



## Full wwPDB EM Validation Report ⓘ

May 26, 2024 – 07:40 AM EDT

PDB ID : 7S4K  
EMDB ID : EMD-24829  
Title : CryoEM structure of Methylococcus capsulatus (Bath) pMMO in a native lipid nanodisc at 2.34 Angstrom resolution  
Authors : Koo, C.W.; Rosenzweig, A.C.  
Deposited on : 2021-09-09  
Resolution : 2.36 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (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 : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

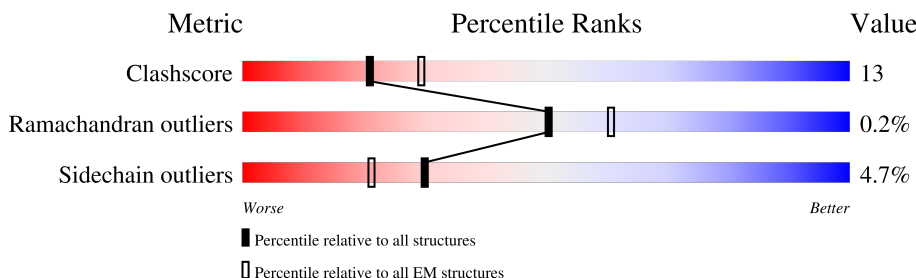
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.36 Å.

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




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	414	
1	E	414	
1	I	414	
2	C	260	
2	G	260	
2	K	260	
3	B	247	
3	F	247	

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Mol	Chain	Length	Quality of chain
3	J	247	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CU	C	301	-	-	X	-
4	CU	G	302	-	-	X	-
4	CU	K	301	-	-	X	-
5	D10	B	305	-	-	X	-
5	D10	F	306	-	-	X	-
5	D10	J	309	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 25049 atoms, of which 2460 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 Particulate methane monooxygenase alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		
1	E	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		
1	I	382	Total	C	N	O	S	0	0
			3017	1938	513	551	15		

- Molecule 2 is a protein called Ammonia monooxygenase/methane monooxygenase, subunit C family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	236	Total	C	N	O	S	0	0
			1972	1339	299	329	5		
2	G	236	Total	C	N	O	S	0	0
			1972	1339	299	329	5		
2	K	236	Total	C	N	O	S	0	0
			1972	1339	299	329	5		

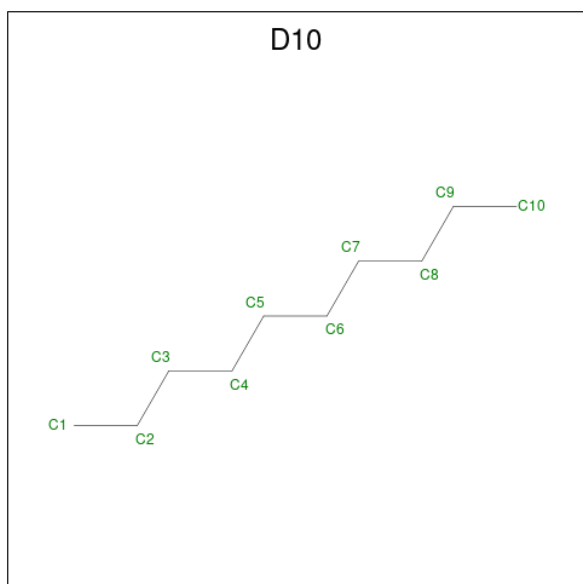
- Molecule 3 is a protein called Particulate methane monooxygenase beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	241	Total	C	N	O	S	0	0
			1977	1329	315	322	11		
3	F	241	Total	C	N	O	S	0	0
			1977	1329	315	322	11		
3	J	241	Total	C	N	O	S	0	0
			1977	1329	315	322	11		

- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total 2	Cu 2	0
4	C	1	Total 1	Cu 1	0
4	G	1	Total 1	Cu 1	0
4	K	1	Total 1	Cu 1	0
4	E	2	Total 2	Cu 2	0
4	I	2	Total 2	Cu 2	0

- Molecule 5 is DECANE (three-letter code: D10) (formula: C<sub>10</sub>H<sub>22</sub>) (labeled as "Ligand of Interest" by depositor).



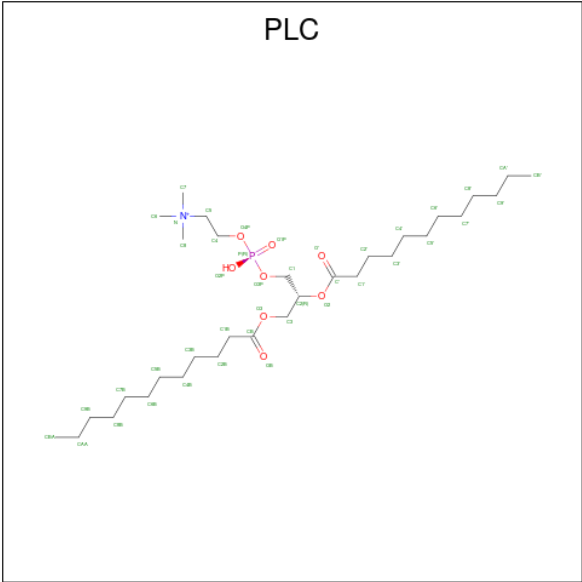
Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total 32	C 10	H 22	0
5	C	1	Total 32	C 10	H 22	0
5	B	1	Total 32	C 10	H 22	0
5	B	1	Total 32	C 10	H 22	0
5	B	1	Total 32	C 10	H 22	0

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Mol	Chain	Residues	Atoms			AltConf
5	B	1	Total 32	C 10	H 22	0
5	G	1	Total 32	C 10	H 22	0
5	K	1	Total 32	C 10	H 22	0
5	E	1	Total 32	C 10	H 22	0
5	I	1	Total 32	C 10	H 22	0
5	F	1	Total 32	C 10	H 22	0
5	F	1	Total 32	C 10	H 22	0
5	F	1	Total 32	C 10	H 22	0
5	F	1	Total 32	C 10	H 22	0
5	J	1	Total 32	C 10	H 22	0
5	J	1	Total 32	C 10	H 22	0
5	J	1	Total 32	C 10	H 22	0
5	J	1	Total 32	C 10	H 22	0

- Molecule 6 is DIUNDECYL PHOSPHATIDYL CHOLINE (three-letter code: PLC) (formula:  $C_{32}H_{65}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



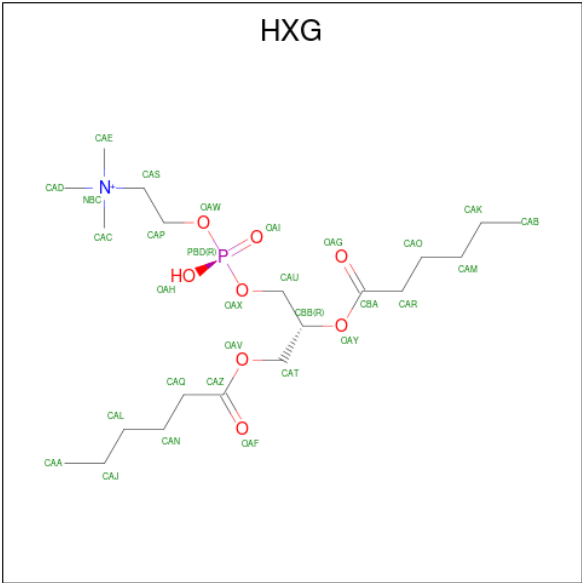
Mol	Chain	Residues	Atoms						AltConf
6	C	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	C	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	B	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	G	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	G	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	G	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	K	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	F	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	F	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	

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Mol	Chain	Residues	Atoms						AltConf
6	J	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	J	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	J	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	
6	J	1	Total	C	H	N	O	P	0
			106	32	64	1	8	1	

- Molecule 7 is 1,2-dihexanoyl-sn-glycero-3-phosphocholine (three-letter code: HXG) (formula: C<sub>20</sub>H<sub>41</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).

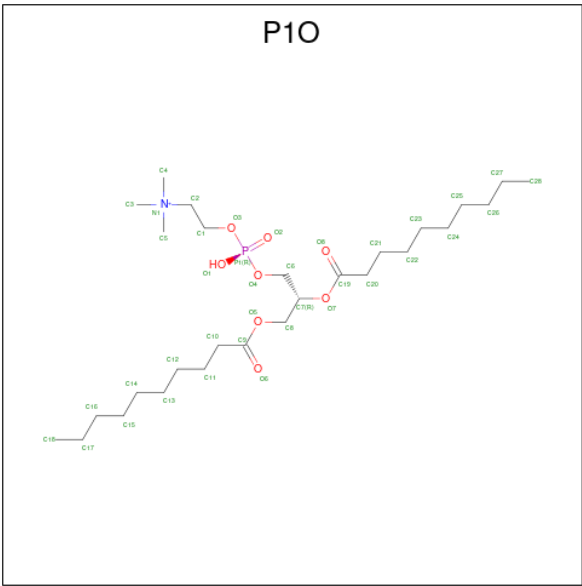


Mol	Chain	Residues	Atoms						AltConf
7	C	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
7	C	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
7	G	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
7	G	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
7	K	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	
7	K	1	Total	C	H	N	O	P	0
			70	20	40	1	8	1	

- Molecule 8 is 1,2-DIDECANOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter



code: P1O) (formula: C<sub>28</sub>H<sub>57</sub>NO<sub>8</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
8	C	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	C	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	B	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	B	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	G	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	G	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	K	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	K	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	F	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	F	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	J	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	
8	J	1	Total	C	H	N	O	P	0
			94	28	56	1	8	1	

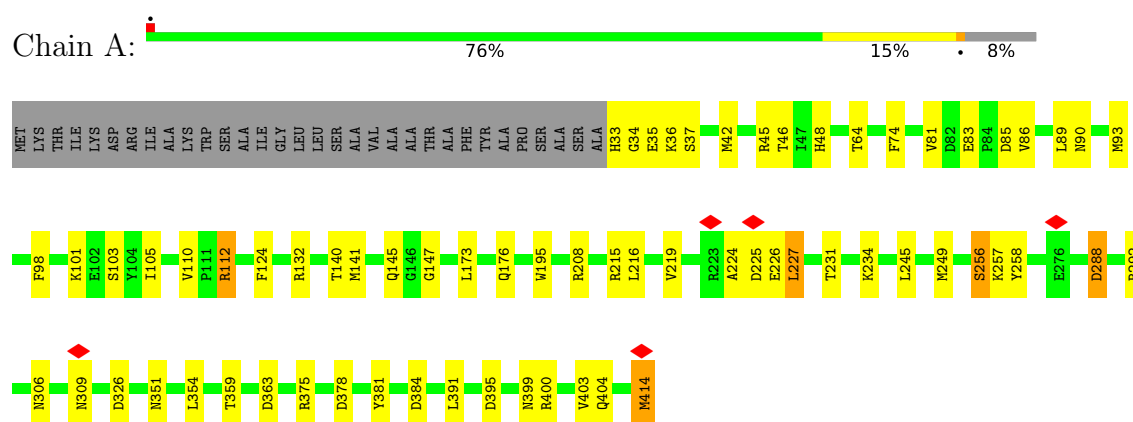
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		AltConf
9	A	17	Total 17	O 17	0
9	C	4	Total 4	O 4	0
9	B	12	Total 12	O 12	0
9	G	4	Total 4	O 4	0
9	K	4	Total 4	O 4	0
9	E	23	Total 23	O 23	0
9	I	24	Total 24	O 24	0
9	F	9	Total 9	O 9	0
9	J	13	Total 13	O 13	0

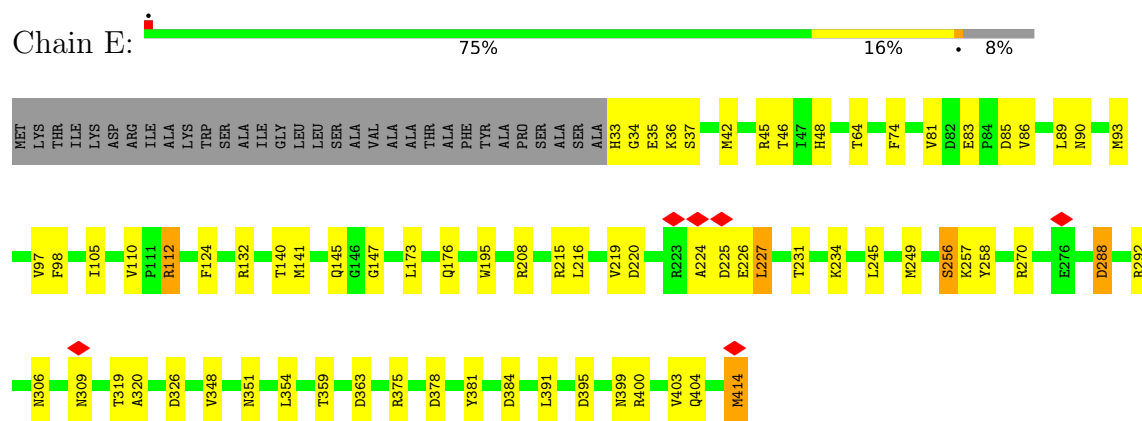
### 3 Residue-property plots

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

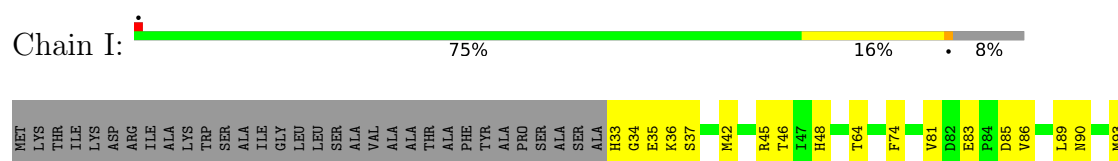
- Molecule 1: Particulate methane monooxygenase alpha subunit

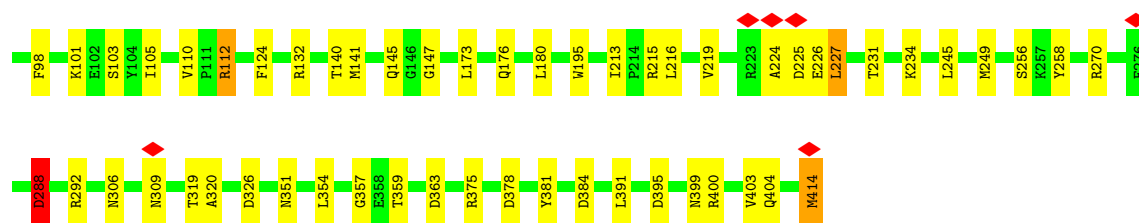


- Molecule 1: Particulate methane monooxygenase alpha subunit

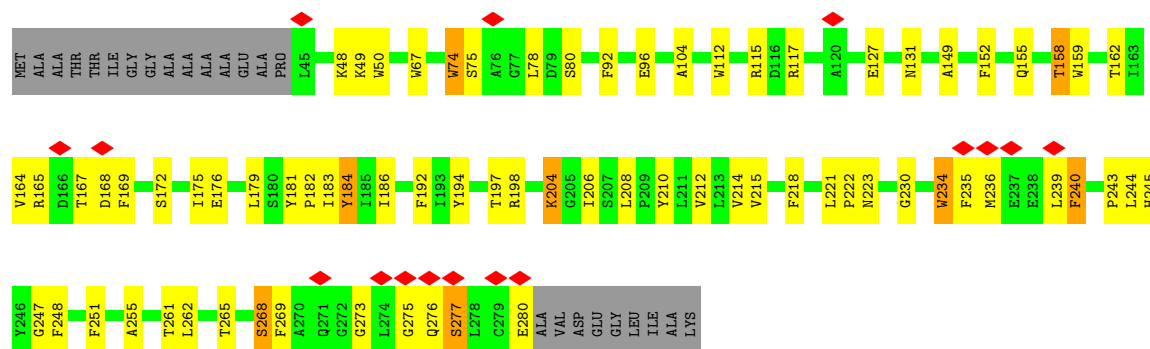


- Molecule 1: Particulate methane monooxygenase alpha subunit

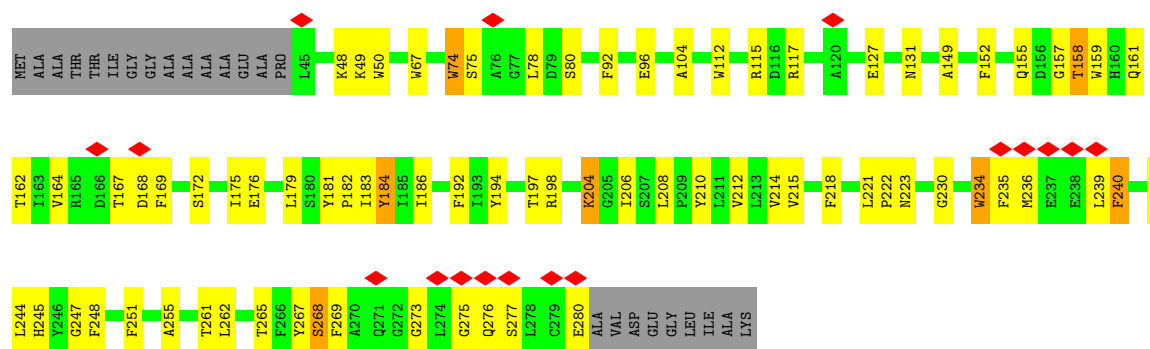




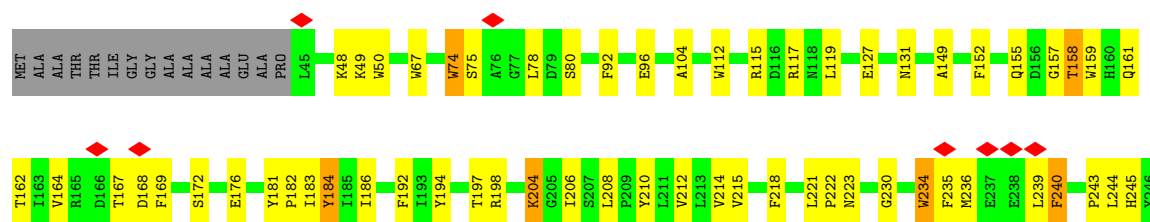
- Molecule 2: Ammonia monooxygenase/methane monooxygenase, subunit C family protein

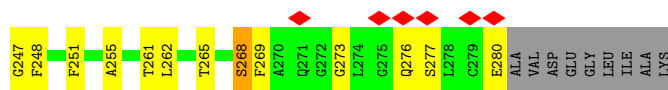


- Molecule 2: Ammonia monooxygenase/methane monooxygenase, subunit C family protein

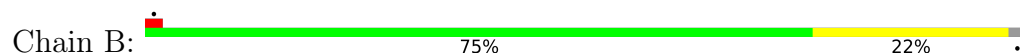


- Molecule 2: Ammonia monooxygenase/methane monooxygenase, subunit C family protein

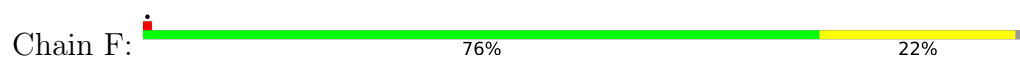




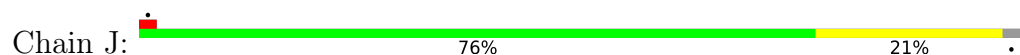
- Molecule 3: Particulate methane monooxygenase beta subunit



- Molecule 3: Particulate methane monooxygenase beta subunit



- Molecule 3: Particulate methane monooxygenase beta subunit



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	546332	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 ( $e^-/\text{\AA}^2$ )	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0237	Depositor
Map size (Å)	204.0, 204.0, 204.0	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.4722222, 0.4722222, 0.4722222	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: HXG, D10, CU, PLC, P1O

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.31	0/3099	0.51	0/4215
1	E	0.31	0/3099	0.51	0/4215
1	I	0.31	0/3099	0.51	0/4215
2	C	0.35	0/2051	0.57	0/2810
2	G	0.35	0/2051	0.57	0/2810
2	K	0.35	0/2051	0.57	0/2810
3	B	0.31	0/2053	0.48	0/2810
3	F	0.31	0/2053	0.48	0/2810
3	J	0.31	0/2053	0.48	0/2810
All	All	0.32	0/21609	0.52	0/29505

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3017	0	2980	44	0
1	E	3017	0	2980	48	0
1	I	3017	0	2980	50	0
2	C	1972	0	1904	96	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1972	0	1904	95	0
2	K	1972	0	1904	96	0
3	B	1977	0	1936	71	0
3	F	1977	0	1936	67	0
3	J	1977	0	1936	69	0
4	A	2	0	0	0	0
4	C	1	0	0	2	0
4	E	2	0	0	0	0
4	G	1	0	0	2	0
4	I	2	0	0	0	0
4	K	1	0	0	2	0
5	A	10	22	22	0	0
5	B	40	88	88	11	0
5	C	10	22	22	1	0
5	E	10	22	22	0	0
5	F	40	88	88	11	0
5	G	10	22	22	1	0
5	I	10	22	22	0	0
5	J	40	88	88	11	0
5	K	10	22	22	1	0
6	B	168	256	256	12	0
6	C	168	256	256	13	0
6	F	84	128	128	8	0
6	G	126	192	192	11	0
6	J	168	256	256	16	0
6	K	42	64	64	4	0
7	C	60	80	80	29	0
7	G	60	80	80	29	0
7	K	60	80	80	29	0
8	B	76	112	112	11	0
8	C	76	112	112	26	0
8	F	76	112	112	10	0
8	G	76	112	112	26	0
8	J	76	112	112	10	0
8	K	76	112	112	25	0
9	A	17	0	0	1	0
9	B	12	0	0	2	0
9	C	4	0	0	0	0
9	E	23	0	0	1	0
9	F	9	0	0	1	0
9	G	4	0	0	0	0
9	I	24	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J	13	0	0	2	0
9	K	4	0	0	0	0
All	All	22589	2460	22920	604	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (604) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:236:MET:H	7:G:303:HXG:H37	1.00	1.15
2:C:236:MET:H	7:C:303:HXG:H37	1.00	1.12
2:K:236:MET:H	7:K:302:HXG:H37	1.00	1.11
2:G:67:TRP:HA	7:G:306:HXG:CAC	1.84	1.08
2:C:67:TRP:HA	7:C:306:HXG:CAC	1.84	1.07
2:G:67:TRP:CD1	7:G:306:HXG:H41	1.90	1.06
2:K:67:TRP:HA	7:K:304:HXG:CAC	1.84	1.06
2:K:67:TRP:HA	7:K:304:HXG:H39	1.07	1.06
2:G:67:TRP:HA	7:G:306:HXG:H39	1.07	1.06
2:C:67:TRP:HA	7:C:306:HXG:H39	1.07	1.06
2:C:67:TRP:CD1	7:C:306:HXG:H41	1.90	1.04
2:K:67:TRP:CD1	7:K:304:HXG:H41	1.90	1.04
2:K:67:TRP:CA	7:K:304:HXG:H39	1.92	0.99
2:G:67:TRP:CA	7:G:306:HXG:H39	1.92	0.99
2:C:67:TRP:CA	7:C:306:HXG:H39	1.92	0.98
2:G:236:MET:N	7:G:303:HXG:H37	1.79	0.98
2:C:236:MET:N	7:C:303:HXG:H37	1.79	0.97
2:K:236:MET:N	7:K:302:HXG:H37	1.79	0.97
2:G:67:TRP:CD1	7:G:306:HXG:CAC	2.49	0.96
2:C:67:TRP:CD1	7:C:306:HXG:CAC	2.49	0.96
2:K:67:TRP:CD1	7:K:304:HXG:CAC	2.49	0.95
2:C:245:HIS:HE2	4:C:301:CU:CU	0.62	0.94
3:F:138:SER:HA	8:F:303:P1O:O8	1.68	0.94
2:G:245:HIS:HE2	4:G:302:CU:CU	0.62	0.93
3:B:138:SER:HA	8:B:302:P1O:O8	1.68	0.92
2:K:236:MET:H	7:K:302:HXG:CAE	1.81	0.92
2:K:245:HIS:HE2	4:K:301:CU:CU	0.62	0.92
3:J:138:SER:HA	8:J:306:P1O:O8	1.68	0.92
2:C:236:MET:H	7:C:303:HXG:CAE	1.81	0.91
2:C:50:TRP:CE3	8:C:308:P1O:H39	2.07	0.90
2:G:236:MET:H	7:G:303:HXG:CAE	1.81	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:50:TRP:CE3	8:K:306:P1O:H39	2.07	0.89
2:G:67:TRP:HD1	7:G:306:HXG:H41	1.37	0.89
2:C:67:TRP:HD1	7:C:306:HXG:H41	1.37	0.89
2:G:50:TRP:CE3	8:G:308:P1O:H39	2.07	0.89
7:C:303:HXG:H9	5:C:304:D10:H42	1.56	0.88
7:K:302:HXG:H9	5:K:303:D10:H42	1.56	0.87
7:G:303:HXG:H9	5:G:304:D10:H42	1.56	0.87
7:G:306:HXG:H37	7:G:306:HXG:H26	1.58	0.86
3:J:161:TRP:CZ2	6:J:305:PLC:H73	2.11	0.86
3:F:161:TRP:CZ2	6:F:302:PLC:H73	2.10	0.86
3:B:161:TRP:CZ2	6:B:301:PLC:H73	2.11	0.85
2:K:67:TRP:HD1	7:K:304:HXG:H41	1.37	0.85
7:K:304:HXG:H37	7:K:304:HXG:H26	1.58	0.84
7:C:306:HXG:H37	7:C:306:HXG:H26	1.58	0.84
8:J:306:P1O:O8	8:J:306:P1O:H20	1.79	0.83
8:F:303:P1O:O8	8:F:303:P1O:H20	1.79	0.82
2:C:112:TRP:CH2	8:C:309:P1O:H2	2.14	0.82
8:B:302:P1O:O8	8:B:302:P1O:H20	1.79	0.82
2:K:112:TRP:CH2	8:K:307:P1O:H2	2.14	0.81
2:G:112:TRP:CH2	8:G:309:P1O:H2	2.14	0.81
2:K:67:TRP:CB	7:K:304:HXG:H40	2.11	0.81
2:K:67:TRP:HB2	7:K:304:HXG:H40	1.63	0.81
2:K:245:HIS:NE2	4:K:301:CU:CU	1.45	0.80
2:C:67:TRP:CB	7:C:306:HXG:H40	2.11	0.80
2:G:67:TRP:HB2	7:G:306:HXG:H40	1.63	0.80
2:C:67:TRP:HB2	7:C:306:HXG:H40	1.63	0.79
2:G:67:TRP:CB	7:G:306:HXG:H40	2.11	0.79
2:C:245:HIS:NE2	4:C:301:CU:CU	1.45	0.79
2:C:67:TRP:CA	7:C:306:HXG:CAC	2.57	0.78
2:G:245:HIS:NE2	4:G:302:CU:CU	1.45	0.78
2:G:234:TRP:CZ2	7:G:303:HXG:H18	2.19	0.78
2:K:234:TRP:CZ2	7:K:302:HXG:H18	2.19	0.78
8:J:306:P1O:H38	8:J:306:P1O:H48	1.66	0.78
2:C:234:TRP:CZ2	7:C:303:HXG:H18	2.19	0.77
8:B:302:P1O:H38	8:B:302:P1O:H48	1.66	0.76
2:G:112:TRP:CH2	8:G:309:P1O:C1	2.69	0.76
8:F:303:P1O:H38	8:F:303:P1O:H48	1.66	0.76
2:K:112:TRP:CH2	8:K:307:P1O:C1	2.69	0.76
1:A:81:VAL:HG13	1:A:147:GLY:HA3	1.69	0.75
2:C:112:TRP:CH2	8:C:309:P1O:C1	2.69	0.75
3:F:237:TRP:HE1	5:F:306:D10:H32	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:199:MET:SD	6:J:303:PLC:H2	2.27	0.74
3:J:237:TRP:HE1	5:J:309:D10:H32	1.50	0.74
3:B:237:TRP:HE1	5:B:305:D10:H32	1.51	0.74
3:J:138:SER:HB2	8:J:306:P1O:O8	1.87	0.74
2:C:234:TRP:HZ2	7:C:303:HXG:H18	1.53	0.74
3:F:138:SER:HB2	8:F:303:P1O:O8	1.87	0.73
1:E:81:VAL:HG13	1:E:147:GLY:HA3	1.69	0.73
2:K:67:TRP:CA	7:K:304:HXG:CAC	2.57	0.73
6:C:310:PLC:H2	3:B:199:MET:SD	2.28	0.73
2:K:234:TRP:HZ2	7:K:302:HXG:H18	1.53	0.73
2:G:234:TRP:HZ2	7:G:303:HXG:H18	1.53	0.73
3:B:138:SER:HB2	8:B:302:P1O:O8	1.87	0.73
2:G:67:TRP:CA	7:G:306:HXG:CAC	2.57	0.73
2:K:67:TRP:HD1	7:K:304:HXG:CAC	1.97	0.73
1:I:81:VAL:HG13	1:I:147:GLY:HA3	1.69	0.72
2:K:48:LYS:HD3	2:K:50:TRP:HD1	1.54	0.72
2:K:162:THR:HG21	3:J:112:THR:HG21	1.70	0.72
2:G:162:THR:HG21	3:F:112:THR:HG21	1.72	0.71
3:F:138:SER:CA	8:F:303:P1O:O8	2.38	0.71
2:G:48:LYS:HD3	2:G:50:TRP:HD1	1.54	0.71
2:K:67:TRP:CB	7:K:304:HXG:CAC	2.68	0.71
2:G:67:TRP:CB	7:G:306:HXG:CAC	2.68	0.71
2:C:48:LYS:HD3	2:C:50:TRP:HD1	1.54	0.71
3:B:138:SER:CA	8:B:302:P1O:O8	2.38	0.71
2:C:67:TRP:CB	7:C:306:HXG:CAC	2.68	0.70
2:G:235:PHE:H	7:G:303:HXG:H41	1.57	0.69
3:J:138:SER:CA	8:J:306:P1O:O8	2.38	0.69
2:C:235:PHE:H	7:C:303:HXG:H41	1.57	0.68
3:J:138:SER:CB	8:J:306:P1O:O8	2.42	0.68
2:C:162:THR:HG21	3:B:112:THR:HG21	1.74	0.68
3:F:138:SER:CB	8:F:303:P1O:O8	2.41	0.68
2:C:67:TRP:HD1	7:C:306:HXG:CAC	1.97	0.68
6:G:301:PLC:H2	3:F:199:MET:SD	2.34	0.68
2:K:235:PHE:H	7:K:302:HXG:H41	1.57	0.68
3:B:138:SER:CB	8:B:302:P1O:O8	2.41	0.68
2:G:67:TRP:HD1	7:G:306:HXG:CAC	1.97	0.68
1:E:326:ASP:OD2	1:E:351:ASN:ND2	2.27	0.67
2:K:162:THR:HG22	3:J:114:PHE:HE2	1.60	0.67
3:B:161:TRP:CZ2	6:B:301:PLC:C7	2.78	0.66
3:J:161:TRP:CZ2	6:J:305:PLC:C7	2.78	0.66
1:A:326:ASP:OD2	1:A:351:ASN:ND2	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:161:TRP:CZ2	6:F:302:PLC:C7	2.78	0.66
6:G:301:PLC:H32	6:G:301:PLC:H1'2	1.78	0.66
2:K:67:TRP:CG	7:K:304:HXG:CAC	2.79	0.66
1:I:326:ASP:OD2	1:I:351:ASN:ND2	2.28	0.66
2:C:67:TRP:CG	7:C:306:HXG:CAC	2.79	0.65
2:G:67:TRP:CG	7:G:306:HXG:CAC	2.79	0.65
7:G:306:HXG:H37	7:G:306:HXG:CAU	2.26	0.65
6:J:303:PLC:H32	6:J:303:PLC:H1'2	1.78	0.65
7:C:306:HXG:H37	7:C:306:HXG:CAU	2.26	0.65
2:C:261:THR:O	2:C:265:THR:HG23	1.97	0.65
6:C:310:PLC:H32	6:C:310:PLC:H1'2	1.78	0.65
7:K:304:HXG:H37	7:K:304:HXG:CAU	2.26	0.65
2:K:261:THR:O	2:K:265:THR:HG23	1.97	0.64
2:C:74:TRP:HA	2:C:78:LEU:HG	1.79	0.64
2:C:162:THR:HG22	3:B:114:PHE:HE2	1.60	0.64
8:C:309:P1O:C10	3:B:247:THR:HG21	2.27	0.64
3:B:210:LYS:HA	1:I:381:TYR:CZ	2.33	0.64
2:K:50:TRP:CZ3	8:K:306:P1O:H39	2.33	0.64
2:G:74:TRP:HA	2:G:78:LEU:HG	1.79	0.63
2:G:261:THR:O	2:G:265:THR:HG23	1.97	0.63
1:E:381:TYR:CZ	3:J:210:LYS:HA	2.33	0.63
2:K:74:TRP:HA	2:K:78:LEU:HG	1.79	0.63
3:B:237:TRP:HE1	5:B:305:D10:C3	2.11	0.63
1:A:93:MET:HE1	1:A:98:PHE:HB2	1.81	0.63
2:G:162:THR:HG22	3:F:114:PHE:HE2	1.64	0.63
3:J:237:TRP:HE1	5:J:309:D10:C3	2.11	0.62
2:C:50:TRP:CZ3	8:C:308:P1O:H39	2.33	0.62
8:G:308:P1O:H18	8:G:308:P1O:H24	1.82	0.62
3:F:237:TRP:HE1	5:F:306:D10:C3	2.10	0.62
1:A:90:ASN:HB3	1:A:141:MET:HG3	1.82	0.62
2:G:50:TRP:CZ3	8:G:308:P1O:H39	2.33	0.62
3:J:138:SER:OG	3:J:138:SER:O	2.17	0.62
1:E:90:ASN:HB3	1:E:141:MET:HG3	1.82	0.62
1:I:173:LEU:HD12	3:J:170:PRO:HB2	1.82	0.62
8:G:309:P1O:O8	8:G:309:P1O:H7	1.99	0.61
1:E:215:ARG:HG2	1:E:227:LEU:HD22	1.82	0.61
8:C:308:P1O:H18	8:C:308:P1O:H24	1.82	0.61
1:A:45:ARG:HB3	1:A:74:PHE:CD2	2.36	0.61
8:C:309:P1O:O8	8:C:309:P1O:H7	1.99	0.61
3:F:138:SER:OG	3:F:138:SER:O	2.18	0.61
8:K:306:P1O:H18	8:K:306:P1O:H24	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:307:P1O:H7	8:K:307:P1O:O8	1.99	0.61
1:E:173:LEU:HD12	3:F:170:PRO:HB2	1.83	0.61
2:G:48:LYS:HD3	2:G:50:TRP:CD1	2.35	0.61
1:I:45:ARG:HB3	1:I:74:PHE:CD2	2.36	0.61
1:E:93:MET:HE1	1:E:98:PHE:HB2	1.83	0.61
2:K:48:LYS:HD3	2:K:50:TRP:CD1	2.35	0.61
2:K:50:TRP:CD2	8:K:306:P1O:H16	2.36	0.61
1:A:381:TYR:CZ	3:F:210:LYS:HA	2.36	0.60
2:C:112:TRP:CZ2	8:C:309:P1O:C1	2.84	0.60
1:A:215:ARG:HG2	1:A:227:LEU:HD22	1.82	0.60
2:C:48:LYS:HD3	2:C:50:TRP:CD1	2.35	0.60
3:F:237:TRP:NE1	5:F:306:D10:H32	2.16	0.60
3:B:138:SER:O	3:B:138:SER:OG	2.18	0.60
1:E:45:ARG:HB3	1:E:74:PHE:CD2	2.36	0.60
3:F:237:TRP:NE1	5:F:306:D10:H51	2.16	0.60
1:I:90:ASN:HB3	1:I:141:MET:HG3	1.82	0.60
1:I:215:ARG:HG2	1:I:227:LEU:HD22	1.82	0.60
2:G:112:TRP:CZ2	8:G:309:P1O:C1	2.84	0.60
2:C:235:PHE:HA	7:C:303:HXG:H41	1.84	0.60
3:J:237:TRP:NE1	5:J:309:D10:H51	2.16	0.60
8:C:308:P1O:O2	8:C:308:P1O:H4	2.02	0.60
2:K:112:TRP:CZ2	8:K:307:P1O:C1	2.84	0.60
3:B:237:TRP:NE1	5:B:305:D10:H51	2.17	0.60
2:C:50:TRP:CD2	8:C:308:P1O:H16	2.36	0.59
3:B:237:TRP:NE1	5:B:305:D10:H32	2.16	0.59
2:C:67:TRP:CD1	7:C:306:HXG:H40	2.36	0.59
2:G:50:TRP:CD2	8:G:308:P1O:H16	2.36	0.59
8:G:308:P1O:H4	8:G:308:P1O:O2	2.02	0.59
8:K:306:P1O:H4	8:K:306:P1O:O2	2.02	0.59
1:A:173:LEU:HD12	3:B:170:PRO:HB2	1.83	0.59
2:G:67:TRP:CD1	7:G:306:HXG:H40	2.36	0.59
2:K:235:PHE:HA	7:K:302:HXG:H41	1.84	0.59
3:J:237:TRP:NE1	5:J:309:D10:H32	2.16	0.59
1:I:93:MET:HE1	1:I:98:PHE:HB2	1.85	0.58
8:G:309:P1O:C10	3:F:247:THR:HG21	2.33	0.58
3:F:143:PHE:CD2	8:F:303:P1O:H26	2.39	0.58
2:G:235:PHE:HA	7:G:303:HXG:H41	1.84	0.58
3:J:143:PHE:CD2	8:J:306:P1O:H26	2.39	0.58
3:B:143:PHE:CD2	8:B:302:P1O:H26	2.39	0.58
8:C:308:P1O:O2	8:C:308:P1O:H6	2.04	0.58
2:K:112:TRP:CH2	8:K:307:P1O:H1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:112:TRP:O	2:G:115:ARG:NH1	2.36	0.57
2:C:239:LEU:HD11	3:B:199:MET:HE2	1.87	0.57
8:G:308:P1O:O2	8:G:308:P1O:H6	2.04	0.57
8:K:306:P1O:O2	8:K:306:P1O:H6	2.04	0.57
2:K:67:TRP:CD1	7:K:304:HXG:H40	2.36	0.57
2:G:112:TRP:CH2	8:G:309:P1O:H1	2.39	0.57
2:K:112:TRP:O	2:K:115:ARG:NH1	2.36	0.57
2:C:112:TRP:O	2:C:115:ARG:NH1	2.36	0.57
2:C:255:ALA:HB3	3:B:36:SER:HB3	1.87	0.57
1:I:292:ARG:NH1	1:I:414:MET:O	2.37	0.56
2:C:112:TRP:CH2	8:C:309:P1O:H1	2.39	0.56
1:I:309:ASN:OD1	1:I:309:ASN:N	2.38	0.56
3:J:67:VAL:HG12	6:J:302:PLC:HEA3	1.87	0.56
8:C:309:P1O:H20	3:B:247:THR:HG21	1.87	0.56
2:G:235:PHE:N	7:G:303:HXG:H41	2.20	0.56
3:B:67:VAL:HG12	6:B:307:PLC:HEA3	1.88	0.56
1:E:391:LEU:HB2	1:E:403:VAL:HG13	1.88	0.56
2:K:255:ALA:HB3	3:J:36:SER:HB3	1.87	0.56
2:C:235:PHE:CZ	2:C:243:PRO:HD2	2.41	0.56
2:G:112:TRP:CZ2	8:G:309:P1O:C3	2.89	0.56
1:A:309:ASN:OD1	1:A:309:ASN:N	2.38	0.55
2:C:235:PHE:N	7:C:303:HXG:H41	2.21	0.55
2:G:255:ALA:HB3	3:F:36:SER:HB3	1.88	0.55
6:G:301:PLC:H63	6:G:301:PLC:O4P	2.06	0.55
2:K:235:PHE:N	7:K:302:HXG:H41	2.21	0.55
1:E:86:VAL:HB	1:E:145:GLN:HB2	1.88	0.55
1:A:391:LEU:HB2	1:A:403:VAL:HG13	1.88	0.55
2:K:112:TRP:CZ2	8:K:307:P1O:C3	2.89	0.55
3:B:213:ALA:HB3	6:B:301:PLC:C1	2.37	0.55
1:A:375:ARG:HH12	3:F:209:GLY:HA2	1.72	0.55
2:C:112:TRP:CZ2	8:C:309:P1O:C3	2.89	0.55
1:E:309:ASN:N	1:E:309:ASN:OD1	2.38	0.55
1:A:86:VAL:HB	1:A:145:GLN:HB2	1.88	0.55
1:I:391:LEU:HB2	1:I:403:VAL:HG13	1.88	0.55
3:J:213:ALA:HB3	6:J:305:PLC:C1	2.37	0.55
1:E:219:VAL:HA	1:E:224:ALA:HB2	1.89	0.55
1:I:86:VAL:HB	1:I:145:GLN:HB2	1.88	0.55
2:G:235:PHE:CZ	2:G:243:PRO:HD2	2.42	0.54
6:C:310:PLC:O4P	6:C:310:PLC:H63	2.06	0.54
1:E:375:ARG:HH12	3:J:209:GLY:HA2	1.71	0.54
3:F:213:ALA:HB3	6:F:302:PLC:C1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:213:ALA:HB3	6:J:305:PLC:H11	1.89	0.54
2:K:235:PHE:CZ	2:K:243:PRO:HD2	2.41	0.54
6:J:303:PLC:O4P	6:J:303:PLC:H63	2.06	0.54
8:K:307:P1O:C10	3:J:247:THR:HG21	2.37	0.54
1:I:219:VAL:HA	1:I:224:ALA:HB2	1.89	0.54
1:A:219:VAL:HA	1:A:224:ALA:HB2	1.89	0.54
3:F:213:ALA:HB3	6:F:302:PLC:H11	1.89	0.54
1:A:292:ARG:NH1	1:A:414:MET:O	2.37	0.53
2:C:92:PHE:HA	6:C:307:PLC:OB	2.09	0.53
3:B:213:ALA:HB3	6:B:301:PLC:H11	1.89	0.53
1:E:292:ARG:NH1	1:E:414:MET:O	2.37	0.53
6:C:310:PLC:C2	3:B:199:MET:SD	2.97	0.53
2:K:192:PHE:HB2	2:K:214:VAL:HG21	1.91	0.52
2:C:155:GLN:HA	2:C:158:THR:HG23	1.92	0.52
2:C:183:ILE:HG12	6:C:307:PLC:HEA3	1.91	0.52
2:G:92:PHE:HA	6:G:307:PLC:OB	2.09	0.52
3:F:233:PHE:CG	5:F:304:D10:H51	2.44	0.52
2:C:192:PHE:HB2	2:C:214:VAL:HG21	1.91	0.52
2:G:155:GLN:HA	2:G:158:THR:HG23	1.92	0.52
3:B:233:PHE:CG	5:B:303:D10:H51	2.44	0.52
3:B:168:HIS:HE1	9:B:411:HOH:O	1.91	0.52
2:G:183:ILE:HG12	6:G:307:PLC:HEA3	1.91	0.52
2:K:92:PHE:HA	6:K:305:PLC:OB	2.09	0.52
2:C:240:PHE:N	3:B:47:ASP:OD2	2.42	0.52
7:K:302:HXG:H17	7:K:302:HXG:H10	1.92	0.52
2:G:192:PHE:HB2	2:G:214:VAL:HG21	1.91	0.52
3:F:194:PRO:HG2	3:F:197:ILE:HG13	1.92	0.52
3:J:233:PHE:CG	5:J:307:D10:H51	2.44	0.52
6:C:302:PLC:HEA3	3:F:67:VAL:HG12	1.92	0.51
2:K:239:LEU:HD11	3:J:199:MET:HE2	1.92	0.51
2:K:155:GLN:HA	2:K:158:THR:HG23	1.92	0.51
1:I:213:ILE:HG13	9:J:401:HOH:O	2.11	0.51
2:C:112:TRP:CZ2	8:C:309:P1O:H7	2.46	0.51
7:G:303:HXG:H17	7:G:303:HXG:H10	1.92	0.51
2:K:183:ILE:HG12	6:K:305:PLC:HEA3	1.91	0.51
1:I:35:GLU:C	1:I:37:SER:H	2.14	0.51
2:G:239:LEU:HD11	3:F:199:MET:HE2	1.92	0.51
1:A:124:PHE:CE2	1:A:140:THR:HG21	2.46	0.51
3:B:194:PRO:HG2	3:B:197:ILE:HG13	1.92	0.51
1:E:35:GLU:C	1:E:37:SER:H	2.14	0.51
2:G:251:PHE:HZ	3:J:226:LEU:HD11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:309:P1O:H20	3:F:247:THR:HG21	1.93	0.51
1:E:124:PHE:CE2	1:E:140:THR:HG21	2.46	0.51
1:I:124:PHE:CE2	1:I:140:THR:HG21	2.46	0.51
1:E:89:LEU:HB2	1:E:105:ILE:HD11	1.93	0.51
3:J:199:MET:SD	6:J:303:PLC:C2	2.97	0.51
7:C:303:HXG:H17	7:C:303:HXG:H10	1.92	0.50
8:C:309:P1O:H12	8:C:309:P1O:H16	1.93	0.50
3:B:209:GLY:HA2	1:I:375:ARG:HH12	1.76	0.50
2:K:112:TRP:CZ2	8:K:307:P1O:H7	2.46	0.50
3:J:194:PRO:HG2	3:J:197:ILE:HG13	1.92	0.50
2:G:112:TRP:CZ2	8:G:309:P1O:H7	2.46	0.50
2:C:75:SER:OG	2:C:75:SER:O	2.30	0.50
8:G:309:P1O:H12	8:G:309:P1O:H16	1.93	0.50
1:E:306:ASN:ND2	1:E:354:LEU:O	2.44	0.50
3:J:66:ILE:HG21	6:J:302:PLC:H6A1	1.92	0.50
3:B:226:LEU:HD11	2:K:251:PHE:HZ	1.76	0.50
1:I:89:LEU:HB2	1:I:105:ILE:HD11	1.93	0.50
2:C:112:TRP:CZ2	8:C:309:P1O:H2	2.47	0.50
2:C:149:ALA:O	3:B:39:ILE:HG12	2.12	0.50
2:K:67:TRP:CG	7:K:304:HXG:H40	2.47	0.50
8:K:307:P1O:H16	8:K:307:P1O:H12	1.93	0.50
1:E:381:TYR:HB2	3:J:210:LYS:HZ2	1.77	0.49
1:A:35:GLU:C	1:A:37:SER:H	2.14	0.49
1:A:89:LEU:HB2	1:A:105:ILE:HD11	1.93	0.49
1:A:306:ASN:ND2	1:A:354:LEU:O	2.44	0.49
2:C:215:VAL:HB	8:B:310:P1O:H54	1.95	0.49
3:B:66:ILE:HG21	6:B:307:PLC:H6A1	1.93	0.49
2:K:112:TRP:HH2	8:K:307:P1O:H1	1.77	0.49
3:B:210:LYS:HZ2	1:I:381:TYR:HB2	1.76	0.49
2:G:96:GLU:HA	6:G:307:PLC:H7A1	1.95	0.49
6:G:301:PLC:OB	6:G:301:PLC:H81	2.12	0.49
6:J:303:PLC:OB	6:J:303:PLC:H81	2.12	0.49
2:C:167:THR:OG1	2:C:168:ASP:N	2.46	0.49
2:G:112:TRP:HH2	8:G:309:P1O:H1	1.77	0.49
2:K:208:LEU:HD13	3:J:244:LEU:HD11	1.95	0.49
2:C:96:GLU:HA	6:C:307:PLC:H7A1	1.95	0.49
3:B:237:TRP:CD1	5:B:305:D10:H51	2.48	0.49
2:G:167:THR:OG1	2:G:168:ASP:N	2.46	0.49
2:K:96:GLU:HA	6:K:305:PLC:H7A1	1.95	0.49
6:C:310:PLC:H81	6:C:310:PLC:OB	2.12	0.49
2:C:112:TRP:CE2	8:C:309:P1O:H6	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:208:LEU:HD13	3:F:244:LEU:HD11	1.94	0.48
2:K:75:SER:OG	2:K:75:SER:O	2.30	0.48
3:F:237:TRP:CD1	5:F:306:D10:H51	2.48	0.48
3:J:237:TRP:CD1	5:J:309:D10:H51	2.48	0.48
2:C:235:PHE:CA	7:C:303:HXG:H41	2.43	0.48
2:C:248:PHE:HB2	3:B:43:LEU:HD12	1.95	0.48
2:K:167:THR:OG1	2:K:168:ASP:N	2.46	0.48
3:B:168:HIS:CE1	9:B:411:HOH:O	2.65	0.48
2:K:240:PHE:N	3:J:47:ASP:OD2	2.46	0.48
1:E:132:ARG:NH1	9:E:601:HOH:O	2.40	0.48
2:C:67:TRP:CG	7:C:306:HXG:H40	2.47	0.48
2:C:112:TRP:HH2	8:C:309:P1O:H1	1.77	0.48
2:C:251:PHE:HZ	3:F:226:LEU:HD11	1.78	0.48
3:B:161:TRP:CE2	6:B:301:PLC:H73	2.48	0.48
2:K:235:PHE:CA	7:K:302:HXG:H41	2.43	0.48
2:G:149:ALA:O	3:F:39:ILE:HG12	2.14	0.48
2:G:235:PHE:CA	7:G:303:HXG:H41	2.43	0.48
1:I:306:ASN:ND2	1:I:354:LEU:O	2.44	0.48
2:G:67:TRP:CG	7:G:306:HXG:H40	2.47	0.47
2:G:164:VAL:HB	1:E:34:GLY:HA3	1.95	0.47
2:G:223:ASN:OD1	2:G:247:GLY:HA3	2.14	0.47
1:I:83:GLU:O	1:I:85:ASP:N	2.44	0.47
1:A:215:ARG:NH2	3:B:84:ARG:O	2.46	0.47
2:C:223:ASN:OD1	2:C:247:GLY:HA3	2.14	0.47
2:G:75:SER:O	2:G:75:SER:OG	2.30	0.47
2:G:112:TRP:CE2	8:G:309:P1O:H6	2.49	0.47
1:E:216:LEU:HB2	3:F:83:TYR:CE2	2.49	0.47
3:J:161:TRP:CE2	6:J:305:PLC:H73	2.48	0.47
2:G:276:GLN:HB3	2:G:280:GLU:HG2	1.96	0.47
2:K:223:ASN:OD1	2:K:247:GLY:HA3	2.14	0.47
2:K:164:VAL:HB	1:I:34:GLY:HA3	1.96	0.47
1:A:216:LEU:HB2	3:B:83:TYR:CE2	2.49	0.47
2:G:131:ASN:OD1	2:G:268:SER:OG	2.31	0.47
2:K:112:TRP:CE2	8:K:307:P1O:H6	2.49	0.47
2:G:215:VAL:HB	8:F:308:P1O:H54	1.97	0.47
2:K:273:GLY:HA2	3:J:7:ALA:HB1	1.97	0.47
2:C:262:LEU:HD12	2:C:262:LEU:HA	1.72	0.47
8:K:307:P1O:H20	3:J:247:THR:HG21	1.96	0.47
6:C:302:PLC:H6A1	3:F:66:ILE:HG21	1.96	0.47
2:K:131:ASN:OD1	2:K:268:SER:OG	2.31	0.47
3:F:236:ARG:HA	3:F:236:ARG:HD3	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:237:TRP:HB2	5:B:304:D10:H51	1.97	0.46
1:E:105:ILE:HG13	1:E:110:VAL:HG21	1.98	0.46
1:I:216:LEU:HB2	3:J:83:TYR:CE2	2.49	0.46
1:I:231:THR:HG22	1:I:234:LYS:HD2	1.98	0.46
3:F:161:TRP:CE2	6:F:302:PLC:H73	2.48	0.46
1:A:395:ASP:OD2	1:A:399:ASN:ND2	2.48	0.46
2:C:276:GLN:HB3	2:C:280:GLU:HG2	1.96	0.46
2:G:112:TRP:CZ2	8:G:309:P1O:H2	2.47	0.46
2:K:276:GLN:HB3	2:K:280:GLU:HG2	1.97	0.46
3:B:210:LYS:HA	1:I:381:TYR:CE2	2.51	0.46
2:C:221:LEU:HG	6:C:305:PLC:HE'3	1.98	0.46
6:B:308:PLC:HE'3	2:K:221:LEU:HG	1.98	0.46
3:J:80:TRP:O	3:J:84:ARG:NH1	2.49	0.46
1:A:105:ILE:HG13	1:A:110:VAL:HG21	1.98	0.46
2:C:131:ASN:OD1	2:C:268:SER:OG	2.31	0.46
2:G:221:LEU:HG	6:G:305:PLC:HE'3	1.98	0.46
1:I:105:ILE:HG13	1:I:110:VAL:HG21	1.98	0.46
3:J:237:TRP:HB2	5:J:308:D10:H51	1.97	0.46
1:A:231:THR:HG22	1:A:234:LYS:HD2	1.98	0.46
2:G:240:PHE:N	3:F:47:ASP:OD2	2.48	0.46
2:K:48:LYS:HE3	2:K:48:LYS:HB2	1.86	0.46
1:A:224:ALA:O	1:A:226:GLU:HG3	2.16	0.46
1:A:384:ASP:OD1	1:E:112:ARG:NH2	2.40	0.46
2:C:198:ARG:HH21	8:C:308:P1O:H2	1.81	0.46
2:K:192:PHE:HZ	2:K:206:ILE:HG23	1.81	0.46
2:K:198:ARG:HH21	8:K:306:P1O:H2	1.81	0.46
1:I:132:ARG:NH1	9:I:601:HOH:O	2.44	0.46
3:F:138:SER:O	3:F:140:SER:N	2.49	0.46
3:F:237:TRP:HB2	5:F:305:D10:H51	1.97	0.46
3:J:138:SER:O	3:J:140:SER:N	2.49	0.46
1:I:215:ARG:NH2	3:J:84:ARG:O	2.48	0.45
1:I:395:ASP:OD2	1:I:399:ASN:ND2	2.48	0.45
3:F:194:PRO:HD2	3:F:197:ILE:HD12	1.99	0.45
3:J:245:GLN:HB2	8:J:301:P1O:H1	1.98	0.45
3:B:138:SER:O	3:B:140:SER:N	2.49	0.45
2:C:183:ILE:HG12	6:C:307:PLC:CBA	2.47	0.45
2:C:230:GLY:O	2:C:244:LEU:HD22	2.17	0.45
2:G:198:ARG:HH21	8:G:308:P1O:H2	1.81	0.45
3:J:231:TRP:HA	3:J:234:ILE:HB	1.99	0.45
2:G:104:ALA:HB2	2:G:186:ILE:HG12	1.99	0.45
2:K:248:PHE:HB2	3:J:43:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:80:TRP:O	3:F:84:ARG:NH1	2.49	0.45
2:C:104:ALA:HB2	2:C:186:ILE:HG12	1.99	0.45
2:C:192:PHE:HZ	2:C:206:ILE:HG23	1.81	0.45
2:K:104:ALA:HB2	2:K:186:ILE:HG12	1.99	0.45
2:K:112:TRP:HH2	8:K:307:P1O:C1	2.26	0.45
1:I:288:ASP:HA	9:I:605:HOH:O	2.17	0.45
1:A:83:GLU:O	1:A:85:ASP:N	2.44	0.45
2:K:117:ARG:HG2	2:K:117:ARG:HH11	1.82	0.45
2:K:183:ILE:HG12	6:K:305:PLC:CBA	2.47	0.45
1:E:395:ASP:OD2	1:E:399:ASN:ND2	2.48	0.45
1:I:145:GLN:HA	3:J:196:TYR:CE1	2.52	0.45
3:J:194:PRO:HD2	3:J:197:ILE:HD12	1.98	0.45
1:A:292:ARG:HE	1:A:292:ARG:HB3	1.53	0.45
3:B:194:PRO:HD2	3:B:197:ILE:HD12	1.99	0.45
2:G:183:ILE:HG12	6:G:307:PLC:CBA	2.47	0.45
1:E:83:GLU:O	1:E:85:ASP:N	2.44	0.45
3:B:80:TRP:O	3:B:84:ARG:NH1	2.49	0.45
1:E:224:ALA:O	1:E:226:GLU:HG3	2.16	0.45
3:F:231:TRP:HA	3:F:234:ILE:HB	1.99	0.45
6:G:301:PLC:C2	3:F:199:MET:SD	3.04	0.45
1:E:231:THR:HG22	1:E:234:LYS:HD2	1.98	0.45
2:C:273:GLY:HA2	3:B:7:ALA:HB1	1.98	0.45
3:B:237:TRP:CD2	5:B:305:D10:H72	2.52	0.45
2:G:248:PHE:HB2	3:F:43:LEU:HD12	1.99	0.45
1:E:45:ARG:HB3	1:E:74:PHE:CE2	2.52	0.45
2:C:208:LEU:HD13	3:B:244:LEU:HD11	1.98	0.44
2:G:117:ARG:HG2	2:G:117:ARG:HH11	1.82	0.44
2:G:230:GLY:O	2:G:244:LEU:HD22	2.17	0.44
2:G:267:TYR:OH	1:E:220:ASP:OD2	2.30	0.44
2:K:230:GLY:O	2:K:244:LEU:HD22	2.17	0.44
1:I:45:ARG:HB3	1:I:74:PHE:CE2	2.52	0.44
3:J:237:TRP:CD2	5:J:309:D10:H72	2.53	0.44
2:C:117:ARG:HG2	2:C:117:ARG:HH11	1.82	0.44
3:B:231:TRP:HA	3:B:234:ILE:HB	1.99	0.44
2:G:50:TRP:CE2	8:G:308:P1O:H16	2.53	0.44
2:G:273:GLY:HA2	3:F:7:ALA:HB1	1.97	0.44
1:I:224:ALA:O	1:I:226:GLU:HG3	2.16	0.44
1:A:34:GLY:HA3	2:C:164:VAL:HB	1.99	0.44
1:E:381:TYR:CE2	3:J:210:LYS:HA	2.52	0.44
1:A:208:ARG:HE	1:A:208:ARG:HB2	1.50	0.44
2:K:149:ALA:O	3:J:39:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:218:PHE:O	2:G:222:PRO:HD2	2.18	0.44
2:K:50:TRP:CE2	8:K:306:P1O:H16	2.53	0.44
2:K:218:PHE:O	2:K:222:PRO:HD2	2.18	0.44
3:F:237:TRP:NE1	5:F:306:D10:C3	2.78	0.44
1:A:258:TYR:CE2	3:B:166:PRO:HG3	2.53	0.44
3:B:236:ARG:HA	3:B:236:ARG:HD3	1.69	0.44
1:E:258:TYR:CE2	3:F:166:PRO:HG3	2.52	0.44
1:E:384:ASP:OD1	1:I:112:ARG:NH2	2.40	0.44
2:C:50:TRP:CE2	8:C:308:P1O:H16	2.53	0.44
2:G:181:TYR:HB2	2:G:182:PRO:HD3	2.00	0.44
3:F:237:TRP:CD2	5:F:306:D10:H72	2.53	0.44
2:C:181:TYR:HB2	2:C:182:PRO:HD3	2.00	0.44
2:G:192:PHE:HZ	2:G:206:ILE:HG23	1.82	0.44
3:J:161:TRP:CE2	6:J:305:PLC:C7	3.01	0.44
2:C:162:THR:HG22	3:B:114:PHE:CE2	2.48	0.43
3:B:161:TRP:CE2	6:B:301:PLC:C7	3.01	0.43
2:G:152:PHE:HB3	2:G:176:GLU:HB2	2.00	0.43
2:K:181:TYR:HB2	2:K:182:PRO:HD3	2.00	0.43
1:E:145:GLN:HA	3:F:196:TYR:CE1	2.53	0.43
1:A:45:ARG:HB3	1:A:74:PHE:CE2	2.52	0.43
2:C:204:LYS:HD2	2:C:204:LYS:O	2.17	0.43
5:B:306:D10:H103	5:F:307:D10:H103	2.00	0.43
2:G:204:LYS:HD2	2:G:204:LYS:O	2.17	0.43
2:K:235:PHE:H	7:K:302:HXG:CAC	2.28	0.43
2:C:152:PHE:HB3	2:C:176:GLU:HB2	2.00	0.43
2:C:181:TYR:HA	2:C:184:TYR:CE2	2.53	0.43
2:G:212:VAL:HA	8:F:308:P1O:C28	2.49	0.43
2:K:115:ARG:HB2	2:K:197:THR:HB	2.00	0.43
1:A:145:GLN:HA	3:B:196:TYR:CE1	2.53	0.43
2:C:115:ARG:HB2	2:C:197:THR:HB	2.00	0.43
3:B:54:TRP:CH2	3:B:197:ILE:HG22	2.54	0.43
2:C:218:PHE:O	2:C:222:PRO:HD2	2.18	0.43
1:E:215:ARG:NH2	3:F:84:ARG:O	2.48	0.43
3:F:161:TRP:CE2	6:F:302:PLC:C7	3.01	0.43
2:K:204:LYS:HD2	2:K:204:LYS:O	2.17	0.43
1:I:224:ALA:O	1:I:226:GLU:N	2.52	0.43
2:G:48:LYS:HE3	2:G:48:LYS:HB2	1.86	0.43
2:G:112:TRP:HH2	8:G:309:P1O:C1	2.26	0.43
2:G:235:PHE:H	7:G:303:HXG:CAC	2.28	0.43
2:K:215:VAL:HB	8:J:301:P1O:H54	2.00	0.43
1:I:292:ARG:HE	1:I:292:ARG:HB3	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:213:ALA:CB	6:F:302:PLC:H12	2.49	0.43
3:J:72:PRO:HB3	3:J:89:ALA:HA	2.01	0.43
1:A:381:TYR:HB2	3:F:210:LYS:HZ2	1.84	0.43
3:B:72:PRO:HB3	3:B:89:ALA:HA	2.01	0.43
3:B:226:LEU:HD11	2:K:251:PHE:CZ	2.54	0.43
2:G:115:ARG:HB2	2:G:197:THR:HB	2.00	0.43
2:G:251:PHE:CZ	3:J:226:LEU:HD11	2.53	0.43
1:A:224:ALA:O	1:A:226:GLU:N	2.52	0.43
2:K:119:LEU:HD23	2:K:119:LEU:HA	1.91	0.43
3:F:54:TRP:CH2	3:F:197:ILE:HG22	2.54	0.43
3:F:245:GLN:HB2	8:F:308:P1O:H1	2.00	0.43
1:A:195:TRP:HB3	3:B:125:VAL:HB	2.01	0.43
3:B:213:ALA:CB	6:B:301:PLC:H12	2.49	0.43
1:I:180:LEU:HD23	1:I:180:LEU:HA	1.83	0.43
3:F:72:PRO:HB3	3:F:89:ALA:HA	2.01	0.43
3:B:138:SER:HA	8:B:302:P1O:C19	2.46	0.42
3:B:237:TRP:NE1	5:B:305:D10:C3	2.78	0.42
2:G:275:GLY:HA3	2:G:276:GLN:HA	1.70	0.42
2:K:181:TYR:HA	2:K:184:TYR:CE2	2.53	0.42
1:E:224:ALA:O	1:E:226:GLU:N	2.52	0.42
3:F:104:ARG:HA	3:F:104:ARG:HD3	1.88	0.42
2:K:112:TRP:CZ2	8:K:307:P1O:H2	2.47	0.42
5:F:307:D10:H103	5:J:310:D10:H103	2.00	0.42
3:J:54:TRP:CH2	3:J:197:ILE:HG22	2.54	0.42
2:C:275:GLY:HA3	2:C:276:GLN:HA	1.70	0.42
2:G:112:TRP:CE2	8:G:309:P1O:C3	3.03	0.42
2:G:181:TYR:HA	2:G:184:TYR:CE2	2.53	0.42
2:K:152:PHE:HB3	2:K:176:GLU:HB2	2.00	0.42
2:K:262:LEU:HD12	2:K:262:LEU:HA	1.72	0.42
1:A:101:LYS:HD2	1:A:101:LYS:HA	1.57	0.42
3:B:59:LEU:HD13	3:B:59:LEU:HA	1.94	0.42
1:I:101:LYS:HD2	1:I:101:LYS:HA	1.57	0.42
3:J:68:LEU:HD23	3:J:68:LEU:HA	1.80	0.42
3:F:104:ARG:HA	3:F:108:PHE:HB2	2.02	0.42
3:J:201:GLU:O	9:J:402:HOH:O	2.22	0.42
3:J:213:ALA:CB	6:J:305:PLC:H12	2.49	0.42
1:A:132:ARG:NH1	9:A:601:HOH:O	2.48	0.42
2:C:212:VAL:HA	8:B:310:P1O:C28	2.50	0.42
3:B:52:SER:HA	3:B:55:LYS:HG3	2.02	0.42
2:G:112:TRP:CZ2	8:G:309:P1O:H6	2.55	0.42
2:K:112:TRP:CZ2	8:K:307:P1O:H6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:ARG:HE	1:E:208:ARG:HB2	1.50	0.42
2:C:235:PHE:H	7:C:303:HXG:CAC	2.28	0.42
6:B:301:PLC:P	6:B:301:PLC:H62	2.60	0.42
6:F:302:PLC:P	6:F:302:PLC:H62	2.60	0.42
3:J:237:TRP:NE1	5:J:309:D10:C3	2.78	0.42
1:A:112:ARG:NH2	1:I:384:ASP:OD1	2.42	0.42
1:E:48:HIS:HE1	1:E:404:GLN:HE21	1.68	0.42
2:C:158:THR:HG22	3:B:108:PHE:CE2	2.54	0.42
3:B:104:ARG:HA	3:B:108:PHE:HB2	2.02	0.42
3:B:155:ILE:HA	3:B:158:PRO:HG2	2.02	0.42
2:K:262:LEU:HD23	3:J:29:VAL:HG23	2.01	0.42
1:I:48:HIS:HE1	1:I:404:GLN:HE21	1.68	0.42
2:C:112:TRP:HB2	8:C:309:P1O:H40	2.02	0.41
3:B:204:THR:HB	2:K:236:MET:SD	2.60	0.41
2:K:112:TRP:CE2	8:K:307:P1O:C3	3.03	0.41
2:K:112:TRP:HB2	8:K:307:P1O:H40	2.02	0.41
2:K:212:VAL:HA	8:J:301:P1O:C28	2.50	0.41
2:K:245:HIS:HB3	3:J:43:LEU:HD13	2.02	0.41
1:I:195:TRP:HB3	3:J:125:VAL:HB	2.02	0.41
3:J:104:ARG:HA	3:J:108:PHE:HB2	2.02	0.41
6:J:305:PLC:P	6:J:305:PLC:H62	2.60	0.41
3:J:52:SER:HA	3:J:55:LYS:HG3	2.02	0.41
2:C:251:PHE:CZ	3:F:226:LEU:HD11	2.54	0.41
2:G:112:TRP:HB2	8:G:309:P1O:H40	2.02	0.41
1:E:195:TRP:HB3	3:F:125:VAL:HB	2.02	0.41
1:I:180:LEU:HD21	3:J:180:ILE:HG23	2.02	0.41
3:F:52:SER:HA	3:F:55:LYS:HG3	2.02	0.41
3:F:150:MET:HA	3:F:221:ALA:HB1	2.03	0.41
1:A:245:LEU:O	1:A:249:MET:HG2	2.21	0.41
2:C:262:LEU:HD23	3:B:29:VAL:HG23	2.02	0.41
1:E:245:LEU:O	1:E:249:MET:HG2	2.21	0.41
2:G:169:PHE:HE2	6:G:305:PLC:H32	1.86	0.41
1:E:97:VAL:HA	1:E:132:ARG:HB2	2.03	0.41
2:C:112:TRP:CE2	8:C:309:P1O:C3	3.03	0.41
8:C:308:P1O:H7	8:C:308:P1O:H1	1.85	0.41
1:E:348:VAL:HB	1:E:351:ASN:HB2	2.03	0.41
1:I:245:LEU:O	1:I:249:MET:HG2	2.21	0.41
1:I:258:TYR:CE2	3:J:166:PRO:HG3	2.55	0.41
1:A:83:GLU:OE2	1:E:270:ARG:NH2	2.53	0.41
1:A:381:TYR:CE2	3:F:210:LYS:HA	2.55	0.41
7:G:303:HXG:OAW	7:G:303:HXG:H40	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:302:HXG:H40	7:K:302:HXG:OAW	2.21	0.41
1:A:48:HIS:HE1	1:A:404:GLN:HE21	1.68	0.41
2:C:112:TRP:CZ2	8:C:309:P1O:H6	2.55	0.41
2:C:175:ILE:O	2:C:179:LEU:HB3	2.21	0.41
7:C:303:HXG:H40	7:C:303:HXG:OAW	2.21	0.41
2:G:175:ILE:O	2:G:179:LEU:HB3	2.21	0.41
2:G:262:LEU:HD23	3:F:29:VAL:HG23	2.02	0.41
2:K:157:GLY:O	2:K:161:GLN:HG2	2.21	0.41
2:K:194:TYR:CE2	2:K:198:ARG:HG3	2.56	0.41
1:I:93:MET:HE3	1:I:93:MET:HB3	1.90	0.41
3:F:30:PHE:O	3:F:34:VAL:HG23	2.21	0.41
3:J:150:MET:HA	3:J:221:ALA:HB1	2.03	0.41
3:J:155:ILE:HA	3:J:158:PRO:HG2	2.02	0.41
2:C:112:TRP:HZ2	8:C:309:P1O:H4	1.86	0.41
2:G:194:TYR:CE2	2:G:198:ARG:HG3	2.56	0.41
1:I:306:ASN:O	1:I:357:GLY:N	2.43	0.41
3:B:205:LEU:HB2	1:I:147:GLY:O	2.21	0.40
2:G:157:GLY:O	2:G:161:GLN:HG2	2.21	0.40
1:E:35:GLU:C	1:E:37:SER:N	2.74	0.40
1:E:83:GLU:OE2	1:I:270:ARG:NH2	2.53	0.40
1:E:319:THR:HG23	1:E:320:ALA:H	1.87	0.40
1:I:103:SER:N	3:J:186:TYR:OH	2.54	0.40
3:F:155:ILE:HA	3:F:158:PRO:HG2	2.02	0.40
3:J:213:ALA:HB1	6:J:305:PLC:O'	2.21	0.40
1:A:103:SER:N	3:B:186:TYR:OH	2.55	0.40
2:C:169:PHE:HE2	6:C:305:PLC:H32	1.86	0.40
5:B:306:D10:H103	5:J:310:D10:H103	2.03	0.40
1:A:256:SER:OG	1:A:257:LYS:N	2.55	0.40
2:C:165:ARG:HE	3:F:206:ARG:HH21	1.70	0.40
2:C:194:TYR:CE2	2:C:198:ARG:HG3	2.56	0.40
6:B:308:PLC:H32	2:K:169:PHE:HE2	1.86	0.40
1:I:319:THR:HG23	1:I:320:ALA:H	1.87	0.40
2:C:277:SER:H	2:C:280:GLU:HG2	1.87	0.40
3:B:150:MET:HA	3:B:221:ALA:HB1	2.03	0.40
2:G:112:TRP:HZ2	8:G:309:P1O:H4	1.86	0.40
8:B:302:P1O:H2	8:B:302:P1O:H12	1.85	0.40
2:K:158:THR:HG22	3:J:108:PHE:CE2	2.57	0.40
1:E:256:SER:OG	1:E:257:LYS:N	2.55	0.40
1:E:292:ARG:HE	1:E:292:ARG:HB3	1.53	0.40
3:F:55:LYS:NZ	9:F:401:HOH:O	2.33	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	380/414 (92%)	366 (96%)	13 (3%)	1 (0%)	41	47
1	E	380/414 (92%)	366 (96%)	13 (3%)	1 (0%)	41	47
1	I	380/414 (92%)	366 (96%)	13 (3%)	1 (0%)	41	47
2	C	234/260 (90%)	211 (90%)	22 (9%)	1 (0%)	34	38
2	G	234/260 (90%)	211 (90%)	22 (9%)	1 (0%)	34	38
2	K	234/260 (90%)	211 (90%)	22 (9%)	1 (0%)	34	38
3	B	239/247 (97%)	228 (95%)	11 (5%)	0	100	100
3	F	239/247 (97%)	228 (95%)	11 (5%)	0	100	100
3	J	239/247 (97%)	228 (95%)	11 (5%)	0	100	100
All	All	2559/2763 (93%)	2415 (94%)	138 (5%)	6 (0%)	50	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	277	SER
2	G	277	SER
2	K	277	SER
1	A	288	ASP
1	E	288	ASP
1	I	288	ASP

### 5.3.2 Protein sidechains

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/345 (94%)	307 (95%)	16 (5%)	24	28
1	E	323/345 (94%)	307 (95%)	16 (5%)	24	28
1	I	323/345 (94%)	307 (95%)	16 (5%)	24	28
2	C	200/212 (94%)	186 (93%)	14 (7%)	15	15
2	G	200/212 (94%)	186 (93%)	14 (7%)	15	15
2	K	200/212 (94%)	186 (93%)	14 (7%)	15	15
3	B	206/210 (98%)	202 (98%)	4 (2%)	57	68
3	F	206/210 (98%)	202 (98%)	4 (2%)	57	68
3	J	206/210 (98%)	202 (98%)	4 (2%)	57	68
All	All	2187/2301 (95%)	2085 (95%)	102 (5%)	30	31

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	36	LYS
1	A	42	MET
1	A	46	THR
1	A	64	THR
1	A	112	ARG
1	A	176	GLN
1	A	225	ASP
1	A	227	LEU
1	A	256	SER
1	A	288	ASP
1	A	359	THR
1	A	363	ASP
1	A	378	ASP
1	A	400	ARG
1	A	414	MET
2	C	49	LYS
2	C	74	TRP
2	C	80	SER
2	C	127	GLU
2	C	158	THR
2	C	159	TRP
2	C	172	SER
2	C	184	TYR
2	C	204	LYS
2	C	210	TYR

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Mol	Chain	Res	Type
2	C	234	TRP
2	C	240	PHE
2	C	268	SER
2	C	269	PHE
3	B	45	MET
3	B	124	LEU
3	B	180	ILE
3	B	195	GLU
2	G	49	LYS
2	G	74	TRP
2	G	80	SER
2	G	127	GLU
2	G	158	THR
2	G	159	TRP
2	G	172	SER
2	G	184	TYR
2	G	204	LYS
2	G	210	TYR
2	G	234	TRP
2	G	240	PHE
2	G	268	SER
2	G	269	PHE
2	K	49	LYS
2	K	74	TRP
2	K	80	SER
2	K	127	GLU
2	K	158	THR
2	K	159	TRP
2	K	172	SER
2	K	184	TYR
2	K	204	LYS
2	K	210	TYR
2	K	234	TRP
2	K	240	PHE
2	K	268	SER
2	K	269	PHE
1	E	33	HIS
1	E	36	LYS
1	E	42	MET
1	E	46	THR
1	E	64	THR
1	E	112	ARG

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Mol	Chain	Res	Type
1	E	176	GLN
1	E	225	ASP
1	E	227	LEU
1	E	256	SER
1	E	288	ASP
1	E	359	THR
1	E	363	ASP
1	E	378	ASP
1	E	400	ARG
1	E	414	MET
1	I	33	HIS
1	I	36	LYS
1	I	42	MET
1	I	46	THR
1	I	64	THR
1	I	112	ARG
1	I	176	GLN
1	I	225	ASP
1	I	227	LEU
1	I	256	SER
1	I	288	ASP
1	I	359	THR
1	I	363	ASP
1	I	378	ASP
1	I	400	ARG
1	I	414	MET
3	F	45	MET
3	F	124	LEU
3	F	180	ILE
3	F	195	GLU
3	J	45	MET
3	J	124	LEU
3	J	180	ILE
3	J	195	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	161	GLN
2	G	161	GLN
2	K	161	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 63 ligands modelled in this entry, 9 are monoatomic - leaving 54 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	$\# Z  > 2$
5	D10	F	305	-	9,9,9	0.21	0	8,8,8	0.56	0
5	D10	F	306	-	9,9,9	0.22	0	8,8,8	0.55	0
8	P1O	B	310	-	37,37,37	0.85	0	43,45,45	0.55	0
5	D10	K	303	-	9,9,9	0.21	0	8,8,8	0.56	0
5	D10	E	503	-	9,9,9	0.21	0	8,8,8	0.55	0
6	PLC	B	308	-	41,41,41	0.84	0	47,49,49	0.58	1 (2%)
7	HXG	C	303	-	29,29,29	0.35	0	35,37,37	0.36	0
6	PLC	F	302	-	41,41,41	1.06	2 (4%)	47,49,49	1.11	3 (6%)
7	HXG	G	303	-	29,29,29	0.35	0	35,37,37	0.36	0
5	D10	B	304	-	9,9,9	0.21	0	8,8,8	0.55	0
8	P1O	G	308	-	37,37,37	1.11	2 (5%)	43,45,45	1.11	3 (6%)
8	P1O	J	301	-	37,37,37	0.86	0	43,45,45	0.55	0
5	D10	J	310	-	9,9,9	0.21	0	8,8,8	0.56	0
5	D10	I	503	-	9,9,9	0.22	0	8,8,8	0.56	0
6	PLC	G	305	-	41,41,41	0.84	0	47,49,49	0.58	1 (2%)
5	D10	B	305	-	9,9,9	0.22	0	8,8,8	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	PLC	J	302	-	41,41,41	0.84	0	47,49,49	0.68	1 (2%)
7	HXG	K	304	-	29,29,29	0.35	0	35,37,37	0.36	0
5	D10	J	307	-	9,9,9	0.21	0	8,8,8	0.56	0
8	P1O	G	309	-	37,37,37	1.12	2 (5%)	43,45,45	1.12	3 (6%)
6	PLC	G	307	-	41,41,41	0.85	0	47,49,49	0.68	2 (4%)
6	PLC	F	301	-	41,41,41	0.81	0	47,49,49	0.74	1 (2%)
7	HXG	K	302	-	29,29,29	0.34	0	35,37,37	0.36	0
5	D10	J	308	-	9,9,9	0.21	0	8,8,8	0.55	0
6	PLC	J	305	-	41,41,41	1.06	2 (4%)	47,49,49	1.11	3 (6%)
5	D10	F	307	-	9,9,9	0.21	0	8,8,8	0.56	0
5	D10	J	309	-	9,9,9	0.22	0	8,8,8	0.55	0
5	D10	F	304	-	9,9,9	0.21	0	8,8,8	0.56	0
6	PLC	B	301	-	41,41,41	1.06	2 (4%)	47,49,49	1.11	3 (6%)
5	D10	A	503	-	9,9,9	0.21	0	8,8,8	0.55	0
8	P1O	K	307	-	37,37,37	1.12	2 (5%)	43,45,45	1.12	3 (6%)
6	PLC	G	301	-	41,41,41	1.05	2 (4%)	47,49,49	1.04	3 (6%)
8	P1O	F	308	-	37,37,37	0.85	0	43,45,45	0.55	0
8	P1O	K	306	-	37,37,37	1.11	2 (5%)	43,45,45	1.11	3 (6%)
8	P1O	F	303	-	37,37,37	1.11	2 (5%)	43,45,45	1.10	3 (6%)
6	PLC	J	304	-	41,41,41	0.81	0	47,49,49	0.74	1 (2%)
8	P1O	C	308	-	37,37,37	1.11	2 (5%)	43,45,45	1.11	3 (6%)
6	PLC	C	302	-	41,41,41	0.83	0	47,49,49	0.68	1 (2%)
5	D10	G	304	-	9,9,9	0.21	0	8,8,8	0.56	0
8	P1O	J	306	-	37,37,37	1.11	2 (5%)	43,45,45	1.10	3 (6%)
6	PLC	C	305	-	41,41,41	0.84	0	47,49,49	0.58	1 (2%)
6	PLC	C	310	-	41,41,41	1.05	2 (4%)	47,49,49	1.04	3 (6%)
6	PLC	C	307	-	41,41,41	0.85	0	47,49,49	0.68	2 (4%)
6	PLC	B	309	-	41,41,41	0.81	0	47,49,49	0.74	1 (2%)
5	D10	B	306	-	9,9,9	0.21	0	8,8,8	0.56	0
7	HXG	C	306	-	29,29,29	0.35	0	35,37,37	0.36	0
8	P1O	C	309	-	37,37,37	1.11	2 (5%)	43,45,45	1.12	3 (6%)
8	P1O	B	302	-	37,37,37	1.11	2 (5%)	43,45,45	1.10	3 (6%)
6	PLC	B	307	-	41,41,41	0.84	0	47,49,49	0.68	1 (2%)
5	D10	B	303	-	9,9,9	0.21	0	8,8,8	0.56	0
6	PLC	K	305	-	41,41,41	0.85	0	47,49,49	0.68	2 (4%)
7	HXG	G	306	-	29,29,29	0.35	0	35,37,37	0.36	0
5	D10	C	304	-	9,9,9	0.21	0	8,8,8	0.56	0
6	PLC	J	303	-	41,41,41	1.05	2 (4%)	47,49,49	1.04	3 (6%)

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
5	D10	F	305	-	-	2/7/7/7	-
5	D10	F	306	-	-	6/7/7/7	-
8	P1O	B	310	-	-	13/41/41/41	-
5	D10	K	303	-	-	0/7/7/7	-
5	D10	E	503	-	-	0/7/7/7	-
6	PLC	B	308	-	-	9/45/45/45	-
7	HXG	C	303	-	-	9/33/33/33	-
6	PLC	F	302	-	-	29/45/45/45	-
7	HXG	G	303	-	-	9/33/33/33	-
5	D10	B	304	-	-	2/7/7/7	-
8	P1O	G	308	-	-	19/41/41/41	-
8	P1O	J	301	-	-	13/41/41/41	-
5	D10	J	310	-	-	5/7/7/7	-
5	D10	I	503	-	-	0/7/7/7	-
6	PLC	G	305	-	-	9/45/45/45	-
5	D10	B	305	-	-	6/7/7/7	-
6	PLC	J	302	-	-	13/45/45/45	-
7	HXG	K	304	-	-	7/33/33/33	-
5	D10	J	307	-	-	0/7/7/7	-
8	P1O	G	309	-	-	26/41/41/41	-
6	PLC	G	307	-	-	17/45/45/45	-
6	PLC	F	301	-	-	14/45/45/45	-
7	HXG	K	302	-	-	9/33/33/33	-
5	D10	J	308	-	-	2/7/7/7	-
6	PLC	J	305	-	-	29/45/45/45	-
5	D10	F	307	-	-	5/7/7/7	-
5	D10	J	309	-	-	6/7/7/7	-
5	D10	F	304	-	-	0/7/7/7	-
6	PLC	B	301	-	-	28/45/45/45	-
5	D10	A	503	-	-	0/7/7/7	-
8	P1O	K	307	-	-	26/41/41/41	-
6	PLC	G	301	-	-	26/45/45/45	-
8	P1O	F	308	-	-	13/41/41/41	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	P1O	K	306	-	-	18/41/41/41	-
8	P1O	F	303	-	-	25/41/41/41	-
6	PLC	J	304	-	-	14/45/45/45	-
8	P1O	C	308	-	-	19/41/41/41	-
6	PLC	C	302	-	-	12/45/45/45	-
5	D10	G	304	-	-	0/7/7/7	-
8	P1O	J	306	-	-	25/41/41/41	-
6	PLC	C	305	-	-	9/45/45/45	-
6	PLC	C	310	-	-	26/45/45/45	-
6	PLC	C	307	-	-	17/45/45/45	-
6	PLC	B	309	-	-	14/45/45/45	-
5	D10	B	306	-	-	5/7/7/7	-
7	HXG	C	306	-	-	7/33/33/33	-
8	P1O	C	309	-	-	26/41/41/41	-
8	P1O	B	302	-	-	25/41/41/41	-
6	PLC	B	307	-	-	12/45/45/45	-
5	D10	B	303	-	-	0/7/7/7	-
6	PLC	K	305	-	-	17/45/45/45	-
7	HXG	G	306	-	-	7/33/33/33	-
5	D10	C	304	-	-	0/7/7/7	-
6	PLC	J	303	-	-	26/45/45/45	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	306	P1O	O5-C9	4.31	1.45	1.33
8	B	302	P1O	O5-C9	4.30	1.45	1.33
8	G	308	P1O	O5-C9	4.30	1.45	1.33
8	F	303	P1O	O5-C9	4.29	1.45	1.33
6	J	303	PLC	O3-CB	4.29	1.45	1.33
8	K	306	P1O	O5-C9	4.29	1.45	1.33
6	C	310	PLC	O3-CB	4.28	1.45	1.33
6	G	301	PLC	O3-CB	4.28	1.45	1.33
8	C	308	P1O	O5-C9	4.28	1.45	1.33
6	B	301	PLC	O3-CB	4.27	1.45	1.33
6	F	302	PLC	O3-CB	4.26	1.45	1.33
8	G	309	P1O	O5-C9	4.26	1.45	1.33
6	J	305	PLC	O3-CB	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	K	307	P1O	O5-C9	4.24	1.45	1.33
8	C	309	P1O	O5-C9	4.23	1.45	1.33
8	G	309	P1O	O7-C19	4.15	1.46	1.34
6	F	302	PLC	O2-C'	4.15	1.46	1.34
6	J	305	PLC	O2-C'	4.14	1.46	1.34
8	K	307	P1O	O7-C19	4.14	1.46	1.34
8	C	309	P1O	O7-C19	4.13	1.46	1.34
6	B	301	PLC	O2-C'	4.12	1.45	1.34
8	F	303	P1O	O7-C19	4.09	1.45	1.34
6	C	310	PLC	O2-C'	4.09	1.45	1.34
6	G	301	PLC	O2-C'	4.09	1.45	1.34
8	B	302	P1O	O7-C19	4.08	1.45	1.34
6	J	303	PLC	O2-C'	4.08	1.45	1.34
8	K	306	P1O	O7-C19	4.07	1.45	1.34
8	J	306	P1O	O7-C19	4.06	1.45	1.34
8	G	308	P1O	O7-C19	4.05	1.45	1.34
8	C	308	P1O	O7-C19	4.05	1.45	1.34

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	309	P1O	O7-C19-C20	4.17	120.49	111.50
8	G	309	P1O	O7-C19-C20	4.16	120.47	111.50
8	J	306	P1O	O7-C19-C20	4.16	120.46	111.50
8	K	307	P1O	O7-C19-C20	4.15	120.45	111.50
8	C	308	P1O	O7-C19-C20	4.15	120.44	111.50
8	F	303	P1O	O7-C19-C20	4.14	120.43	111.50
8	K	306	P1O	O7-C19-C20	4.14	120.42	111.50
8	B	302	P1O	O7-C19-C20	4.13	120.41	111.50
8	G	308	P1O	O7-C19-C20	4.13	120.41	111.50
6	C	310	PLC	O2-C'-C1'	4.09	120.31	111.50
6	J	303	PLC	O2-C'-C1'	4.08	120.30	111.50
6	G	301	PLC	O2-C'-C1'	4.08	120.29	111.50
6	B	301	PLC	O2-C'-C1'	3.95	120.02	111.50
6	J	305	PLC	O2-C'-C1'	3.94	120.00	111.50
6	F	302	PLC	O2-C'-C1'	3.94	119.99	111.50
6	B	309	PLC	O2-C'-C1'	3.70	119.47	111.50
6	F	301	PLC	O2-C'-C1'	3.68	119.44	111.50
6	J	304	PLC	O2-C'-C1'	3.68	119.42	111.50
6	C	302	PLC	O2-C'-C1'	3.10	118.18	111.50
6	B	307	PLC	O2-C'-C1'	3.10	118.17	111.50
6	J	302	PLC	O2-C'-C1'	3.08	118.14	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	307	PLC	O2-C'-C1'	2.98	117.91	111.50
6	K	305	PLC	O2-C'-C1'	2.97	117.91	111.50
6	C	307	PLC	O2-C'-C1'	2.96	117.88	111.50
6	F	302	PLC	CB'-CA'-C9'	2.79	134.60	113.42
6	B	301	PLC	CB'-CA'-C9'	2.79	134.58	113.42
6	J	305	PLC	CB'-CA'-C9'	2.78	134.53	113.42
6	F	302	PLC	O3-CB-C1B	2.70	120.37	111.91
6	B	301	PLC	O3-CB-C1B	2.69	120.36	111.91
8	F	303	P1O	O5-C9-C10	2.69	120.36	111.91
6	J	305	PLC	O3-CB-C1B	2.69	120.33	111.91
8	J	306	P1O	O5-C9-C10	2.69	120.33	111.91
8	B	302	P1O	O5-C9-C10	2.68	120.33	111.91
6	J	303	PLC	O3-CB-C1B	2.68	120.33	111.91
6	C	310	PLC	O3-CB-C1B	2.68	120.31	111.91
6	G	301	PLC	O3-CB-C1B	2.67	120.29	111.91
8	G	308	P1O	O5-C9-C10	2.67	120.28	111.91
8	C	308	P1O	O5-C9-C10	2.67	120.28	111.91
8	K	306	P1O	O5-C9-C10	2.66	120.27	111.91
8	G	309	P1O	O5-C9-C10	2.62	120.14	111.91
8	K	307	P1O	O5-C9-C10	2.62	120.12	111.91
8	C	309	P1O	O5-C9-C10	2.61	120.11	111.91
8	G	309	P1O	C7-O7-C19	-2.40	111.88	117.79
8	C	309	P1O	C7-O7-C19	-2.39	111.92	117.79
8	K	307	P1O	C7-O7-C19	-2.39	111.92	117.79
6	B	308	PLC	O2-C'-C1'	2.37	116.61	111.50
6	C	305	PLC	O2-C'-C1'	2.37	116.61	111.50
6	G	305	PLC	O2-C'-C1'	2.36	116.58	111.50
8	J	306	P1O	C7-O7-C19	-2.32	112.08	117.79
8	B	302	P1O	C7-O7-C19	-2.32	112.09	117.79
8	F	303	P1O	C7-O7-C19	-2.31	112.10	117.79
6	G	307	PLC	O2-C'-O'	-2.24	118.28	123.70
6	K	305	PLC	O2-C'-O'	-2.24	118.28	123.70
8	K	306	P1O	C7-O7-C19	-2.23	112.29	117.79
6	C	307	PLC	O2-C'-O'	-2.22	118.34	123.70
8	C	308	P1O	C7-O7-C19	-2.22	112.33	117.79
8	G	308	P1O	C7-O7-C19	-2.20	112.37	117.79
6	J	303	PLC	C2-O2-C'	-2.11	112.61	117.79
6	G	301	PLC	C2-O2-C'	-2.10	112.63	117.79
6	C	310	PLC	C2-O2-C'	-2.10	112.63	117.79

There are no chirality outliers.

All (656) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	302	PLC	O4P-C4-C5-N
6	C	302	PLC	C1'-C'-O2-C2
6	C	307	PLC	C1'-C'-O2-C2
6	C	307	PLC	O'-C'-O2-C2
6	C	307	PLC	C1-O3P-P-O1P
6	C	310	PLC	C1'-C'-O2-C2
6	C	310	PLC	C4-O4P-P-O3P
6	B	301	PLC	C4-O4P-P-O2P
6	B	307	PLC	O4P-C4-C5-N
6	B	307	PLC	C1'-C'-O2-C2
6	B	309	PLC	C1'-C'-O2-C2
6	B	309	PLC	C1-O3P-P-O1P
6	B	309	PLC	C4-O4P-P-O1P
6	G	301	PLC	C1'-C'-O2-C2
6	G	301	PLC	C4-O4P-P-O3P
6	G	307	PLC	C1'-C'-O2-C2
6	G	307	PLC	O'-C'-O2-C2
6	G	307	PLC	C1-O3P-P-O1P
6	K	305	PLC	C1'-C'-O2-C2
6	K	305	PLC	O'-C'-O2-C2
6	K	305	PLC	C1-O3P-P-O1P
6	F	301	PLC	C1'-C'-O2-C2
6	F	301	PLC	C1-O3P-P-O1P
6	F	301	PLC	C4-O4P-P-O1P
6	F	302	PLC	C4-O4P-P-O2P
6	J	302	PLC	O4P-C4-C5-N
6	J	302	PLC	C1'-C'-O2-C2
6	J	303	PLC	C1'-C'-O2-C2
6	J	303	PLC	C4-O4P-P-O3P
6	J	304	PLC	C1'-C'-O2-C2
6	J	304	PLC	C1-O3P-P-O1P
6	J	304	PLC	C4-O4P-P-O1P
6	J	305	PLC	C4-O4P-P-O2P
7	C	303	HXG	CAU-OAX-PBD-OAW
7	C	306	HXG	OAW-CAP-CAS-NBC
7	G	303	HXG	CAU-OAX-PBD-OAW
7	G	306	HXG	OAW-CAP-CAS-NBC
7	K	302	HXG	CAU-OAX-PBD-OAW
7	K	304	HXG	OAW-CAP-CAS-NBC
8	C	308	P1O	C1-O3-P1-O1
8	C	308	P1O	C2-C1-O3-P1
8	C	308	P1O	O3-C1-C2-N1
8	C	308	P1O	O6-C9-O5-C8

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Mol	Chain	Res	Type	Atoms
8	C	308	P1O	C10-C9-O5-C8
8	C	308	P1O	O8-C19-O7-C7
8	C	309	P1O	C1-O3-P1-O1
8	C	309	P1O	C1-O3-P1-O2
8	C	309	P1O	C6-O4-P1-O1
8	C	309	P1O	C6-O4-P1-O2
8	B	302	P1O	C1-O3-P1-O1
8	B	302	P1O	C1-O3-P1-O2
8	B	302	P1O	C1-O3-P1-O4
8	B	302	P1O	C6-O4-P1-O1
8	B	302	P1O	C6-O4-P1-O2
8	B	310	P1O	C20-C19-O7-C7
8	G	308	P1O	C1-O3-P1-O1
8	G	308	P1O	C2-C1-O3-P1
8	G	308	P1O	O3-C1-C2-N1
8	G	308	P1O	O6-C9-O5-C8
8	G	308	P1O	C10-C9-O5-C8
8	G	308	P1O	O8-C19-O7-C7
8	G	309	P1O	C1-O3-P1-O1
8	G	309	P1O	C1-O3-P1-O2
8	G	309	P1O	C6-O4-P1-O1
8	G	309	P1O	C6-O4-P1-O2
8	K	306	P1O	C1-O3-P1-O1
8	K	306	P1O	C2-C1-O3-P1
8	K	306	P1O	O3-C1-C2-N1
8	K	306	P1O	O6-C9-O5-C8
8	K	306	P1O	C10-C9-O5-C8
8	K	306	P1O	O8-C19-O7-C7
8	K	307	P1O	C1-O3-P1-O1
8	K	307	P1O	C1-O3-P1-O2
8	K	307	P1O	C6-O4-P1-O1
8	K	307	P1O	C6-O4-P1-O2
8	F	303	P1O	C1-O3-P1-O1
8	F	303	P1O	C1-O3-P1-O2
8	F	303	P1O	C1-O3-P1-O4
8	F	303	P1O	C6-O4-P1-O1
8	F	303	P1O	C6-O4-P1-O2
8	F	308	P1O	C20-C19-O7-C7
8	J	301	P1O	C20-C19-O7-C7
8	J	306	P1O	C1-O3-P1-O1
8	J	306	P1O	C1-O3-P1-O2
8	J	306	P1O	C1-O3-P1-O4

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Mol	Chain	Res	Type	Atoms
8	J	306	P1O	C6-O4-P1-O1
8	J	306	P1O	C6-O4-P1-O2
6	C	302	PLC	OB-CB-O3-C3
6	C	307	PLC	OB-CB-O3-C3
6	B	301	PLC	OB-CB-O3-C3
6	B	307	PLC	OB-CB-O3-C3
6	G	307	PLC	OB-CB-O3-C3
6	K	305	PLC	OB-CB-O3-C3
6	F	302	PLC	OB-CB-O3-C3
6	J	302	PLC	OB-CB-O3-C3
6	J	305	PLC	OB-CB-O3-C3
6	C	302	PLC	C1B-CB-O3-C3
6	C	307	PLC	C1B-CB-O3-C3
6	B	301	PLC	C1B-CB-O3-C3
6	B	307	PLC	C1B-CB-O3-C3
6	G	307	PLC	C1B-CB-O3-C3
6	K	305	PLC	C1B-CB-O3-C3
6	F	302	PLC	C1B-CB-O3-C3
6	J	302	PLC	C1B-CB-O3-C3
6	J	305	PLC	C1B-CB-O3-C3
8	B	302	P1O	C10-C9-O5-C8
8	F	303	P1O	C10-C9-O5-C8
8	J	306	P1O	C10-C9-O5-C8
6	B	309	PLC	OB-CB-O3-C3
6	F	301	PLC	OB-CB-O3-C3
6	J	304	PLC	OB-CB-O3-C3
8	B	302	P1O	O6-C9-O5-C8
8	F	303	P1O	O6-C9-O5-C8
8	J	306	P1O	O6-C9-O5-C8
6	C	302	PLC	O'-C'-O2-C2
6	C	305	PLC	O'-C'-O2-C2
6	C	310	PLC	O'-C'-O2-C2
6	B	307	PLC	O'-C'-O2-C2
6	B	308	PLC	O'-C'-O2-C2
6	G	301	PLC	O'-C'-O2-C2
6	G	305	PLC	O'-C'-O2-C2
6	J	302	PLC	O'-C'-O2-C2
6	J	303	PLC	O'-C'-O2-C2
8	B	310	P1O	O8-C19-O7-C7
8	F	308	P1O	O8-C19-O7-C7
8	J	301	P1O	O8-C19-O7-C7
6	B	309	PLC	C1B-CB-O3-C3

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Mol	Chain	Res	Type	Atoms
6	F	301	PLC	C1B-CB-O3-C3
6	J	304	PLC	C1B-CB-O3-C3
6	C	305	PLC	C1'-C'-O2-C2
6	B	308	PLC	C1'-C'-O2-C2
6	G	305	PLC	C1'-C'-O2-C2
8	C	308	P1O	C20-C19-O7-C7
8	G	308	P1O	C20-C19-O7-C7
8	K	306	P1O	C20-C19-O7-C7
6	B	309	PLC	O'-C'-O2-C2
6	F	301	PLC	O'-C'-O2-C2
6	J	304	PLC	O'-C'-O2-C2
6	C	305	PLC	OB-CB-O3-C3
6	B	308	PLC	OB-CB-O3-C3
6	G	305	PLC	OB-CB-O3-C3
6	C	310	PLC	C4-C5-N-C6
6	G	301	PLC	C4-C5-N-C6
6	C	305	PLC	C1B-CB-O3-C3
6	B	308	PLC	C1B-CB-O3-C3
6	G	305	PLC	C1B-CB-O3-C3
6	J	303	PLC	C4-C5-N-C6
6	C	310	PLC	C1B-CB-O3-C3
6	G	301	PLC	C1B-CB-O3-C3
6	J	303	PLC	C1B-CB-O3-C3
8	B	310	P1O	C10-C9-O5-C8
8	F	308	P1O	C10-C9-O5-C8
8	J	301	P1O	C10-C9-O5-C8
8	C	308	P1O	C9-C10-C11-C12
8	G	308	P1O	C9-C10-C11-C12
8	K	306	P1O	C9-C10-C11-C12
7	C	303	HXG	CAL-CAN-CAQ-CAZ
7	G	303	HXG	CAL-CAN-CAQ-CAZ
7	K	302	HXG	CAL-CAN-CAQ-CAZ
8	C	309	P1O	C10-C9-O5-C8
8	G	309	P1O	C10-C9-O5-C8
8	K	307	P1O	C10-C9-O5-C8
6	B	301	PLC	CB-C1B-C2B-C3B
6	F	302	PLC	CB-C1B-C2B-C3B
6	J	305	PLC	CB-C1B-C2B-C3B
7	C	306	HXG	CAM-CAO-CAR-CBA
7	G	306	HXG	CAM-CAO-CAR-CBA
7	K	304	HXG	CAM-CAO-CAR-CBA
8	C	309	P1O	C7-C6-O4-P1

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Mol	Chain	Res	Type	Atoms
8	G	309	P1O	C7-C6-O4-P1
8	K	307	P1O	C7-C6-O4-P1
6	C	310	PLC	OB-CB-O3-C3
6	G	301	PLC	OB-CB-O3-C3
6	J	303	PLC	OB-CB-O3-C3
8	B	310	P1O	O6-C9-O5-C8
8	F	308	P1O	O6-C9-O5-C8
8	J	301	P1O	O6-C9-O5-C8
6	C	305	PLC	C4-O4P-P-O3P
6	B	301	PLC	C4-O4P-P-O3P
6	B	308	PLC	C4-O4P-P-O3P
6	G	305	PLC	C4-O4P-P-O3P
6	F	302	PLC	C4-O4P-P-O3P
6	J	305	PLC	C4-O4P-P-O3P
7	C	303	HXG	CAP-OAW-PBD-OAX
7	G	303	HXG	CAP-OAW-PBD-OAX
7	K	302	HXG	CAP-OAW-PBD-OAX
8	C	308	P1O	C1-O3-P1-O4
8	C	308	P1O	C6-O4-P1-O3
8	C	309	P1O	C1-O3-P1-O4
8	C	309	P1O	C6-O4-P1-O3
8	B	302	P1O	C6-O4-P1-O3
8	G	308	P1O	C1-O3-P1-O4
8	G	308	P1O	C6-O4-P1-O3
8	G	309	P1O	C1-O3-P1-O4
8	G	309	P1O	C6-O4-P1-O3
8	K	306	P1O	C1-O3-P1-O4
8	K	306	P1O	C6-O4-P1-O3
8	K	307	P1O	C1-O3-P1-O4
8	K	307	P1O	C6-O4-P1-O3
8	F	303	P1O	C6-O4-P1-O3
8	J	306	P1O	C6-O4-P1-O3
6	C	310	PLC	CB-C1B-C2B-C3B
6	G	301	PLC	CB-C1B-C2B-C3B
6	J	303	PLC	CB-C1B-C2B-C3B
6	C	310	PLC	C4-C5-N-C7
6	G	301	PLC	C4-C5-N-C7
6	J	303	PLC	C4-C5-N-C7
8	B	302	P1O	C20-C19-O7-C7
8	F	303	P1O	C20-C19-O7-C7
8	J	306	P1O	C20-C19-O7-C7
6	C	310	PLC	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
6	G	301	PLC	C2B-C3B-C4B-C5B
6	J	303	PLC	C2B-C3B-C4B-C5B
8	C	308	P1O	C21-C22-C23-C24
8	C	309	P1O	C13-C14-C15-C16
8	B	302	P1O	C11-C12-C13-C14
8	G	308	P1O	C21-C22-C23-C24
8	K	306	P1O	C21-C22-C23-C24
8	K	307	P1O	C13-C14-C15-C16
8	F	303	P1O	C11-C12-C13-C14
8	J	306	P1O	C11-C12-C13-C14
6	B	301	PLC	C7'-C8'-C9'-CA'
6	F	302	PLC	C7'-C8'-C9'-CA'
6	J	305	PLC	C7'-C8'-C9'-CA'
8	G	309	P1O	C13-C14-C15-C16
8	B	302	P1O	O8-C19-O7-C7
8	F	303	P1O	O8-C19-O7-C7
8	J	306	P1O	O8-C19-O7-C7
6	B	301	PLC	C3B-C4B-C5B-C6B
6	F	302	PLC	C3B-C4B-C5B-C6B
6	J	305	PLC	C3B-C4B-C5B-C6B
8	C	309	P1O	O6-C9-O5-C8
8	G	309	P1O	O6-C9-O5-C8
8	K	307	P1O	O6-C9-O5-C8
5	B	305	D10	C5-C6-C7-C8
5	F	306	D10	C5-C6-C7-C8
5	J	309	D10	C5-C6-C7-C8
6	C	310	PLC	C3B-C4B-C5B-C6B
6	G	301	PLC	C3B-C4B-C5B-C6B
6	J	303	PLC	C3B-C4B-C5B-C6B
8	C	309	P1O	C24-C25-C26-C27
8	B	302	P1O	C21-C22-C23-C24
8	G	309	P1O	C24-C25-C26-C27
8	F	303	P1O	C21-C22-C23-C24
8	J	306	P1O	C21-C22-C23-C24
8	K	307	P1O	C24-C25-C26-C27
8	J	306	P1O	C13-C14-C15-C16
6	B	301	PLC	O'-C'-O2-C2
6	F	302	PLC	O'-C'-O2-C2
6	J	305	PLC	O'-C'-O2-C2
6	B	301	PLC	C1'-C'-O2-C2
6	F	302	PLC	C1'-C'-O2-C2
6	J	305	PLC	C1'-C'-O2-C2

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Mol	Chain	Res	Type	Atoms
8	B	302	P1O	C13-C14-C15-C16
8	F	303	P1O	C13-C14-C15-C16
6	B	309	PLC	C'-C1'-C2'-C3'
6	F	301	PLC	C'-C1'-C2'-C3'
6	J	304	PLC	C'-C1'-C2'-C3'
6	C	310	PLC	C4-C5-N-C8
6	G	301	PLC	C4-C5-N-C8
6	J	303	PLC	C4-C5-N-C8
6	G	301	PLC	C4B-C5B-C6B-C7B
6	C	310	PLC	C4B-C5B-C6B-C7B
6	J	303	PLC	C4B-C5B-C6B-C7B
6	C	310	PLC	C6'-C7'-C8'-C9'
6	B	301	PLC	C1'-C2'-C3'-C4'
6	G	301	PLC	C6'-C7'-C8'-C9'
6	J	303	PLC	C6'-C7'-C8'-C9'
6	F	302	PLC	C1'-C2'-C3'-C4'
6	J	305	PLC	C1'-C2'-C3'-C4'
7	C	303	HXG	CAR-CBA-OAY-CBB
7	G	303	HXG	CAR-CBA-OAY-CBB
7	K	302	HXG	CAR-CBA-OAY-CBB
5	B	306	D10	C5-C6-C7-C8
5	F	307	D10	C5-C6-C7-C8
5	J	310	D10	C5-C6-C7-C8
8	G	309	P1O	C21-C22-C23-C24
8	K	307	P1O	C21-C22-C23-C24
8	C	309	P1O	C21-C22-C23-C24
8	C	309	P1O	C12-C13-C14-C15
8	G	309	P1O	C12-C13-C14-C15
8	K	307	P1O	C12-C13-C14-C15
6	C	310	PLC	C4'-C5'-C6'-C7'
6	B	301	PLC	C1B-C2B-C3B-C4B
6	G	301	PLC	C4'-C5'-C6'-C7'
6	F	302	PLC	C1B-C2B-C3B-C4B
6	J	303	PLC	C4'-C5'-C6'-C7'
6	J	305	PLC	C1B-C2B-C3B-C4B
8	B	302	P1O	C23-C24-C25-C26
8	F	303	P1O	C23-C24-C25-C26
8	J	306	P1O	C23-C24-C25-C26
8	C	309	P1O	C10-C11-C12-C13
8	G	309	P1O	C10-C11-C12-C13
8	K	307	P1O	C10-C11-C12-C13
7	C	303	HXG	OAG-CBA-OAY-CBB

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Mol	Chain	Res	Type	Atoms
7	G	303	HXG	OAG-CBA-OAY-CBB
7	K	302	HXG	OAG-CBA-OAY-CBB
8	C	309	P1O	C20-C19-O7-C7
8	G	309	P1O	C20-C19-O7-C7
8	K	307	P1O	C20-C19-O7-C7
6	C	307	PLC	C4'-C5'-C6'-C7'
6	K	305	PLC	C4'-C5'-C6'-C7'
6	G	307	PLC	C4'-C5'-C6'-C7'
8	C	309	P1O	O8-C19-O7-C7
8	G	309	P1O	O8-C19-O7-C7
8	K	307	P1O	O8-C19-O7-C7
5	B	304	D10	C5-C6-C7-C8
5	B	305	D10	C4-C5-C6-C7
5	B	306	D10	C4-C5-C6-C7
5	F	305	D10	C5-C6-C7-C8
5	F	306	D10	C4-C5-C6-C7
5	F	307	D10	C4-C5-C6-C7
5	J	308	D10	C5-C6-C7-C8
5	J	309	D10	C4-C5-C6-C7
5	J	310	D10	C4-C5-C6-C7
8	B	310	P1O	C22-C23-C24-C25
6	C	302	PLC	C1-O3P-P-O4P
6	B	307	PLC	C1-O3P-P-O4P
6	J	302	PLC	C1-O3P-P-O4P
8	F	308	P1O	C22-C23-C24-C25
8	J	301	P1O	C22-C23-C24-C25
8	C	308	P1O	C22-C23-C24-C25
8	G	308	P1O	C22-C23-C24-C25
7	C	303	HXG	OAX-CAU-CBB-CAT
7	G	303	HXG	OAX-CAU-CBB-CAT
7	K	302	HXG	OAX-CAU-CBB-CAT
8	B	302	P1O	C20-C21-C22-C23
8	K	306	P1O	C22-C23-C24-C25
8	F	303	P1O	C20-C21-C22-C23
8	J	306	P1O	C20-C21-C22-C23
6	B	301	PLC	C2'-C3'-C4'-C5'
5	B	306	D10	C6-C7-C8-C9
5	F	307	D10	C6-C7-C8-C9
5	J	310	D10	C6-C7-C8-C9
6	F	302	PLC	C2'-C3'-C4'-C5'
6	J	305	PLC	C2'-C3'-C4'-C5'
6	J	303	PLC	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
6	C	310	PLC	C6B-C7B-C8B-C9B
6	G	301	PLC	C6B-C7B-C8B-C9B
6	B	301	PLC	C5'-C6'-C7'-C8'
6	F	302	PLC	C5'-C6'-C7'-C8'
6	J	305	PLC	C5'-C6'-C7'-C8'
6	C	307	PLC	C7'-C8'-C9'-CA'
6	G	307	PLC	C7'-C8'-C9'-CA'
6	K	305	PLC	C7'-C8'-C9'-CA'
5	J	310	D10	C2-C3-C4-C5
6	C	307	PLC	C1B-C2B-C3B-C4B
6	G	307	PLC	C1B-C2B-C3B-C4B
5	B	305	D10	C2-C3-C4-C5
5	B	306	D10	C2-C3-C4-C5
5	F	306	D10	C2-C3-C4-C5
5	F	307	D10	C2-C3-C4-C5
5	J	309	D10	C2-C3-C4-C5
6	K	305	PLC	C1B-C2B-C3B-C4B
6	C	310	PLC	C7B-C8B-C9B-CAA
6	G	301	PLC	C7B-C8B-C9B-CAA
6	J	303	PLC	C7B-C8B-C9B-CAA
5	F	306	D10	C6-C7-C8-C9
5	J	309	D10	C6-C7-C8-C9
5	B	305	D10	C6-C7-C8-C9
6	B	301	PLC	O3P-C1-C2-C3
6	F	302	PLC	O3P-C1-C2-C3
6	J	305	PLC	O3P-C1-C2-C3
8	C	309	P1O	O4-C6-C7-C8
8	G	309	P1O	O4-C6-C7-C8
8	K	307	P1O	O4-C6-C7-C8
8	B	310	P1O	C7-C6-O4-P1
8	F	308	P1O	C7-C6-O4-P1
8	J	301	P1O	C7-C6-O4-P1
8	C	309	P1O	C19-C20-C21-C22
8	G	309	P1O	C19-C20-C21-C22
8	K	307	P1O	C19-C20-C21-C22
8	B	302	P1O	C12-C13-C14-C15
8	F	303	P1O	C12-C13-C14-C15
8	J	306	P1O	C12-C13-C14-C15
6	B	301	PLC	C4'-C5'-C6'-C7'
6	F	302	PLC	C4'-C5'-C6'-C7'
6	J	305	PLC	C4'-C5'-C6'-C7'
8	C	309	P1O	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
8	K	307	P1O	C15-C16-C17-C18
8	G	309	P1O	C15-C16-C17-C18
5	B	305	D10	C3-C4-C5-C6
5	F	306	D10	C3-C4-C5-C6
5	J	309	D10	C3-C4-C5-C6
6	C	307	PLC	C2-C1-O3P-P
6	G	307	PLC	C2-C1-O3P-P
6	K	305	PLC	C2-C1-O3P-P
6	C	310	PLC	O3P-C1-C2-C3
6	G	301	PLC	O3P-C1-C2-C3
6	J	303	PLC	O3P-C1-C2-C3
8	C	309	P1O	C14-C15-C16-C17
8	C	309	P1O	C22-C23-C24-C25
8	G	309	P1O	C14-C15-C16-C17
8	G	309	P1O	C22-C23-C24-C25
8	K	307	P1O	C14-C15-C16-C17
8	K	307	P1O	C22-C23-C24-C25
8	C	308	P1O	C11-C12-C13-C14
8	G	308	P1O	C11-C12-C13-C14
8	K	306	P1O	C11-C12-C13-C14
6	C	310	PLC	C3-C2-O2-C'
6	G	301	PLC	C3-C2-O2-C'
6	J	303	PLC	C3-C2-O2-C'
7	C	306	HXG	CAT-CBB-OAY-CBA
7	G	306	HXG	CAT-CBB-OAY-CBA
7	K	304	HXG	CAT-CBB-OAY-CBA
8	B	310	P1O	C6-C7-O7-C19
8	F	308	P1O	C6-C7-O7-C19
8	J	301	P1O	C6-C7-O7-C19
8	J	306	P1O	C9-C10-C11-C12
8	F	303	P1O	C9-C10-C11-C12
6	C	310	PLC	O3P-C1-C2-O2
6	B	301	PLC	O3P-C1-C2-O2
6	G	301	PLC	O3P-C1-C2-O2
6	F	302	PLC	O3P-C1-C2-O2
6	J	303	PLC	O3P-C1-C2-O2
6	J	305	PLC	O3P-C1-C2-O2
8	C	309	P1O	O4-C6-C7-O7
8	G	309	P1O	O4-C6-C7-O7
8	K	307	P1O	O4-C6-C7-O7
8	B	302	P1O	C9-C10-C11-C12
8	F	303	P1O	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
8	C	309	P1O	O7-C7-C8-O5
8	G	309	P1O	O7-C7-C8-O5
8	K	307	P1O	O7-C7-C8-O5
8	B	302	P1O	C24-C25-C26-C27
8	J	306	P1O	C24-C25-C26-C27
8	B	302	P1O	C15-C16-C17-C18
8	F	303	P1O	C15-C16-C17-C18
8	J	306	P1O	C15-C16-C17-C18
6	C	302	PLC	C1B-C2B-C3B-C4B
6	B	307	PLC	C1B-C2B-C3B-C4B
6	J	302	PLC	C1B-C2B-C3B-C4B
6	C	307	PLC	C1-O3P-P-O4P
6	B	309	PLC	C1-O3P-P-O4P
6	G	307	PLC	C1-O3P-P-O4P
6	K	305	PLC	C1-O3P-P-O4P
6	F	301	PLC	C1-O3P-P-O4P
6	J	304	PLC	C1-O3P-P-O4P
6	C	302	PLC	C1-O3P-P-O2P
6	C	305	PLC	C4-O4P-P-O1P
6	C	310	PLC	C4-O4P-P-O2P
6	B	301	PLC	C4-O4P-P-O1P
6	B	307	PLC	C1-O3P-P-O2P
6	B	308	PLC	C4-O4P-P-O1P
6	G	301	PLC	C4-O4P-P-O2P
6	G	305	PLC	C4-O4P-P-O1P
6	F	302	PLC	C4-O4P-P-O1P
6	J	302	PLC	C1-O3P-P-O2P
6	J	303	PLC	C4-O4P-P-O2P
6	J	305	PLC	C4-O4P-P-O1P
7	C	303	HXG	CAU-OAX-PBD-OAH
7	C	303	HXG	CAP-OAW-PBD-OAI
7	G	303	HXG	CAU-OAX-PBD-OAH
7	G	303	HXG	CAP-OAW-PBD-OAI
7	K	302	HXG	CAU-OAX-PBD-OAH
7	K	302	HXG	CAP-OAW-PBD-OAI
8	C	308	P1O	C6-O4-P1-O2
8	B	302	P1O	C1-C2-N1-C5
8	G	308	P1O	C6-O4-P1-O2
8	K	306	P1O	C6-O4-P1-O2
8	F	303	P1O	C1-C2-N1-C5
8	J	306	P1O	C1-C2-N1-C5
6	C	302	PLC	C5-C4-O4P-P

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Mol	Chain	Res	Type	Atoms
6	C	307	PLC	C5-C4-O4P-P
6	B	307	PLC	C5-C4-O4P-P
6	B	309	PLC	C5-C4-O4P-P
6	G	307	PLC	C5-C4-O4P-P
6	K	305	PLC	C5-C4-O4P-P
6	F	301	PLC	C5-C4-O4P-P
6	J	302	PLC	C5-C4-O4P-P
6	J	304	PLC	C5-C4-O4P-P
6	J	304	PLC	C1'-C2'-C3'-C4'
6	F	301	PLC	C1'-C2'-C3'-C4'
5	B	306	D10	C3-C4-C5-C6
5	F	307	D10	C3-C4-C5-C6
5	J	310	D10	C3-C4-C5-C6
6	B	309	PLC	C1'-C2'-C3'-C4'
8	B	302	P1O	C10-C11-C12-C13
8	J	306	P1O	C10-C11-C12-C13
7	C	303	HXG	OAX-CAU-CBB-OAY
7	G	303	HXG	OAX-CAU-CBB-OAY
7	K	302	HXG	OAX-CAU-CBB-OAY
8	F	303	P1O	C10-C11-C12-C13
6	C	305	PLC	C2B-C1B-CB-O3
6	B	308	PLC	C2B-C1B-CB-O3
6	G	305	PLC	C2B-C1B-CB-O3
8	B	302	P1O	C1-C2-N1-C4
8	F	303	P1O	C1-C2-N1-C4
8	J	306	P1O	C1-C2-N1-C4
8	B	310	P1O	C19-C20-C21-C22
8	F	308	P1O	C19-C20-C21-C22
6	B	301	PLC	C1-C2-C3-O3
6	B	309	PLC	O4P-C4-C5-N
6	B	309	PLC	C7B-C8B-C9B-CAA
6	F	301	PLC	O4P-C4-C5-N
6	F	301	PLC	C7B-C8B-C9B-CAA
6	F	302	PLC	C1-C2-C3-O3
6	J	304	PLC	O4P-C4-C5-N
6	J	304	PLC	C7B-C8B-C9B-CAA
6	J	305	PLC	C1-C2-C3-O3
6	B	301	PLC	O2-C2-C3-O3
6	B	309	PLC	O2-C2-C3-O3
6	F	301	PLC	O2-C2-C3-O3
6	F	302	PLC	O2-C2-C3-O3
6	J	304	PLC	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	J	305	PLC	O2-C2-C3-O3
6	J	303	PLC	C3'-C4'-C5'-C6'
8	J	301	P1O	C19-C20-C21-C22
6	C	310	PLC	C3'-C4'-C5'-C6'
6	G	301	PLC	C3'-C4'-C5'-C6'
7	C	306	HXG	CBB-CAU-OAX-PBD
7	G	306	HXG	CBB-CAU-OAX-PBD
7	K	304	HXG	CBB-CAU-OAX-PBD
6	C	302	PLC	C5B-C6B-C7B-C8B
6	J	302	PLC	C5B-C6B-C7B-C8B
6	B	307	PLC	C5B-C6B-C7B-C8B
6	C	305	PLC	C3-C2-O2-C'
6	B	308	PLC	C3-C2-O2-C'
6	G	305	PLC	C3-C2-O2-C'
8	K	306	P1O	C24-C25-C26-C27
8	C	308	P1O	C24-C25-C26-C27
8	G	308	P1O	C24-C25-C26-C27
6	B	301	PLC	C1-O3P-P-O4P
6	F	302	PLC	C1-O3P-P-O4P
6	J	305	PLC	C1-O3P-P-O4P
8	B	310	P1O	C1-O3-P1-O4
8	B	310	P1O	C6-O4-P1-O3
8	F	308	P1O	C1-O3-P1-O4
8	F	308	P1O	C6-O4-P1-O3
8	J	301	P1O	C1-O3-P1-O4
8	J	301	P1O	C6-O4-P1-O3
8	C	309	P1O	C6-C7-C8-O5
8	G	309	P1O	C6-C7-C8-O5
8	K	307	P1O	C6-C7-C8-O5
6	C	302	PLC	C3'-C4'-C5'-C6'
6	F	302	PLC	C6'-C7'-C8'-C9'
6	J	302	PLC	C3'-C4'-C5'-C6'
6	B	301	PLC	C6'-C7'-C8'-C9'
6	J	305	PLC	C6'-C7'-C8'-C9'
6	B	307	PLC	C3'-C4'-C5'-C6'
6	C	310	PLC	C5'-C6'-C7'-C8'
6	G	301	PLC	C5'-C6'-C7'-C8'
5	F	306	D10	C7-C8-C9-C10
5	J	309	D10	C7-C8-C9-C10
6	J	303	PLC	C5'-C6'-C7'-C8'
5	B	305	D10	C7-C8-C9-C10
7	C	306	HXG	OAV-CAT-CBB-OAY

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Mol	Chain	Res	Type	Atoms
7	G	306	HXG	OAV-CAT-CBB-OAY
7	K	304	HXG	OAV-CAT-CBB-OAY
8	B	302	P1O	O7-C7-C8-O5
8	F	303	P1O	O7-C7-C8-O5
8	J	306	P1O	O7-C7-C8-O5
6	B	301	PLC	C4B-C5B-C6B-C7B
6	F	302	PLC	C4B-C5B-C6B-C7B
6	J	305	PLC	C4B-C5B-C6B-C7B
8	C	309	P1O	C23-C24-C25-C26
8	G	309	P1O	C23-C24-C25-C26
8	K	307	P1O	C23-C24-C25-C26
6	C	307	PLC	C3-C2-O2-C'
6	B	301	PLC	C3-C2-O2-C'
6	B	309	PLC	C1-C2-O2-C'
6	G	307	PLC	C3-C2-O2-C'
6	K	305	PLC	C3-C2-O2-C'
6	F	301	PLC	C1-C2-O2-C'
6	F	302	PLC	C3-C2-O2-C'
6	J	304	PLC	C1-C2-O2-C'
6	J	305	PLC	C3-C2-O2-C'
8	B	302	P1O	C1-C2-N1-C3
8	F	303	P1O	C1-C2-N1-C3
8	J	306	P1O	C1-C2-N1-C3
6	B	301	PLC	C4-C5-N-C6
6	F	302	PLC	C4-C5-N-C6
6	J	305	PLC	C4-C5-N-C6
8	C	309	P1O	C9-C10-C11-C12
8	G	309	P1O	C9-C10-C11-C12
8	K	307	P1O	C9-C10-C11-C12
6	F	302	PLC	C3'-C4'-C5'-C6'
6	J	305	PLC	C3'-C4'-C5'-C6'
6	B	301	PLC	C3'-C4'-C5'-C6'
6	C	310	PLC	C1-O3P-P-O4P
6	G	301	PLC	C1-O3P-P-O4P
6	J	303	PLC	C1-O3P-P-O4P
6	C	307	PLC	C1-C2-O2-C'
6	G	307	PLC	C1-C2-O2-C'
6	K	305	PLC	C1-C2-O2-C'
6	G	307	PLC	C6B-C7B-C8B-C9B
6	C	307	PLC	C6B-C7B-C8B-C9B
6	K	305	PLC	C6B-C7B-C8B-C9B
6	C	307	PLC	O2-C'-C1'-C2'

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Mol	Chain	Res	Type	Atoms
6	G	307	PLC	O2-C'-C1'-C2'
6	K	305	PLC	O2-C'-C1'-C2'
6	G	305	PLC	C5B-C6B-C7B-C8B
6	C	305	PLC	C5B-C6B-C7B-C8B
6	B	308	PLC	C5B-C6B-C7B-C8B
6	C	307	PLC	C'-C1'-C2'-C3'
6	G	307	PLC	C'-C1'-C2'-C3'
6	K	305	PLC	C'-C1'-C2'-C3'
6	C	310	PLC	C2B-C1B-CB-O3
6	G	301	PLC	C2B-C1B-CB-O3
6	J	303	PLC	C2B-C1B-CB-O3
7	K	304	HXG	OAG-CBA-OAY-CBB
5	F	305	D10	C7-C8-C9-C10
5	B	304	D10	C7-C8-C9-C10
5	J	308	D10	C7-C8-C9-C10
6	B	301	PLC	O2-C'-C1'-C2'
6	F	302	PLC	O2-C'-C1'-C2'
6	J	305	PLC	O2-C'-C1'-C2'
8	G	308	P1O	C10-C11-C12-C13
8	K	306	P1O	C10-C11-C12-C13
8	C	308	P1O	C10-C11-C12-C13
8	B	310	P1O	C23-C24-C25-C26
8	F	308	P1O	C23-C24-C25-C26
7	C	306	HXG	OAG-CBA-OAY-CBB
7	G	306	HXG	OAG-CBA-OAY-CBB
8	C	308	P1O	C7-C6-O4-P1
8	G	308	P1O	C7-C6-O4-P1
8	K	306	P1O	C7-C6-O4-P1
8	J	301	P1O	C23-C24-C25-C26
7	C	306	HXG	CAU-OAX-PBD-OAI
7	G	306	HXG	CAU-OAX-PBD-OAI
7	K	304	HXG	CAU-OAX-PBD-OAI
8	B	310	P1O	C1-O3-P1-O2
8	B	310	P1O	C6-O4-P1-O2
8	F	308	P1O	C1-O3-P1-O2
8	F	308	P1O	C6-O4-P1-O2
8	J	301	P1O	C1-O3-P1-O2
8	J	301	P1O	C6-O4-P1-O2
8	C	308	P1O	C11-C10-C9-O5
8	G	308	P1O	C11-C10-C9-O5
8	K	306	P1O	C11-C10-C9-O5
6	C	307	PLC	O'-C'-C1'-C2'

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Mol	Chain	Res	Type	Atoms
6	G	307	PLC	O'-C'-C1'-C2'
6	K	305	PLC	O'-C'-C1'-C2'
6	C	310	PLC	C2B-C1B-CB-OB
8	B	302	P1O	C11-C10-C9-O5
8	F	303	P1O	C11-C10-C9-O5
8	J	306	P1O	C11-C10-C9-O5
6	F	302	PLC	O'-C'-C1'-C2'
6	B	301	PLC	O'-C'-C1'-C2'
6	G	301	PLC	C2B-C1B-CB-OB
6	J	303	PLC	C2B-C1B-CB-OB
6	C	302	PLC	C2B-C1B-CB-O3
6	B	307	PLC	C2B-C1B-CB-O3
6	J	305	PLC	O'-C'-C1'-C2'
6	C	310	PLC	O2-C'-C1'-C2'
6	G	301	PLC	O2-C'-C1'-C2'
6	J	303	PLC	O2-C'-C1'-C2'
6	J	302	PLC	C2B-C1B-CB-O3
6	B	301	PLC	C4-C5-N-C8
6	F	302	PLC	C4-C5-N-C7
6	F	302	PLC	C4-C5-N-C8
6	J	305	PLC	C4-C5-N-C7
6	J	305	PLC	C4-C5-N-C8
6	J	302	PLC	C2B-C1B-CB-OB
8	C	308	P1O	C11-C10-C9-O6
8	G	308	P1O	C11-C10-C9-O6

There are no ring outliers.

48 monomers are involved in 289 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	305	D10	1	0
5	F	306	D10	7	0
8	B	310	P1O	2	0
5	K	303	D10	1	0
6	B	308	PLC	2	0
7	C	303	HXG	13	0
6	F	302	PLC	8	0
7	G	303	HXG	13	0
5	B	304	D10	1	0
8	G	308	P1O	8	0
8	J	301	P1O	3	0
5	J	310	D10	2	0

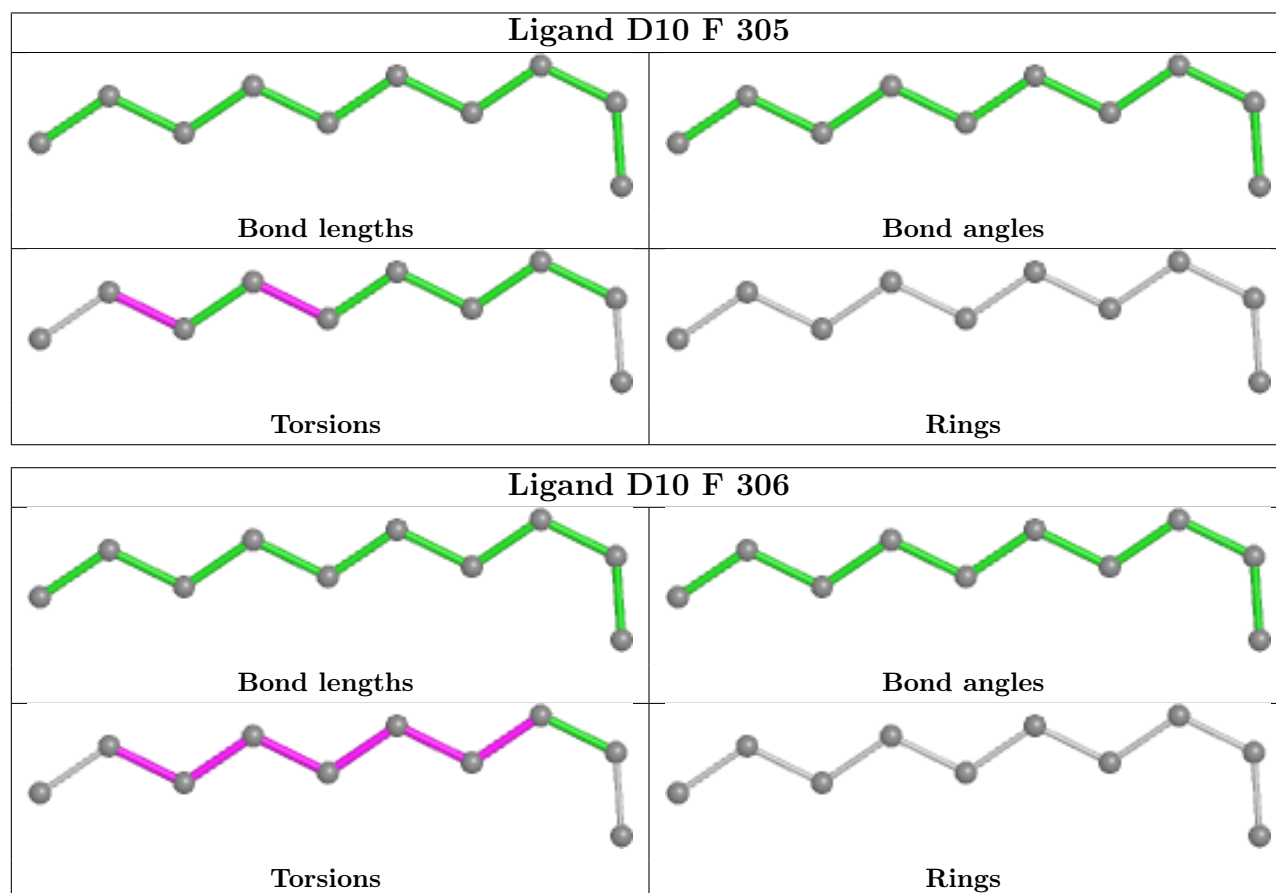
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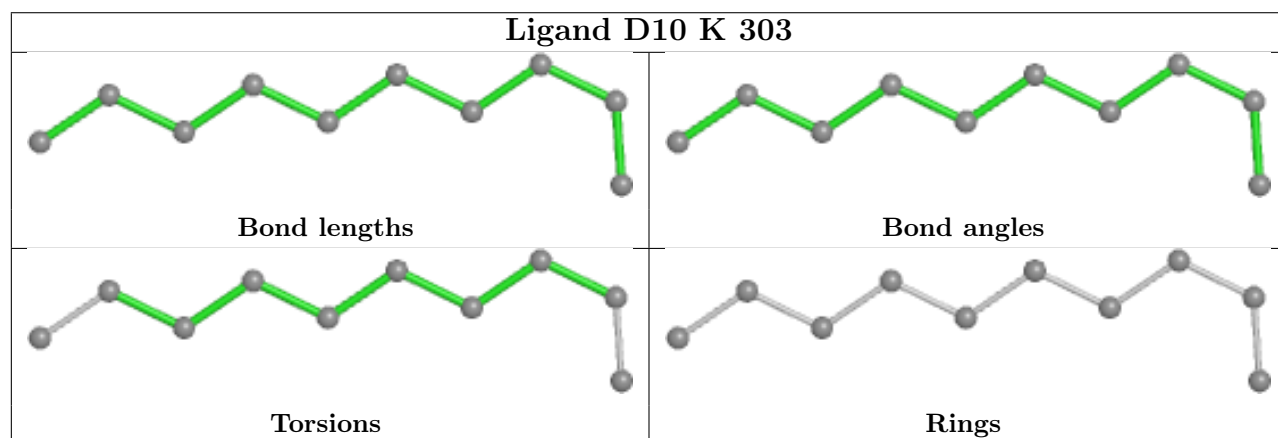
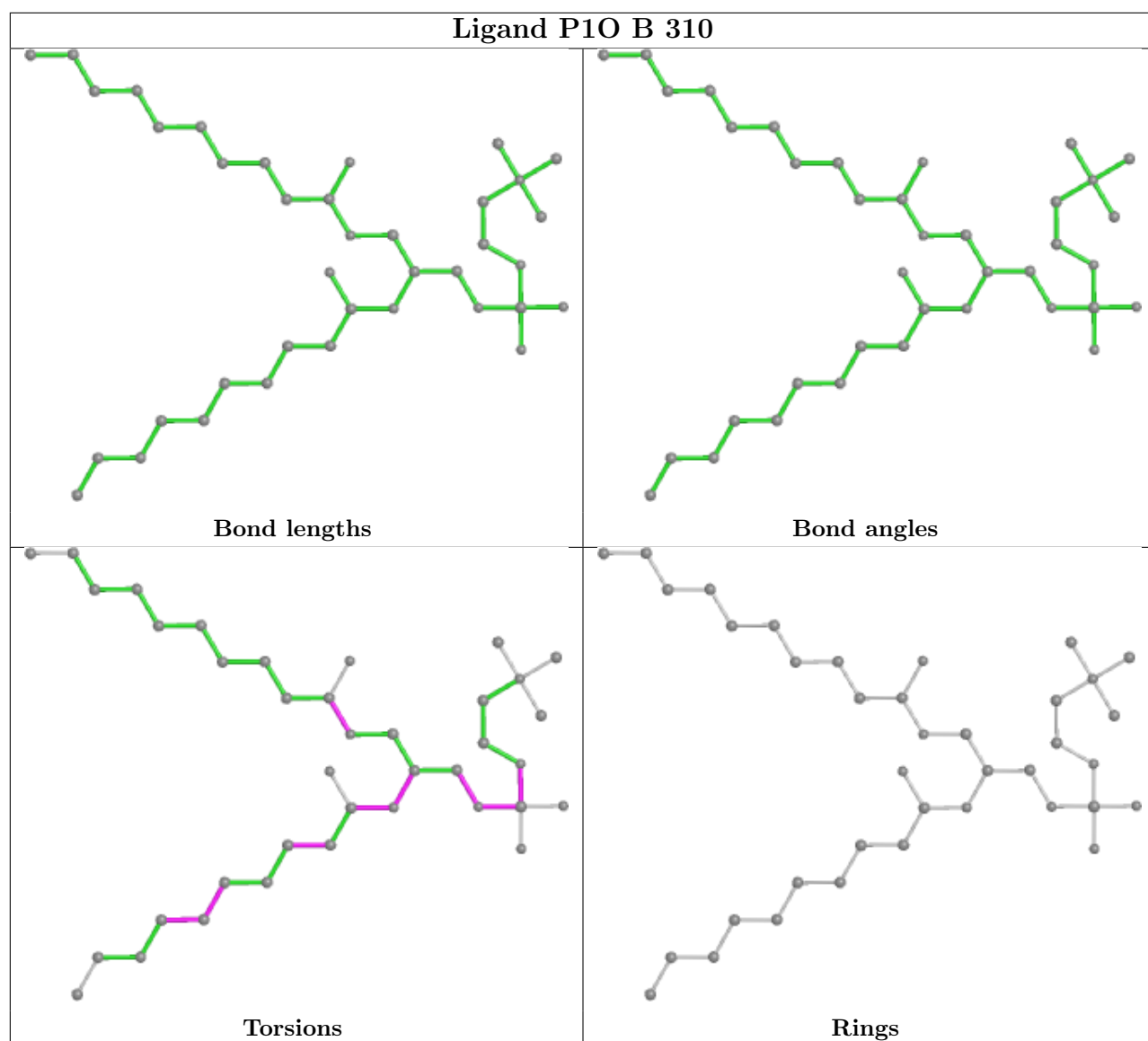
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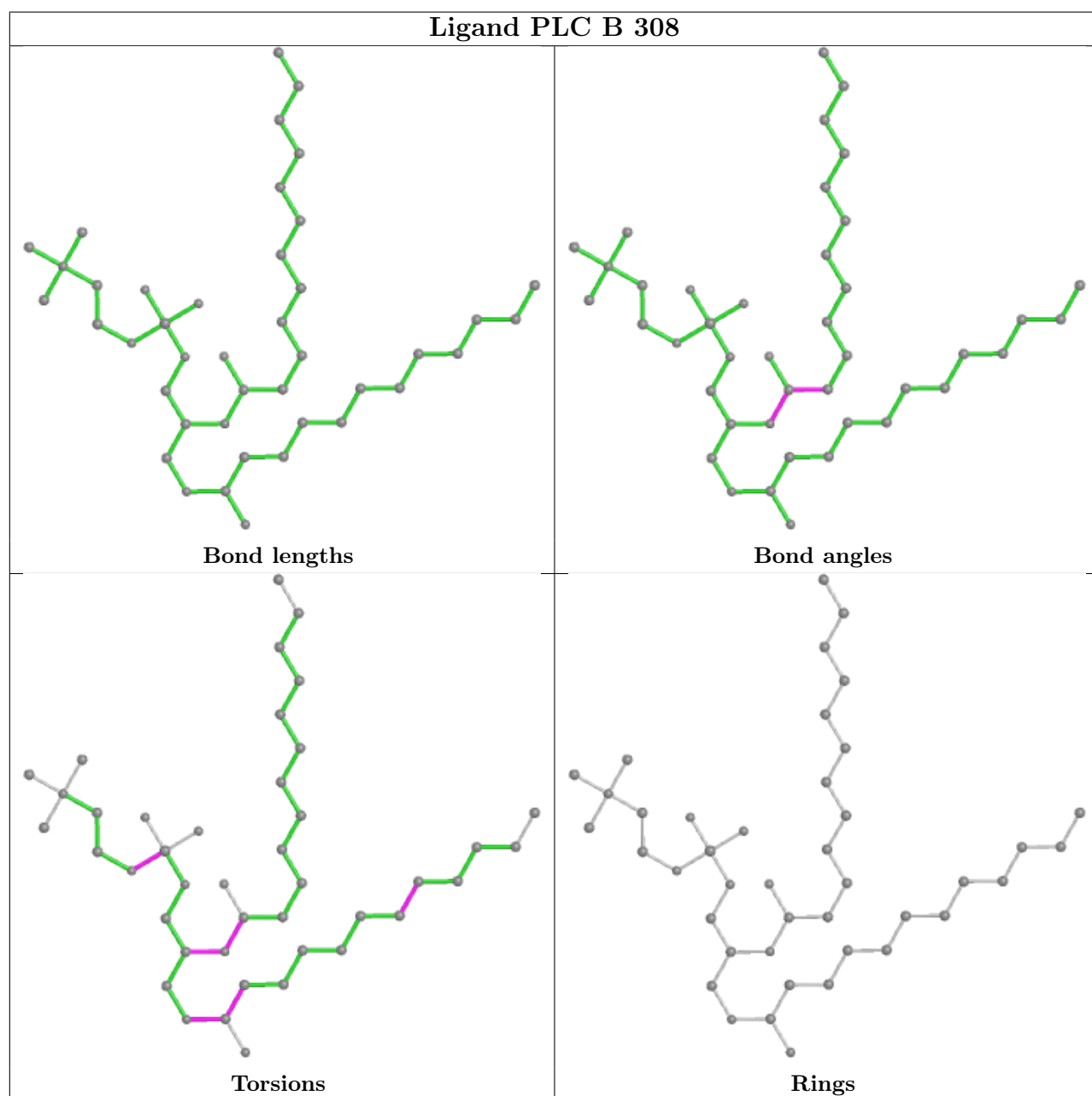
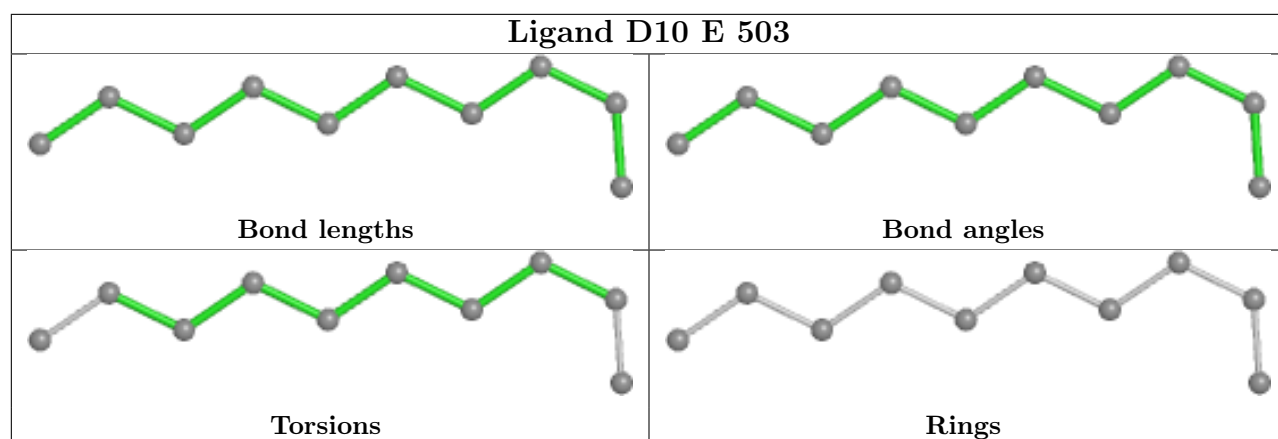
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	305	PLC	2	0
5	B	305	D10	7	0
6	J	302	PLC	2	0
7	K	304	HXG	16	0
5	J	307	D10	1	0
8	G	309	P1O	18	0
6	G	307	PLC	4	0
7	K	302	HXG	13	0
5	J	308	D10	1	0
6	J	305	PLC	9	0
5	F	307	D10	2	0
5	J	309	D10	7	0
5	F	304	D10	1	0
6	B	301	PLC	8	0
8	K	307	P1O	17	0
6	G	301	PLC	5	0
8	F	308	P1O	3	0
8	K	306	P1O	8	0
8	F	303	P1O	7	0
8	C	308	P1O	9	0
6	C	302	PLC	2	0
5	G	304	D10	1	0
8	J	306	P1O	7	0
6	C	305	PLC	2	0
6	C	310	PLC	5	0
6	C	307	PLC	4	0
5	B	306	D10	2	0
7	C	306	HXG	16	0
8	C	309	P1O	17	0
8	B	302	P1O	9	0
6	B	307	PLC	2	0
5	B	303	D10	1	0
6	K	305	PLC	4	0
7	G	306	HXG	16	0
5	C	304	D10	1	0
6	J	303	PLC	5	0

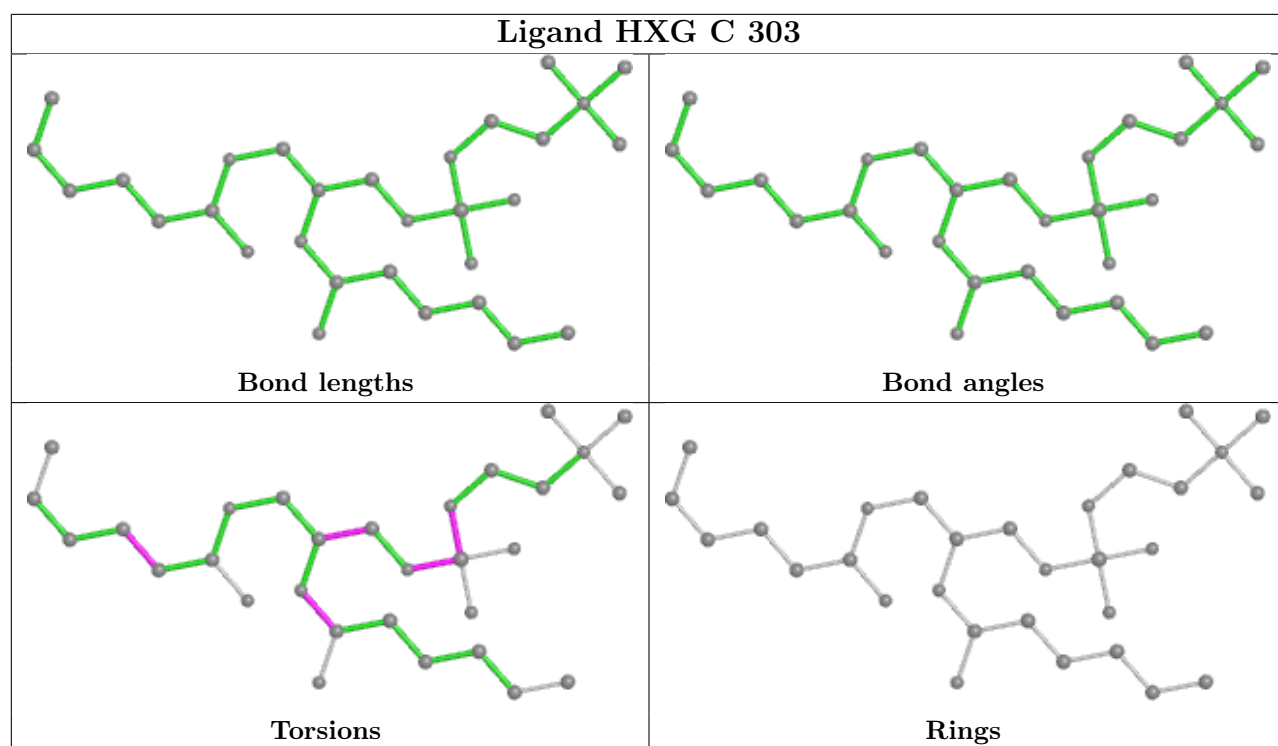
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

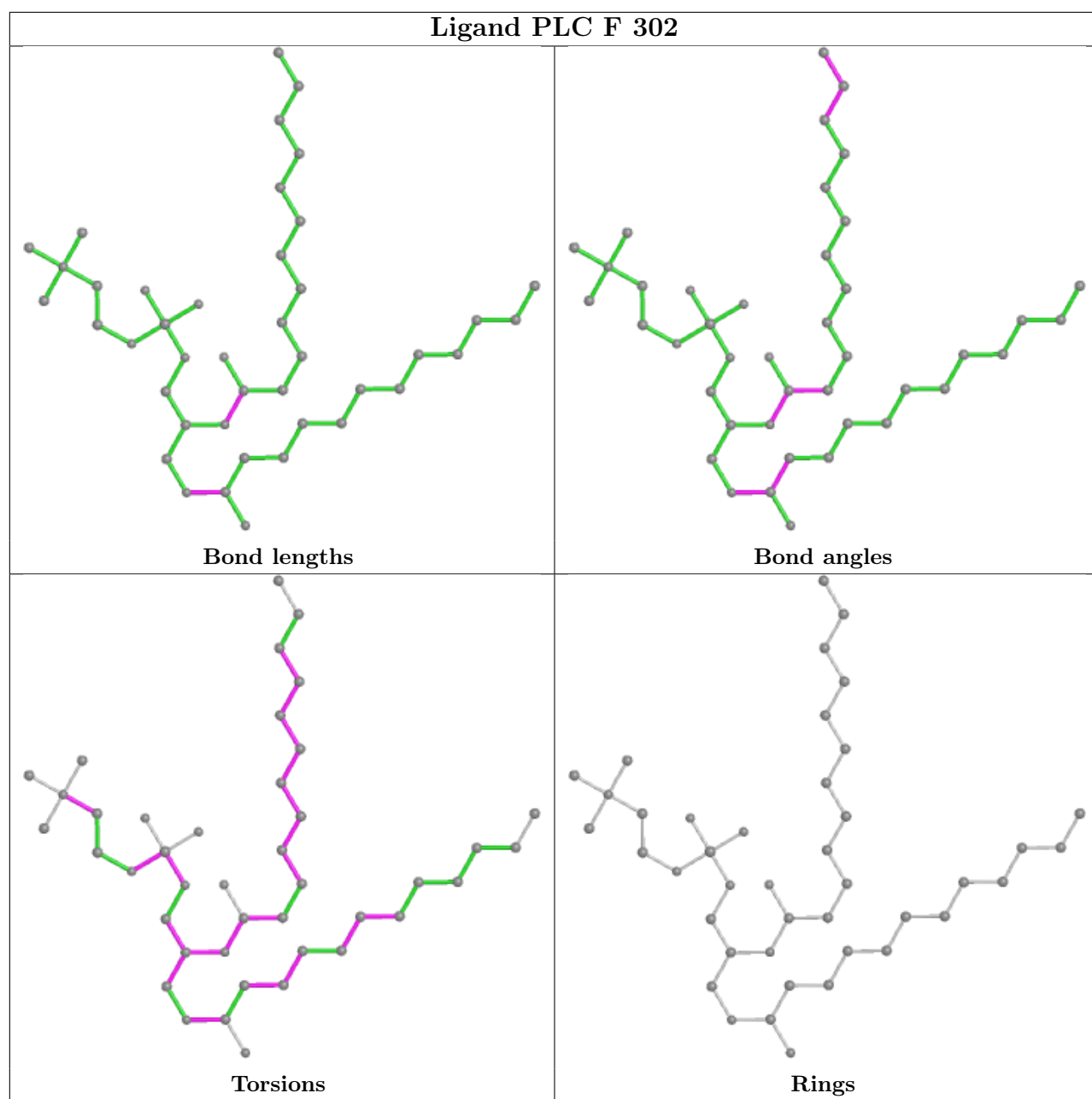
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

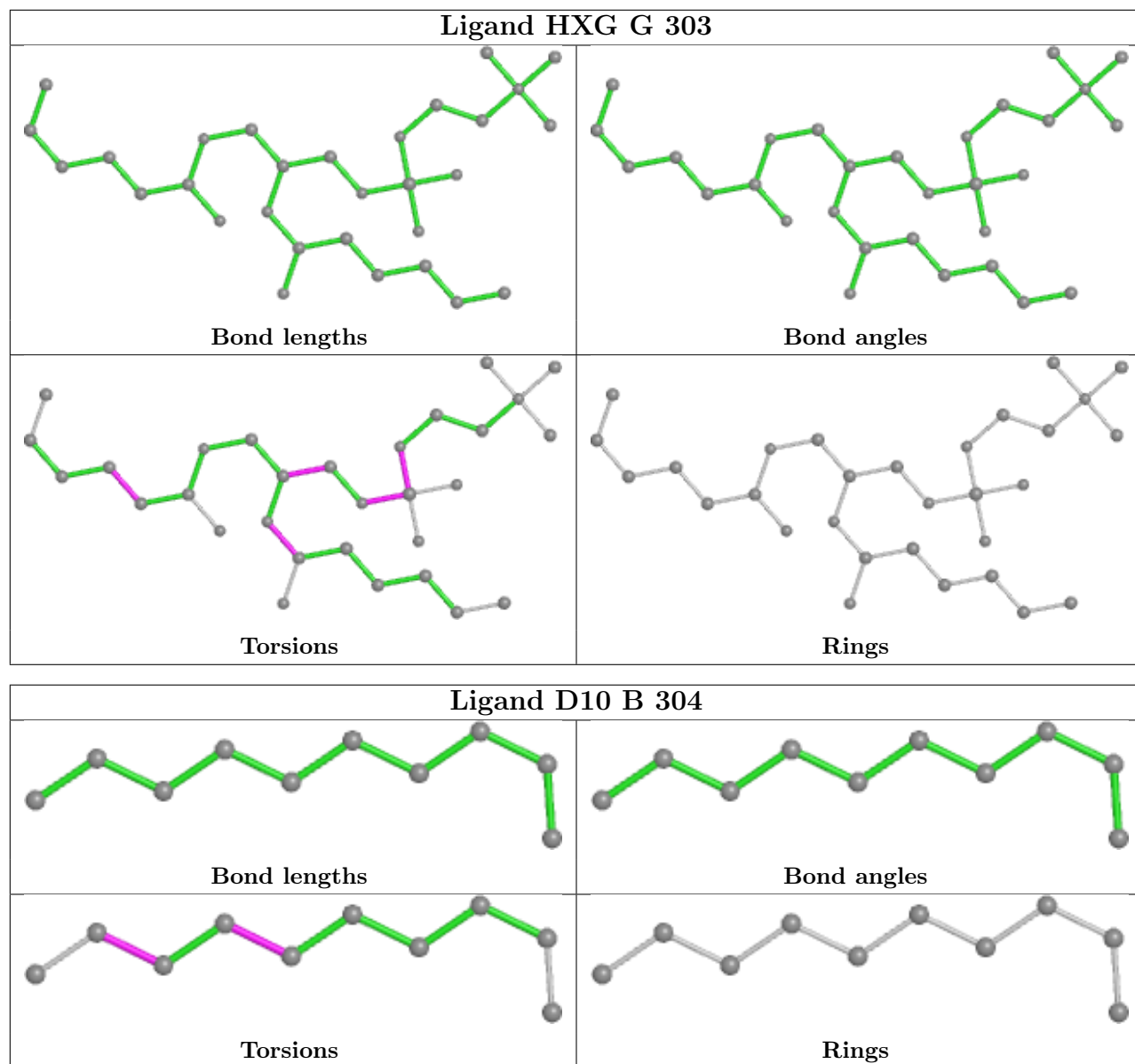




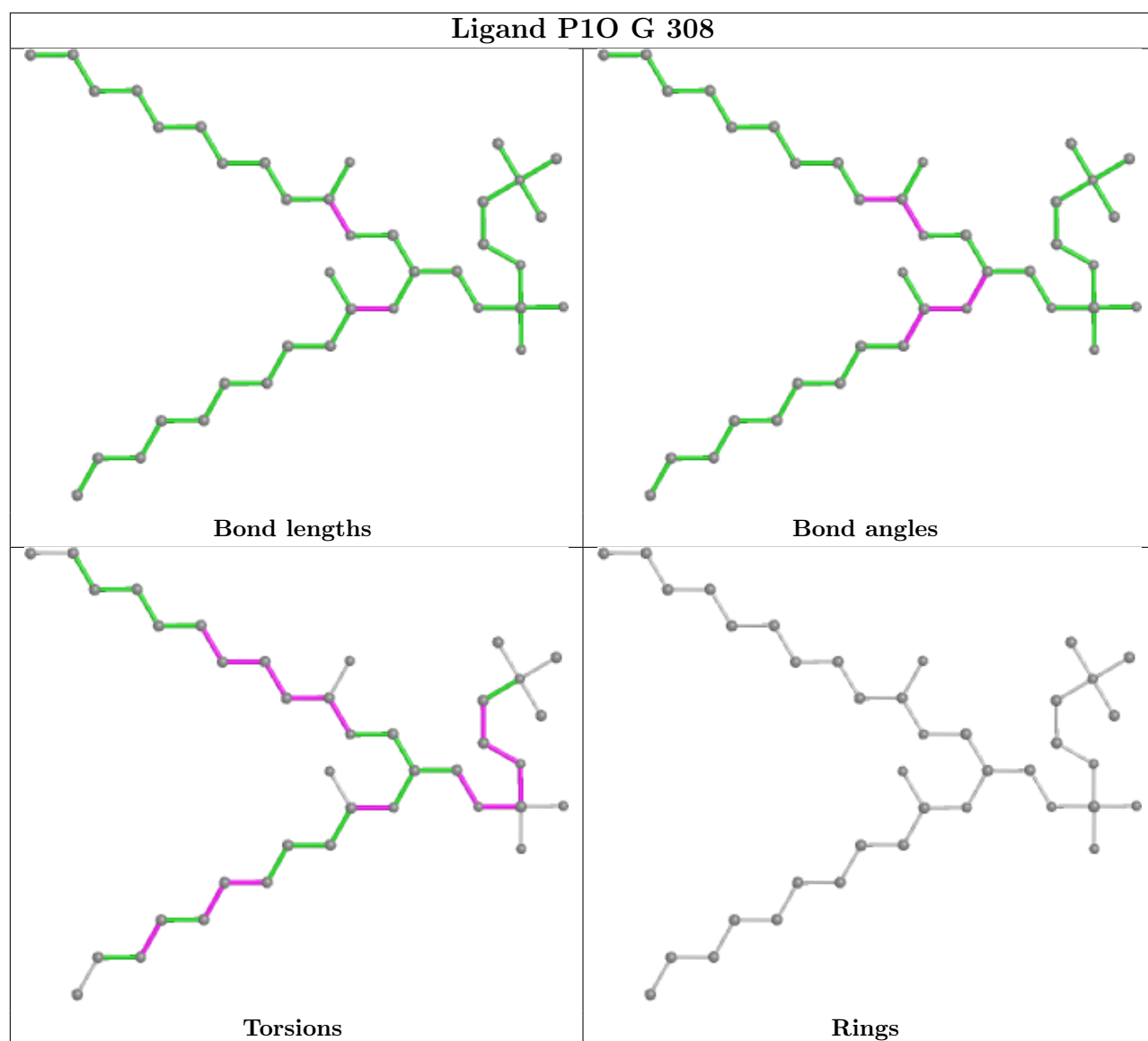


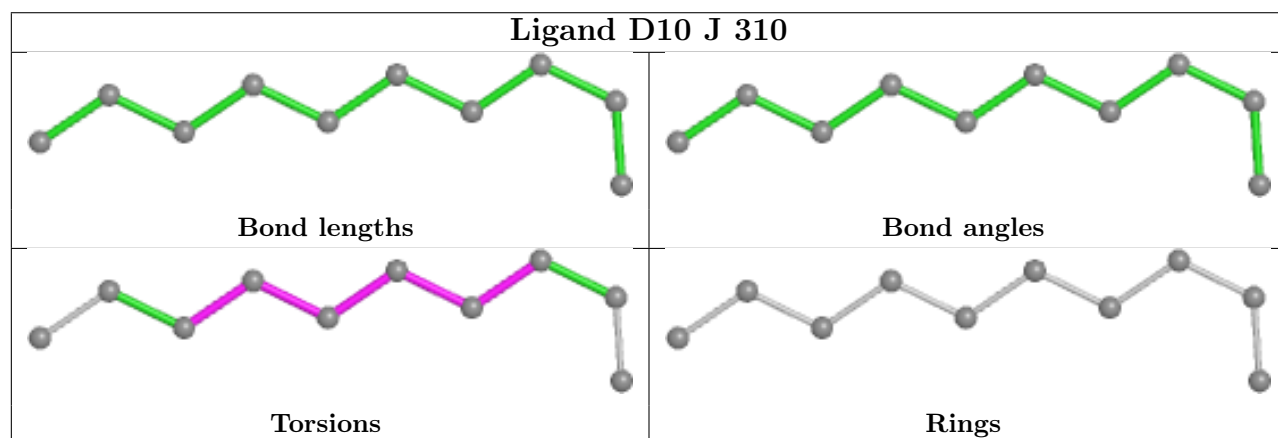
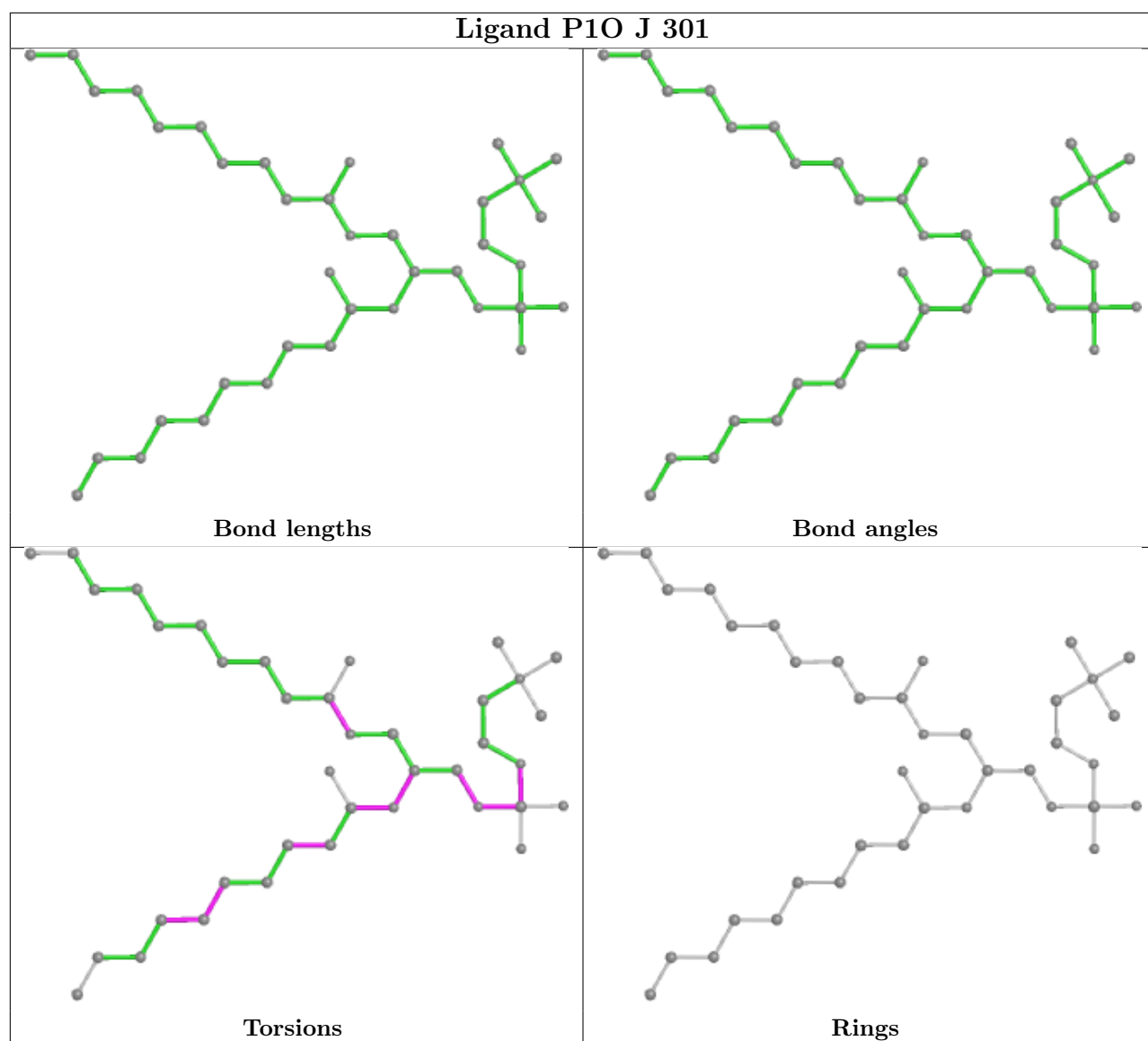


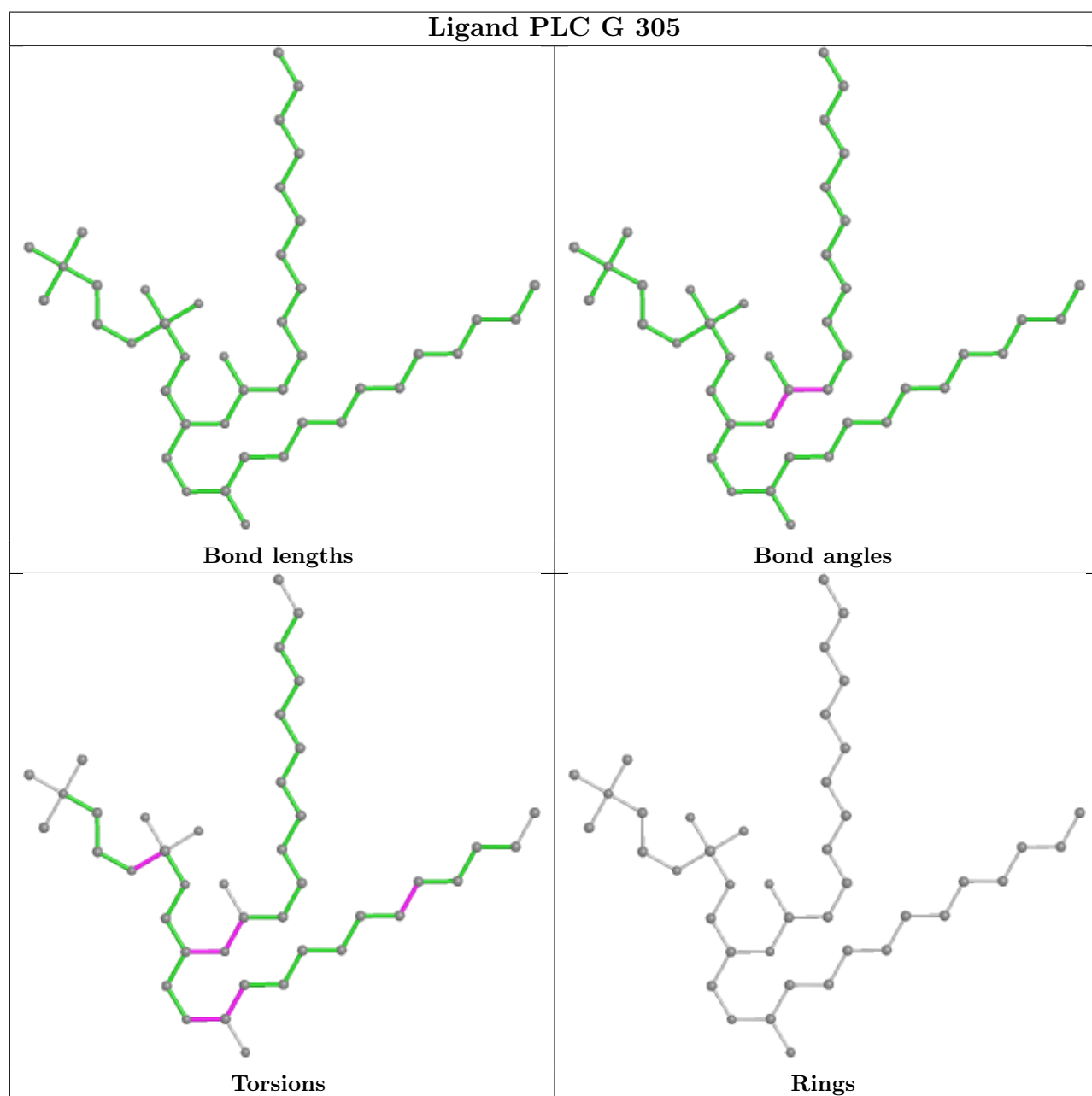
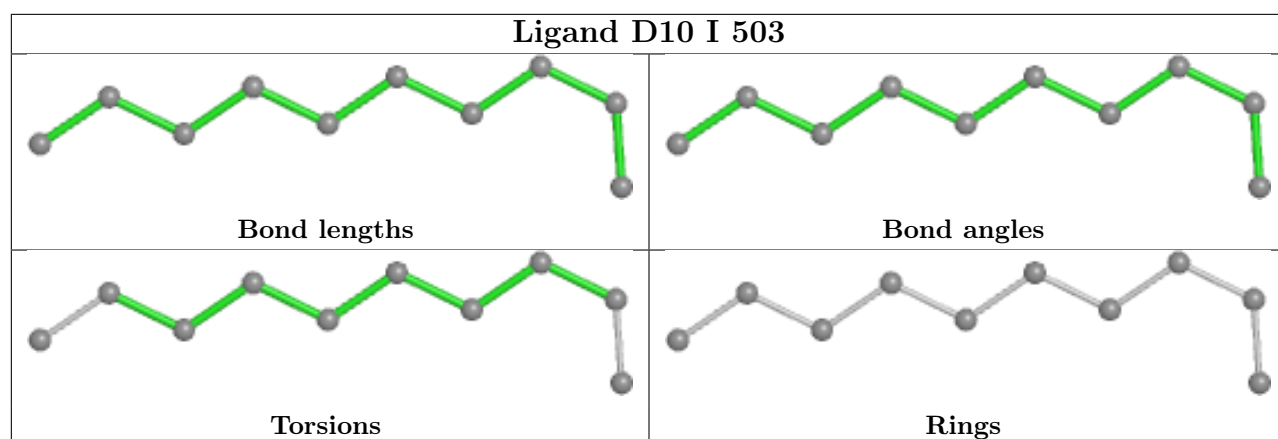


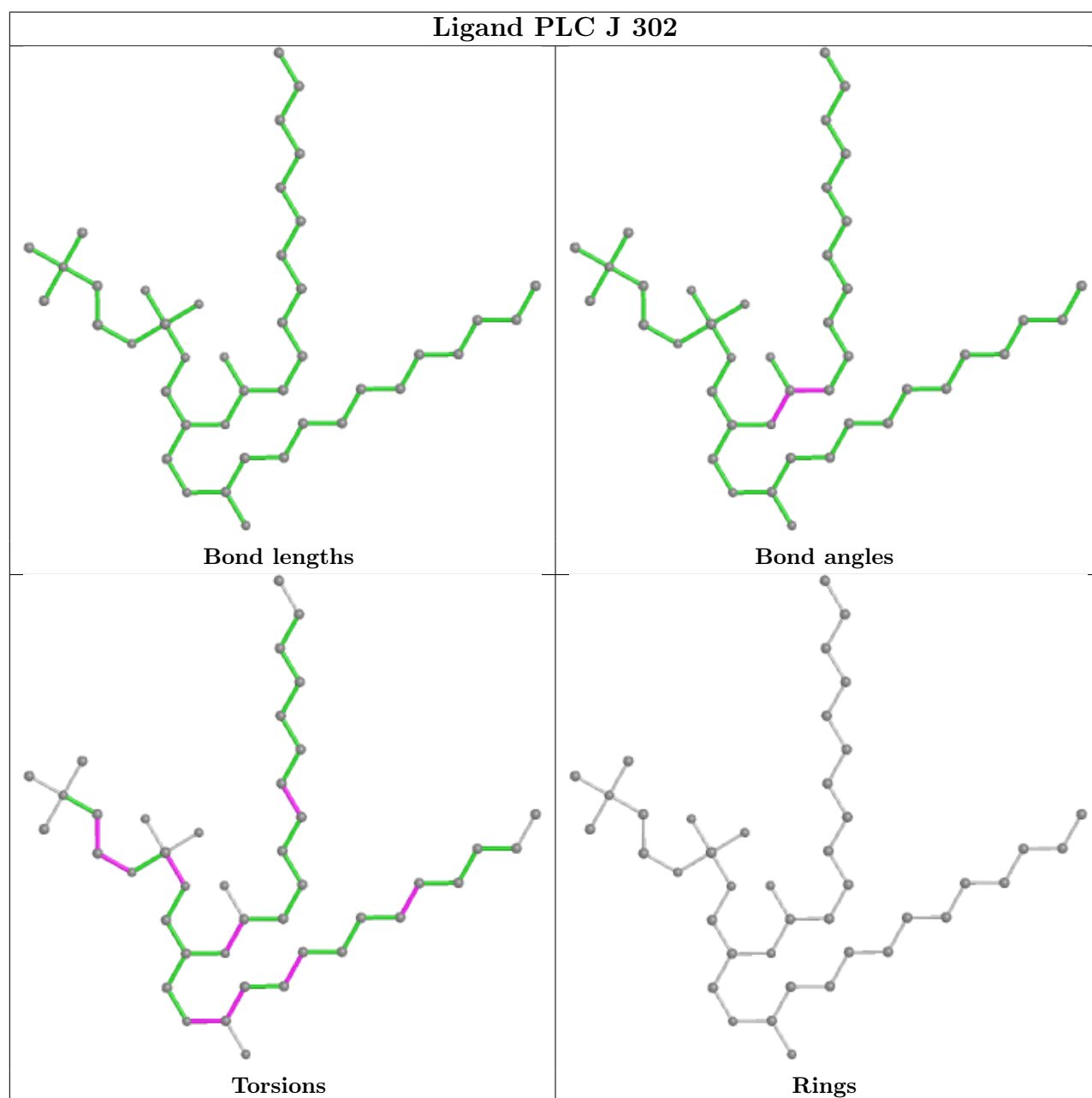
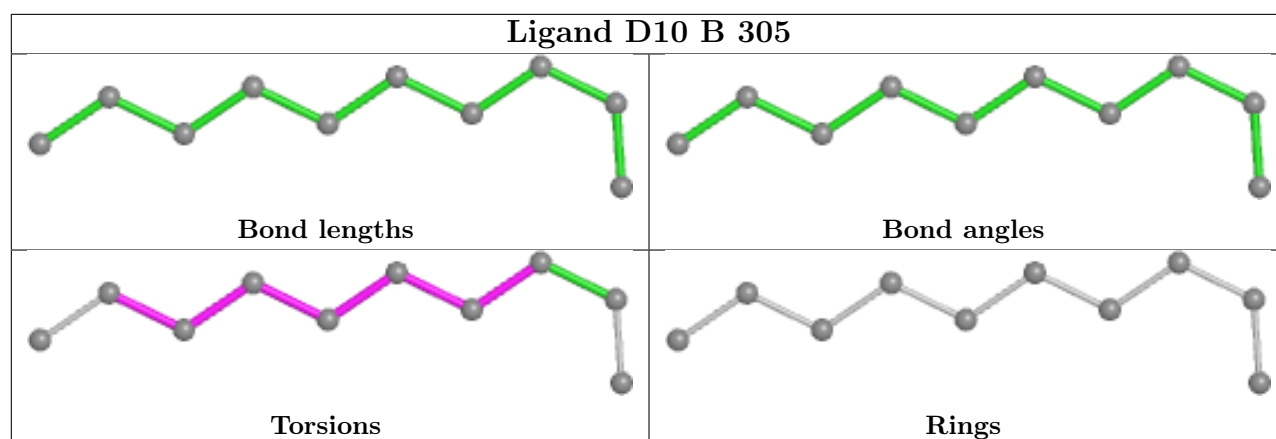


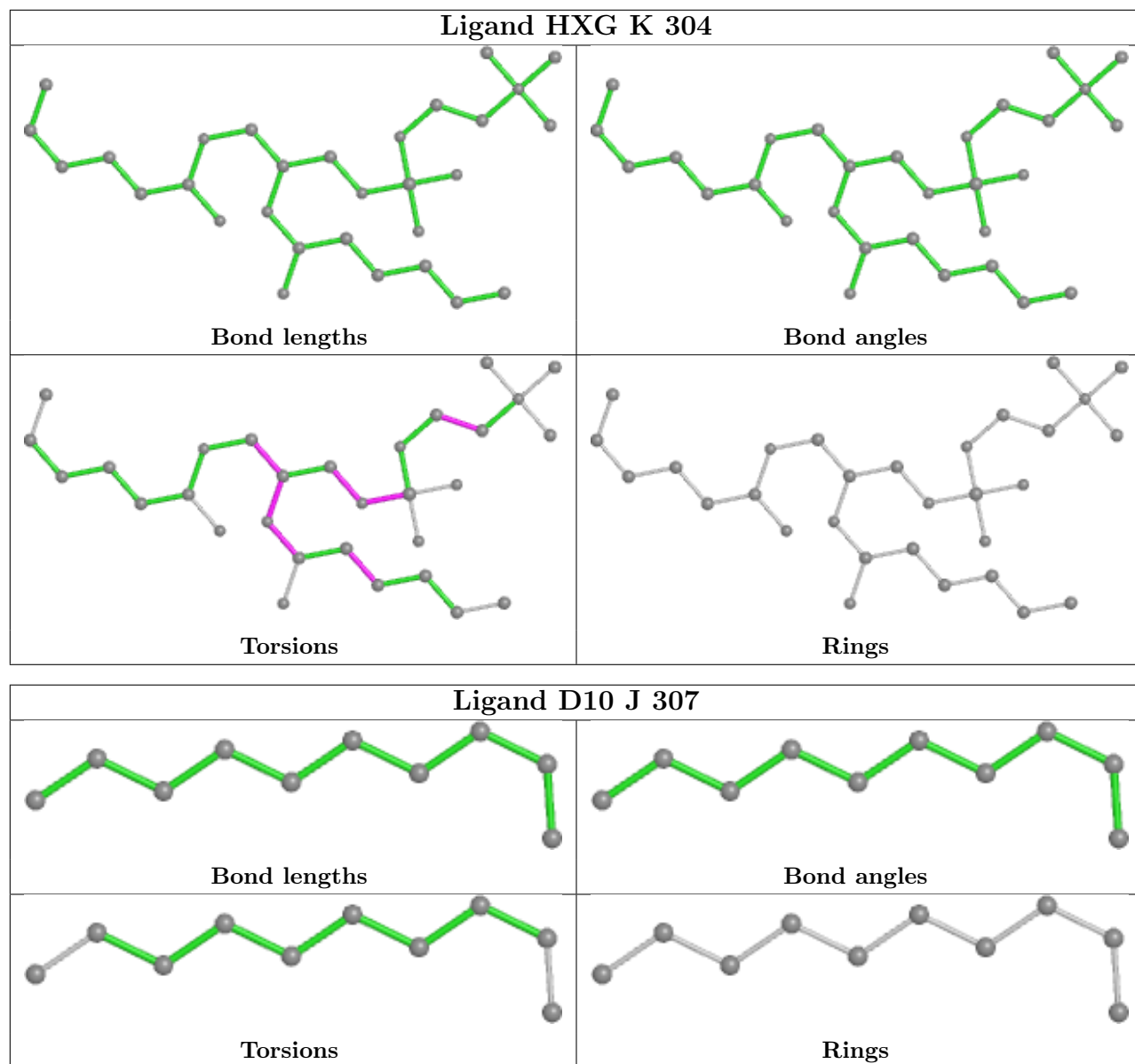


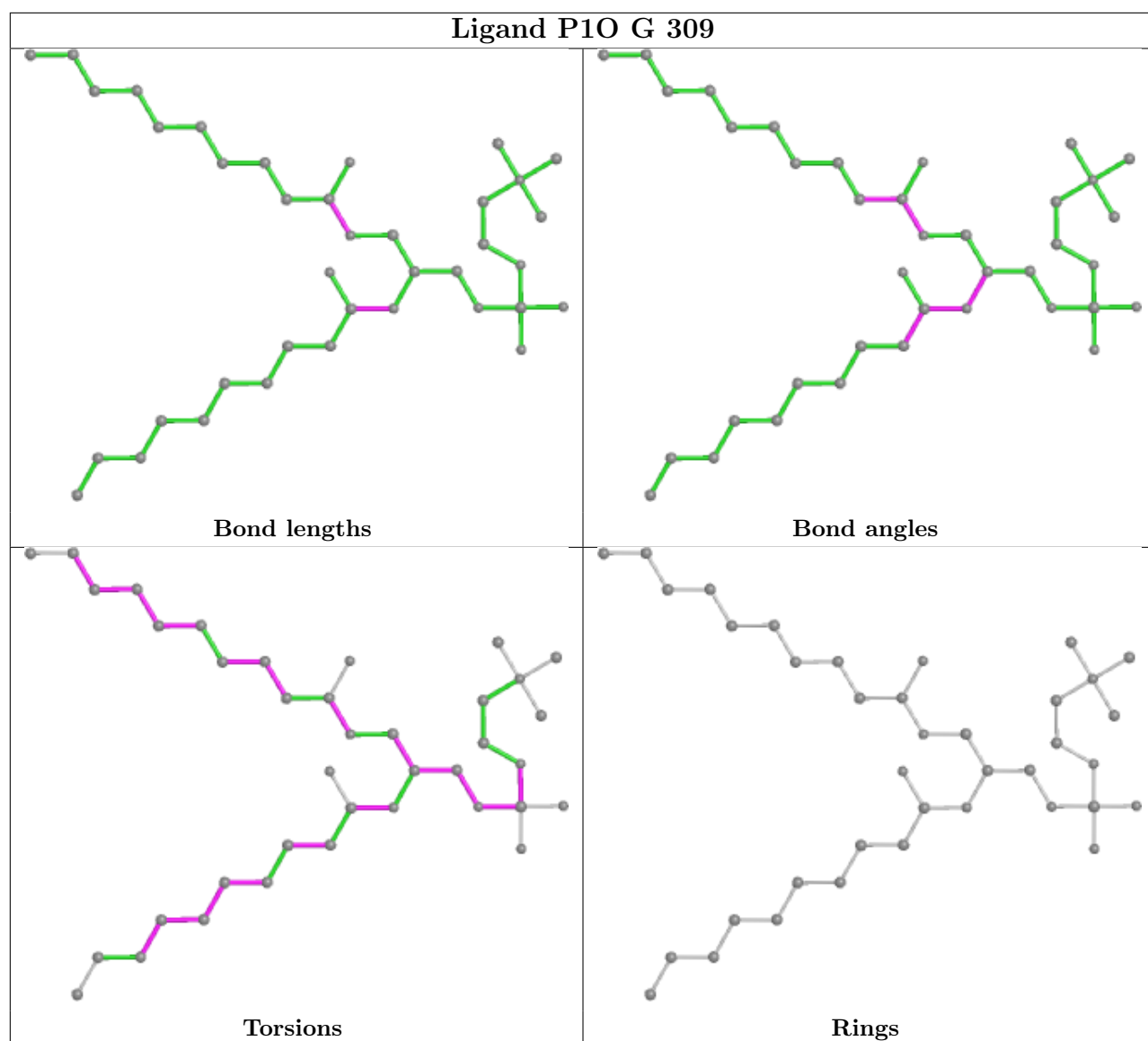


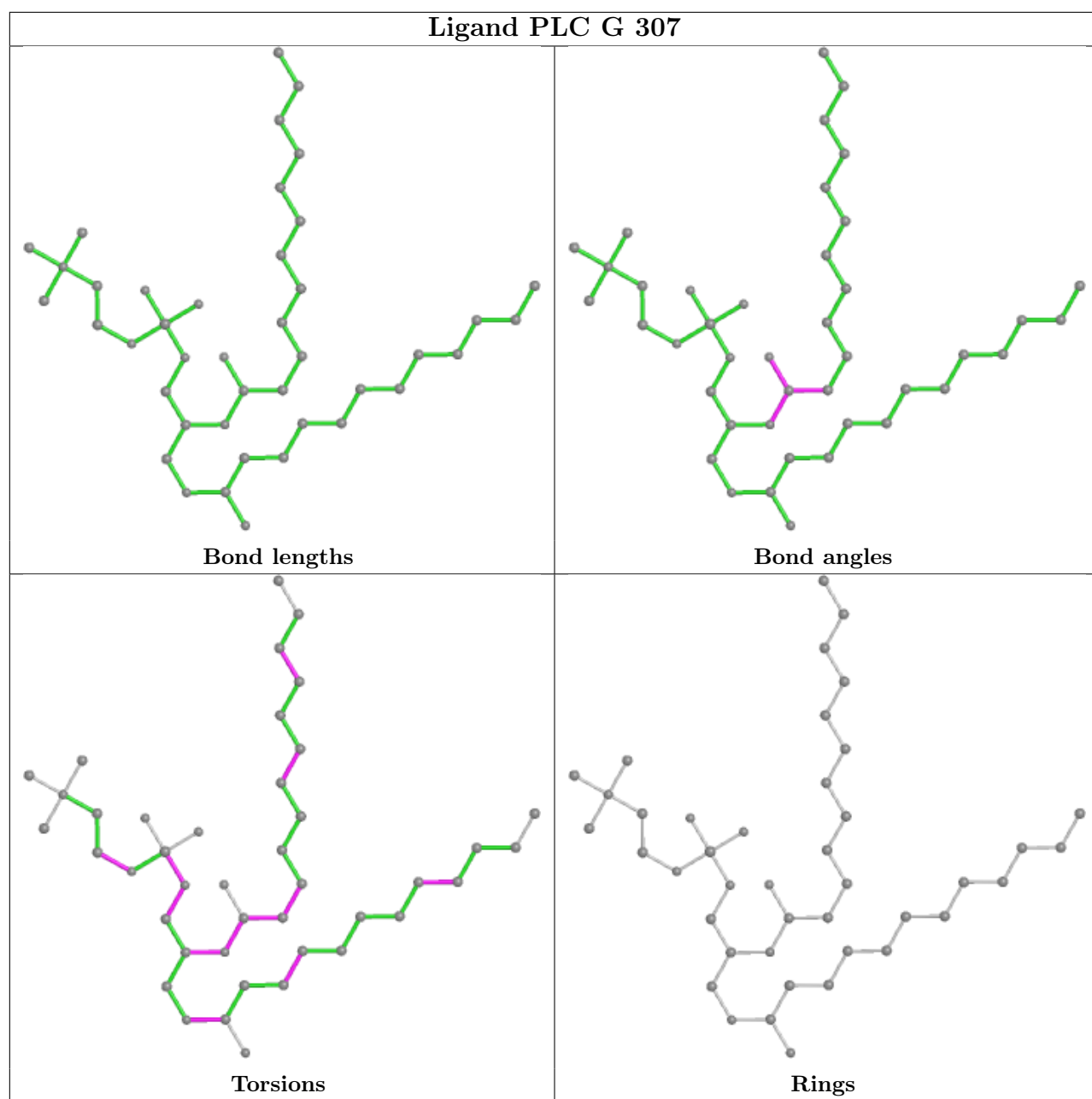


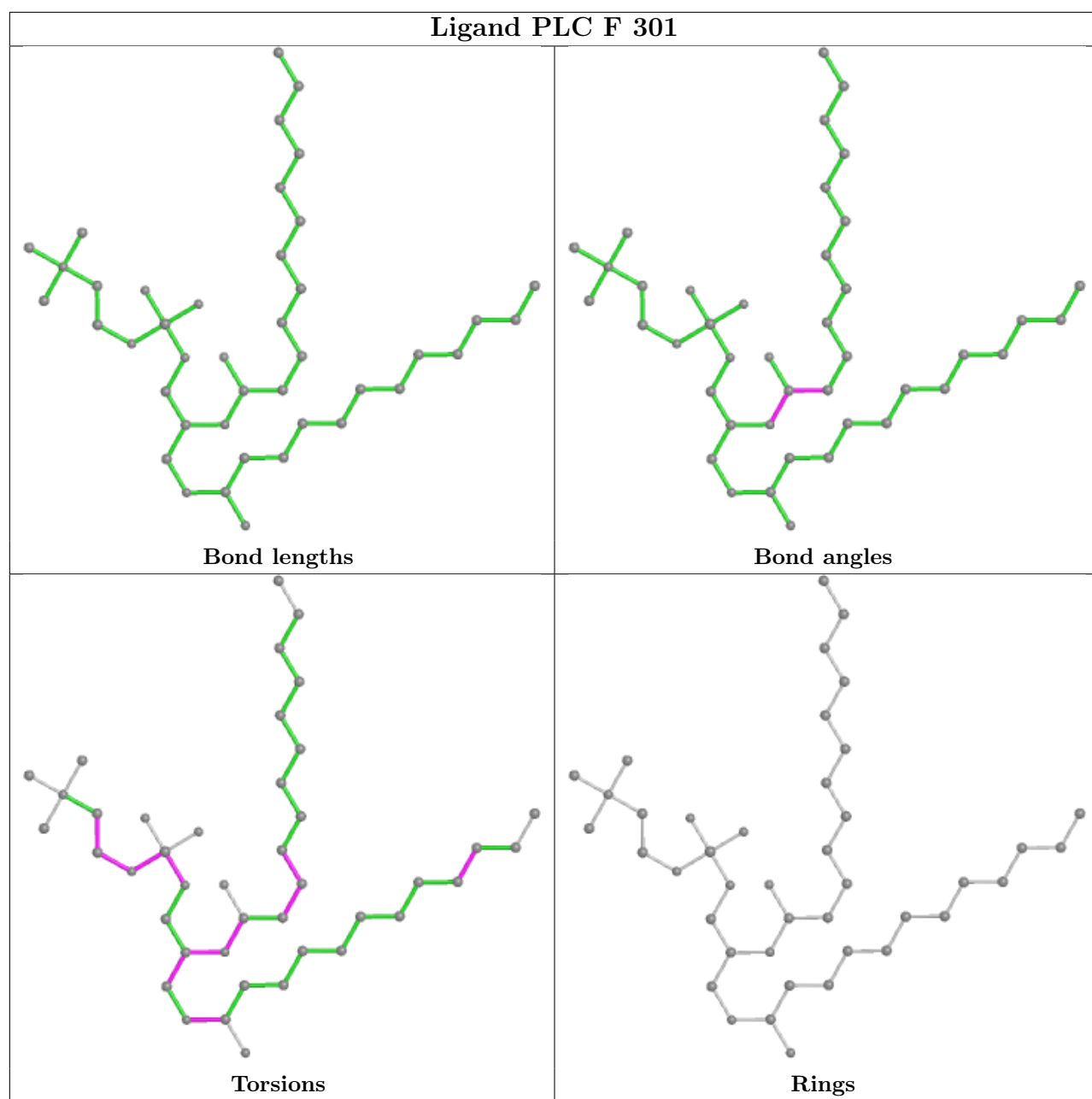




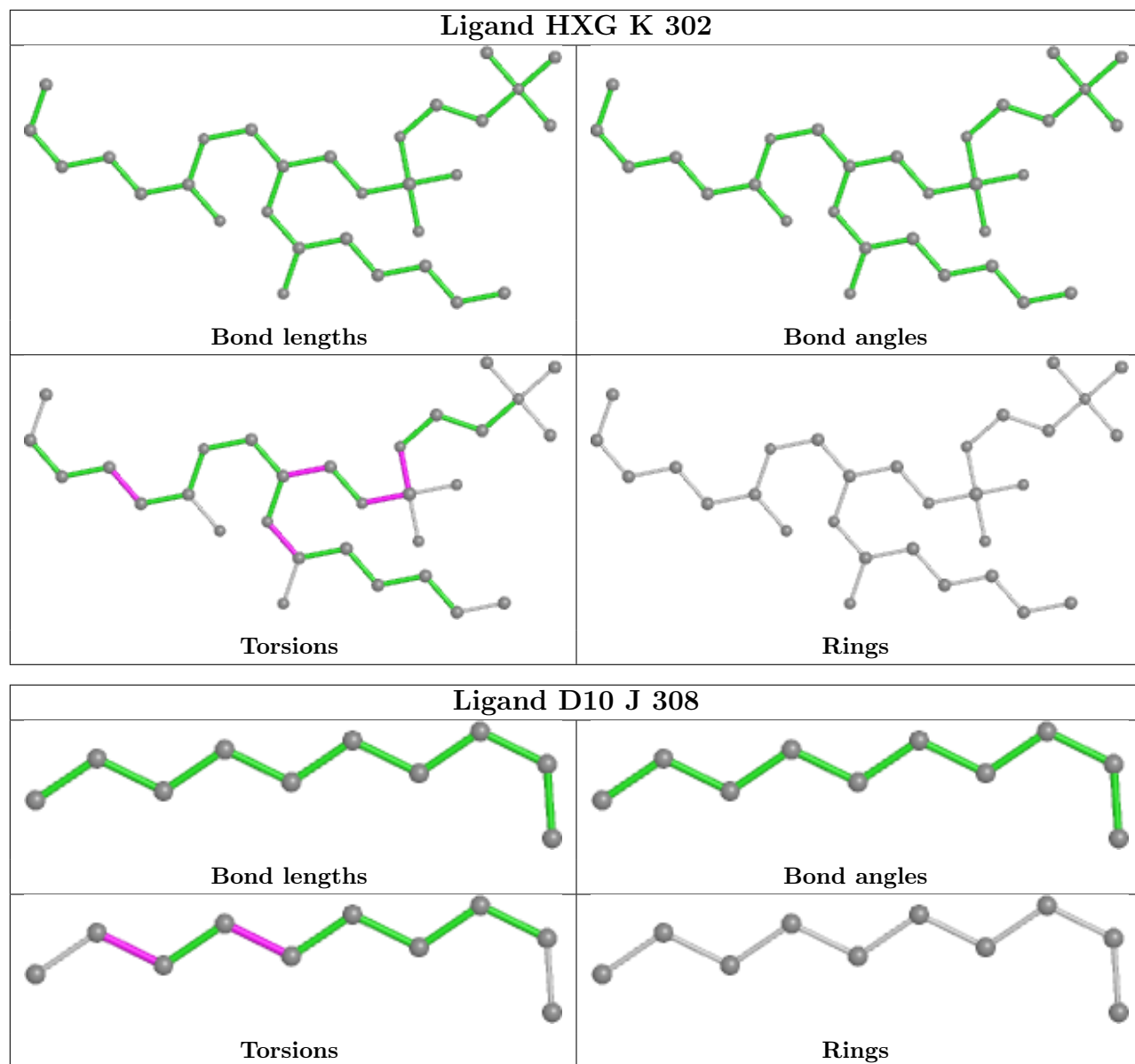


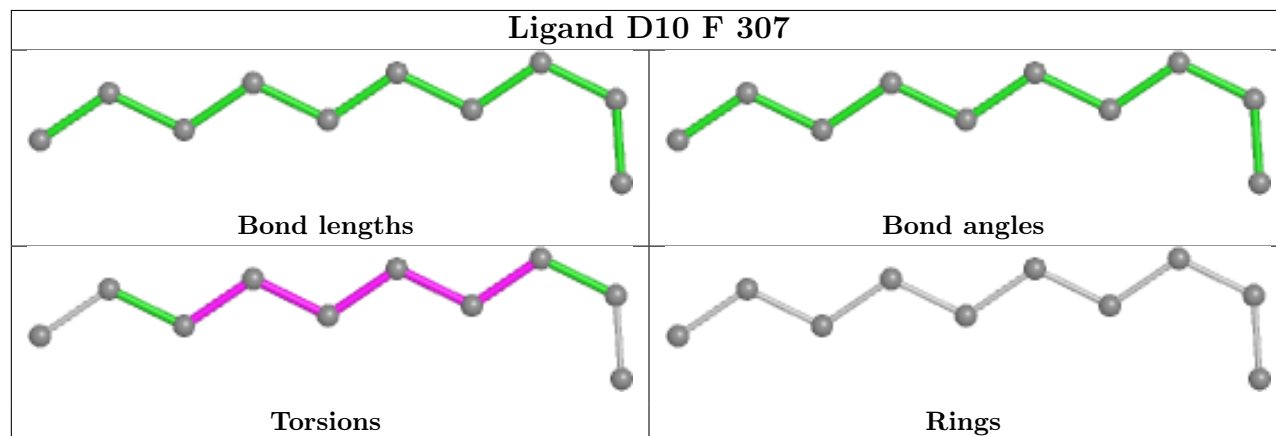
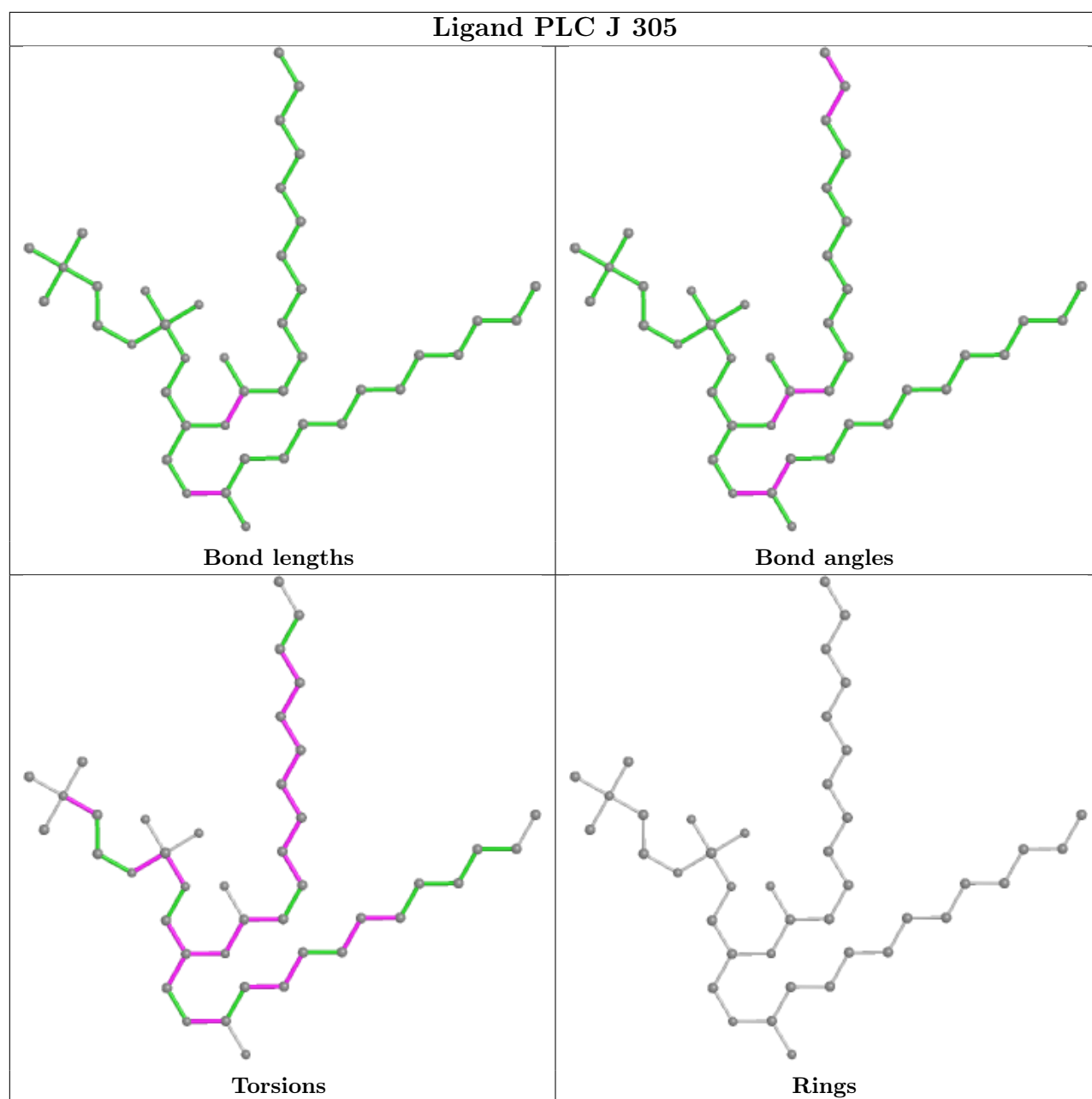


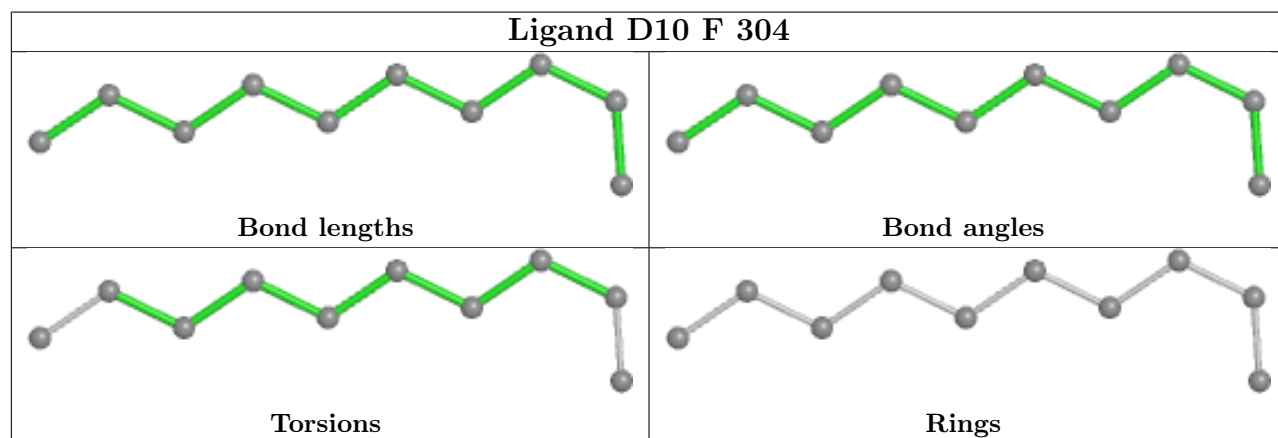
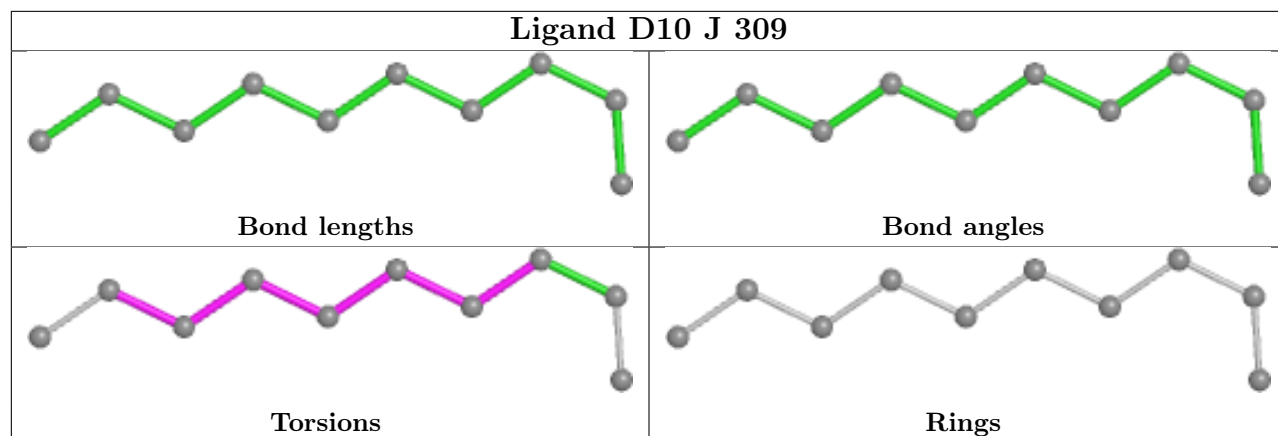


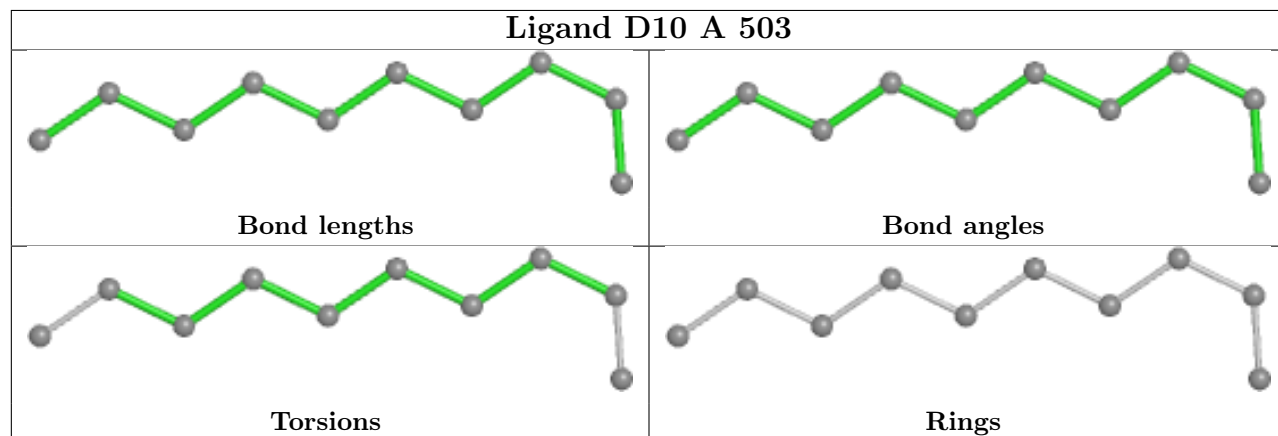
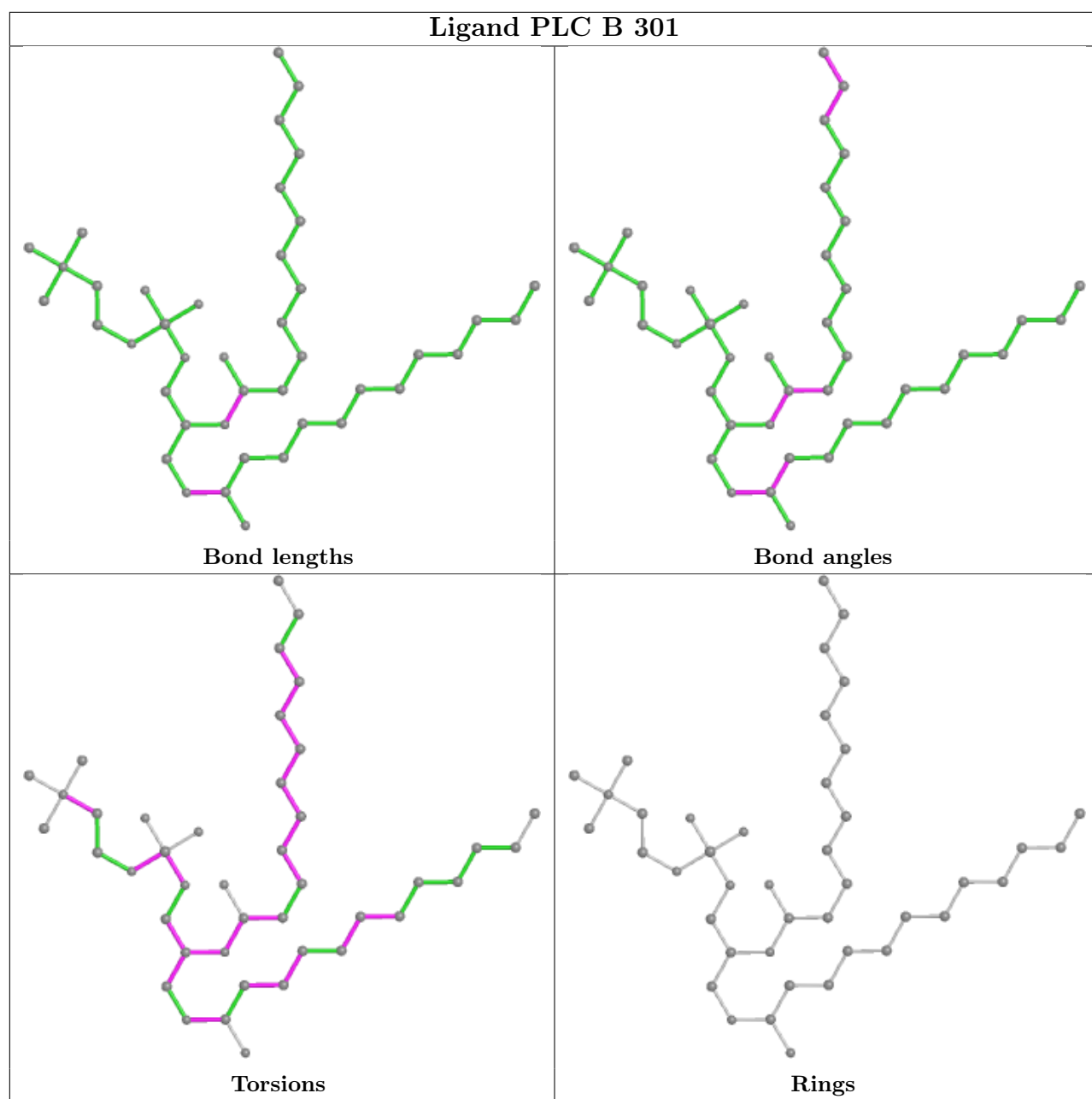


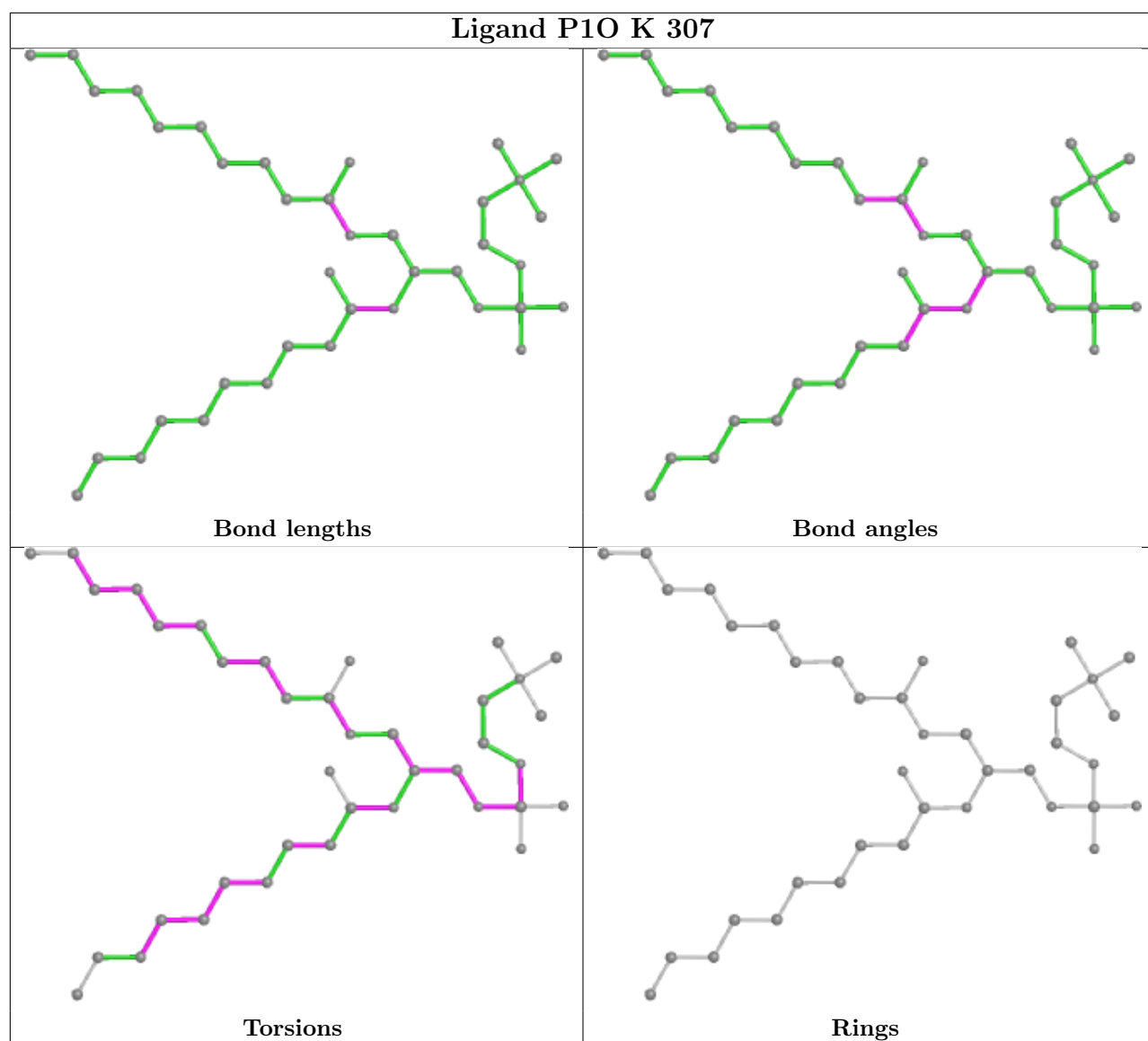


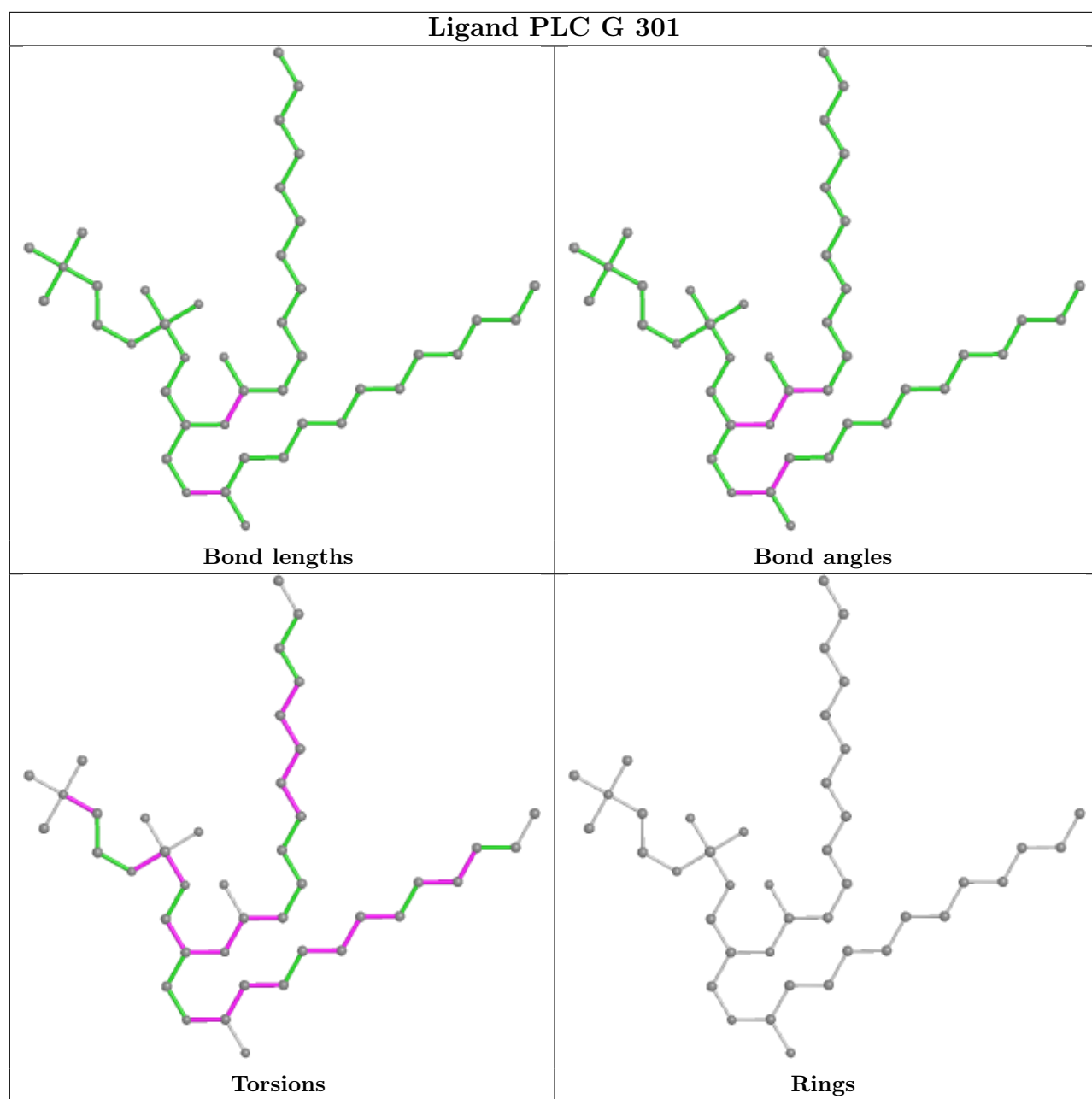


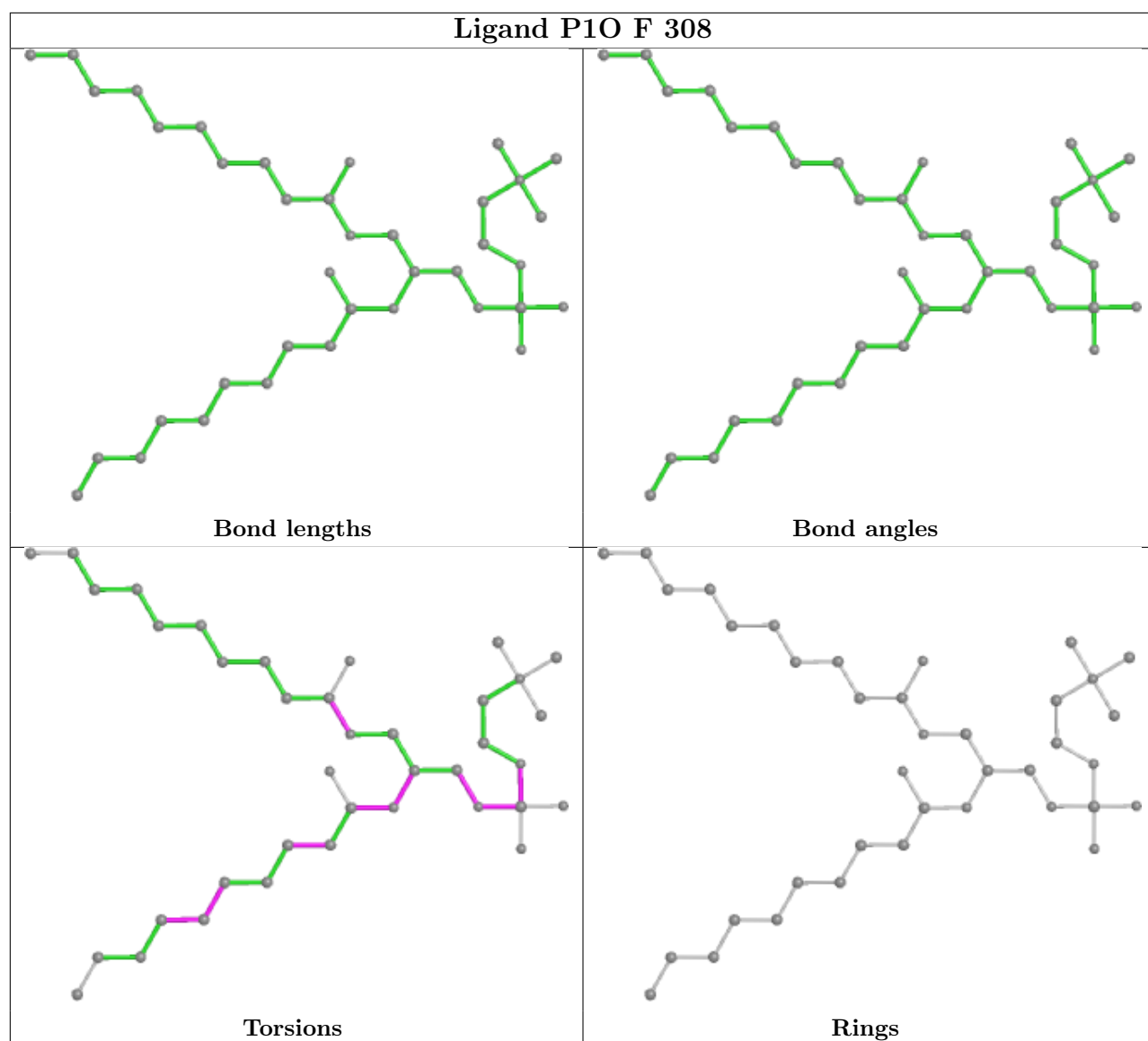


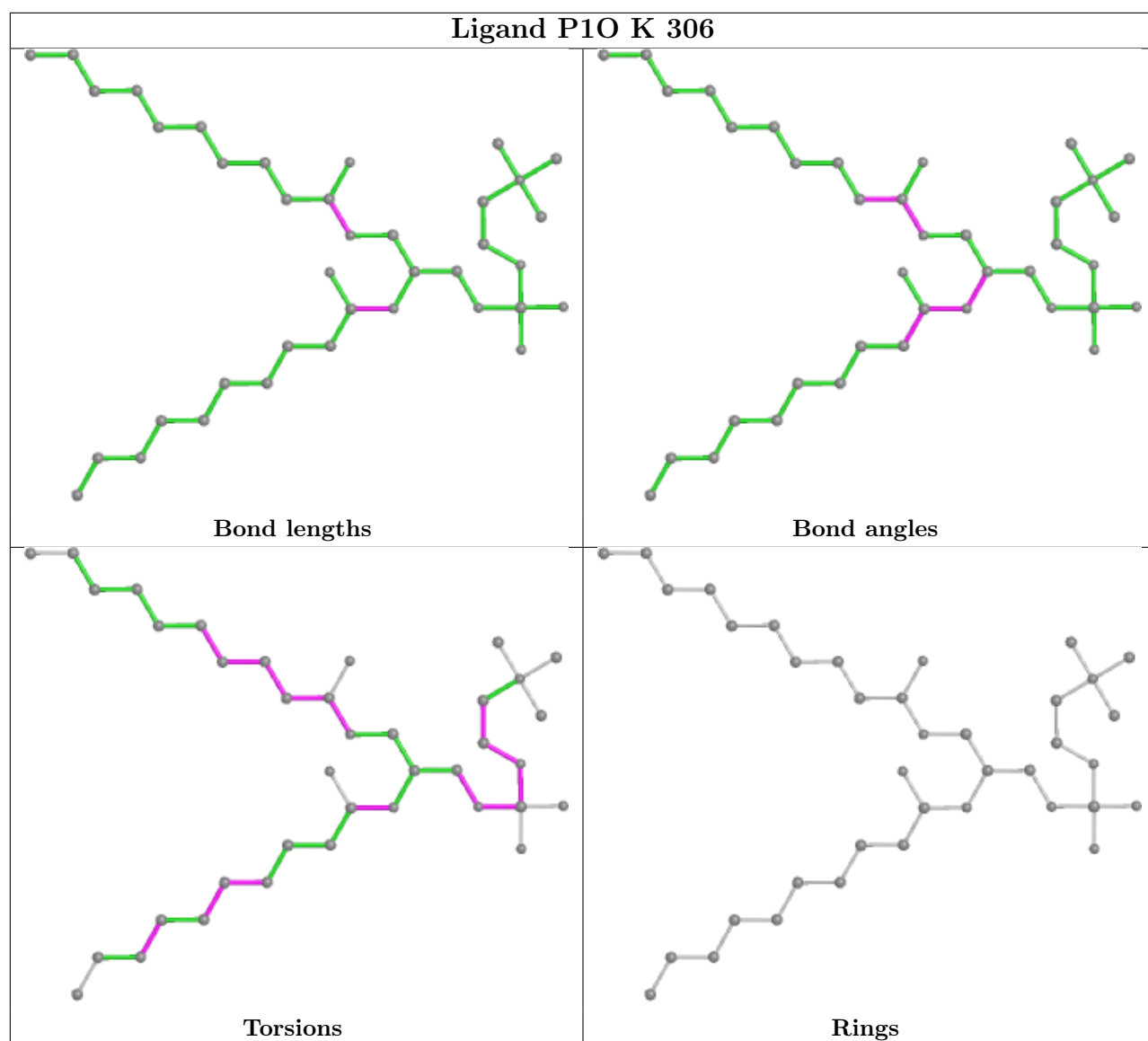




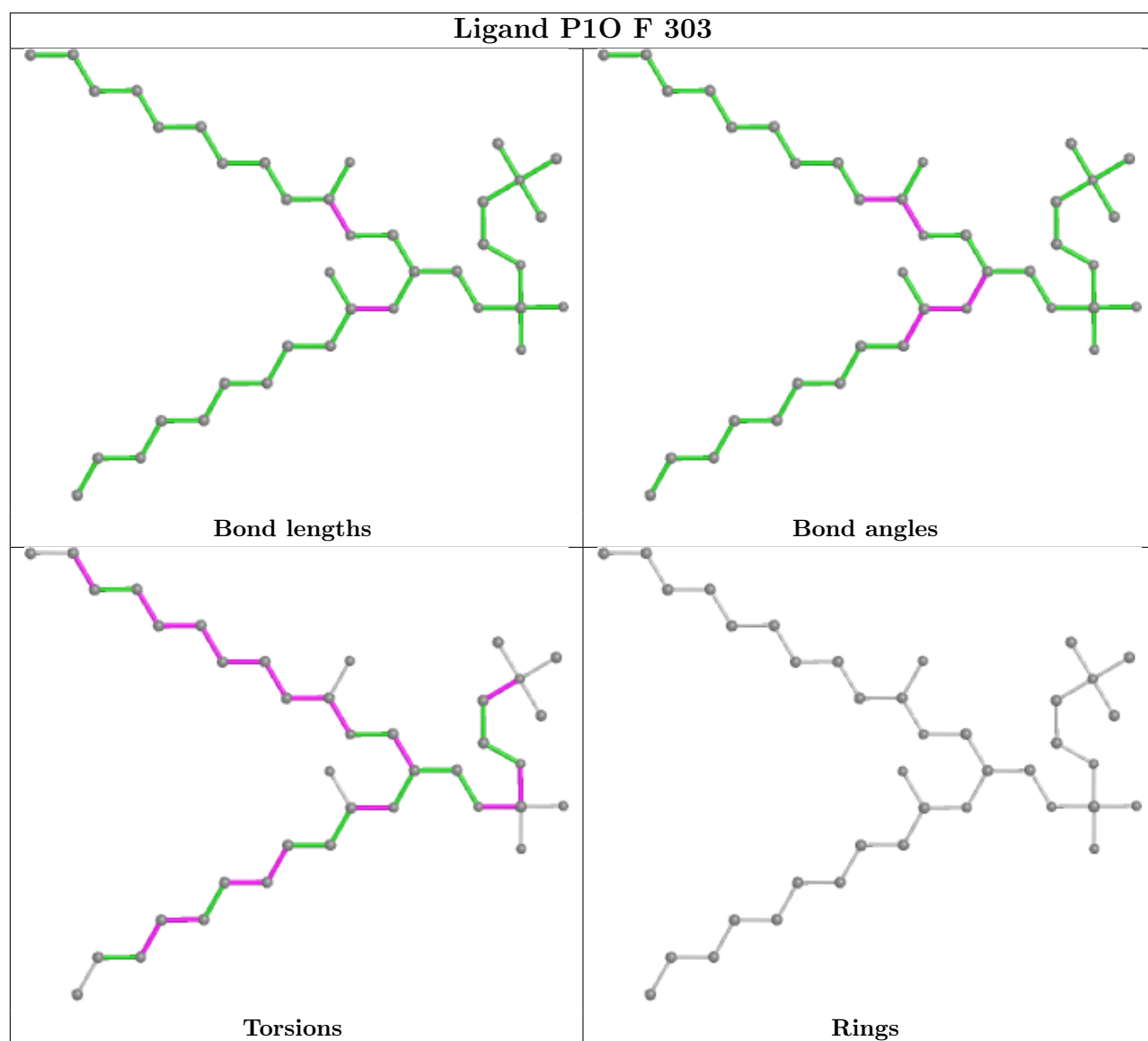


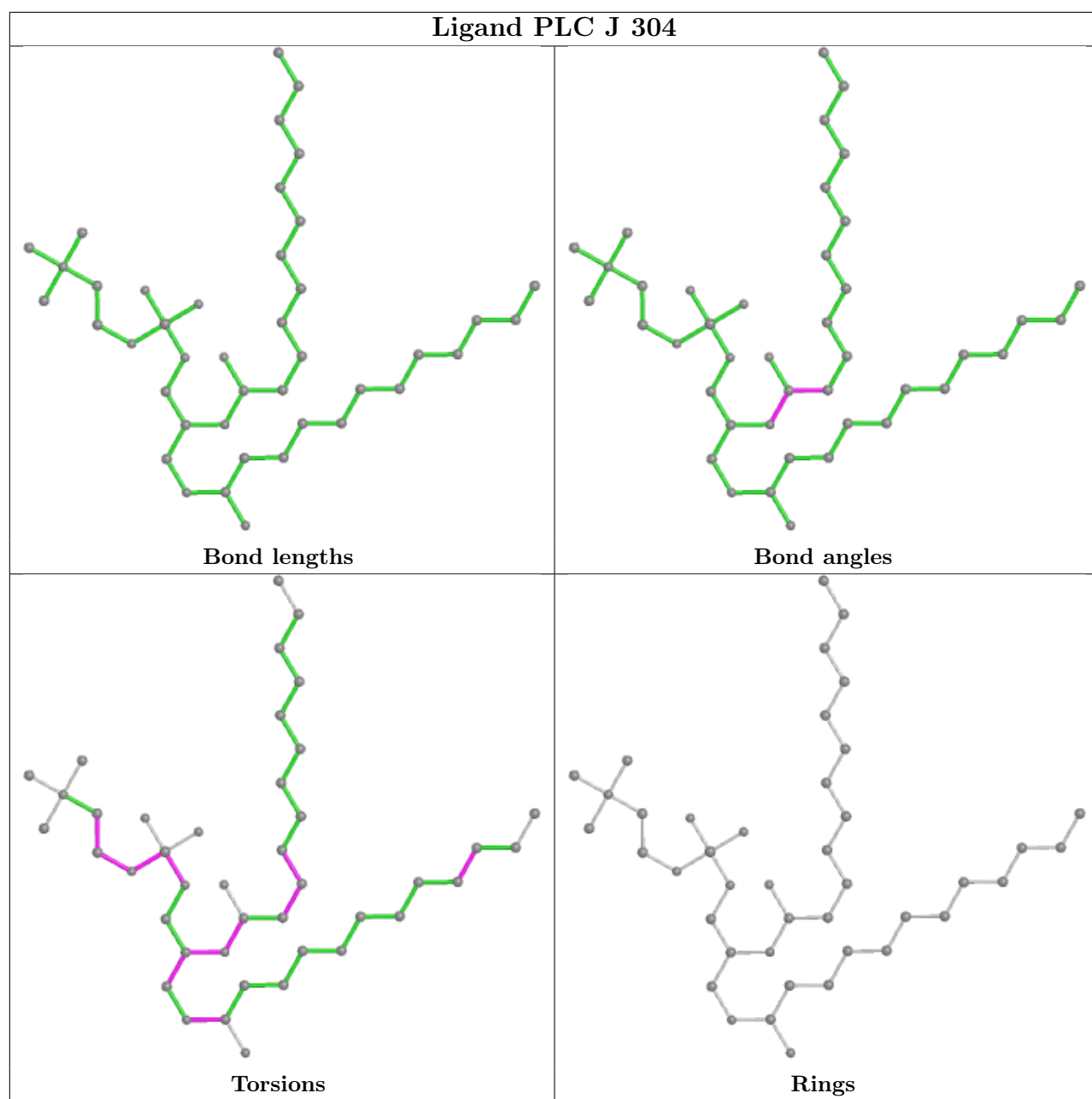


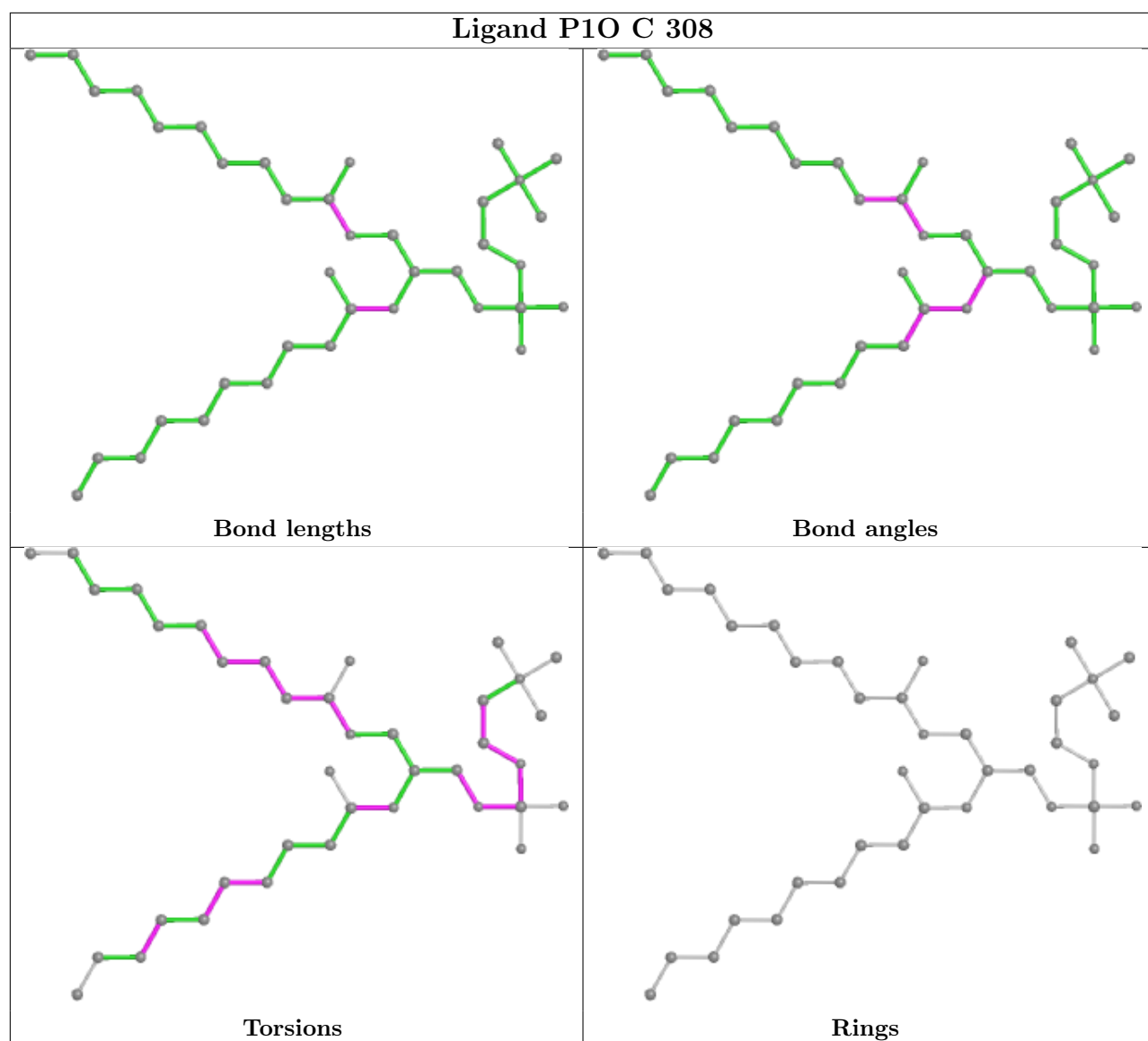


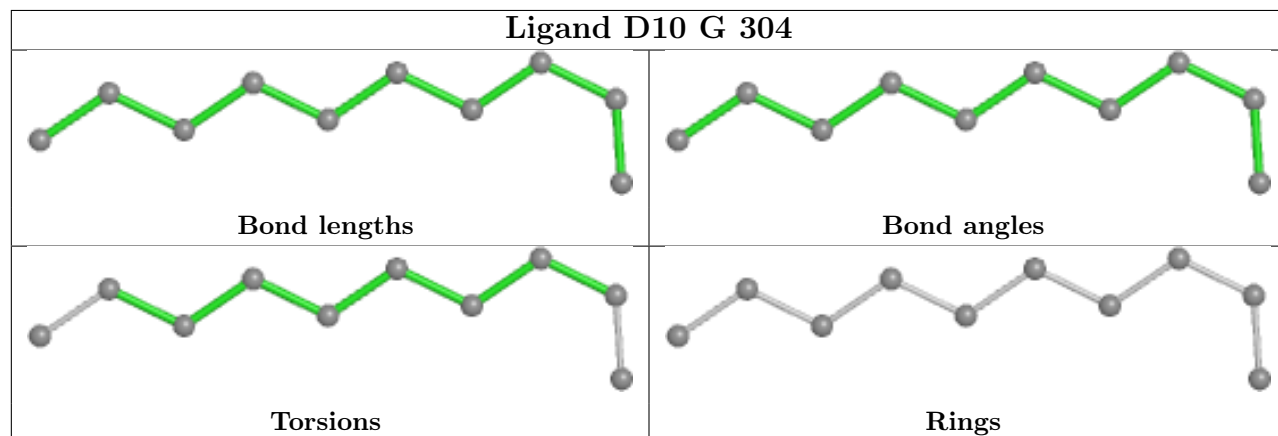
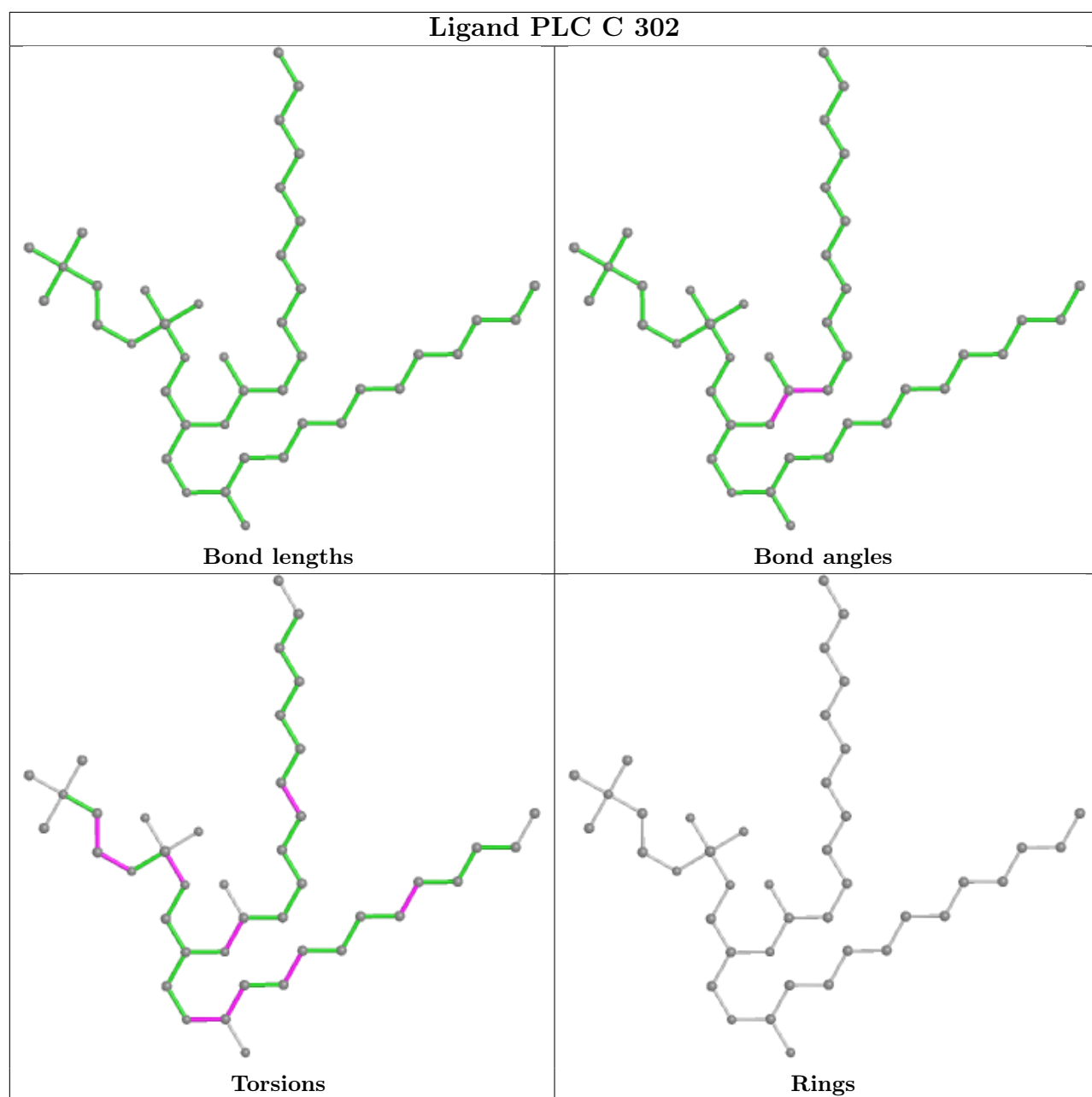


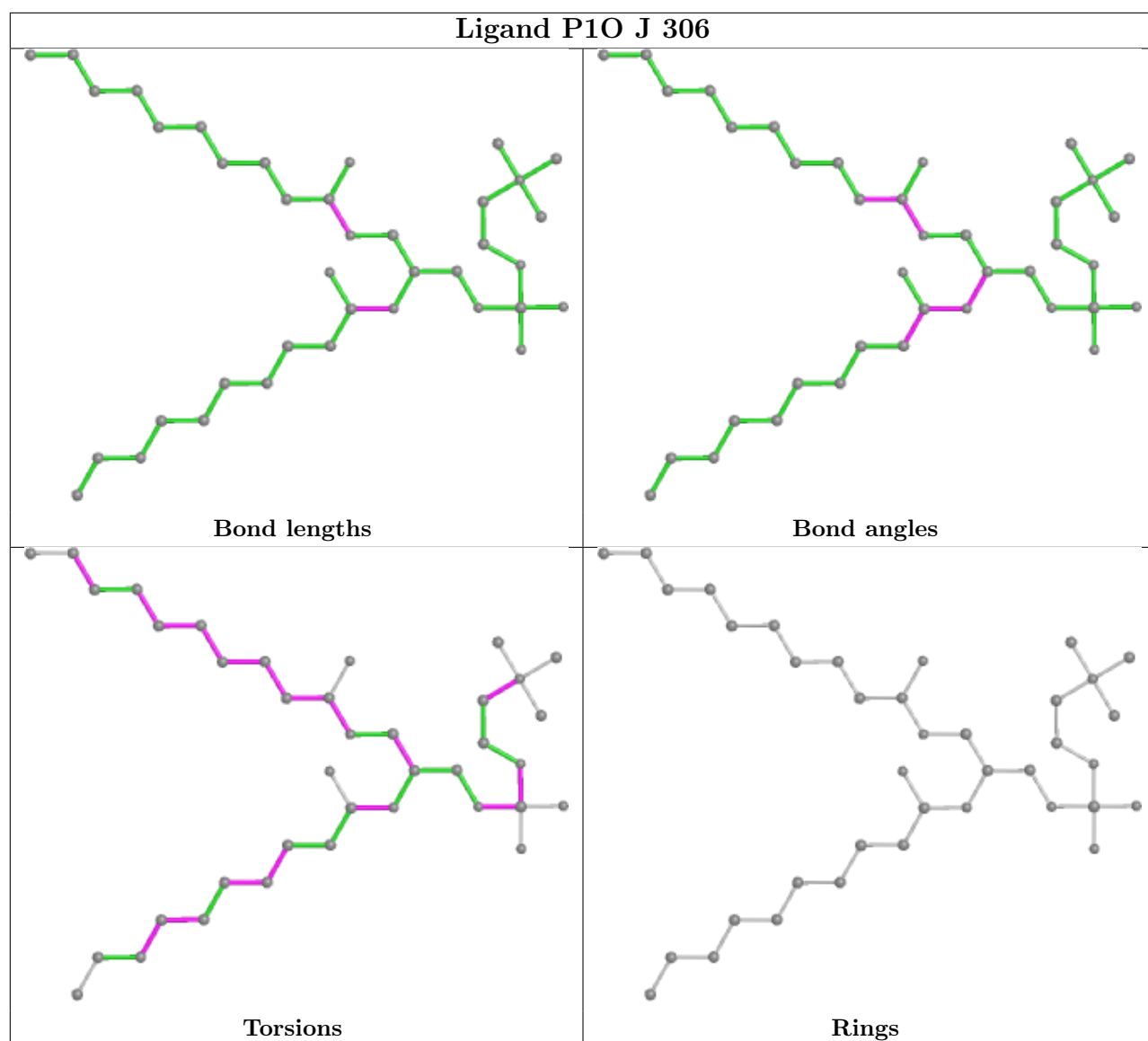


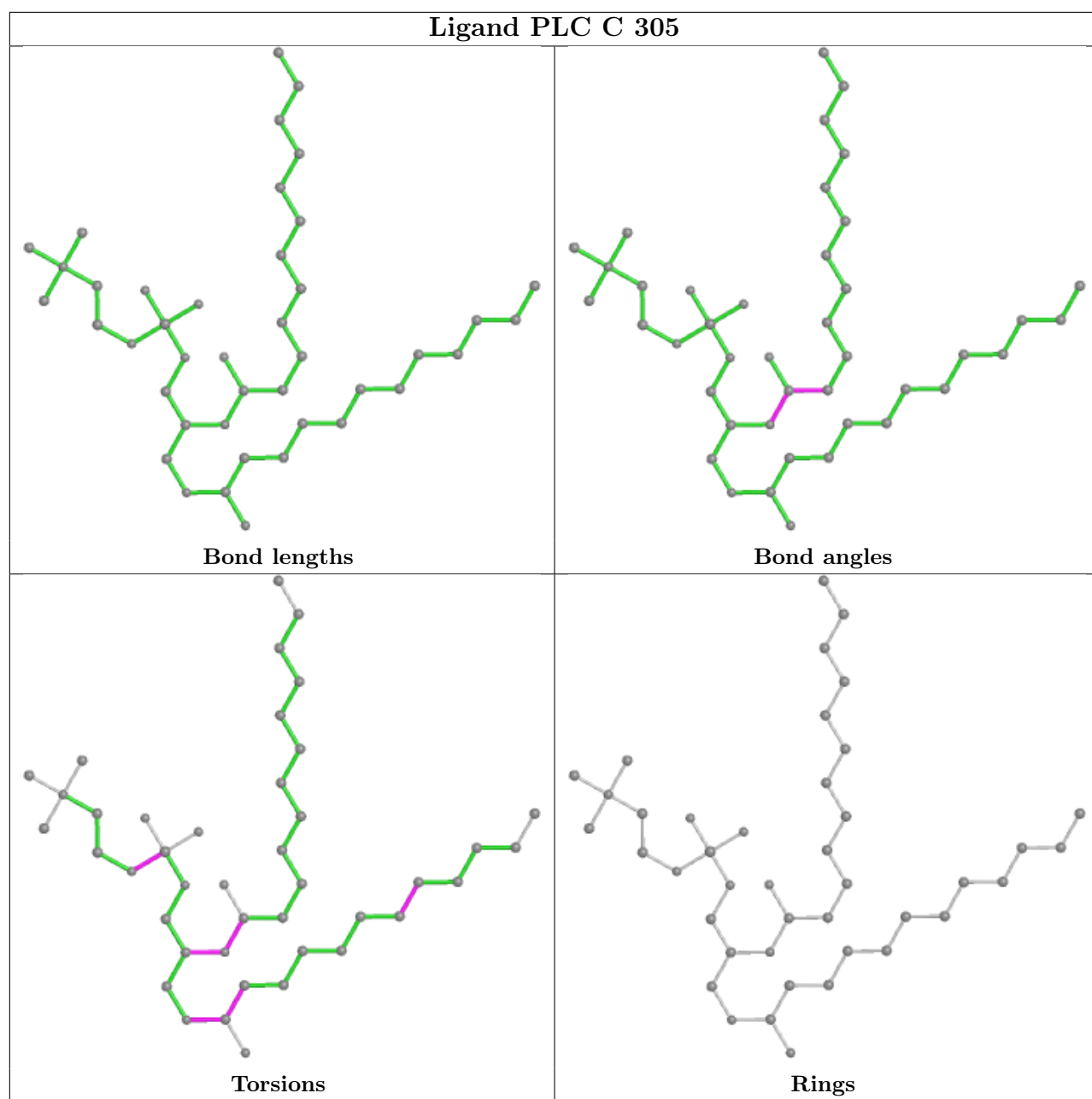


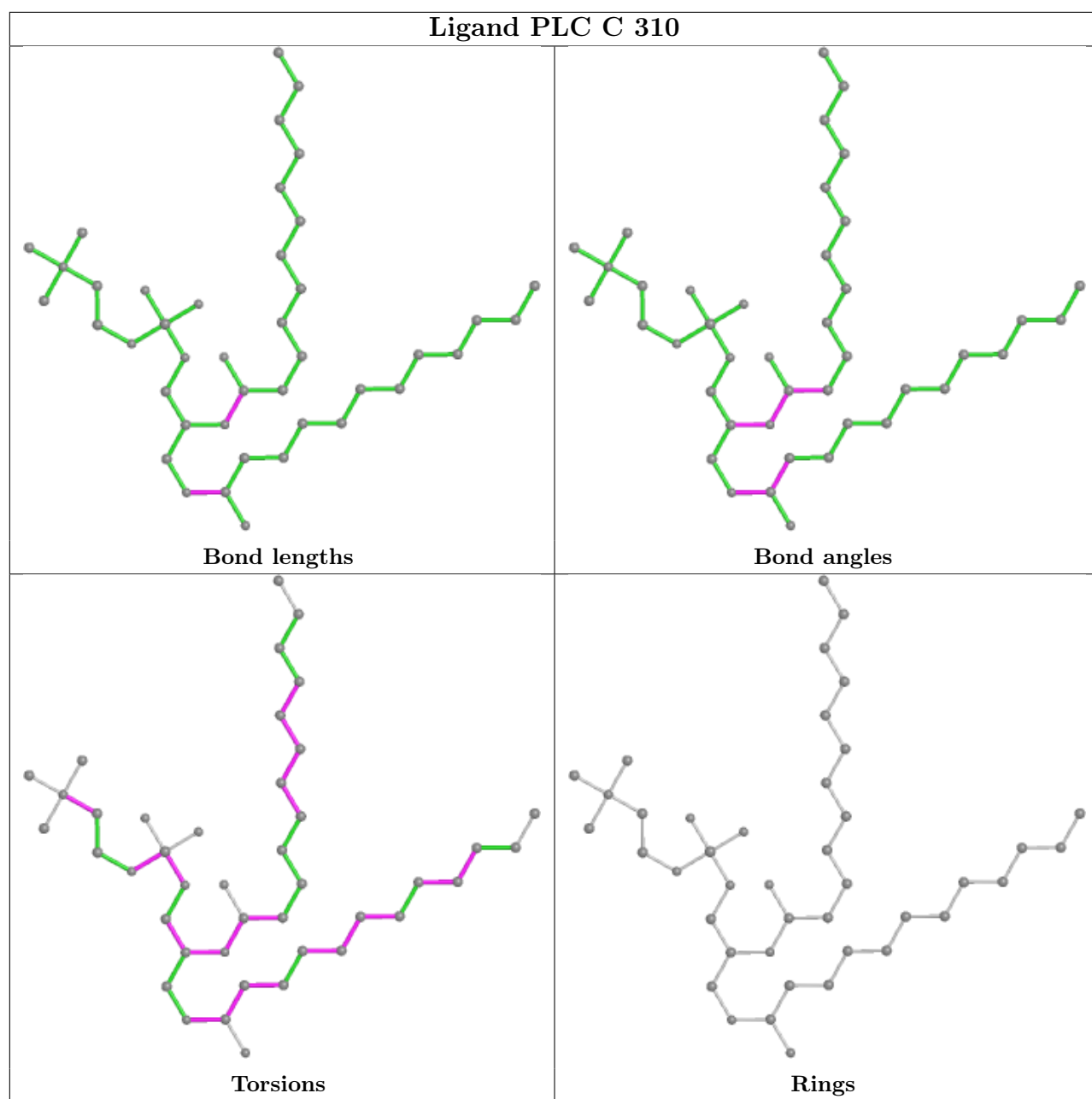


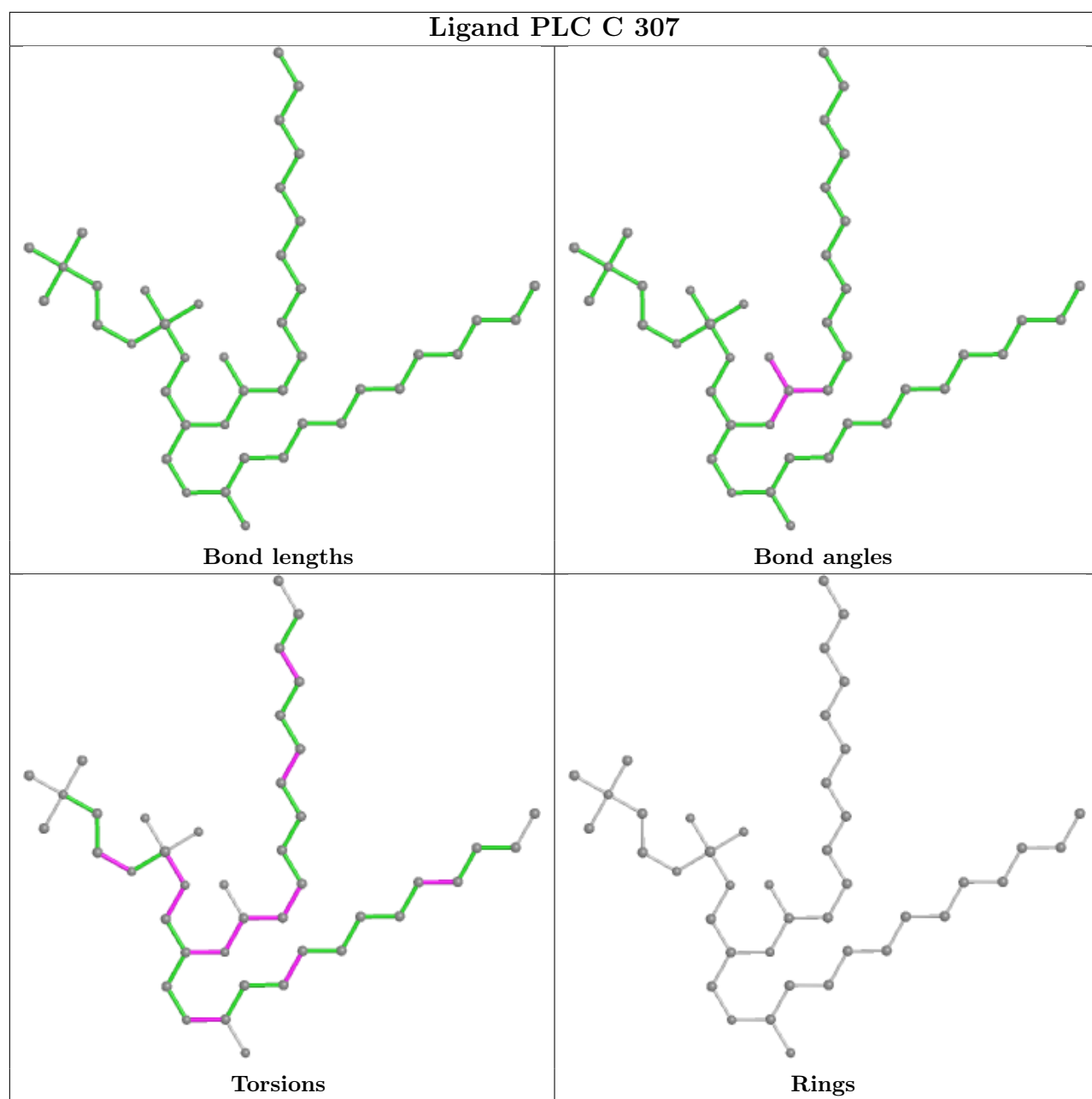




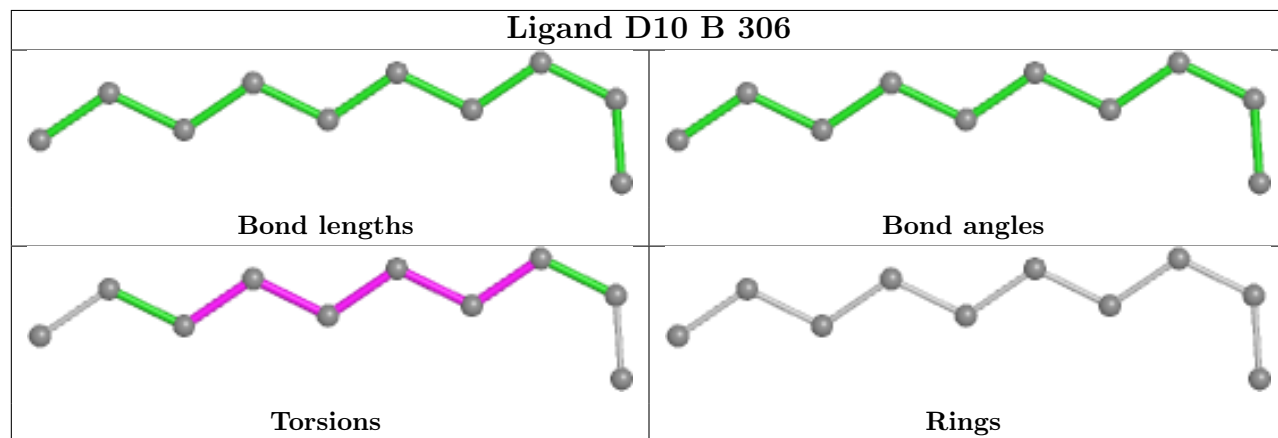
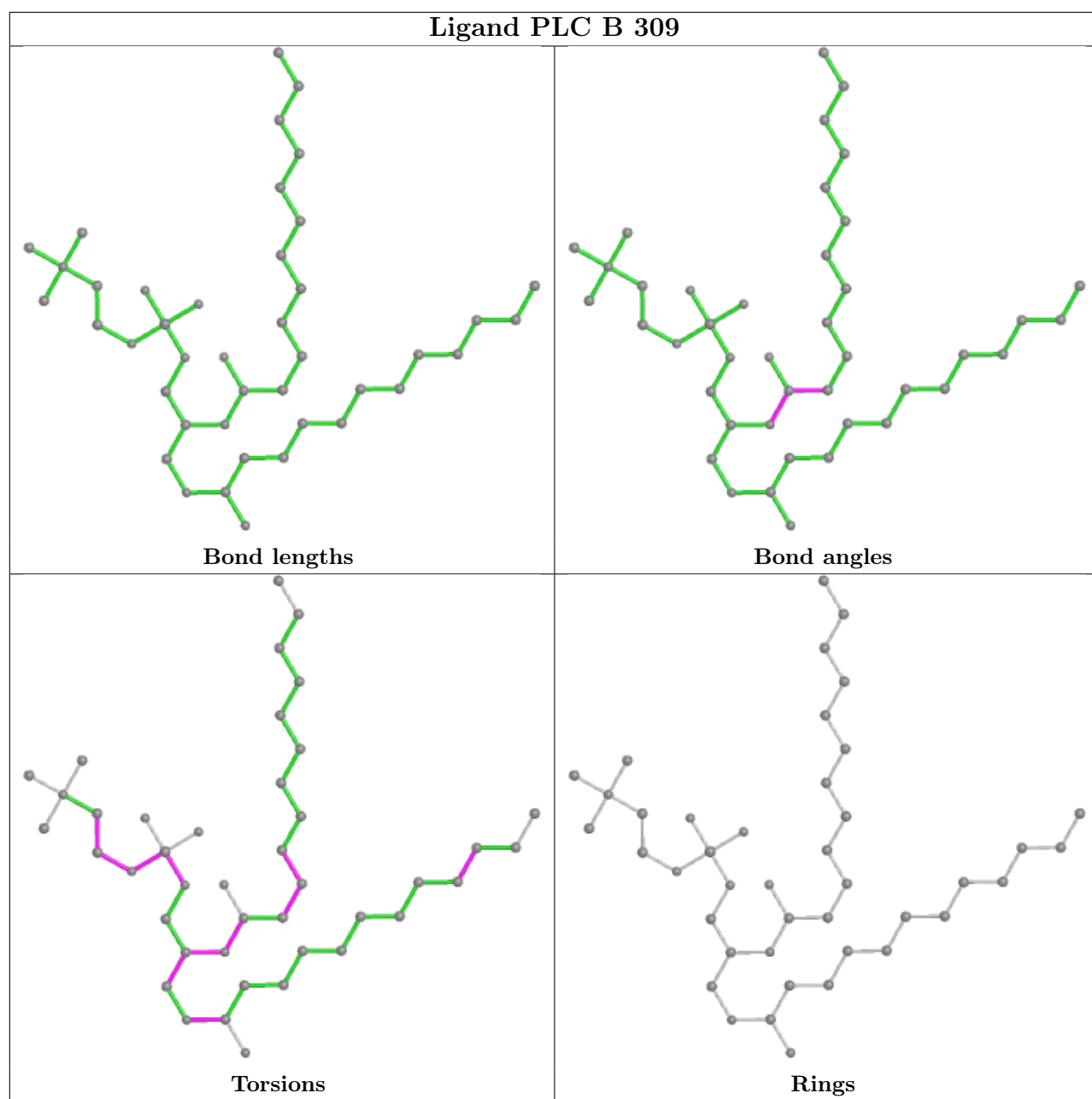


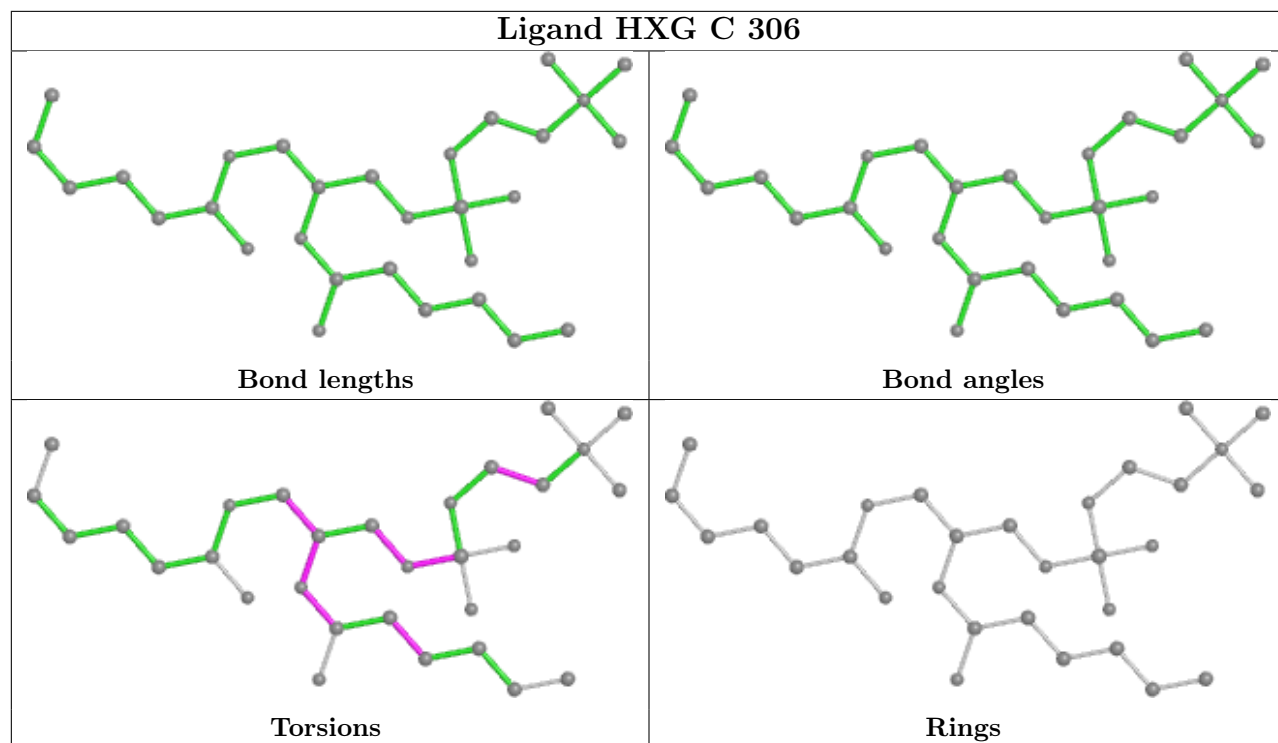


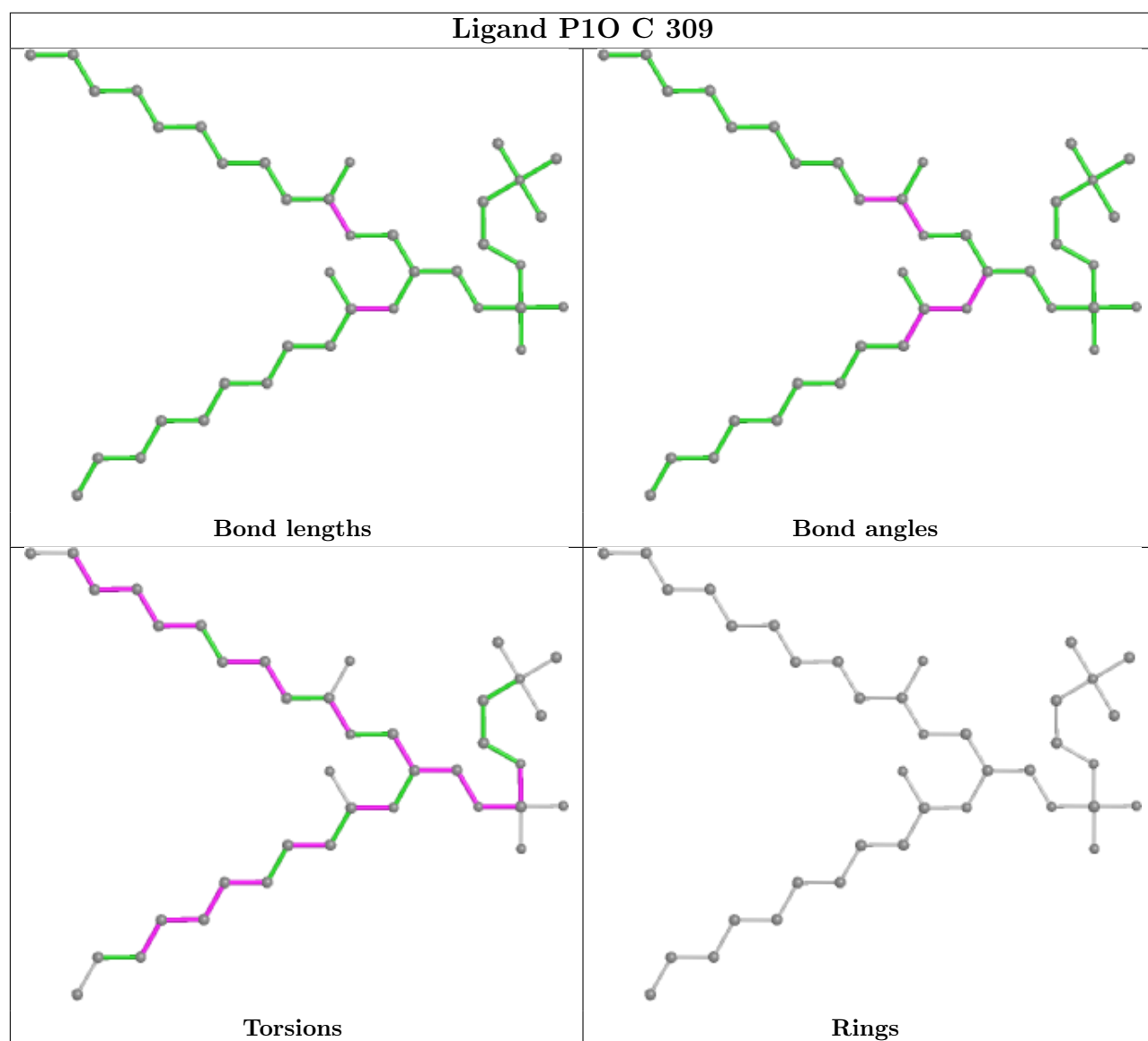


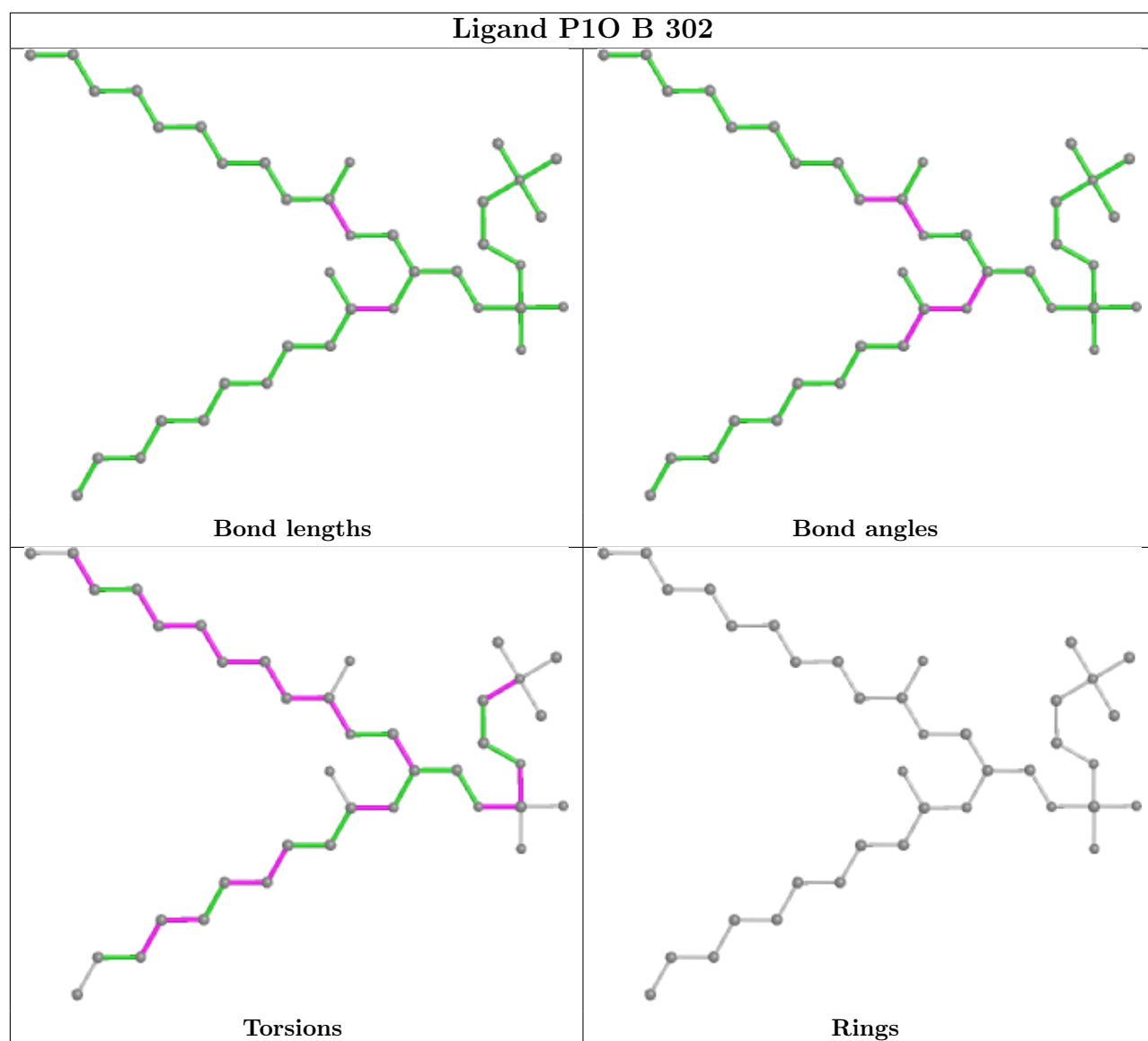


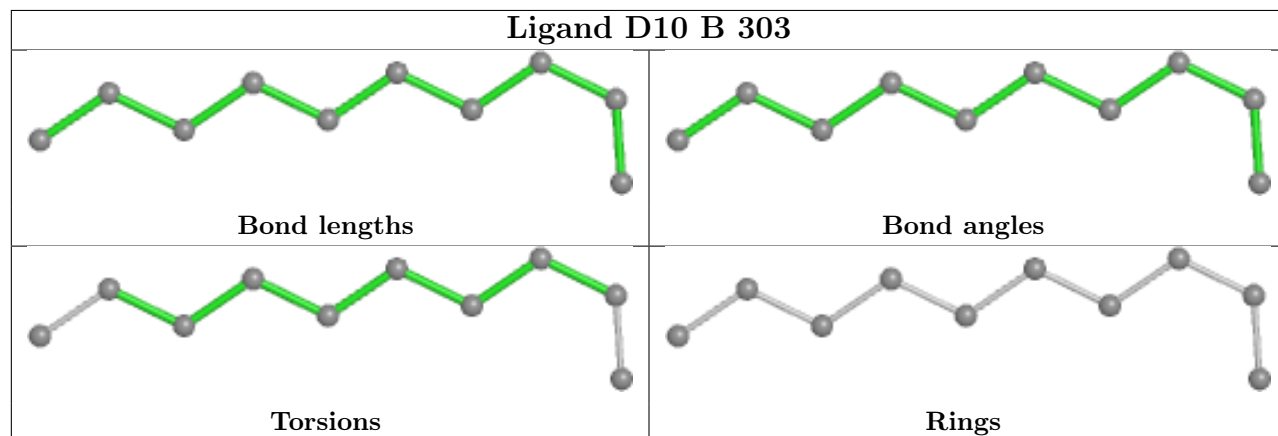
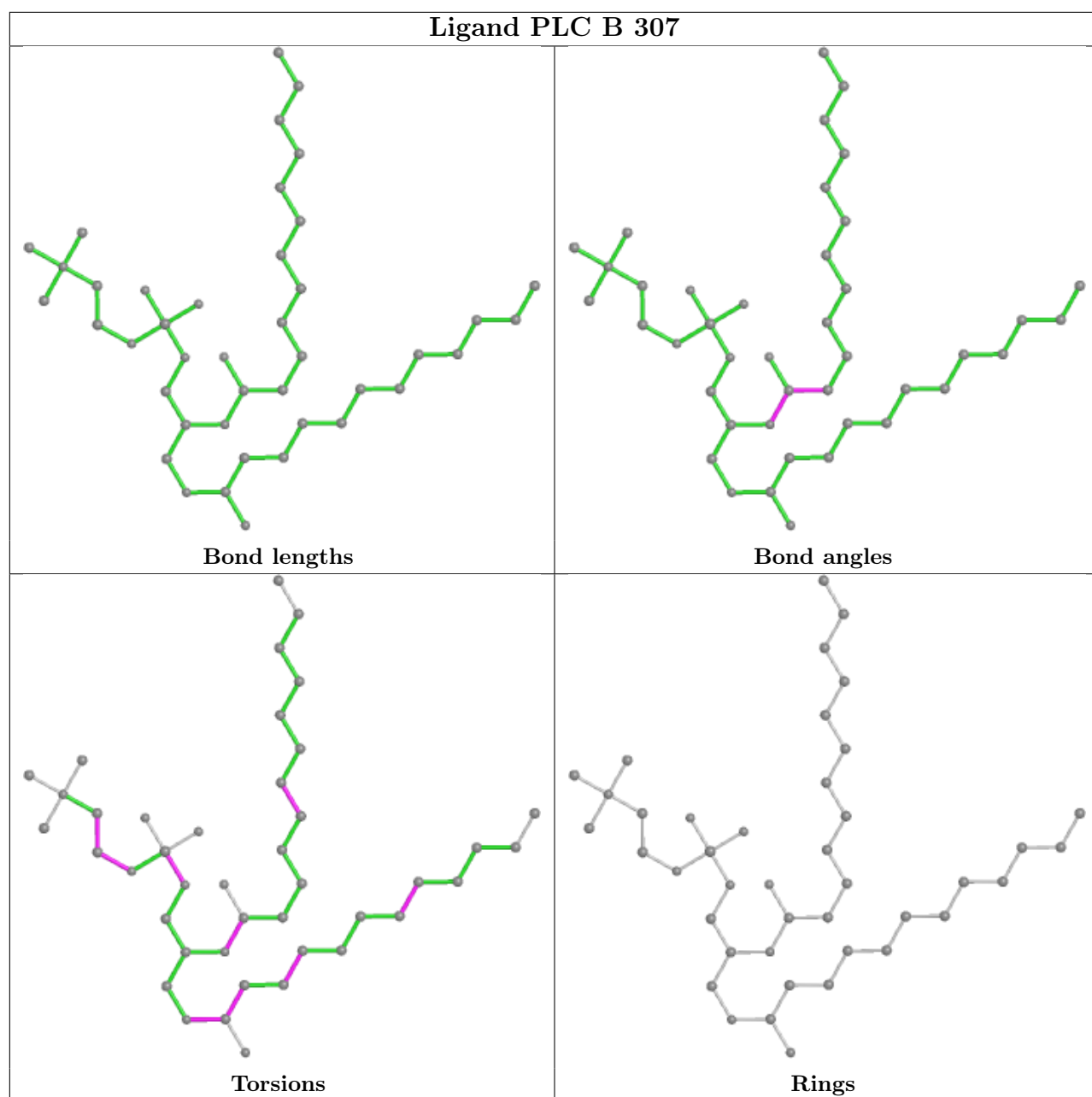


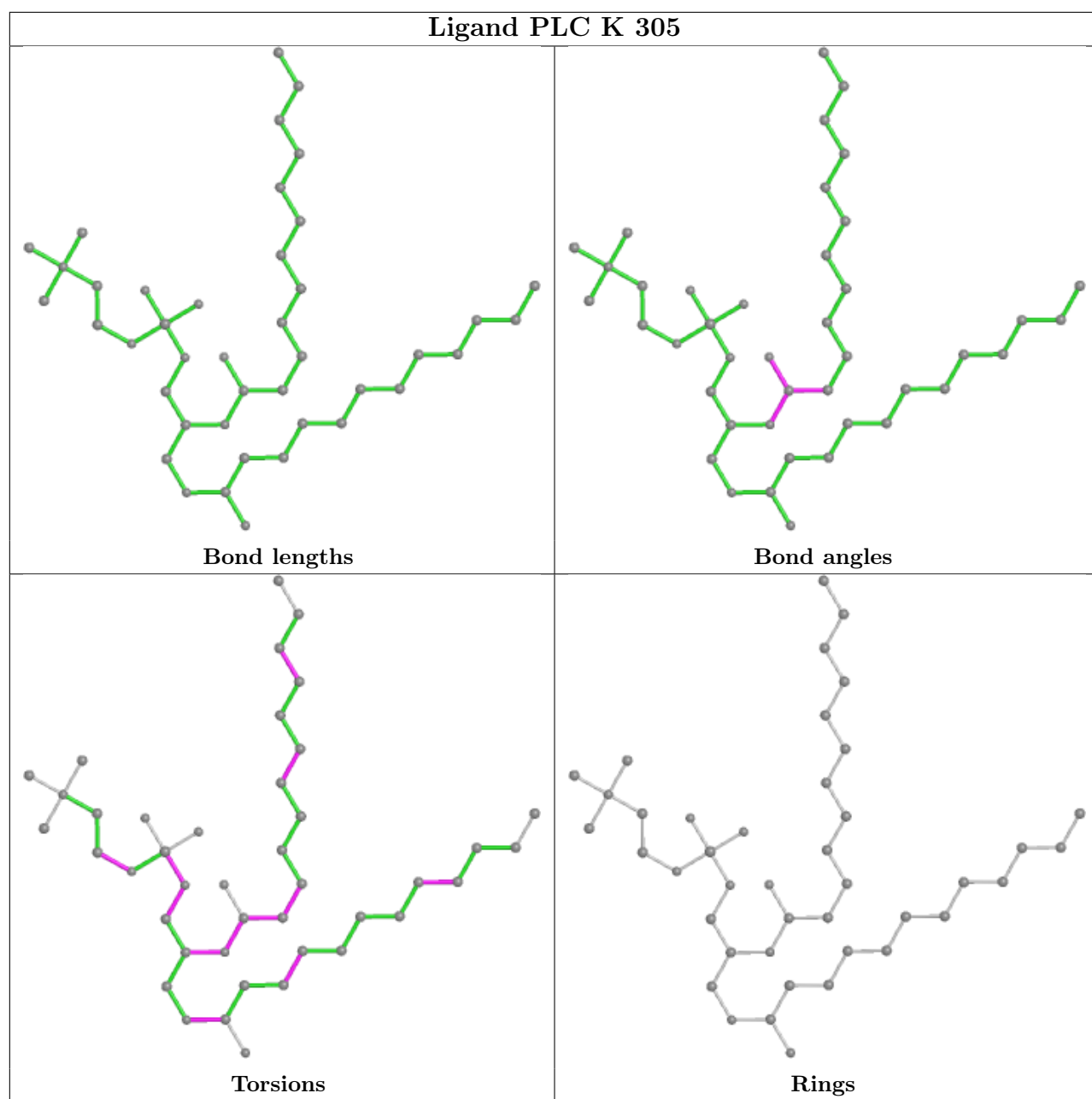


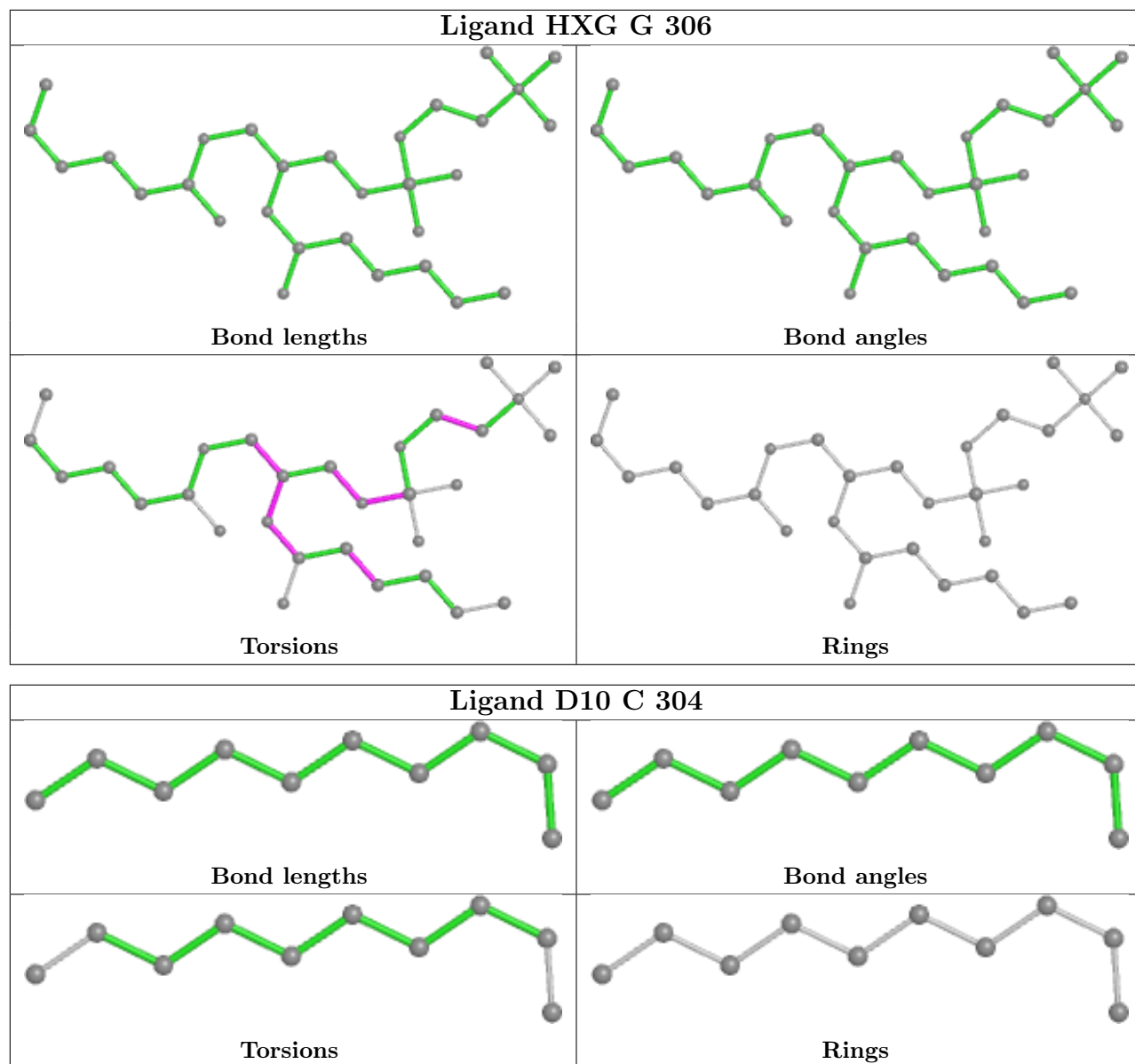


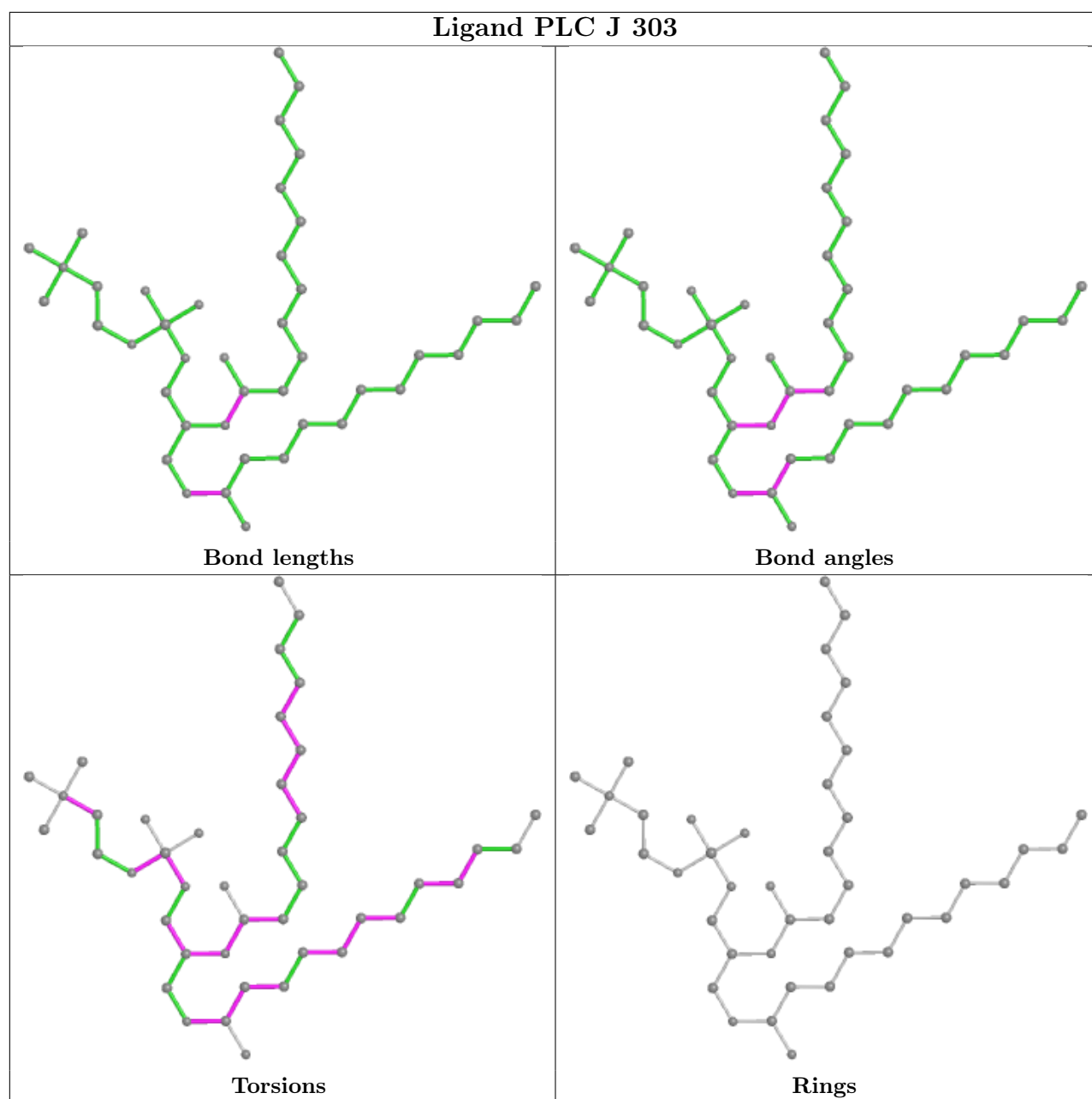












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



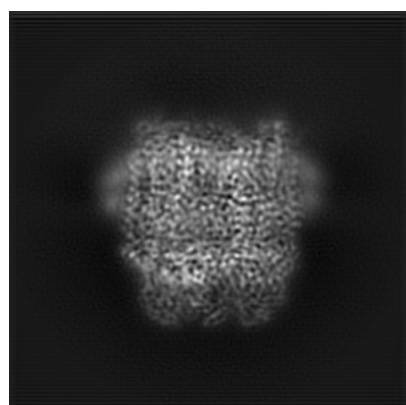
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24829. These allow visual inspection of the internal detail of the map and identification of artifacts.

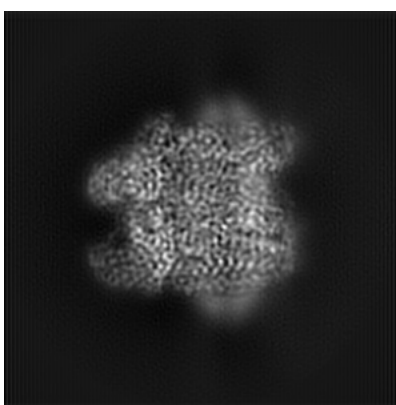
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

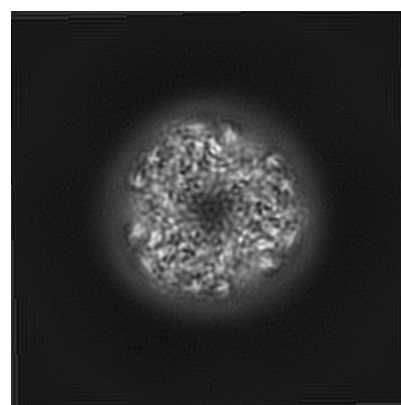
#### 6.1.1 Primary map



X



Y

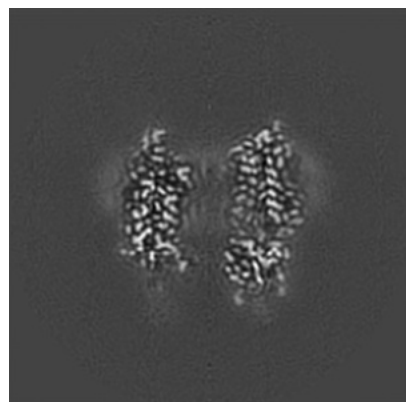


Z

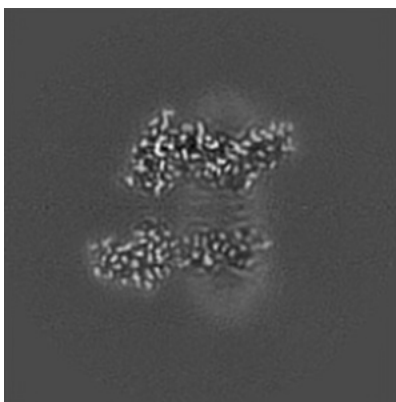
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

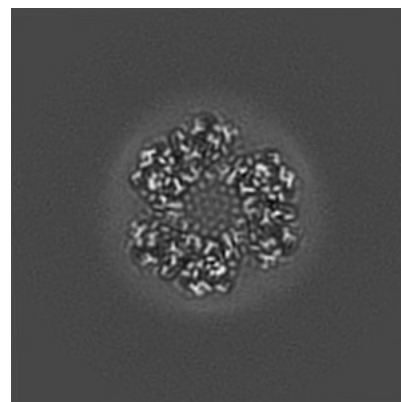
#### 6.2.1 Primary map



X Index: 216



Y Index: 216

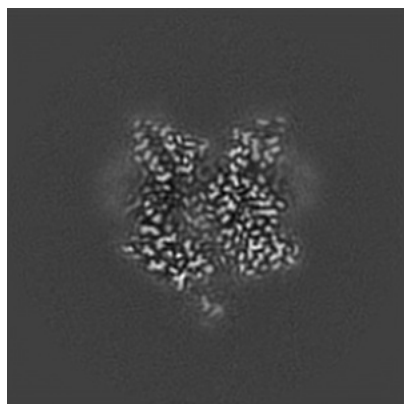


Z Index: 216

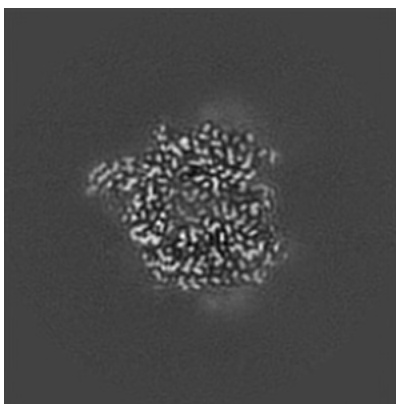
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

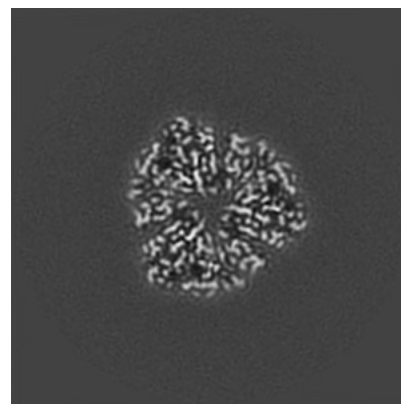
### 6.3.1 Primary map



X Index: 179



Y Index: 253

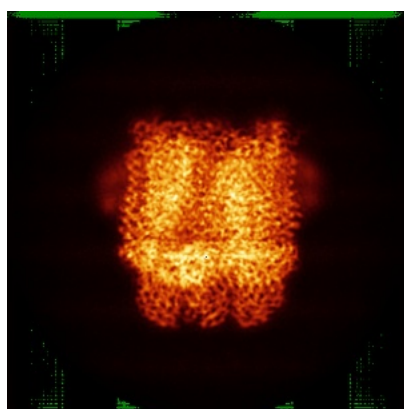


Z Index: 167

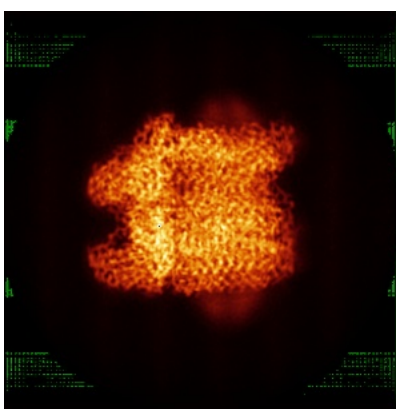
The images above show the largest variance slices of the map in three orthogonal directions.

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

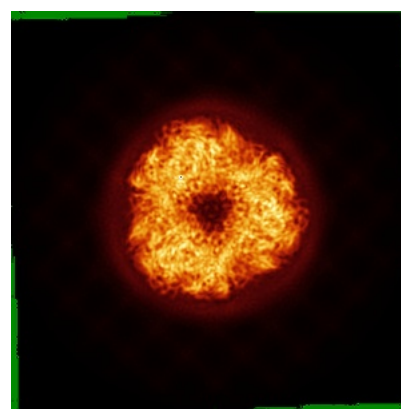
### 6.4.1 Primary map



X



Y

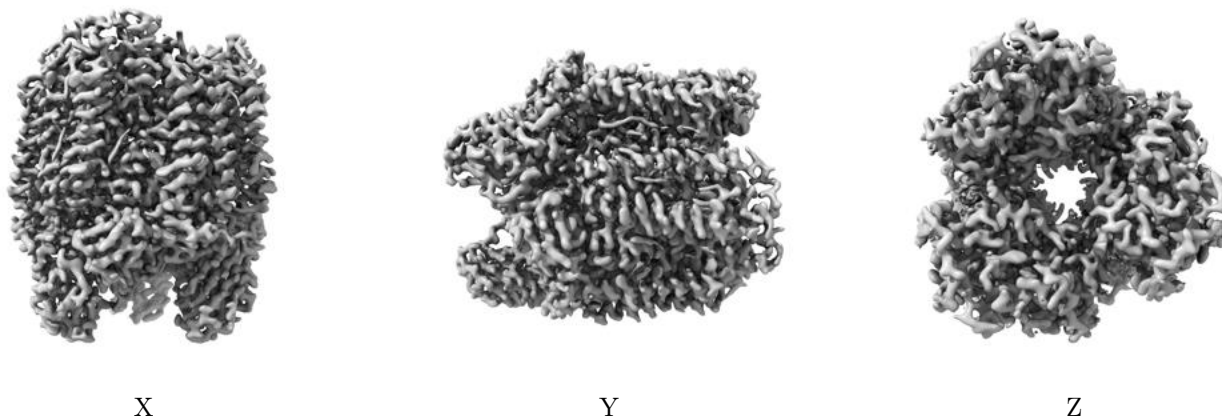


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0237. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

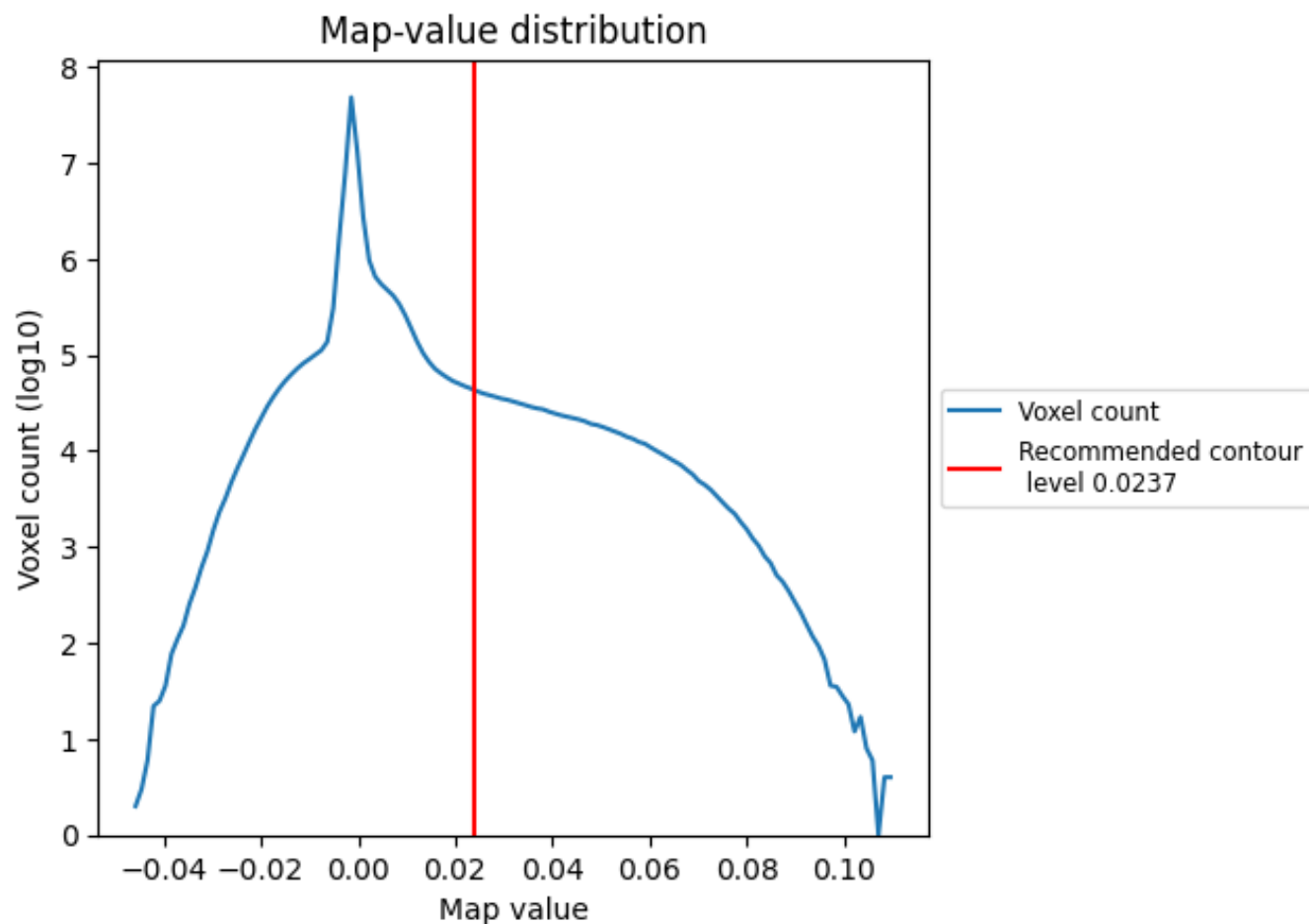
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

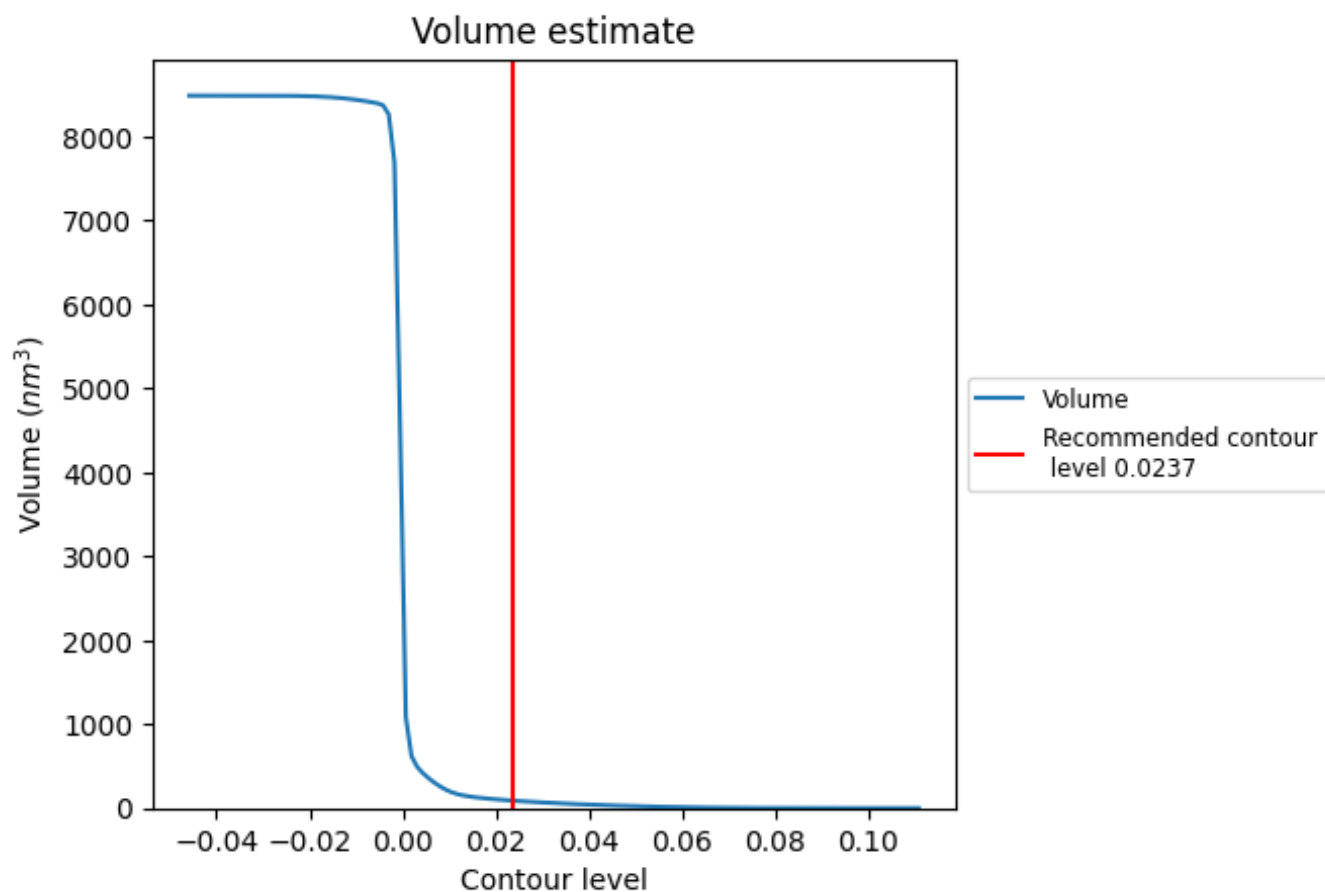
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

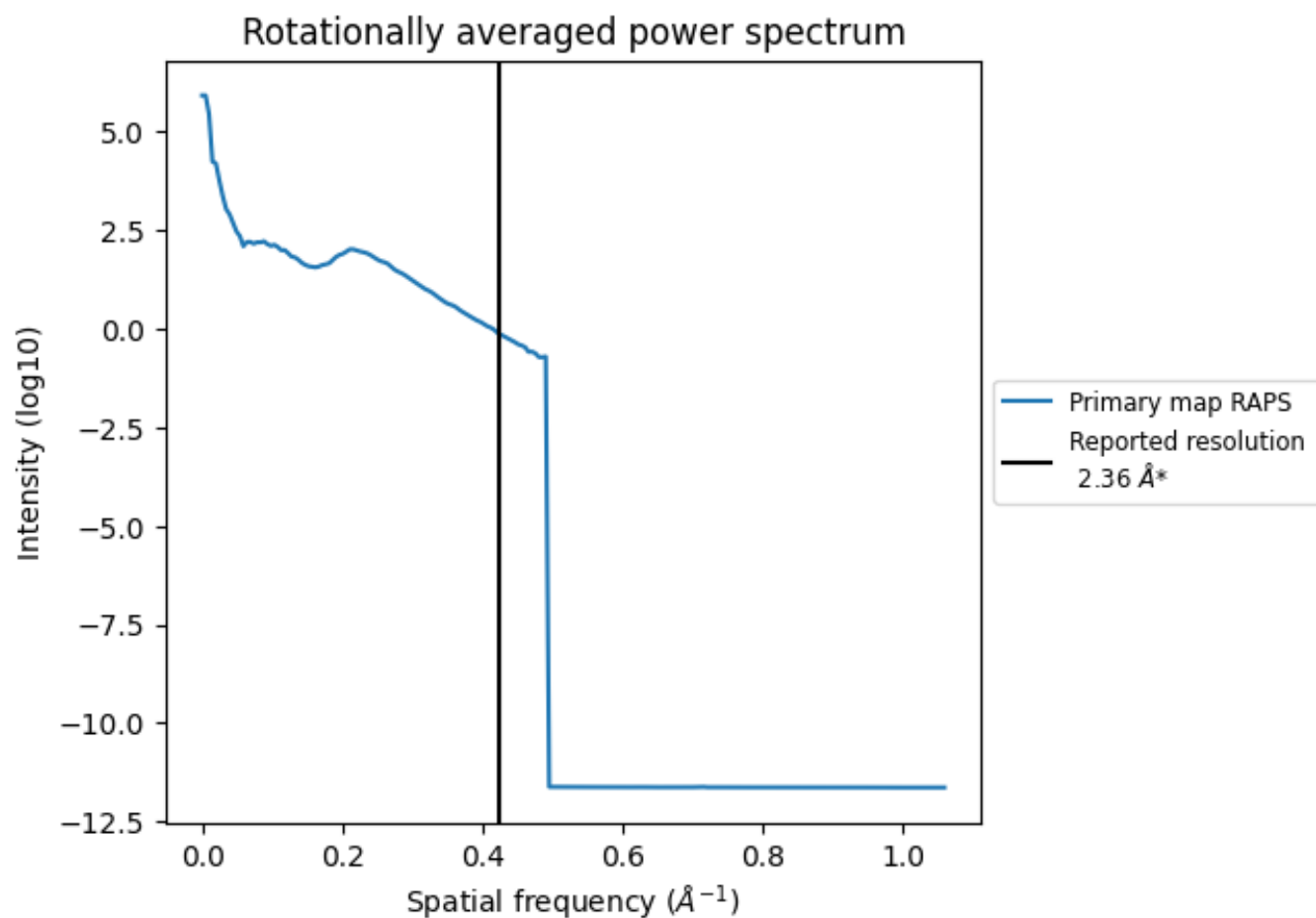
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89  $\text{nm}^3$ ; this corresponds to an approximate mass of 81 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

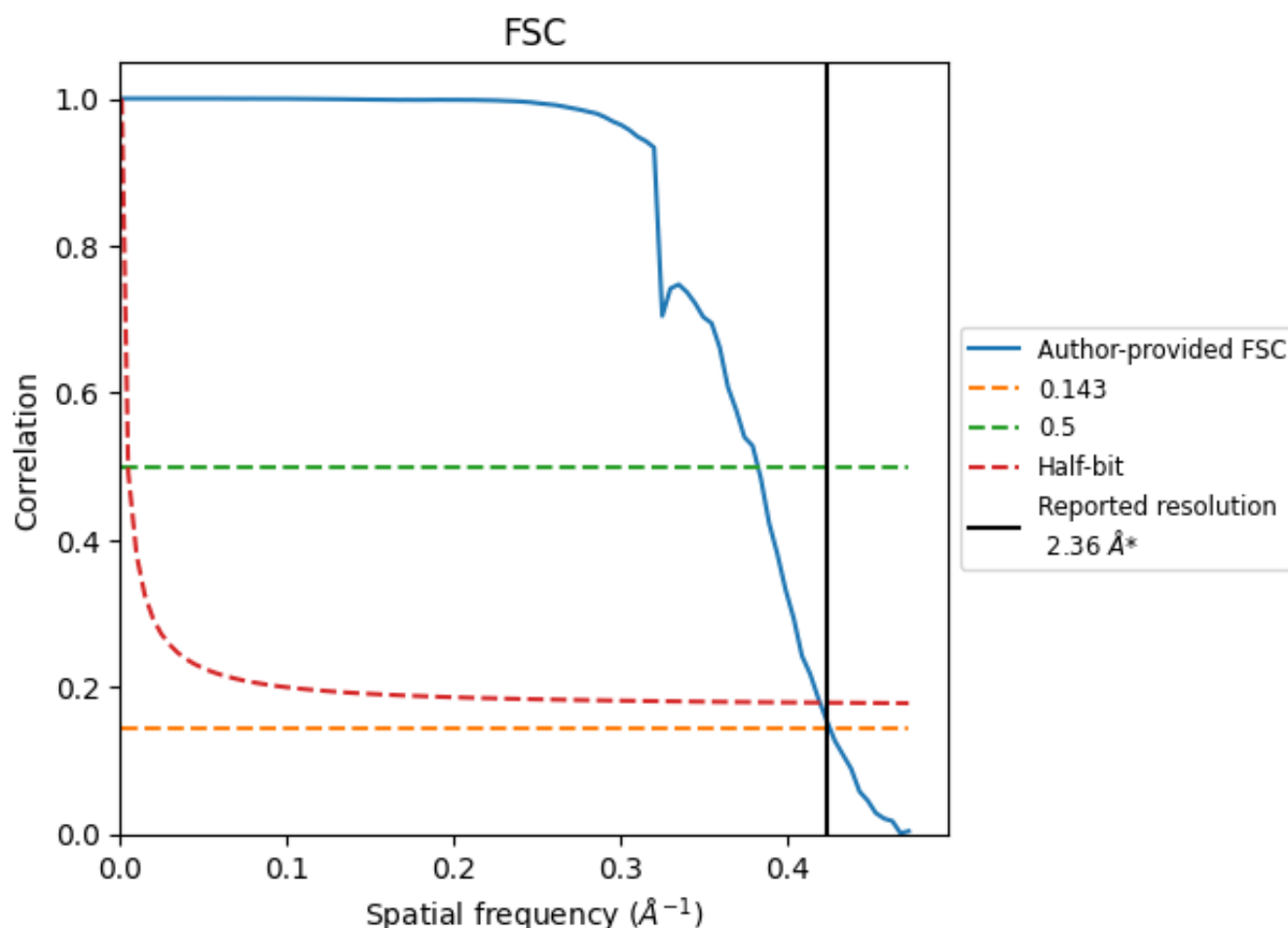


\*Reported resolution corresponds to spatial frequency of 0.424 Å<sup>-1</sup>

## 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 0.424 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.36	-	-
Author-provided FSC curve	2.35	2.61	2.38
Unmasked-calculated*	-	-	-

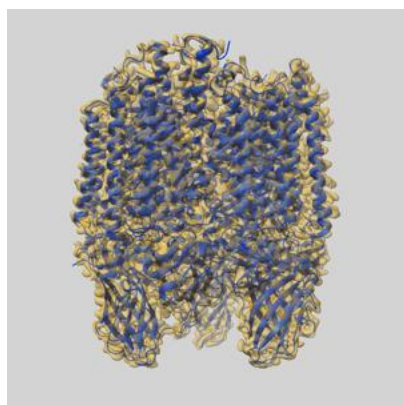
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



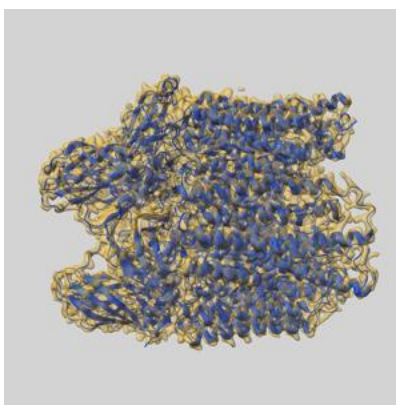
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24829 and PDB model 7S4K. Per-residue inclusion information can be found in section [3](#) on page [11](#).

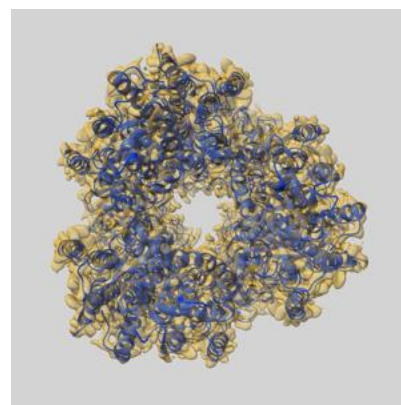
### 9.1 Map-model overlay [i](#)



X



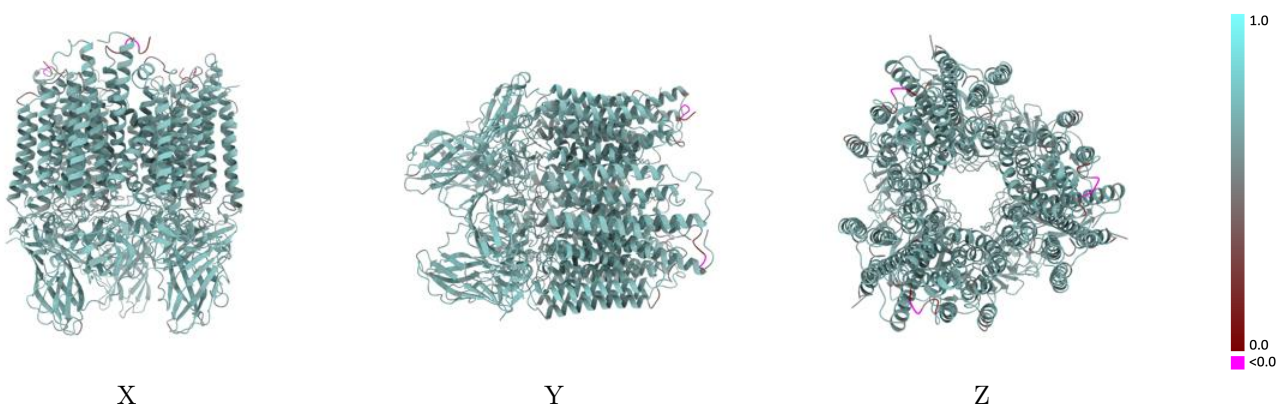
Y



Z

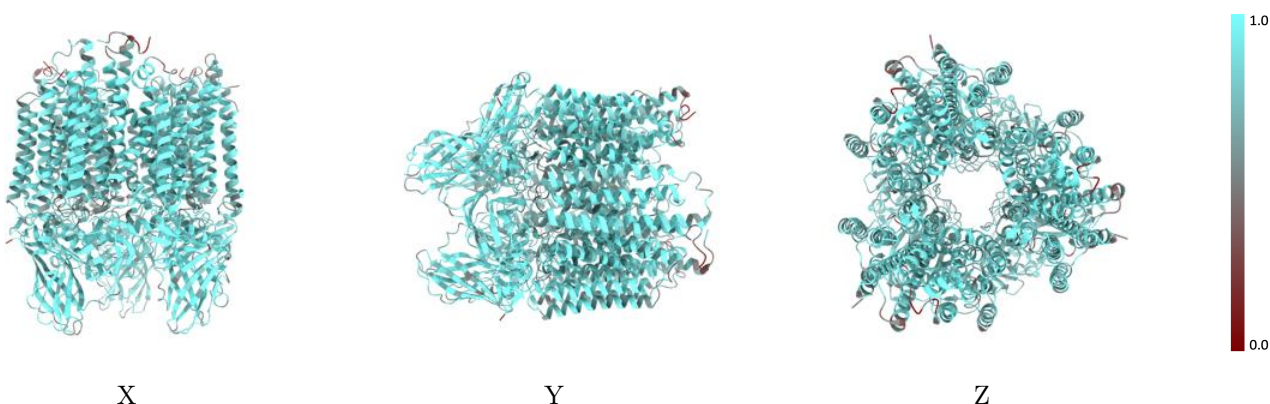
The images above show the 3D surface view of the map at the recommended contour level 0.0237 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



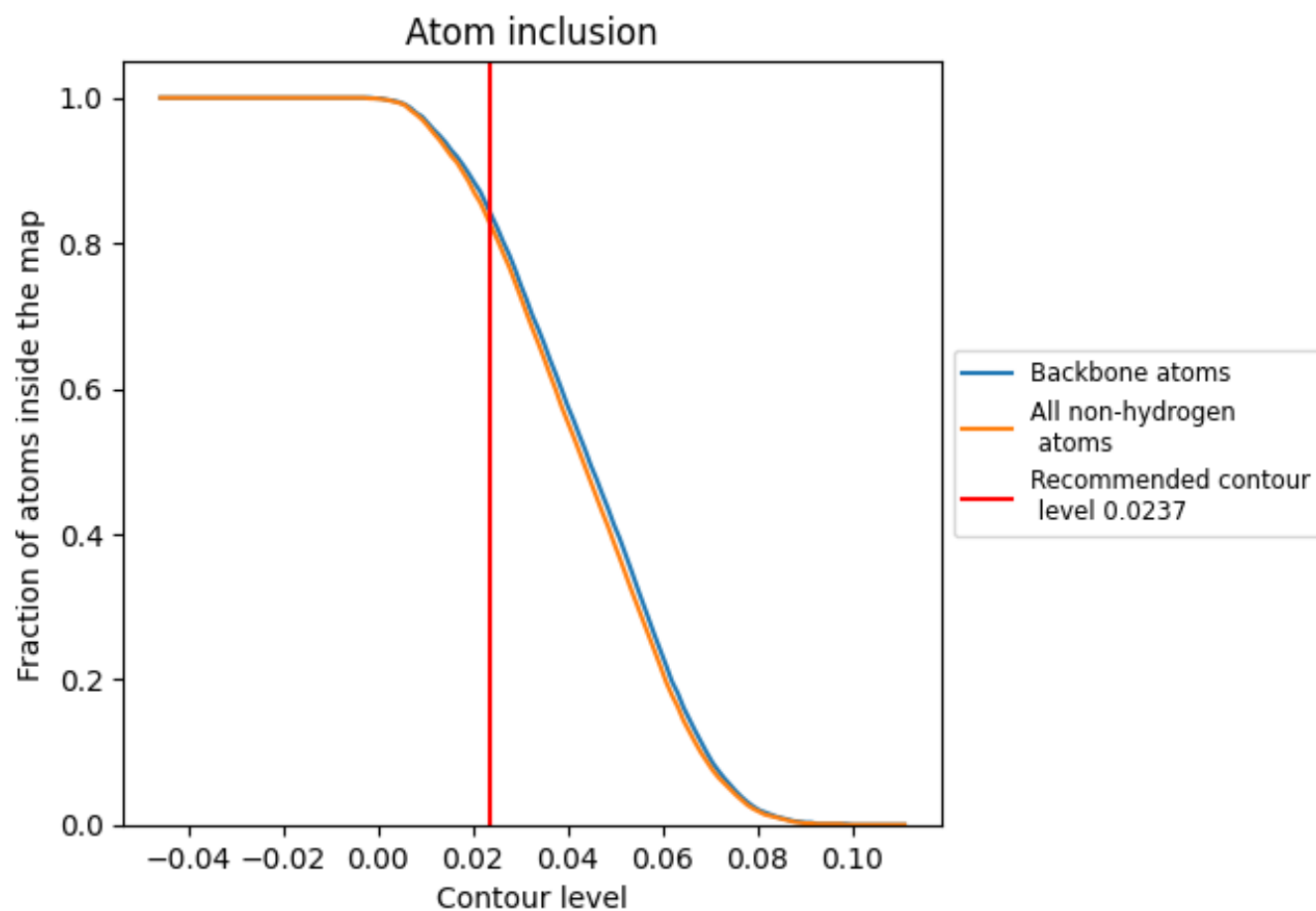
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0237).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.0237) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8250	<div><div></div></div> 0.6360
A	<div><div></div></div> 0.8710	<div><div></div></div> 0.6540
B	<div><div></div></div> 0.8160	<div><div></div></div> 0.6420
C	<div><div></div></div> 0.7370	<div><div></div></div> 0.6040
E	<div><div></div></div> 0.8780	<div><div></div></div> 0.6520
F	<div><div></div></div> 0.8470	<div><div></div></div> 0.6460
G	<div><div></div></div> 0.7400	<div><div></div></div> 0.6070
I	<div><div></div></div> 0.8740	<div><div></div></div> 0.6520
J	<div><div></div></div> 0.8220	<div><div></div></div> 0.6370
K	<div><div></div></div> 0.7810	<div><div></div></div> 0.6130

1.0

0.0

<0.0