



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:29 AM UTC

PDB ID : 9GJ8 / pdb_00009gj8
EMDB ID : EMD-51384
Title : Structure of Sticholisin II in large unilamellar vesicles.
Authors : Santiago, C.; Martin-Benito, J.; Arranz, R.; Masiulis, S.
Deposited on : 2024-08-21
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

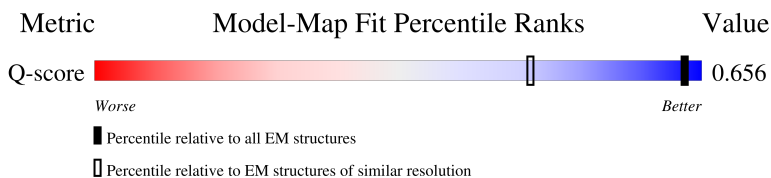
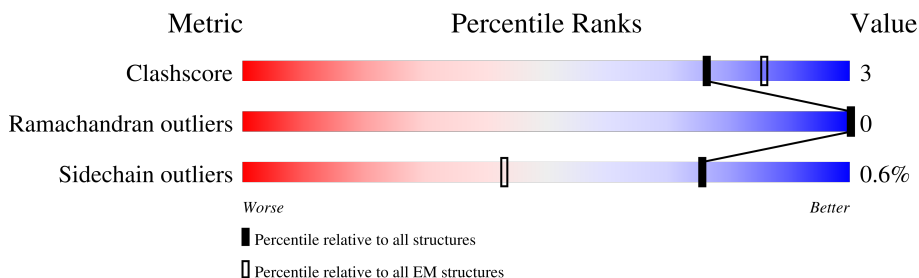
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.10 Å.

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







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2317 (1.60 - 2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	175	
1	B	175	
1	C	175	
1	E	175	

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Mol	Chain	Length	Quality of chain
1	G	175	 92% 8%
1	I	175	 93% 7%
1	J	175	 93% 7%
1	L	175	 93% 7%

2 Entry composition

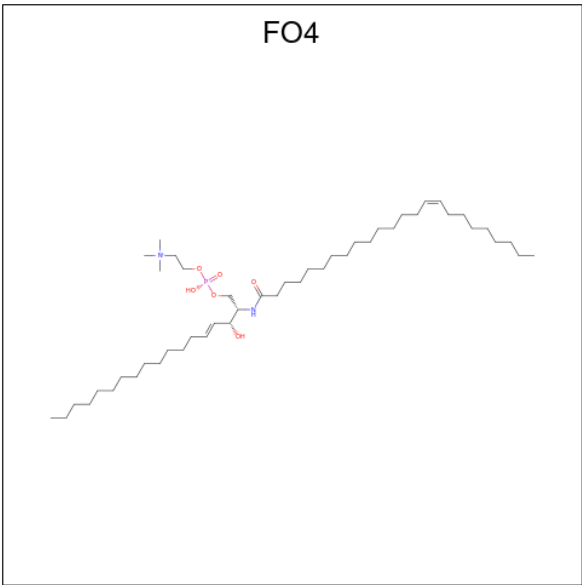
There are 3 unique types of molecules in this entry. The entry contains 13072 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DELTA-stichotoxin-She4b.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	175	Total	C	N	O	S	0	0
			1361	871	229	255	6		
1	A	175	Total	C	N	O	S	0	0
			1361	871	229	255	6		
1	B	175	Total	C	N	O	S	0	0
			1361	871	229	255	6		
1	E	175	Total	C	N	O	S	0	0
			1361	871	229	255	6		
1	G	175	Total	C	N	O	S	0	0
			1361	871	229	255	6		
1	I	175	Total	C	N	O	S	0	0
			1361	871	229	255	6		
1	J	175	Total	C	N	O	S	0	0
			1361	871	229	255	6		
1	L	175	Total	C	N	O	S	0	0
			1361	871	229	255	6		

- Molecule 2 is sphingomyelin (CCD ID: FO4) (formula: $C_{47}H_{94}N_2O_6P$) (labeled as "Ligand of Interest" by depositor).



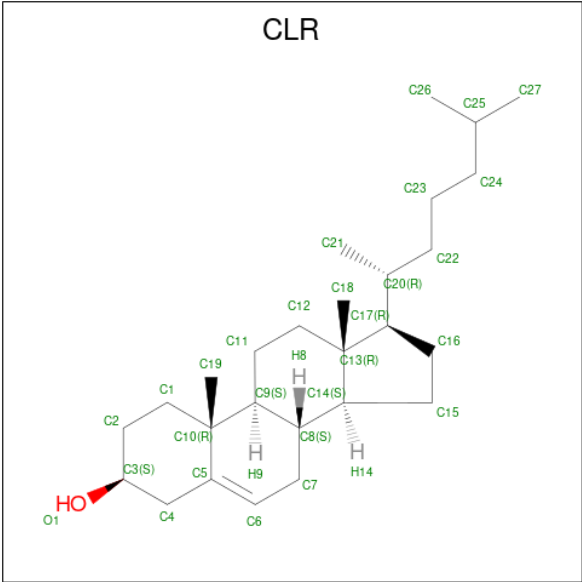
Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			32	23	2	6	1	
2	C	1	Total	C	N	O	P	0
			42	33	2	6	1	
2	C	1	Total	C	N	O	P	0
			35	26	2	6	1	
2	A	1	Total	C	N	O	P	0
			52	43	2	6	1	
2	A	1	Total	C	N	O	P	0
			52	43	2	6	1	
2	A	1	Total	C	N	O	P	0
			32	23	2	6	1	
2	A	1	Total	C	N	O	P	0
			42	33	2	6	1	
2	A	1	Total	C	N	O	P	0
			35	26	2	6	1	
2	B	1	Total	C	N	O	P	0
			52	43	2	6	1	
2	B	1	Total	C	N	O	P	0
			32	23	2	6	1	
2	B	1	Total	C	N	O	P	0
			42	33	2	6	1	
2	B	1	Total	C	N	O	P	0
			35	26	2	6	1	
2	E	1	Total	C	N	O	P	0
			52	43	2	6	1	
2	E	1	Total	C	N	O	P	0
			32	23	2	6	1	

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Mol	Chain	Residues	Atoms					AltConf
2	E	1	Total	C	N	O	P	0
			42	33	2	6	1	
2	E	1	Total	C	N	O	P	0
			35	26	2	6	1	
2	G	1	Total	C	N	O	P	0
			52	43	2	6	1	
2	G	1	Total	C	N	O	P	0
			32	23	2	6	1	
2	G	1	Total	C	N	O	P	0
			42	33	2	6	1	
2	G	1	Total	C	N	O	P	0
			35	26	2	6	1	
2	I	1	Total	C	N	O	P	0
			52	43	2	6	1	
2	I	1	Total	C	N	O	P	0
			32	23	2	6	1	
2	I	1	Total	C	N	O	P	0
			42	33	2	6	1	
2	I	1	Total	C	N	O	P	0
			35	26	2	6	1	
2	J	1	Total	C	N	O	P	0
			52	43	2	6	1	
2	J	1	Total	C	N	O	P	0
			32	23	2	6	1	
2	J	1	Total	C	N	O	P	0
			42	33	2	6	1	
2	J	1	Total	C	N	O	P	0
			35	26	2	6	1	
2	L	1	Total	C	N	O	P	0
			52	43	2	6	1	
2	L	1	Total	C	N	O	P	0
			32	23	2	6	1	
2	L	1	Total	C	N	O	P	0
			42	33	2	6	1	
2	L	1	Total	C	N	O	P	0
			35	26	2	6	1	

- Molecule 3 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
3	C	1	Total	C	O	0
			28	27	1	
3	C	1	Total	C	O	0
			28	27	1	
3	C	1	Total	C	O	0
			28	27	1	
3	C	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	A	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	B	1	Total	C	O	0
			28	27	1	
3	E	1	Total	C	O	0
			28	27	1	
3	E	1	Total	C	O	0
			28	27	1	

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Mol	Chain	Residues	Atoms			AltConf
3	E	1	Total	C	O	0
			28	27	1	
3	E	1	Total	C	O	0
			28	27	1	
3	G	1	Total	C	O	0
			28	27	1	
3	G	1	Total	C	O	0
			28	27	1	
3	G	1	Total	C	O	0
			28	27	1	
3	G	1	Total	C	O	0
			28	27	1	
3	I	1	Total	C	O	0
			28	27	1	
3	I	1	Total	C	O	0
			28	27	1	
3	I	1	Total	C	O	0
			28	27	1	
3	I	1	Total	C	O	0
			28	27	1	
3	J	1	Total	C	O	0
			28	27	1	
3	J	1	Total	C	O	0
			28	27	1	
3	J	1	Total	C	O	0
			28	27	1	
3	J	1	Total	C	O	0
			28	27	1	
3	L	1	Total	C	O	0
			28	27	1	
3	L	1	Total	C	O	0
			28	27	1	
3	L	1	Total	C	O	0
			28	27	1	
3	L	1	Total	C	O	0
			28	27	1	

3 Residue-property plots [i](#)

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

- Molecule 1: DELTA-stichotoxin-She4b

Chain C:  93% 7%



- Molecule 1: DELTA-stichotoxin-She4b

Chain A:  91% 9%




- Molecule 1: DELTA-stichotoxin-She4b

Chain B:  91% 9%



- Molecule 1: DELTA-stichotoxin-She4b

Chain E:  90% 10%




- Molecule 1: DELTA-stichotoxin-She4b

Chain G:  92% 8%



- Molecule 1: DELTA-stichotoxin-She4b

Chain I:  93% 7%



- Molecule 1: DELTA-stichotoxin-She4b

Chain J:  93% 7%



- Molecule 1: DELTA-stichotoxin-She4b

Chain L:  93% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	180000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.080	Depositor
Minimum map value	-0.308	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	127.75, 127.75, 127.75	wwPDB
Map dimensions	140, 140, 140	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9125, 0.9125, 0.9125	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: CLR, FO4

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	0.20	0/1394	0.34	0/1885
1	B	0.20	0/1394	0.35	0/1885
1	C	0.20	0/1394	0.34	0/1885
1	E	0.20	0/1394	0.34	0/1885
1	G	0.20	0/1394	0.35	0/1885
1	I	0.20	0/1394	0.35	0/1885
1	J	0.20	0/1394	0.34	0/1885
1	L	0.20	0/1394	0.35	0/1885
All	All	0.20	0/11152	0.35	0/15080

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	1361	0	1334	8	0
1	B	1361	0	1334	10	0
1	C	1361	0	1334	7	0
1	E	1361	0	1334	9	0
1	G	1361	0	1334	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1361	0	1334	8	0
1	J	1361	0	1334	7	0
1	L	1361	0	1334	7	0
2	A	213	0	0	0	0
2	B	161	0	0	0	0
2	C	109	0	0	0	0
2	E	161	0	0	0	0
2	G	161	0	0	0	0
2	I	161	0	0	0	0
2	J	161	0	0	0	0
2	L	161	0	0	0	0
3	A	112	0	184	2	0
3	B	112	0	184	2	0
3	C	112	0	184	2	0
3	E	112	0	184	2	0
3	G	112	0	184	2	0
3	I	112	0	184	2	0
3	J	112	0	184	2	0
3	L	112	0	184	2	0
All	All	13072	0	12144	76	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (76) 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)
1:A:3:ALA:O	1:A:7:ILE:HG13	2.00	0.61
1:E:3:ALA:O	1:E:7:ILE:HG13	2.02	0.60
3:J:707:CLR:H211	3:J:707:CLR:H263	1.88	0.56
3:C:206:CLR:H263	3:C:206:CLR:H211	1.88	0.56
3:G:707:CLR:H263	3:G:707:CLR:H211	1.88	0.54
3:B:707:CLR:H211	3:B:707:CLR:H263	1.88	0.54
1:G:169:MET:HE3	1:G:171:ILE:HD11	1.90	0.53
1:I:19:LYS:NZ	1:J:18:ASP:OD1	2.42	0.53
1:C:18:ASP:OD1	1:L:19:LYS:NZ	2.42	0.52
1:B:43:TRP:CD1	1:B:92:MET:HG2	2.45	0.52
1:A:19:LYS:NZ	1:B:18:ASP:OD1	2.43	0.52
1:J:43:TRP:CD1	1:J:92:MET:HG2	2.45	0.51
3:A:708:CLR:H211	3:A:708:CLR:H263	1.92	0.51
1:B:169:MET:HE3	1:B:171:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:707:CLR:H211	3:I:707:CLR:H263	1.93	0.50
1:E:19:LYS:NZ	1:G:18:ASP:OD1	2.43	0.50
3:A:708:CLR:H17	3:A:709:CLR:H181	1.93	0.50
3:E:707:CLR:H263	3:E:707:CLR:H211	1.93	0.50
3:E:707:CLR:H17	3:E:708:CLR:H181	1.94	0.50
3:L:707:CLR:H263	3:L:707:CLR:H211	1.92	0.49
3:L:707:CLR:H17	3:L:708:CLR:H181	1.94	0.49
3:I:707:CLR:H17	3:I:708:CLR:H181	1.95	0.49
1:A:101:MET:HE2	1:A:135:TYR:HA	1.96	0.48
1:L:101:MET:HE2	1:L:135:TYR:HA	1.96	0.48
1:J:118:LYS:HD2	1:J:120:TYR:CZ	2.49	0.47
1:C:118:LYS:HD2	1:C:120:TYR:CZ	2.49	0.47
1:G:118:LYS:HD2	1:G:120:TYR:CZ	2.50	0.47
1:C:118:LYS:HG2	1:C:119:ILE:N	2.30	0.46
1:G:155:LEU:HD23	1:G:175:ARG:HB2	1.97	0.46
1:B:118:LYS:HD2	1:B:120:TYR:CZ	2.50	0.46
1:E:101:MET:HE2	1:E:135:TYR:HA	1.96	0.46
1:B:118:LYS:HG2	1:B:119:ILE:N	2.31	0.46
1:A:118:LYS:HD2	1:A:120:TYR:CZ	2.50	0.46
1:L:75:LYS:HE2	1:L:82:THR:O	2.16	0.46
1:C:155:LEU:HD23	1:C:175:ARG:HB2	1.98	0.46
1:B:155:LEU:HD23	1:B:175:ARG:HB2	1.98	0.45
1:A:75:LYS:HE2	1:A:82:THR:O	2.16	0.45
1:E:118:LYS:HD2	1:E:120:TYR:CZ	2.50	0.45
1:G:19:LYS:HE2	1:G:23:GLU:OE2	2.17	0.45
1:C:3:ALA:O	1:C:7:ILE:HG13	2.17	0.45
1:B:19:LYS:HE2	1:B:23:GLU:OE2	2.17	0.45
1:I:75:LYS:HE2	1:I:82:THR:O	2.16	0.45
1:J:155:LEU:HD23	1:J:175:ARG:HB2	1.98	0.45
1:I:118:LYS:HD2	1:I:120:TYR:CZ	2.52	0.45
1:L:118:LYS:HD2	1:L:120:TYR:CZ	2.52	0.45
3:C:206:CLR:H17	3:C:207:CLR:H181	1.99	0.45
1:A:43:TRP:CD1	1:A:92:MET:HG2	2.52	0.44
3:B:707:CLR:H17	3:B:708:CLR:H181	1.99	0.44
1:E:43:TRP:CD1	1:E:92:MET:HG2	2.52	0.44
1:E:75:LYS:HE2	1:E:82:THR:O	2.16	0.44
1:A:155:LEU:HD23	1:A:175:ARG:HB2	1.99	0.44
1:I:43:TRP:CD1	1:I:92:MET:HG2	2.52	0.44
1:I:155:LEU:HD23	1:I:175:ARG:HB2	1.99	0.44
1:J:118:LYS:HG2	1:J:119:ILE:N	2.33	0.44
1:L:43:TRP:CD1	1:L:92:MET:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:707:CLR:H17	3:G:708:CLR:H181	2.00	0.43
1:E:31:ILE:HD12	1:E:161:MET:HE3	2.00	0.43
1:E:155:LEU:HD23	1:E:175:ARG:HB2	1.99	0.43
1:G:43:TRP:CD1	1:G:92:MET:HG2	2.53	0.43
1:L:155:LEU:HD23	1:L:175:ARG:HB2	1.99	0.43
1:A:31:ILE:HD12	1:A:161:MET:HE3	2.00	0.43
1:I:31:ILE:HD12	1:I:161:MET:HE3	2.00	0.43
1:C:43:TRP:CD1	1:C:92:MET:HG2	2.54	0.43
3:J:707:CLR:H17	3:J:708:CLR:H181	2.01	0.43
1:B:19:LYS:HA	1:B:19:LYS:HD2	1.81	0.42
1:G:19:LYS:HA	1:G:19:LYS:HD2	1.80	0.42
1:G:118:LYS:HG2	1:G:119:ILE:N	2.34	0.42
1:I:157:MET:HE3	1:I:157:MET:HB3	1.94	0.42
1:J:3:ALA:O	1:J:7:ILE:HG13	2.20	0.42
1:L:31:ILE:HD12	1:L:161:MET:HE3	2.01	0.41
1:B:19:LYS:NZ	1:E:18:ASP:OD1	2.53	0.41
1:G:169:MET:HE3	1:G:171:ILE:CD1	2.50	0.41
1:C:153:TYR:O	1:C:175:ARG:NH2	2.54	0.41
1:B:3:ALA:O	1:B:7:ILE:HG13	2.20	0.41
1:J:153:TYR:O	1:J:175:ARG:NH2	2.54	0.41
1:G:19:LYS:NZ	1:I:18:ASP:OD1	2.53	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
1	B	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
1	C	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
1	E	173/175 (99%)	169 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
1	I	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
1	J	173/175 (99%)	168 (97%)	5 (3%)	0	100	100
1	L	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
All	All	1384/1400 (99%)	1348 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	138/138 (100%)	138 (100%)	0	100	100
1	B	138/138 (100%)	137 (99%)	1 (1%)	76	83
1	C	138/138 (100%)	137 (99%)	1 (1%)	76	83
1	E	138/138 (100%)	137 (99%)	1 (1%)	76	83
1	G	138/138 (100%)	136 (99%)	2 (1%)	59	67
1	I	138/138 (100%)	138 (100%)	0	100	100
1	J	138/138 (100%)	136 (99%)	2 (1%)	59	67
1	L	138/138 (100%)	138 (100%)	0	100	100
All	All	1104/1104 (100%)	1097 (99%)	7 (1%)	76	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	121	SER
1	B	121	SER
1	E	17	LEU
1	G	17	LEU
1	G	121	SER
1	J	17	LEU

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Mol	Chain	Res	Type
1	J	121	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	15	GLN
1	C	144	ASN
1	C	150	ASN
1	A	15	GLN
1	A	144	ASN
1	B	15	GLN
1	B	144	ASN
1	B	150	ASN
1	E	15	GLN
1	E	144	ASN
1	G	15	GLN
1	G	144	ASN
1	G	150	ASN
1	I	15	GLN
1	I	144	ASN
1	J	15	GLN
1	J	144	ASN
1	J	150	ASN
1	L	15	GLN
1	L	144	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

64 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CLR	C	204	-	31,31,31	0.37	0	48,48,48	0.70	0
2	FO4	J	703	-	40,41,55	0.58	1 (2%)	46,49,63	0.65	1 (2%)
2	FO4	A	701	-	50,51,55	0.52	1 (2%)	56,59,63	0.47	0
2	FO4	L	703	-	40,41,55	0.58	1 (2%)	46,49,63	0.66	1 (2%)
3	CLR	B	707	-	31,31,31	0.41	0	48,48,48	0.74	0
2	FO4	I	703	-	40,41,55	0.58	1 (2%)	46,49,63	0.66	1 (2%)
3	CLR	G	706	-	31,31,31	0.40	0	48,48,48	0.60	0
3	CLR	I	705	-	31,31,31	0.38	0	48,48,48	0.69	0
3	CLR	I	707	-	31,31,31	0.42	0	48,48,48	0.77	1 (2%)
3	CLR	L	706	-	31,31,31	0.40	0	48,48,48	0.62	0
2	FO4	B	702	-	30,31,55	0.70	1 (3%)	35,39,63	1.93	5 (14%)
2	FO4	B	704	-	33,34,55	0.65	1 (3%)	39,42,63	0.63	0
3	CLR	E	706	-	31,31,31	0.40	0	48,48,48	0.62	0
3	CLR	B	705	-	31,31,31	0.37	0	48,48,48	0.70	0
2	FO4	J	701	-	50,51,55	0.52	1 (2%)	56,59,63	0.47	0
2	FO4	A	704	-	40,41,55	0.58	1 (2%)	46,49,63	0.66	1 (2%)
3	CLR	C	205	-	31,31,31	0.41	0	48,48,48	0.60	0
3	CLR	G	707	-	31,31,31	0.41	0	48,48,48	0.75	0
3	CLR	I	708	-	31,31,31	0.40	0	48,48,48	0.86	0
3	CLR	L	707	-	31,31,31	0.42	0	48,48,48	0.77	1 (2%)
2	FO4	L	701	-	50,51,55	0.53	1 (2%)	56,59,63	0.52	0
2	FO4	B	701	-	50,51,55	0.52	1 (2%)	56,59,63	0.47	0
3	CLR	J	708	-	31,31,31	0.40	0	48,48,48	0.83	0
2	FO4	E	704	-	33,34,55	0.65	1 (3%)	39,42,63	0.61	0
3	CLR	I	706	-	31,31,31	0.40	0	48,48,48	0.62	0
3	CLR	B	708	-	31,31,31	0.40	0	48,48,48	0.84	0
2	FO4	C	202	-	40,41,55	0.58	1 (2%)	46,49,63	0.65	1 (2%)
3	CLR	J	706	-	31,31,31	0.40	0	48,48,48	0.60	0
3	CLR	A	709	-	31,31,31	0.40	0	48,48,48	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FO4	G	702	-	30,31,55	0.70	1 (3%)	35,39,63	1.92	5 (14%)
2	FO4	A	705	-	33,34,55	0.65	1 (3%)	39,42,63	0.61	0
2	FO4	L	702	-	30,31,55	0.71	1 (3%)	35,39,63	1.90	5 (14%)
2	FO4	L	704	-	33,34,55	0.65	1 (3%)	39,42,63	0.61	0
3	CLR	A	708	-	31,31,31	0.42	0	48,48,48	0.77	1 (2%)
2	FO4	C	201	-	30,31,55	0.69	1 (3%)	35,39,63	1.92	5 (14%)
3	CLR	C	206	-	31,31,31	0.41	0	48,48,48	0.74	0
3	CLR	J	707	-	31,31,31	0.41	0	48,48,48	0.74	0
2	FO4	G	703	-	40,41,55	0.58	1 (2%)	46,49,63	0.65	1 (2%)
2	FO4	G	704	-	33,34,55	0.65	1 (3%)	39,42,63	0.64	0
3	CLR	L	705	-	31,31,31	0.38	0	48,48,48	0.69	0
2	FO4	E	702	-	30,31,55	0.71	1 (3%)	35,39,63	1.91	5 (14%)
3	CLR	G	705	-	31,31,31	0.38	0	48,48,48	0.70	0
3	CLR	E	705	-	31,31,31	0.38	0	48,48,48	0.69	0
2	FO4	J	702	-	30,31,55	0.70	1 (3%)	35,39,63	1.92	5 (14%)
2	FO4	J	704	-	33,34,55	0.65	1 (3%)	39,42,63	0.64	0
3	CLR	J	705	-	31,31,31	0.37	0	48,48,48	0.70	0
3	CLR	L	708	-	31,31,31	0.40	0	48,48,48	0.86	0
2	FO4	A	703	-	30,31,55	0.71	1 (3%)	35,39,63	1.91	5 (14%)
2	FO4	E	703	-	40,41,55	0.58	1 (2%)	46,49,63	0.65	1 (2%)
2	FO4	I	701	-	50,51,55	0.53	1 (2%)	56,59,63	0.52	0
3	CLR	E	707	-	31,31,31	0.42	0	48,48,48	0.77	1 (2%)
3	CLR	G	708	-	31,31,31	0.40	0	48,48,48	0.84	0
2	FO4	G	701	-	50,51,55	0.53	1 (2%)	56,59,63	0.47	0
3	CLR	A	706	-	31,31,31	0.38	0	48,48,48	0.69	0
3	CLR	A	707	-	31,31,31	0.40	0	48,48,48	0.61	0
2	FO4	E	701	-	50,51,55	0.53	1 (2%)	56,59,63	0.52	0
2	FO4	A	702	-	50,51,55	0.53	1 (2%)	56,59,63	0.52	0
3	CLR	B	706	-	31,31,31	0.41	0	48,48,48	0.60	0
3	CLR	C	207	-	31,31,31	0.40	0	48,48,48	0.83	0
2	FO4	C	203	-	33,34,55	0.65	1 (3%)	39,42,63	0.64	0
2	FO4	B	703	-	40,41,55	0.58	1 (2%)	46,49,63	0.65	1 (2%)
3	CLR	E	708	-	31,31,31	0.40	0	48,48,48	0.86	0
2	FO4	I	702	-	30,31,55	0.71	1 (3%)	35,39,63	1.91	5 (14%)
2	FO4	I	704	-	33,34,55	0.65	1 (3%)	39,42,63	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CLR	C	204	-	-	1/10/68/68	0/4/4/4
2	FO4	J	703	-	-	17/46/46/60	-
2	FO4	A	701	-	-	10/56/56/60	-
2	FO4	L	703	-	-	18/46/46/60	-
3	CLR	B	707	-	-	6/10/68/68	0/4/4/4
2	FO4	I	703	-	-	17/46/46/60	-
3	CLR	G	706	-	-	3/10/68/68	0/4/4/4
3	CLR	I	705	-	-	1/10/68/68	0/4/4/4
3	CLR	I	707	-	-	5/10/68/68	0/4/4/4
3	CLR	L	706	-	-	3/10/68/68	0/4/4/4
2	FO4	B	702	-	-	13/36/36/60	-
2	FO4	B	704	-	-	16/39/39/60	-
3	CLR	E	706	-	-	3/10/68/68	0/4/4/4
3	CLR	B	705	-	-	1/10/68/68	0/4/4/4
2	FO4	J	701	-	-	10/56/56/60	-
2	FO4	A	704	-	-	17/46/46/60	-
3	CLR	C	205	-	-	3/10/68/68	0/4/4/4
3	CLR	G	707	-	-	6/10/68/68	0/4/4/4
3	CLR	I	708	-	-	3/10/68/68	0/4/4/4
3	CLR	L	707	-	-	5/10/68/68	0/4/4/4
2	FO4	L	701	-	-	9/56/56/60	-
2	FO4	B	701	-	-	10/56/56/60	-
3	CLR	J	708	-	-	2/10/68/68	0/4/4/4
2	FO4	E	704	-	-	15/39/39/60	-
3	CLR	I	706	-	-	3/10/68/68	0/4/4/4
3	CLR	B	708	-	-	2/10/68/68	0/4/4/4
2	FO4	C	202	-	-	17/46/46/60	-
3	CLR	J	706	-	-	3/10/68/68	0/4/4/4
3	CLR	A	709	-	-	3/10/68/68	0/4/4/4
2	FO4	G	702	-	-	13/36/36/60	-
2	FO4	A	705	-	-	16/39/39/60	-
2	FO4	L	702	-	-	13/36/36/60	-
2	FO4	L	704	-	-	16/39/39/60	-
3	CLR	A	708	-	-	5/10/68/68	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FO4	C	201	-	-	13/36/36/60	-
3	CLR	C	206	-	-	6/10/68/68	0/4/4/4
3	CLR	J	707	-	-	6/10/68/68	0/4/4/4
2	FO4	G	703	-	-	17/46/46/60	-
2	FO4	G	704	-	-	16/39/39/60	-
3	CLR	L	705	-	-	1/10/68/68	0/4/4/4
2	FO4	E	702	-	-	13/36/36/60	-
3	CLR	G	705	-	-	1/10/68/68	0/4/4/4
3	CLR	E	705	-	-	1/10/68/68	0/4/4/4
2	FO4	J	702	-	-	13/36/36/60	-
2	FO4	J	704	-	-	15/39/39/60	-
3	CLR	J	705	-	-	1/10/68/68	0/4/4/4
3	CLR	L	708	-	-	3/10/68/68	0/4/4/4
2	FO4	A	703	-	-	13/36/36/60	-
2	FO4	E	703	-	-	17/46/46/60	-
2	FO4	I	701	-	-	9/56/56/60	-
3	CLR	E	707	-	-	5/10/68/68	0/4/4/4
3	CLR	G	708	-	-	2/10/68/68	0/4/4/4
2	FO4	G	701	-	-	10/56/56/60	-
3	CLR	A	706	-	-	1/10/68/68	0/4/4/4
3	CLR	A	707	-	-	3/10/68/68	0/4/4/4
2	FO4	E	701	-	-	9/56/56/60	-
2	FO4	A	702	-	-	9/56/56/60	-
3	CLR	B	706	-	-	3/10/68/68	0/4/4/4
3	CLR	C	207	-	-	2/10/68/68	0/4/4/4
2	FO4	C	203	-	-	16/39/39/60	-
2	FO4	B	703	-	-	17/46/46/60	-
3	CLR	E	708	-	-	3/10/68/68	0/4/4/4
2	FO4	I	702	-	-	13/36/36/60	-
2	FO4	I	704	-	-	15/39/39/60	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	701	FO4	O-C	-2.38	1.39	1.43
2	I	702	FO4	O-C	-2.38	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FO4	O-C	-2.38	1.39	1.43
2	A	701	FO4	O-C	-2.38	1.39	1.43
2	A	703	FO4	O-C	-2.38	1.39	1.43
2	E	702	FO4	O-C	-2.38	1.39	1.43
2	L	702	FO4	O-C	-2.38	1.39	1.43
2	J	701	FO4	O-C	-2.37	1.39	1.43
2	I	704	FO4	O-C	-2.37	1.39	1.43
2	E	704	FO4	O-C	-2.37	1.39	1.43
2	A	705	FO4	O-C	-2.37	1.39	1.43
2	L	704	FO4	O-C	-2.37	1.39	1.43
2	G	702	FO4	O-C	-2.36	1.39	1.43
2	B	702	FO4	O-C	-2.36	1.39	1.43
2	G	704	FO4	O-C	-2.36	1.39	1.43
2	J	702	FO4	O-C	-2.36	1.39	1.43
2	J	704	FO4	O-C	-2.35	1.39	1.43
2	C	203	FO4	O-C	-2.35	1.39	1.43
2	C	201	FO4	O-C	-2.35	1.39	1.43
2	B	704	FO4	O-C	-2.35	1.39	1.43
2	I	703	FO4	O-C	-2.35	1.39	1.43
2	L	703	FO4	O-C	-2.35	1.39	1.43
2	J	703	FO4	O-C	-2.34	1.39	1.43
2	E	703	FO4	O-C	-2.34	1.39	1.43
2	A	704	FO4	O-C	-2.34	1.39	1.43
2	A	702	FO4	O-C	-2.34	1.39	1.43
2	B	703	FO4	O-C	-2.34	1.39	1.43
2	C	202	FO4	O-C	-2.34	1.39	1.43
2	L	701	FO4	O-C	-2.34	1.39	1.43
2	G	703	FO4	O-C	-2.34	1.39	1.43
2	E	701	FO4	O-C	-2.34	1.39	1.43
2	I	701	FO4	O-C	-2.33	1.39	1.43

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	703	FO4	C16-N-C17	7.80	136.40	123.40
2	I	702	FO4	C16-N-C17	7.79	136.39	123.40
2	E	702	FO4	C16-N-C17	7.79	136.39	123.40
2	L	702	FO4	C16-N-C17	7.79	136.38	123.40
2	B	702	FO4	C16-N-C17	7.75	136.33	123.40
2	G	702	FO4	C16-N-C17	7.74	136.30	123.40
2	C	201	FO4	C16-N-C17	7.73	136.29	123.40
2	J	702	FO4	C16-N-C17	7.73	136.29	123.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	FO4	C-C1-C2	3.88	132.72	124.69
2	B	702	FO4	C-C1-C2	3.88	132.72	124.69
2	G	702	FO4	C-C1-C2	3.87	132.71	124.69
2	J	702	FO4	C-C1-C2	3.86	132.68	124.69
2	L	702	FO4	C-C1-C2	3.80	132.55	124.69
2	I	702	FO4	C-C1-C2	3.79	132.54	124.69
2	E	702	FO4	C-C1-C2	3.79	132.53	124.69
2	A	703	FO4	C-C1-C2	3.78	132.51	124.69
2	I	702	FO4	C41-C16-N	3.28	114.33	109.66
2	E	702	FO4	C41-C16-N	3.27	114.31	109.66
2	B	702	FO4	C18-C17-N	3.26	121.61	115.86
2	L	702	FO4	C41-C16-N	3.26	114.30	109.66
2	E	702	FO4	C18-C17-N	3.26	121.61	115.86
2	A	703	FO4	C41-C16-N	3.26	114.30	109.66
2	A	703	FO4	C18-C17-N	3.24	121.58	115.86
2	G	702	FO4	C18-C17-N	3.24	121.58	115.86
2	I	702	FO4	C18-C17-N	3.24	121.58	115.86
2	J	702	FO4	C18-C17-N	3.24	121.57	115.86
2	C	201	FO4	C18-C17-N	3.24	121.57	115.86
2	J	702	FO4	C-C16-N	3.24	115.14	109.66
2	L	702	FO4	C18-C17-N	3.24	121.57	115.86
2	G	702	FO4	C-C16-N	3.23	115.14	109.66
2	B	702	FO4	C-C16-N	3.23	115.14	109.66
2	C	201	FO4	C-C16-N	3.22	115.12	109.66
2	G	702	FO4	C41-C16-N	2.92	113.81	109.66
2	C	201	FO4	C41-C16-N	2.91	113.81	109.66
2	J	702	FO4	C41-C16-N	2.91	113.80	109.66
2	B	702	FO4	C41-C16-N	2.91	113.80	109.66
2	A	703	FO4	C-C16-N	2.76	114.34	109.66
2	L	702	FO4	C-C16-N	2.75	114.33	109.66
2	E	702	FO4	C-C16-N	2.75	114.32	109.66
2	I	702	FO4	C-C16-N	2.75	114.32	109.66
3	A	708	CLR	C15-C14-C13	2.10	106.31	103.84
3	E	707	CLR	C15-C14-C13	2.09	106.30	103.84
3	L	707	CLR	C15-C14-C13	2.09	106.30	103.84
2	A	704	FO4	C16-N-C17	2.07	126.85	123.40
3	I	707	CLR	C15-C14-C13	2.07	106.27	103.84
2	E	703	FO4	C16-N-C17	2.06	126.84	123.40
2	L	703	FO4	C16-N-C17	2.06	126.83	123.40
2	B	703	FO4	C16-N-C17	2.05	126.83	123.40
2	I	703	FO4	C16-N-C17	2.05	126.82	123.40
2	C	202	FO4	C16-N-C17	2.03	126.79	123.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	703	FO4	C16-N-C17	2.03	126.78	123.40
2	J	703	FO4	C16-N-C17	2.02	126.77	123.40

There are no chirality outliers.

All (538) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	201	FO4	C41-C16-N-C17
2	C	201	FO4	N-C16-C41-O2
2	C	201	FO4	C-C16-C41-O2
2	C	201	FO4	C1-C-C16-C41
2	C	201	FO4	O-C-C16-C41
2	C	202	FO4	C42-O4-P-O5
2	C	202	FO4	C42-O4-P-O3
2	C	202	FO4	C42-O4-P-O2
2	C	202	FO4	C41-O2-P-O5
2	C	202	FO4	C41-O2-P-O3
2	C	202	FO4	C41-O2-P-O4
2	C	203	FO4	C42-O4-P-O3
2	C	203	FO4	C42-O4-P-O2
2	C	203	FO4	N-C16-C41-O2
2	C	203	FO4	C-C16-C41-O2
2	C	203	FO4	C1-C-C16-N
2	C	203	FO4	O-C-C16-N
2	C	203	FO4	C1-C-C16-C41
2	C	203	FO4	O-C-C16-C41
2	A	703	FO4	C41-C16-N-C17
2	A	703	FO4	N-C16-C41-O2
2	A	703	FO4	C-C16-C41-O2
2	A	703	FO4	C1-C-C16-C41
2	A	703	FO4	O-C-C16-C41
2	A	704	FO4	C-C16-N-C17
2	A	704	FO4	C42-O4-P-O5
2	A	704	FO4	C42-O4-P-O3
2	A	704	FO4	C42-O4-P-O2
2	A	704	FO4	C41-O2-P-O3
2	A	704	FO4	C41-O2-P-O4
2	A	705	FO4	C42-O4-P-O3
2	A	705	FO4	C42-O4-P-O2
2	A	705	FO4	N-C16-C41-O2
2	A	705	FO4	C-C16-C41-O2
2	A	705	FO4	C1-C-C16-N

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Mol	Chain	Res	Type	Atoms
2	A	705	FO4	O-C-C16-N
2	A	705	FO4	C1-C-C16-C41
2	A	705	FO4	O-C-C16-C41
2	B	702	FO4	C41-C16-N-C17
2	B	702	FO4	N-C16-C41-O2
2	B	702	FO4	C-C16-C41-O2
2	B	702	FO4	C1-C-C16-C41
2	B	702	FO4	O-C-C16-C41
2	B	703	FO4	C42-O4-P-O5
2	B	703	FO4	C42-O4-P-O3
2	B	703	FO4	C42-O4-P-O2
2	B	703	FO4	C41-O2-P-O5
2	B	703	FO4	C41-O2-P-O3
2	B	703	FO4	C41-O2-P-O4
2	B	704	FO4	C42-O4-P-O3
2	B	704	FO4	C42-O4-P-O2
2	B	704	FO4	N-C16-C41-O2
2	B	704	FO4	C-C16-C41-O2
2	B	704	FO4	C1-C-C16-N
2	B	704	FO4	O-C-C16-N
2	B	704	FO4	C1-C-C16-C41
2	B	704	FO4	O-C-C16-C41
2	E	702	FO4	C41-C16-N-C17
2	E	702	FO4	N-C16-C41-O2
2	E	702	FO4	C-C16-C41-O2
2	E	702	FO4	C1-C-C16-C41
2	E	702	FO4	O-C-C16-C41
2	E	703	FO4	C-C16-N-C17
2	E	703	FO4	C42-O4-P-O5
2	E	703	FO4	C42-O4-P-O3
2	E	703	FO4	C42-O4-P-O2
2	E	703	FO4	C41-O2-P-O3
2	E	703	FO4	C41-O2-P-O4
2	E	704	FO4	C42-O4-P-O3
2	E	704	FO4	C42-O4-P-O2
2	E	704	FO4	N-C16-C41-O2
2	E	704	FO4	C-C16-C41-O2
2	E	704	FO4	C1-C-C16-N
2	E	704	FO4	O-C-C16-N
2	E	704	FO4	C1-C-C16-C41
2	E	704	FO4	O-C-C16-C41
2	G	702	FO4	C41-C16-N-C17

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Mol	Chain	Res	Type	Atoms
2	G	702	FO4	N-C16-C41-O2
2	G	702	FO4	C-C16-C41-O2
2	G	702	FO4	C1-C-C16-C41
2	G	702	FO4	O-C-C16-C41
2	G	703	FO4	C42-O4-P-O5
2	G	703	FO4	C42-O4-P-O3
2	G	703	FO4	C42-O4-P-O2
2	G	703	FO4	C41-O2-P-O5
2	G	703	FO4	C41-O2-P-O3
2	G	703	FO4	C41-O2-P-O4
2	G	704	FO4	C42-O4-P-O3
2	G	704	FO4	C42-O4-P-O2
2	G	704	FO4	N-C16-C41-O2
2	G	704	FO4	C-C16-C41-O2
2	G	704	FO4	C1-C-C16-N
2	G	704	FO4	O-C-C16-N
2	G	704	FO4	C1-C-C16-C41
2	G	704	FO4	O-C-C16-C41
2	I	702	FO4	C41-C16-N-C17
2	I	702	FO4	N-C16-C41-O2
2	I	702	FO4	C-C16-C41-O2
2	I	702	FO4	C1-C-C16-C41
2	I	702	FO4	O-C-C16-C41
2	I	703	FO4	C-C16-N-C17
2	I	703	FO4	C42-O4-P-O5
2	I	703	FO4	C42-O4-P-O3
2	I	703	FO4	C42-O4-P-O2
2	I	703	FO4	C41-O2-P-O3
2	I	703	FO4	C41-O2-P-O4
2	I	704	FO4	C42-O4-P-O3
2	I	704	FO4	C42-O4-P-O2
2	I	704	FO4	N-C16-C41-O2
2	I	704	FO4	C-C16-C41-O2
2	I	704	FO4	C1-C-C16-N
2	I	704	FO4	O-C-C16-N
2	I	704	FO4	C1-C-C16-C41
2	I	704	FO4	O-C-C16-C41
2	J	702	FO4	C41-C16-N-C17
2	J	702	FO4	N-C16-C41-O2
2	J	702	FO4	C-C16-C41-O2
2	J	702	FO4	C1-C-C16-C41
2	J	702	FO4	O-C-C16-C41

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Mol	Chain	Res	Type	Atoms
2	J	703	FO4	C42-O4-P-O5
2	J	703	FO4	C42-O4-P-O3
2	J	703	FO4	C42-O4-P-O2
2	J	703	FO4	C41-O2-P-O5
2	J	703	FO4	C41-O2-P-O3
2	J	703	FO4	C41-O2-P-O4
2	J	704	FO4	C42-O4-P-O3
2	J	704	FO4	C42-O4-P-O2
2	J	704	FO4	N-C16-C41-O2
2	J	704	FO4	C-C16-C41-O2
2	J	704	FO4	C1-C-C16-N
2	J	704	FO4	O-C-C16-N
2	J	704	FO4	C1-C-C16-C41
2	J	704	FO4	O-C-C16-C41
2	L	702	FO4	C41-C16-N-C17
2	L	702	FO4	N-C16-C41-O2
2	L	702	FO4	C-C16-C41-O2
2	L	702	FO4	C1-C-C16-C41
2	L	702	FO4	O-C-C16-C41
2	L	703	FO4	C-C16-N-C17
2	L	703	FO4	C42-O4-P-O5
2	L	703	FO4	C42-O4-P-O3
2	L	703	FO4	C42-O4-P-O2
2	L	703	FO4	C41-O2-P-O3
2	L	703	FO4	C41-O2-P-O4
2	L	704	FO4	C42-O4-P-O3
2	L	704	FO4	C42-O4-P-O2
2	L	704	FO4	N-C16-C41-O2
2	L	704	FO4	C-C16-C41-O2
2	L	704	FO4	C1-C-C16-N
2	L	704	FO4	O-C-C16-N
2	L	704	FO4	C1-C-C16-C41
2	L	704	FO4	O-C-C16-C41
2	C	201	FO4	C18-C17-N-C16
2	A	703	FO4	C18-C17-N-C16
2	B	702	FO4	C18-C17-N-C16
2	E	702	FO4	C18-C17-N-C16
2	G	702	FO4	C18-C17-N-C16
2	I	702	FO4	C18-C17-N-C16
2	J	702	FO4	C18-C17-N-C16
2	L	702	FO4	C18-C17-N-C16
2	C	201	FO4	C42-C43-N1-C44

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Mol	Chain	Res	Type	Atoms
2	B	702	FO4	C42-C43-N1-C44
2	G	702	FO4	C42-C43-N1-C44
2	J	702	FO4	C42-C43-N1-C44
2	C	201	FO4	O1-C17-N-C16
2	A	703	FO4	O1-C17-N-C16
2	B	702	FO4	O1-C17-N-C16
2	E	702	FO4	O1-C17-N-C16
2	G	702	FO4	O1-C17-N-C16
2	I	702	FO4	O1-C17-N-C16
2	J	702	FO4	O1-C17-N-C16
2	L	702	FO4	O1-C17-N-C16
3	C	207	CLR	C21-C20-C22-C23
3	A	709	CLR	C21-C20-C22-C23
3	E	708	CLR	C21-C20-C22-C23
3	I	708	CLR	C21-C20-C22-C23
3	J	708	CLR	C21-C20-C22-C23
3	L	708	CLR	C21-C20-C22-C23
3	C	207	CLR	C17-C20-C22-C23
3	A	709	CLR	C17-C20-C22-C23
3	B	708	CLR	C17-C20-C22-C23
3	E	708	CLR	C17-C20-C22-C23
3	G	708	CLR	C17-C20-C22-C23
3	I	708	CLR	C17-C20-C22-C23
3	J	708	CLR	C17-C20-C22-C23
3	L	708	CLR	C17-C20-C22-C23
3	B	708	CLR	C21-C20-C22-C23
3	G	708	CLR	C21-C20-C22-C23
3	E	707	CLR	C17-C20-C22-C23
3	I	707	CLR	C17-C20-C22-C23
2	A	704	FO4	C2-C3-C4-C5
2	E	703	FO4	C2-C3-C4-C5
2	I	703	FO4	C2-C3-C4-C5
2	L	703	FO4	C2-C3-C4-C5
3	A	708	CLR	C17-C20-C22-C23
3	L	707	CLR	C17-C20-C22-C23
2	C	201	FO4	C42-C43-N1-C46
2	A	703	FO4	C42-C43-N1-C46
2	A	703	FO4	C42-C43-N1-C45
2	A	703	FO4	C42-C43-N1-C44
2	B	702	FO4	C42-C43-N1-C46
2	E	702	FO4	C42-C43-N1-C46
2	E	702	FO4	C42-C43-N1-C45

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Mol	Chain	Res	Type	Atoms
2	E	702	FO4	C42-C43-N1-C44
2	G	702	FO4	C42-C43-N1-C46
2	I	702	FO4	C42-C43-N1-C46
2	I	702	FO4	C42-C43-N1-C45
2	I	702	FO4	C42-C43-N1-C44
2	J	702	FO4	C42-C43-N1-C46
2	L	702	FO4	C42-C43-N1-C46
2	L	702	FO4	C42-C43-N1-C45
2	L	702	FO4	C42-C43-N1-C44
2	C	202	FO4	C2-C3-C4-C5
2	B	703	FO4	C2-C3-C4-C5
2	G	703	FO4	C2-C3-C4-C5
2	J	703	FO4	C2-C3-C4-C5
3	C	206	CLR	C17-C20-C22-C23
2	C	202	FO4	O-C-C1-C2
2	B	703	FO4	O-C-C1-C2
2	G	703	FO4	O-C-C1-C2
2	J	703	FO4	O-C-C1-C2
3	B	707	CLR	C17-C20-C22-C23
2	A	702	FO4	C17-C18-C19-C20
2	E	701	FO4	C17-C18-C19-C20
2	I	701	FO4	C17-C18-C19-C20
2	L	701	FO4	C17-C18-C19-C20
2	C	201	FO4	C42-C43-N1-C45
2	B	702	FO4	C42-C43-N1-C45
2	G	702	FO4	C42-C43-N1-C45
2	J	702	FO4	C42-C43-N1-C45
3	G	707	CLR	C17-C20-C22-C23
3	J	707	CLR	C17-C20-C22-C23
3	C	205	CLR	C20-C22-C23-C24
3	J	706	CLR	C20-C22-C23-C24
2	A	704	FO4	C21-C22-C23-C24
2	E	703	FO4	C21-C22-C23-C24
2	I	703	FO4	C21-C22-C23-C24
2	L	703	FO4	C21-C22-C23-C24
2	B	703	FO4	C21-C22-C23-C24
3	B	706	CLR	C20-C22-C23-C24
3	G	706	CLR	C20-C22-C23-C24
2	G	703	FO4	C21-C22-C23-C24
2	C	202	FO4	C21-C22-C23-C24
2	A	702	FO4	C11-C12-C13-C14
2	J	703	FO4	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
2	E	701	FO4	C11-C12-C13-C14
2	I	701	FO4	C11-C12-C13-C14
2	L	701	FO4	C11-C12-C13-C14
2	B	701	FO4	C11-C12-C13-C14
2	G	701	FO4	C11-C12-C13-C14
2	A	701	FO4	C11-C12-C13-C14
2	J	701	FO4	C11-C12-C13-C14
3	A	708	CLR	C21-C20-C22-C23
3	E	707	CLR	C21-C20-C22-C23
3	I	707	CLR	C21-C20-C22-C23
3	L	707	CLR	C21-C20-C22-C23
2	G	701	FO4	C28-C29-C30-C31
2	C	202	FO4	C41-C16-N-C17
2	B	703	FO4	C41-C16-N-C17
2	E	703	FO4	C41-C16-N-C17
2	G	703	FO4	C41-C16-N-C17
2	I	703	FO4	C41-C16-N-C17
2	J	703	FO4	C41-C16-N-C17
2	E	703	FO4	C22-C23-C24-C25
2	G	704	FO4	C19-C20-C21-C22
2	A	704	FO4	C22-C23-C24-C25
2	C	203	FO4	C19-C20-C21-C22
2	L	703	FO4	C22-C23-C24-C25
2	I	703	FO4	C22-C23-C24-C25
2	J	704	FO4	C19-C20-C21-C22
2	A	701	FO4	C28-C29-C30-C31
2	A	702	FO4	C28-C29-C30-C31
2	B	701	FO4	C28-C29-C30-C31
2	I	701	FO4	C28-C29-C30-C31
2	J	701	FO4	C28-C29-C30-C31
2	L	701	FO4	C28-C29-C30-C31
2	E	701	FO4	C28-C29-C30-C31
2	C	202	FO4	C-C16-N-C17
2	B	703	FO4	C-C16-N-C17
2	G	703	FO4	C-C16-N-C17
2	J	703	FO4	C-C16-N-C17
3	I	706	CLR	C20-C22-C23-C24
3	A	707	CLR	C20-C22-C23-C24
3	E	706	CLR	C20-C22-C23-C24
3	I	707	CLR	C20-C22-C23-C24
3	L	706	CLR	C20-C22-C23-C24
3	L	707	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
2	B	704	FO4	C19-C20-C21-C22
3	A	708	CLR	C20-C22-C23-C24
3	E	707	CLR	C20-C22-C23-C24
3	C	206	CLR	C21-C20-C22-C23
2	G	703	FO4	C22-C23-C24-C25
2	J	703	FO4	C22-C23-C24-C25
2	C	202	FO4	C22-C23-C24-C25
2	B	703	FO4	C22-C23-C24-C25
3	B	707	CLR	C21-C20-C22-C23
2	G	701	FO4	C18-C19-C20-C21
2	E	704	FO4	C19-C20-C21-C22
2	J	701	FO4	C18-C19-C20-C21
2	A	701	FO4	C18-C19-C20-C21
2	B	701	FO4	C18-C19-C20-C21
2	I	703	FO4	C11-C10-C9-C8
2	E	703	FO4	C11-C10-C9-C8
2	L	703	FO4	C11-C10-C9-C8
2	A	704	FO4	C11-C10-C9-C8
2	B	704	FO4	C18-C19-C20-C21
2	A	705	FO4	C19-C20-C21-C22
2	I	704	FO4	C19-C20-C21-C22
2	L	704	FO4	C19-C20-C21-C22
2	J	703	FO4	C11-C10-C9-C8
2	C	202	FO4	C11-C10-C9-C8
2	B	703	FO4	C11-C10-C9-C8
3	G	707	CLR	C21-C20-C22-C23
3	J	707	CLR	C21-C20-C22-C23
2	E	704	FO4	C18-C19-C20-C21
2	G	703	FO4	C11-C10-C9-C8
3	A	707	CLR	C17-C20-C22-C23
3	E	706	CLR	C17-C20-C22-C23
3	I	706	CLR	C17-C20-C22-C23
3	L	706	CLR	C17-C20-C22-C23
2	L	704	FO4	C18-C19-C20-C21
2	A	705	FO4	C18-C19-C20-C21
2	J	704	FO4	C18-C19-C20-C21
2	I	704	FO4	C18-C19-C20-C21
2	J	703	FO4	C7-C8-C9-C10
2	G	703	FO4	C7-C8-C9-C10
2	C	202	FO4	C7-C8-C9-C10
3	C	206	CLR	C20-C22-C23-C24
3	B	707	CLR	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
3	G	707	CLR	C20-C22-C23-C24
3	J	707	CLR	C20-C22-C23-C24
2	B	703	FO4	C7-C8-C9-C10
2	A	704	FO4	C7-C8-C9-C10
2	G	704	FO4	C18-C19-C20-C21
2	E	703	FO4	C7-C8-C9-C10
2	L	703	FO4	C7-C8-C9-C10
2	B	703	FO4	C24-C25-C26-C27
2	I	703	FO4	C7-C8-C9-C10
2	I	703	FO4	C24-C25-C26-C27
2	C	202	FO4	C24-C25-C26-C27
2	A	702	FO4	C18-C19-C20-C21
2	A	704	FO4	C24-C25-C26-C27
2	E	701	FO4	C18-C19-C20-C21
2	I	701	FO4	C18-C19-C20-C21
2	L	701	FO4	C18-C19-C20-C21
2	E	703	FO4	C24-C25-C26-C27
2	G	703	FO4	C24-C25-C26-C27
2	J	703	FO4	C24-C25-C26-C27
2	L	703	FO4	C24-C25-C26-C27
2	C	203	FO4	C18-C19-C20-C21
2	A	704	FO4	C41-C16-N-C17
2	L	703	FO4	C41-C16-N-C17
2	B	702	FO4	C1-C2-C3-C4
2	G	702	FO4	C1-C2-C3-C4
2	J	702	FO4	C1-C2-C3-C4
3	C	206	CLR	C23-C24-C25-C26
3	B	707	CLR	C23-C24-C25-C26
3	G	707	CLR	C23-C24-C25-C26
2	J	701	FO4	C21-C22-C23-C24
2	G	701	FO4	C21-C22-C23-C24
2	C	201	FO4	O-C-C16-N
2	A	703	FO4	O-C-C16-N
2	B	702	FO4	O-C-C16-N
2	E	702	FO4	O-C-C16-N
2	G	702	FO4	O-C-C16-N
2	I	702	FO4	O-C-C16-N
2	J	702	FO4	O-C-C16-N
2	L	702	FO4	O-C-C16-N
3	J	707	CLR	C23-C24-C25-C26
2	A	701	FO4	C21-C22-C23-C24
2	B	701	FO4	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
2	L	701	FO4	C3-C4-C5-C6
2	A	702	FO4	C3-C4-C5-C6
2	L	701	FO4	C22-C23-C24-C25
2	I	701	FO4	C3-C4-C5-C6
2	I	701	FO4	C22-C23-C24-C25
3	J	705	CLR	C22-C23-C24-C25
2	E	701	FO4	C3-C4-C5-C6
2	E	701	FO4	C22-C23-C24-C25
2	A	702	FO4	C22-C23-C24-C25
3	B	706	CLR	C17-C20-C22-C23
3	A	708	CLR	C23-C24-C25-C26
3	E	707	CLR	C23-C24-C25-C26
3	I	707	CLR	C23-C24-C25-C26
3	L	707	CLR	C23-C24-C25-C26
3	G	705	CLR	C22-C23-C24-C25
2	J	701	FO4	C3-C4-C5-C6
2	A	701	FO4	C3-C4-C5-C6
2	G	701	FO4	C3-C4-C5-C6
2	B	701	FO4	C3-C4-C5-C6
2	G	703	FO4	C20-C21-C22-C23
2	C	201	FO4	C42-O4-P-O5
2	C	203	FO4	C42-O4-P-O5
2	A	703	FO4	C42-O4-P-O5
2	A	704	FO4	C41-O2-P-O5
2	A	705	FO4	C42-O4-P-O5
2	B	702	FO4	C42-O4-P-O5
2	B	704	FO4	C42-O4-P-O5
2	E	702	FO4	C42-O4-P-O5
2	E	703	FO4	C41-O2-P-O5
2	E	704	FO4	C42-O4-P-O5
2	G	702	FO4	C42-O4-P-O5
2	G	704	FO4	C42-O4-P-O5
2	I	702	FO4	C42-O4-P-O5
2	I	703	FO4	C41-O2-P-O5
2	I	704	FO4	C42-O4-P-O5
2	J	702	FO4	C42-O4-P-O5
2	J	704	FO4	C42-O4-P-O5
2	L	702	FO4	C42-O4-P-O5
2	L	703	FO4	C41-O2-P-O5
2	L	704	FO4	C42-O4-P-O5
2	J	703	FO4	C20-C21-C22-C23
3	C	205	CLR	C17-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
3	G	706	CLR	C17-C20-C22-C23
2	C	202	FO4	C20-C21-C22-C23
2	B	703	FO4	C20-C21-C22-C23
3	A	707	CLR	C21-C20-C22-C23
3	E	706	CLR	C21-C20-C22-C23
3	I	706	CLR	C21-C20-C22-C23
3	L	706	CLR	C21-C20-C22-C23
3	G	707	CLR	C23-C24-C25-C27
3	J	707	CLR	C23-C24-C25-C27
3	C	206	CLR	C23-C24-C25-C27
3	B	707	CLR	C23-C24-C25-C27
3	C	204	CLR	C22-C23-C24-C25
2	C	201	FO4	C1-C2-C3-C4
2	A	703	FO4	C1-C2-C3-C4
2	E	702	FO4	C1-C2-C3-C4
2	I	702	FO4	C1-C2-C3-C4
2	L	702	FO4	C1-C2-C3-C4
3	J	706	CLR	C17-C20-C22-C23
3	G	707	CLR	C22-C23-C24-C25
3	J	707	CLR	C22-C23-C24-C25
2	A	701	FO4	C17-C18-C19-C20
2	I	703	FO4	C20-C21-C22-C23
2	B	701	FO4	C17-C18-C19-C20
3	B	707	CLR	C22-C23-C24-C25
2	L	703	FO4	C20-C21-C22-C23
3	C	206	CLR	C22-C23-C24-C25
2	J	701	FO4	C17-C18-C19-C20
2	G	701	FO4	C17-C18-C19-C20
3	B	705	CLR	C22-C23-C24-C25
2	E	703	FO4	C20-C21-C22-C23
2	A	701	FO4	C27-C28-C29-C30
2	I	701	FO4	C21-C22-C23-C24
2	I	703	FO4	O-C-C1-C2
2	L	703	FO4	O-C-C1-C2
2	L	701	FO4	C21-C22-C23-C24
2	E	701	FO4	C21-C22-C23-C24
2	A	704	FO4	C20-C21-C22-C23
3	L	705	CLR	C22-C23-C24-C25
2	A	702	FO4	C21-C22-C23-C24
3	I	705	CLR	C22-C23-C24-C25
2	B	701	FO4	C27-C28-C29-C30
2	E	701	FO4	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
2	A	702	FO4	C27-C28-C29-C30
2	I	701	FO4	C27-C28-C29-C30
2	L	701	FO4	C27-C28-C29-C30
2	B	701	FO4	C22-C23-C24-C25
2	G	701	FO4	C22-C23-C24-C25
2	B	703	FO4	C1-C2-C3-C4
2	E	703	FO4	C1-C2-C3-C4
2	J	701	FO4	C22-C23-C24-C25
2	A	704	FO4	C1-C2-C3-C4
2	G	703	FO4	C1-C2-C3-C4
2	I	703	FO4	C1-C2-C3-C4
2	L	703	FO4	C1-C2-C3-C4
2	A	701	FO4	C22-C23-C24-C25
3	B	706	CLR	C21-C20-C22-C23
3	G	706	CLR	C21-C20-C22-C23
2	B	704	FO4	C17-C18-C19-C20
2	A	701	FO4	O-C-C16-C41
2	B	701	FO4	O-C-C16-C41
2	G	701	FO4	O-C-C16-C41
2	J	701	FO4	O-C-C16-C41
2	A	704	FO4	O-C-C1-C2
2	E	703	FO4	O-C-C1-C2
2	J	701	FO4	C27-C28-C29-C30
2	C	202	FO4	C1-C2-C3-C4
2	J	703	FO4	C1-C2-C3-C4
3	C	205	CLR	C21-C20-C22-C23
2	J	704	FO4	C42-C43-N1-C46
3	J	706	CLR	C21-C20-C22-C23
2	G	701	FO4	C27-C28-C29-C30
2	C	203	FO4	O4-C42-C43-N1
2	A	705	FO4	O4-C42-C43-N1
2	B	704	FO4	O4-C42-C43-N1
2	E	704	FO4	O4-C42-C43-N1
2	G	704	FO4	O4-C42-C43-N1
2	I	704	FO4	O4-C42-C43-N1
2	J	704	FO4	O4-C42-C43-N1
2	L	704	FO4	O4-C42-C43-N1
2	C	203	FO4	C42-C43-N1-C46
2	C	203	FO4	C42-C43-N1-C44
2	B	704	FO4	C42-C43-N1-C46
2	B	704	FO4	C42-C43-N1-C44
2	G	704	FO4	C42-C43-N1-C46

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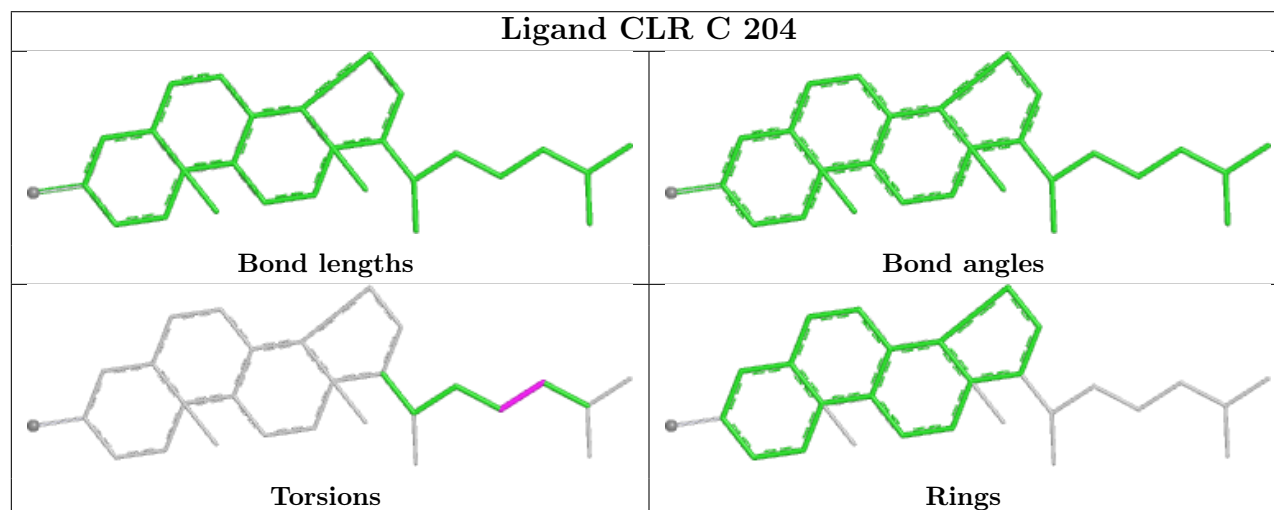
Mol	Chain	Res	Type	Atoms
2	G	704	FO4	C42-C43-N1-C44
2	J	704	FO4	C42-C43-N1-C44
3	A	708	CLR	C22-C23-C24-C25
3	E	707	CLR	C22-C23-C24-C25
2	E	701	FO4	C23-C24-C25-C26
2	J	701	FO4	C6-C7-C8-C9
3	I	707	CLR	C22-C23-C24-C25
3	L	707	CLR	C22-C23-C24-C25
2	I	701	FO4	C23-C24-C25-C26
2	A	702	FO4	C23-C24-C25-C26
2	G	701	FO4	C6-C7-C8-C9
2	C	203	FO4	O1-C17-C18-C19
2	G	704	FO4	O1-C17-C18-C19
2	L	701	FO4	C23-C24-C25-C26
3	E	705	CLR	C22-C23-C24-C25
2	B	701	FO4	C6-C7-C8-C9
2	A	705	FO4	C42-C43-N1-C44
2	I	704	FO4	C42-C43-N1-C44
2	L	704	FO4	C42-C43-N1-C44
2	A	701	FO4	C6-C7-C8-C9
3	E	708	CLR	C22-C23-C24-C25
3	I	708	CLR	C22-C23-C24-C25
2	C	203	FO4	N-C17-C18-C19
2	A	705	FO4	C42-C43-N1-C46
2	E	704	FO4	C42-C43-N1-C44
2	I	704	FO4	C42-C43-N1-C46
2	L	704	FO4	C42-C43-N1-C46
3	A	706	CLR	C22-C23-C24-C25
2	B	704	FO4	O1-C17-C18-C19
2	E	704	FO4	O1-C17-C18-C19
2	J	704	FO4	O1-C17-C18-C19
3	L	708	CLR	C22-C23-C24-C25
2	G	704	FO4	N-C17-C18-C19
2	A	705	FO4	O1-C17-C18-C19
2	I	704	FO4	O1-C17-C18-C19
2	E	704	FO4	C42-C43-N1-C46
3	A	709	CLR	C22-C23-C24-C25
2	L	703	FO4	C-C16-C41-O2
2	L	704	FO4	O1-C17-C18-C19
2	A	705	FO4	C17-C18-C19-C20
2	L	704	FO4	C17-C18-C19-C20

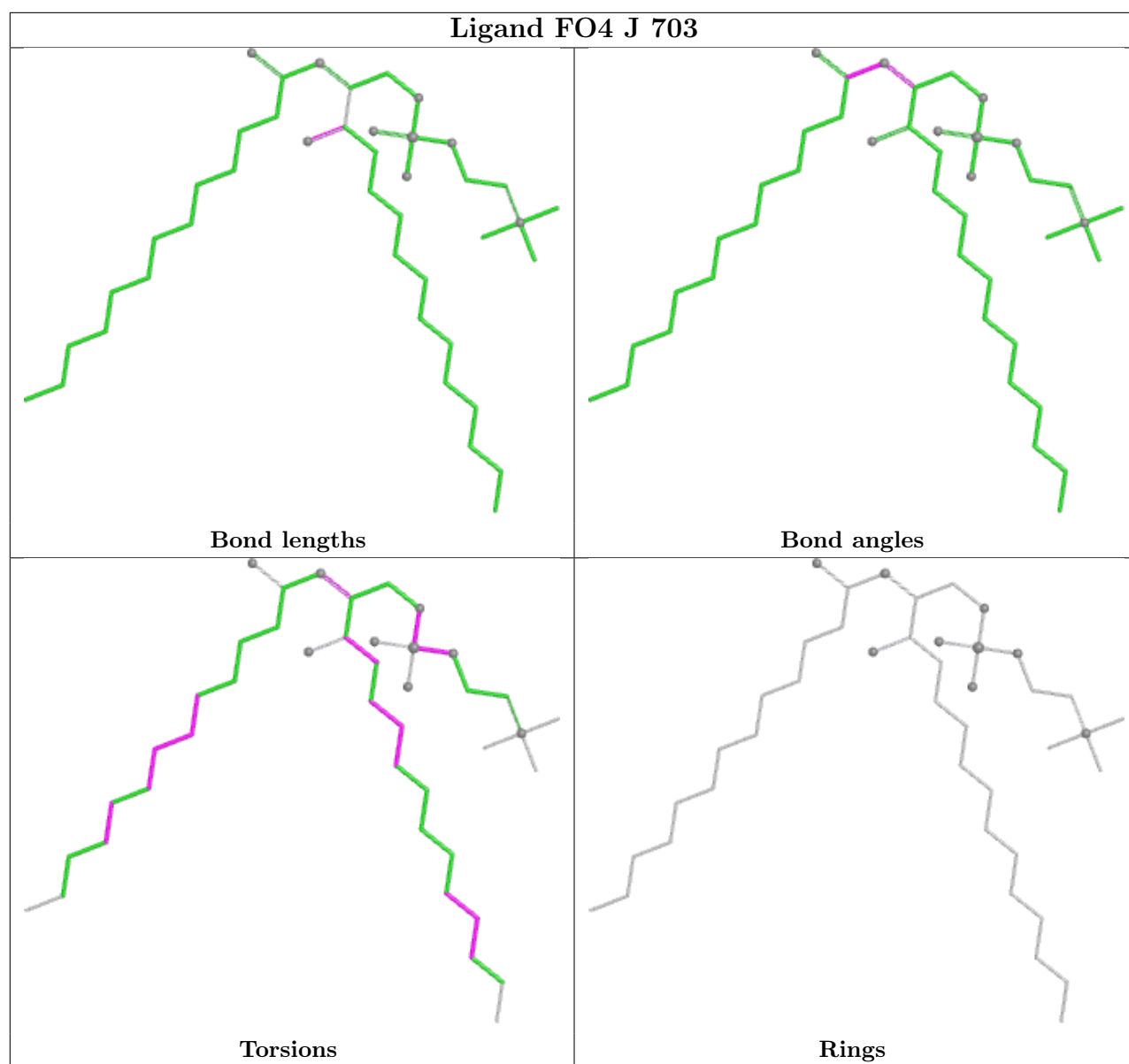
There are no ring outliers.

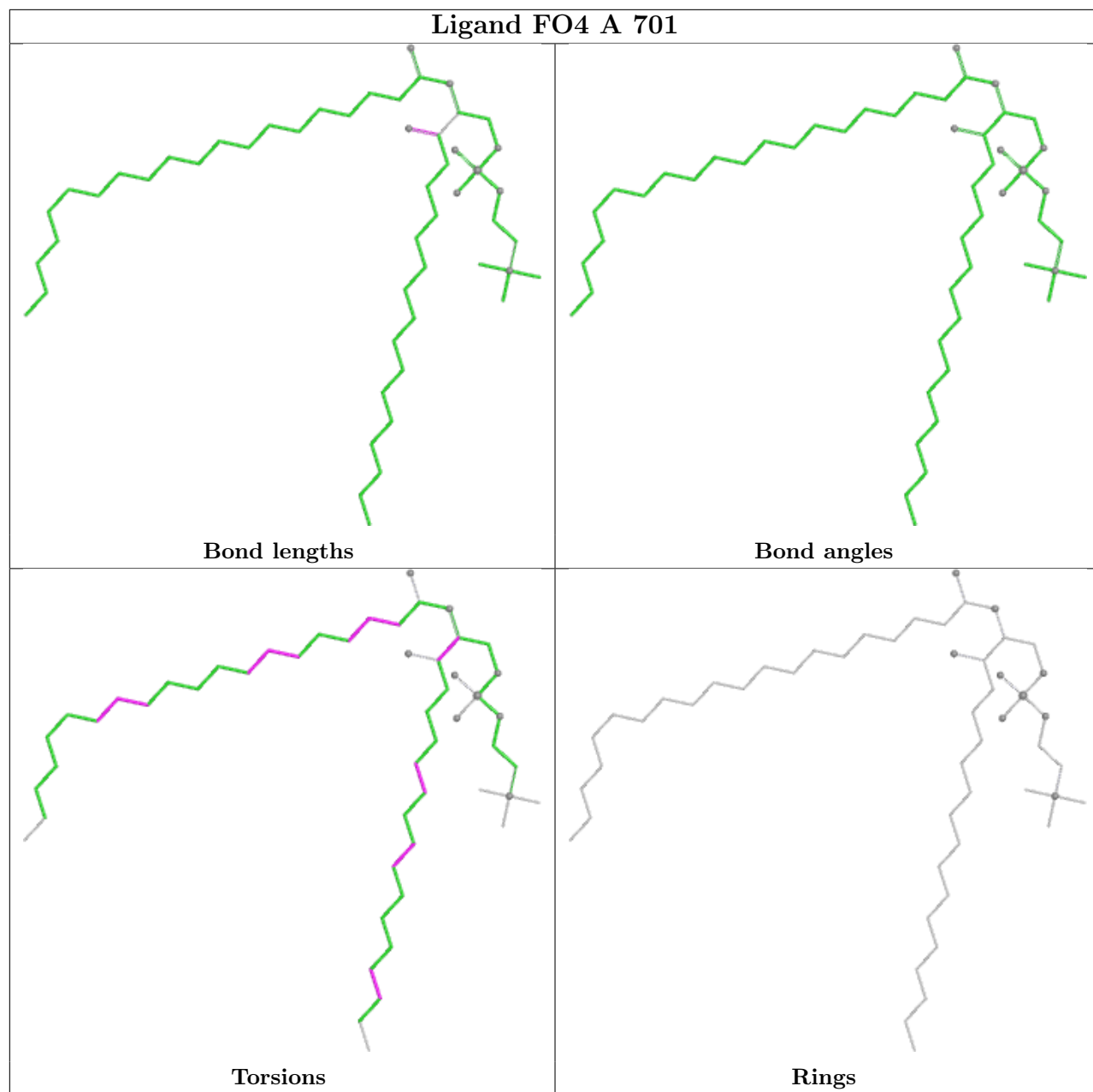
16 monomers are involved in 16 short contacts:

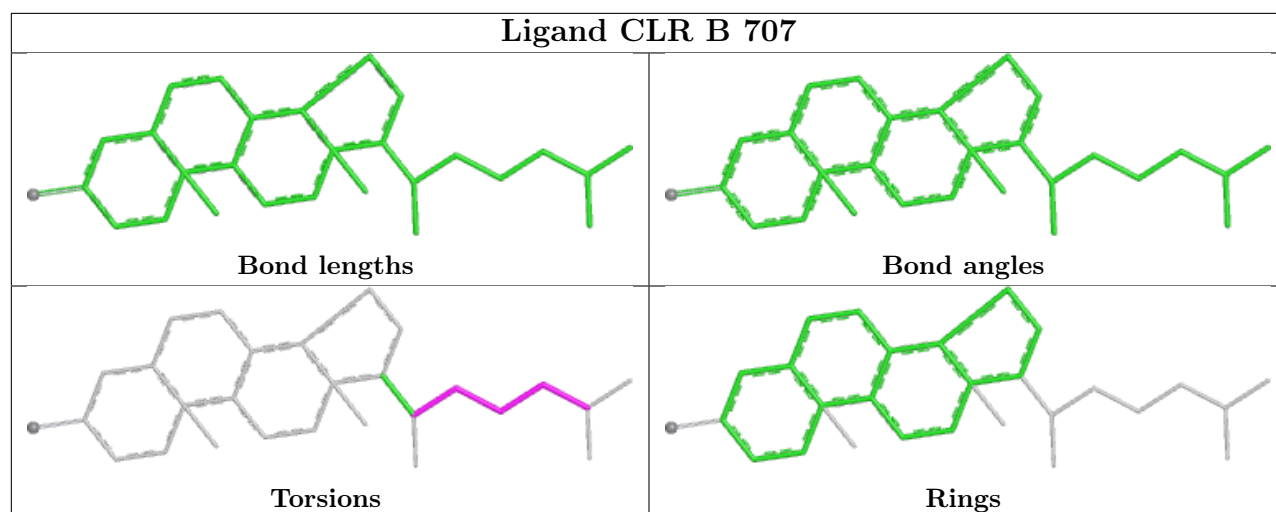
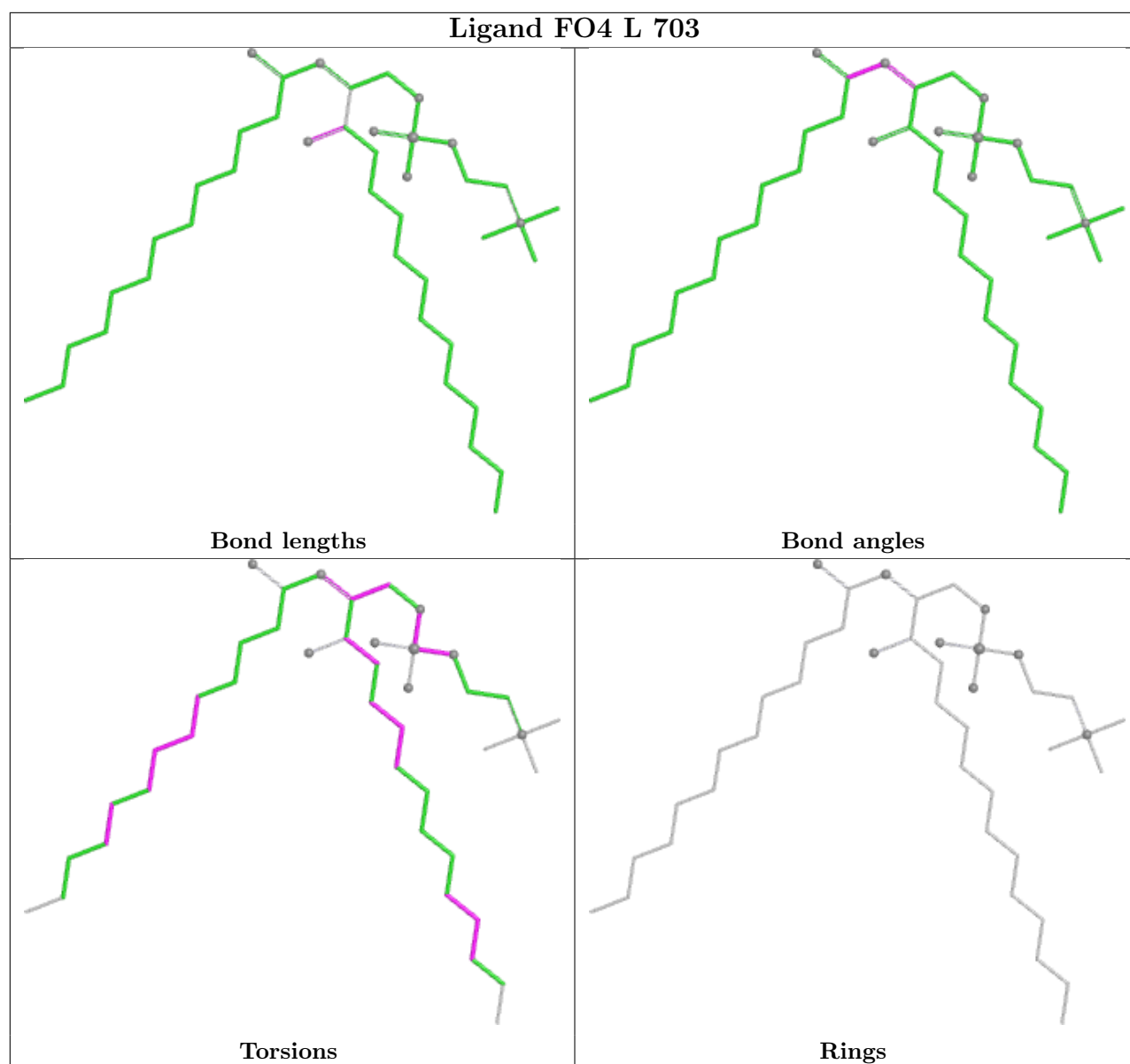
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	707	CLR	2	0
3	I	707	CLR	2	0
3	G	707	CLR	2	0
3	I	708	CLR	1	0
3	L	707	CLR	2	0
3	J	708	CLR	1	0
3	B	708	CLR	1	0
3	A	709	CLR	1	0
3	A	708	CLR	2	0
3	C	206	CLR	2	0
3	J	707	CLR	2	0
3	L	708	CLR	1	0
3	E	707	CLR	2	0
3	G	708	CLR	1	0
3	C	207	CLR	1	0
3	E	708	CLR	1	0

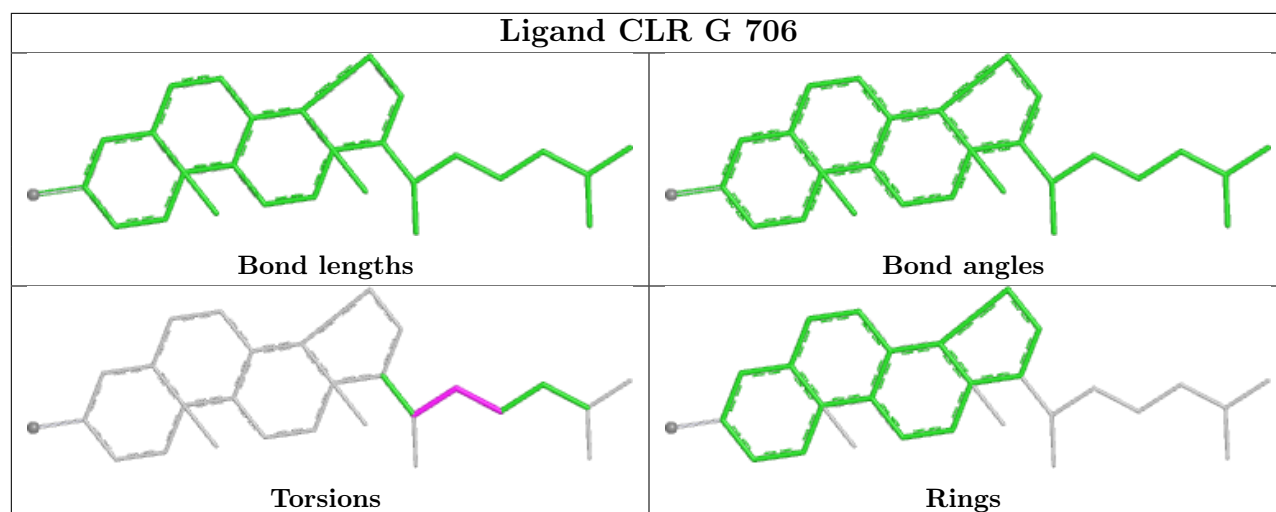
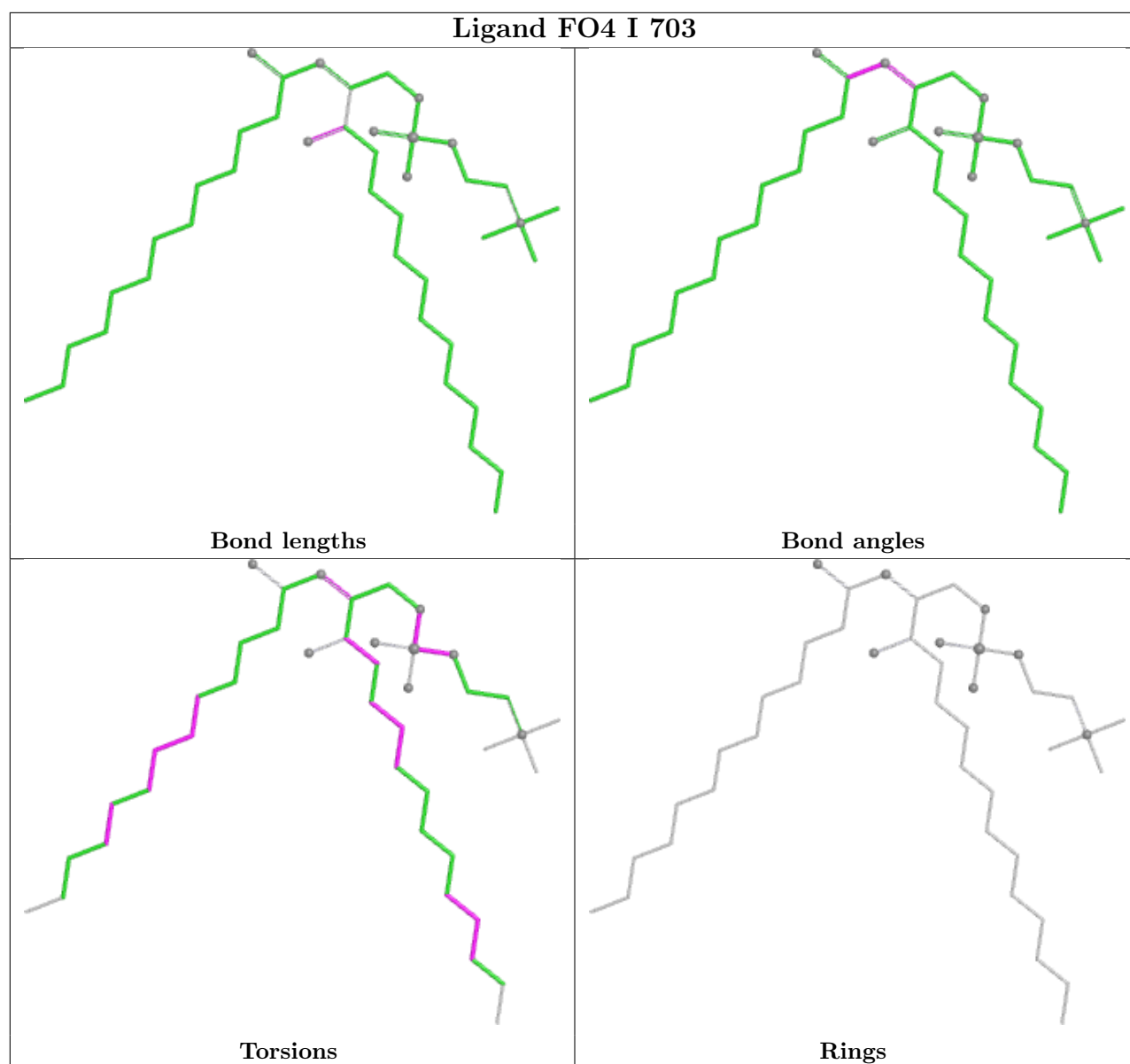
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

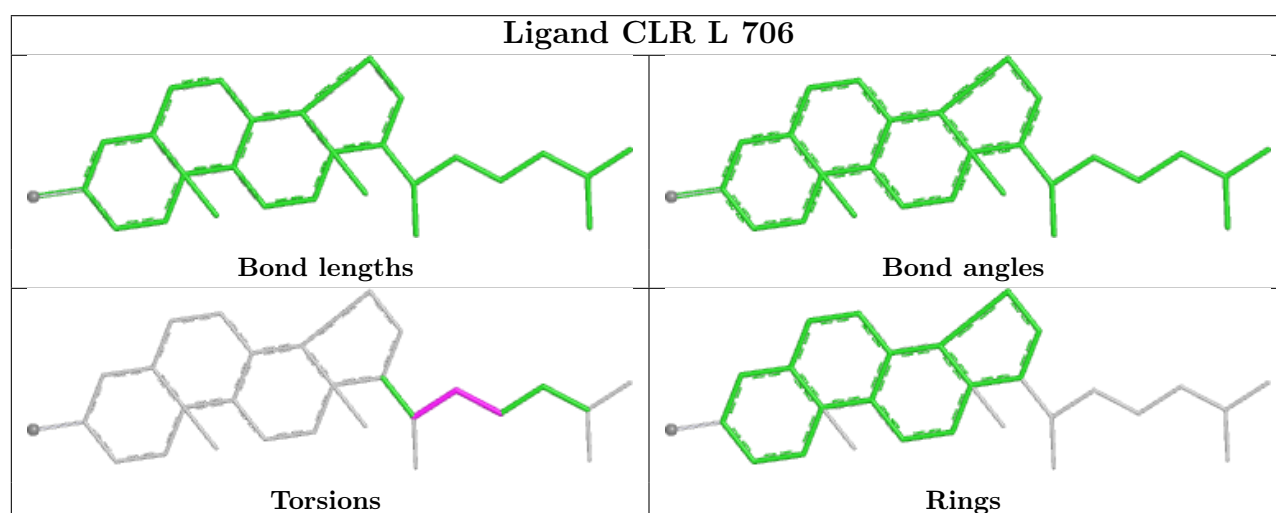
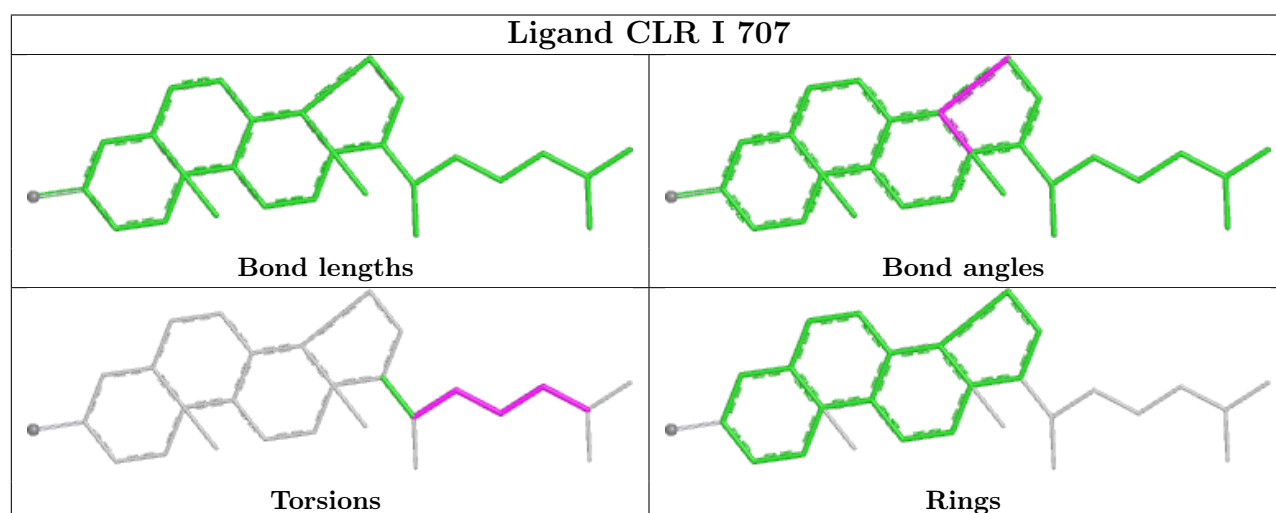
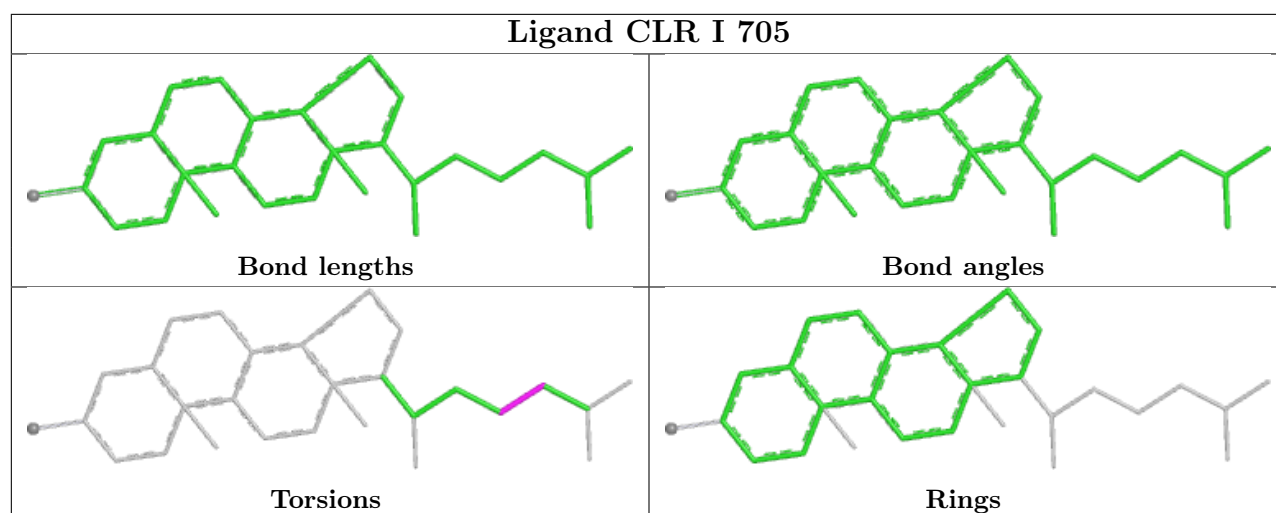


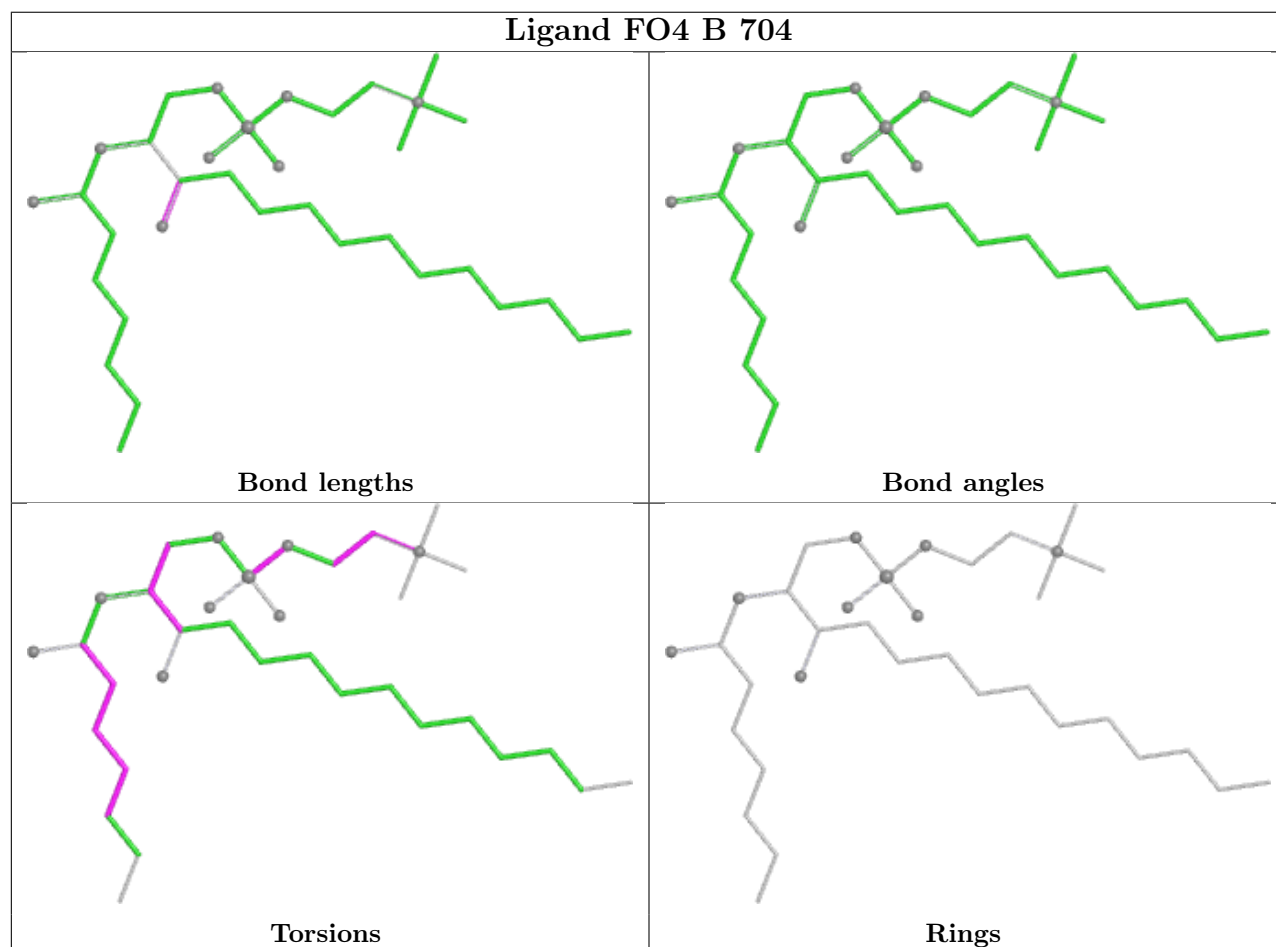
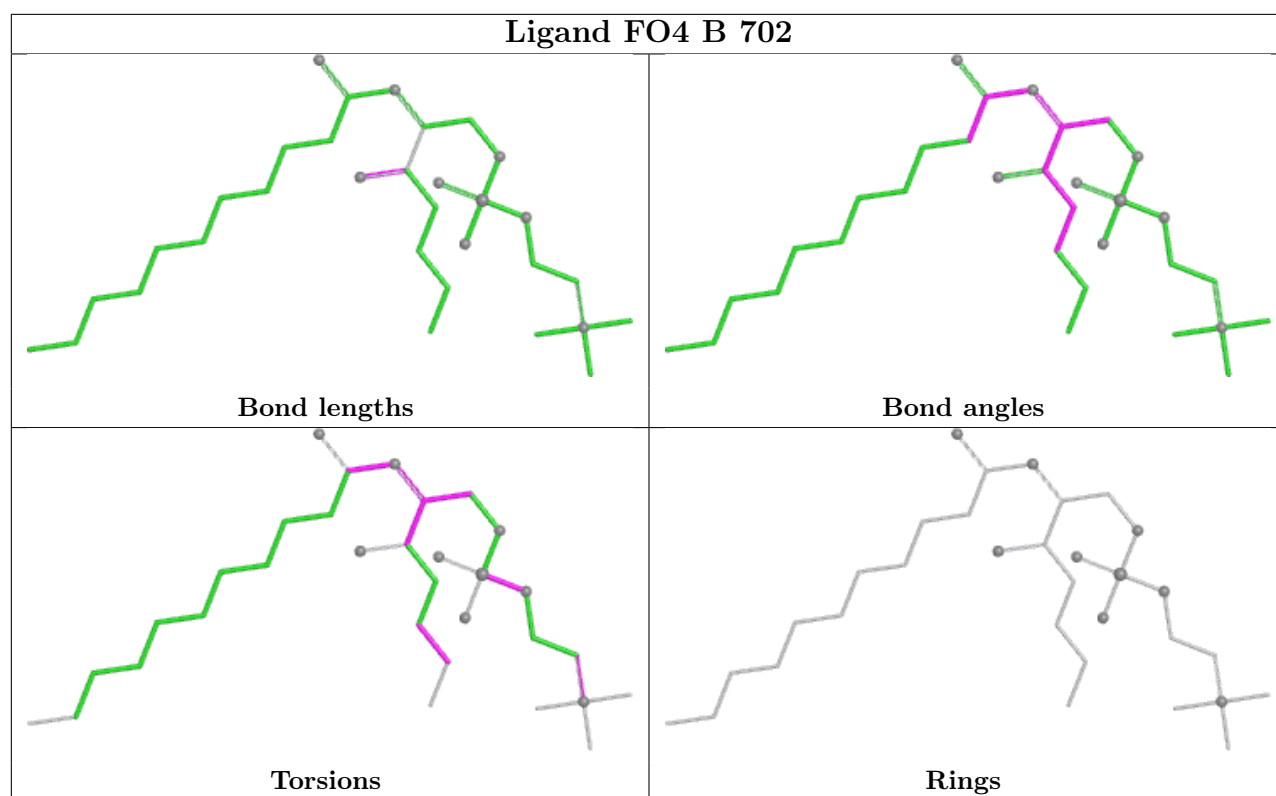


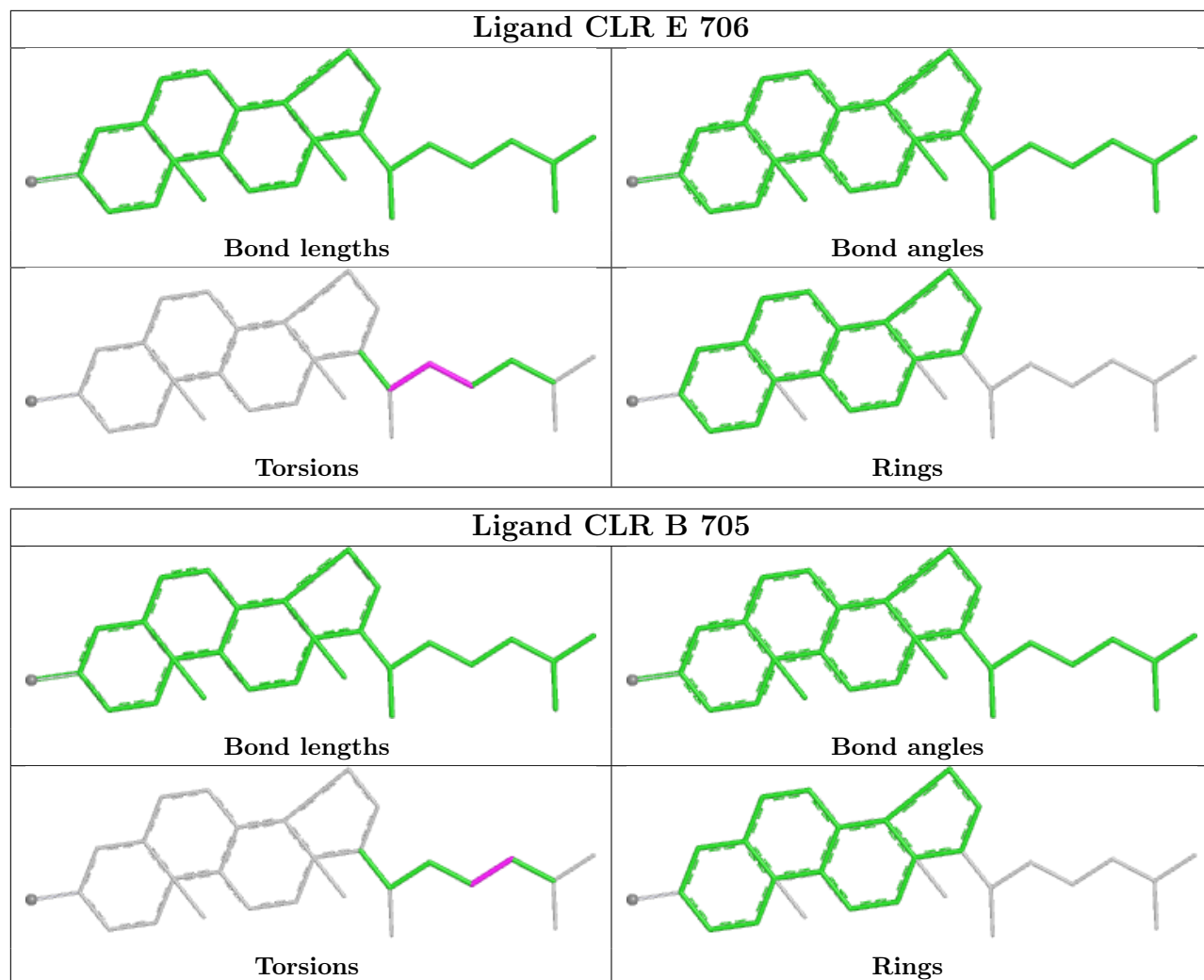


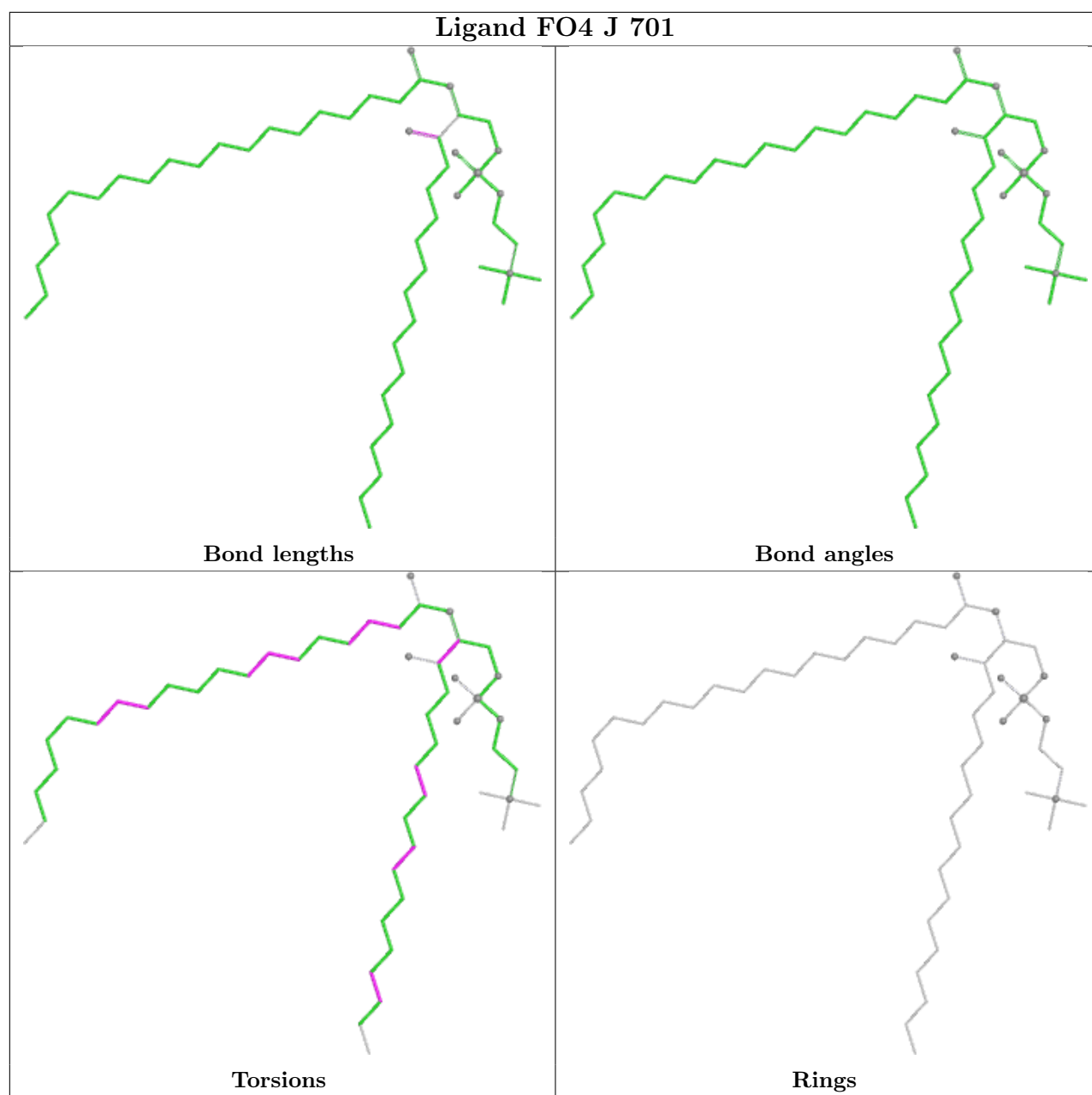


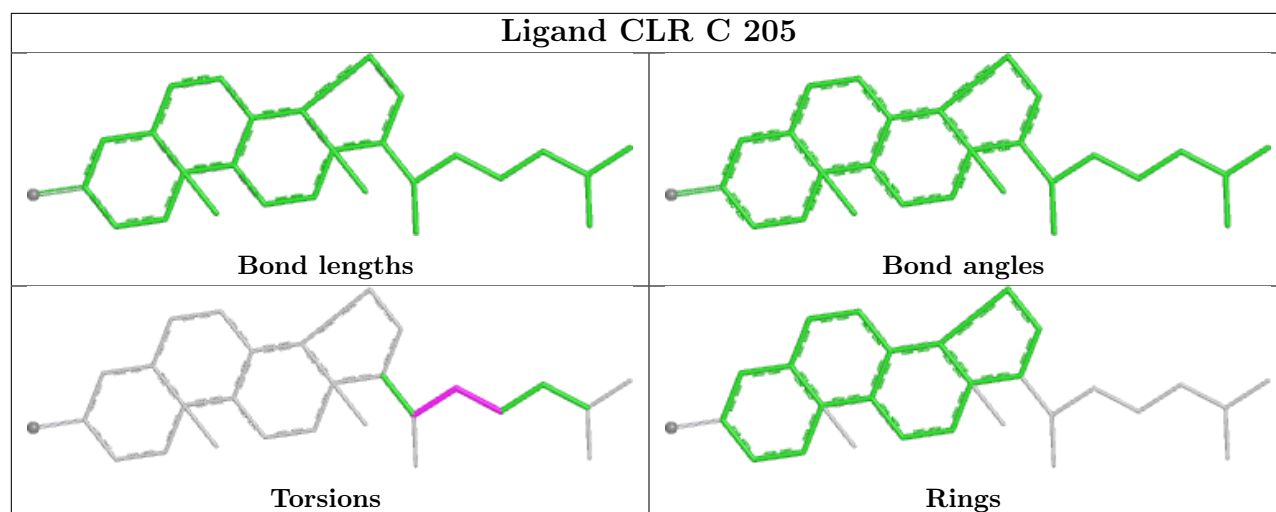
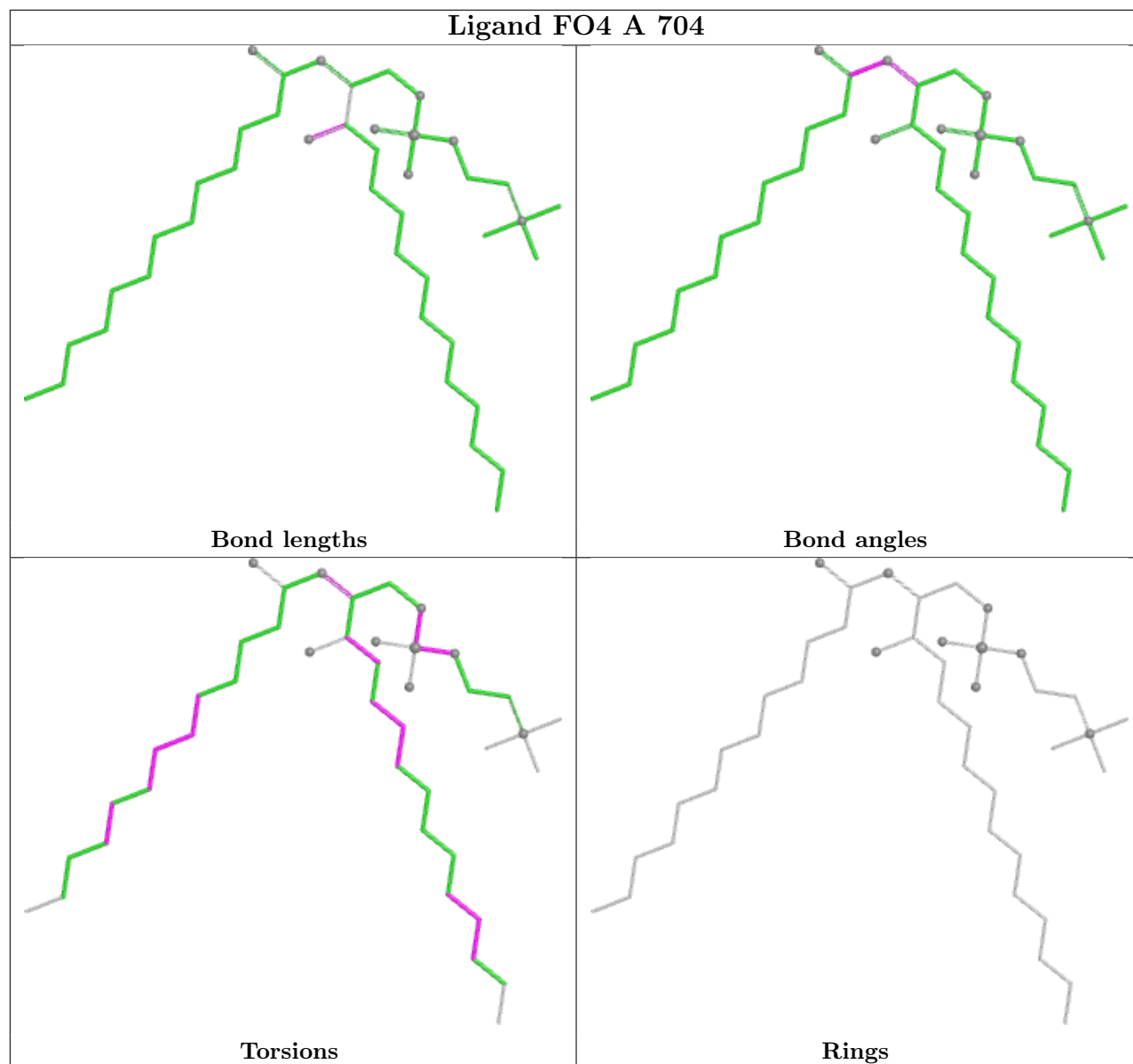


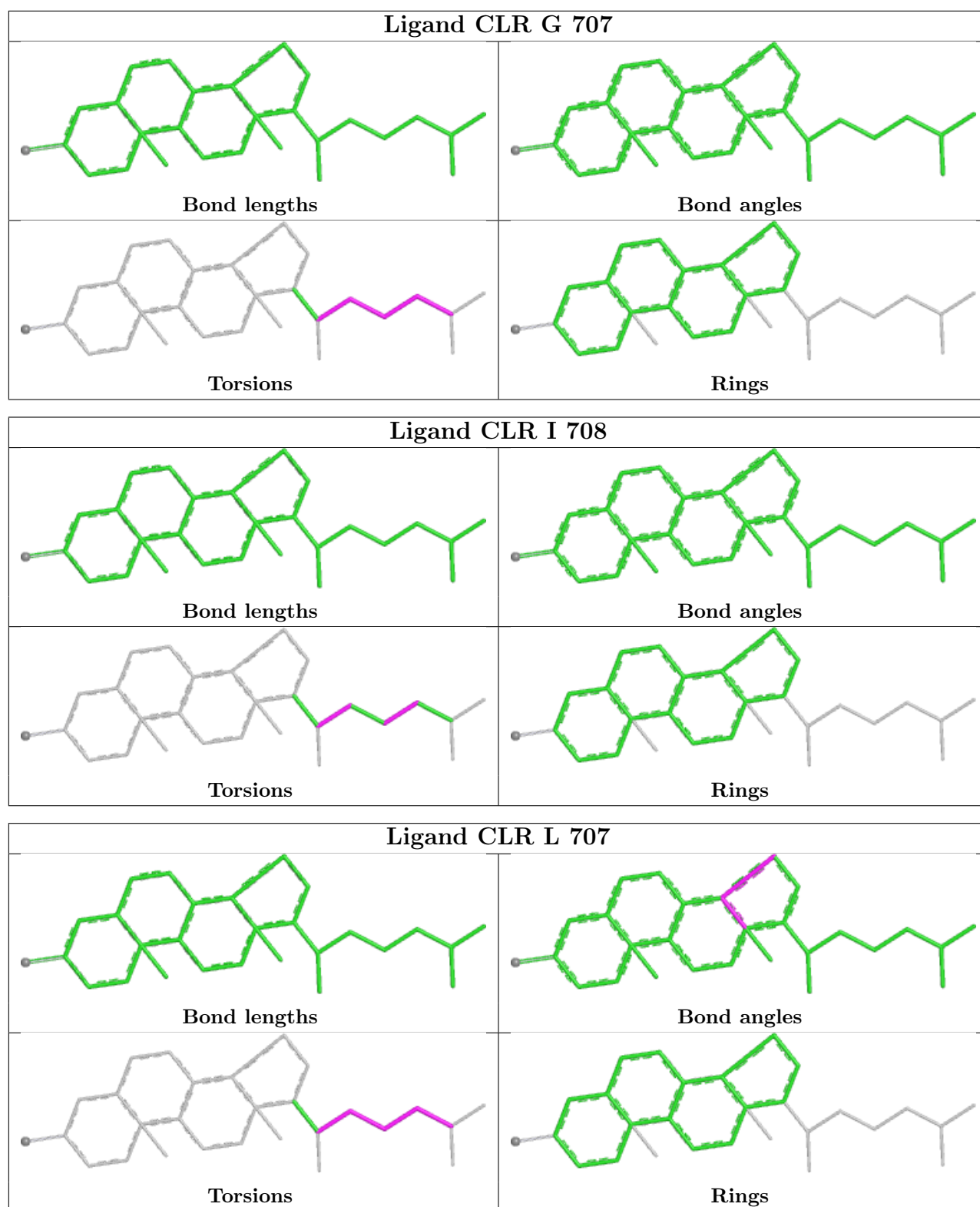


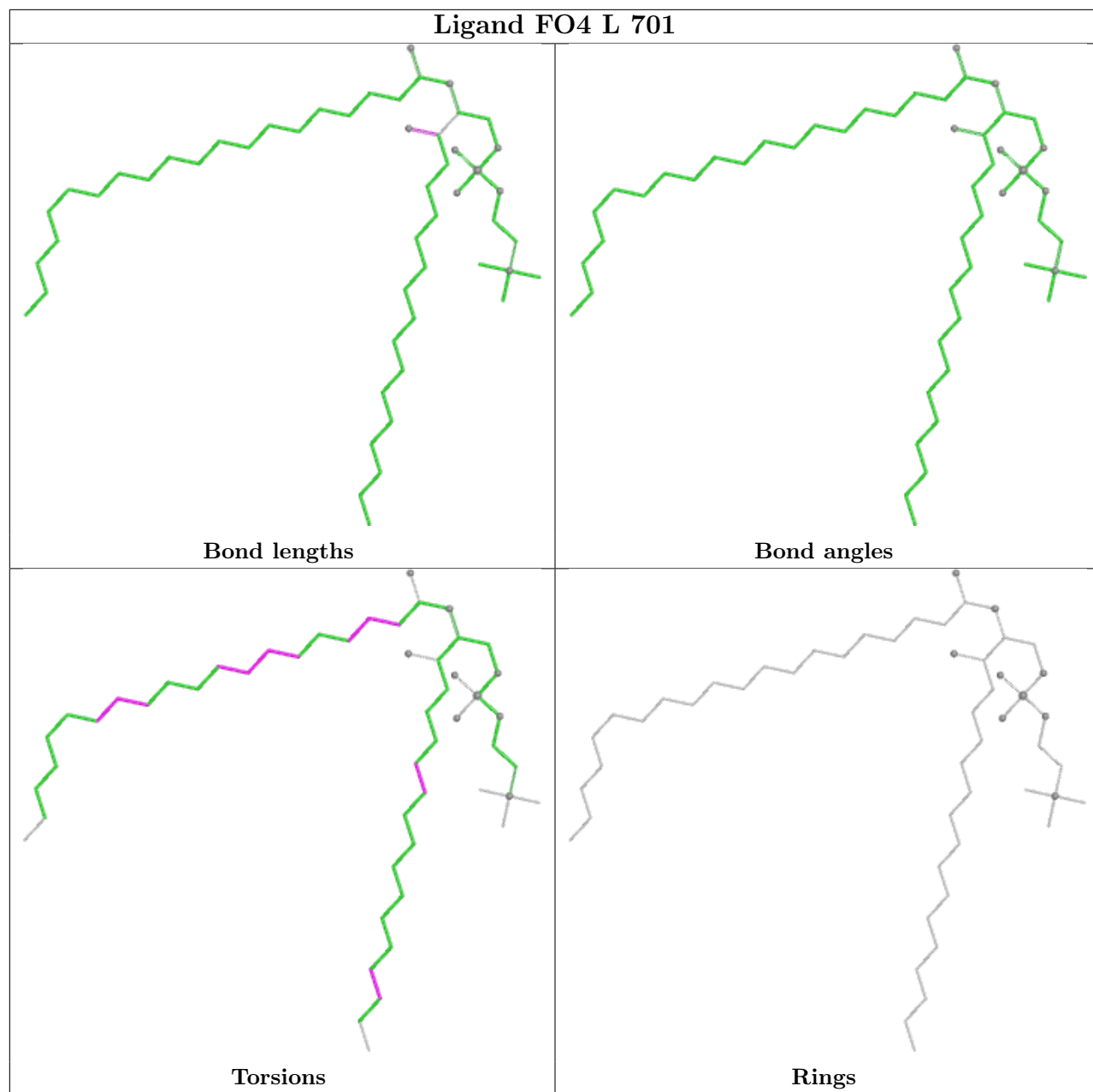


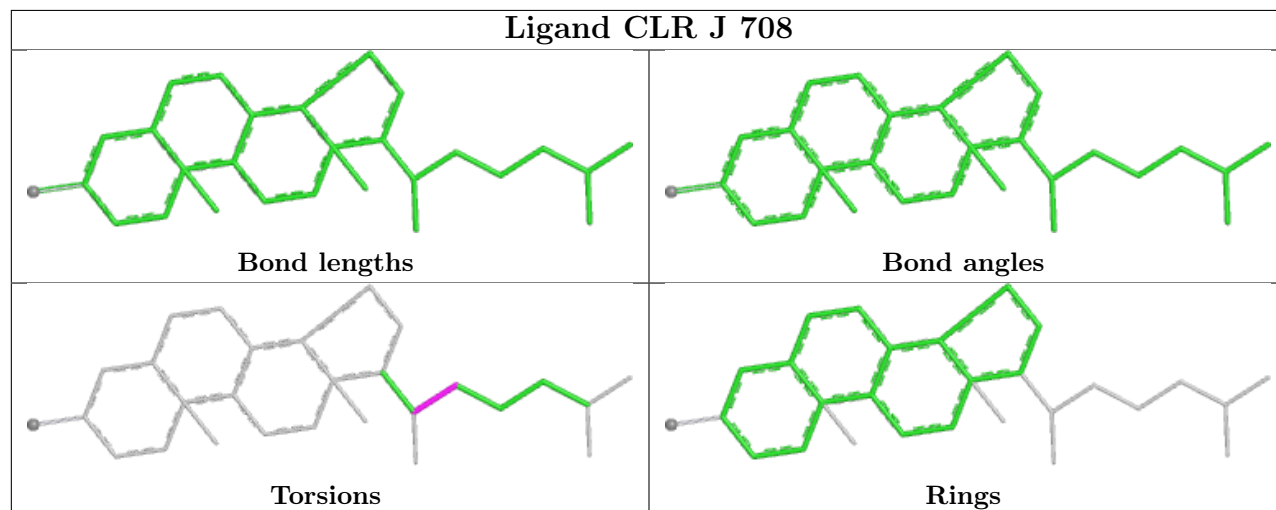
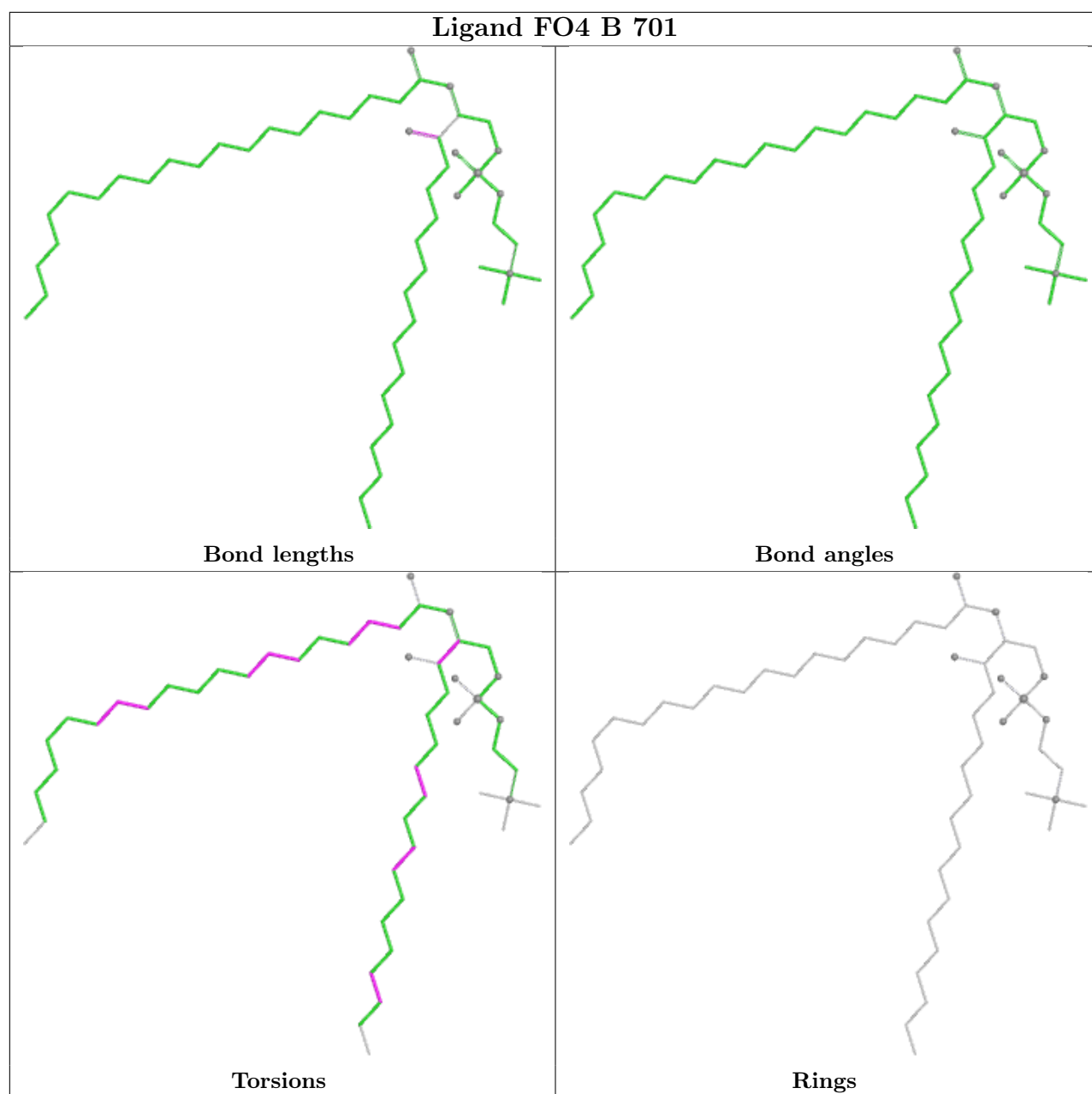




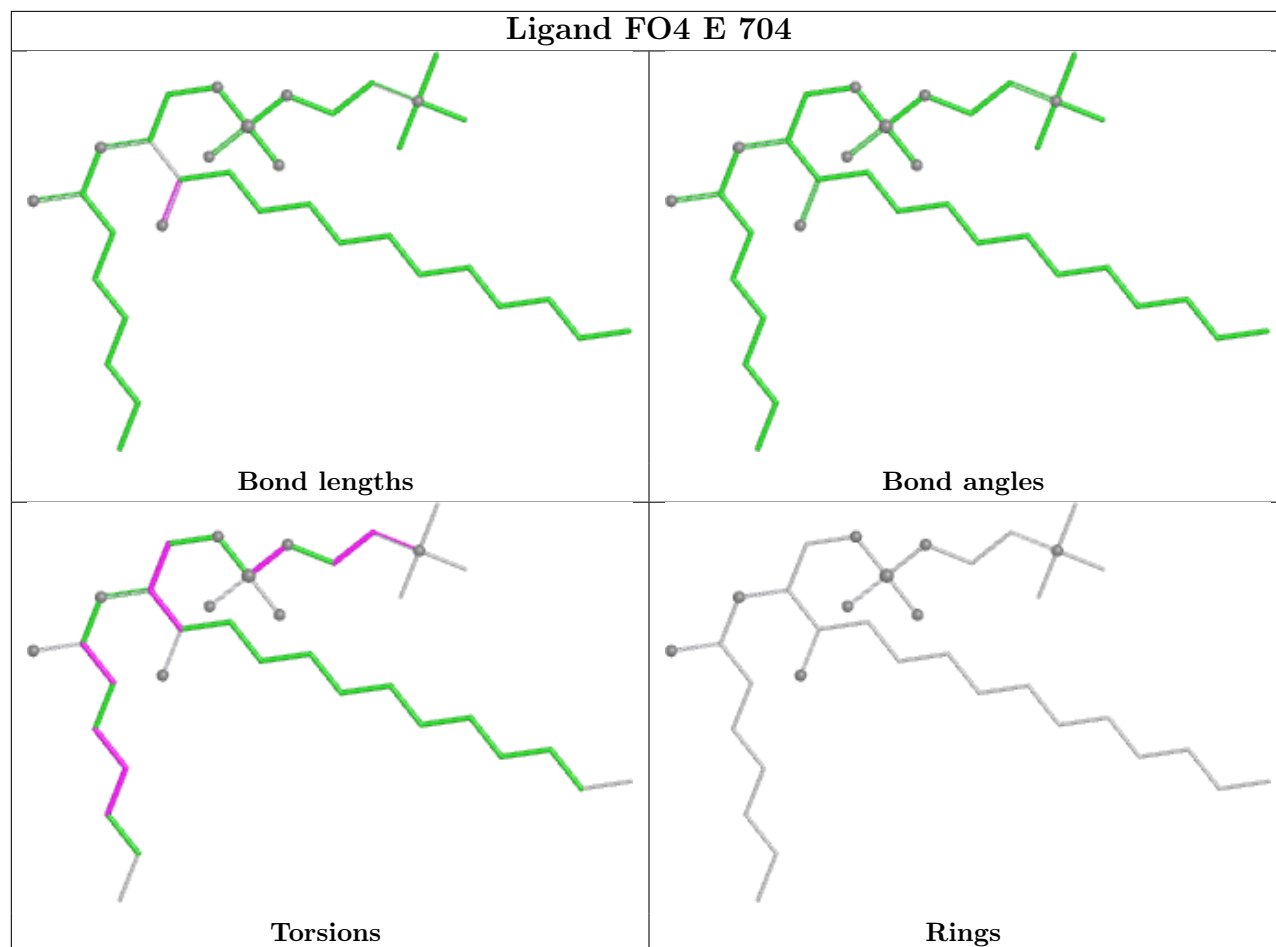




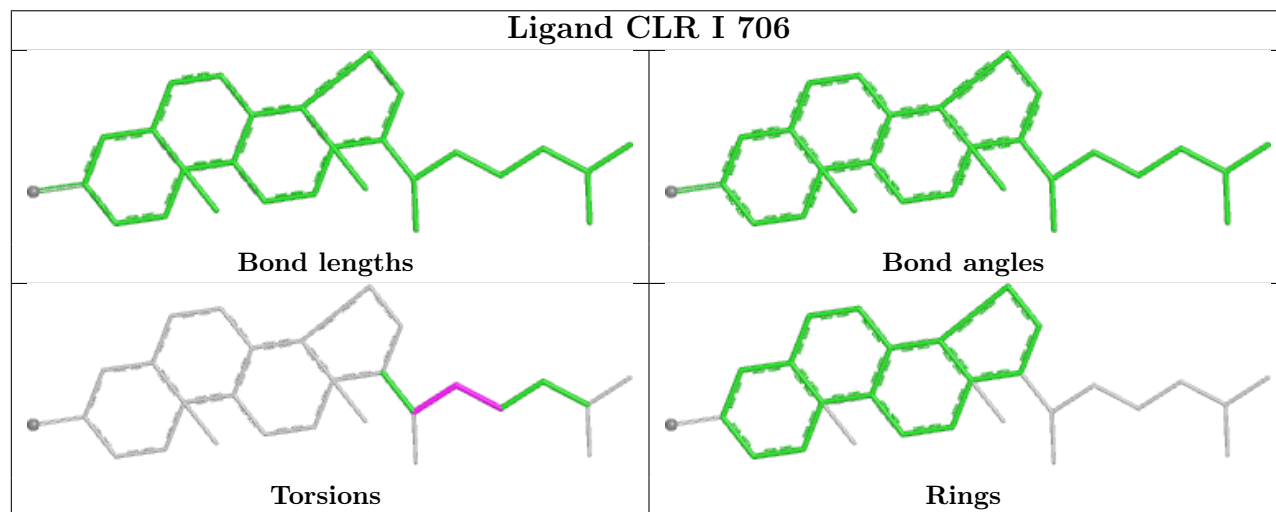


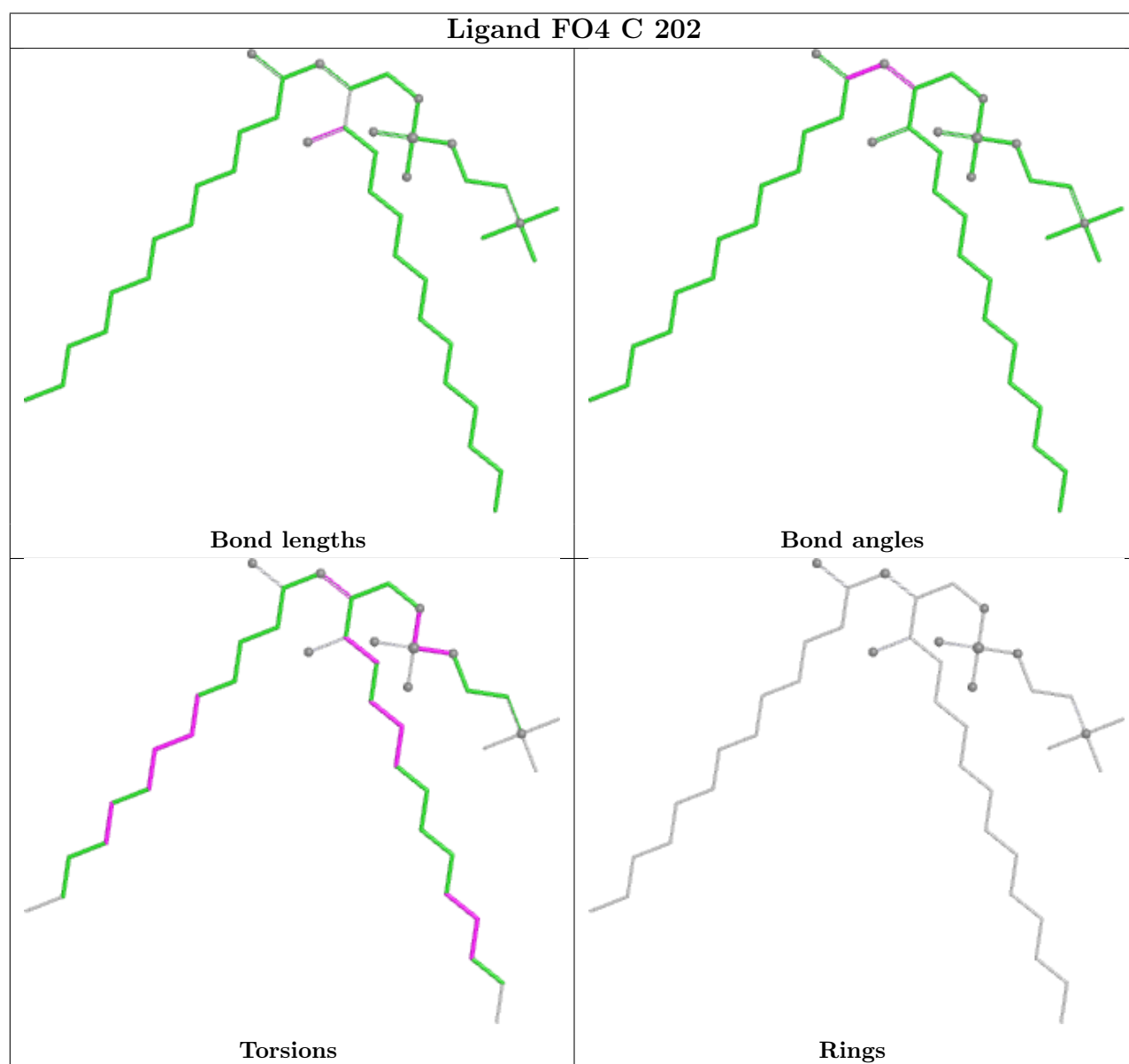
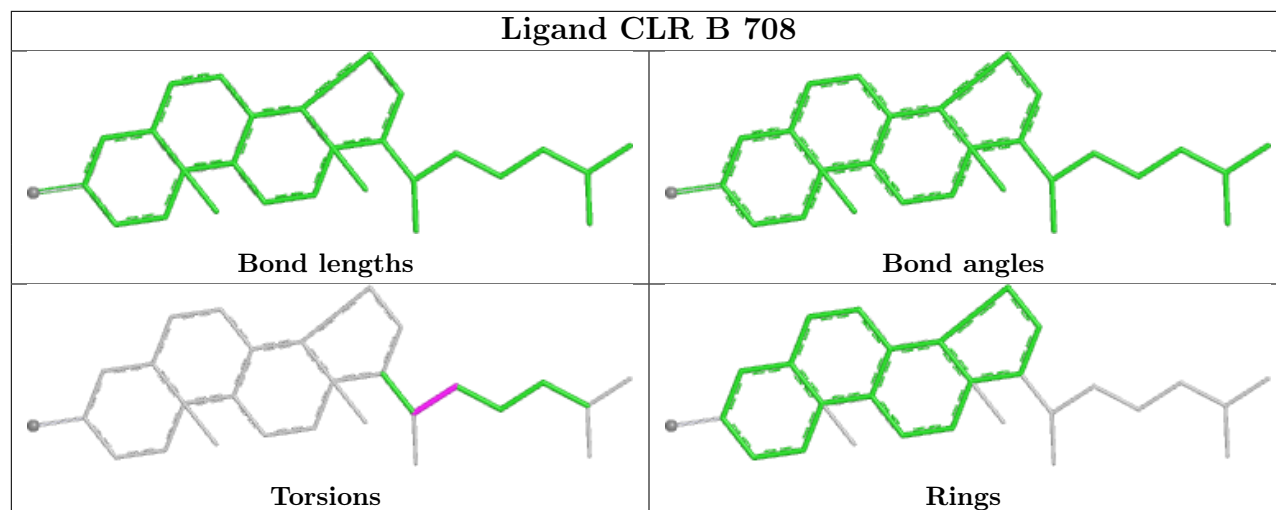


Ligand FO4 E 704

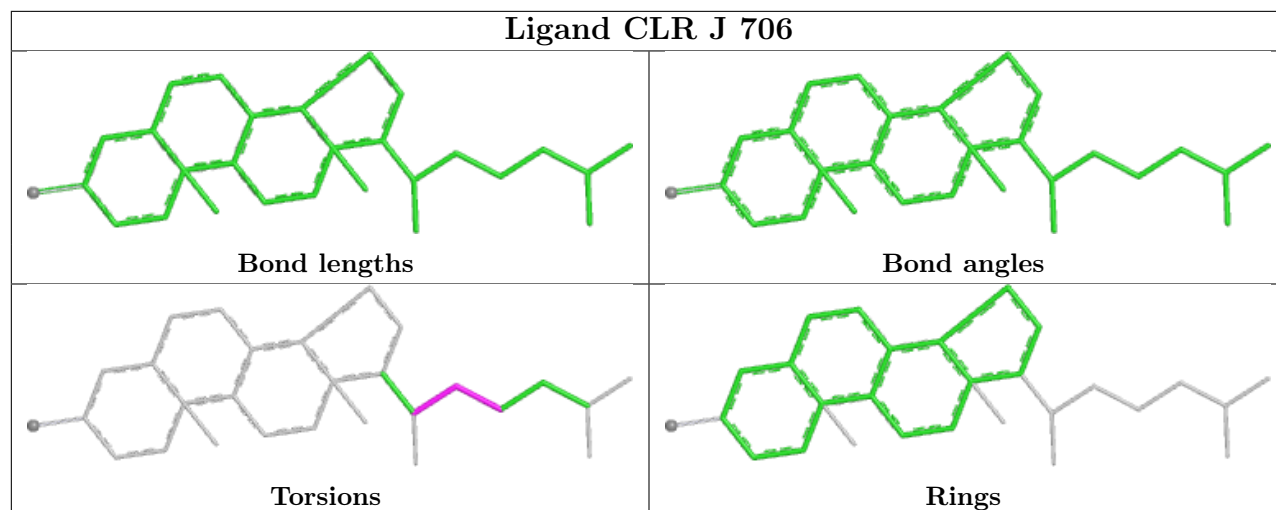


Ligand CLR I 706

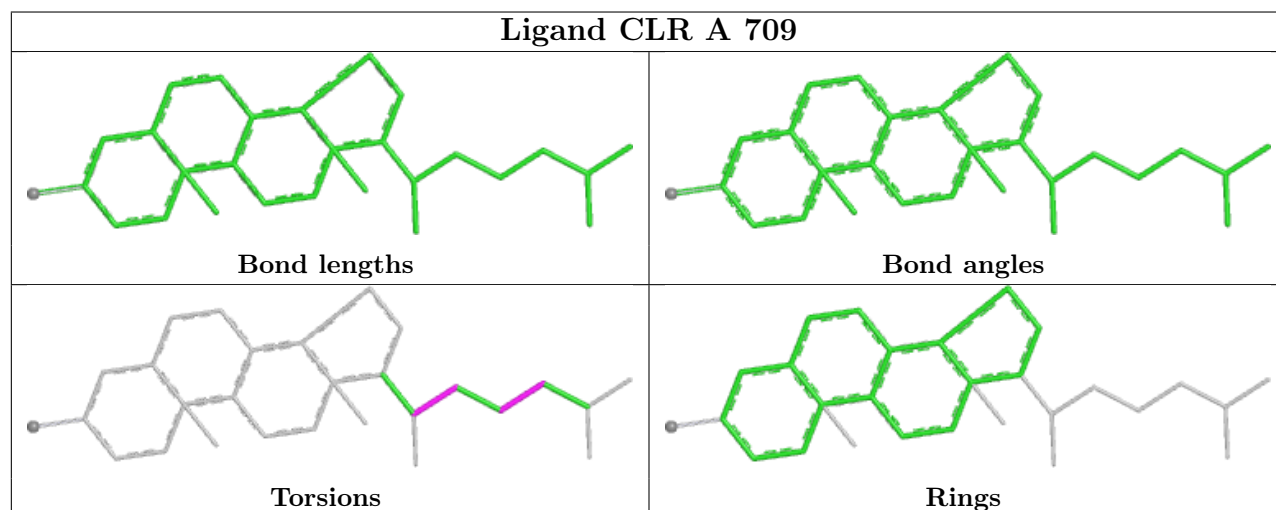


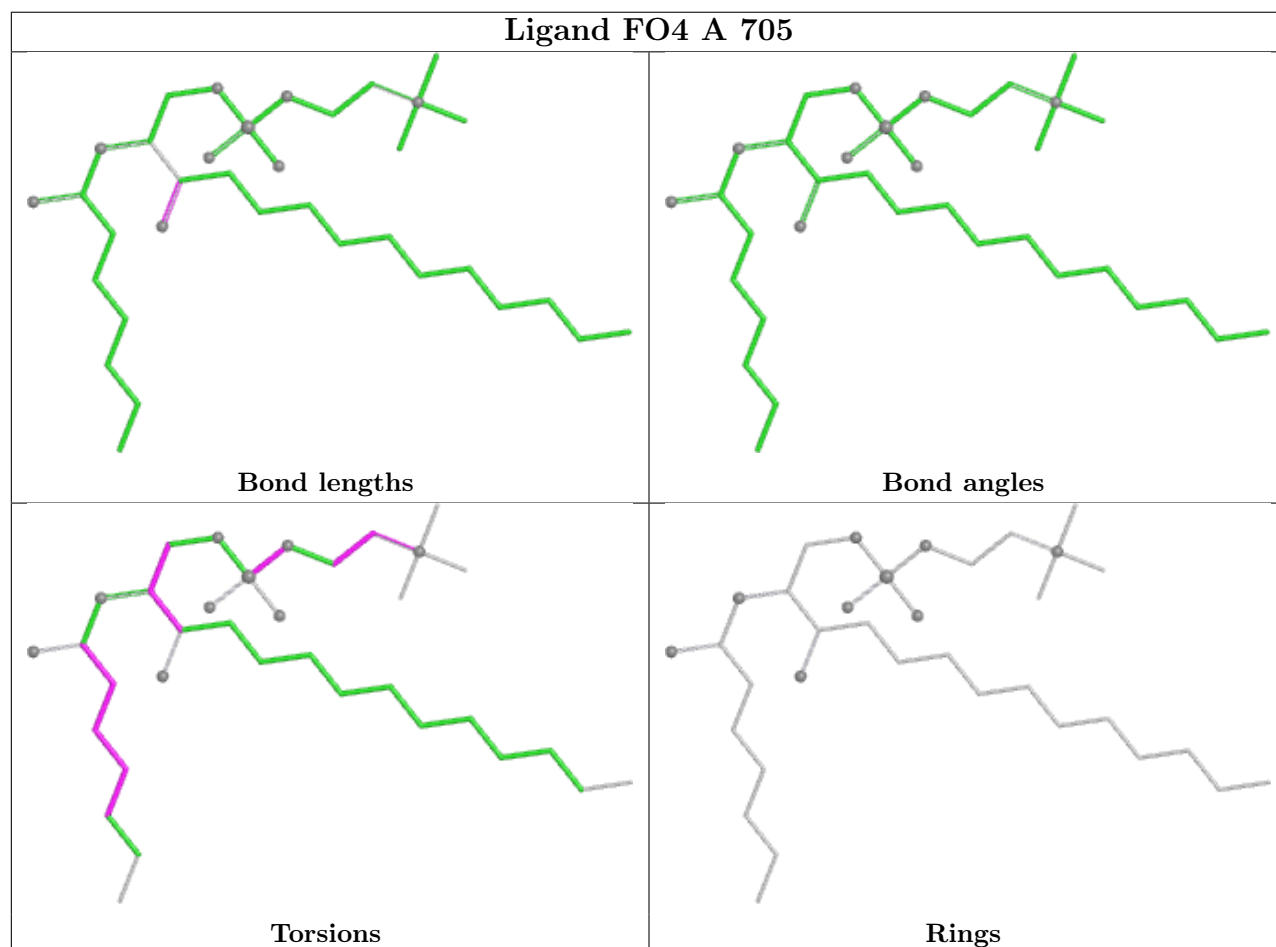
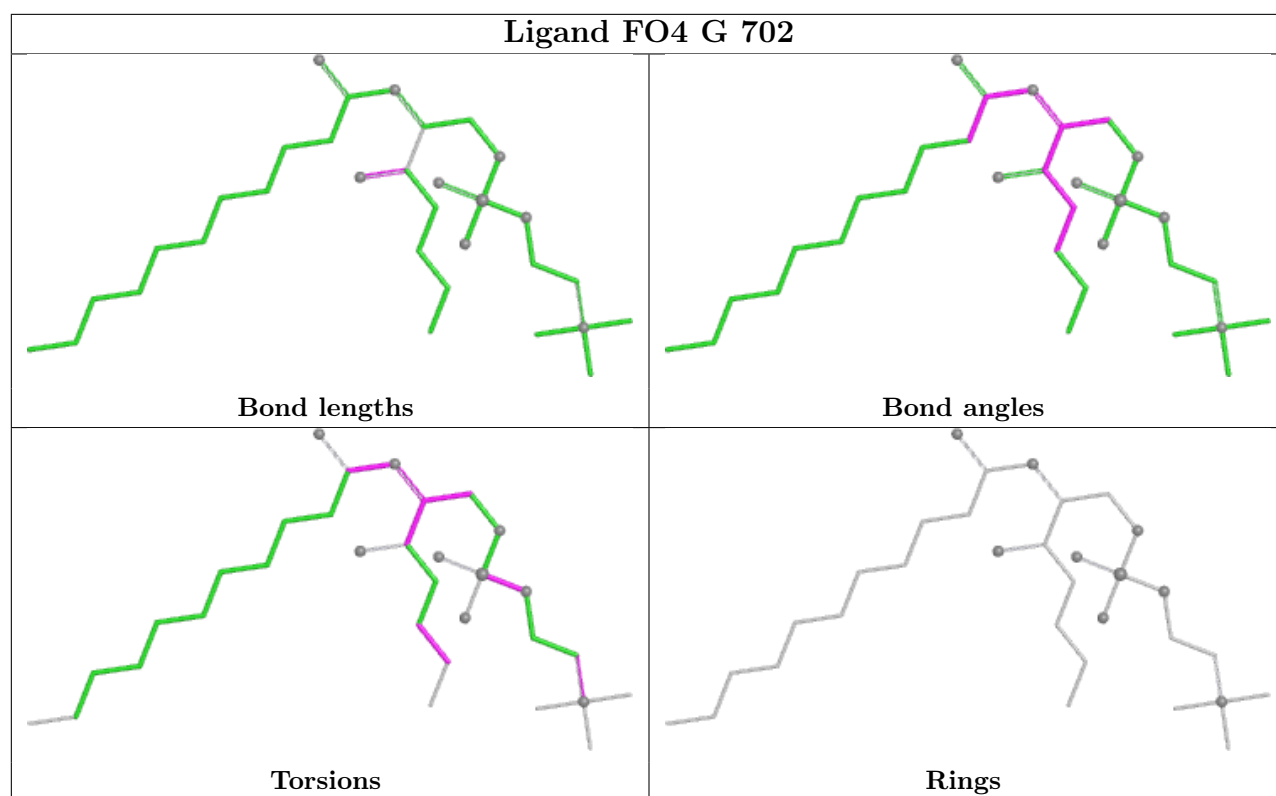


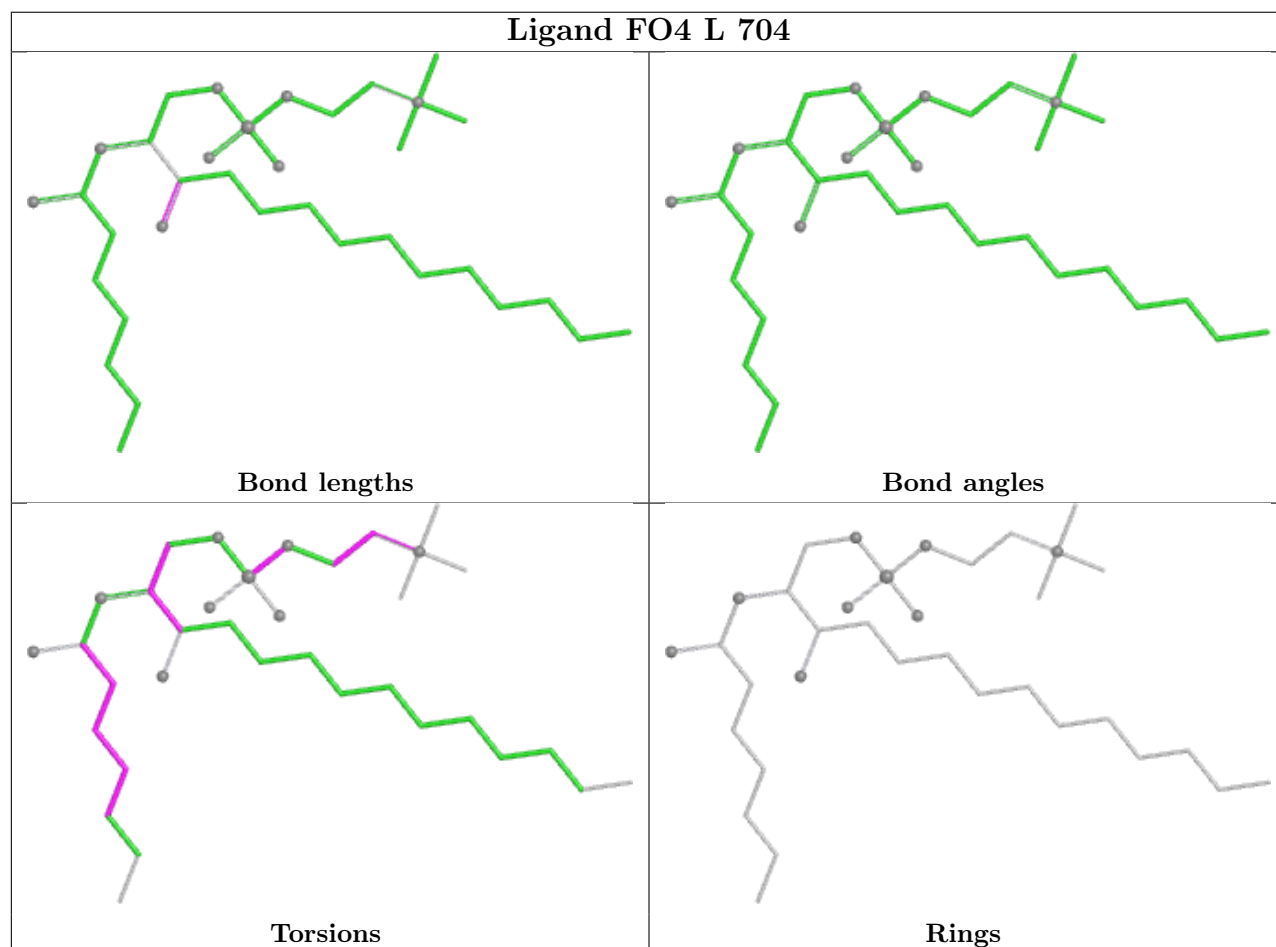
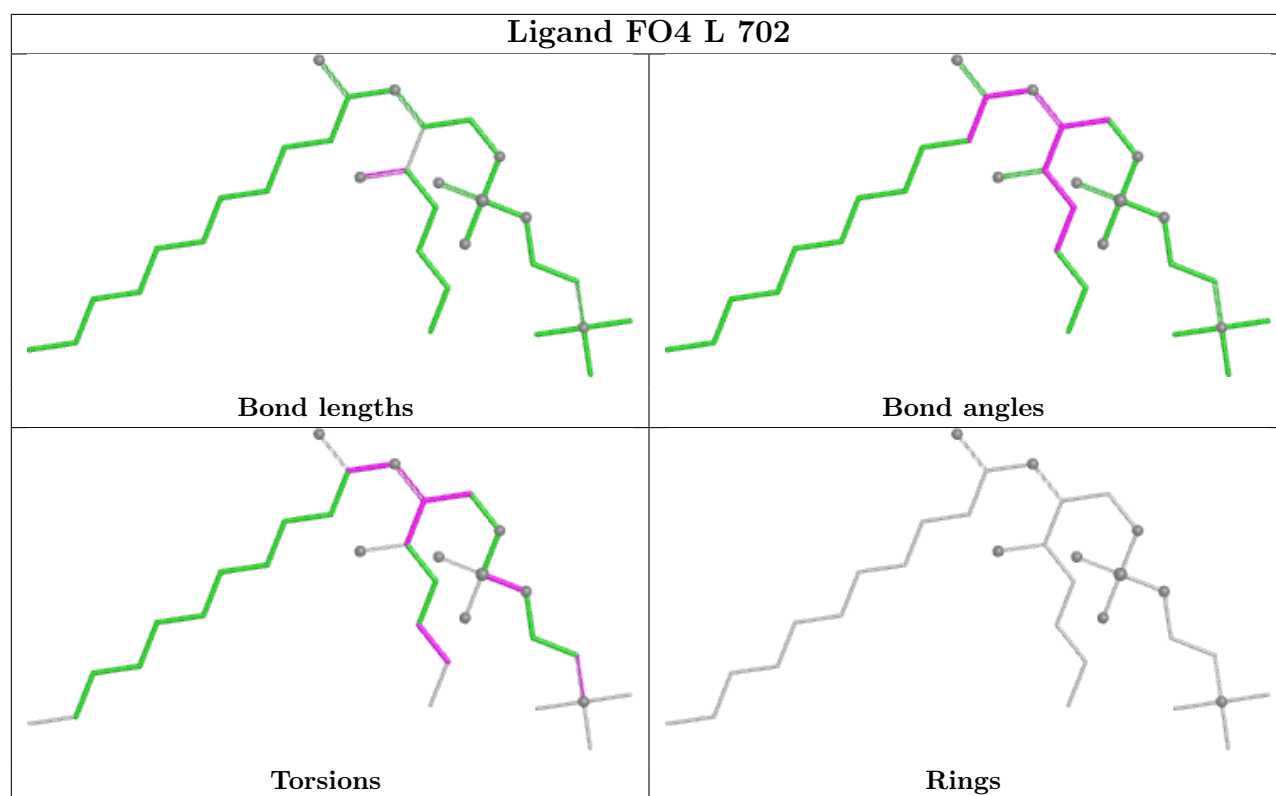
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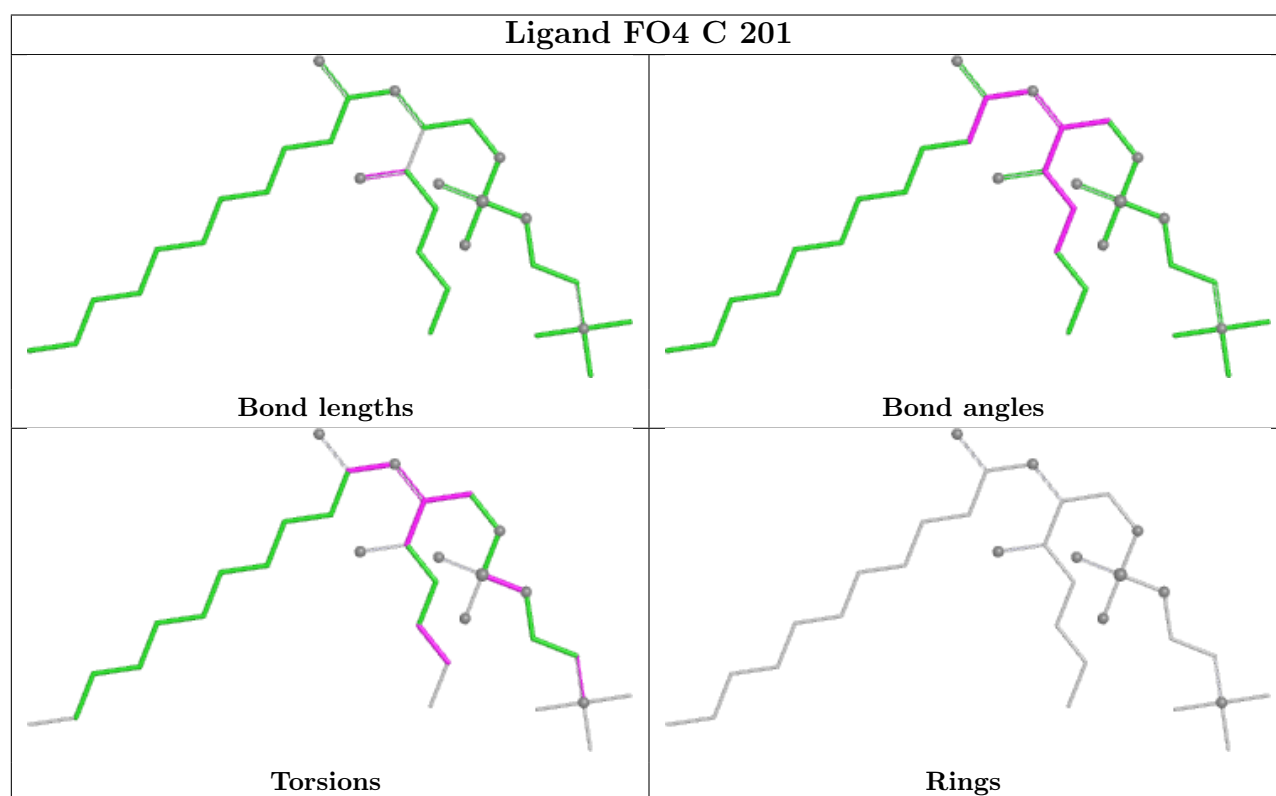
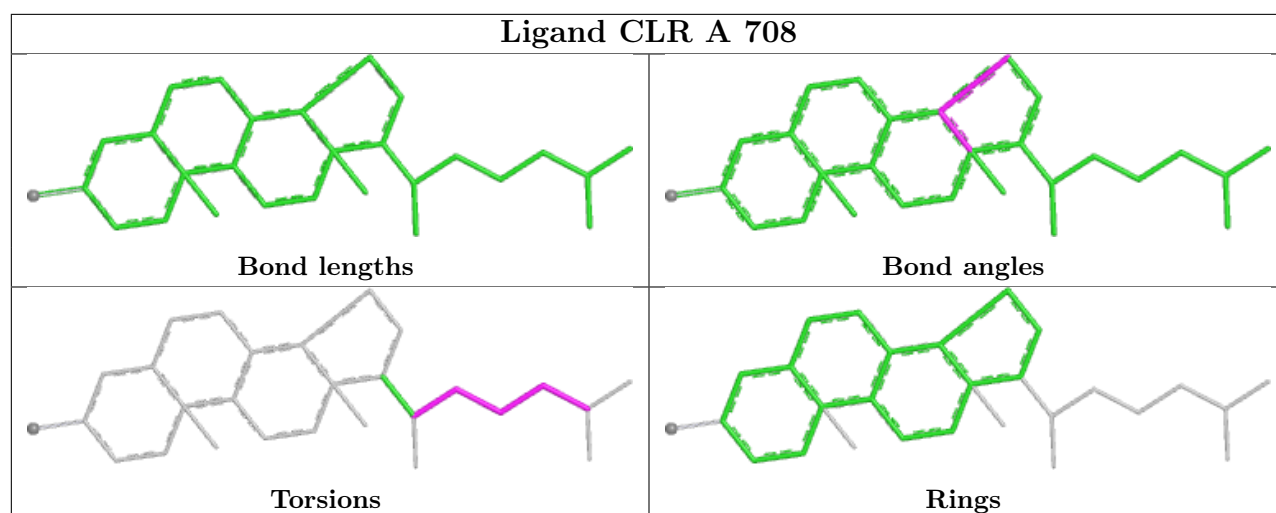


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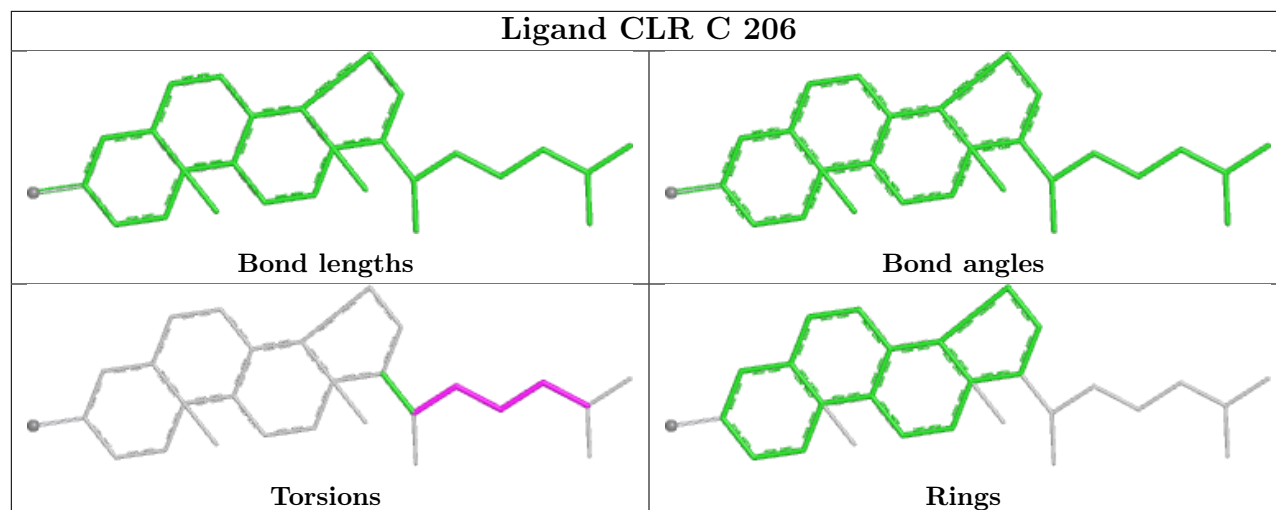




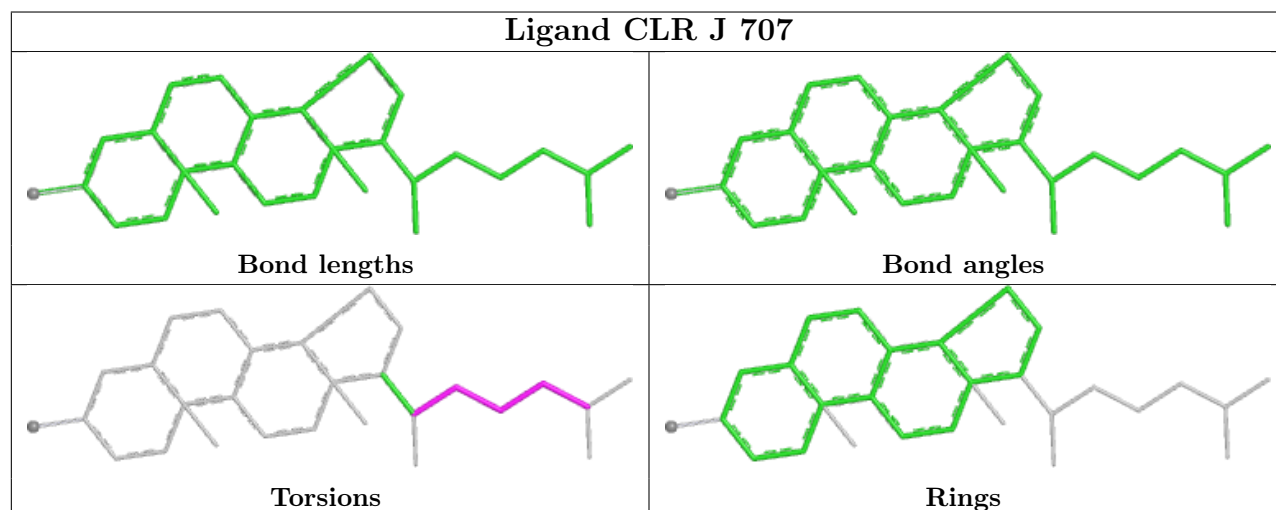


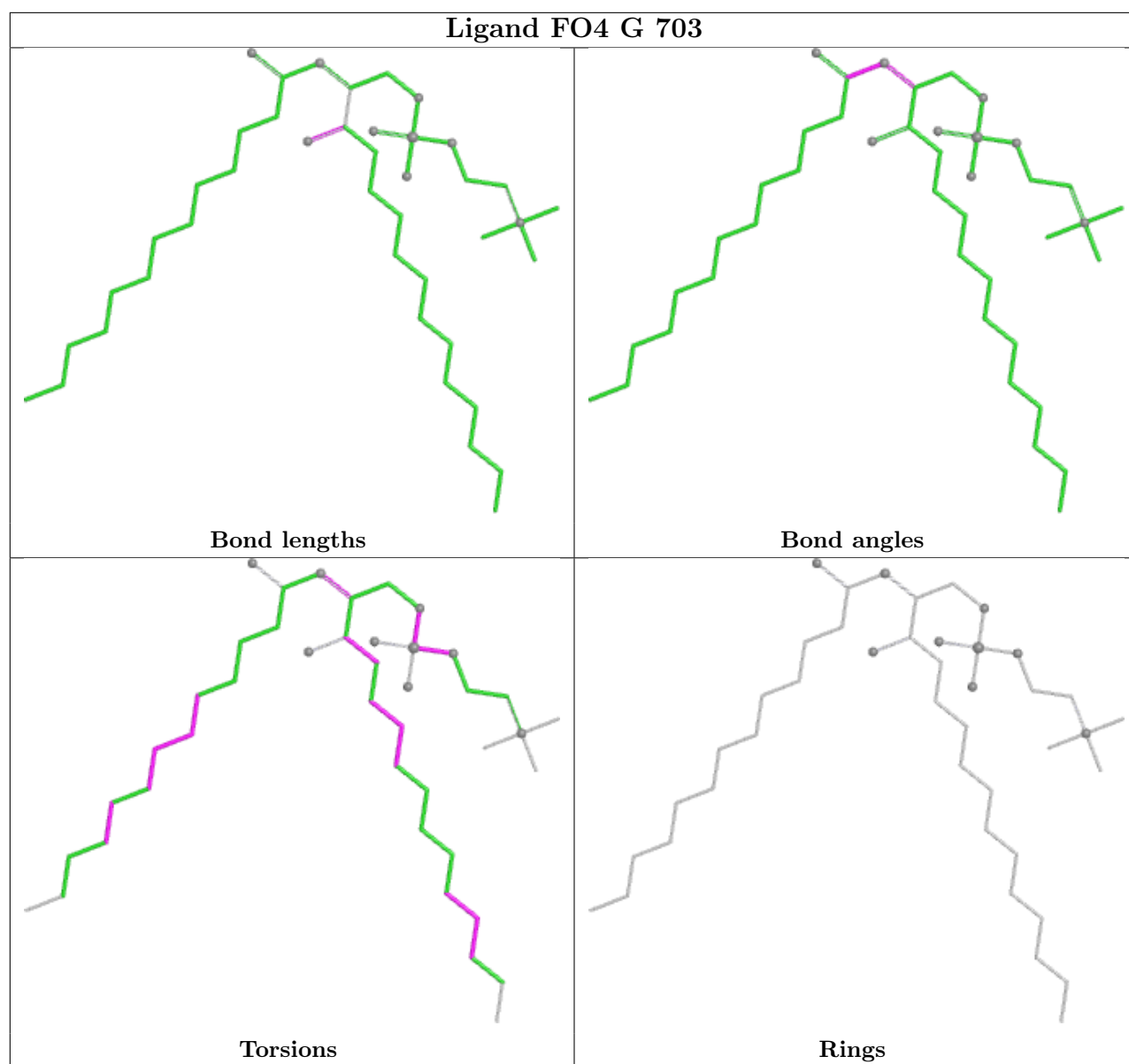


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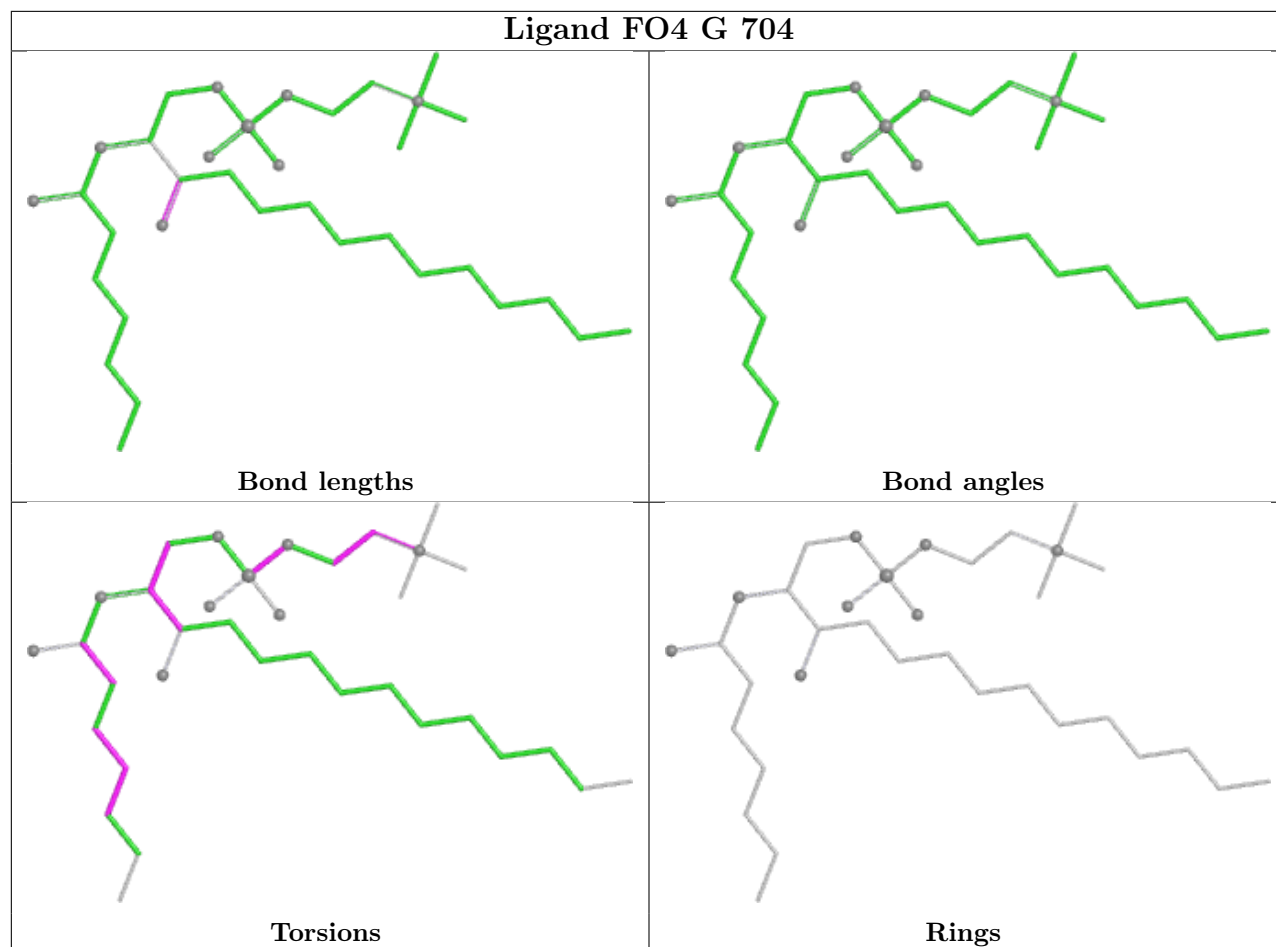


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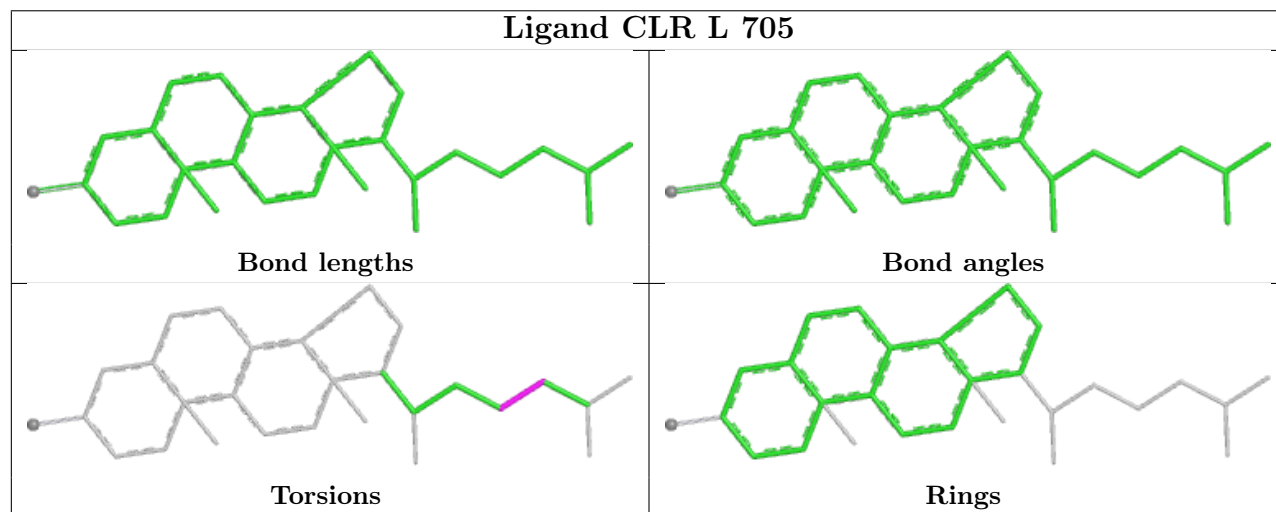


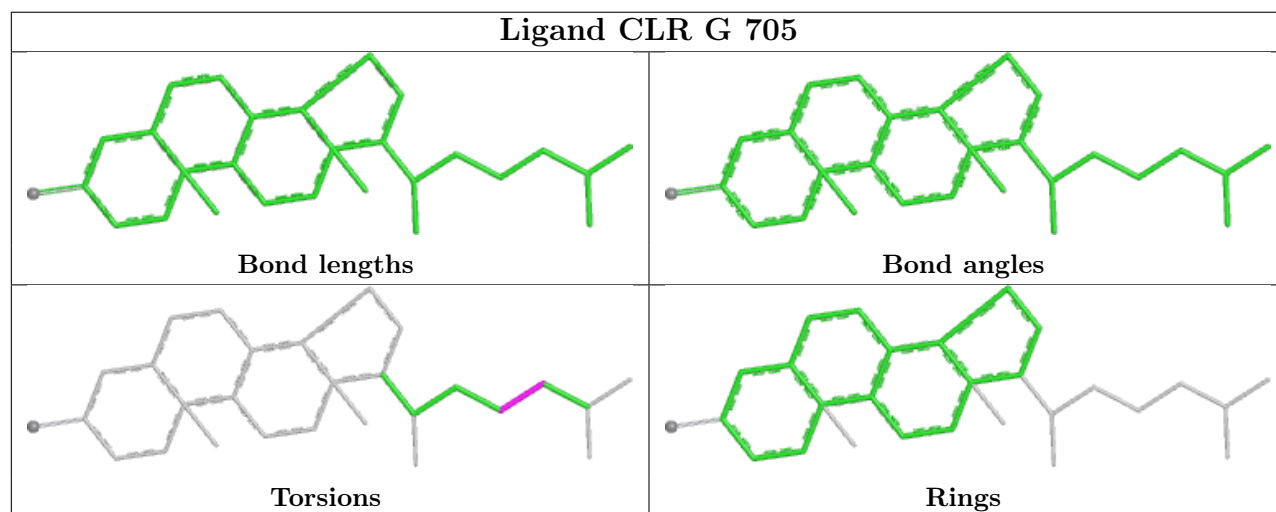
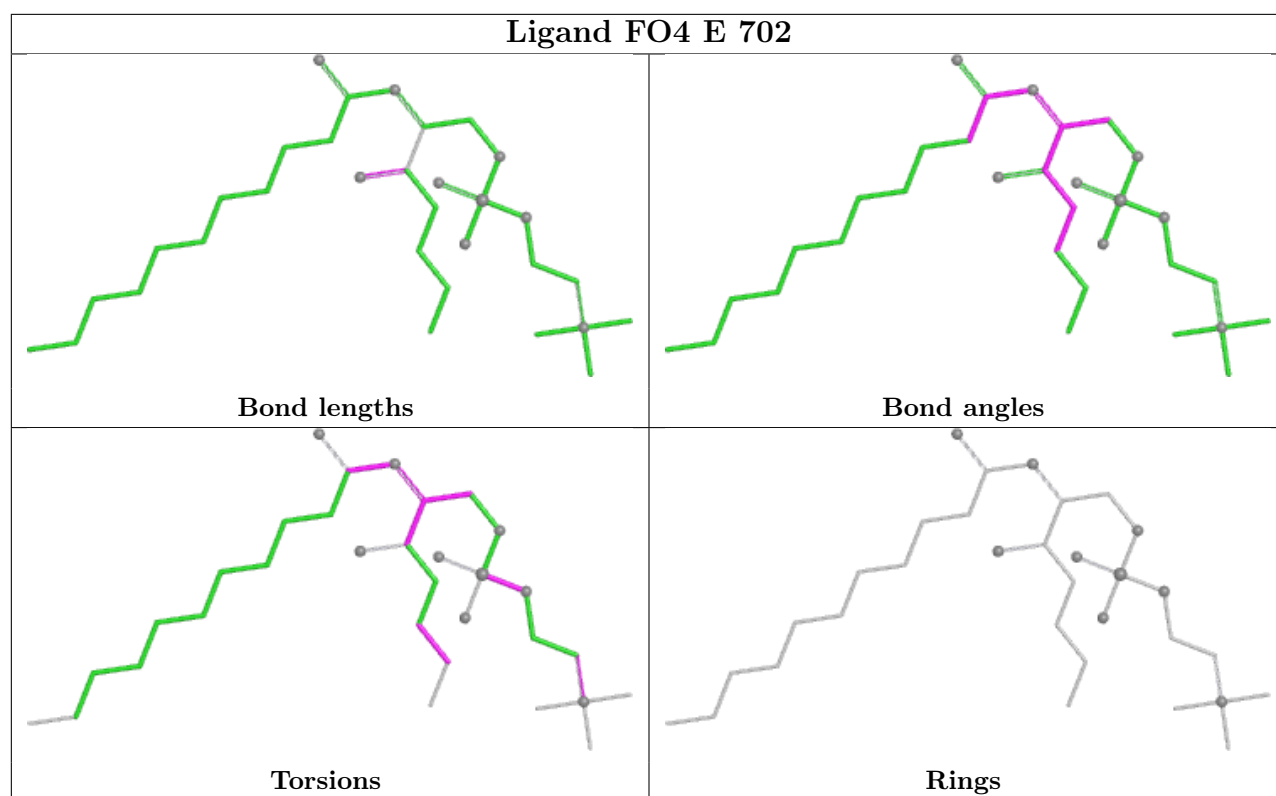


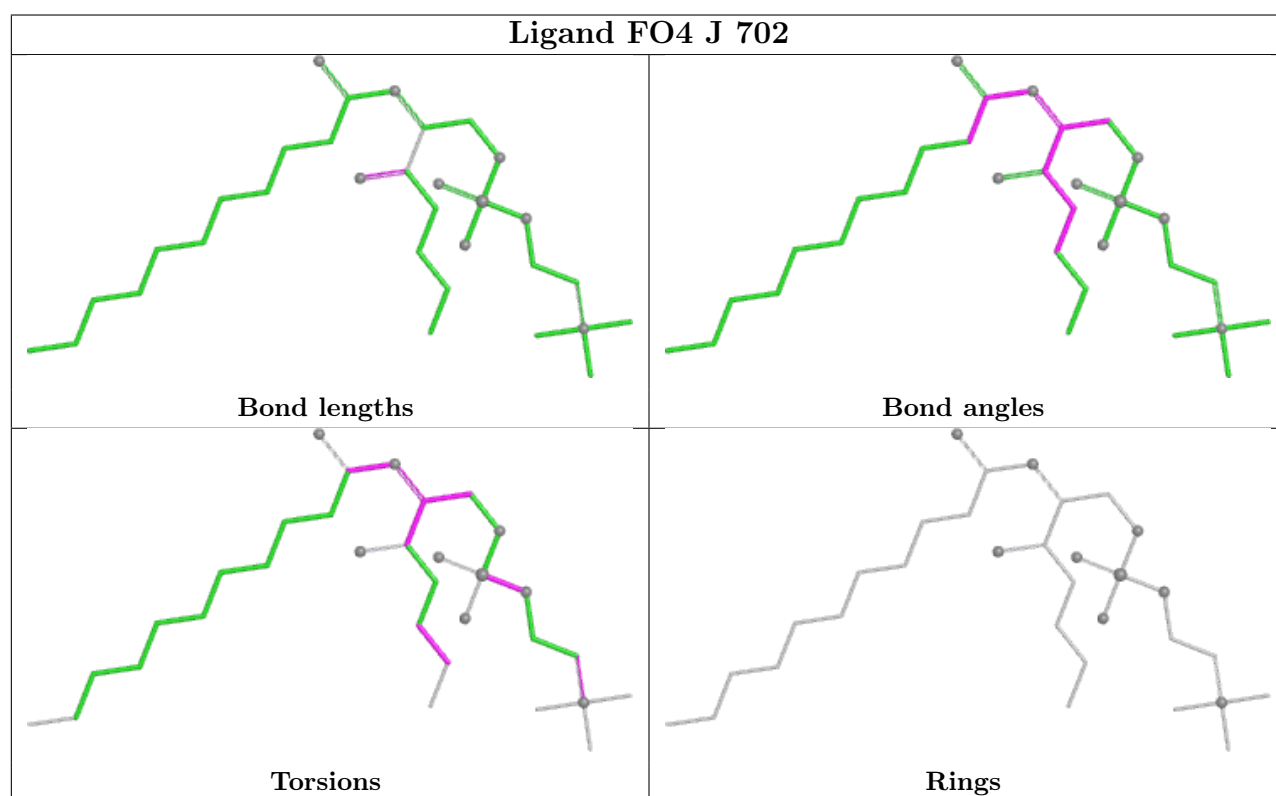
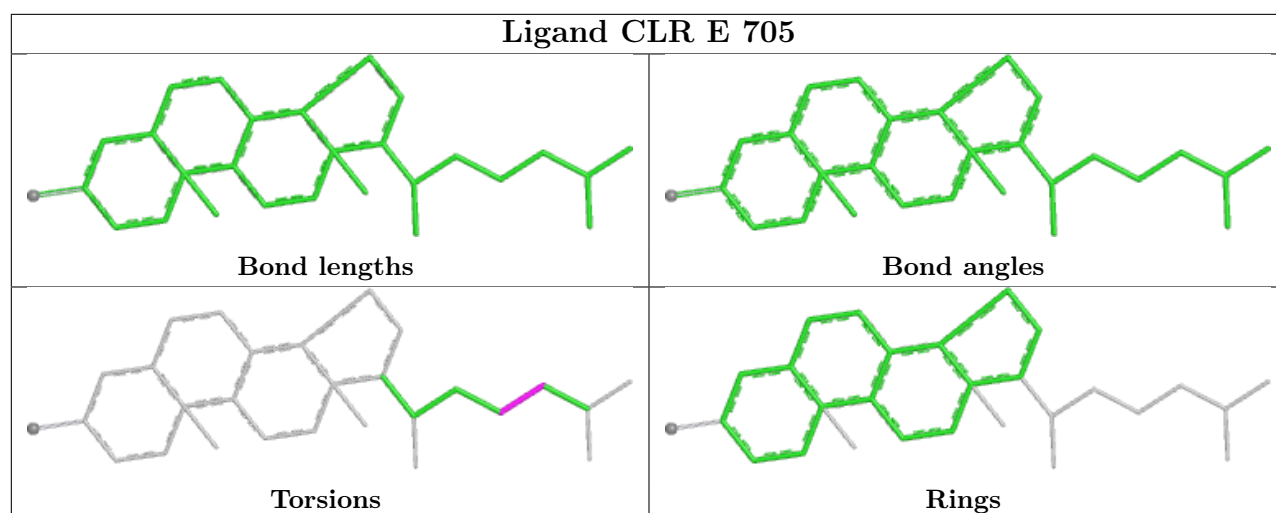
Ligand FO4 G 704

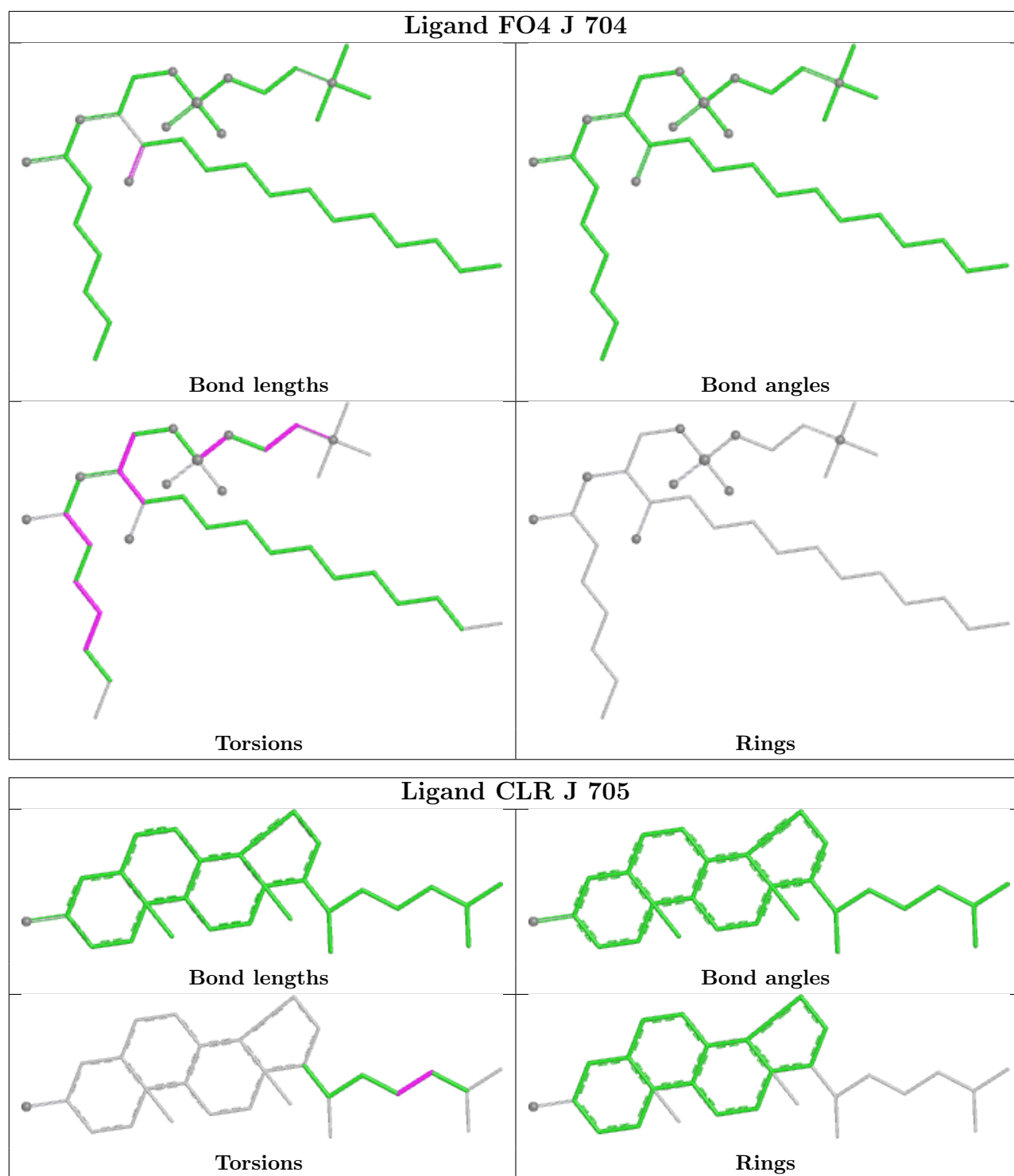


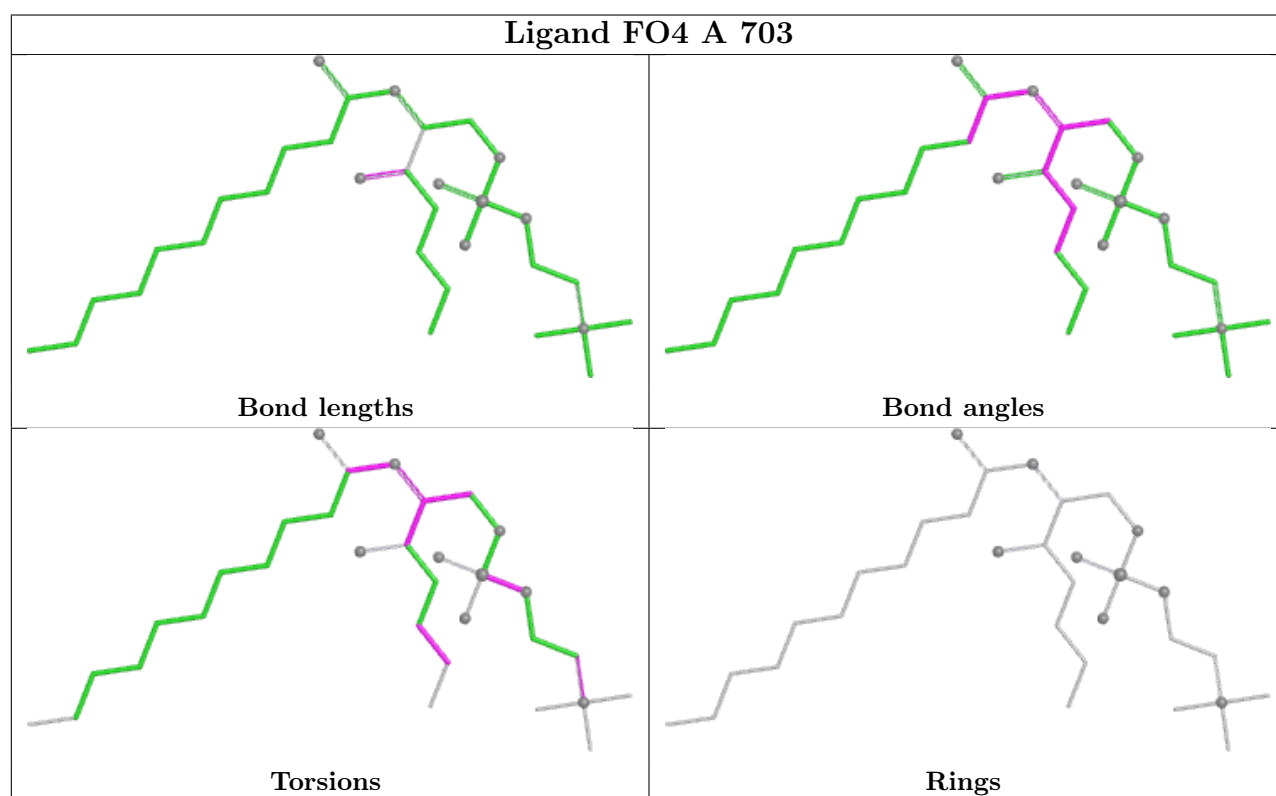
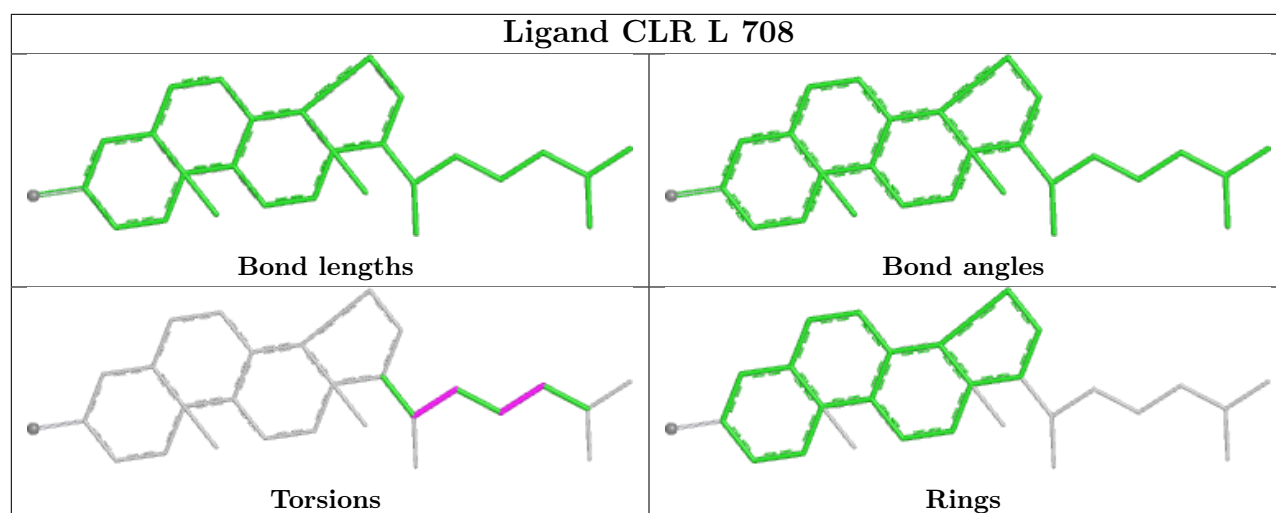
Ligand CLR L 705

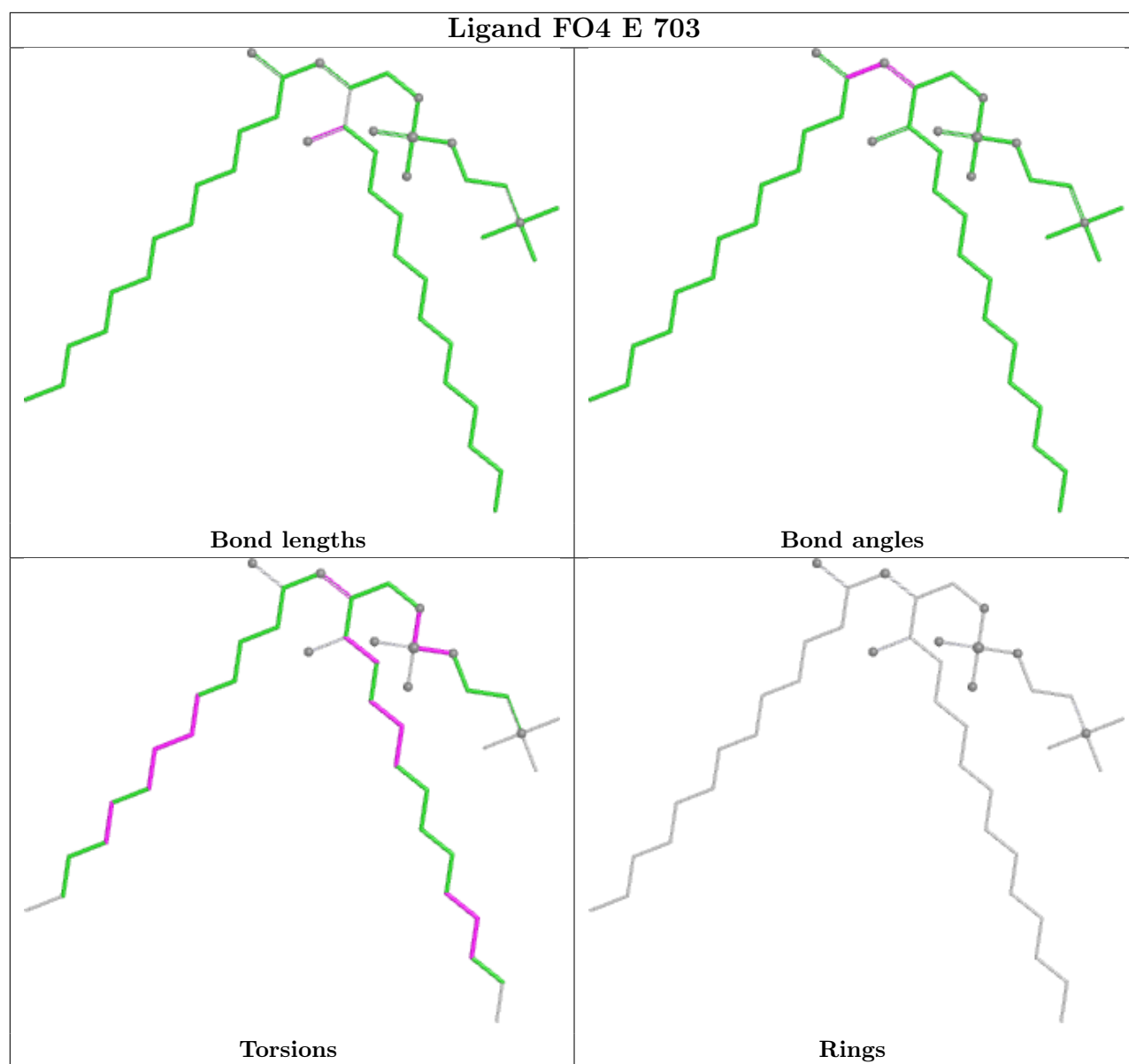


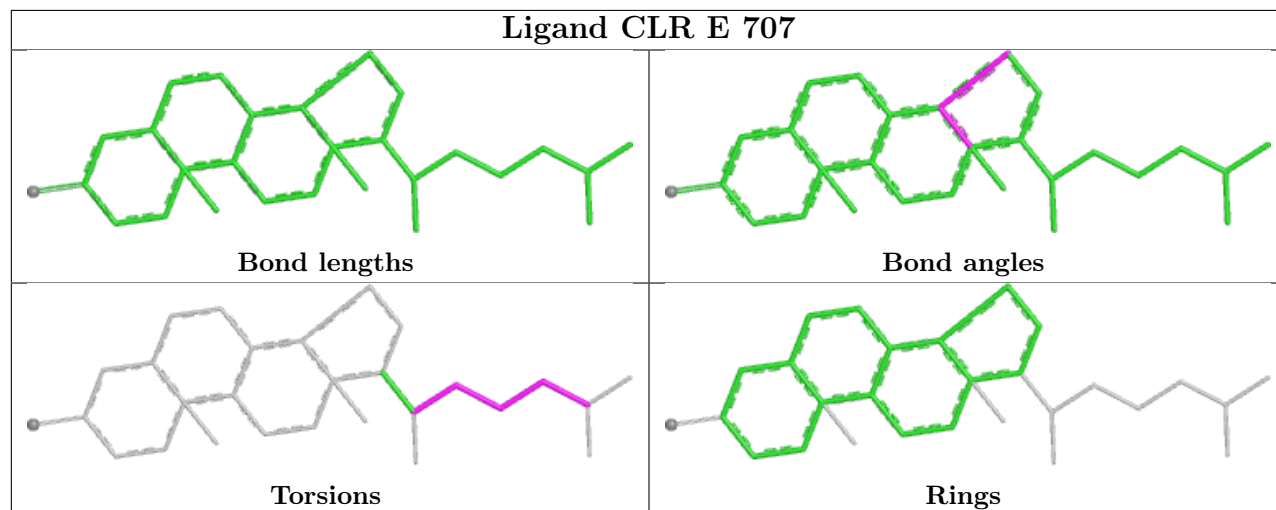
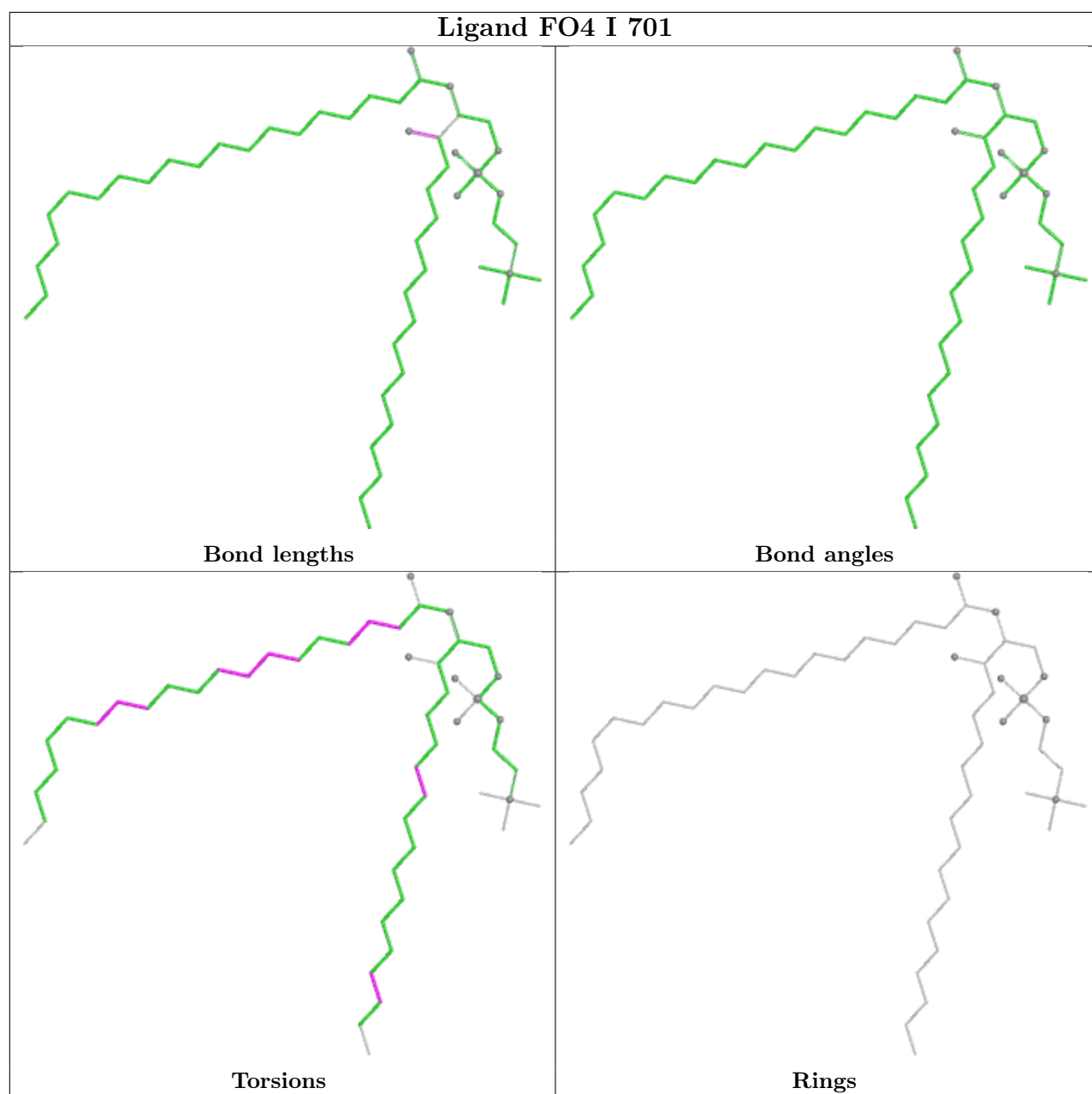


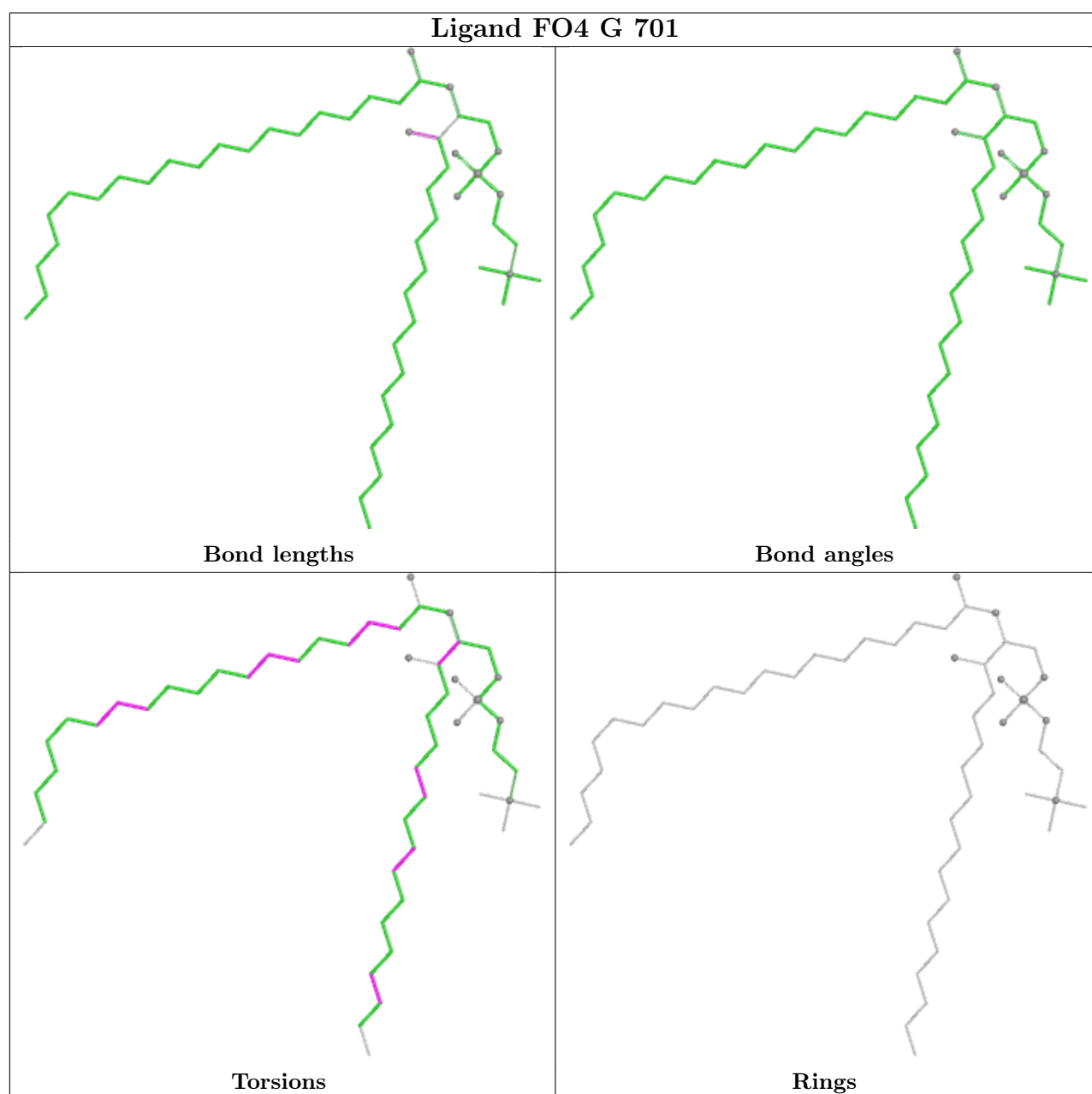
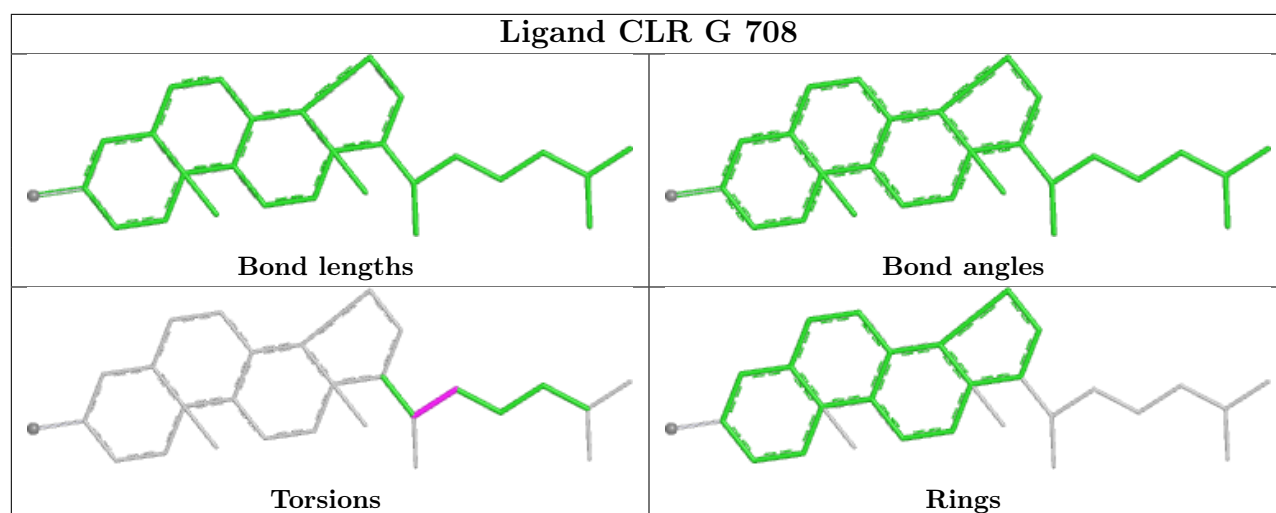


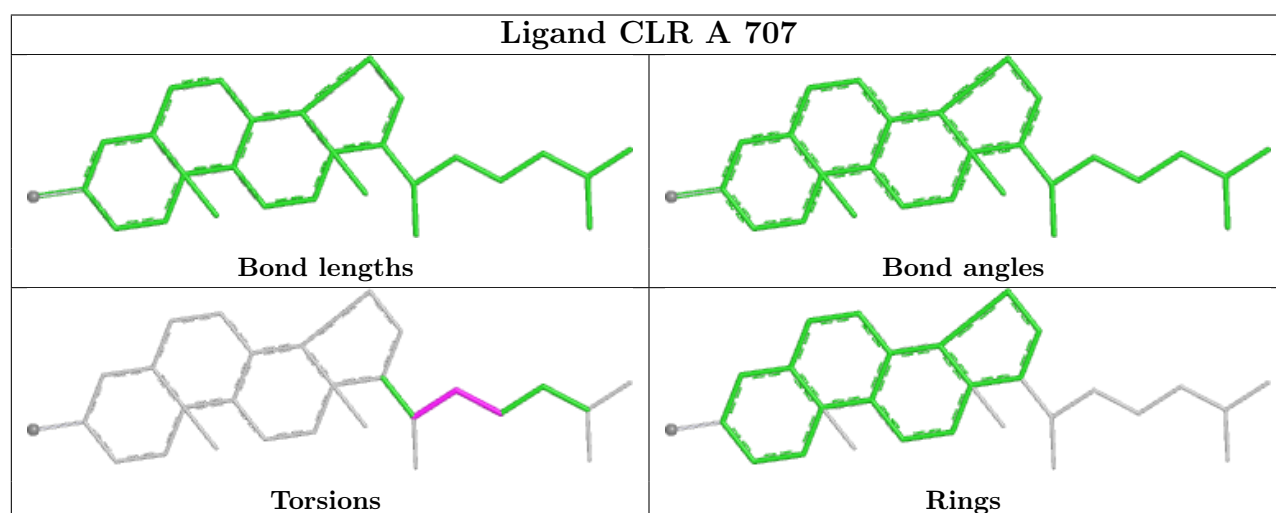
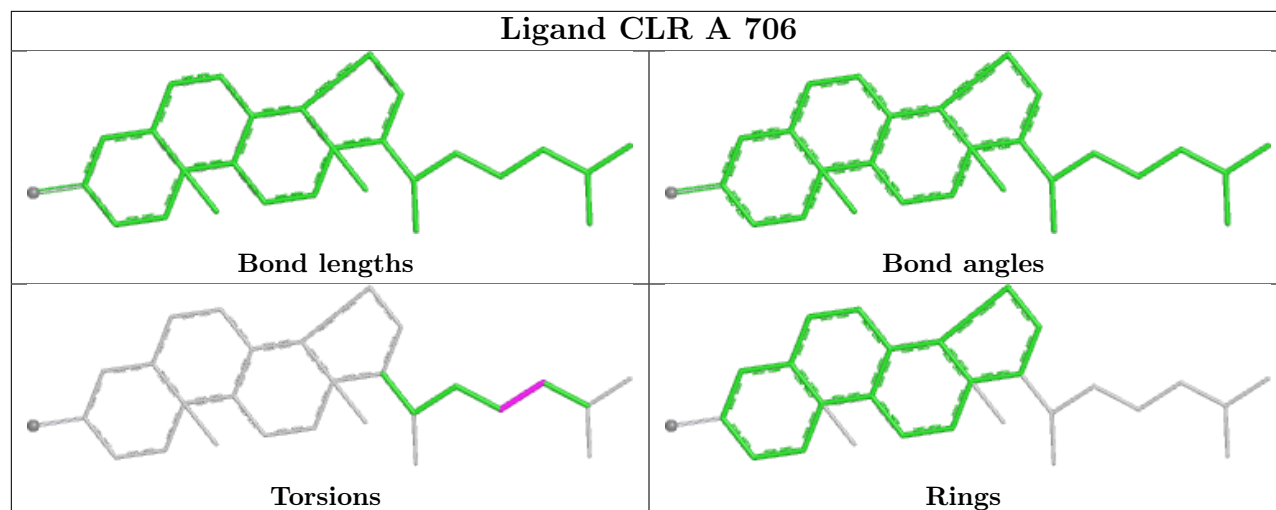


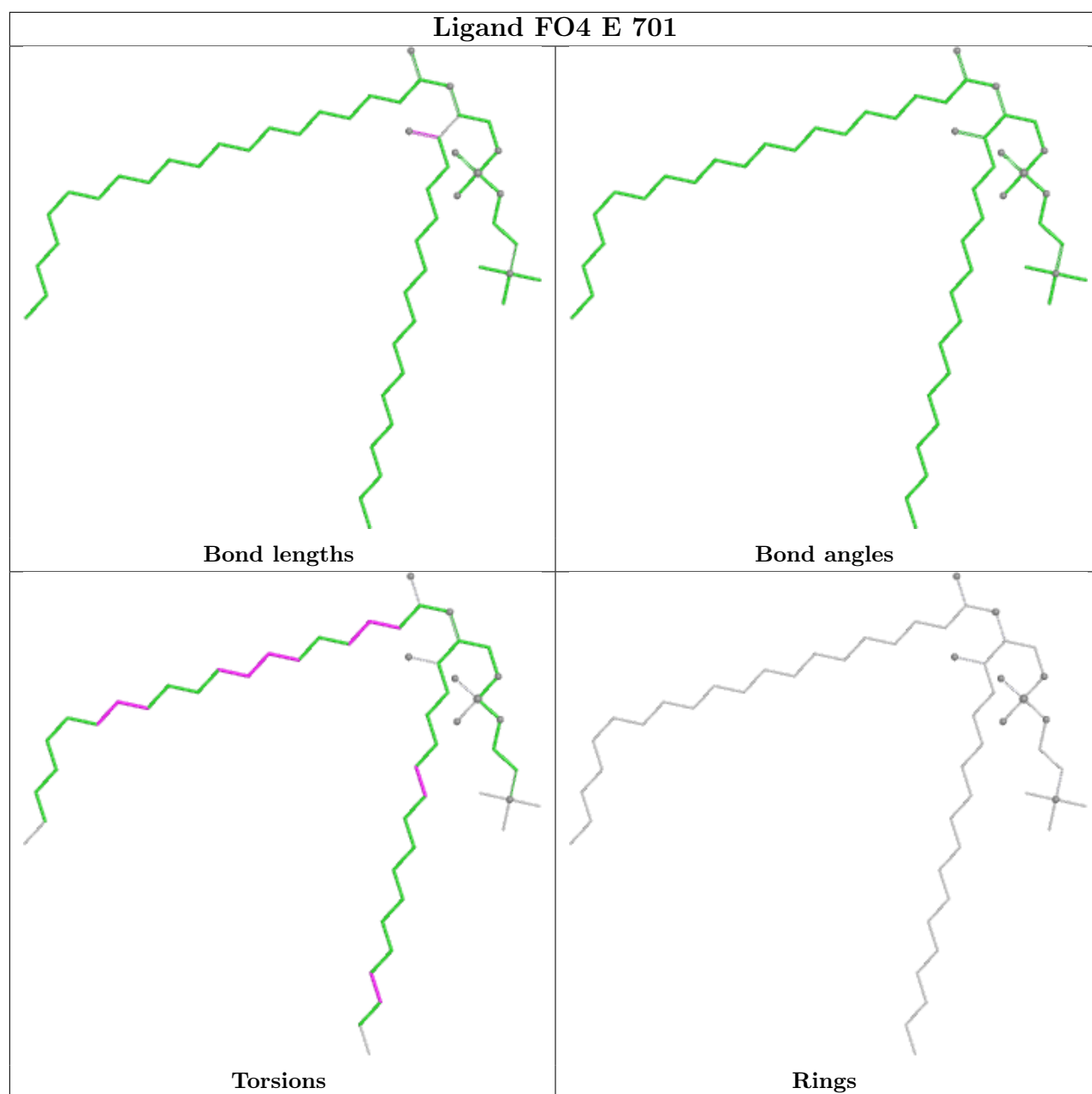


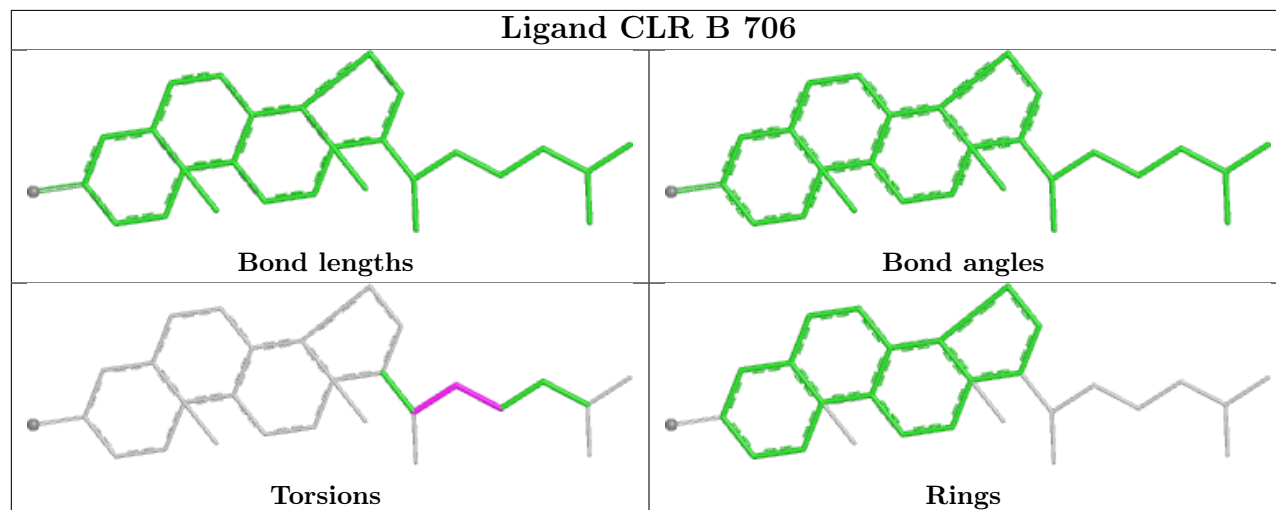
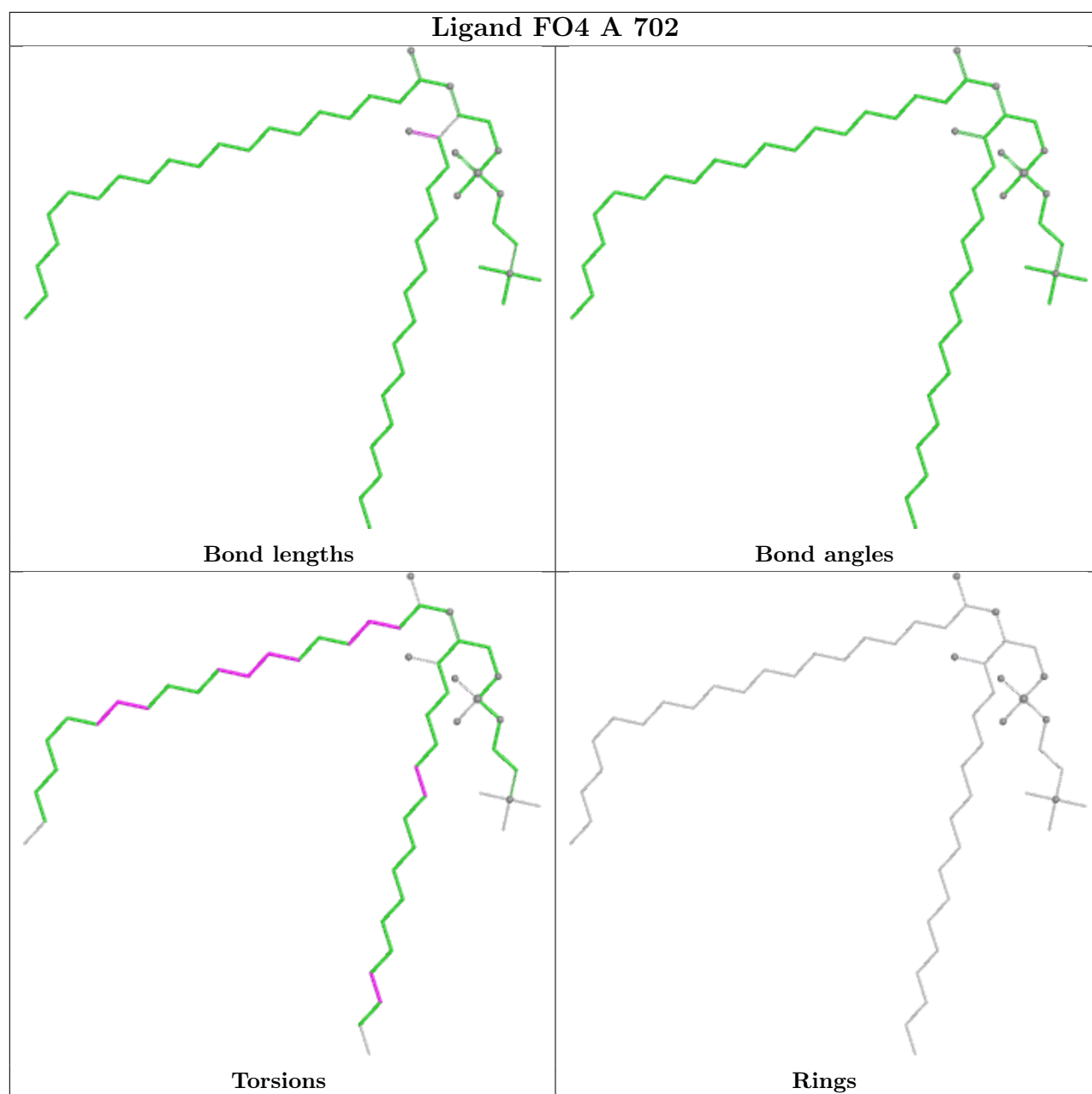


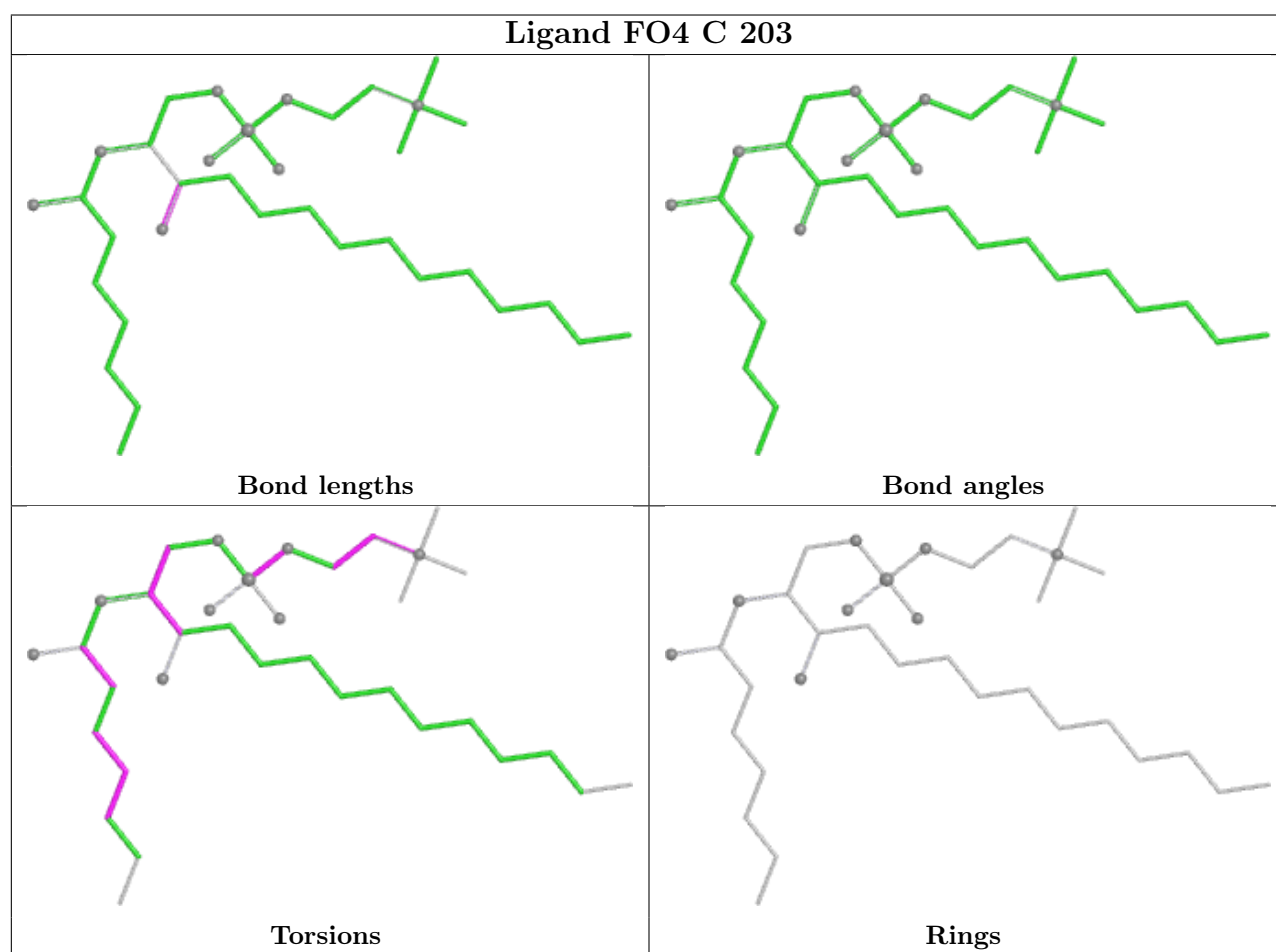
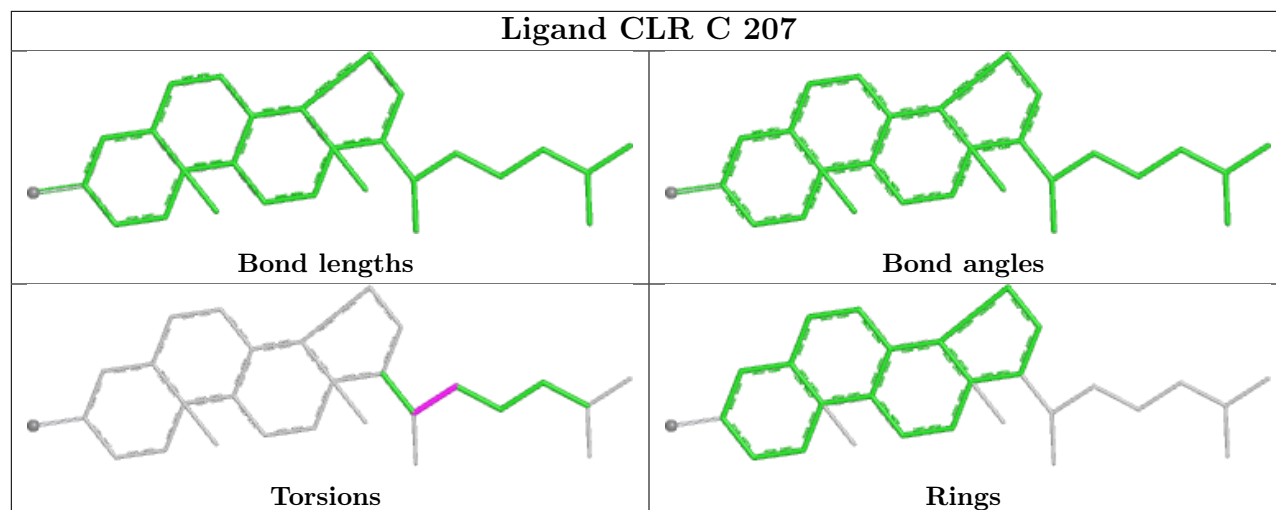


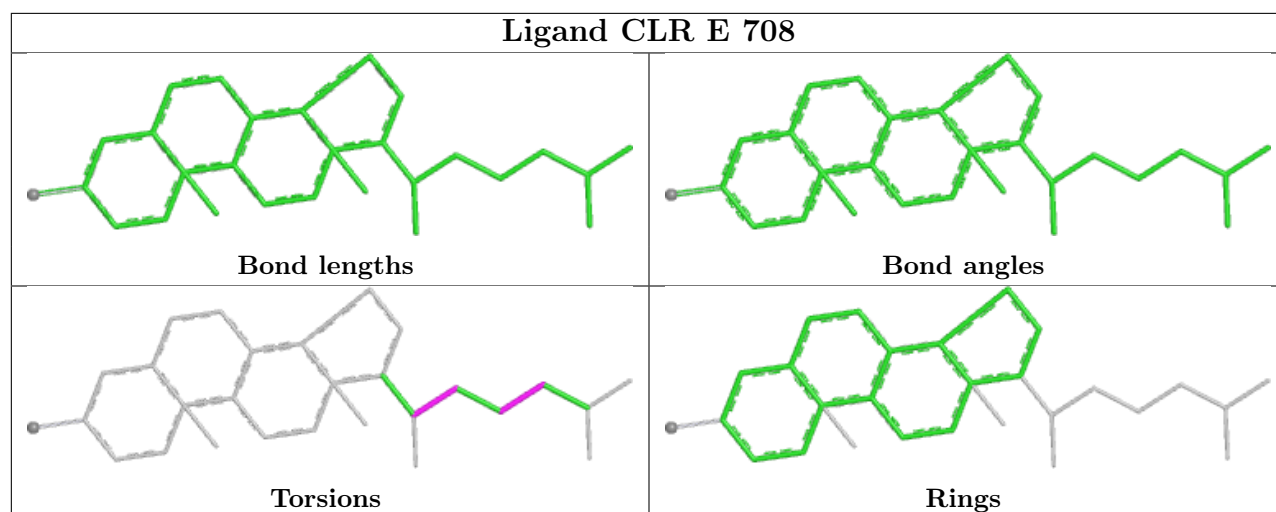
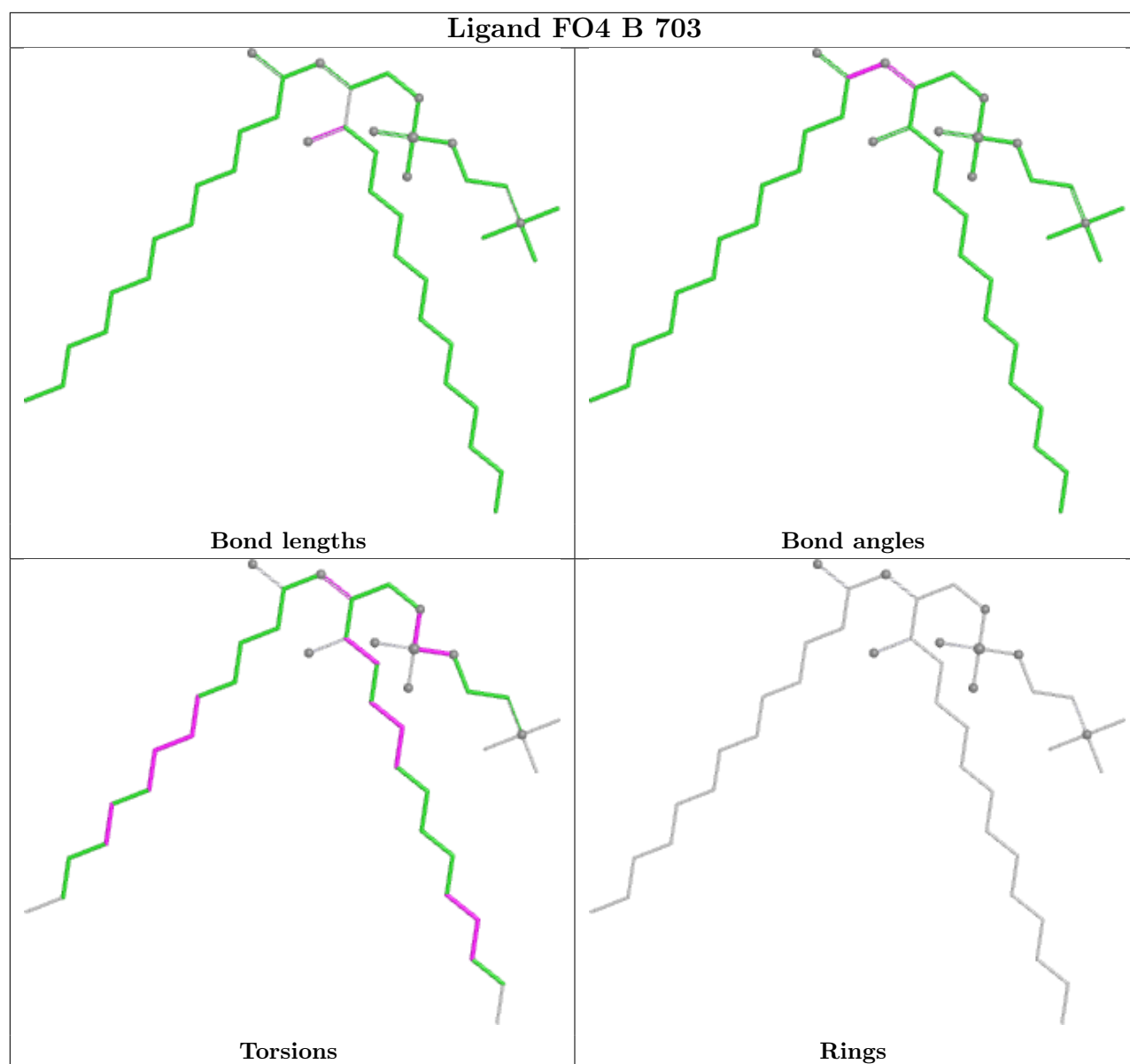


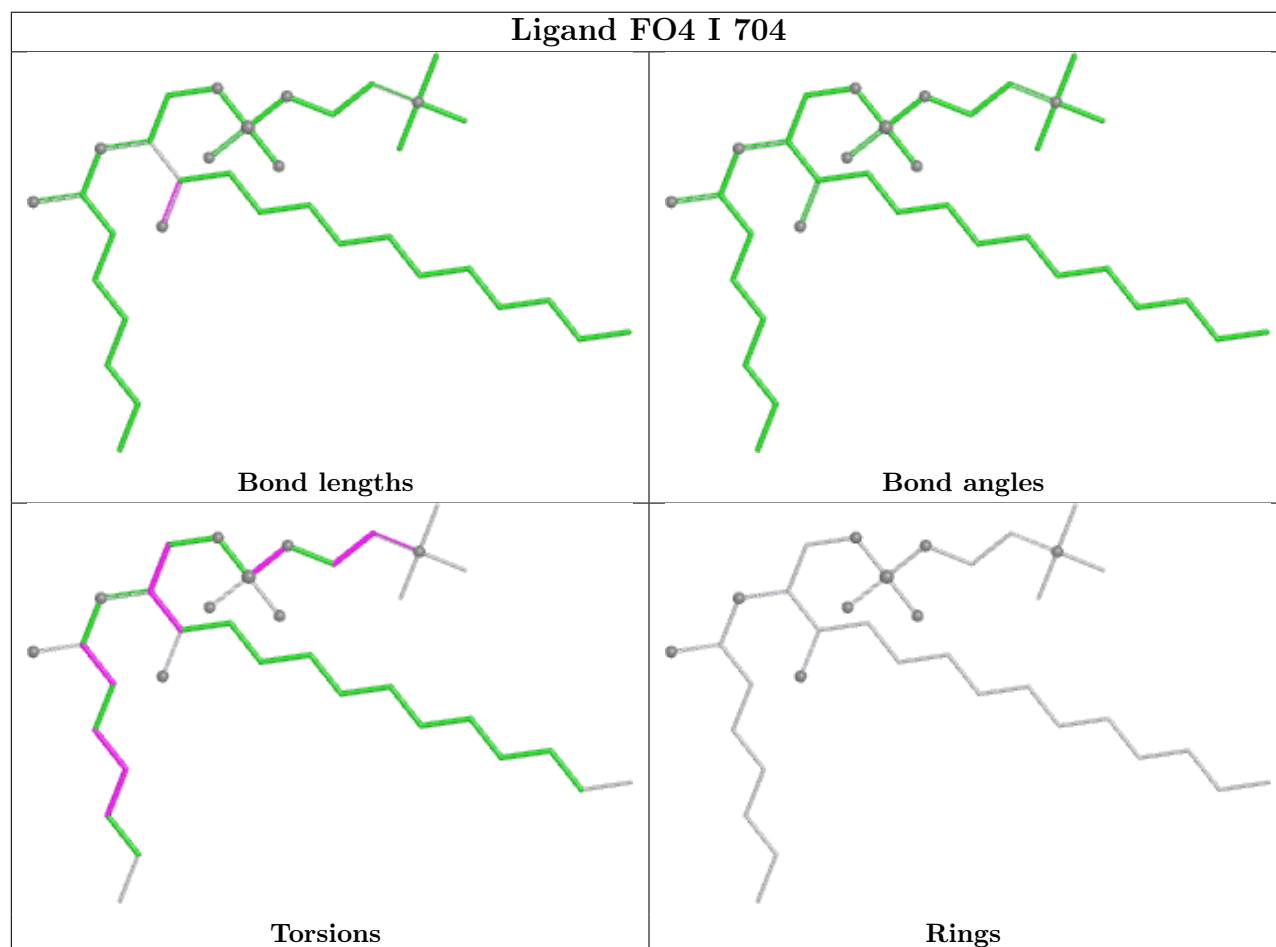
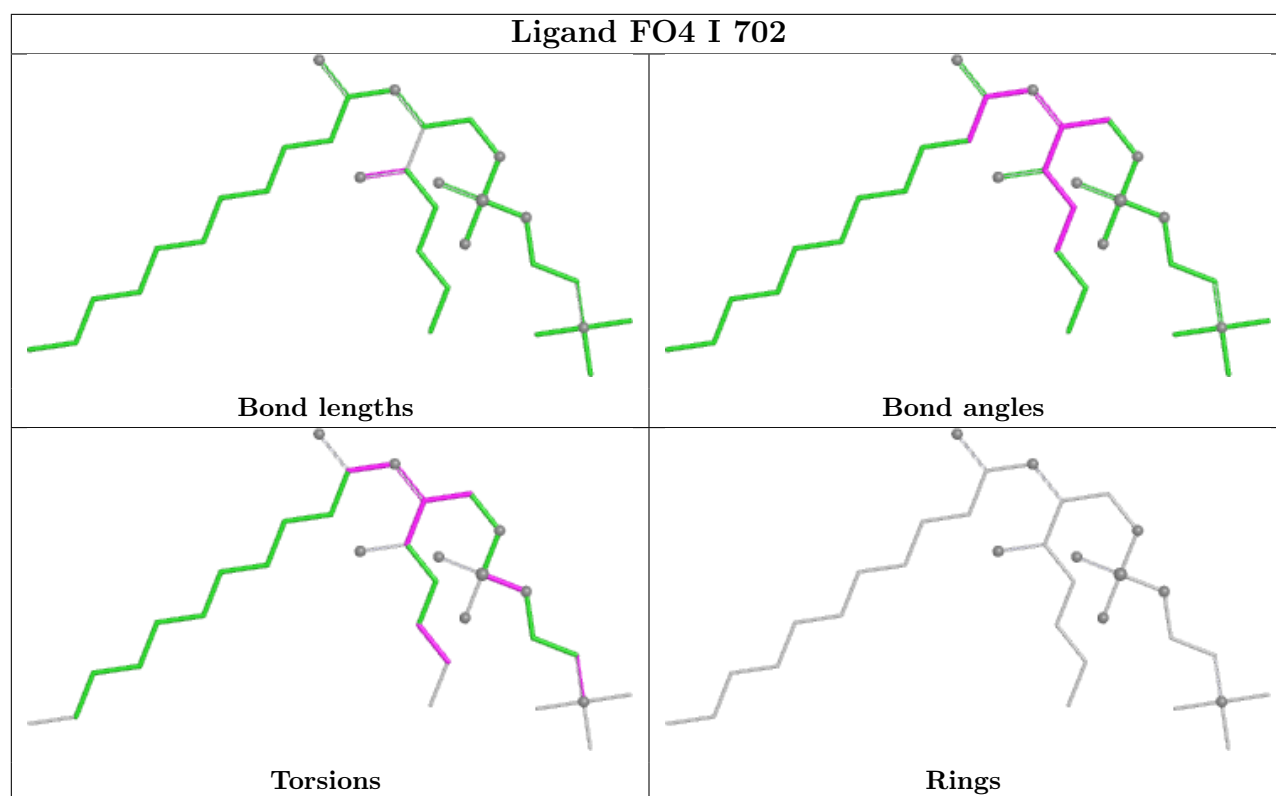












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

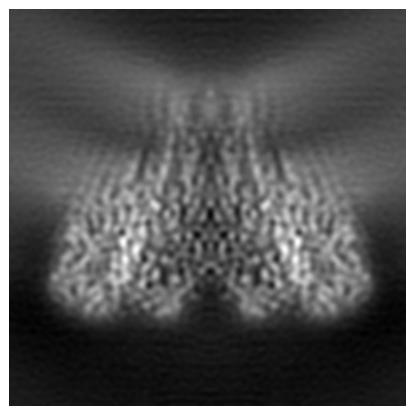
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51384. These allow visual inspection of the internal detail of the map and identification of artifacts.

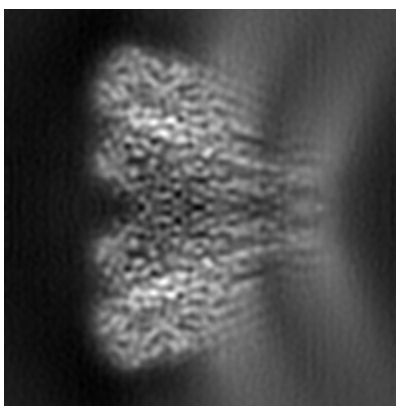
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

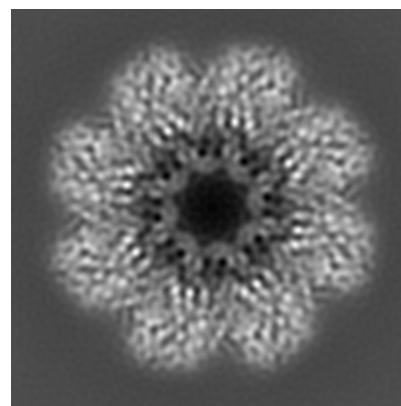
6.1.1 Primary map



X

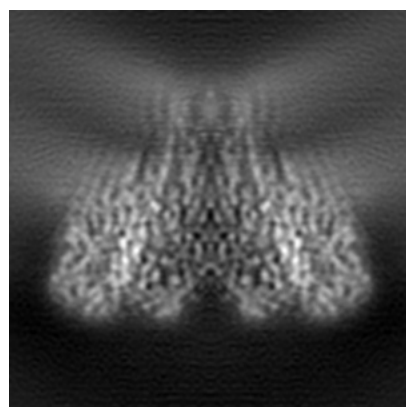


Y

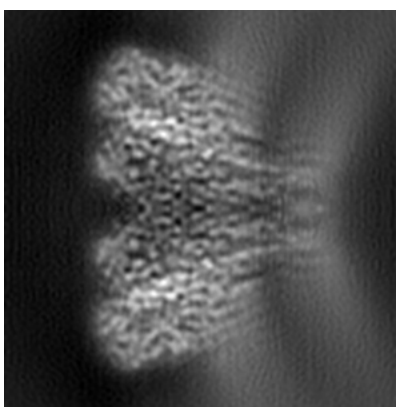


Z

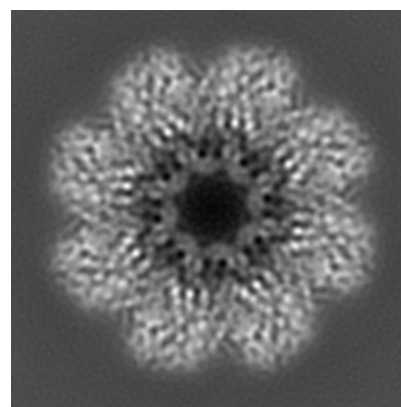
6.1.2 Raw map



X



Y

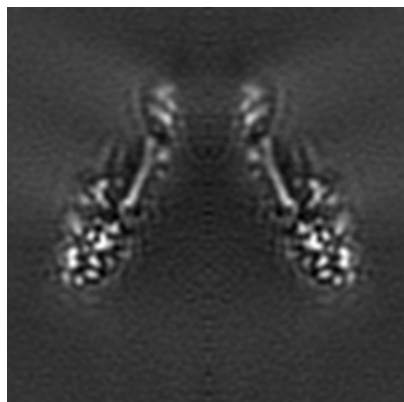


Z

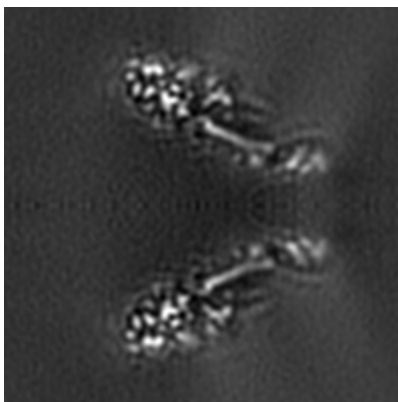
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

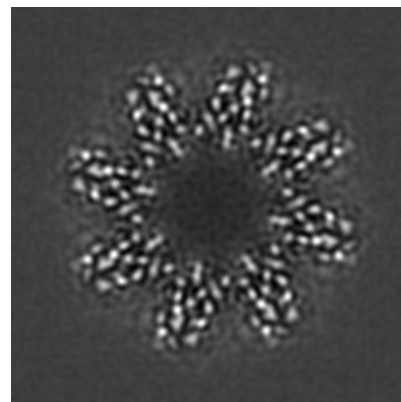
6.2.1 Primary map



X Index: 70

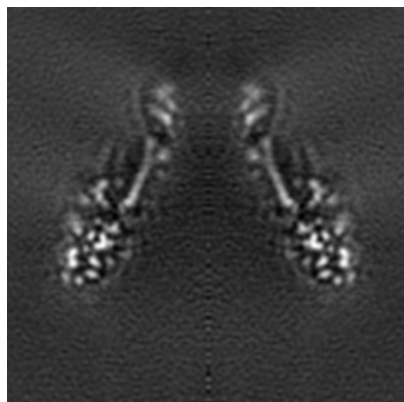


Y Index: 70

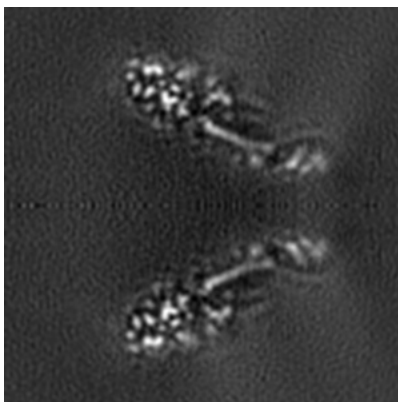


Z Index: 70

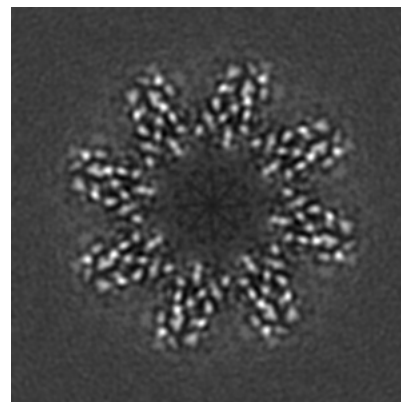
6.2.2 Raw map



X Index: 70



Y Index: 70

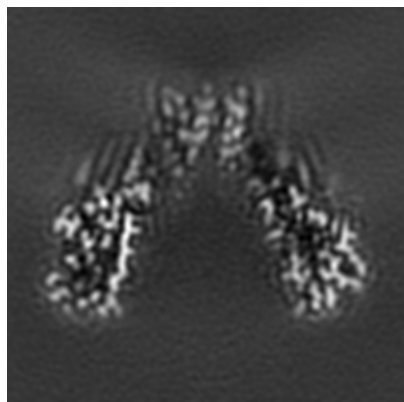


Z Index: 70

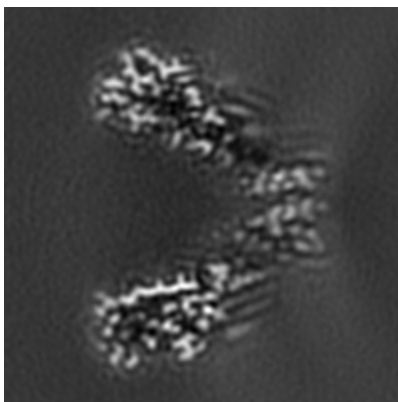
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

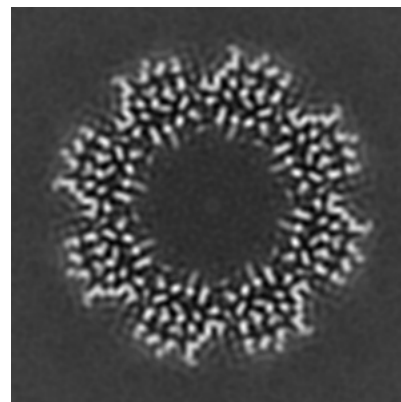
6.3.1 Primary map



X Index: 57

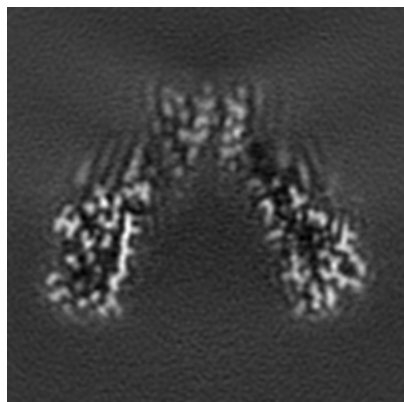


Y Index: 83

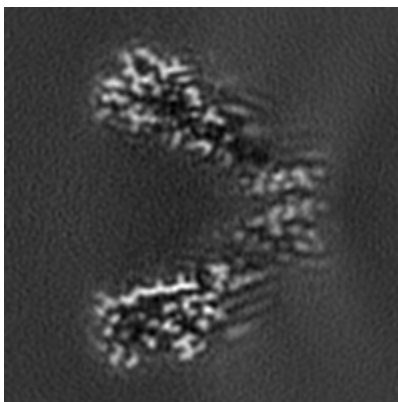


Z Index: 59

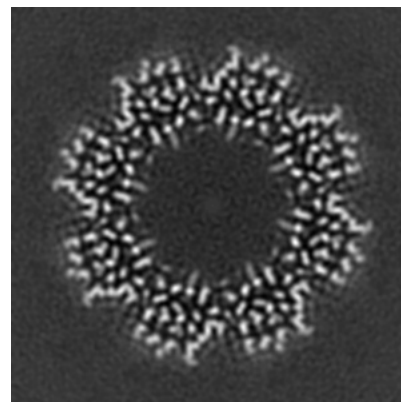
6.3.2 Raw map



X Index: 57



Y Index: 83

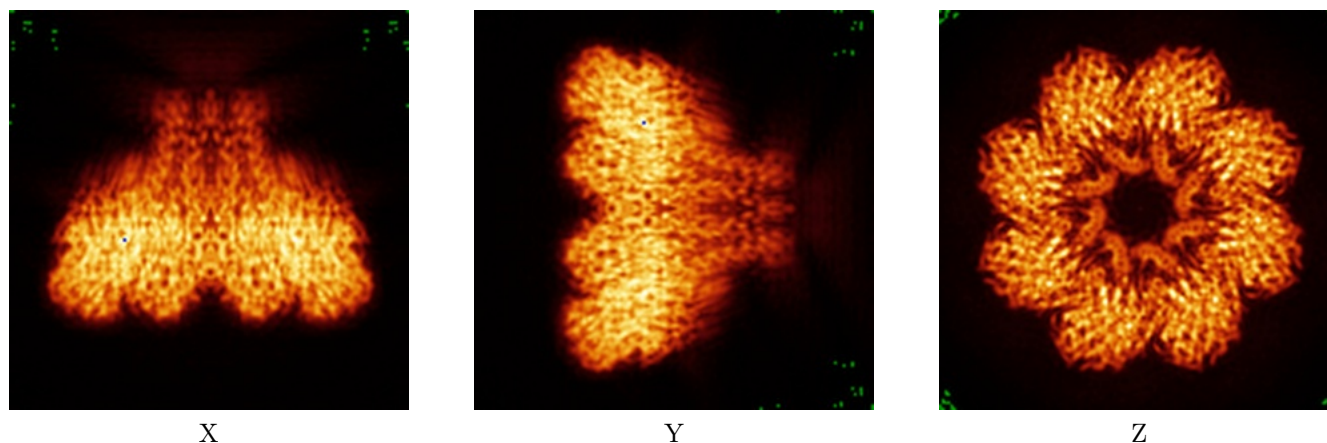


Z Index: 59

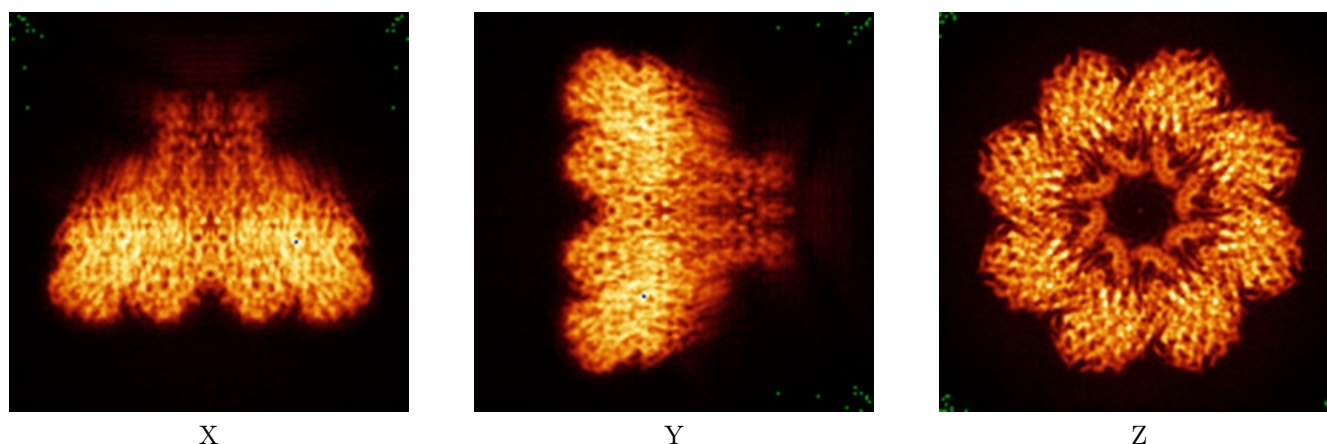
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

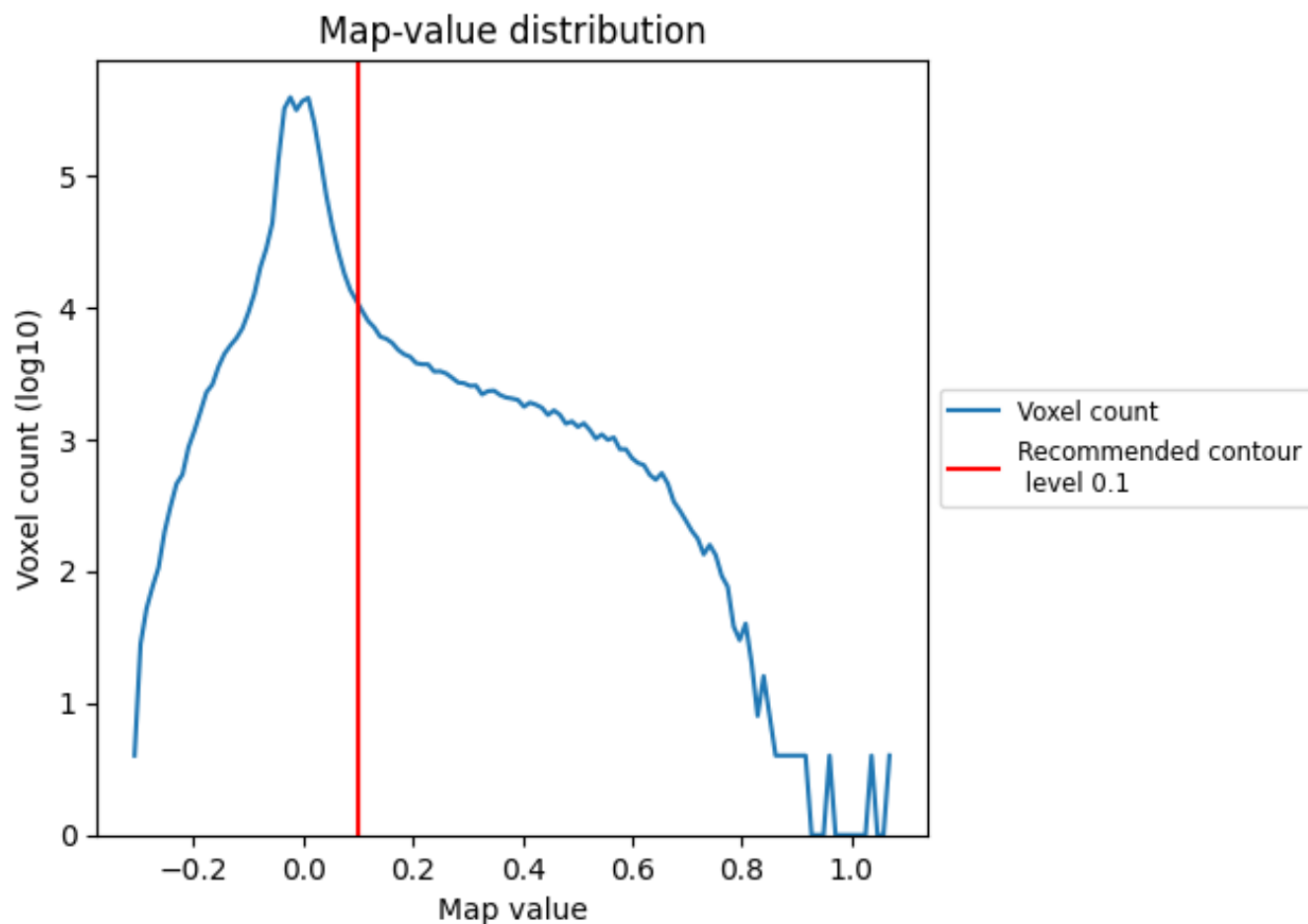
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

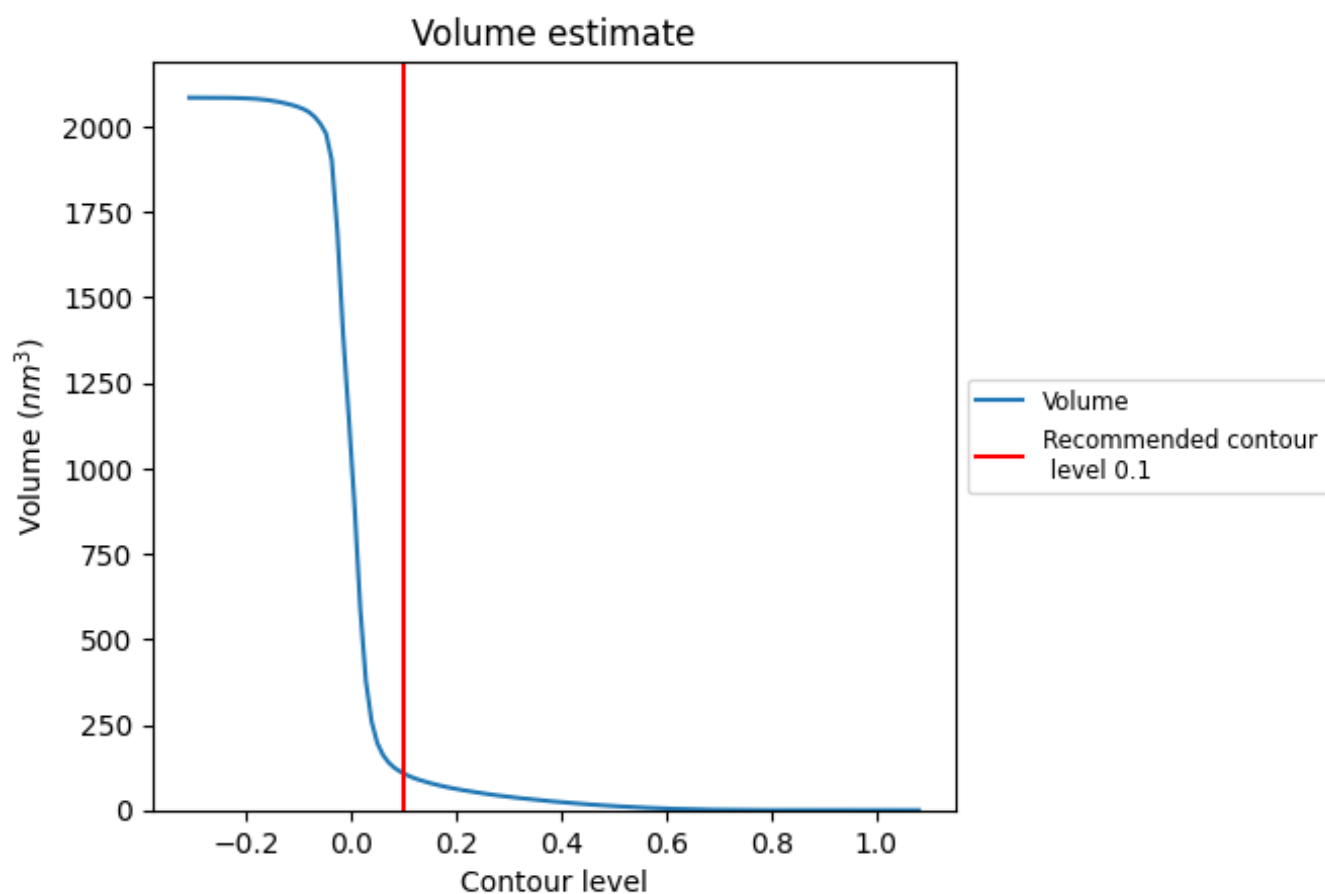
This section contains the results of statistical analysis of the map.

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.

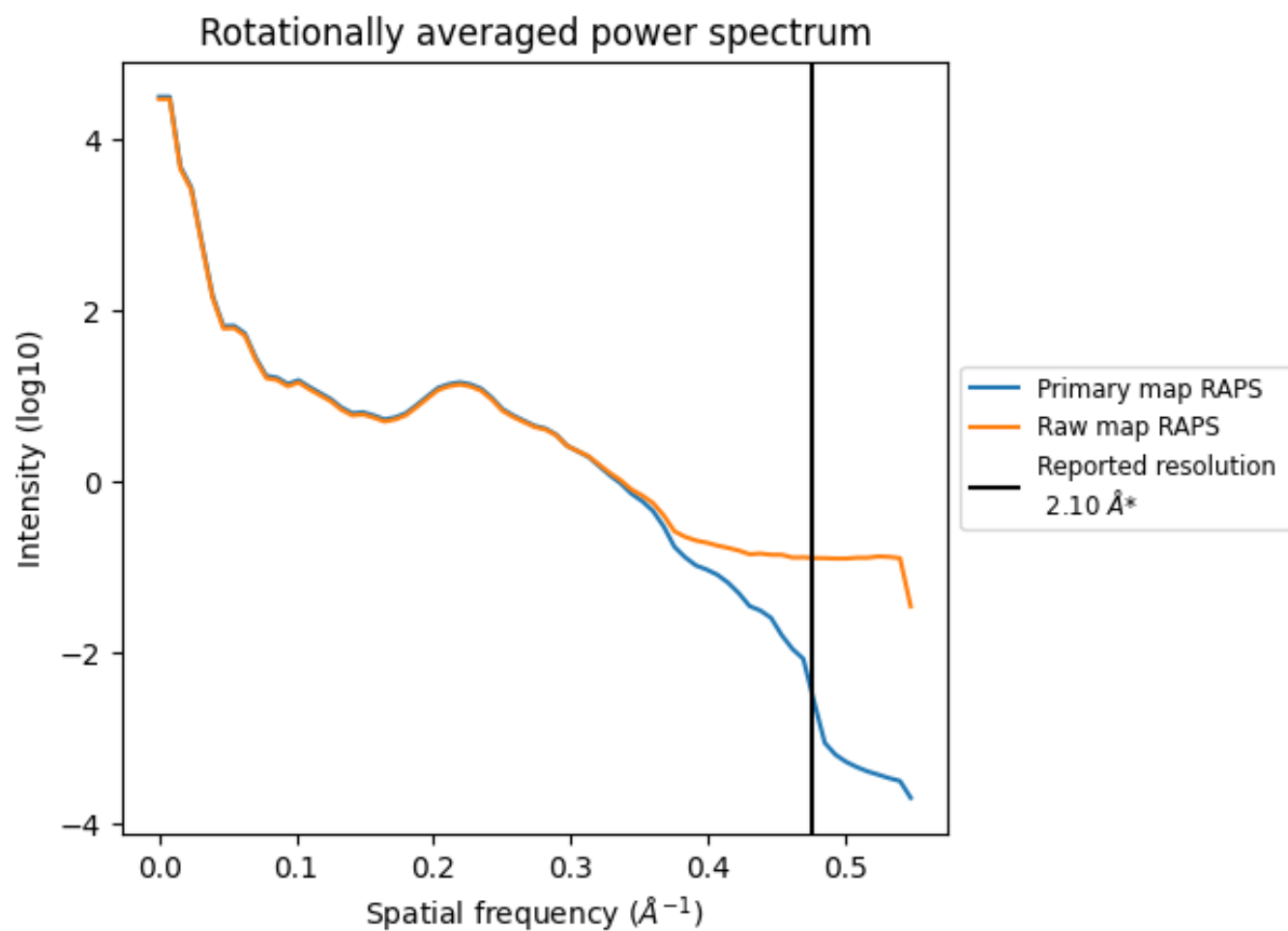
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm^3 ; this corresponds to an approximate mass of 97 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 ⓘ

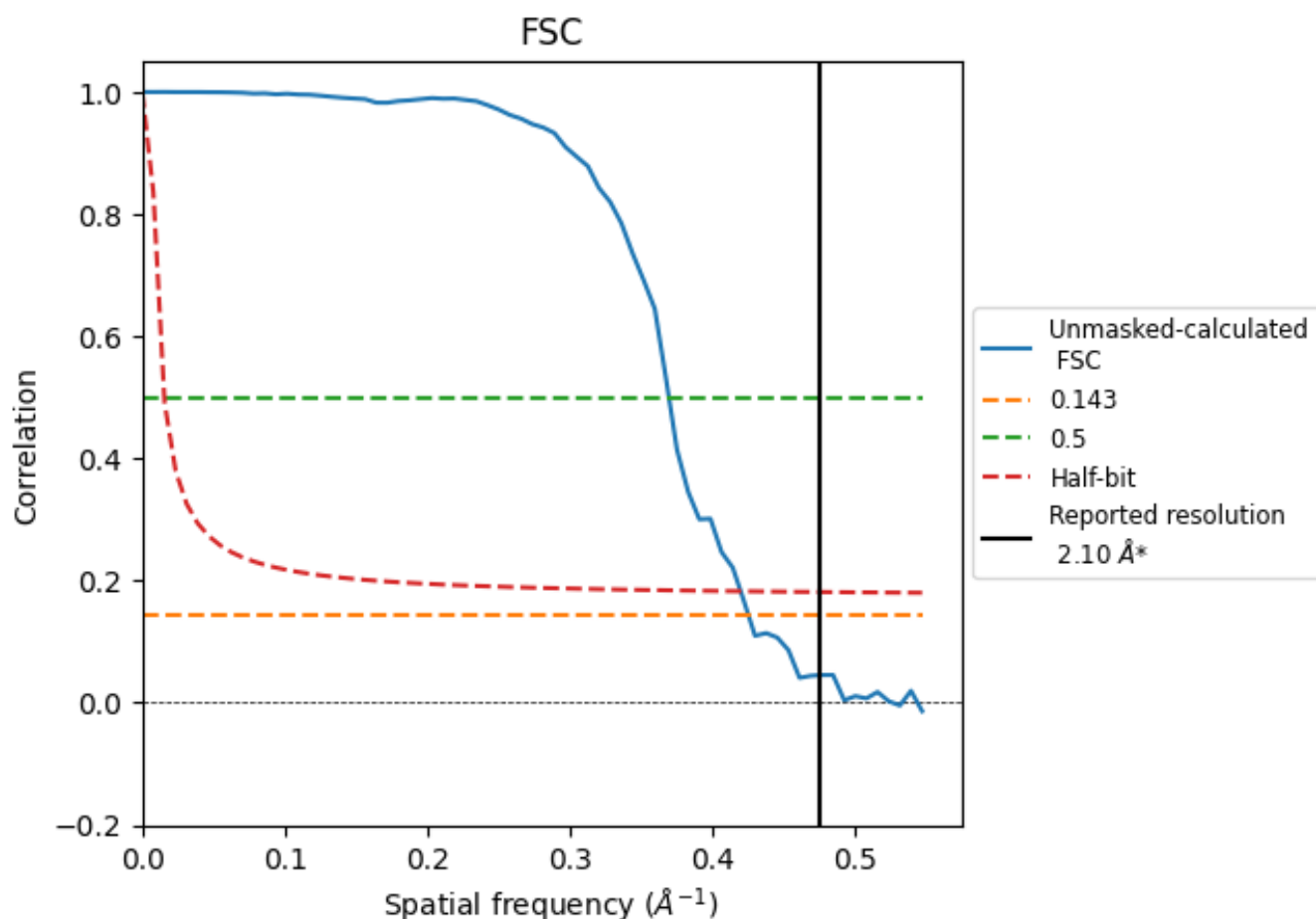


*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.476 \AA^{-1}

8.2 Resolution estimates [i](#)

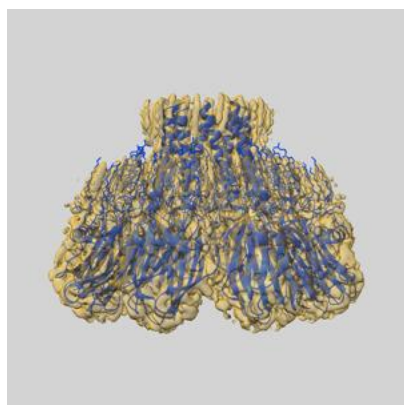
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.35	2.70	2.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.35 differs from the reported value 2.1 by more than 10 %

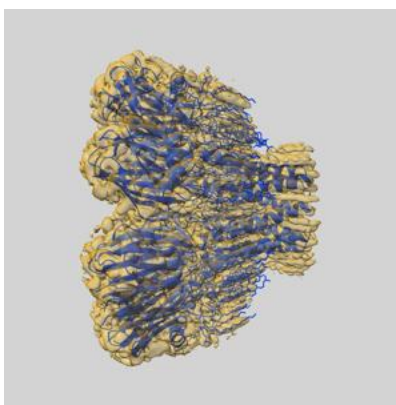
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-51384 and PDB model 9GJ8. Per-residue inclusion information can be found in section [3](#) on page [9](#).

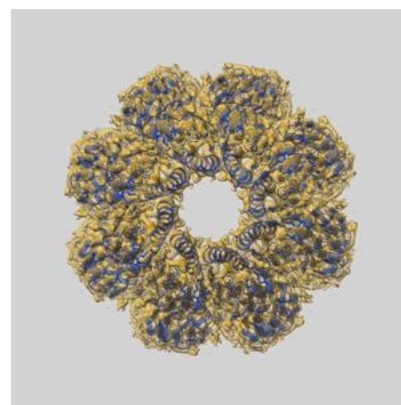
9.1 Map-model overlay [i](#)



X



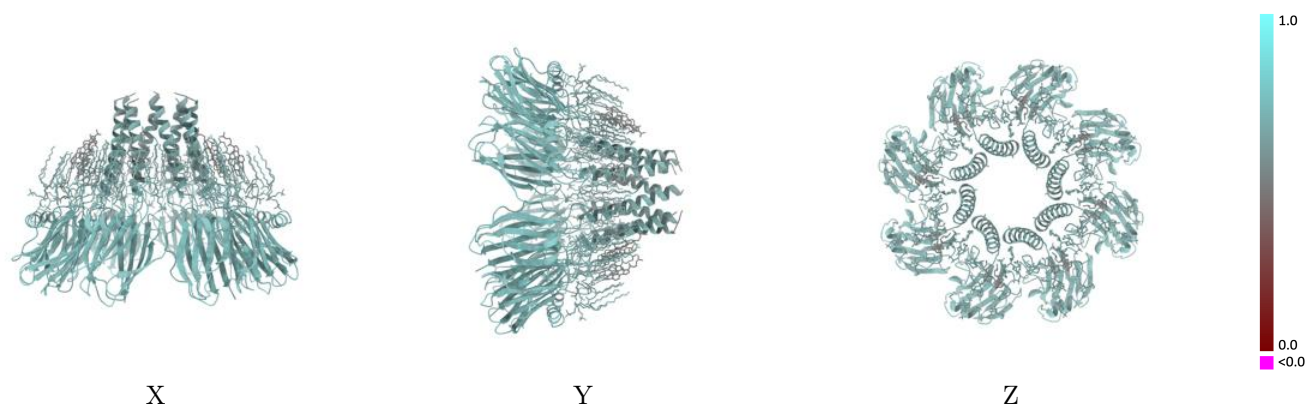
Y



Z

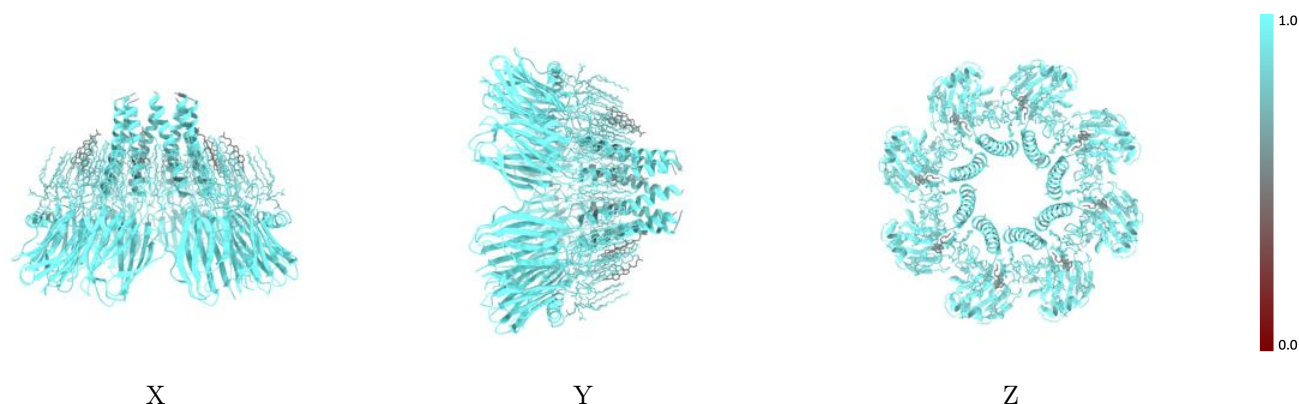
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



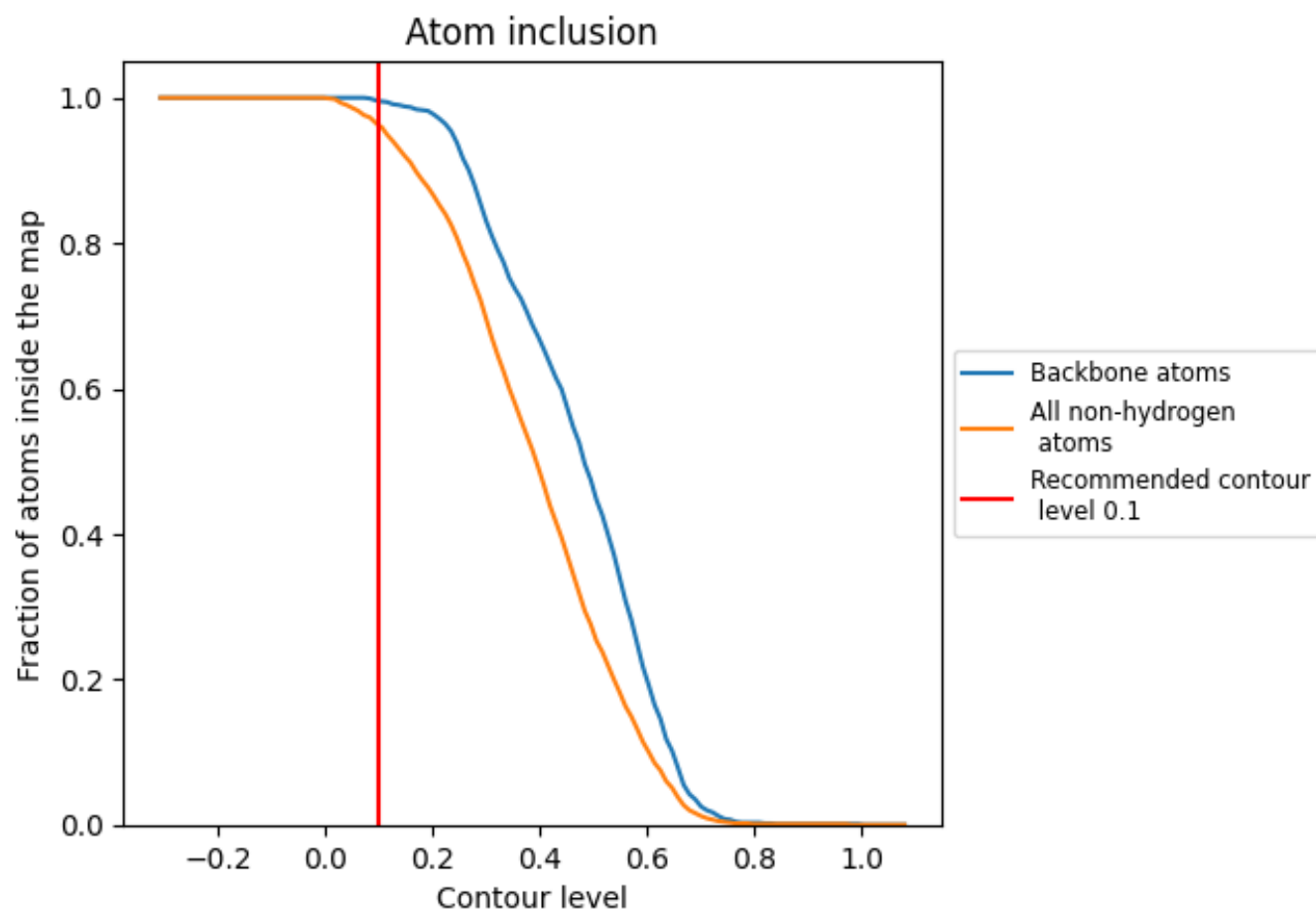
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 96% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9610</div>	<div><div></div>0.6560</div>
A	<div><div></div>0.9620</div>	<div><div></div>0.6550</div>
B	<div><div></div>0.9610</div>	<div><div></div>0.6550</div>
C	<div><div></div>0.9610</div>	<div><div></div>0.6560</div>
E	<div><div></div>0.9610</div>	<div><div></div>0.6560</div>
G	<div><div></div>0.9610</div>	<div><div></div>0.6560</div>
I	<div><div></div>0.9610</div>	<div><div></div>0.6570</div>
J	<div><div></div>0.9610</div>	<div><div></div>0.6570</div>
L	<div><div></div>0.9610</div>	<div><div></div>0.6560</div>

1.0

0.0

<0.0