01	2.13	2.06
6	K	101	BCL	MG-NC	2.97	2.13	2.06
6	U	101	BCL	C1B-NB	2.97	1.37	1.35
6	1	101	BCL	MG-NC	2.95	2.13	2.06
6	Y	101	BCL	CBD-CGD	-2.95	1.43	1.52
6	W	101	BCL	C1B-NB	2.90	1.37	1.35
6	1	101	BCL	C1B-NB	2.89	1.37	1.35
6	Q	101	BCL	MG-NC	2.87	2.13	2.06
6	I	101	BCL	MG-NC	2.86	2.13	2.06
6	4	101	BCL	MG-NC	2.85	2.13	2.06
6	M	404	BCL	MG-NC	2.84	2.13	2.06
6	S	101	BCL	MG-NC	2.81	2.13	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	M	407	SPN	C28-C29	2.81	1.59	1.50
6	U	101	BCL	MG-NC	2.80	2.12	2.06
6	K	101	BCL	C2D-C1D	-2.79	1.36	1.42
6	7	101	BCL	MG-NC	2.77	2.12	2.06
6	W	101	BCL	MG-NC	2.69	2.12	2.06
6	C	101	BCL	CBD-CGD	-2.68	1.44	1.52
6	W	101	BCL	CBD-CGD	-2.68	1.44	1.52
6	4	101	BCL	OBD-CAD	2.66	1.26	1.22
6	7	101	BCL	CBD-CGD	-2.65	1.44	1.52
6	F	101	BCL	C4B-NB	2.64	1.37	1.35
6	K	101	BCL	CBD-CGD	-2.61	1.44	1.52
6	S	101	BCL	CBD-CGD	-2.61	1.44	1.52
6	W	101	BCL	C3B-CAB	-2.61	1.42	1.49
6	F	101	BCL	CBD-CGD	-2.60	1.44	1.52
6	5	101	BCL	CBD-CGD	-2.58	1.44	1.52
6	9	101	BCL	CBD-CGD	-2.58	1.44	1.52
6	Q	101	BCL	CBD-CGD	-2.57	1.44	1.52
6	O	101	BCL	CBD-CGD	-2.56	1.44	1.52
6	U	101	BCL	C2D-C1D	-2.54	1.36	1.42
6	L	301	BCL	MG-NC	2.46	2.12	2.06
6	E	101	BCL	CBD-CGD	-2.46	1.44	1.52
6	O	101	BCL	C2D-C1D	-2.43	1.37	1.42
6	Q	101	BCL	C2D-C1D	-2.42	1.37	1.42
10	M	407	SPN	C20-C19	2.41	1.58	1.50
6	O	101	BCL	MG-NC	2.38	2.11	2.06
6	T	101	BCL	C3D-CAD	-2.38	1.40	1.46
6	E	102	BCL	C3D-CAD	-2.38	1.40	1.46
6	t	101	BCL	C3D-CAD	-2.38	1.40	1.46
6	0	101	BCL	C3D-CAD	-2.38	1.40	1.46
6	N	101	BCL	C3D-CAD	-2.38	1.40	1.46
6	Z	101	BCL	C3D-CAD	-2.38	1.40	1.46
6	5	102	BCL	C3D-CAD	-2.38	1.40	1.46
6	B	101	BCL	C3D-CAD	-2.38	1.40	1.46
6	J	101	BCL	C3D-CAD	-2.38	1.40	1.46
6	3	101	BCL	C3D-CAD	-2.38	1.40	1.46
6	P	101	BCL	C3D-CAD	-2.37	1.40	1.46
6	R	101	BCL	C3D-CAD	-2.37	1.40	1.46
6	V	101	BCL	C3D-CAD	-2.37	1.40	1.46
6	G	101	BCL	C3D-CAD	-2.37	1.40	1.46
6	2	101	BCL	C3D-CAD	-2.37	1.40	1.46
6	X	101	BCL	C3D-CAD	-2.37	1.40	1.46
6	8	101	BCL	C3D-CAD	-2.37	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	101	BCL	CBD-CGD	-2.35	1.45	1.52
7	M	405	BPH	CHA-CBD	2.35	1.55	1.52
6	1	101	BCL	C2D-C1D	-2.34	1.37	1.42
7	M	405	BPH	OBD-CAD	2.34	1.25	1.22
6	U	101	BCL	CBD-CGD	-2.29	1.45	1.52
6	C	101	BCL	OBD-CAD	2.29	1.25	1.22
6	U	101	BCL	C4B-NB	2.28	1.37	1.35
8	M	406	U10	C1-C2	-2.27	1.39	1.47
8	L	303	U10	C6-C5	-2.26	1.39	1.47
6	R	101	BCL	MG-NC	2.25	2.11	2.06
6	X	101	BCL	MG-NC	2.25	2.11	2.06
6	N	101	BCL	MG-NC	2.25	2.11	2.06
6	1	101	BCL	CBD-CGD	-2.25	1.45	1.52
6	J	101	BCL	MG-NC	2.25	2.11	2.06
6	0	101	BCL	MG-NC	2.25	2.11	2.06
6	8	101	BCL	MG-NC	2.25	2.11	2.06
6	t	101	BCL	MG-NC	2.25	2.11	2.06
6	5	102	BCL	MG-NC	2.25	2.11	2.06
6	E	102	BCL	MG-NC	2.25	2.11	2.06
6	B	101	BCL	MG-NC	2.25	2.11	2.06
6	T	101	BCL	MG-NC	2.25	2.11	2.06
6	V	101	BCL	MG-NC	2.25	2.11	2.06
6	G	101	BCL	MG-NC	2.25	2.11	2.06
6	2	101	BCL	MG-NC	2.25	2.11	2.06
6	3	101	BCL	MG-NC	2.25	2.11	2.06
6	Z	101	BCL	MG-NC	2.25	2.11	2.06
6	P	101	BCL	MG-NC	2.25	2.11	2.06
6	5	101	BCL	C3B-CAB	-2.25	1.43	1.49
6	9	101	BCL	C4B-NB	2.25	1.37	1.35
6	A	101	BCL	C4B-NB	2.24	1.37	1.35
6	A	101	BCL	CBD-CGD	-2.23	1.45	1.52
6	A	101	BCL	C2D-C1D	-2.23	1.37	1.42
8	M	406	U10	C6-C5	-2.23	1.39	1.47
8	L	303	U10	C1-C2	-2.21	1.39	1.47
6	7	101	BCL	OBD-CAD	2.20	1.25	1.22
6	9	101	BCL	OBD-CAD	2.18	1.25	1.22
6	L	301	BCL	OBD-CAD	2.17	1.25	1.22
6	C	101	BCL	C4B-NB	2.16	1.37	1.35
6	4	101	BCL	C4B-NB	2.16	1.37	1.35
6	Q	101	BCL	C3B-CAB	-2.16	1.43	1.49
6	C	101	BCL	C2D-C1D	-2.13	1.37	1.42
6	5	101	BCL	C2D-C1D	-2.10	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	101	BCL	C4B-NB	2.09	1.37	1.35
6	Q	101	BCL	CAA-C2A	-2.09	1.50	1.54
6	M	403	BCL	OBD-CAD	2.09	1.25	1.22
6	1	101	BCL	C3B-CAB	-2.08	1.43	1.49
6	9	101	BCL	C2D-C1D	-2.07	1.37	1.42
6	F	101	BCL	C2D-C1D	-2.06	1.37	1.42
6	W	101	BCL	O1A-CGA	-2.06	1.15	1.22
6	Y	101	BCL	C4B-NB	2.05	1.37	1.35
6	1	101	BCL	CAA-CBA	-2.04	1.46	1.52
6	S	101	BCL	C4B-NB	2.04	1.37	1.35
6	Q	101	BCL	C4B-NB	2.04	1.37	1.35
6	C	101	BCL	O1A-CGA	-2.02	1.15	1.22
6	B	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	G	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	J	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	8	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	5	102	BCL	CBD-CGD	-2.01	1.46	1.52
6	2	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	0	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	I	101	BCL	C2D-C1D	-2.01	1.38	1.42
6	E	102	BCL	CBD-CGD	-2.01	1.46	1.52
6	R	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	T	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	Z	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	V	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	X	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	N	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	3	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	P	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	t	101	BCL	CBD-CGD	-2.01	1.46	1.52
6	Q	101	BCL	C3D-CAD	-2.01	1.41	1.46
6	S	101	BCL	C2D-C1D	-2.01	1.38	1.42
6	W	101	BCL	C2D-C1D	-2.00	1.38	1.42

All (420) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	101	BCL	OBB-CAB-C3B	-26.10	73.67	119.99
6	E	101	BCL	OBB-CAB-CBB	-17.76	80.21	120.17
6	E	101	BCL	CBB-CAB-C3B	11.30	153.89	120.34
6	L	301	BCL	CAD-C3D-C4D	-8.36	103.81	108.47
10	M	407	SPN	C7-C8-C9	-6.72	111.48	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	404	BCL	CAD-C3D-C4D	-6.44	104.88	108.47
6	M	401	BCL	CAD-C3D-C4D	-6.04	105.10	108.47
6	M	403	BCL	CAD-C3D-C4D	-5.59	105.36	108.47
10	M	407	SPN	CM4-C9-C8	-5.41	109.80	123.68
10	M	407	SPN	C28-C29-C30	-5.38	109.35	127.75
6	O	101	BCL	CMB-C2B-C1B	-5.06	120.69	128.46
6	U	101	BCL	CMB-C2B-C1B	-4.77	121.14	128.46
10	M	407	SPN	CM6-C18-C17	4.63	123.06	115.27
6	4	101	BCL	CAD-C3D-C4D	-4.58	105.92	108.47
6	1	101	BCL	CAD-C3D-C4D	-4.49	105.97	108.47
6	K	101	BCL	CAD-C3D-C4D	-4.49	105.97	108.47
6	K	101	BCL	CMB-C2B-C1B	-4.46	121.60	128.46
6	7	101	BCL	CMB-C2B-C1B	-4.45	121.62	128.46
6	S	101	BCL	CMB-C2B-C1B	-4.43	121.65	128.46
6	4	101	BCL	CMB-C2B-C1B	-4.42	121.67	128.46
6	1	101	BCL	CHA-C1A-NA	-4.39	116.35	126.40
6	U	101	BCL	CAD-C3D-C4D	-4.37	106.03	108.47
6	W	101	BCL	CMB-C2B-C1B	-4.36	121.76	128.46
6	W	101	BCL	OBD-CAD-CBD	-4.34	119.69	125.89
6	7	101	BCL	CAD-C3D-C4D	-4.29	106.08	108.47
6	9	101	BCL	CAD-C3D-C4D	-4.29	106.08	108.47
6	C	101	BCL	CAD-C3D-C4D	-4.24	106.10	108.47
6	Q	101	BCL	CAA-CBA-CGA	-4.22	101.31	112.51
6	S	101	BCL	CAD-C3D-C4D	-4.21	106.12	108.47
6	9	101	BCL	CMB-C2B-C1B	-4.19	122.03	128.46
6	9	101	BCL	CHA-C1A-NA	-4.17	116.85	126.40
6	I	101	BCL	CMB-C2B-C1B	-4.16	122.07	128.46
6	O	101	BCL	OBD-CAD-CBD	-4.15	119.97	125.89
6	U	101	BCL	OBD-CAD-CBD	-4.12	120.00	125.89
6	K	101	BCL	OBD-CAD-CBD	-4.11	120.03	125.89
6	O	101	BCL	CAD-C3D-C4D	-4.10	106.19	108.47
6	F	101	BCL	CMB-C2B-C1B	-4.09	122.17	128.46
6	Q	101	BCL	CMB-C2B-C1B	-4.07	122.20	128.46
10	M	407	SPN	CM5-C13-C14	4.07	122.11	115.27
10	M	407	SPN	CM9-C30-C29	-4.05	110.93	122.65
6	S	101	BCL	OBD-CAD-CBD	-4.02	120.15	125.89
6	Y	101	BCL	CAD-C3D-C4D	-4.01	106.23	108.47
6	A	101	BCL	CMB-C2B-C1B	-4.01	122.30	128.46
6	C	101	BCL	OBD-CAD-CBD	-4.01	120.17	125.89
6	4	101	BCL	OBD-CAD-CBD	-4.00	120.17	125.89
6	C	101	BCL	CMB-C2B-C1B	-4.00	122.32	128.46
6	4	101	BCL	CHA-C1A-NA	-3.98	117.28	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	101	BCL	OBD-CAD-CBD	-3.98	120.20	125.89
6	Q	101	BCL	CHA-C1A-NA	-3.98	117.28	126.40
6	F	101	BCL	OBD-CAD-CBD	-3.96	120.23	125.89
6	Q	101	BCL	CAD-C3D-C4D	-3.95	106.27	108.47
6	5	101	BCL	OBD-CAD-CBD	-3.94	120.26	125.89
6	M	401	BCL	CHA-C1A-NA	-3.94	117.38	126.40
6	1	101	BCL	CBA-CAA-C2A	-3.94	102.25	113.86
6	S	101	BCL	CHA-C1A-NA	-3.92	117.41	126.40
6	7	101	BCL	CHA-C1A-NA	-3.92	117.43	126.40
6	1	101	BCL	OBD-CAD-CBD	-3.91	120.31	125.89
6	5	101	BCL	CMB-C2B-C1B	-3.90	122.46	128.46
6	C	101	BCL	CHA-C1A-NA	-3.89	117.50	126.40
6	Y	101	BCL	OBD-CAD-CBD	-3.87	120.36	125.89
6	F	101	BCL	CAD-C3D-C4D	-3.87	106.31	108.47
6	W	101	BCL	CAD-C3D-C4D	-3.86	106.32	108.47
6	9	101	BCL	OBD-CAD-CBD	-3.82	120.44	125.89
6	7	101	BCL	OBD-CAD-CBD	-3.82	120.44	125.89
6	5	101	BCL	CAD-C3D-C4D	-3.82	106.34	108.47
6	A	101	BCL	OBD-CAD-CBD	-3.82	120.44	125.89
6	M	401	BCL	CMB-C2B-C1B	-3.74	122.71	128.46
6	M	403	BCL	CMB-C2B-C1B	-3.73	122.73	128.46
6	Q	101	BCL	OBD-CAD-CBD	-3.73	120.57	125.89
6	R	101	BCL	CAD-C3D-C4D	-3.72	106.40	108.47
6	2	101	BCL	CAD-C3D-C4D	-3.72	106.40	108.47
10	M	407	SPN	C10-C9-C8	-3.72	113.59	121.12
6	G	101	BCL	CAD-C3D-C4D	-3.72	106.40	108.47
6	Z	101	BCL	CAD-C3D-C4D	-3.72	106.40	108.47
6	8	101	BCL	CAD-C3D-C4D	-3.72	106.40	108.47
6	3	101	BCL	CAD-C3D-C4D	-3.72	106.40	108.47
6	B	101	BCL	CAD-C3D-C4D	-3.71	106.40	108.47
6	5	102	BCL	CAD-C3D-C4D	-3.71	106.40	108.47
6	P	101	BCL	CAD-C3D-C4D	-3.71	106.40	108.47
6	t	101	BCL	CAD-C3D-C4D	-3.71	106.40	108.47
6	9	101	BCL	C2A-C1A-CHA	3.71	130.35	123.86
6	E	101	BCL	CMB-C2B-C1B	-3.71	122.76	128.46
6	E	102	BCL	CAD-C3D-C4D	-3.71	106.40	108.47
6	J	101	BCL	CAD-C3D-C4D	-3.71	106.40	108.47
6	N	101	BCL	CAD-C3D-C4D	-3.71	106.40	108.47
6	T	101	BCL	CAD-C3D-C4D	-3.71	106.40	108.47
6	V	101	BCL	CAD-C3D-C4D	-3.71	106.40	108.47
6	X	101	BCL	CAD-C3D-C4D	-3.71	106.40	108.47
6	0	101	BCL	CAD-C3D-C4D	-3.70	106.40	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	101	BCL	CAD-C3D-C4D	-3.70	106.41	108.47
6	E	101	BCL	OBD-CAD-CBD	-3.69	120.62	125.89
10	M	407	SPN	CM3-C5-C6	3.69	121.47	115.27
6	Y	101	BCL	CHA-C1A-NA	-3.66	118.02	126.40
6	L	301	BCL	CMB-C2B-C1B	-3.63	122.89	128.46
6	A	101	BCL	CAD-C3D-C4D	-3.63	106.45	108.47
6	1	101	BCL	CMB-C2B-C1B	-3.63	122.89	128.46
6	K	101	BCL	CHA-C1A-NA	-3.59	118.18	126.40
6	L	301	BCL	CHA-C1A-NA	-3.58	118.21	126.40
6	5	101	BCL	CHA-C1A-NA	-3.57	118.22	126.40
6	4	101	BCL	C2A-C1A-CHA	3.55	130.07	123.86
6	7	101	BCL	C2A-C1A-CHA	3.54	130.05	123.86
6	C	101	BCL	CAA-CBA-CGA	-3.52	103.17	112.51
6	E	101	BCL	CHA-C1A-NA	-3.51	118.36	126.40
6	5	101	BCL	CHD-C4C-NC	-3.51	121.18	125.08
7	M	405	BPH	C4C-C3C-C2C	-3.51	99.50	102.84
6	M	404	BCL	CHA-C1A-NA	-3.47	118.45	126.40
6	O	101	BCL	CMB-C2B-C3B	3.47	131.17	124.68
6	U	101	BCL	CHA-C1A-NA	-3.45	118.50	126.40
6	M	401	BCL	OBD-CAD-CBD	-3.42	121.01	125.89
6	A	101	BCL	CHA-C1A-NA	-3.38	118.65	126.40
7	L	302	BPH	O2D-CGD-CBD	3.38	115.27	111.00
6	I	101	BCL	CHA-C1A-NA	-3.35	118.72	126.40
6	O	101	BCL	CHA-C1A-NA	-3.35	118.74	126.40
6	K	101	BCL	C2A-C1A-CHA	3.34	129.70	123.86
6	M	404	BCL	CMB-C2B-C1B	-3.33	123.35	128.46
6	E	102	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
6	5	102	BCL	OBD-CAD-CBD	-3.32	121.15	125.89
6	t	101	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
6	N	101	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
6	T	101	BCL	OBD-CAD-CBD	-3.32	121.16	125.89
6	P	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
6	Z	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
6	8	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
6	3	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
6	F	101	BCL	CHA-C1A-NA	-3.31	118.81	126.40
6	G	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
6	J	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
6	V	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
6	0	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
6	B	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
6	R	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	2	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
6	X	101	BCL	OBD-CAD-CBD	-3.31	121.16	125.89
6	E	102	BCL	CHA-C1A-NA	-3.30	118.83	126.40
6	J	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	N	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	V	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	X	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	8	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	0	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	2	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	Z	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	5	102	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	t	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	G	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	P	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	R	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	B	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	3	101	BCL	CHA-C1A-NA	-3.30	118.84	126.40
6	T	101	BCL	CHA-C1A-NA	-3.30	118.85	126.40
6	E	101	BCL	CAD-C3D-C4D	-3.29	106.64	108.47
6	M	403	BCL	CHA-C1A-NA	-3.24	118.97	126.40
6	U	101	BCL	CMB-C2B-C3B	3.24	130.74	124.68
6	Y	101	BCL	CMB-C2B-C1B	-3.24	123.49	128.46
6	W	101	BCL	CHA-C1A-NA	-3.23	119.01	126.40
6	7	101	BCL	CMB-C2B-C3B	3.21	130.69	124.68
6	Q	101	BCL	C2A-C1A-CHA	3.21	129.47	123.86
6	M	403	BCL	C2A-C1A-CHA	3.20	129.46	123.86
6	F	101	BCL	C2A-C1A-CHA	3.20	129.46	123.86
6	I	101	BCL	C4A-NA-C1A	3.20	108.14	106.71
10	M	407	SPN	C15-C14-C13	3.19	121.82	113.45
6	E	101	BCL	CHD-C4C-NC	-3.17	121.56	125.08
6	4	101	BCL	CMB-C2B-C3B	3.17	130.60	124.68
6	M	404	BCL	OBD-CAD-CBD	-3.16	121.38	125.89
6	G	101	BCL	CMB-C2B-C1B	-3.11	123.68	128.46
6	2	101	BCL	CMB-C2B-C1B	-3.11	123.68	128.46
6	3	101	BCL	CMB-C2B-C1B	-3.11	123.68	128.46
6	E	102	BCL	CMB-C2B-C1B	-3.11	123.68	128.46
6	8	101	BCL	CMB-C2B-C1B	-3.11	123.68	128.46
6	t	101	BCL	CMB-C2B-C1B	-3.11	123.68	128.46
6	K	101	BCL	CMB-C2B-C3B	3.11	130.50	124.68
6	B	101	BCL	CMB-C2B-C1B	-3.11	123.68	128.46
6	N	101	BCL	CMB-C2B-C1B	-3.11	123.68	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	101	BCL	CMB-C2B-C1B	-3.11	123.68	128.46
6	Z	101	BCL	CMB-C2B-C1B	-3.11	123.68	128.46
6	P	101	BCL	CMB-C2B-C1B	-3.11	123.68	128.46
6	5	102	BCL	CMB-C2B-C1B	-3.11	123.68	128.46
6	X	101	BCL	CMB-C2B-C1B	-3.11	123.69	128.46
6	R	101	BCL	CMB-C2B-C1B	-3.11	123.69	128.46
6	V	101	BCL	CMB-C2B-C1B	-3.11	123.69	128.46
6	0	101	BCL	CMB-C2B-C1B	-3.11	123.69	128.46
6	J	101	BCL	CMB-C2B-C1B	-3.11	123.69	128.46
6	A	101	BCL	CMD-C2D-C3D	3.10	130.47	124.68
6	5	102	BCL	C2A-C1A-CHA	3.09	129.25	123.86
6	t	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	B	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	X	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	8	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	2	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	E	102	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	S	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	V	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	J	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	N	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	0	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	P	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	3	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	S	101	BCL	CMB-C2B-C3B	3.08	130.44	124.68
6	T	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	Z	101	BCL	C2A-C1A-CHA	3.08	129.25	123.86
6	G	101	BCL	C2A-C1A-CHA	3.08	129.24	123.86
6	R	101	BCL	C2A-C1A-CHA	3.08	129.24	123.86
6	A	101	BCL	C4B-C3B-CAB	-3.08	121.19	127.13
6	W	101	BCL	C2A-C1A-CHA	3.08	129.24	123.86
6	O	101	BCL	C4A-NA-C1A	3.07	108.08	106.71
6	7	101	BCL	CAA-CBA-CGA	-3.04	104.44	112.51
6	9	101	BCL	CMB-C2B-C3B	3.04	130.36	124.68
7	L	302	BPH	C1C-C2C-C3C	-3.03	99.96	102.84
6	1	101	BCL	CMD-C2D-C3D	3.01	130.30	124.68
6	5	101	BCL	CHC-C1C-NC	-2.98	120.39	124.51
6	A	101	BCL	C2A-C1A-CHA	2.96	129.04	123.86
10	M	407	SPN	C17-C18-C19	-2.95	115.14	121.12
6	I	101	BCL	CMB-C2B-C3B	2.95	130.20	124.68
6	5	101	BCL	CBA-CAA-C2A	-2.94	105.17	113.86
6	1	101	BCL	C2A-C1A-CHA	2.93	128.99	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	O	101	BCL	C2A-C1A-CHA	2.93	128.98	123.86
6	O	101	BCL	CMD-C2D-C3D	2.91	130.13	124.68
6	Y	101	BCL	CHD-C4C-NC	-2.89	121.86	125.08
6	5	101	BCL	C2A-C1A-CHA	2.89	128.91	123.86
6	Q	101	BCL	CMB-C2B-C3B	2.89	130.08	124.68
6	C	101	BCL	C2A-C1A-CHA	2.88	128.90	123.86
6	M	403	BCL	OBD-CAD-CBD	-2.88	121.78	125.89
6	U	101	BCL	CMD-C2D-C3D	2.87	130.06	124.68
6	A	101	BCL	CHC-C1C-NC	-2.87	120.54	124.51
6	A	101	BCL	CMB-C2B-C3B	2.86	130.03	124.68
7	M	405	BPH	OBD-CAD-CBD	-2.86	121.63	125.82
6	5	101	BCL	CMD-C2D-C3D	2.86	130.03	124.68
6	W	101	BCL	CMB-C2B-C3B	2.86	130.03	124.68
6	Y	101	BCL	CMD-C2D-C3D	2.85	130.00	124.68
6	E	101	BCL	C2A-C1A-CHA	2.84	128.82	123.86
6	5	101	BCL	C4B-C3B-CAB	-2.83	121.66	127.13
6	L	301	BCL	OBD-CAD-CBD	-2.83	121.86	125.89
6	5	101	BCL	CMB-C2B-C3B	2.81	129.94	124.68
6	Q	101	BCL	CMD-C2D-C3D	2.81	129.94	124.68
6	K	101	BCL	CMD-C2D-C3D	2.81	129.93	124.68
7	L	302	BPH	CAA-CBA-CGA	2.80	119.93	112.51
6	M	403	BCL	CMB-C2B-C3B	2.78	129.88	124.68
6	I	101	BCL	C2A-C1A-CHA	2.78	128.72	123.86
7	M	405	BPH	C1C-C2C-C3C	-2.78	100.20	102.84
6	M	401	BCL	CHD-C4C-NC	-2.77	121.99	125.08
6	K	101	BCL	CAA-CBA-CGA	-2.77	105.14	112.51
6	C	101	BCL	CMB-C2B-C3B	2.77	129.86	124.68
6	M	401	BCL	CMD-C2D-C3D	2.77	129.86	124.68
6	F	101	BCL	CMB-C2B-C3B	2.76	129.84	124.68
7	L	302	BPH	OBD-CAD-CBD	-2.75	121.78	125.82
6	U	101	BCL	C2A-C1A-CHA	2.75	128.68	123.86
6	I	101	BCL	CMD-C2D-C3D	2.73	129.79	124.68
6	M	403	BCL	O2D-CGD-CBD	2.71	116.09	111.27
6	S	101	BCL	CMD-C2D-C3D	2.70	129.72	124.68
6	I	101	BCL	CBA-CAA-C2A	-2.68	105.96	113.86
6	C	101	BCL	CMD-C2D-C3D	2.67	129.67	124.68
6	W	101	BCL	CMD-C2D-C3D	2.67	129.67	124.68
6	Y	101	BCL	C2A-C1A-CHA	2.66	128.51	123.86
6	M	401	BCL	CMB-C2B-C3B	2.66	129.66	124.68
6	9	101	BCL	CMD-C2D-C3D	2.64	129.63	124.68
6	T	101	BCL	C4A-NA-C1A	2.64	107.89	106.71
6	5	102	BCL	C4A-NA-C1A	2.64	107.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	101	BCL	C4A-NA-C1A	2.63	107.89	106.71
6	3	101	BCL	C4A-NA-C1A	2.63	107.89	106.71
6	J	101	BCL	C4A-NA-C1A	2.63	107.89	106.71
6	R	101	BCL	C4A-NA-C1A	2.62	107.89	106.71
6	Z	101	BCL	C4A-NA-C1A	2.62	107.89	106.71
6	G	101	BCL	C4A-NA-C1A	2.62	107.89	106.71
6	P	101	BCL	C4A-NA-C1A	2.62	107.89	106.71
6	X	101	BCL	C4A-NA-C1A	2.62	107.89	106.71
6	8	101	BCL	C4A-NA-C1A	2.62	107.89	106.71
6	0	101	BCL	C4A-NA-C1A	2.62	107.89	106.71
6	t	101	BCL	C4A-NA-C1A	2.62	107.89	106.71
6	N	101	BCL	C4A-NA-C1A	2.62	107.88	106.71
6	2	101	BCL	C4A-NA-C1A	2.62	107.88	106.71
6	A	101	BCL	CHD-C4C-NC	-2.62	122.17	125.08
6	E	102	BCL	C4A-NA-C1A	2.62	107.88	106.71
6	V	101	BCL	C4A-NA-C1A	2.62	107.88	106.71
6	Y	101	BCL	CHC-C1C-NC	-2.61	120.90	124.51
6	4	101	BCL	CMD-C2D-C3D	2.60	129.55	124.68
6	F	101	BCL	CMD-C2D-C3D	2.60	129.54	124.68
10	M	407	SPN	CMB-C30-C29	-2.59	115.17	122.65
6	I	101	BCL	CHD-C4C-NC	-2.58	122.22	125.08
6	I	101	BCL	CHC-C1C-NC	-2.56	120.98	124.51
6	E	101	BCL	CMB-C2B-C3B	2.53	129.42	124.68
6	4	101	BCL	CAA-CBA-CGA	-2.53	105.79	112.51
6	E	101	BCL	CMD-C2D-C3D	2.53	129.41	124.68
6	1	101	BCL	CAA-CBA-CGA	-2.52	105.82	112.51
7	M	405	BPH	CMB-C2B-C3B	2.50	129.35	124.68
6	M	403	BCL	CMD-C2D-C3D	2.49	129.34	124.68
6	U	101	BCL	OBB-CAB-CBB	-2.48	114.58	120.17
6	M	403	BCL	C4B-C3B-CAB	-2.48	122.34	127.13
6	5	101	BCL	C4A-NA-C1A	2.47	107.82	106.71
6	4	101	BCL	OBB-CAB-CBB	-2.47	114.61	120.17
6	M	404	BCL	CMD-C2D-C3D	2.46	129.28	124.68
6	A	101	BCL	O2D-CGD-CBD	2.46	115.63	111.27
6	4	101	BCL	OBD-CAD-C3D	2.45	132.05	127.98
6	C	101	BCL	CMA-C3A-C4A	-2.45	105.18	111.77
6	E	101	BCL	CHC-C1C-NC	-2.44	121.14	124.51
6	W	101	BCL	OBD-CAD-C3D	2.44	132.03	127.98
6	M	404	BCL	OBD-CAD-C3D	2.42	132.00	127.98
6	7	101	BCL	CHC-C1C-NC	-2.42	121.16	124.51
7	L	302	BPH	C4C-C3C-C2C	-2.42	100.54	102.84
10	M	407	SPN	CMB-C30-CM9	-2.41	109.27	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	M	403	BCL	C1C-NC-C4C	2.41	107.79	106.71
6	Y	101	BCL	CBA-CAA-C2A	-2.41	106.74	113.86
6	1	101	BCL	CMB-C2B-C3B	2.39	129.16	124.68
6	L	301	BCL	CMB-C2B-C3B	2.39	129.15	124.68
6	7	101	BCL	CMD-C2D-C3D	2.38	129.14	124.68
6	7	101	BCL	OBB-CAB-CBB	-2.38	114.82	120.17
6	L	301	BCL	CBA-CAA-C2A	2.37	120.86	113.86
6	2	101	BCL	CMB-C2B-C3B	2.37	129.11	124.68
6	B	101	BCL	CMB-C2B-C3B	2.37	129.11	124.68
6	P	101	BCL	CMB-C2B-C3B	2.37	129.11	124.68
6	8	101	BCL	CMB-C2B-C3B	2.37	129.11	124.68
6	E	102	BCL	CMB-C2B-C3B	2.37	129.11	124.68
6	R	101	BCL	CMB-C2B-C3B	2.37	129.11	124.68
6	T	101	BCL	CMB-C2B-C3B	2.37	129.11	124.68
6	Z	101	BCL	CMB-C2B-C3B	2.37	129.11	124.68
6	5	102	BCL	CMB-C2B-C3B	2.37	129.11	124.68
6	G	101	BCL	CMB-C2B-C3B	2.37	129.11	124.68
6	t	101	BCL	CMB-C2B-C3B	2.37	129.11	124.68
6	X	101	BCL	CMB-C2B-C3B	2.37	129.10	124.68
6	0	101	BCL	CMB-C2B-C3B	2.37	129.10	124.68
6	3	101	BCL	CMB-C2B-C3B	2.37	129.10	124.68
6	J	101	BCL	CMB-C2B-C3B	2.37	129.10	124.68
6	N	101	BCL	CMB-C2B-C3B	2.37	129.10	124.68
6	V	101	BCL	CMB-C2B-C3B	2.37	129.10	124.68
6	M	403	BCL	C4A-NA-C1A	2.36	107.77	106.71
6	L	301	BCL	OBB-CAB-CBB	-2.36	114.86	120.17
6	9	101	BCL	CAA-CBA-CGA	-2.35	106.26	112.51
6	U	101	BCL	C4B-C3B-CAB	-2.34	122.61	127.13
6	S	101	BCL	CAA-CBA-CGA	-2.33	106.31	112.51
6	U	101	BCL	CAA-CBA-CGA	-2.33	106.32	112.51
10	M	407	SPN	C3-C4-C5	-2.32	122.93	126.79
10	M	407	SPN	C27-C28-C29	2.30	119.44	111.88
6	L	301	BCL	CMD-C2D-C3D	2.30	128.97	124.68
6	M	401	BCL	OBD-CAD-C3D	2.29	131.78	127.98
6	Y	101	BCL	CMB-C2B-C3B	2.28	128.95	124.68
6	C	101	BCL	OBD-CAD-C3D	2.28	131.77	127.98
6	4	101	BCL	C4B-C3B-CAB	-2.28	122.73	127.13
6	F	101	BCL	C4A-NA-C1A	2.28	107.73	106.71
6	O	101	BCL	OBD-CAD-C3D	2.27	131.75	127.98
6	O	101	BCL	C4B-C3B-CAB	-2.27	122.75	127.13
7	L	302	BPH	CMB-C2B-C3B	2.26	128.91	124.68
6	Y	101	BCL	CHB-C4A-NA	-2.25	121.39	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	101	BCL	OBD-CAD-C3D	2.25	131.71	127.98
6	K	101	BCL	OBD-CAD-C3D	2.25	131.71	127.98
6	O	101	BCL	OBB-CAB-CBB	-2.24	115.12	120.17
6	M	404	BCL	CMB-C2B-C3B	2.24	128.87	124.68
6	9	101	BCL	CHC-C1C-NC	-2.24	121.42	124.51
6	O	101	BCL	CHC-C1C-NC	-2.23	121.42	124.51
6	S	101	BCL	OBD-CAD-C3D	2.23	131.69	127.98
6	9	101	BCL	C4B-C3B-CAB	-2.23	122.82	127.13
7	M	405	BPH	CMD-C2D-C3D	2.23	128.84	124.68
6	7	101	BCL	C4B-C3B-CAB	-2.22	122.83	127.13
6	I	101	BCL	CAC-C3C-C2C	-2.22	108.70	114.26
10	M	407	SPN	CM3-C5-C4	-2.22	117.98	123.68
6	B	101	BCL	O2D-CGD-CBD	2.22	115.21	111.27
6	J	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	4	101	BCL	CHC-C1C-NC	-2.21	121.45	124.51
6	G	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	5	102	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	T	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	3	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	P	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	R	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	2	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	t	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	M	401	BCL	CHB-C4A-NA	-2.21	121.45	124.51
7	L	302	BPH	CMD-C2D-C3D	2.21	128.81	124.68
6	X	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	N	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	V	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	Z	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	8	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	0	101	BCL	O2D-CGD-CBD	2.21	115.20	111.27
6	E	102	BCL	O2D-CGD-CBD	2.21	115.19	111.27
6	M	403	BCL	OBD-CAD-C3D	2.19	131.61	127.98
6	I	101	BCL	OBD-CAD-C3D	2.17	131.58	127.98
6	L	301	BCL	OBD-CAD-C3D	2.17	131.58	127.98
6	U	101	BCL	O2D-CGD-O1D	-2.16	119.62	123.84
6	8	101	BCL	CMD-C2D-C3D	2.15	128.70	124.68
6	P	101	BCL	CMD-C2D-C3D	2.15	128.70	124.68
6	t	101	BCL	CMD-C2D-C3D	2.15	128.70	124.68
6	B	101	BCL	CMD-C2D-C3D	2.15	128.70	124.68
6	E	102	BCL	CMD-C2D-C3D	2.15	128.70	124.68
6	N	101	BCL	CMD-C2D-C3D	2.15	128.70	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	101	BCL	CMD-C2D-C3D	2.15	128.70	124.68
6	J	101	BCL	CMD-C2D-C3D	2.15	128.70	124.68
6	V	101	BCL	CMD-C2D-C3D	2.15	128.70	124.68
6	Z	101	BCL	CMD-C2D-C3D	2.15	128.70	124.68
6	0	101	BCL	CMD-C2D-C3D	2.15	128.70	124.68
6	R	101	BCL	CMD-C2D-C3D	2.15	128.70	124.68
6	X	101	BCL	CMD-C2D-C3D	2.15	128.70	124.68
6	5	102	BCL	CMD-C2D-C3D	2.15	128.70	124.68
6	T	101	BCL	CMD-C2D-C3D	2.15	128.69	124.68
6	2	101	BCL	CMD-C2D-C3D	2.15	128.69	124.68
6	3	101	BCL	CMD-C2D-C3D	2.15	128.69	124.68
6	7	101	BCL	OBD-CAD-C3D	2.14	131.53	127.98
6	K	101	BCL	OBB-CAB-CBB	-2.14	115.36	120.17
6	9	101	BCL	OBD-CAD-C3D	2.13	131.52	127.98
6	M	401	BCL	C2A-C1A-CHA	2.12	127.57	123.86
6	A	101	BCL	C1C-NC-C4C	-2.12	105.75	106.71
6	M	404	BCL	C1C-NC-C4C	2.12	107.66	106.71
6	U	101	BCL	OBD-CAD-C3D	2.11	131.49	127.98
6	C	101	BCL	OBB-CAB-CBB	-2.11	115.43	120.17
6	W	101	BCL	CHC-C1C-NC	-2.10	121.60	124.51
6	Q	101	BCL	CHC-C1C-NC	-2.10	121.61	124.51
6	M	401	BCL	CBA-CAA-C2A	2.09	120.05	113.86
6	F	101	BCL	CAA-CBA-CGA	-2.07	107.01	112.51
6	1	101	BCL	O2D-CGD-O1D	-2.07	119.80	123.84
6	5	101	BCL	CHB-C4A-NA	-2.06	121.66	124.51
6	5	101	BCL	OBD-CAD-C3D	2.05	131.38	127.98
6	M	401	BCL	CAC-C3C-C4C	2.04	117.11	112.58
6	S	101	BCL	CMA-C3A-C4A	-2.04	106.29	111.77
6	C	101	BCL	CHC-C1C-NC	-2.04	121.69	124.51
10	M	407	SPN	C20-C19-C18	-2.02	122.79	127.66
7	M	405	BPH	CMA-C3A-C4A	-2.02	109.95	114.38
8	L	303	U10	O4-C4-C3	-2.02	116.03	123.64
6	L	301	BCL	O2D-CGD-CBD	2.01	114.85	111.27
10	M	407	SPN	CM8-C26-C27	2.01	118.66	115.27
6	Q	101	BCL	C4B-C3B-CAB	-2.01	123.25	127.13
10	M	407	SPN	C11-C12-C13	-2.01	122.83	127.66
6	Q	101	BCL	OBD-CAD-C3D	2.01	131.31	127.98

There are no chirality outliers.

All (205) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	101	BCL	CHA-CBD-CGD-O1D
6	B	101	BCL	CHA-CBD-CGD-O2D
6	E	101	BCL	C4C-C3C-CAC-CBC
6	E	102	BCL	CHA-CBD-CGD-O1D
6	E	102	BCL	CHA-CBD-CGD-O2D
6	F	101	BCL	CHA-CBD-CGD-O1D
6	F	101	BCL	CHA-CBD-CGD-O2D
6	G	101	BCL	CHA-CBD-CGD-O1D
6	G	101	BCL	CHA-CBD-CGD-O2D
6	I	101	BCL	CHA-CBD-CGD-O1D
6	J	101	BCL	CHA-CBD-CGD-O1D
6	J	101	BCL	CHA-CBD-CGD-O2D
6	N	101	BCL	CHA-CBD-CGD-O1D
6	N	101	BCL	CHA-CBD-CGD-O2D
6	P	101	BCL	CHA-CBD-CGD-O1D
6	P	101	BCL	CHA-CBD-CGD-O2D
6	Q	101	BCL	CHA-CBD-CGD-O1D
6	Q	101	BCL	CHA-CBD-CGD-O2D
6	R	101	BCL	CHA-CBD-CGD-O1D
6	R	101	BCL	CHA-CBD-CGD-O2D
6	S	101	BCL	CHA-CBD-CGD-O1D
6	S	101	BCL	CHA-CBD-CGD-O2D
6	T	101	BCL	CHA-CBD-CGD-O1D
6	T	101	BCL	CHA-CBD-CGD-O2D
6	V	101	BCL	CHA-CBD-CGD-O1D
6	V	101	BCL	CHA-CBD-CGD-O2D
6	X	101	BCL	CHA-CBD-CGD-O1D
6	X	101	BCL	CHA-CBD-CGD-O2D
6	Y	101	BCL	C2A-CAA-CBA-CGA
6	Z	101	BCL	CHA-CBD-CGD-O1D
6	Z	101	BCL	CHA-CBD-CGD-O2D
6	1	101	BCL	C4C-C3C-CAC-CBC
6	2	101	BCL	CHA-CBD-CGD-O1D
6	2	101	BCL	CHA-CBD-CGD-O2D
6	7	101	BCL	C2C-C3C-CAC-CBC
6	7	101	BCL	C4C-C3C-CAC-CBC
6	7	101	BCL	CHA-CBD-CGD-O1D
6	7	101	BCL	CHA-CBD-CGD-O2D
6	8	101	BCL	CHA-CBD-CGD-O1D
6	8	101	BCL	CHA-CBD-CGD-O2D
6	9	101	BCL	C2C-C3C-CAC-CBC
6	9	101	BCL	C4C-C3C-CAC-CBC
6	9	101	BCL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
6	9	101	BCL	CHA-CBD-CGD-O2D
6	0	101	BCL	CHA-CBD-CGD-O1D
6	0	101	BCL	CHA-CBD-CGD-O2D
6	4	101	BCL	CHA-CBD-CGD-O1D
6	4	101	BCL	CHA-CBD-CGD-O2D
6	t	101	BCL	CHA-CBD-CGD-O1D
6	t	101	BCL	CHA-CBD-CGD-O2D
6	5	101	BCL	C2C-C3C-CAC-CBC
6	5	102	BCL	CHA-CBD-CGD-O1D
6	5	102	BCL	CHA-CBD-CGD-O2D
6	3	101	BCL	CHA-CBD-CGD-O1D
6	3	101	BCL	CHA-CBD-CGD-O2D
6	M	404	BCL	CHA-CBD-CGD-O1D
6	M	404	BCL	CHA-CBD-CGD-O2D
6	M	404	BCL	CAD-CBD-CGD-O1D
6	M	404	BCL	CAD-CBD-CGD-O2D
10	M	407	SPN	C7-C8-C9-CM4
10	M	407	SPN	C11-C10-C9-CM4
10	M	407	SPN	C19-C20-C21-C22
10	M	407	SPN	C28-C29-C30-CM9
10	M	407	SPN	C14-C15-C16-C17
10	M	407	SPN	CM8-C26-C27-C28
10	M	407	SPN	C25-C26-C27-C28
10	M	407	SPN	C20-C21-C22-C23
10	M	407	SPN	CM3-C5-C6-C7
6	L	301	BCL	C2A-CAA-CBA-CGA
7	M	405	BPH	C2A-CAA-CBA-CGA
6	5	101	BCL	C3A-C2A-CAA-CBA
10	M	407	SPN	C4-C5-C6-C7
6	9	101	BCL	C1A-C2A-CAA-CBA
6	5	101	BCL	C1A-C2A-CAA-CBA
6	E	101	BCL	C2C-C3C-CAC-CBC
6	1	101	BCL	C2C-C3C-CAC-CBC
10	M	407	SPN	C5-C6-C7-C8
10	M	407	SPN	CM1-C1-C2-O2
10	M	407	SPN	CM1-C1-C2-C3
6	9	101	BCL	C3A-C2A-CAA-CBA
10	M	407	SPN	C16-C17-C18-CM6
10	M	407	SPN	C11-C10-C9-C8
10	M	407	SPN	C16-C17-C18-C19
10	M	407	SPN	C22-C23-C24-C25
6	M	404	BCL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
6	I	101	BCL	CHA-CBD-CGD-O2D
6	K	101	BCL	CHA-CBD-CGD-O1D
6	K	101	BCL	CHA-CBD-CGD-O2D
6	5	101	BCL	CHA-CBD-CGD-O1D
6	M	401	BCL	CHA-CBD-CGD-O1D
6	M	401	BCL	CHA-CBD-CGD-O2D
10	M	407	SPN	C20-C21-C22-CM7
10	M	407	SPN	O1-C1-C2-O2
6	M	401	BCL	CAD-CBD-CGD-O1D
8	M	406	U10	C5-C4-O4-C4M
6	A	101	BCL	C2A-CAA-CBA-CGA
6	M	403	BCL	CAA-CBA-CGA-O1A
6	7	101	BCL	CAA-CBA-CGA-O2A
6	5	101	BCL	CAA-CBA-CGA-O1A
10	M	407	SPN	CM2-C1-C2-C3
6	I	101	BCL	CAA-CBA-CGA-O1A
6	U	101	BCL	CAA-CBA-CGA-O1A
8	L	303	U10	C5-C4-O4-C4M
6	5	101	BCL	CAA-CBA-CGA-O2A
6	F	101	BCL	CAA-CBA-CGA-O1A
6	I	101	BCL	CAA-CBA-CGA-O2A
6	W	101	BCL	CAA-CBA-CGA-O1A
6	U	101	BCL	CAA-CBA-CGA-O2A
6	7	101	BCL	CAA-CBA-CGA-O1A
7	M	405	BPH	C2C-C3C-CAC-CBC
6	9	101	BCL	CAA-CBA-CGA-O1A
6	I	101	BCL	C1A-C2A-CAA-CBA
6	W	101	BCL	CAA-CBA-CGA-O2A
6	C	101	BCL	CAA-CBA-CGA-O1A
6	M	403	BCL	CAA-CBA-CGA-O2A
6	O	101	BCL	CAA-CBA-CGA-O1A
6	1	101	BCL	CAA-CBA-CGA-O2A
6	O	101	BCL	CAA-CBA-CGA-O2A
7	L	302	BPH	CAA-CBA-CGA-O1A
6	F	101	BCL	CAA-CBA-CGA-O2A
6	1	101	BCL	CAA-CBA-CGA-O1A
6	C	101	BCL	CAA-CBA-CGA-O2A
6	9	101	BCL	CAA-CBA-CGA-O2A
6	Y	101	BCL	CAA-CBA-CGA-O2A
6	B	101	BCL	CAA-CBA-CGA-O1A
6	E	102	BCL	CAA-CBA-CGA-O1A
6	G	101	BCL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
6	J	101	BCL	CAA-CBA-CGA-O1A
6	N	101	BCL	CAA-CBA-CGA-O1A
6	P	101	BCL	CAA-CBA-CGA-O1A
6	R	101	BCL	CAA-CBA-CGA-O1A
6	T	101	BCL	CAA-CBA-CGA-O1A
6	V	101	BCL	CAA-CBA-CGA-O1A
6	X	101	BCL	CAA-CBA-CGA-O1A
6	Z	101	BCL	CAA-CBA-CGA-O1A
6	8	101	BCL	CAA-CBA-CGA-O1A
6	0	101	BCL	CAA-CBA-CGA-O1A
6	t	101	BCL	CAA-CBA-CGA-O1A
6	5	102	BCL	CAA-CBA-CGA-O1A
6	3	101	BCL	CAA-CBA-CGA-O1A
6	B	101	BCL	CAA-CBA-CGA-O2A
6	E	102	BCL	CAA-CBA-CGA-O2A
6	G	101	BCL	CAA-CBA-CGA-O2A
6	J	101	BCL	CAA-CBA-CGA-O2A
6	N	101	BCL	CAA-CBA-CGA-O2A
6	P	101	BCL	CAA-CBA-CGA-O2A
6	R	101	BCL	CAA-CBA-CGA-O2A
6	T	101	BCL	CAA-CBA-CGA-O2A
6	V	101	BCL	CAA-CBA-CGA-O2A
6	X	101	BCL	CAA-CBA-CGA-O2A
6	Z	101	BCL	CAA-CBA-CGA-O2A
6	2	101	BCL	CAA-CBA-CGA-O1A
6	2	101	BCL	CAA-CBA-CGA-O2A
6	8	101	BCL	CAA-CBA-CGA-O2A
6	0	101	BCL	CAA-CBA-CGA-O2A
6	t	101	BCL	CAA-CBA-CGA-O2A
6	5	102	BCL	CAA-CBA-CGA-O2A
6	3	101	BCL	CAA-CBA-CGA-O2A
10	M	407	SPN	CM5-C13-C14-C15
7	M	405	BPH	CAA-CBA-CGA-O2A
7	M	405	BPH	CAA-CBA-CGA-O1A
7	M	405	BPH	CAD-CBD-CGD-O2D
7	L	302	BPH	CAA-CBA-CGA-O2A
10	M	407	SPN	C26-C27-C28-C29
6	Y	101	BCL	CAA-CBA-CGA-O1A
6	O	101	BCL	CHA-CBD-CGD-O1D
6	O	101	BCL	CHA-CBD-CGD-O2D
6	W	101	BCL	CHA-CBD-CGD-O1D
6	W	101	BCL	CHA-CBD-CGD-O2D

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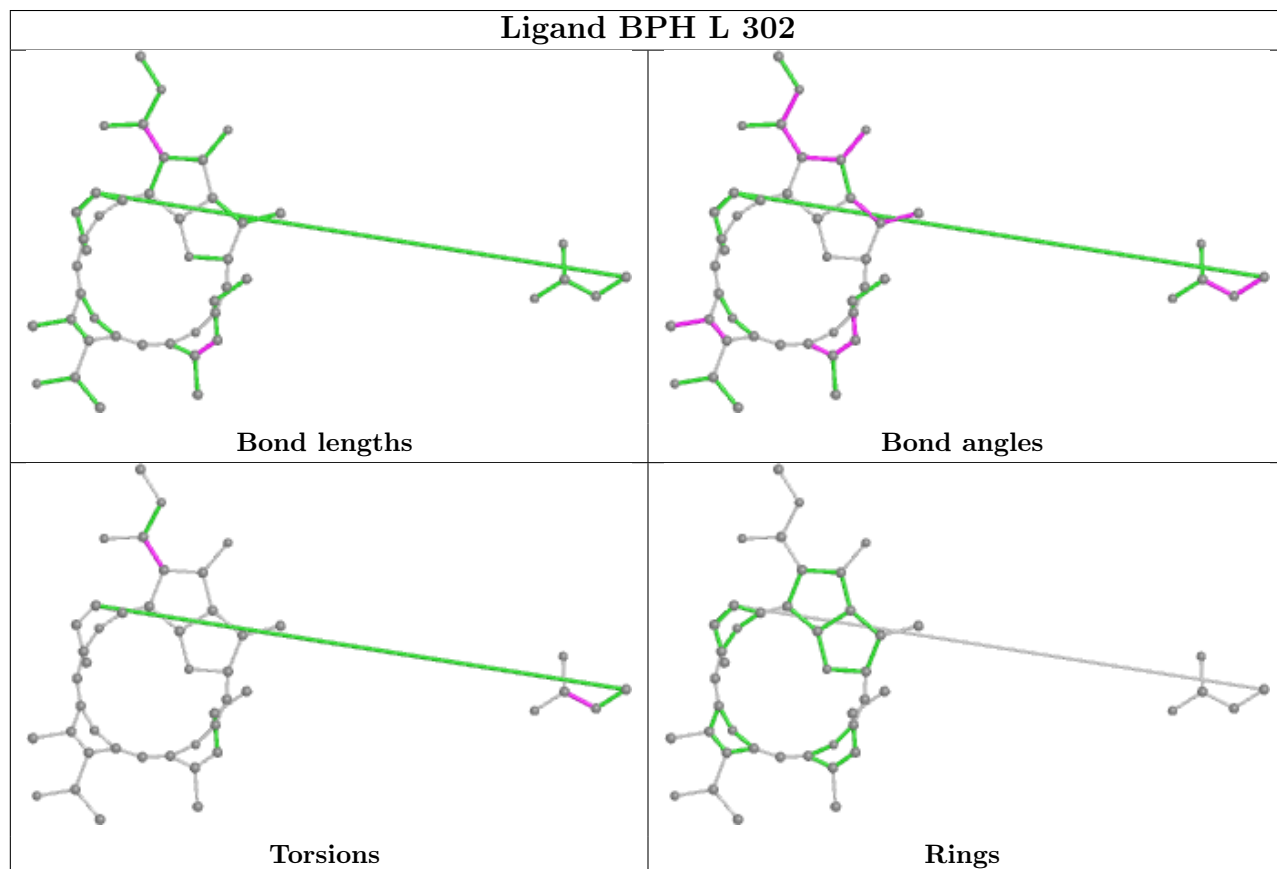
Mol	Chain	Res	Type	Atoms
6	Y	101	BCL	CHA-CBD-CGD-O1D
6	Y	101	BCL	CHA-CBD-CGD-O2D
6	5	101	BCL	CHA-CBD-CGD-O2D
6	C	101	BCL	CHA-CBD-CGD-O1D
6	C	101	BCL	CHA-CBD-CGD-O2D
10	M	407	SPN	C12-C13-C14-C15
10	M	407	SPN	C23-C24-C25-C26
6	B	101	BCL	C1A-C2A-CAA-CBA
6	E	102	BCL	C1A-C2A-CAA-CBA
6	G	101	BCL	C1A-C2A-CAA-CBA
6	J	101	BCL	C1A-C2A-CAA-CBA
6	N	101	BCL	C1A-C2A-CAA-CBA
6	P	101	BCL	C1A-C2A-CAA-CBA
6	R	101	BCL	C1A-C2A-CAA-CBA
6	T	101	BCL	C1A-C2A-CAA-CBA
6	V	101	BCL	C1A-C2A-CAA-CBA
6	X	101	BCL	C1A-C2A-CAA-CBA
6	Z	101	BCL	C1A-C2A-CAA-CBA
6	2	101	BCL	C1A-C2A-CAA-CBA
6	8	101	BCL	C1A-C2A-CAA-CBA
6	0	101	BCL	C1A-C2A-CAA-CBA
6	t	101	BCL	C1A-C2A-CAA-CBA
6	5	102	BCL	C1A-C2A-CAA-CBA
6	3	101	BCL	C1A-C2A-CAA-CBA
6	M	401	BCL	C1A-C2A-CAA-CBA
6	M	404	BCL	C1A-C2A-CAA-CBA
6	L	301	BCL	CAA-CBA-CGA-O2A
8	M	406	U10	C2-C3-O3-C3M
6	W	101	BCL	CAD-CBD-CGD-O1D
6	C	101	BCL	CAD-CBD-CGD-O1D
7	L	302	BPH	CAD-CBD-CGD-O1D
10	M	407	SPN	CM2-C1-C2-O2
6	I	101	BCL	C3A-C2A-CAA-CBA
6	4	101	BCL	CAA-CBA-CGA-O1A
8	M	406	U10	C4-C3-O3-C3M
6	4	101	BCL	CAA-CBA-CGA-O2A

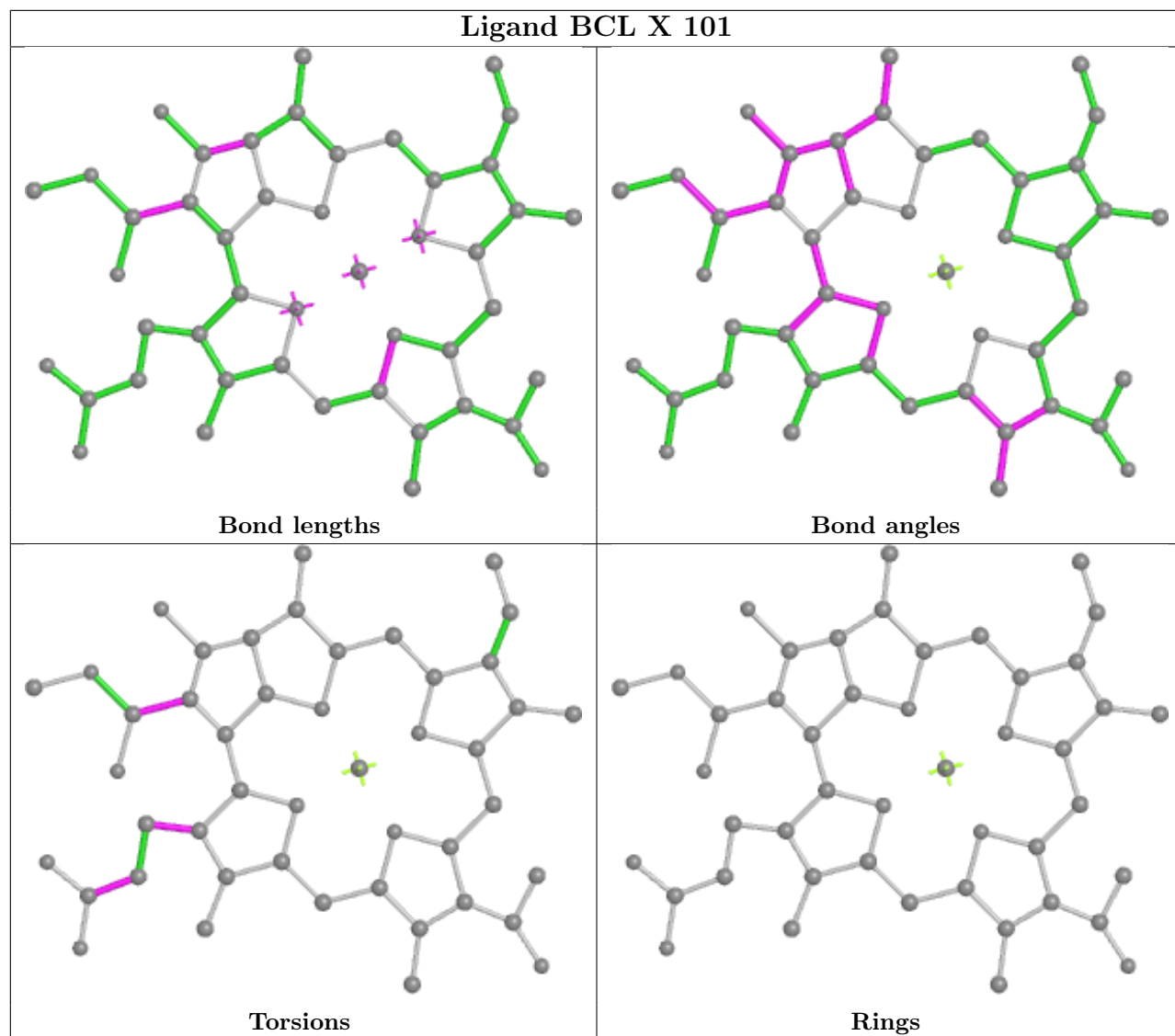
There are no ring outliers.

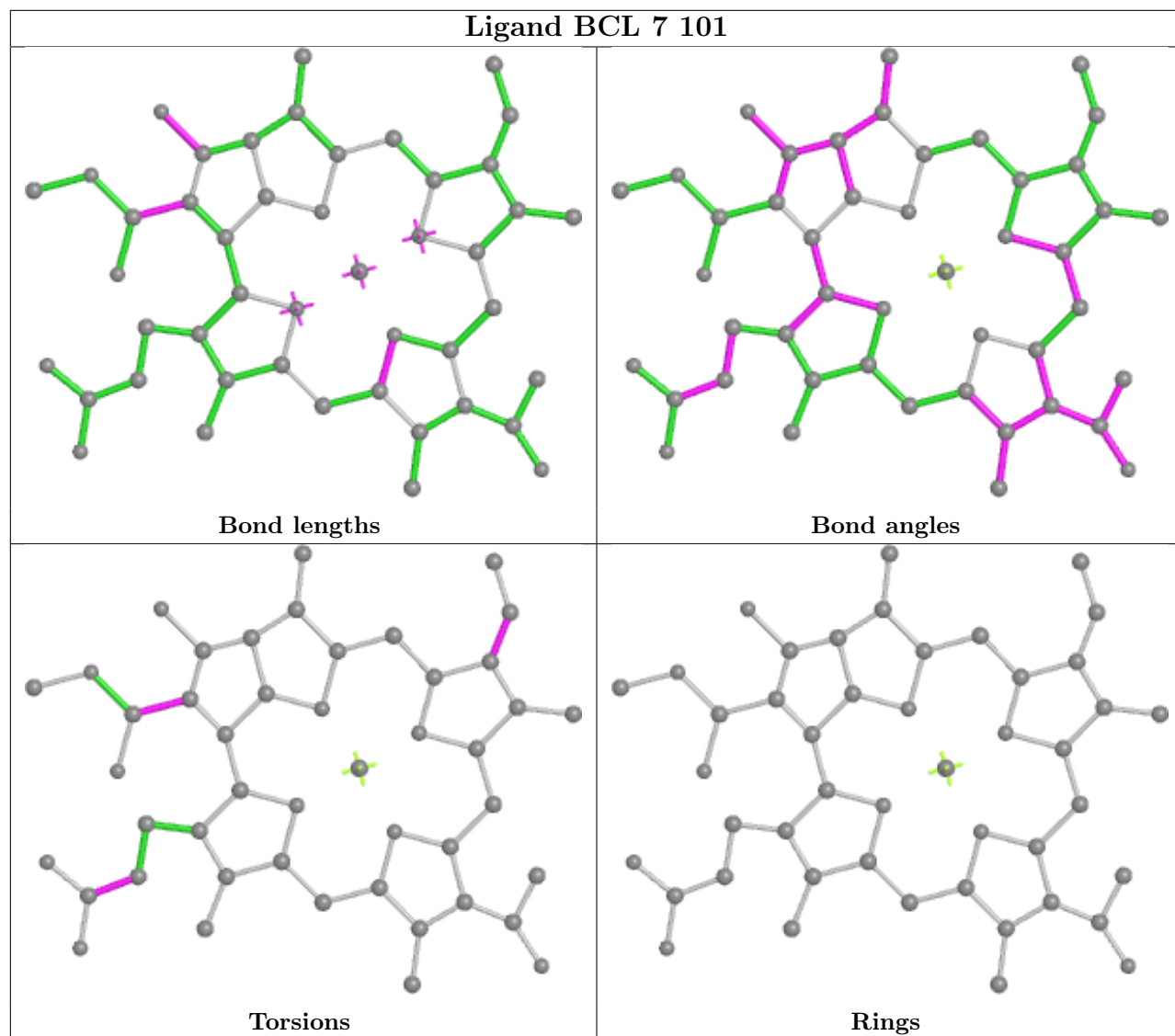
No monomer is involved in short contacts.

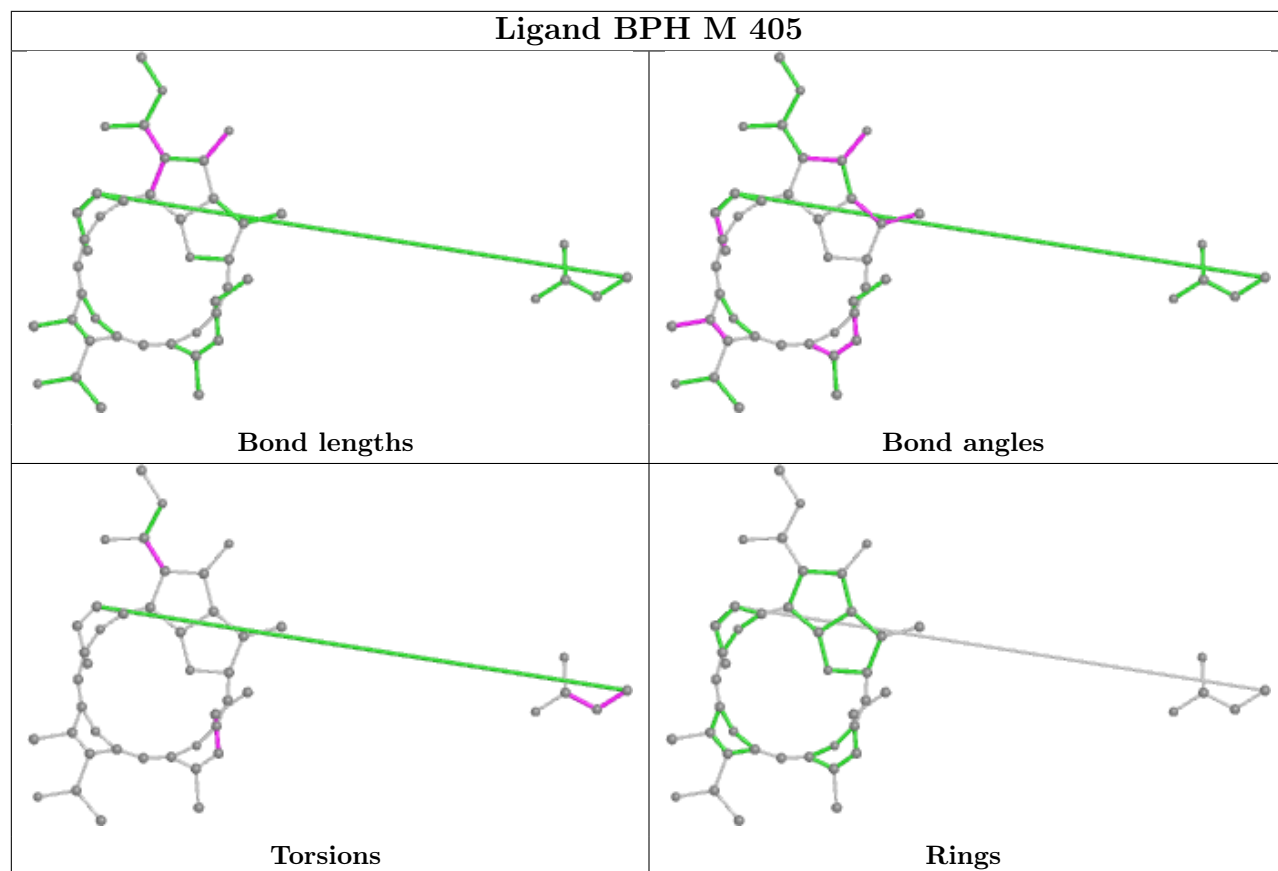
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

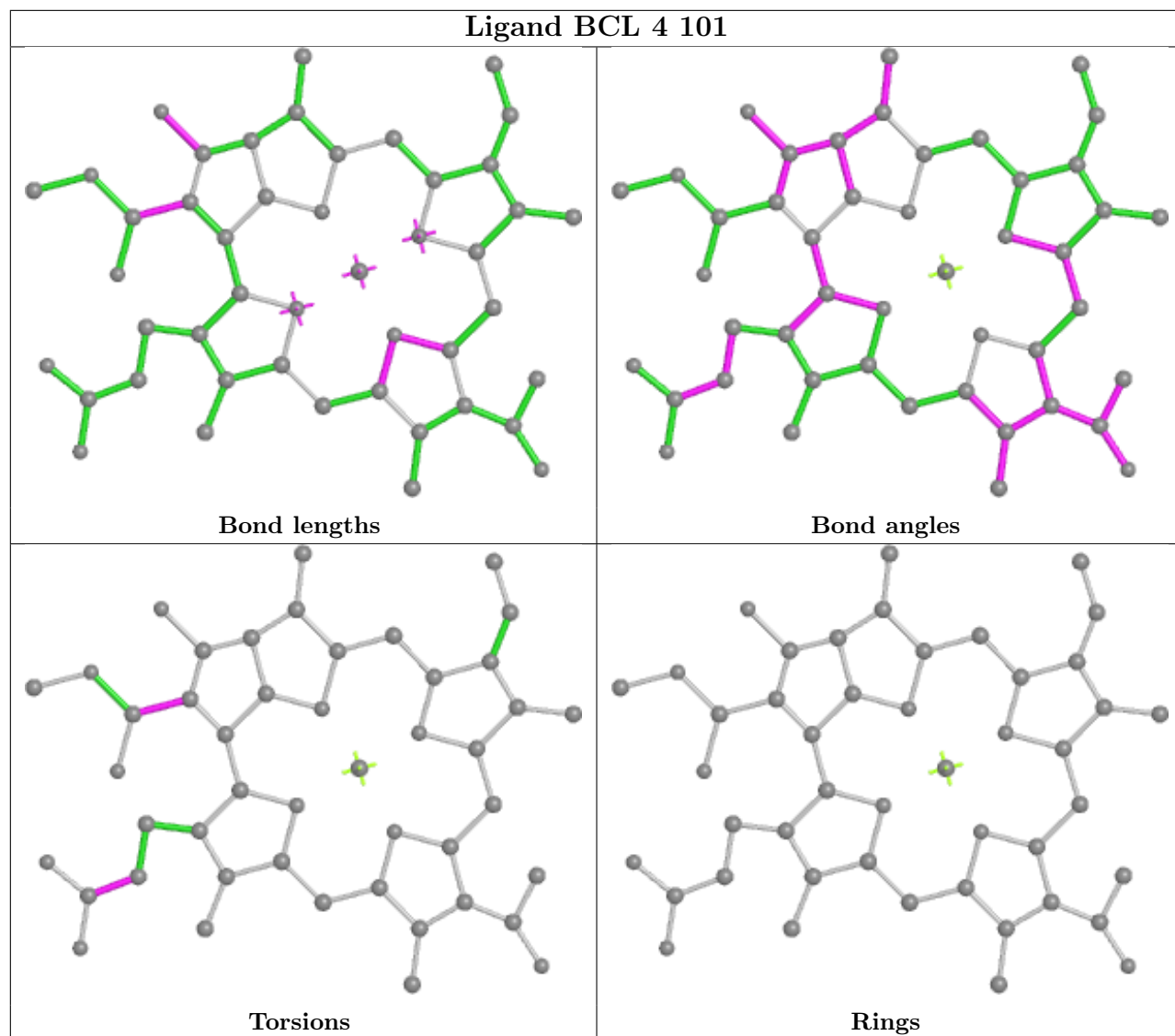
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

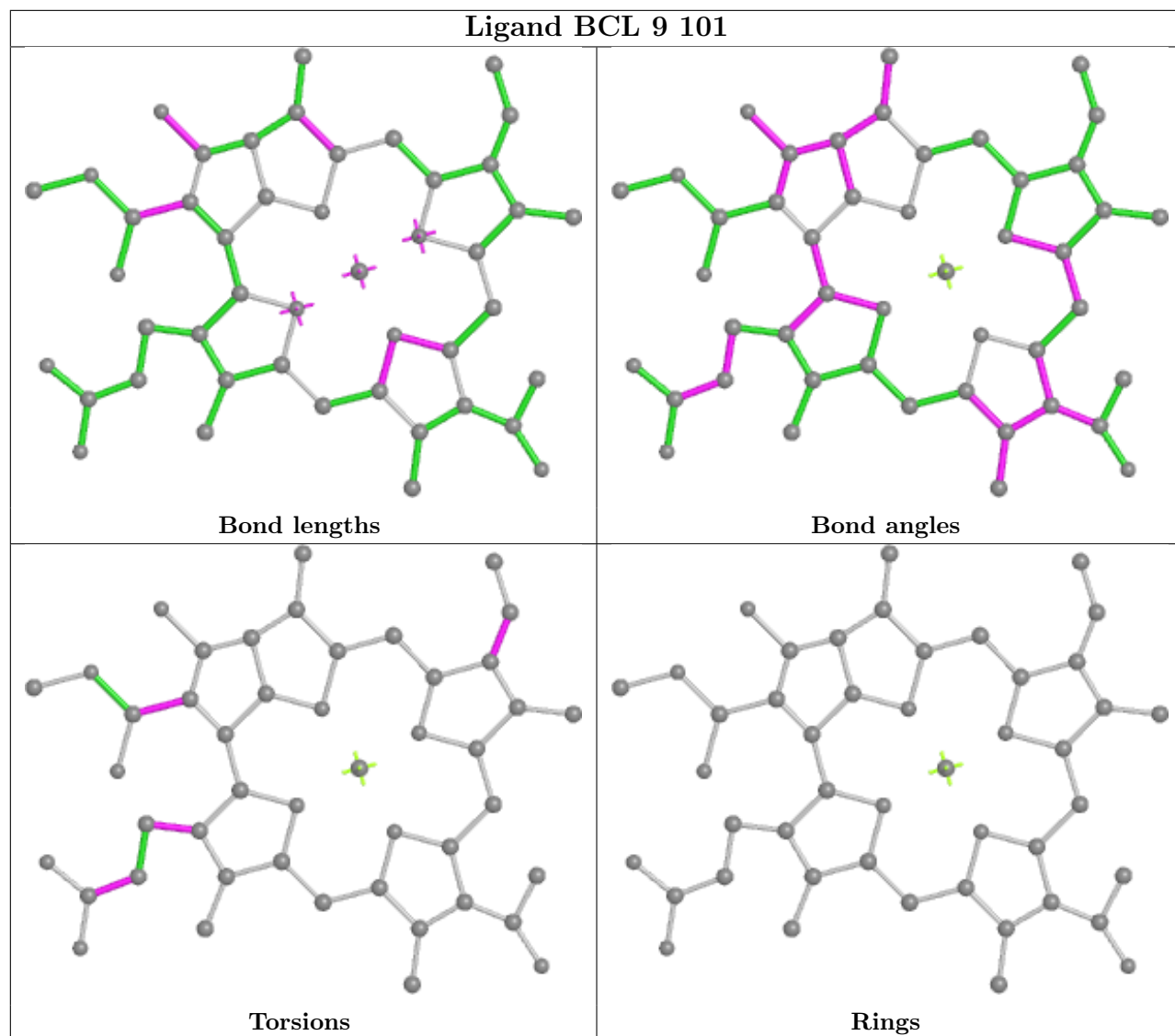


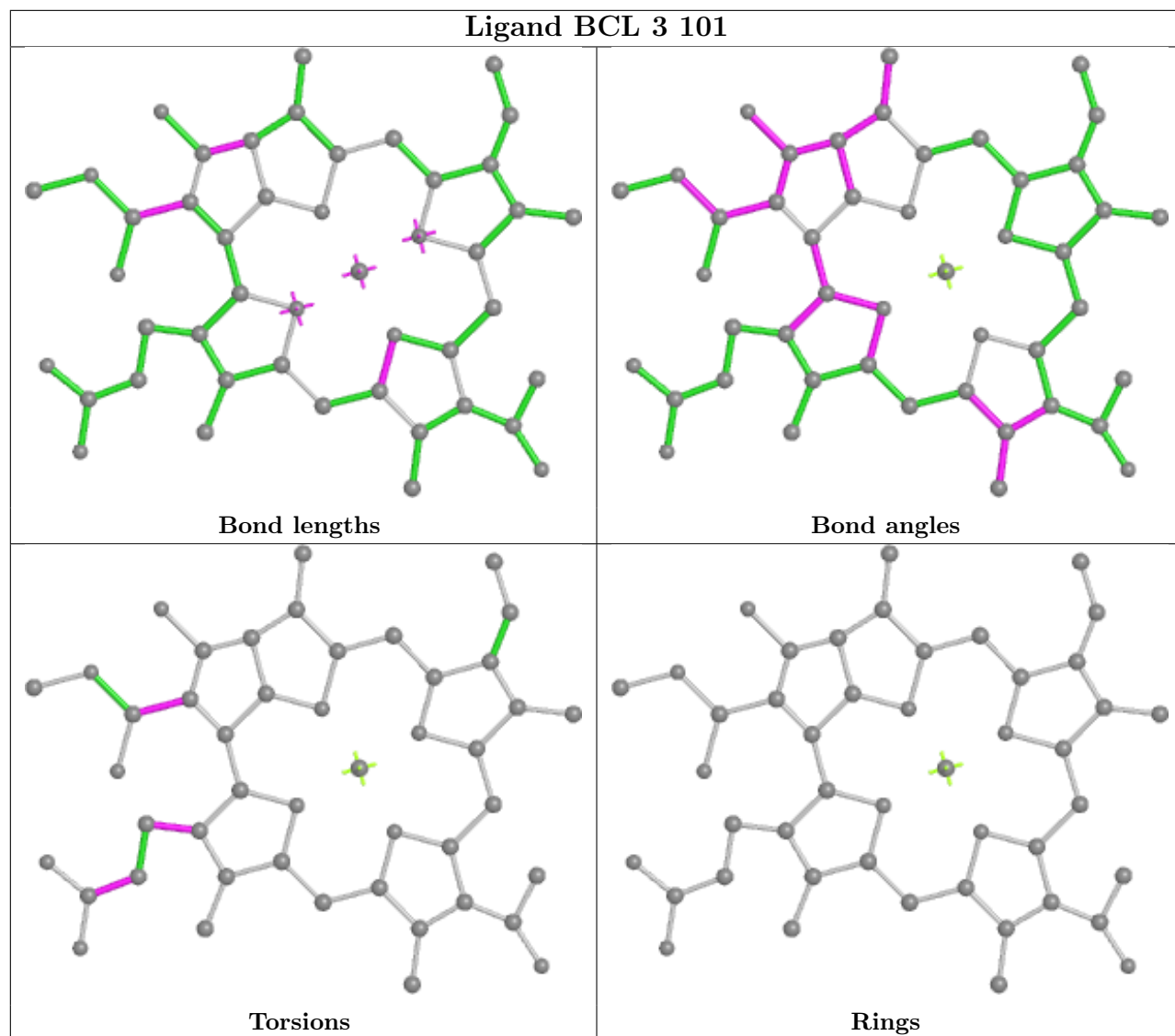


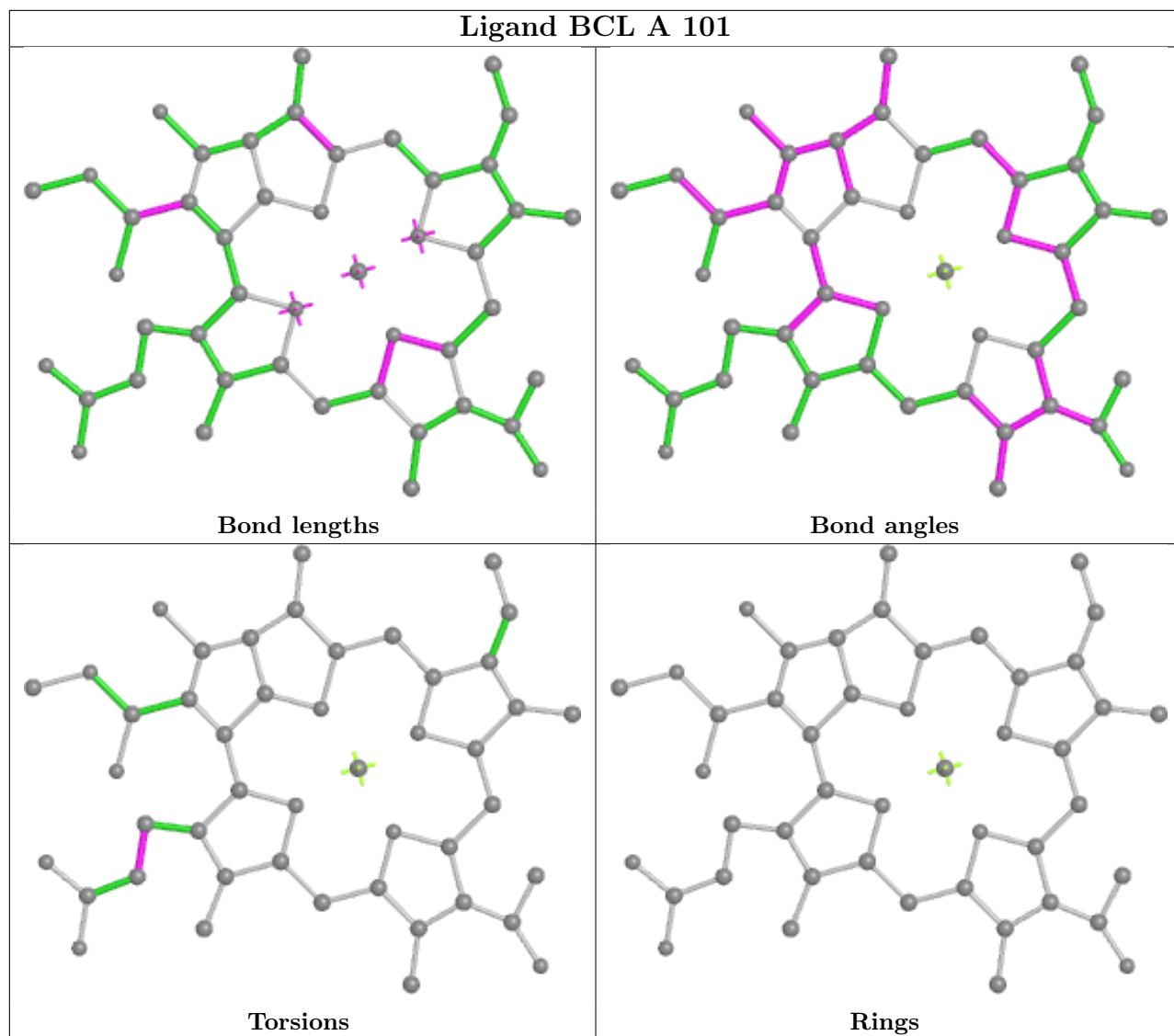


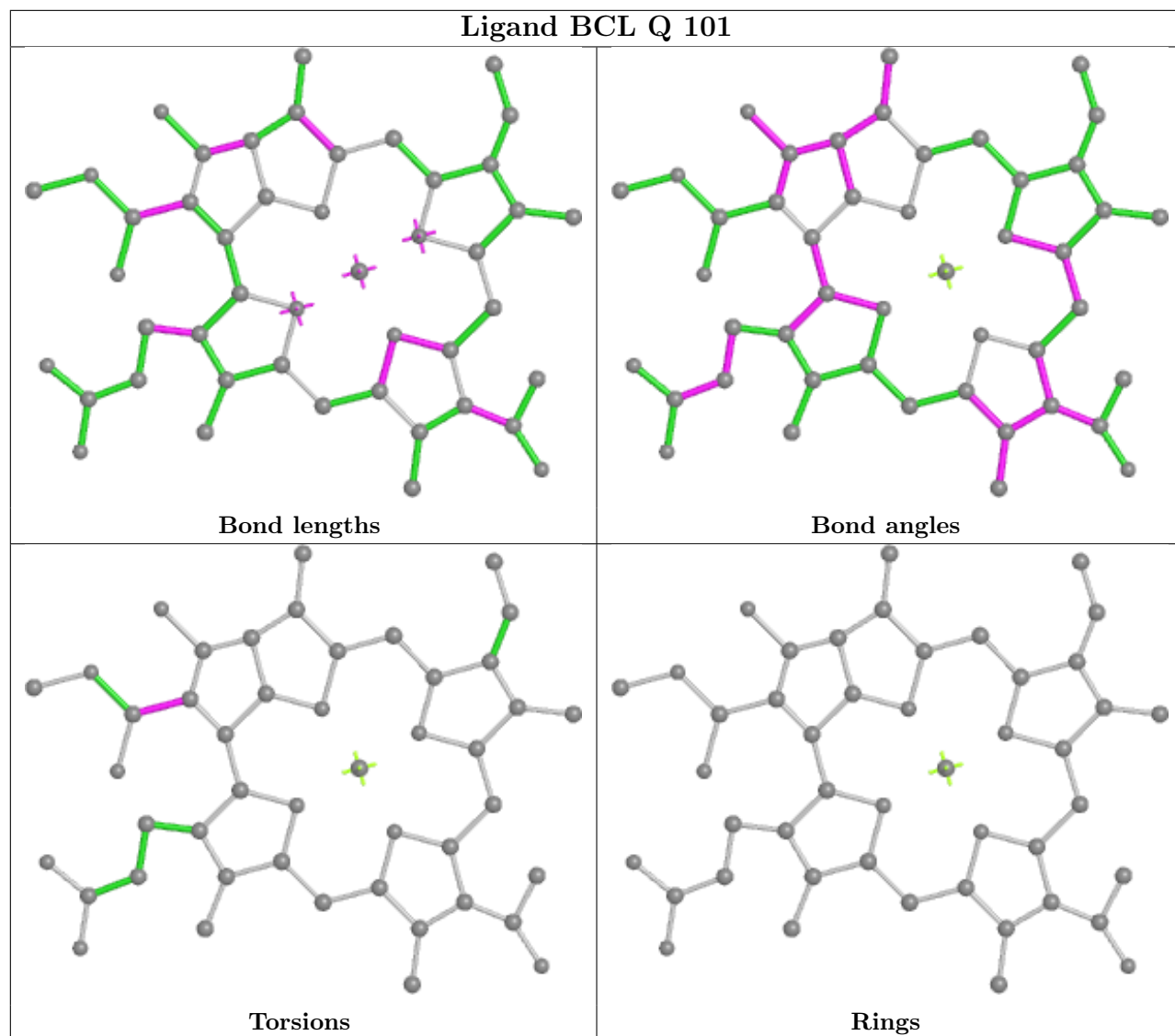


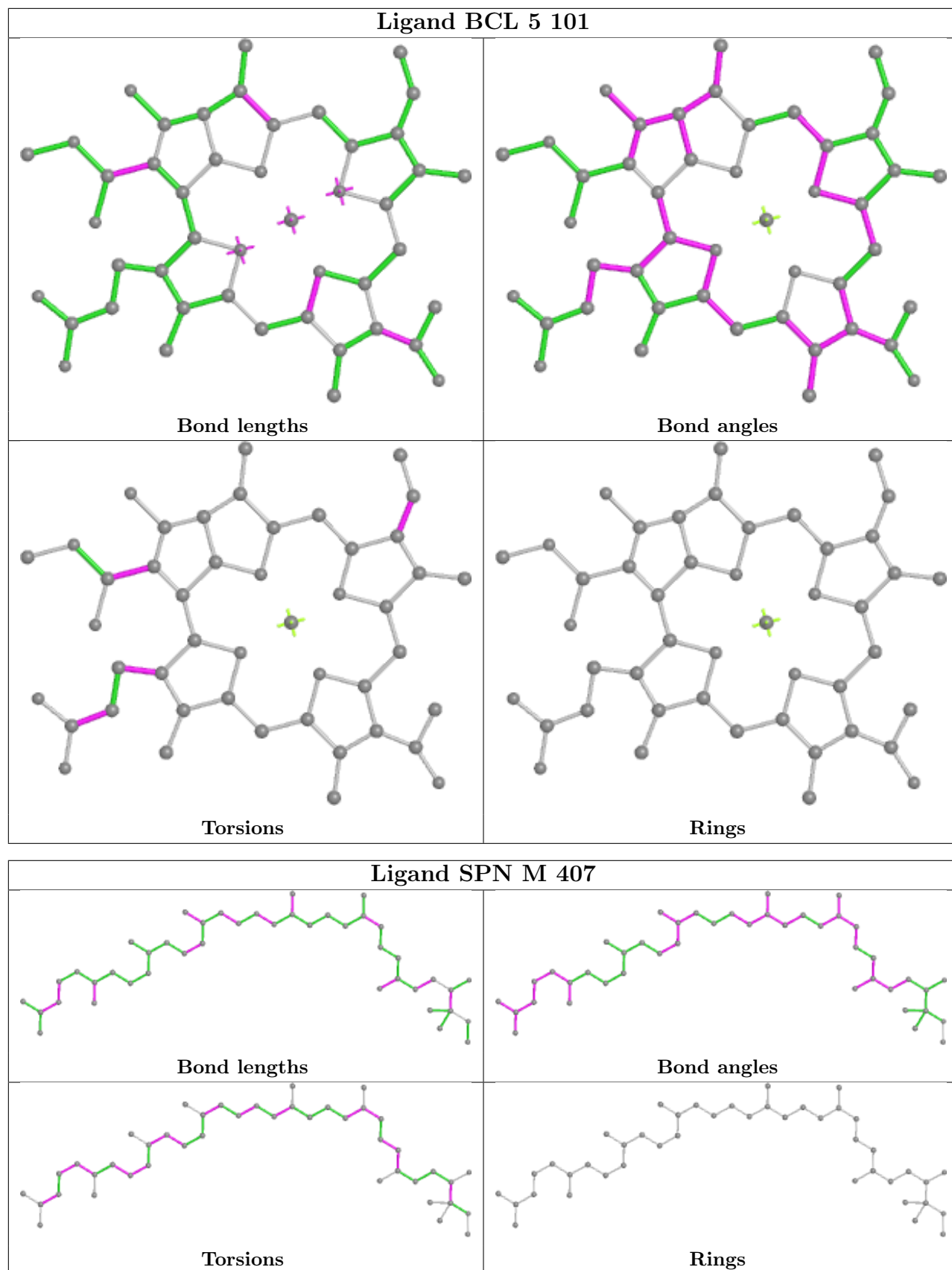


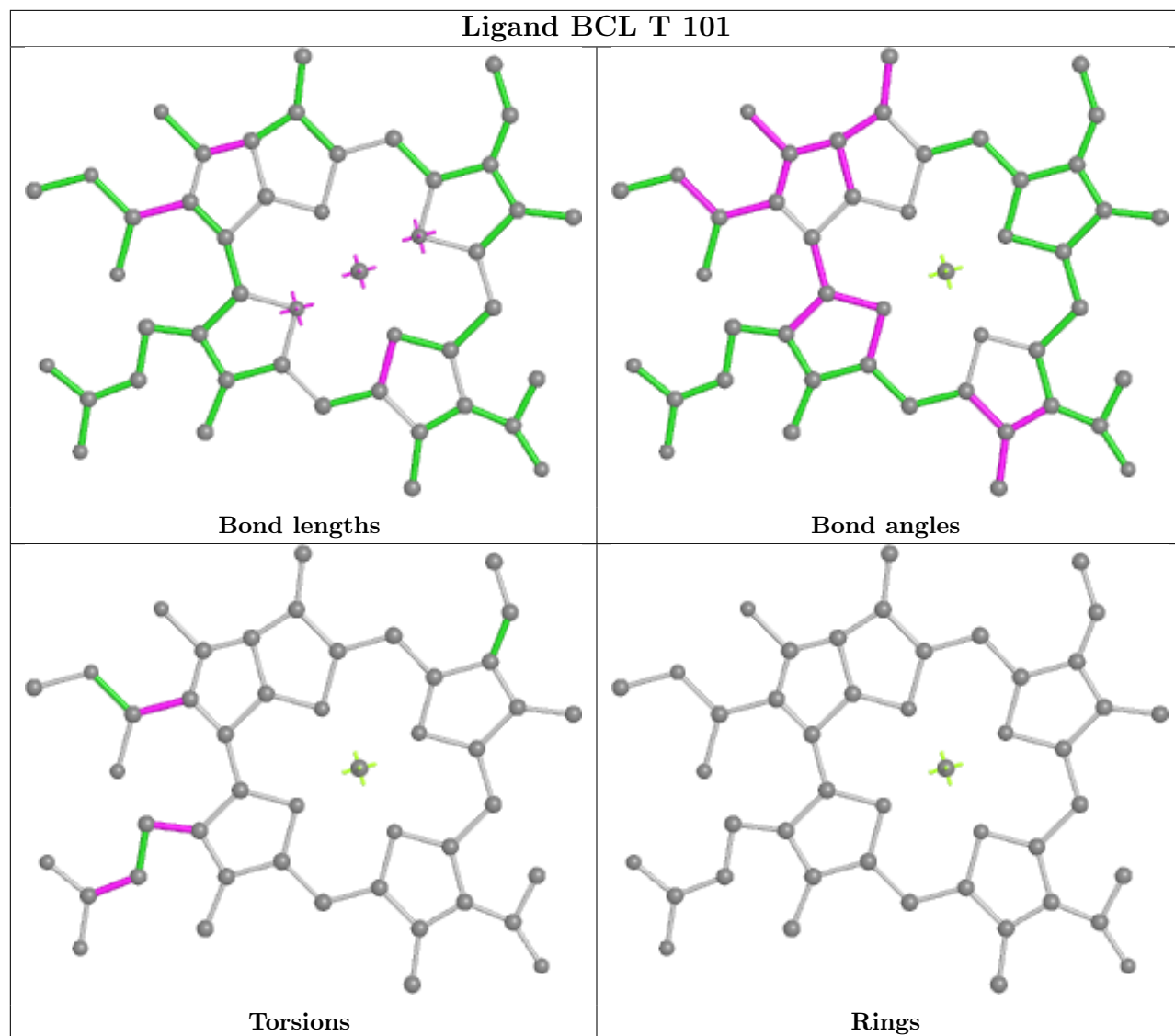


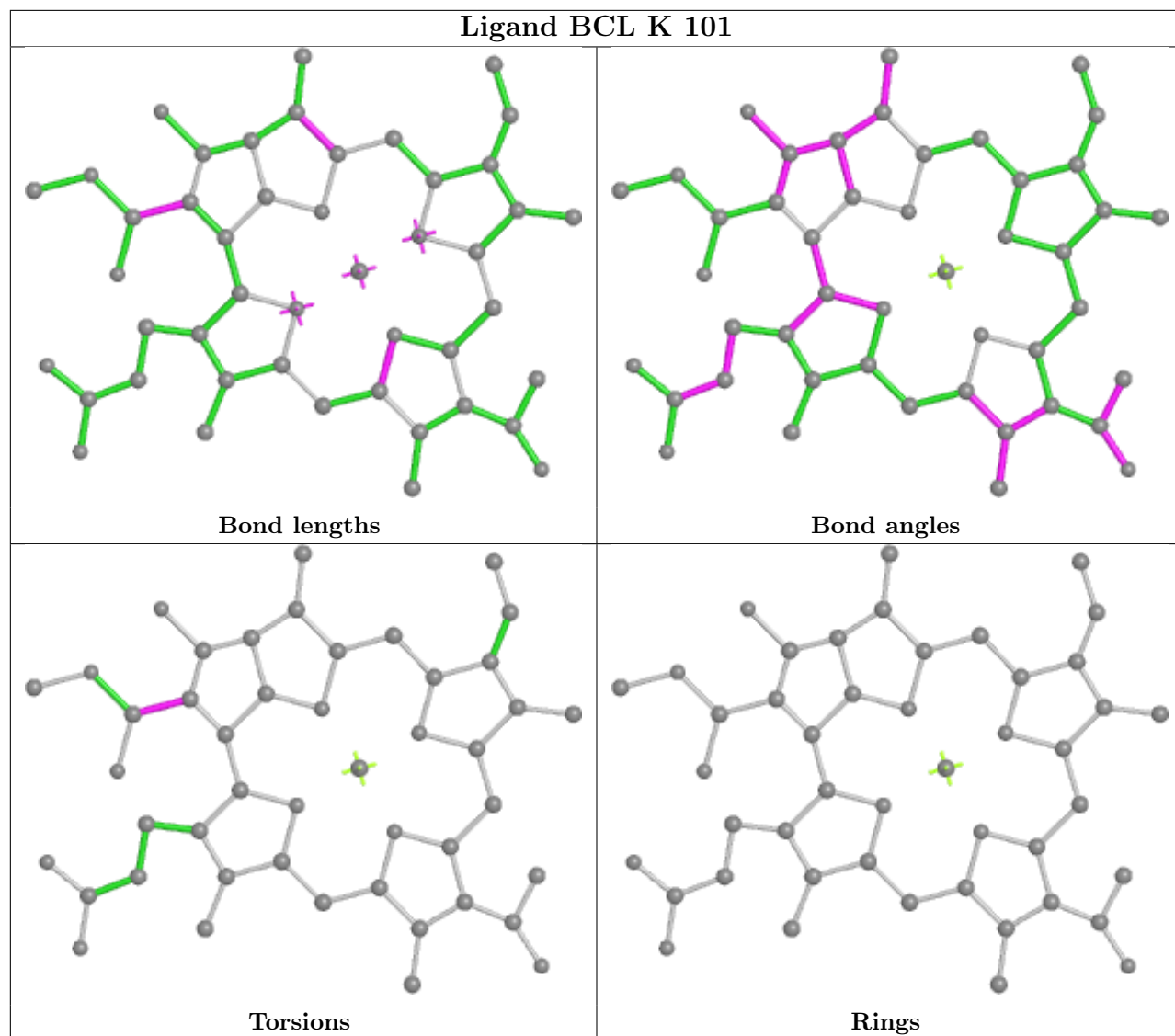


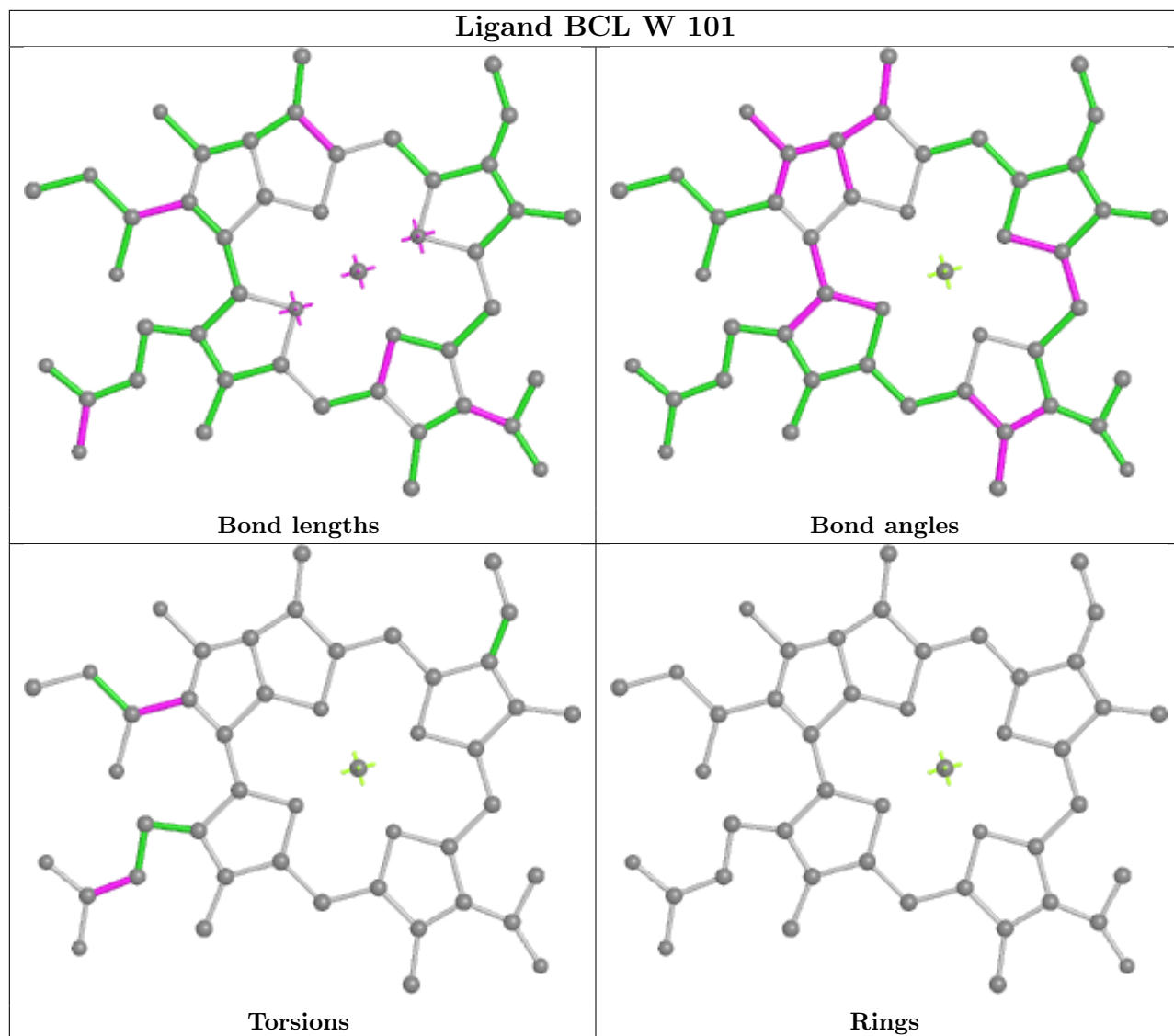


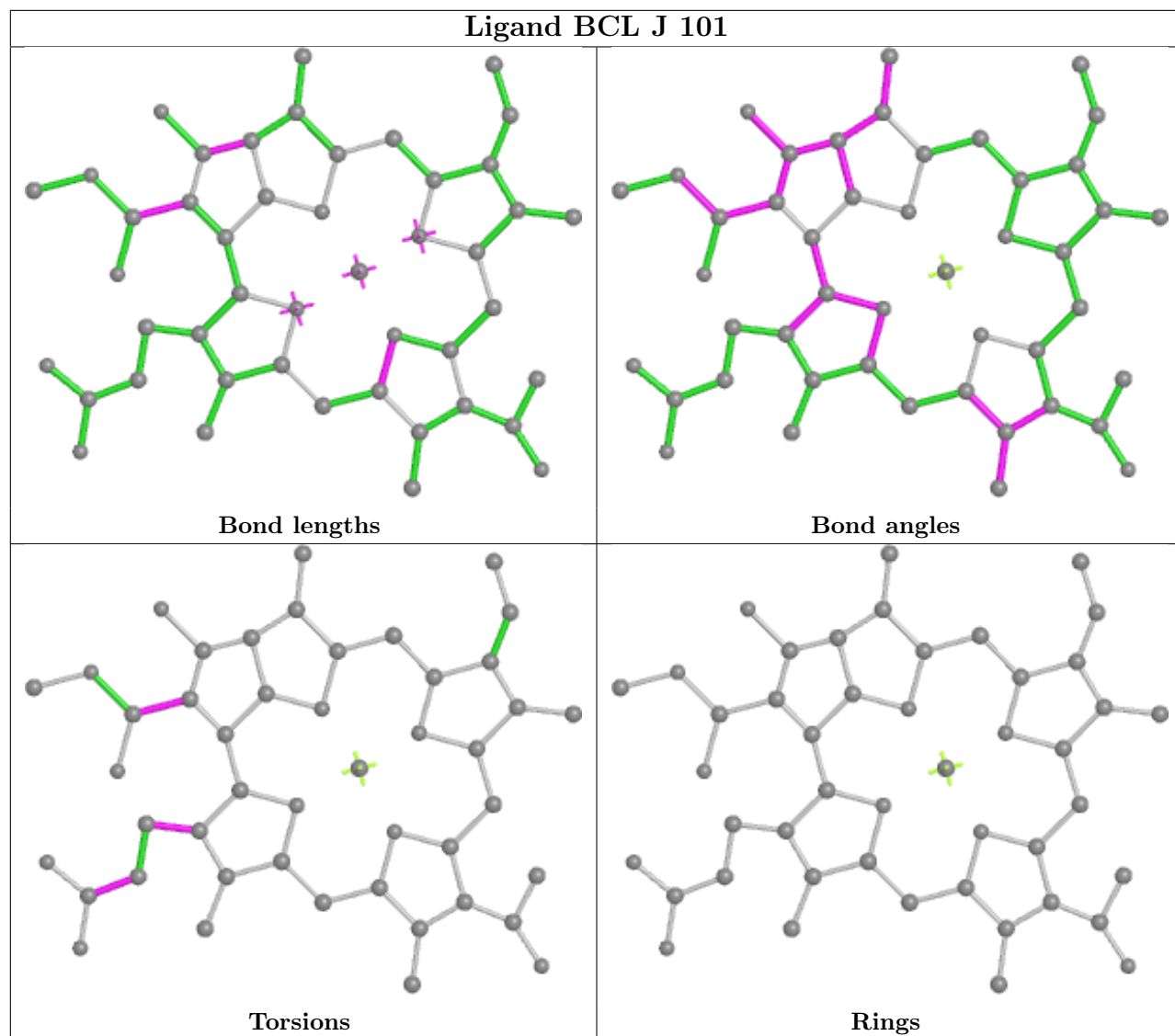


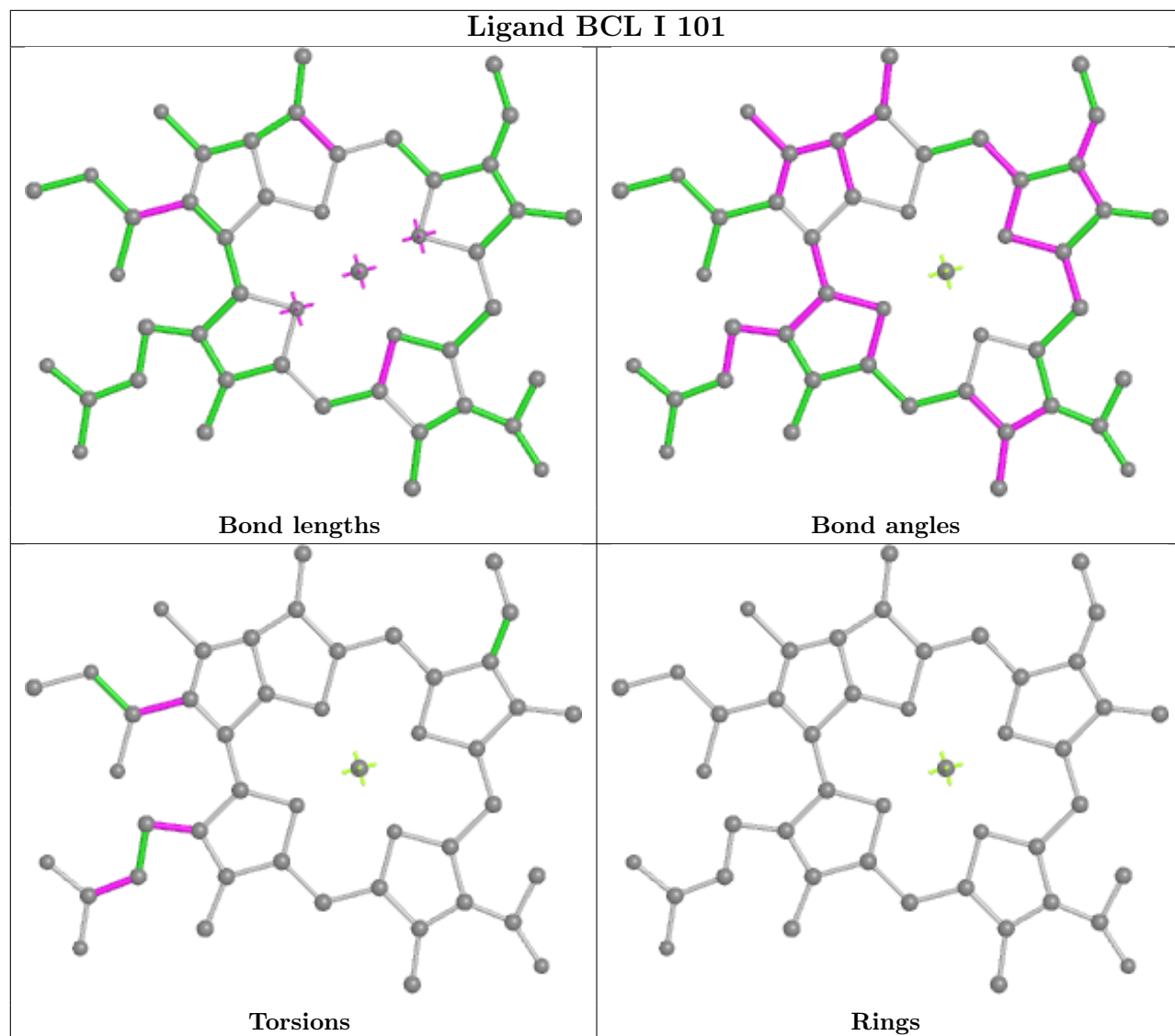


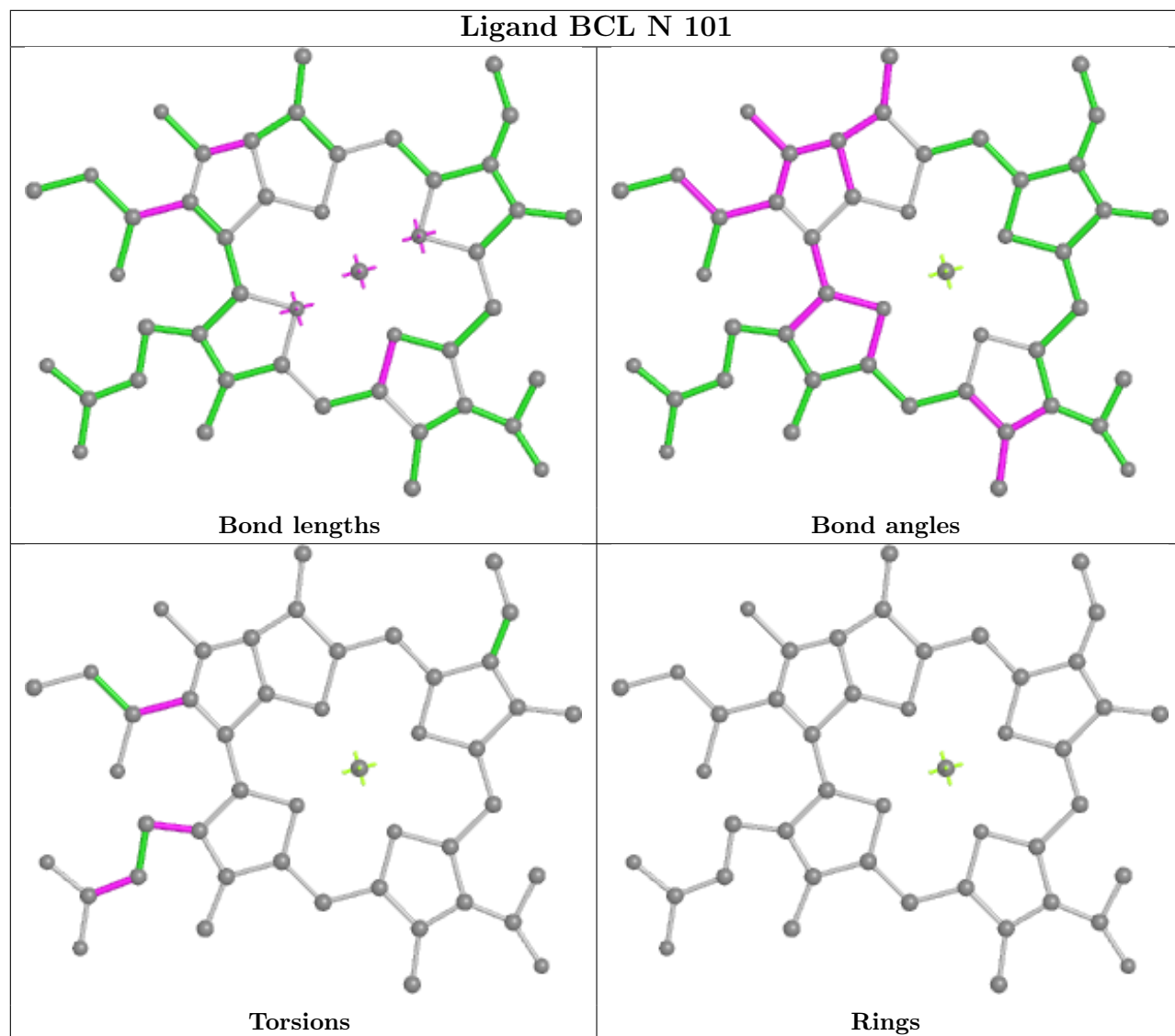


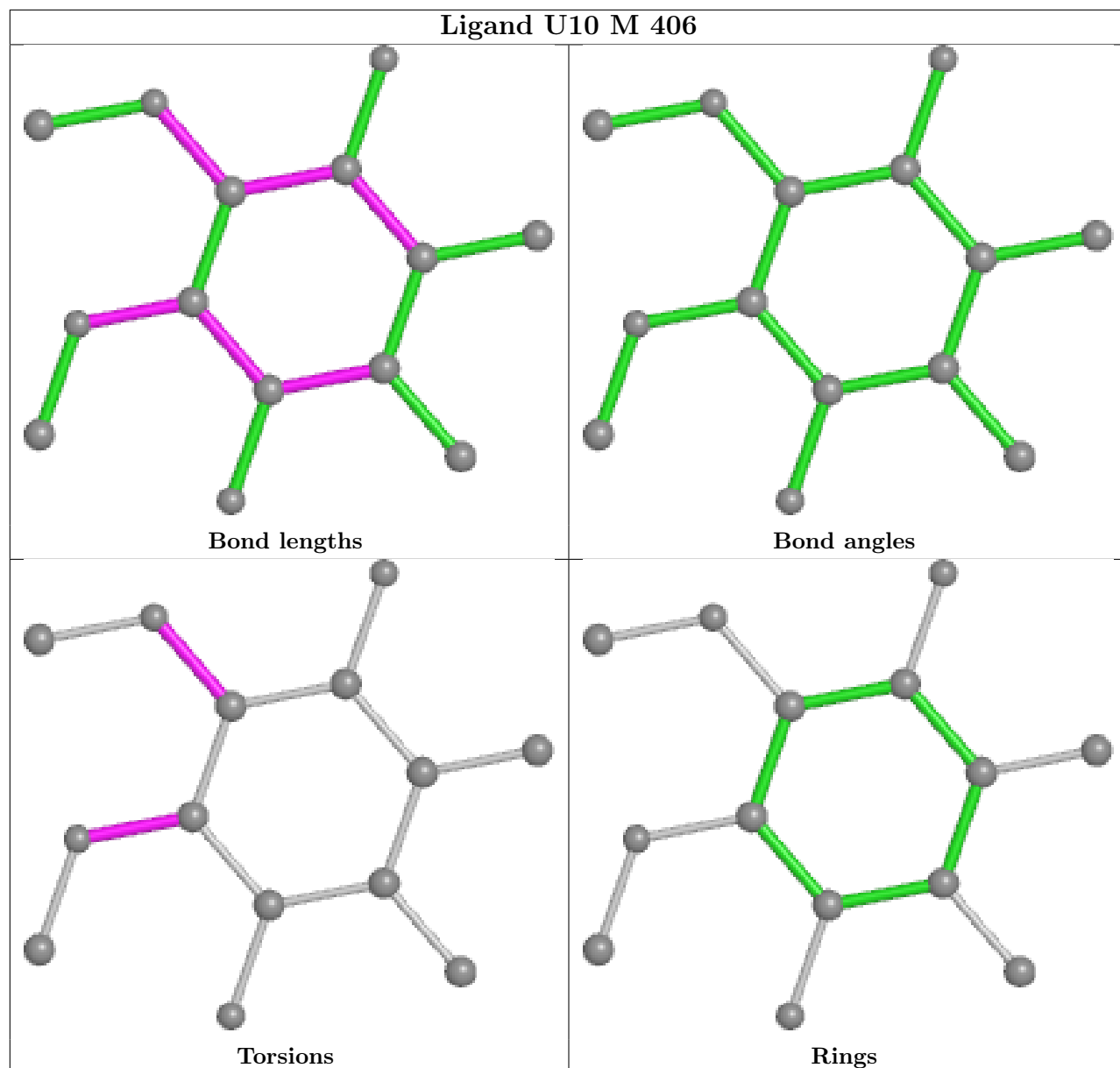


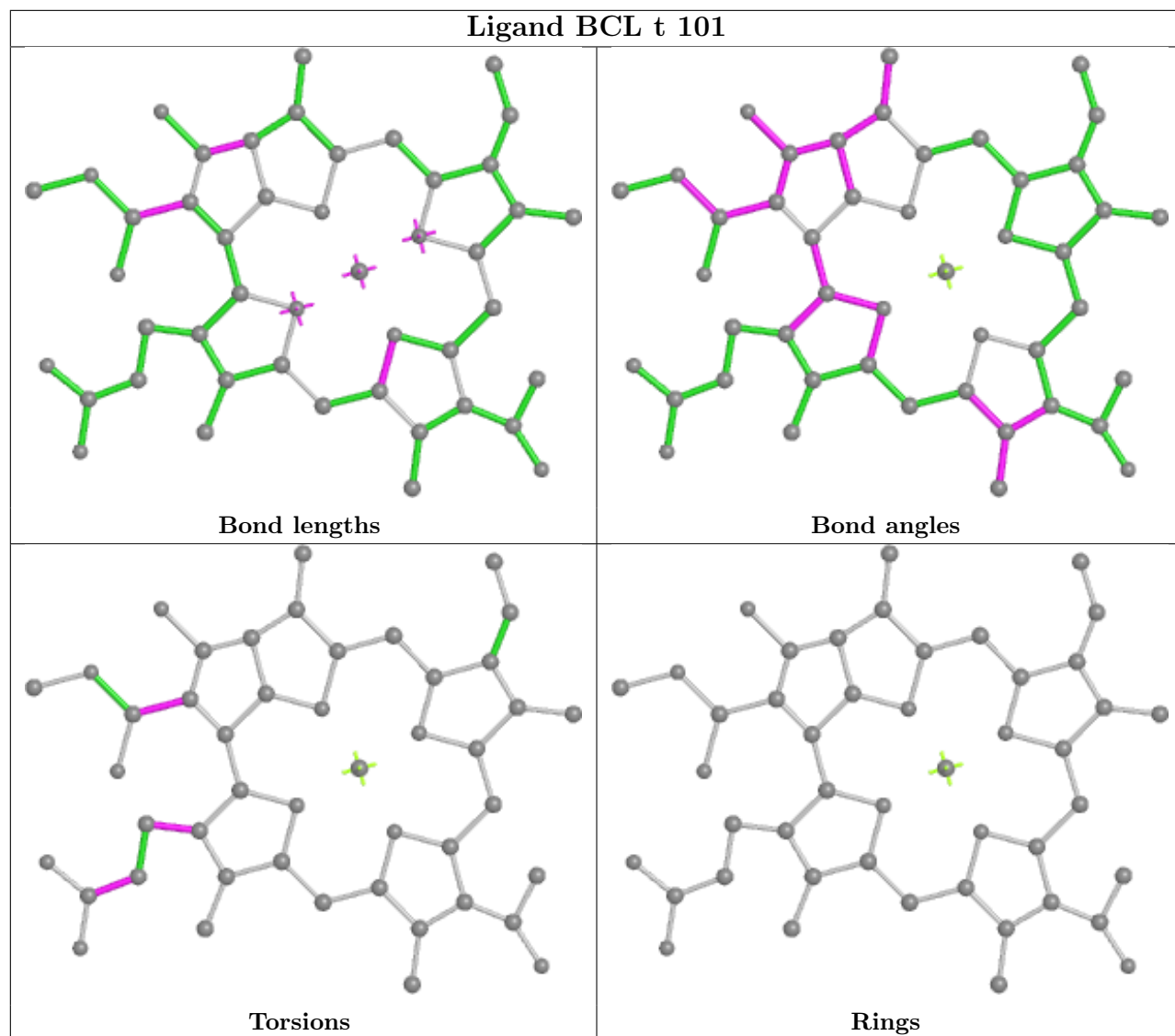


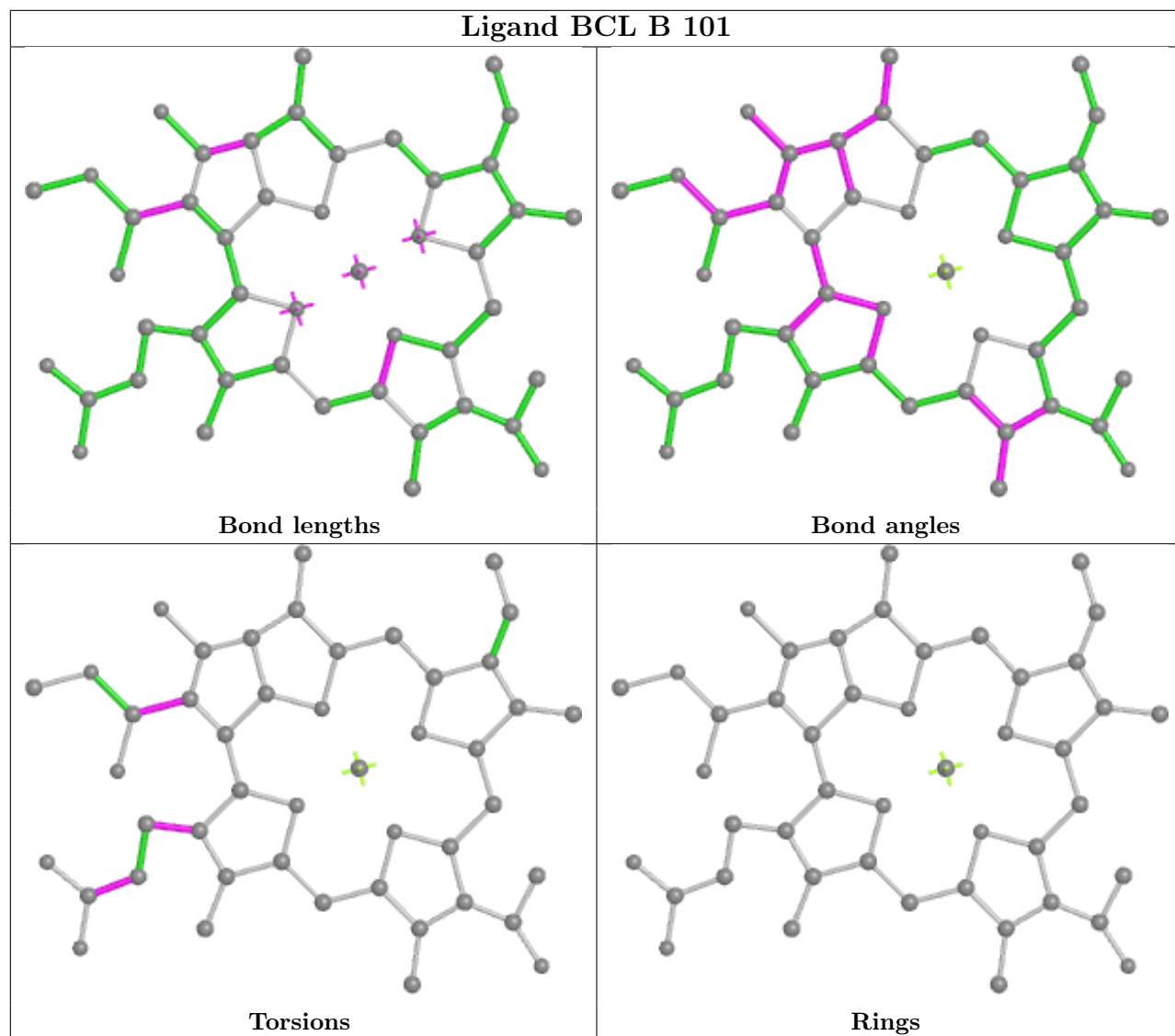


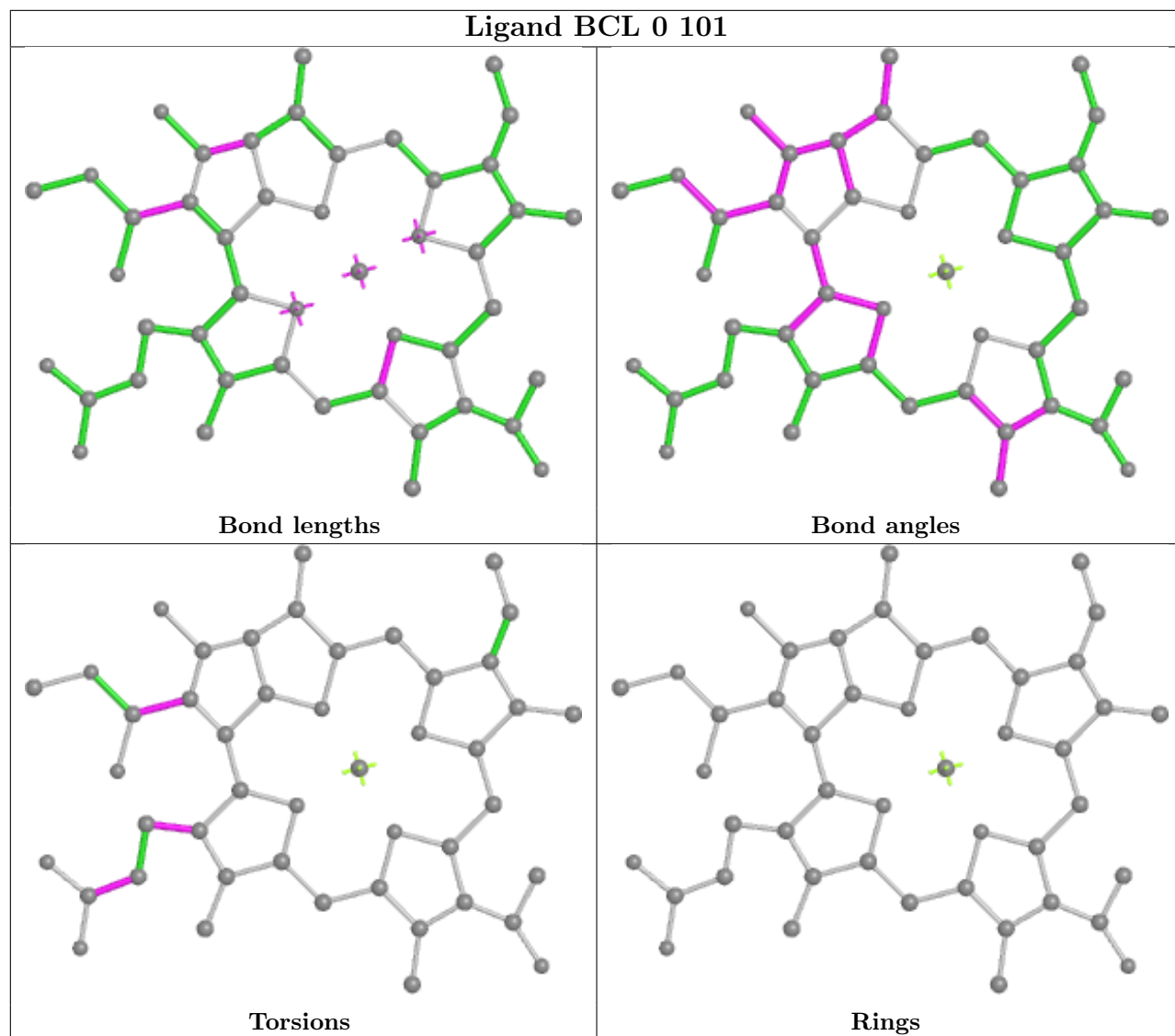


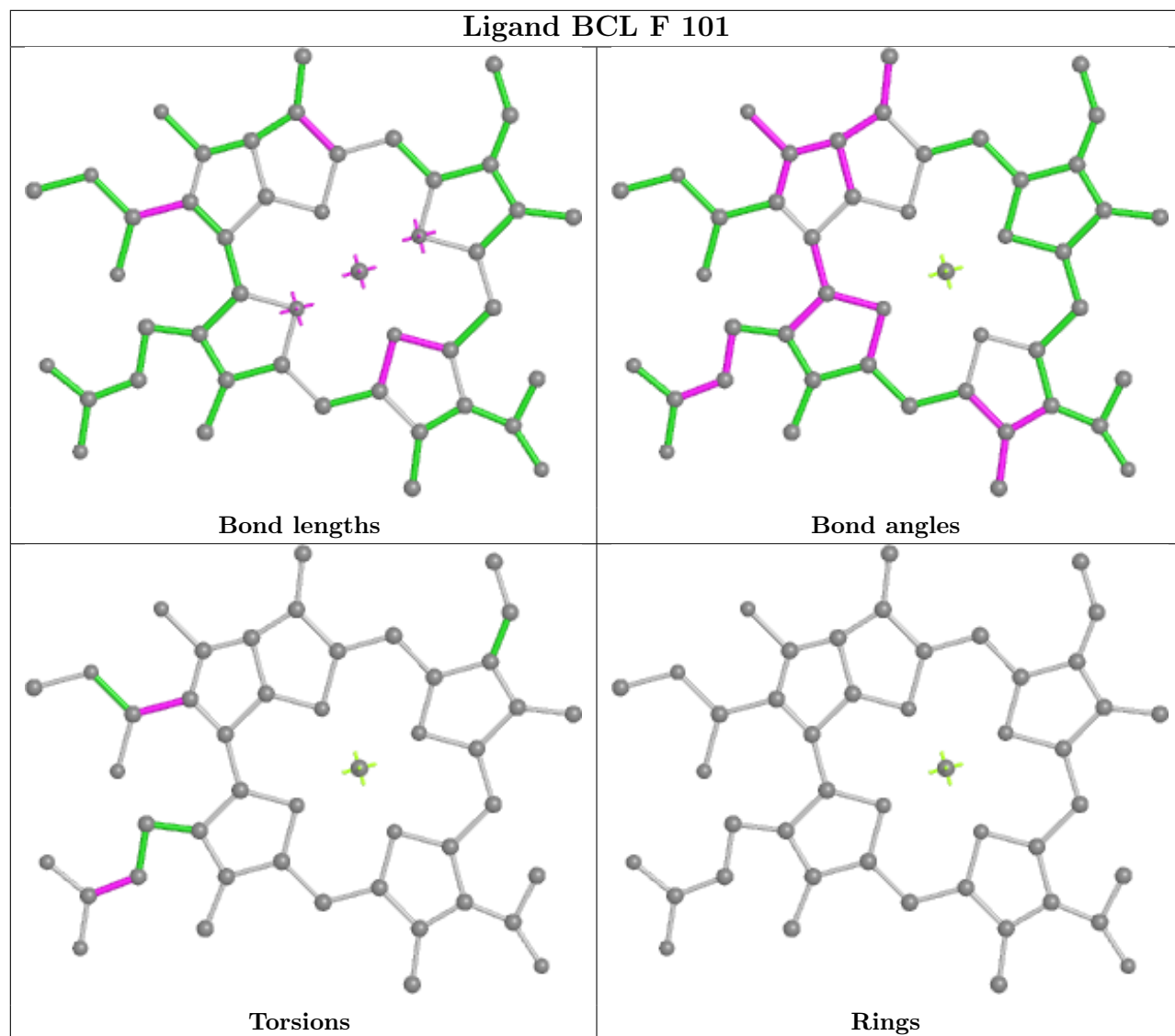


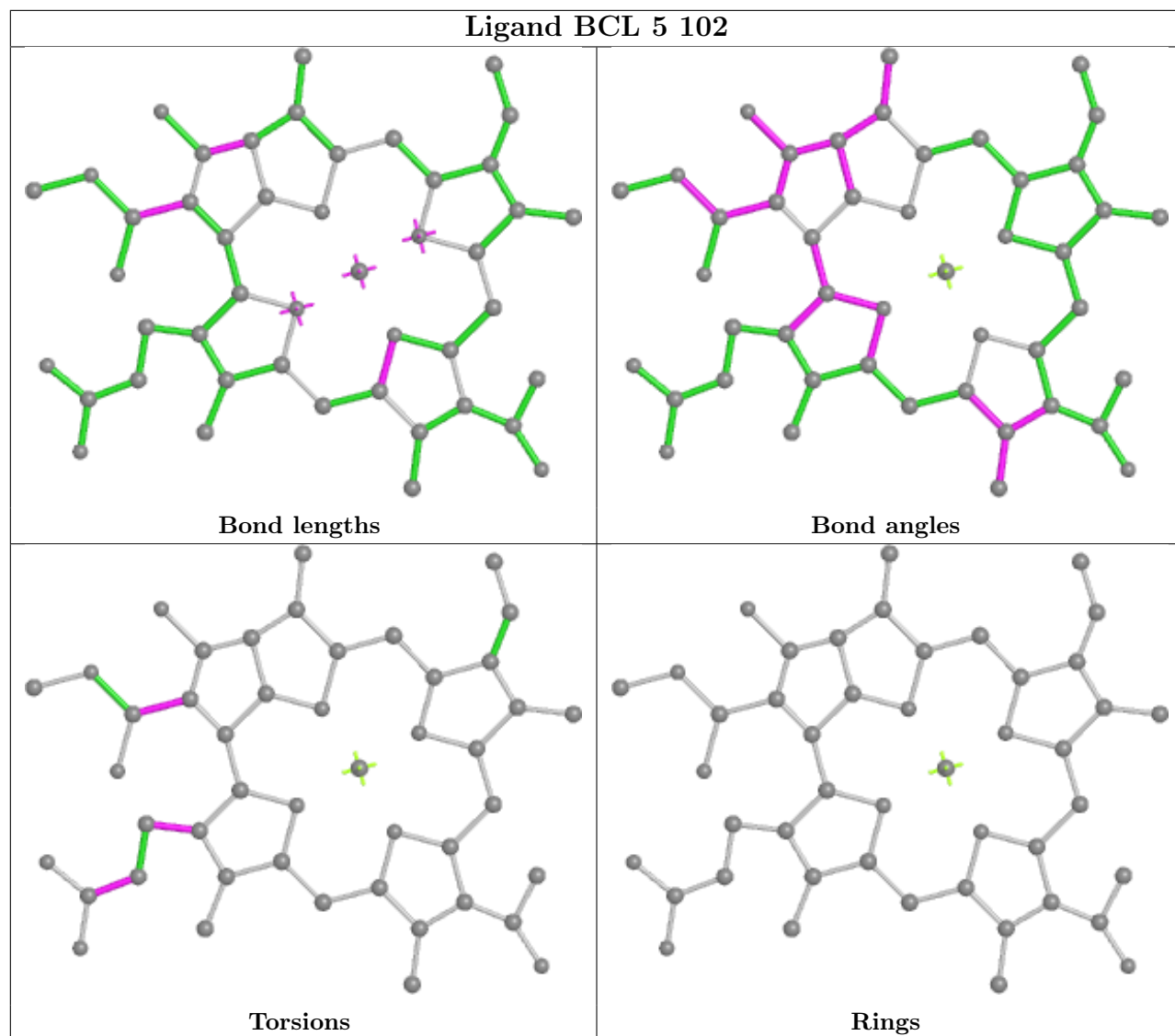


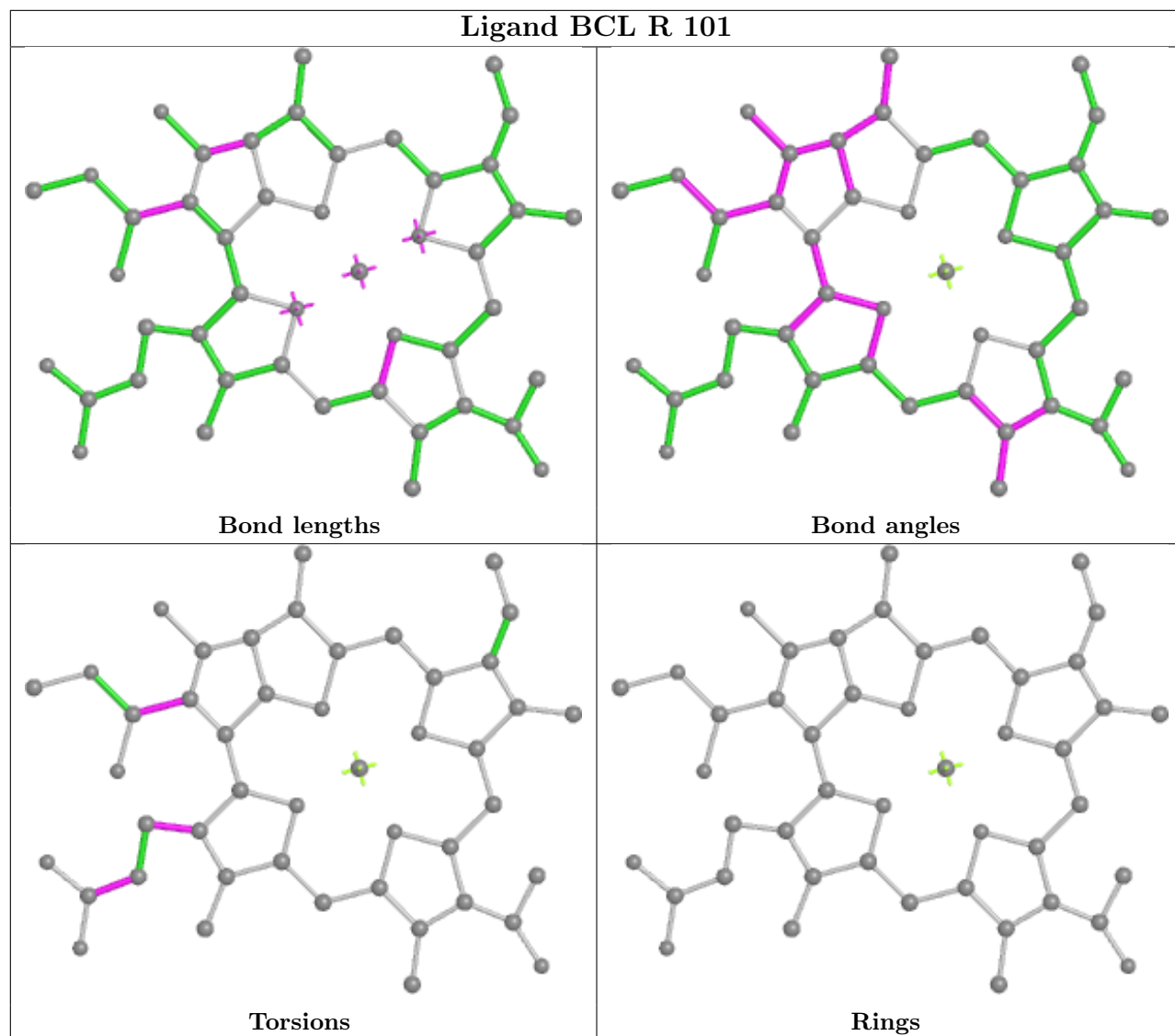


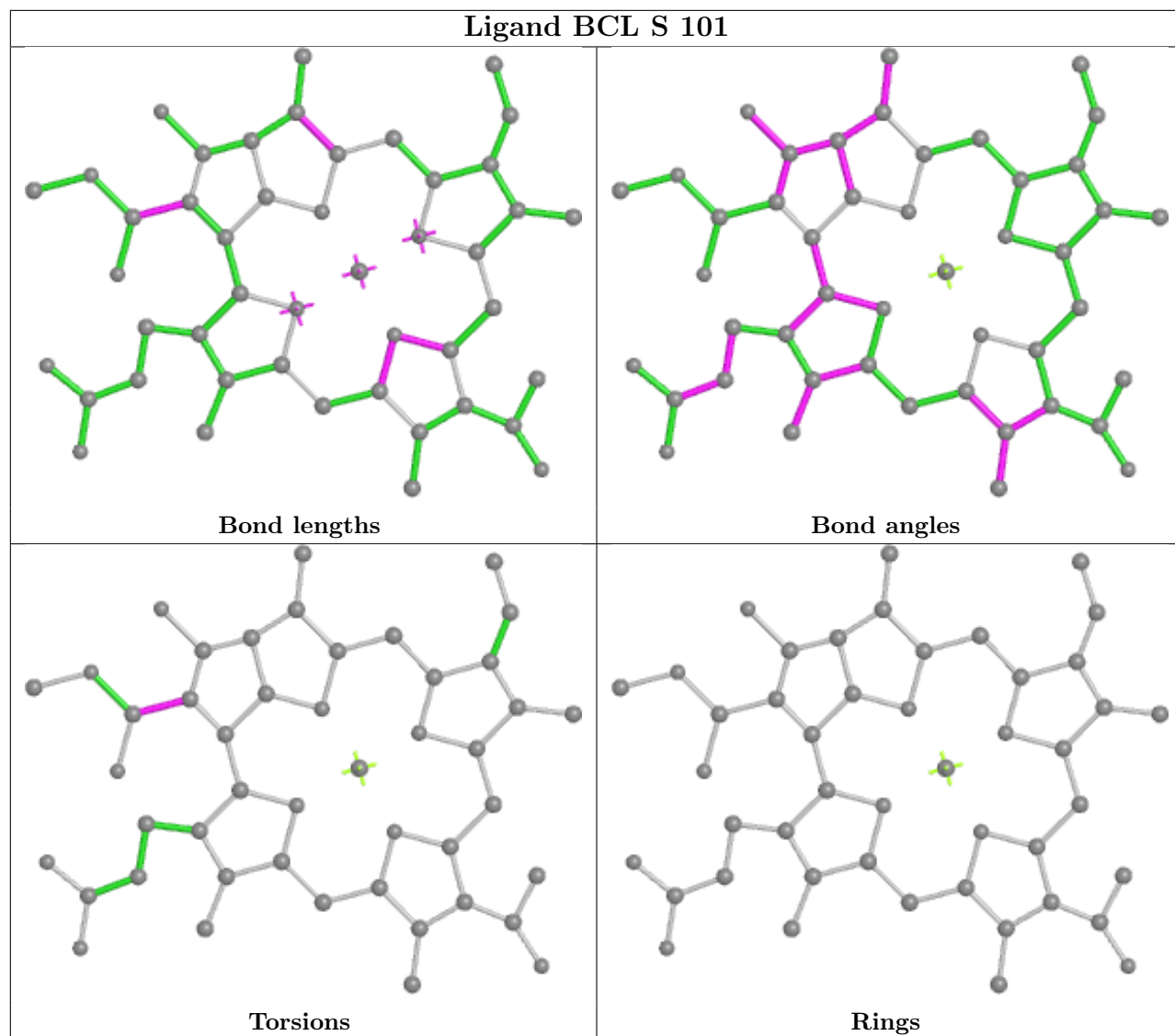


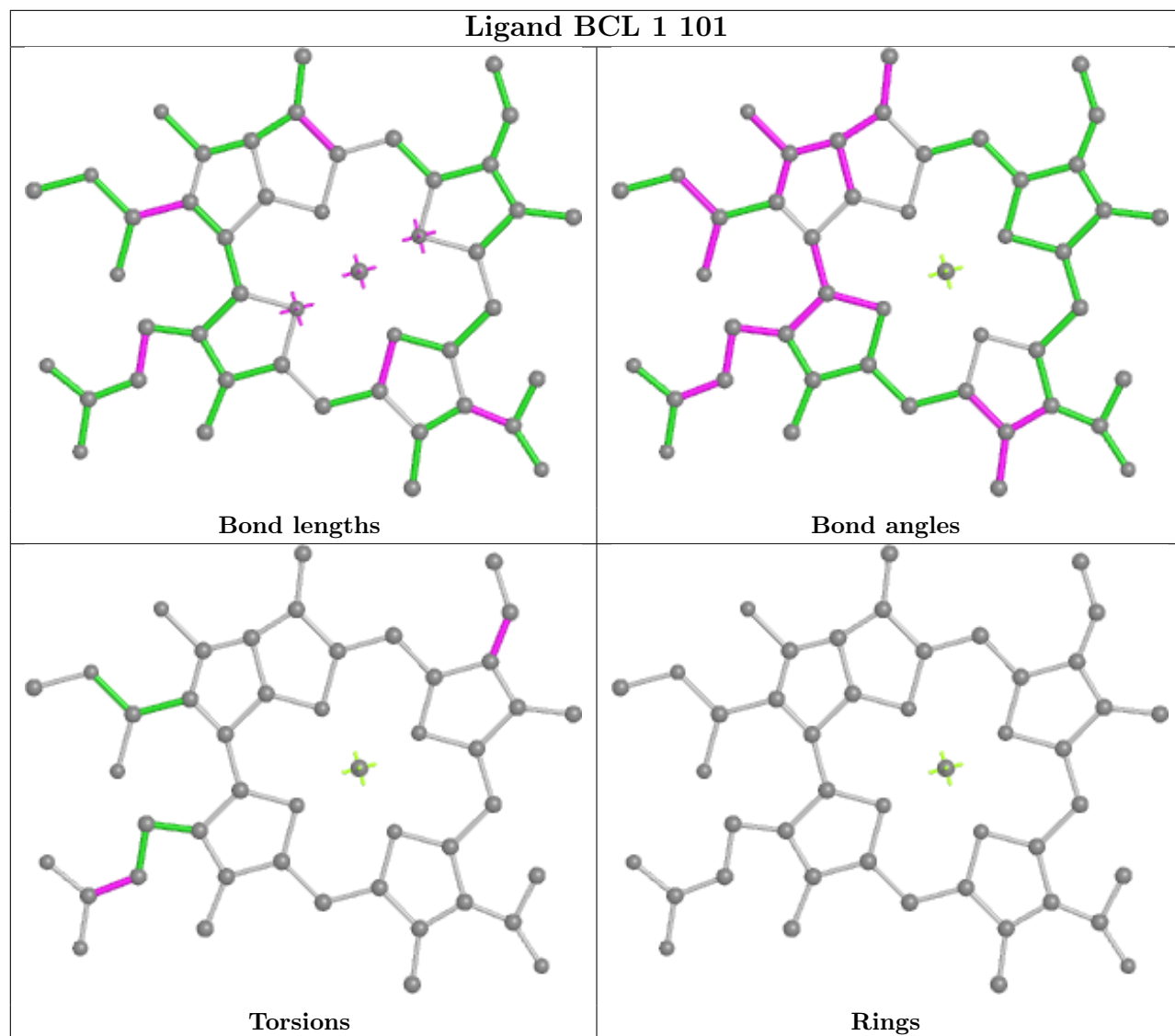


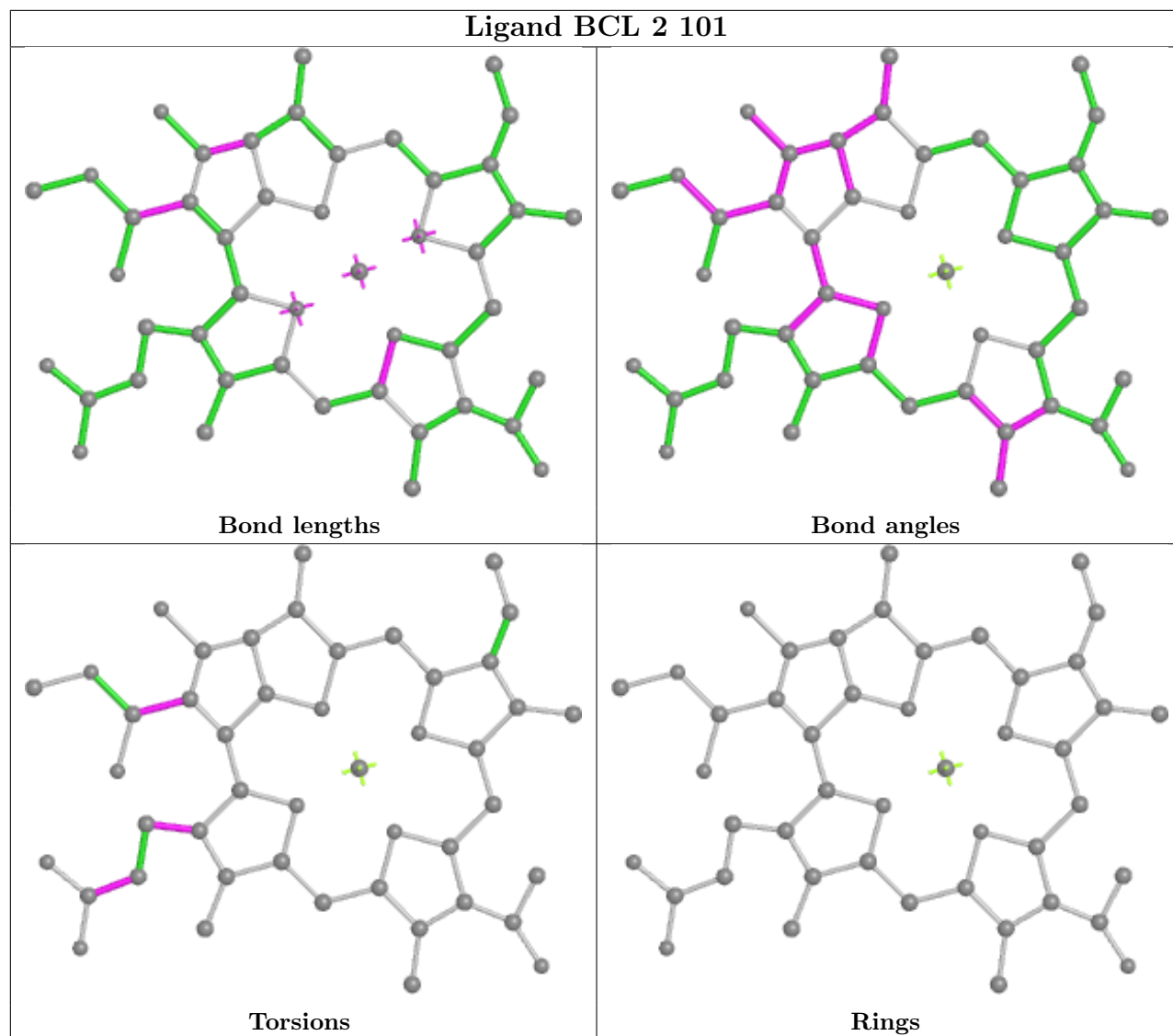


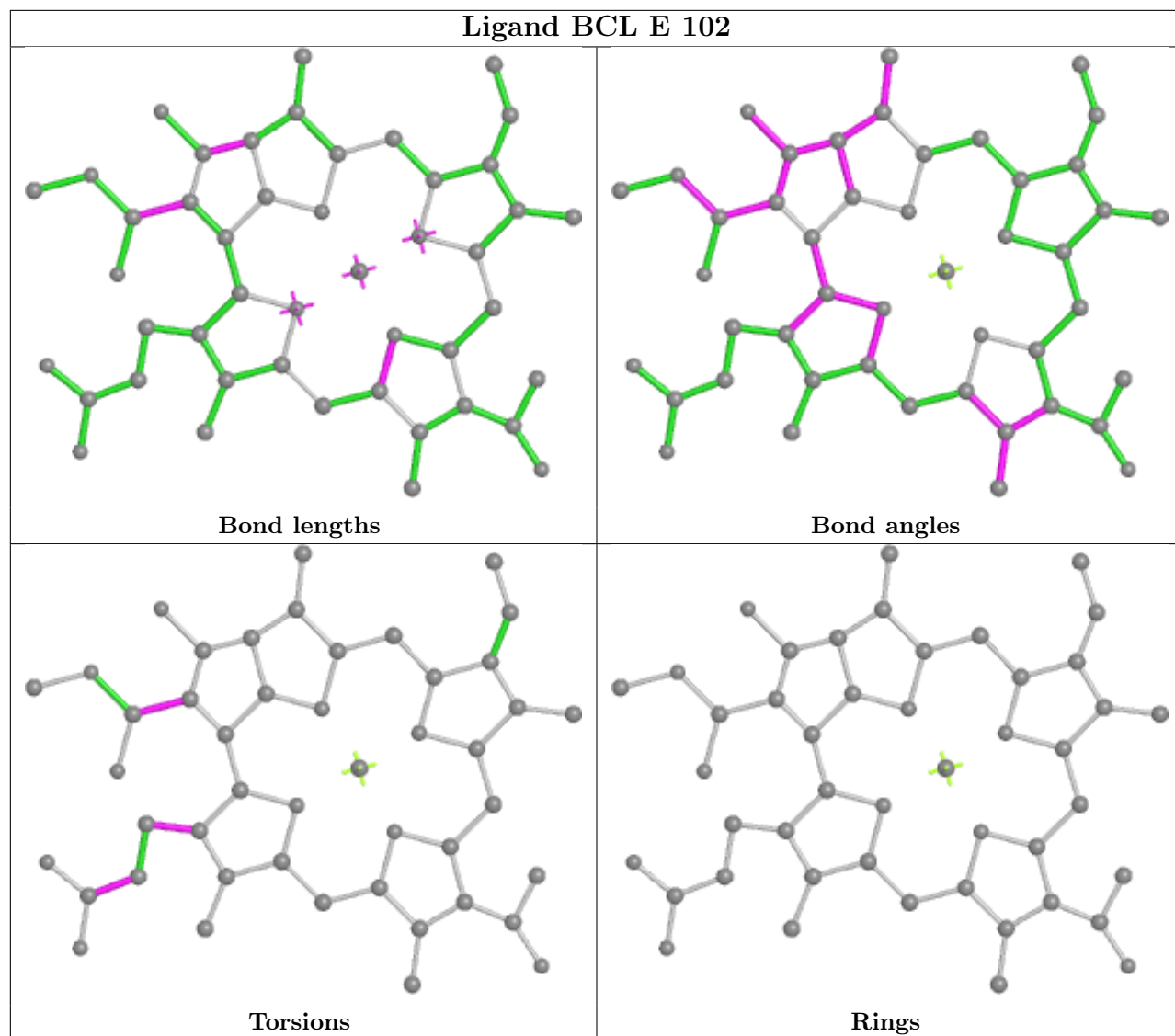


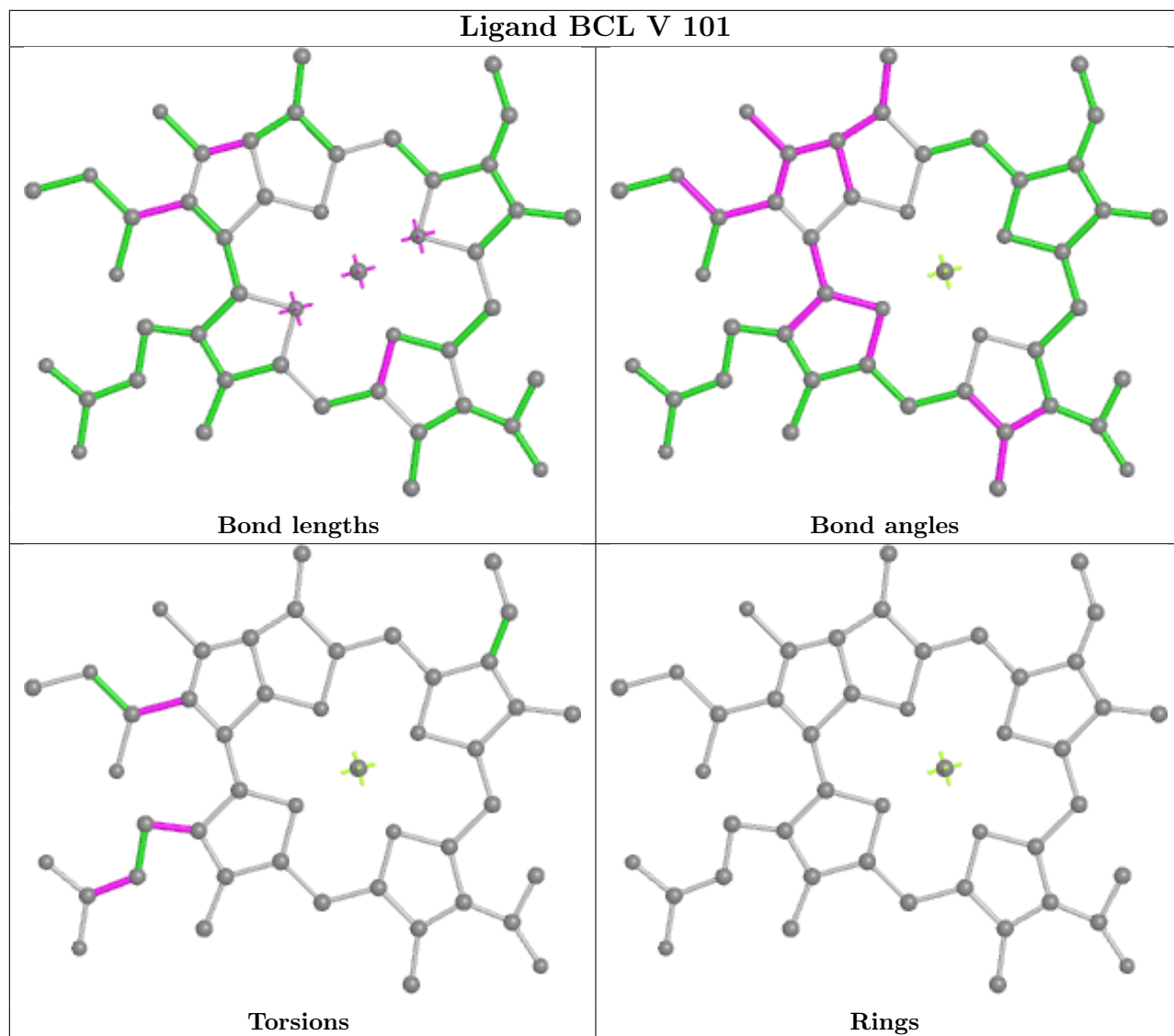


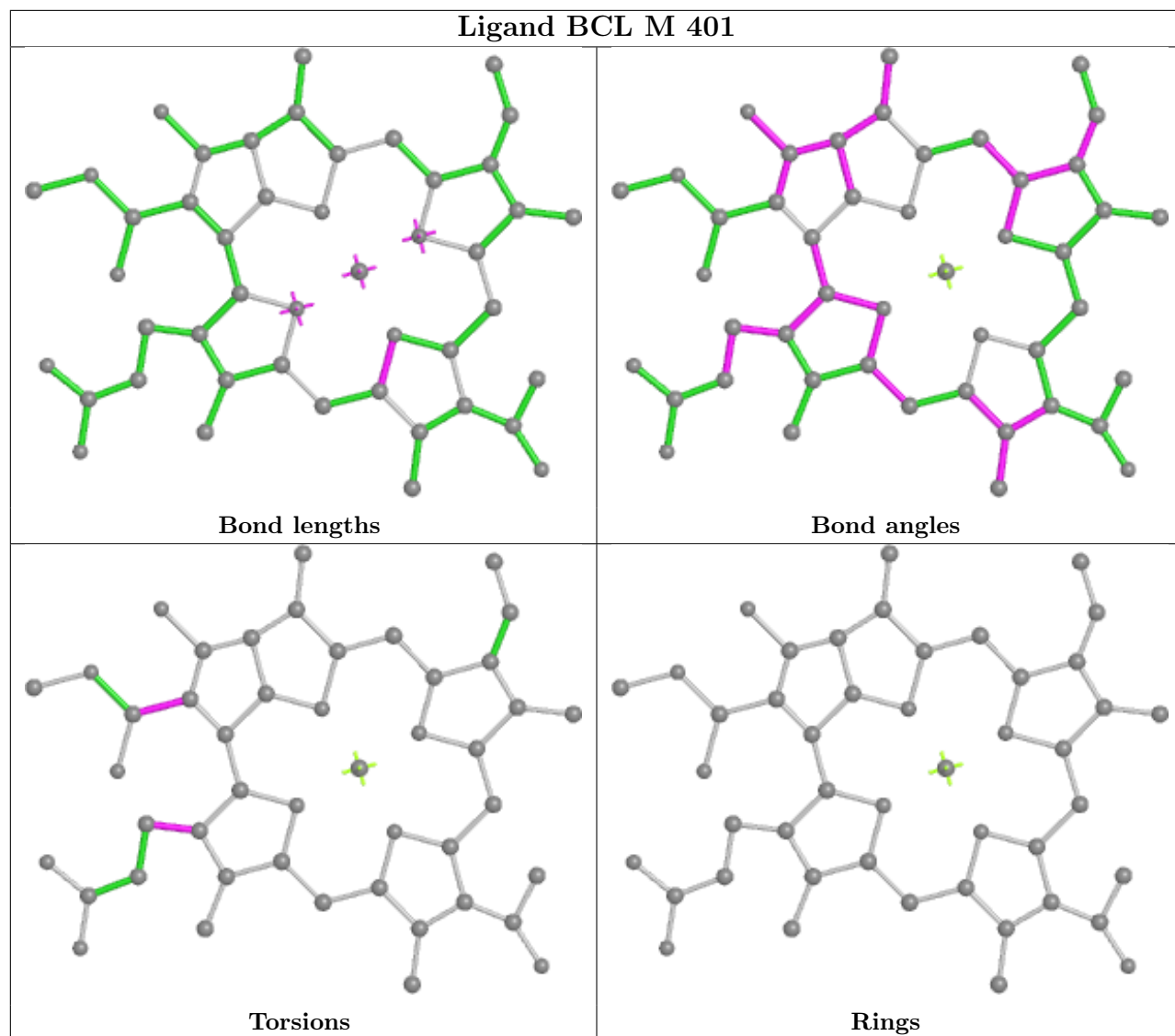


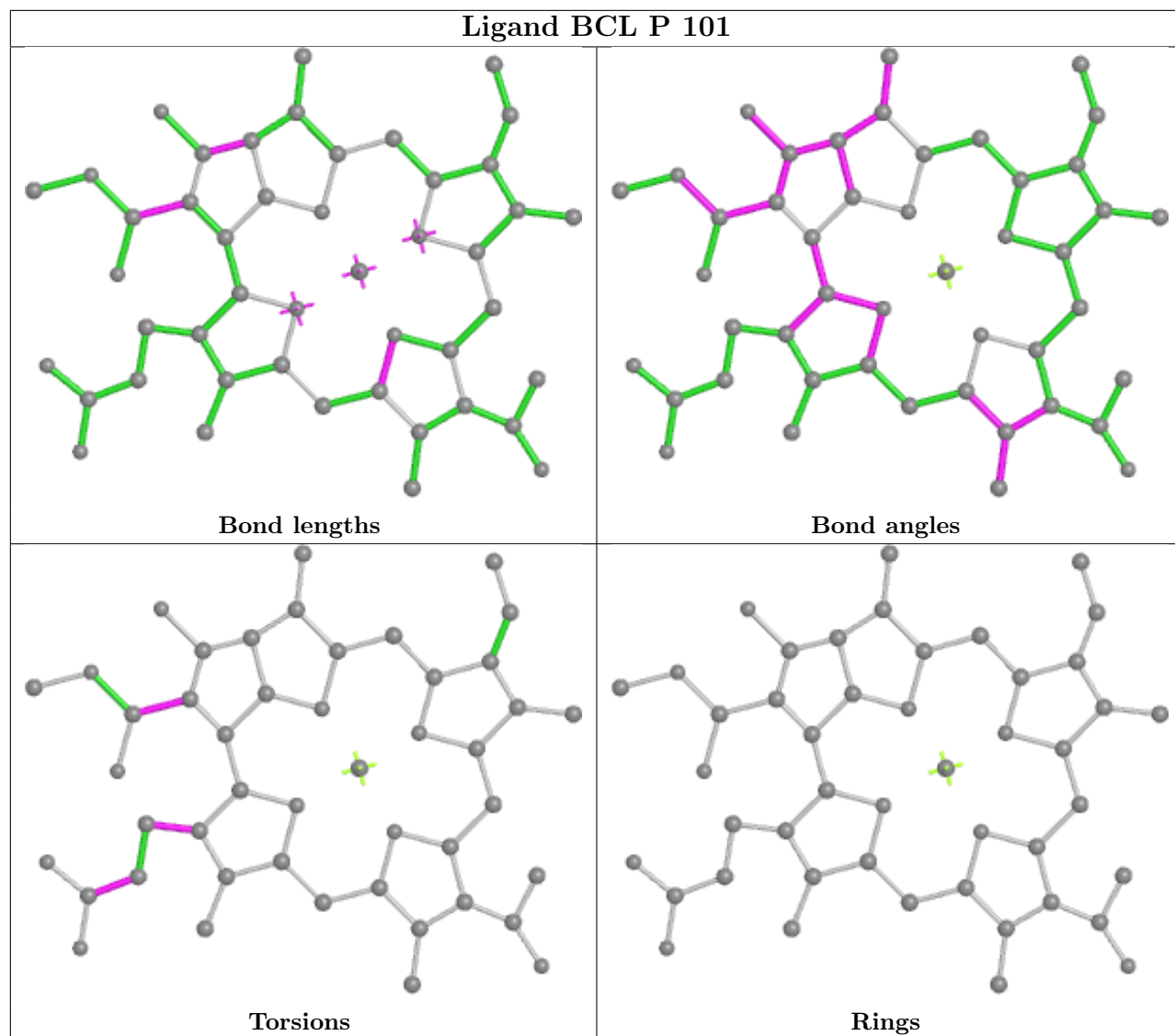


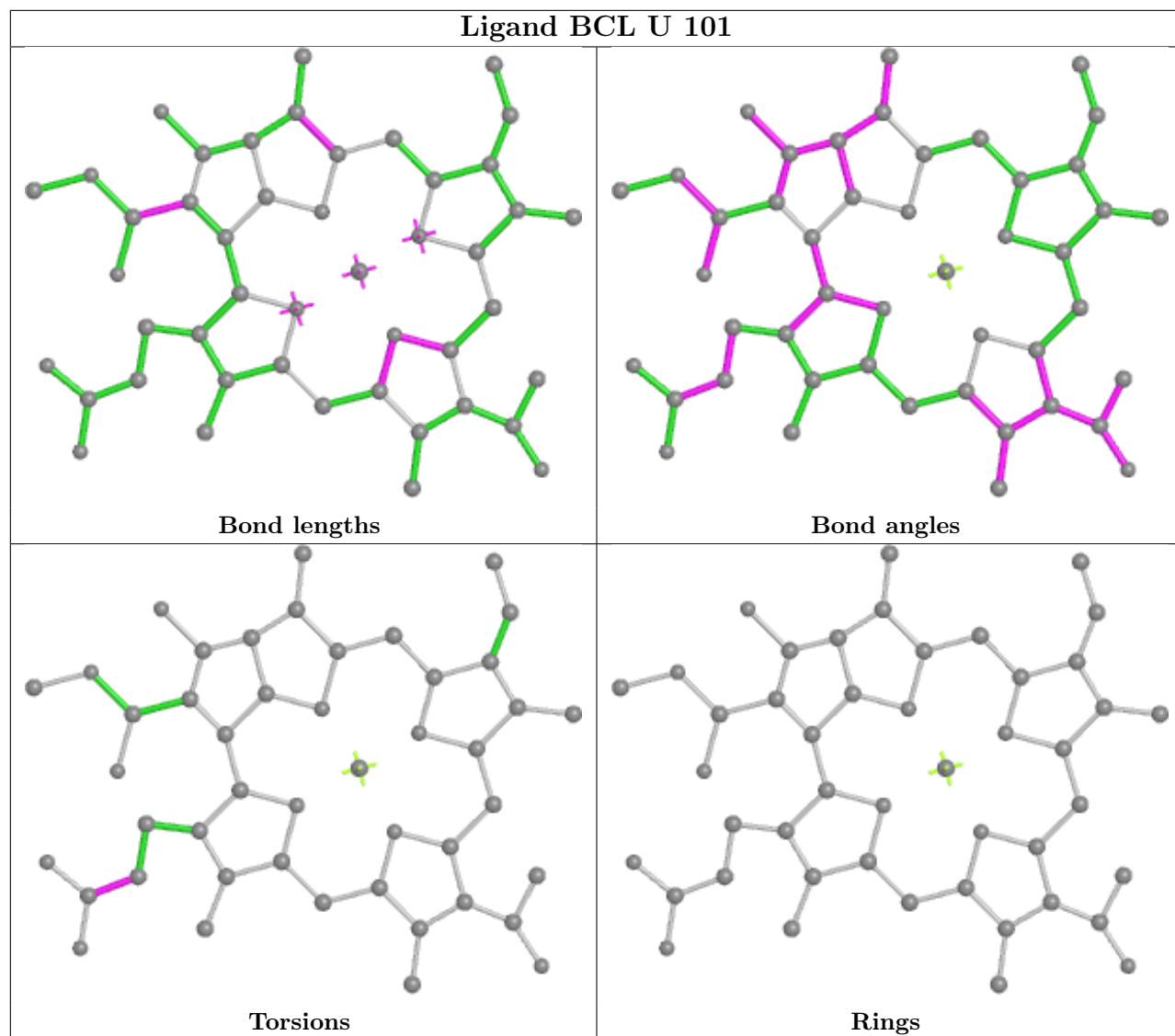


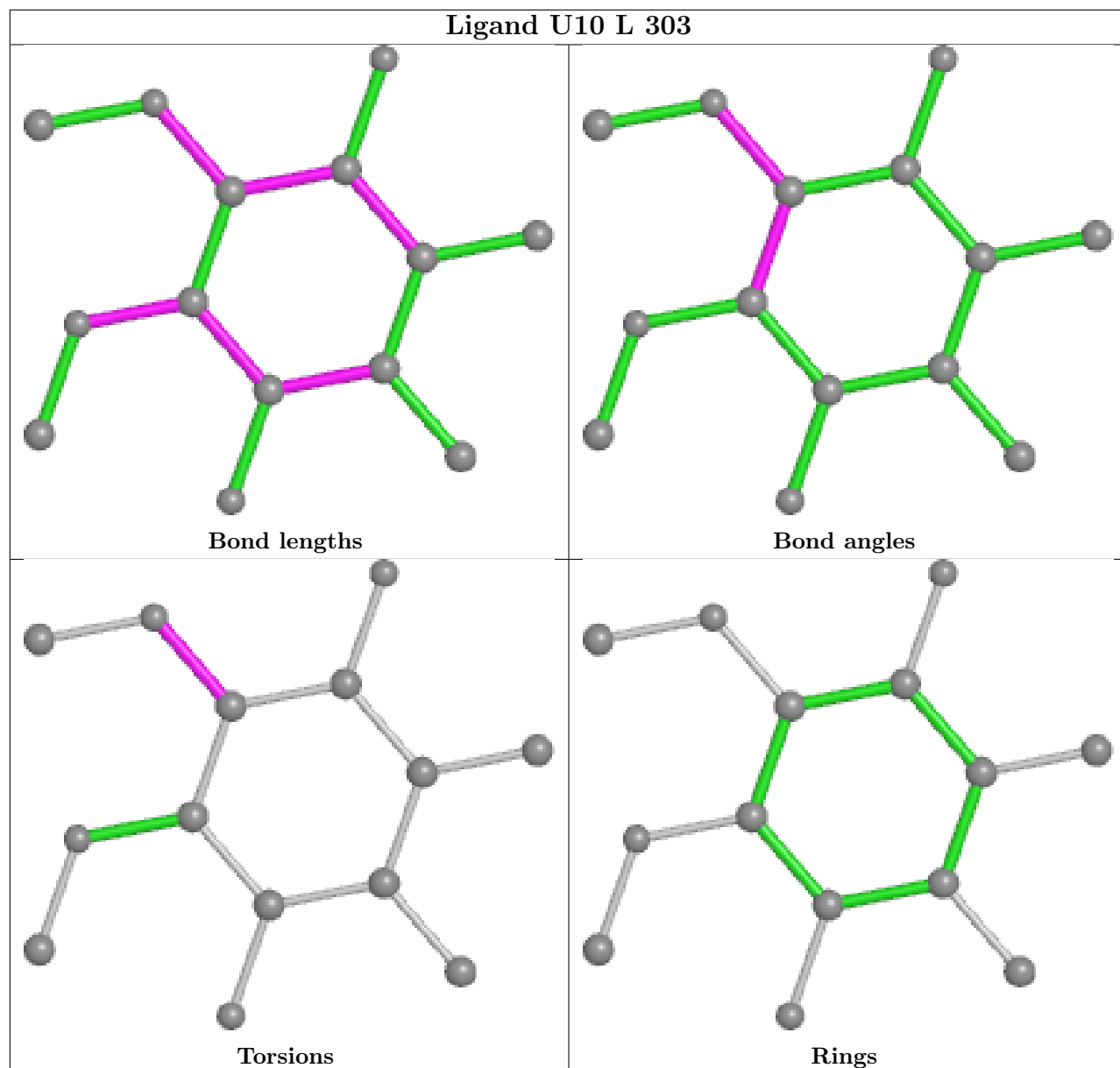


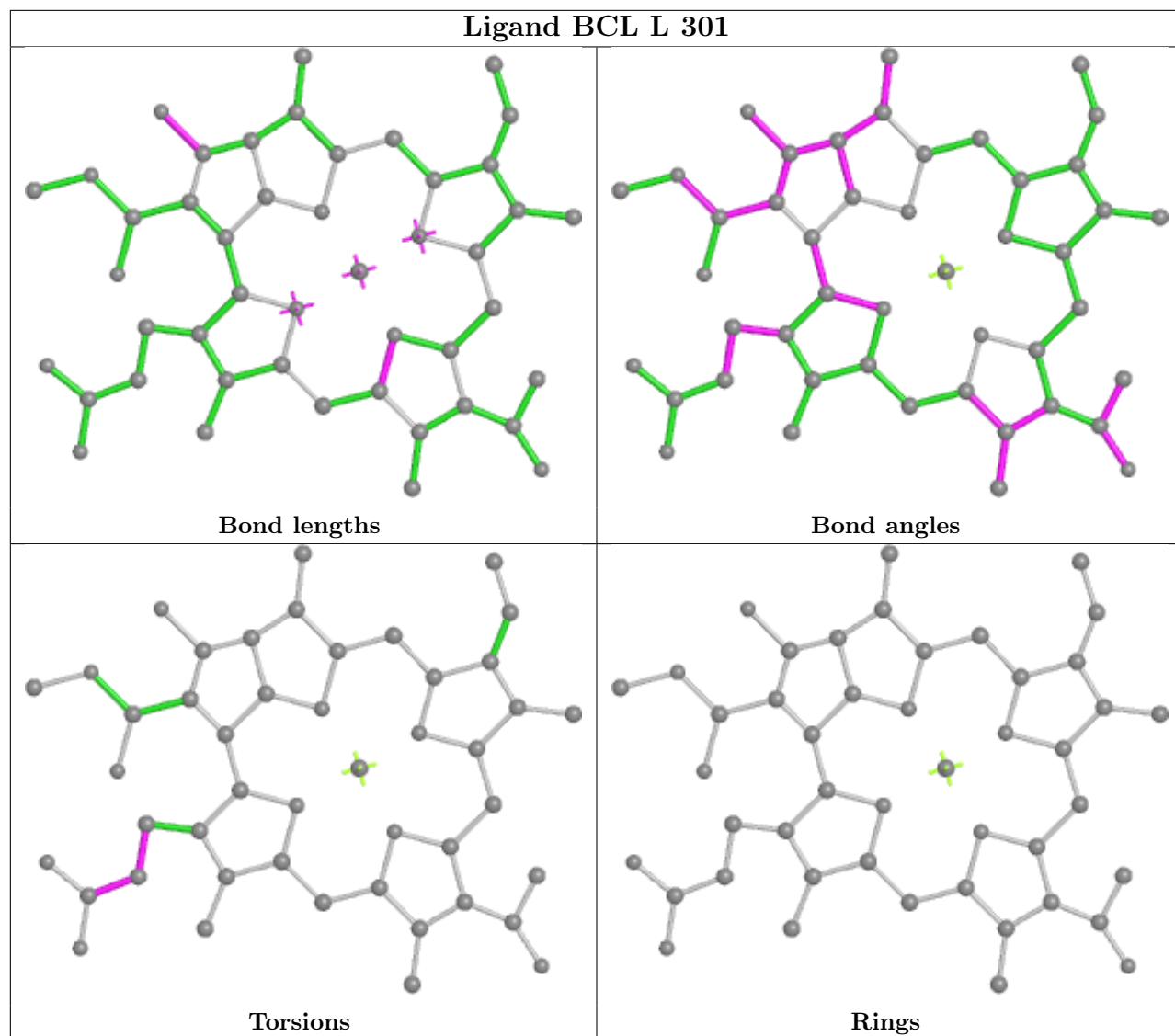


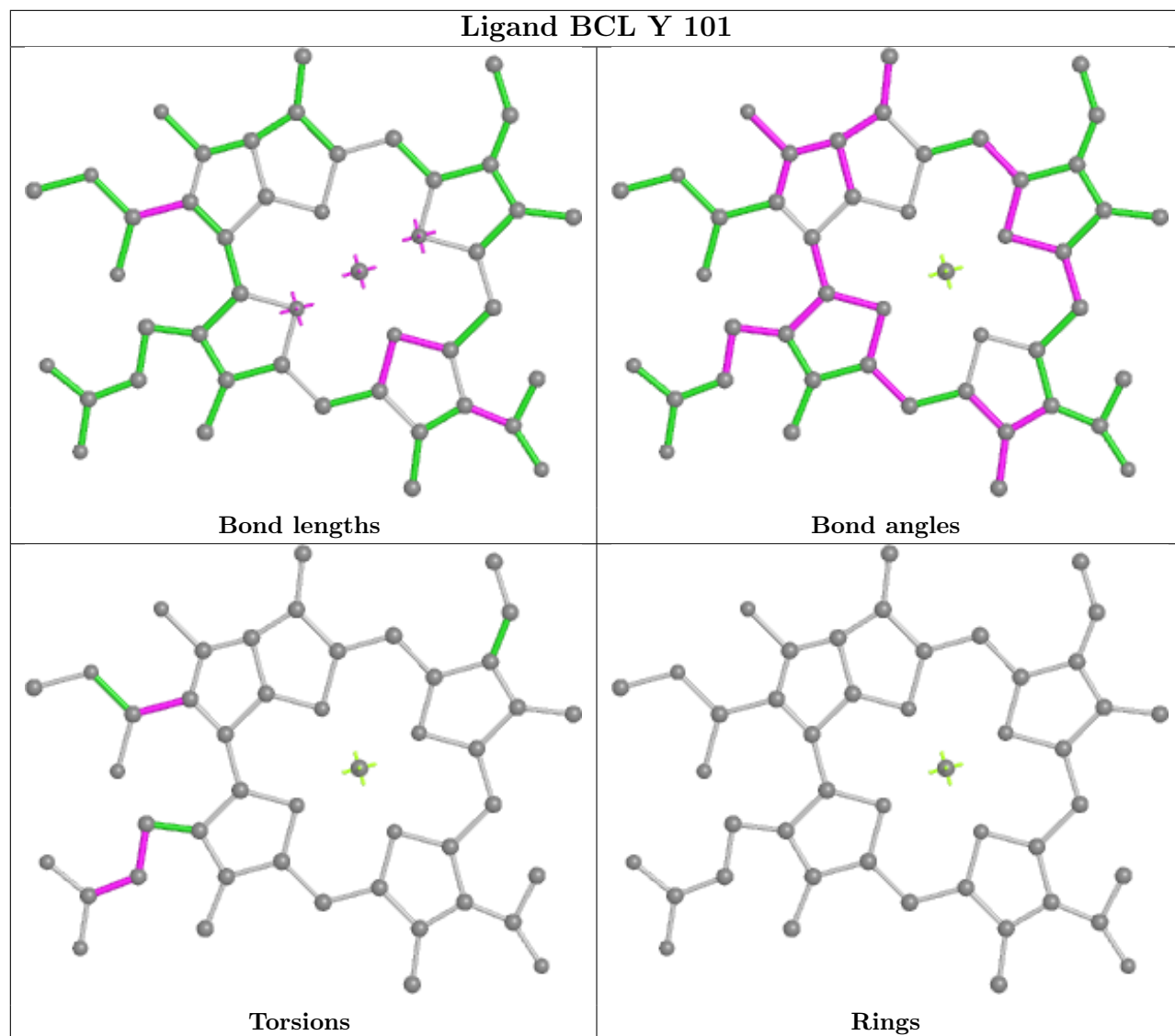


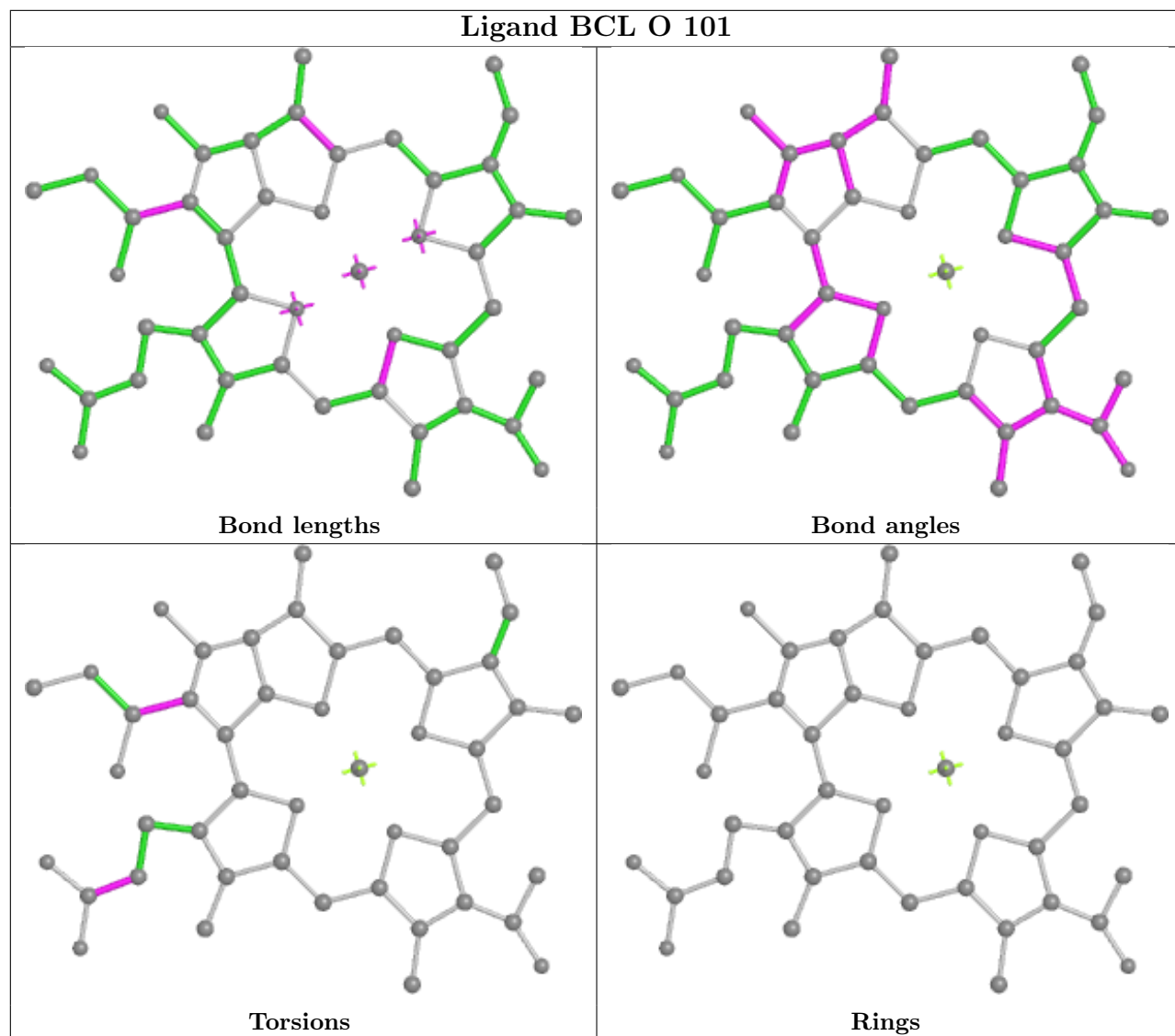


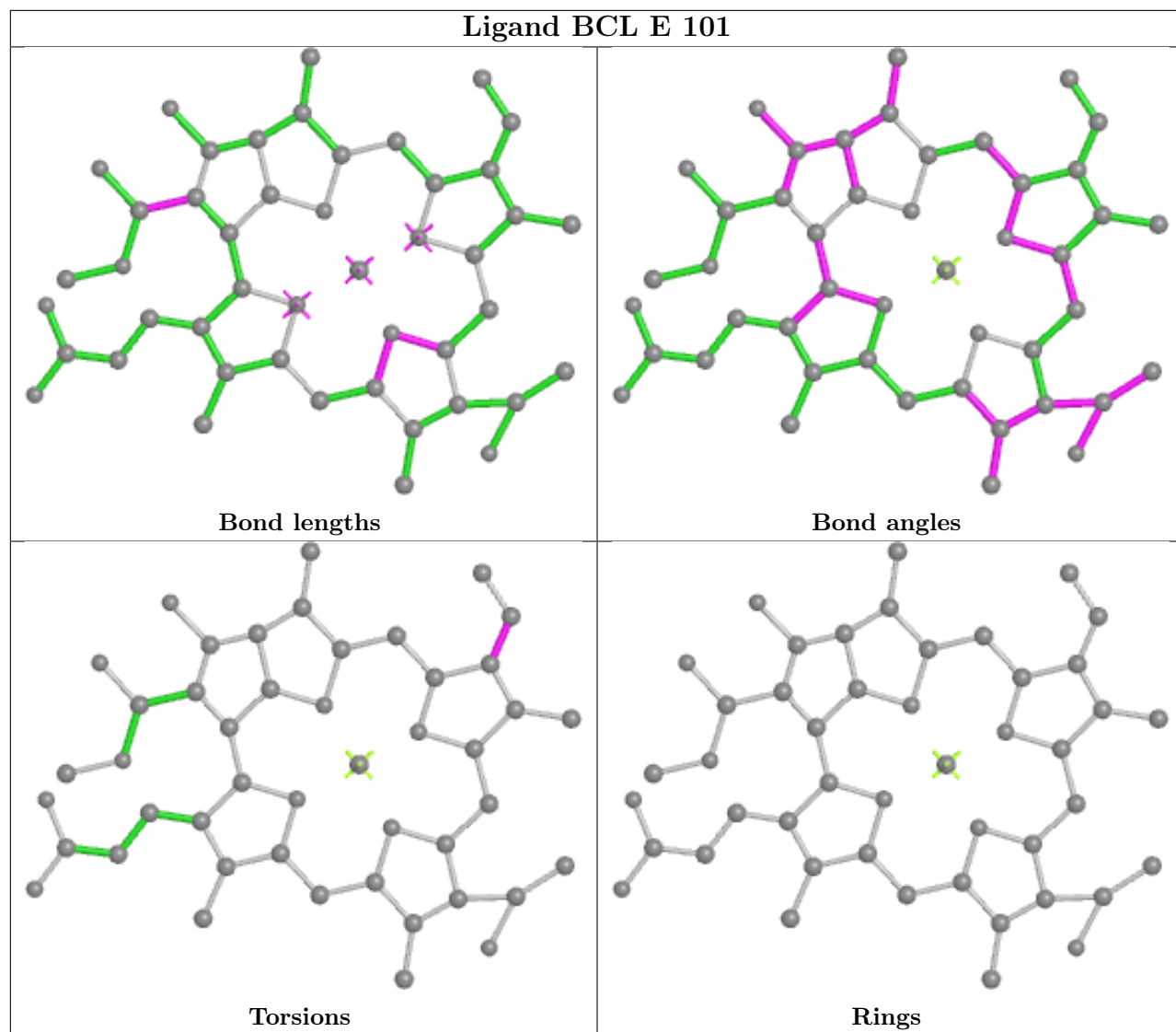


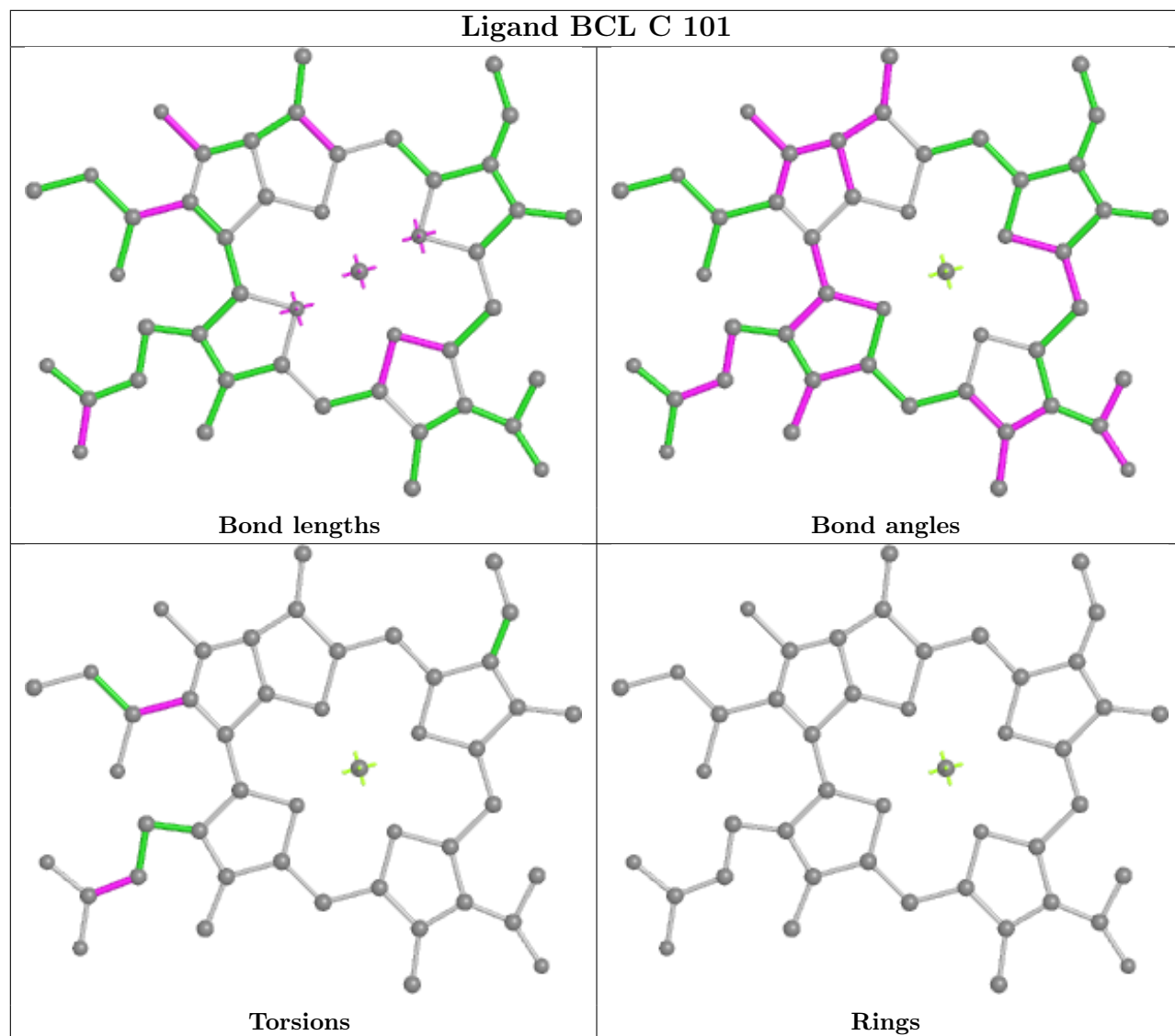


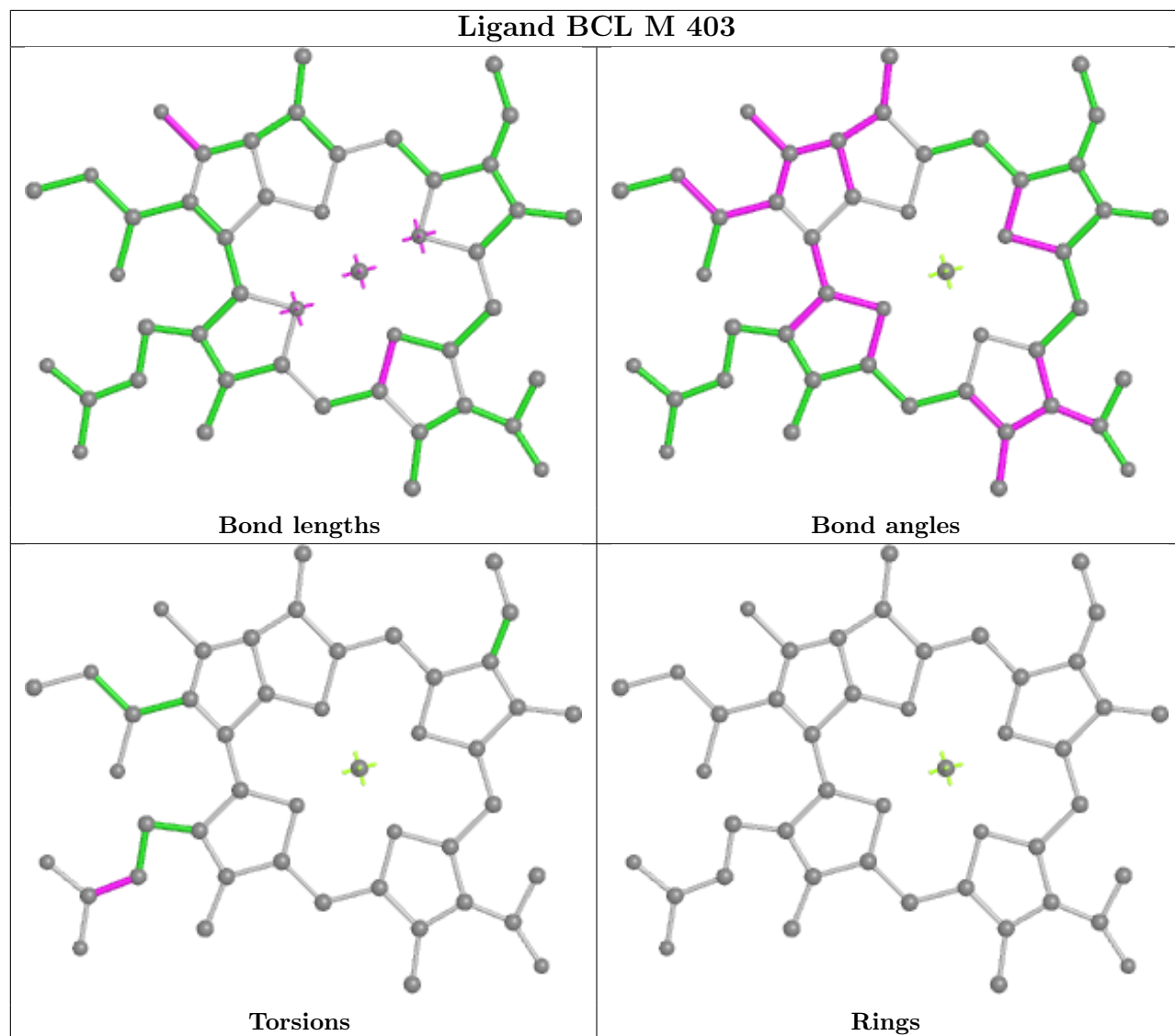


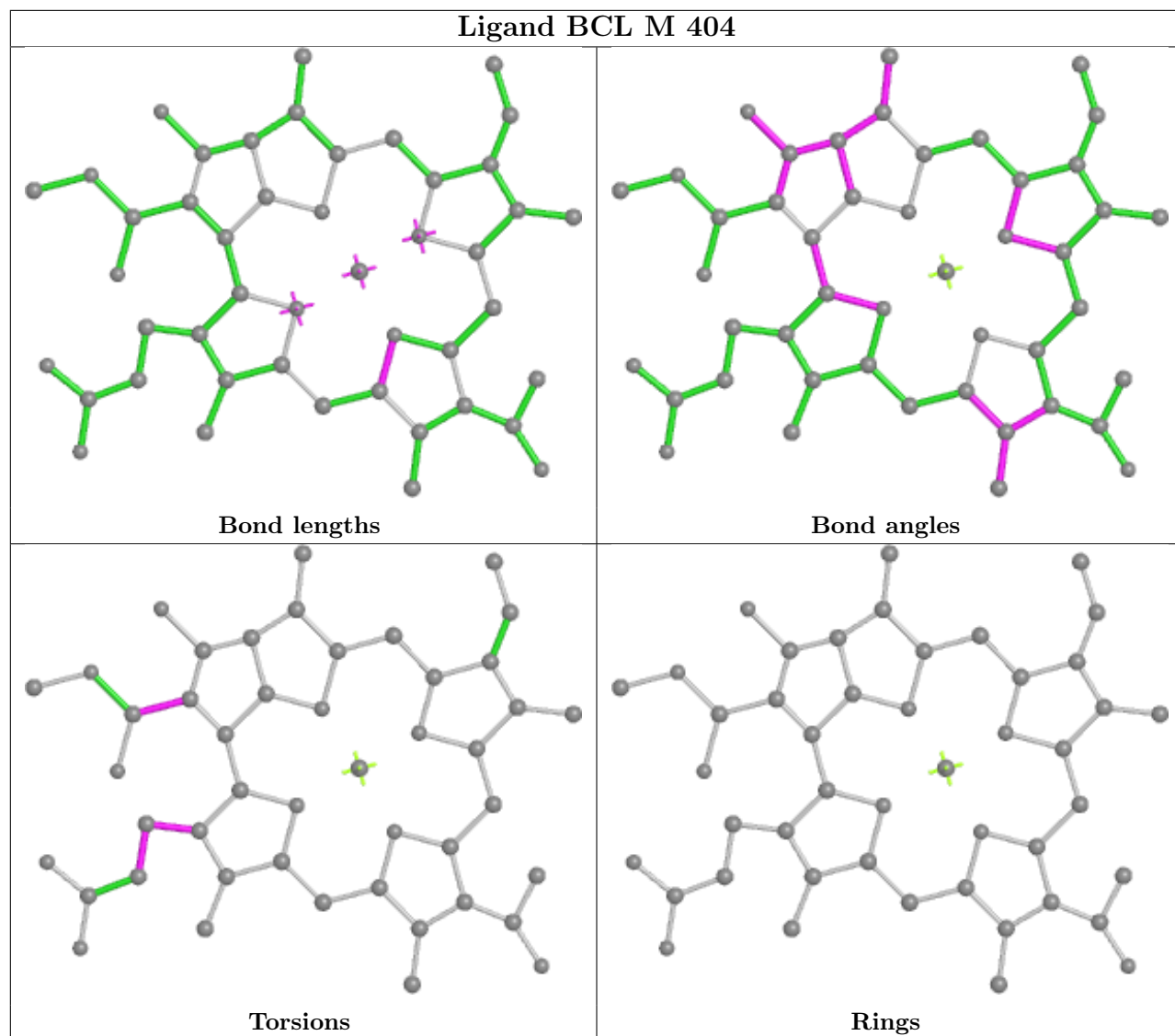


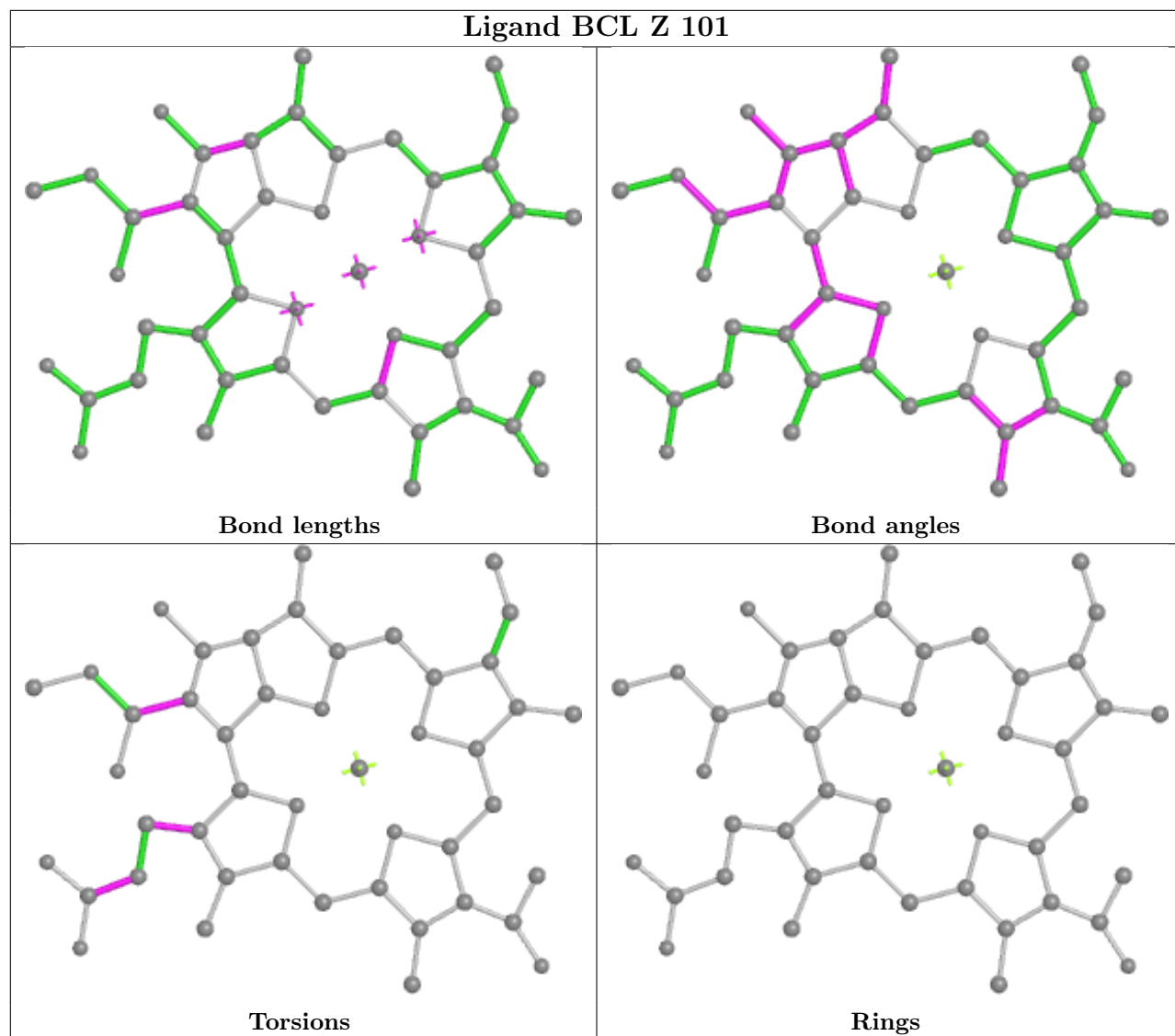


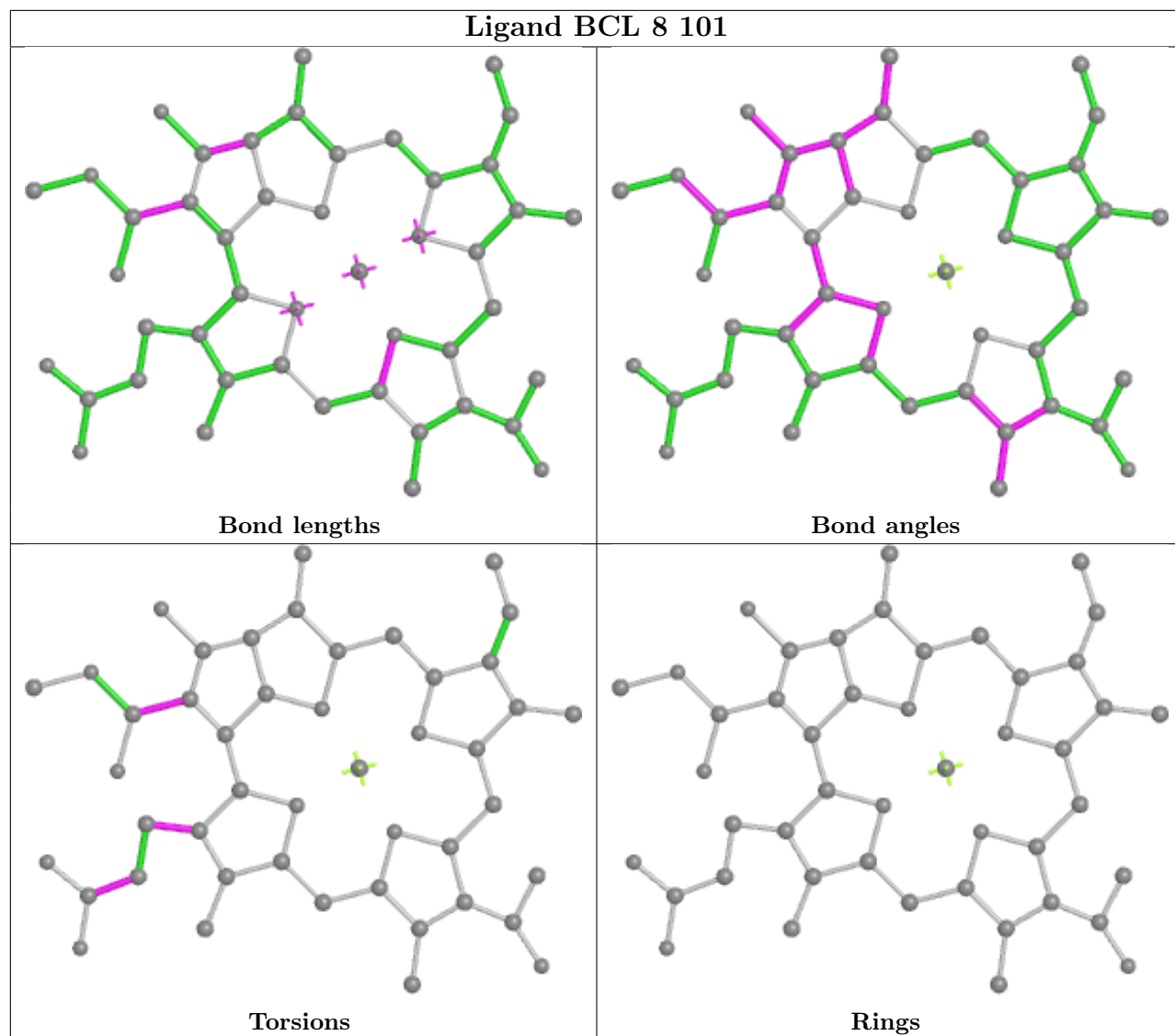


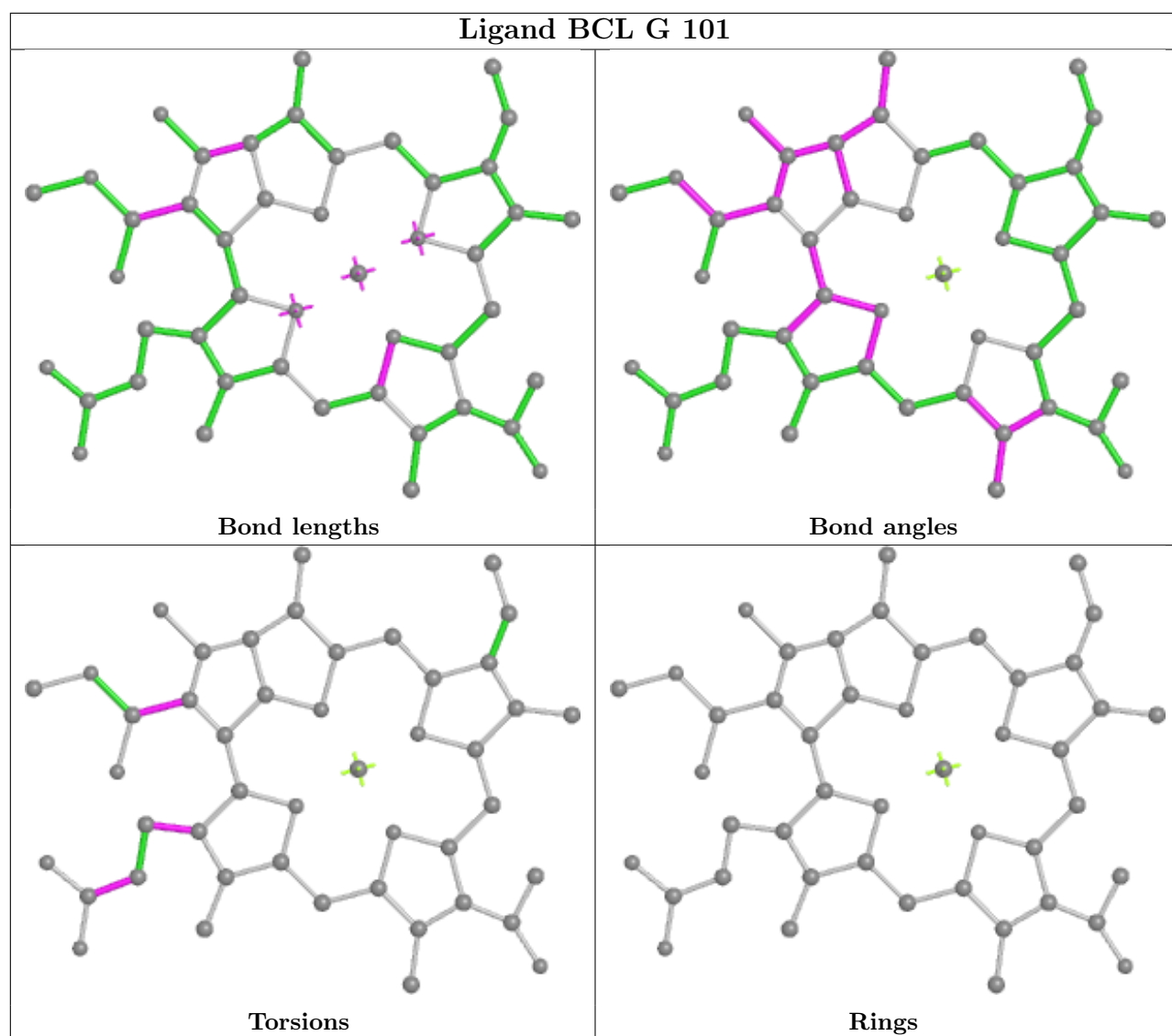












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

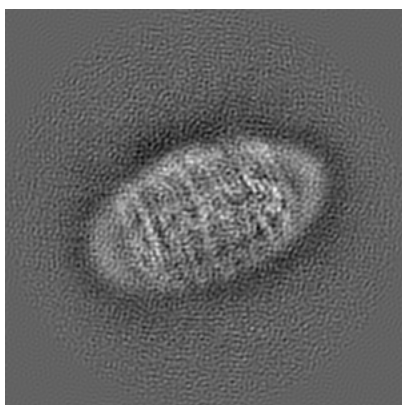
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32062. 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

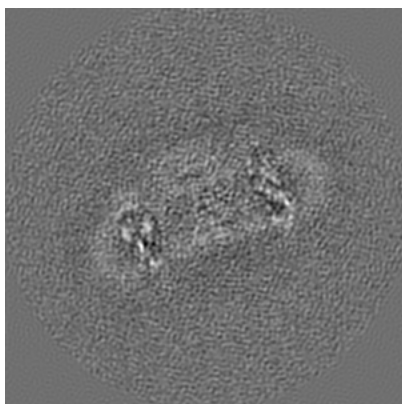


Z

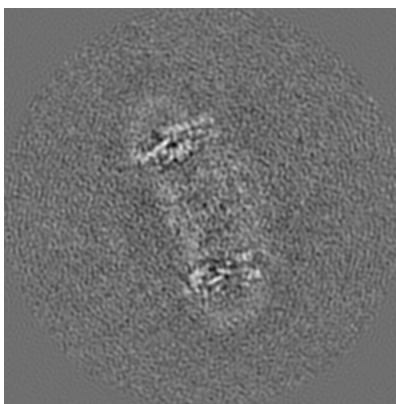
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

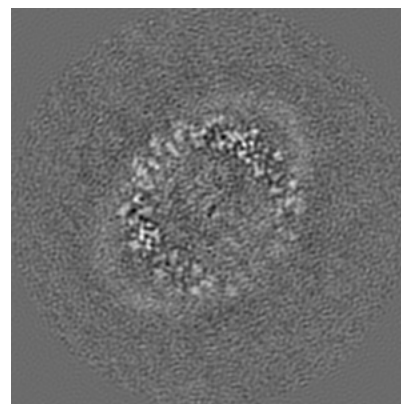
6.2.1 Primary map



X Index: 125



Y Index: 125

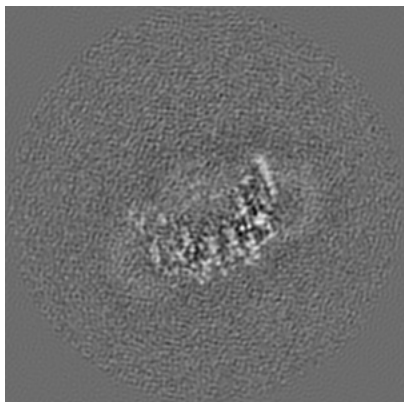


Z Index: 125

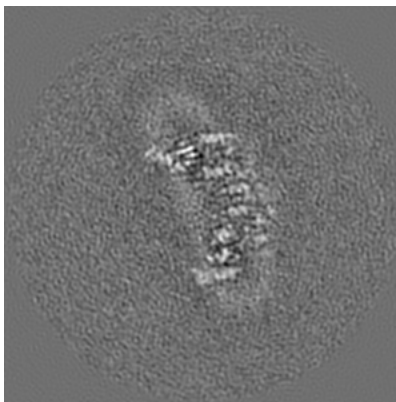
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

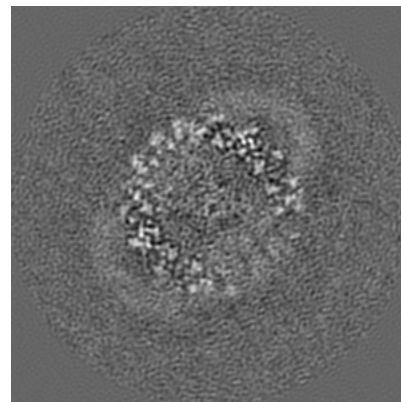
6.3.1 Primary map



X Index: 155



Y Index: 155



Z Index: 124

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0254. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

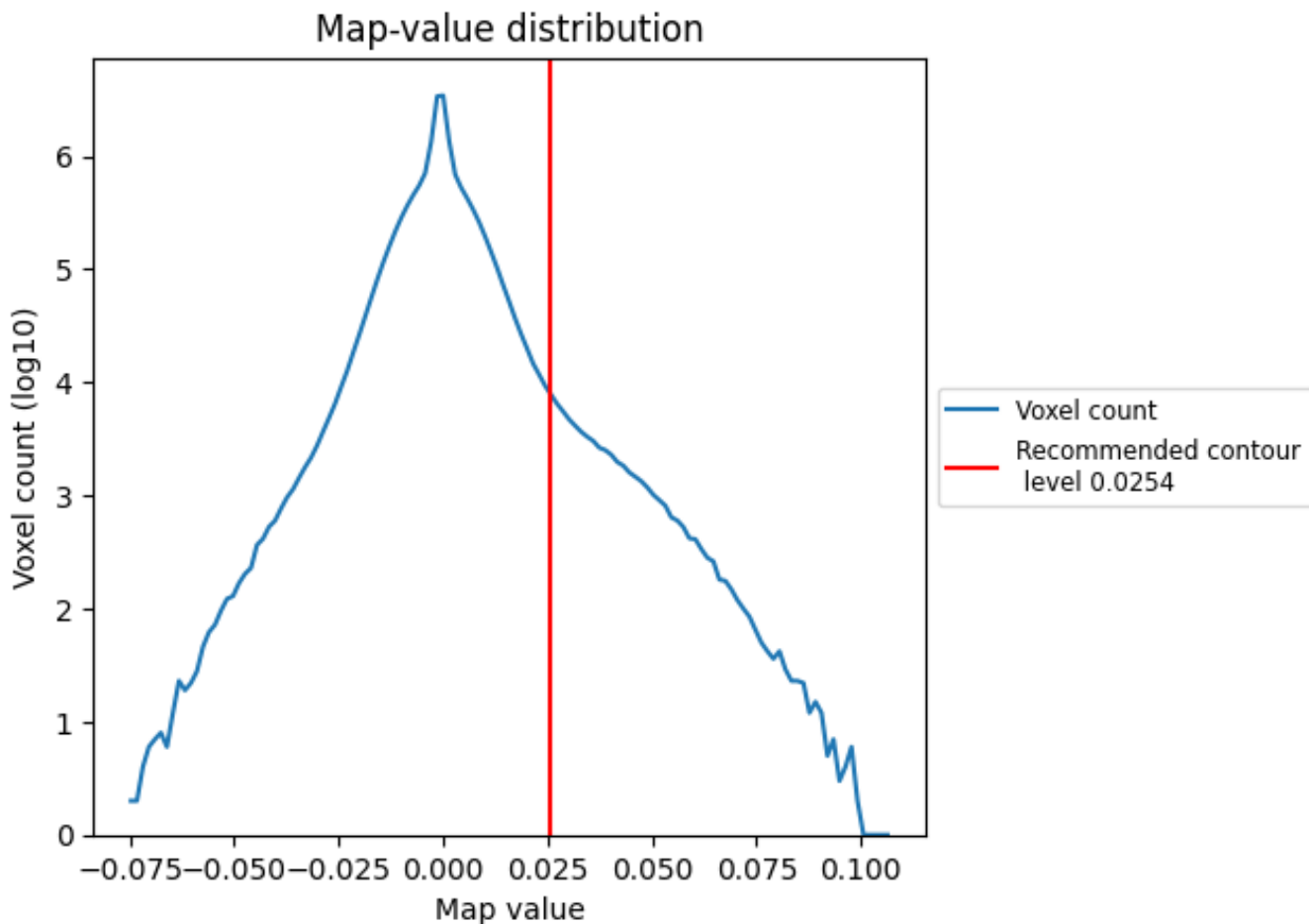
6.5 Mask visualisation

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

7 Map analysis [i](#)

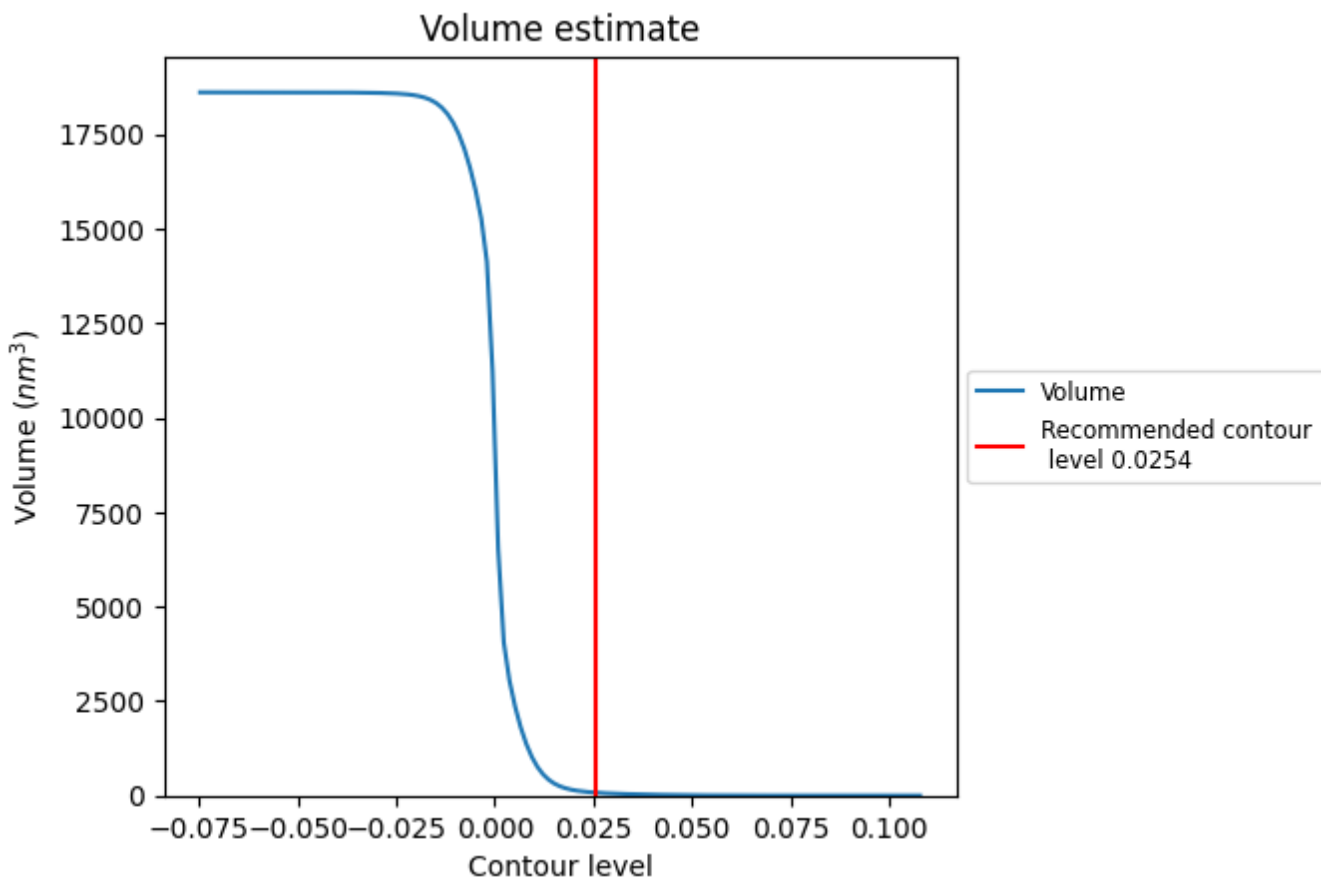
This section contains the results of statistical analysis of the map.

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.

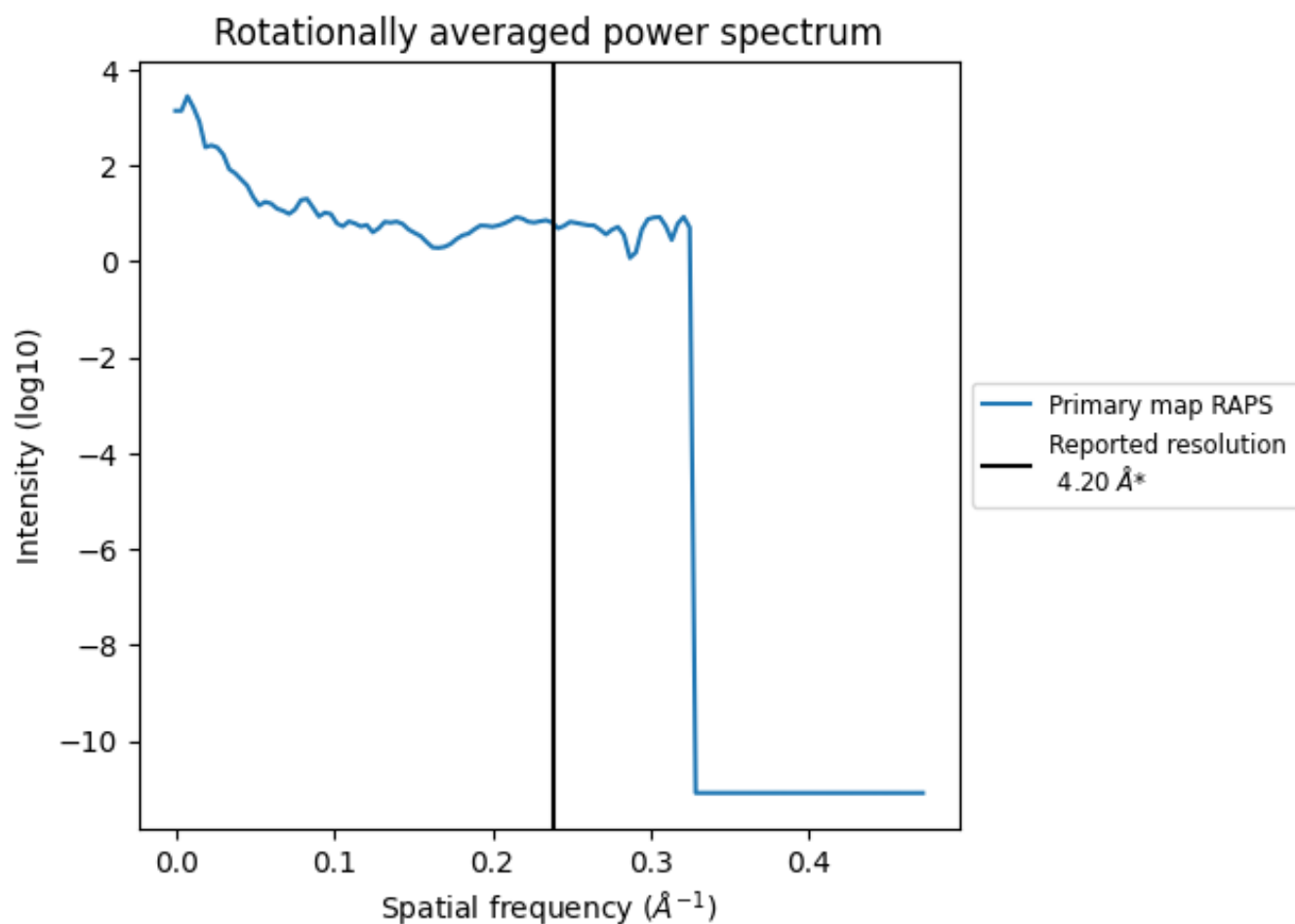
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 79 nm^3 ; this corresponds to an approximate mass of 71 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [\(i\)](#)

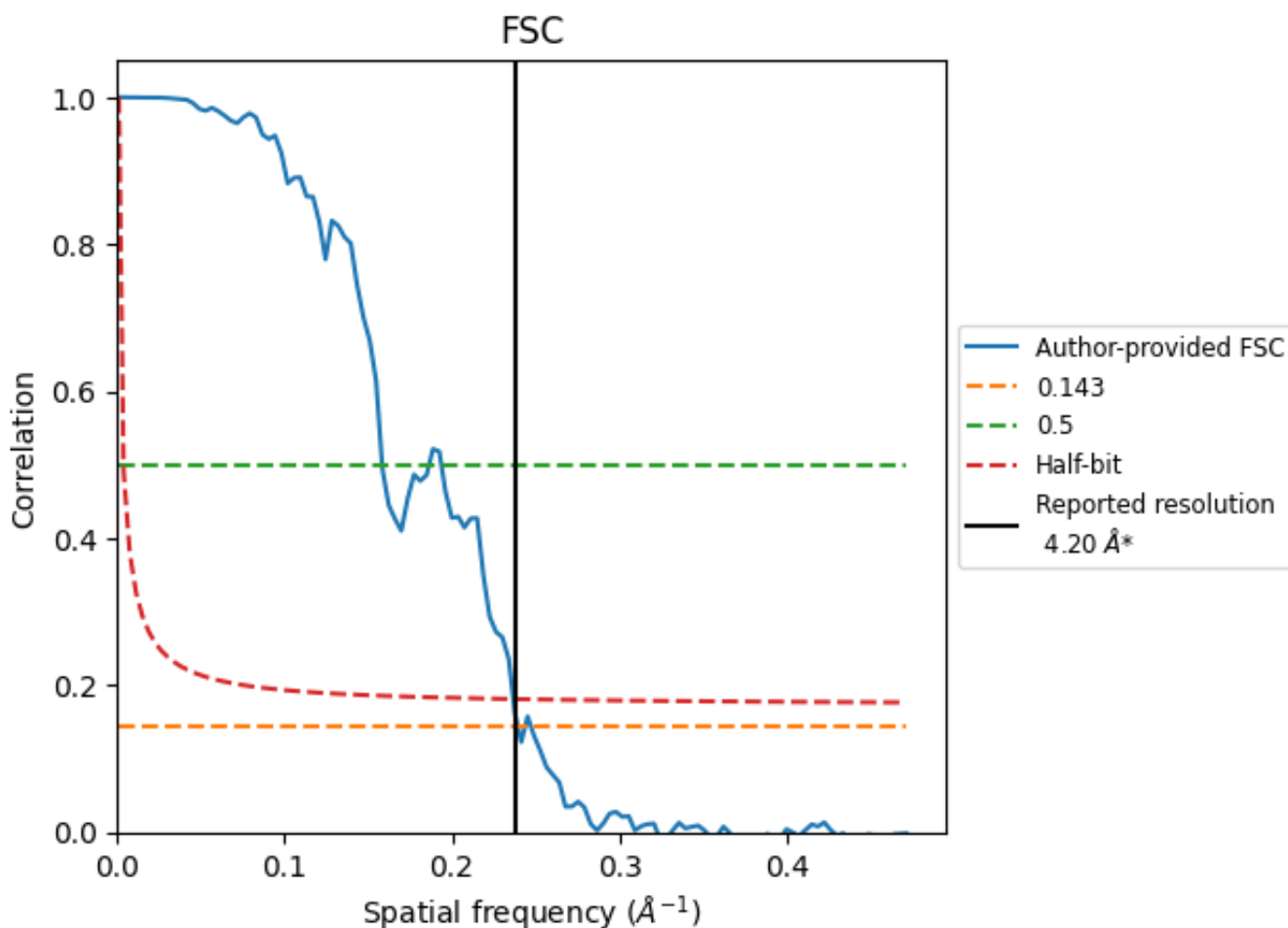


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

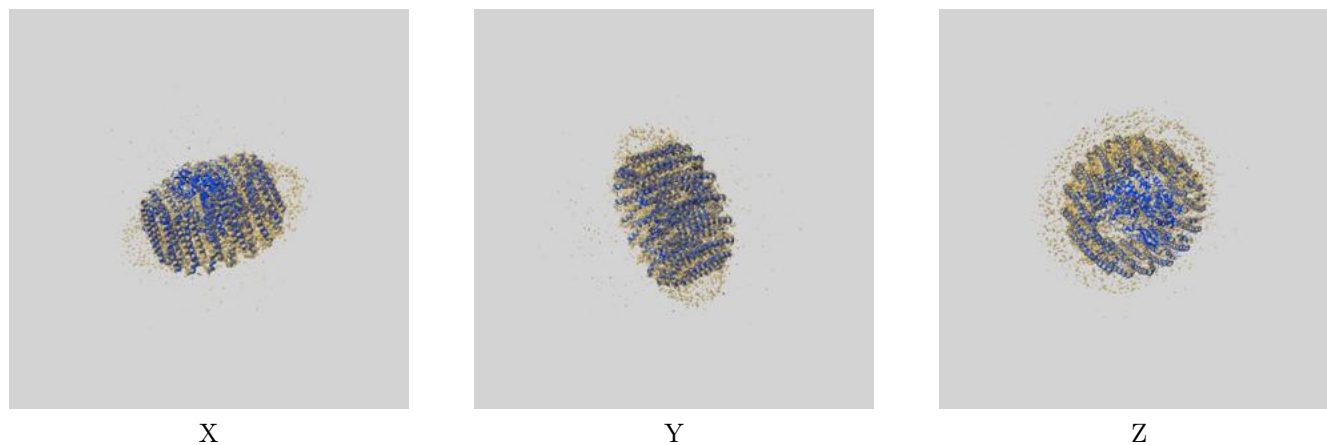
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	6.32	4.22
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

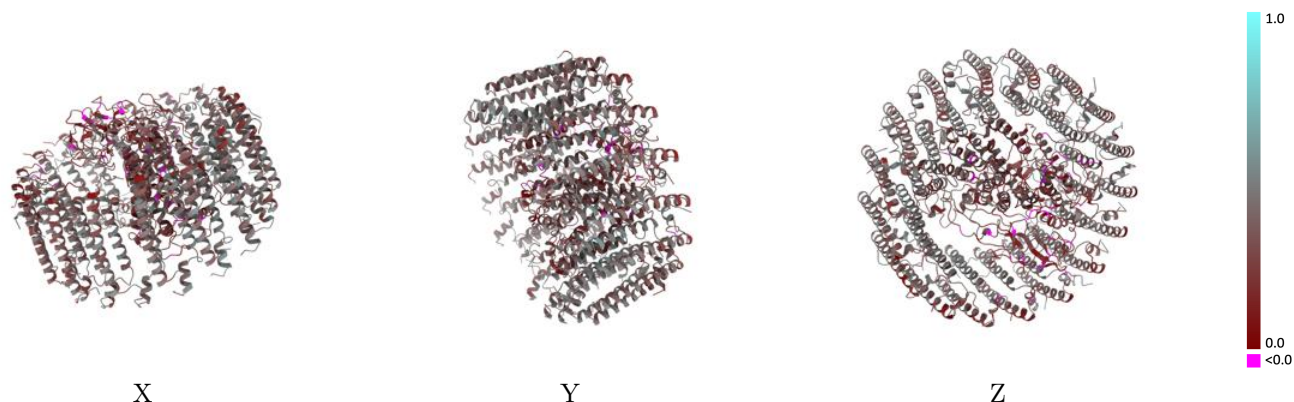
This section contains information regarding the fit between EMDB map EMD-32062 and PDB model 7VOY. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



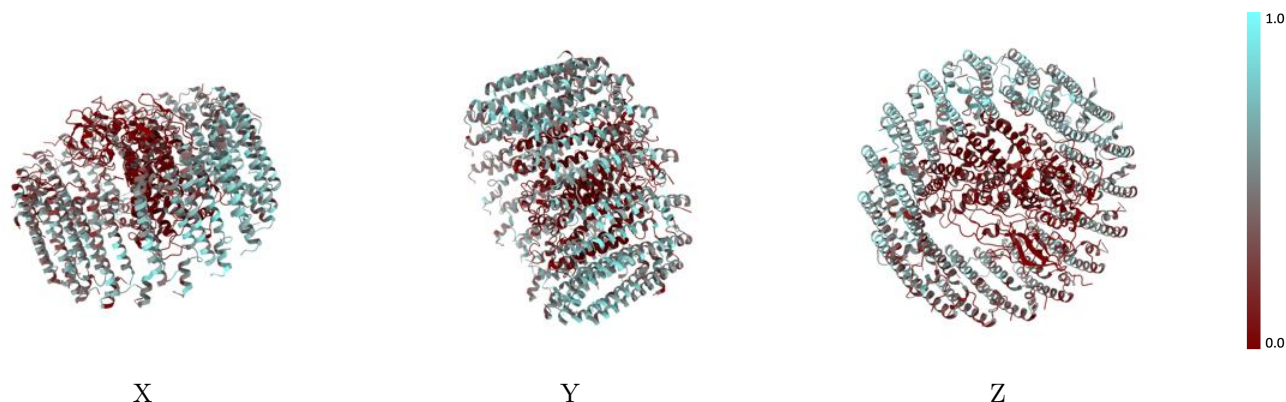
The images above show the 3D surface view of the map at the recommended contour level 0.0254 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



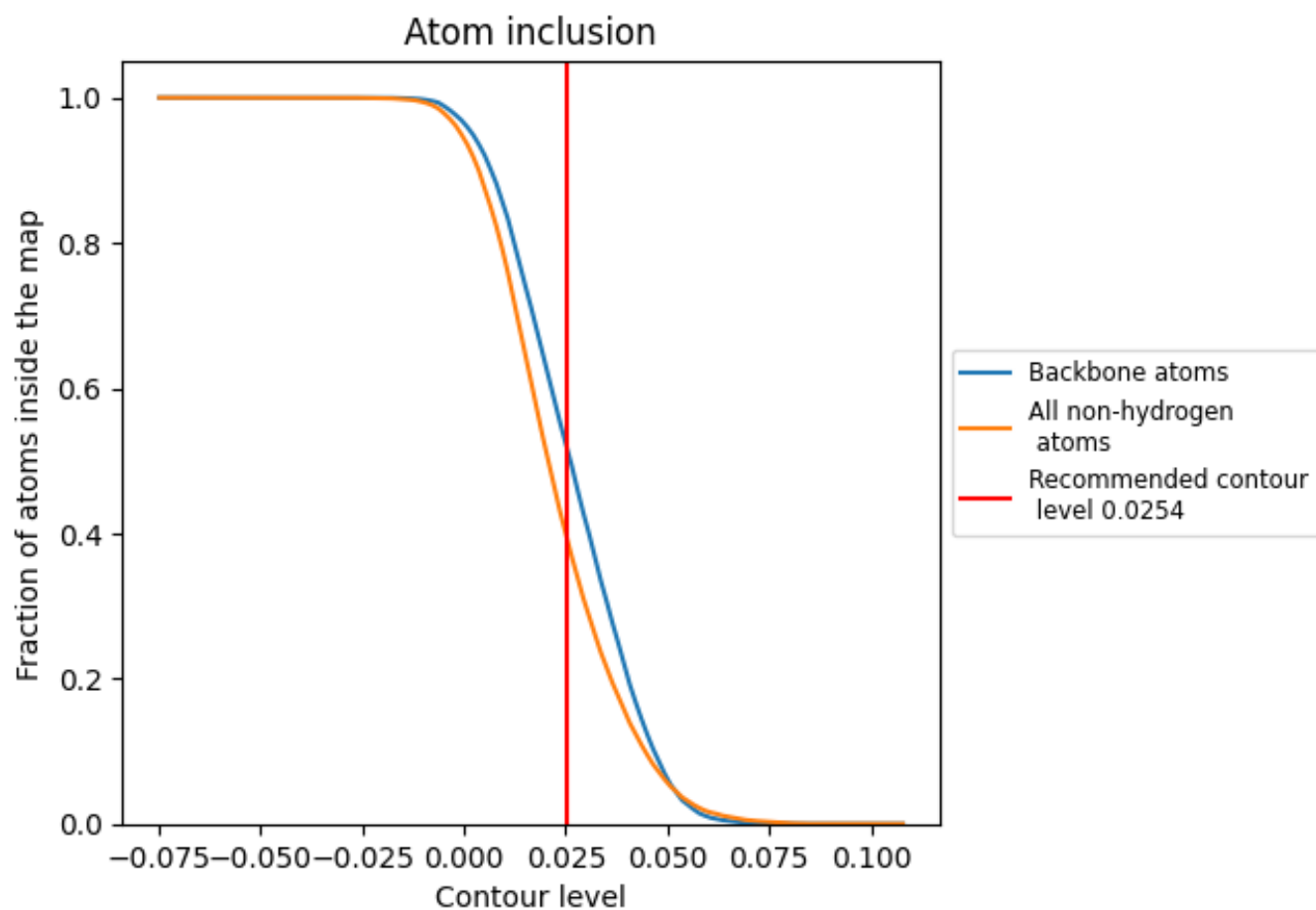
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0254).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 39% 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 (0.0254) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3918	 0.3720
0	 0.4198	 0.3390
1	 0.5879	 0.4410
2	 0.5442	 0.4090
3	 0.4812	 0.3960
4	 0.5041	 0.4300
5	 0.4717	 0.3810
6	 0.5248	 0.4430
7	 0.5117	 0.4320
8	 0.4249	 0.3480
9	 0.4938	 0.4270
A	 0.4547	 0.4190
B	 0.3860	 0.3570
C	 0.5905	 0.4580
D	 0.4257	 0.3990
E	 0.4403	 0.3540
F	 0.4753	 0.4180
G	 0.4623	 0.3790
H	 0.0466	 0.2360
I	 0.5370	 0.4380
J	 0.5299	 0.3840
K	 0.5905	 0.4430
L	 0.0932	 0.2730
M	 0.1007	 0.3040
N	 0.5896	 0.4260
O	 0.6235	 0.4690
P	 0.5948	 0.4060
Q	 0.6255	 0.4520
R	 0.5688	 0.3930
S	 0.6132	 0.4590
T	 0.5636	 0.4030
U	 0.6481	 0.4590
V	 0.5662	 0.4120
W	 0.6152	 0.4600
X	 0.5584	 0.3950



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Chain	Atom inclusion	Q-score
Y	 0.5947	 0.4500
Z	 0.5729	 0.3960
t	 0.4336	 0.3520