



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:12 AM UTC

PDB ID : 9Z9Y / pdb_00009z9y
EMDB ID : EMD-7396
Title : Gated state sheep connexin-50 in DMPC nanodiscs at low pH
Authors : Jarodsky, J.M.; Myers, J.B.; Reichow, S.L.
Deposited on : 2025-11-18
Resolution : 2.30 Å (reported)
Based on initial model : 7jjp

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.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

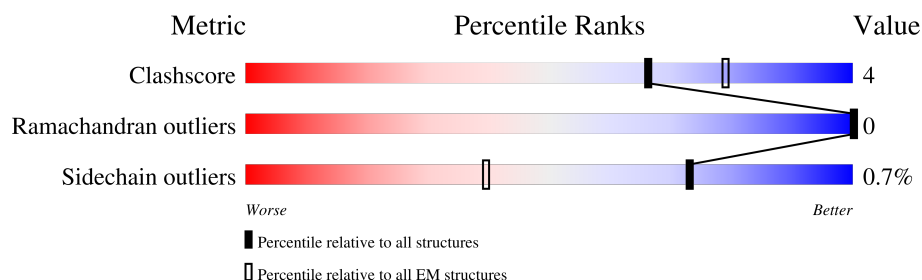
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	440	38% 5% 58%
1	B	440	38% 5% 58%
1	C	440	38% 5% 58%
1	D	440	38% 5% 58%
1	E	440	38% 5% 58%
1	F	440	37% 5% 58%
1	G	440	37% 5% 58%
1	H	440	38% • 58%
1	I	440	38% • 58%

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Mol	Chain	Length	Quality of chain
1	J	440	 38% • 58%
1	K	440	 38% • 58%
1	L	440	 37% 5% 58%

2 Entry composition

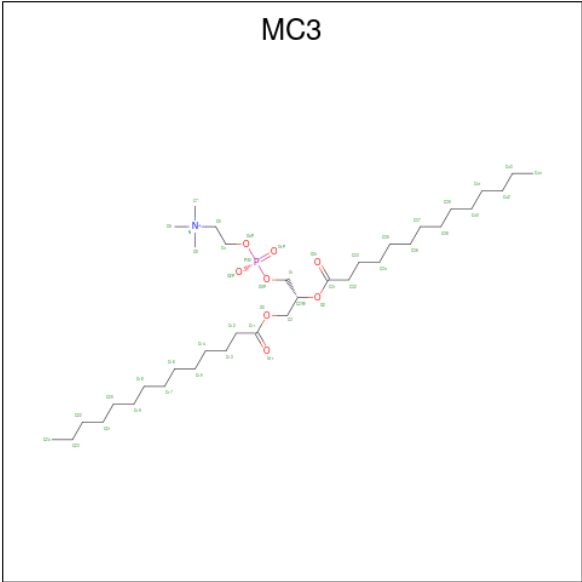
There are 3 unique types of molecules in this entry. The entry contains 47280 atoms, of which 24672 are hydrogens and 0 are deuteriums.

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 Gap junction alpha-8 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	185	Total	C	H	N	O	S	0	0
			2823	953	1384	236	241	9		
1	B	185	Total	C	H	N	O	S	0	0
			2823	953	1384	236	241	9		
1	C	185	Total	C	H	N	O	S	0	0
			2823	953	1384	236	241	9		
1	D	185	Total	C	H	N	O	S	0	0
			2823	953	1384	236	241	9		
1	E	185	Total	C	H	N	O	S	0	0
			2823	953	1384	236	241	9		
1	F	185	Total	C	H	N	O	S	0	0
			2823	953	1384	236	241	9		
1	G	185	Total	C	H	N	O	S	0	0
			2823	953	1384	236	241	9		
1	H	185	Total	C	H	N	O	S	0	0
			2823	953	1384	236	241	9		
1	I	185	Total	C	H	N	O	S	0	0
			2823	953	1384	236	241	9		
1	J	185	Total	C	H	N	O	S	0	0
			2823	953	1384	236	241	9		
1	K	185	Total	C	H	N	O	S	0	0
			2823	953	1384	236	241	9		
1	L	185	Total	C	H	N	O	S	0	0
			2823	953	1384	236	241	9		

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: MC3) (formula: C₃₆H₇₂NO₈P).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H	O	P	0
			76	24	43	8	1	
2	A	1	Total	C	H			0
			39	13	26			
2	A	1	Total	C	H			0
			39	13	26			
2	A	1	Total	C	H			0
			36	12	24			
2	A	1	Total	C	H			0
			36	12	24			
2	A	1	Total	C	H			0
			36	12	24			
2	A	1	Total	C	H			0
			27	9	18			
2	A	1	Total	C	H			0
			21	7	14			
2	A	1	Total	C	H			0
			24	8	16			
2	A	1	Total	C	H			0
			27	9	18			
2	A	1	Total	C	H			0
			18	6	12			
2	A	1	Total	C	H			0
			12	4	8			
2	A	1	Total	C	H			0
			24	8	16			
2	A	1	Total	C	H			0
			36	12	24			

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H			0
			18	6	12			
2	A	1	Total	C	H			0
			21	7	14			
2	A	1	Total	C	H			0
			27	9	18			
2	A	1	Total	C	H	O	P	0
			67	21	37	8	1	
2	A	1	Total	C	H			0
			39	13	26			
2	A	1	Total	C	H			0
			36	12	24			
2	A	1	Total	C	H			0
			36	12	24			
2	A	1	Total	C	H			0
			30	10	20			
2	A	1	Total	C	H			0
			36	12	24			
2	A	1	Total	C	H			0
			39	13	26			
2	A	1	Total	C	H			0
			30	10	20			
2	A	1	Total	C	H			0
			33	11	22			
2	A	1	Total	C	H			0
			18	6	12			
2	A	1	Total	C	H			0
			24	8	16			
2	A	1	Total	C	H			0
			21	7	14			
2	A	1	Total	C	H			0
			18	6	12			
2	A	1	Total	C	H			0
			21	7	14			
2	A	1	Total	C	H			0
			15	5	10			
2	A	1	Total	C	H	N	O	P
			62	18	34	1	8	1
2	B	1	Total	C	H	O	P	0
			76	24	43	8	1	
2	B	1	Total	C	H			0
			39	13	26			

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	H			0
			39	13	26			
2	B	1	Total	C	H			0
			36	12	24			
2	B	1	Total	C	H			0
			36	12	24			
2	B	1	Total	C	H			0
			36	12	24			
2	B	1	Total	C	H			0
			27	9	18			
2	B	1	Total	C	H			0
			21	7	14			
2	B	1	Total	C	H			0
			24	8	16			
2	B	1	Total	C	H			0
			27	9	18			
2	B	1	Total	C	H			0
			18	6	12			
2	B	1	Total	C	H			0
			12	4	8			
2	B	1	Total	C	H			0
			24	8	16			
2	B	1	Total	C	H			0
			36	12	24			
2	B	1	Total	C	H			0
			18	6	12			
2	B	1	Total	C	H			0
			21	7	14			
2	B	1	Total	C	H			0
			27	9	18			
2	B	1	Total	C	H	O	P	0
			67	21	37	8	1	
2	B	1	Total	C	H			0
			39	13	26			
2	B	1	Total	C	H			0
			36	12	24			
2	B	1	Total	C	H			0
			36	12	24			
2	B	1	Total	C	H			0
			30	10	20			
2	B	1	Total	C	H			0
			36	12	24			

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Mol	Chain	Residues	Atoms						AltConf
2	B	1	Total	C	H				0
			39	13	26				
2	B	1	Total	C	H				0
			30	10	20				
2	B	1	Total	C	H				0
			33	11	22				
2	B	1	Total	C	H				0
			18	6	12				
2	B	1	Total	C	H				0
			24	8	16				
2	B	1	Total	C	H				0
			21	7	14				
2	B	1	Total	C	H				0
			18	6	12				
2	B	1	Total	C	H				0
			21	7	14				
2	B	1	Total	C	H				0
			15	5	10				
2	B	1	Total	C	H	N	O	P	0
			62	18	34	1	8	1	
2	C	1	Total	C	H	O	P		0
			76	24	43	8	1		
2	C	1	Total	C	H				0
			39	13	26				
2	C	1	Total	C	H				0
			39	13	26				
2	C	1	Total	C	H				0
			36	12	24				
2	C	1	Total	C	H				0
			36	12	24				
2	C	1	Total	C	H				0
			36	12	24				
2	C	1	Total	C	H				0
			27	9	18				
2	C	1	Total	C	H				0
			21	7	14				
2	C	1	Total	C	H				0
			24	8	16				
2	C	1	Total	C	H				0
			27	9	18				
2	C	1	Total	C	H				0
			18	6	12				

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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	H			0
			12	4	8			
2	C	1	Total	C	H			0
			24	8	16			
2	C	1	Total	C	H			0
			36	12	24			
2	C	1	Total	C	H			0
			18	6	12			
2	C	1	Total	C	H			0
			21	7	14			
2	C	1	Total	C	H			0
			27	9	18			
2	C	1	Total	C	H	O	P	0
			67	21	37	8	1	
2	C	1	Total	C	H			0
			39	13	26			
2	C	1	Total	C	H			0
			36	12	24			
2	C	1	Total	C	H			0
			36	12	24			
2	C	1	Total	C	H			0
			30	10	20			
2	C	1	Total	C	H			0
			36	12	24			
2	C	1	Total	C	H			0
			39	13	26			
2	C	1	Total	C	H			0
			30	10	20			
2	C	1	Total	C	H			0
			33	11	22			
2	C	1	Total	C	H			0
			18	6	12			
2	C	1	Total	C	H			0
			24	8	16			
2	C	1	Total	C	H			0
			21	7	14			
2	C	1	Total	C	H			0
			18	6	12			
2	C	1	Total	C	H			0
			21	7	14			
2	C	1	Total	C	H			0
			15	5	10			

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Mol	Chain	Residues	Atoms					AltConf	
2	C	1	Total 62	C 18	H 34	N 1	O 8	P 1	0
2	D	1	Total 76	C 24	H 43	O 8	P 1		0
2	D	1	Total 39	C 13	H 26				0
2	D	1	Total 39	C 13	H 26				0
2	D	1	Total 36	C 12	H 24				0
2	D	1	Total 36	C 12	H 24				0
2	D	1	Total 36	C 12	H 24				0
2	D	1	Total 27	C 9	H 18				0
2	D	1	Total 21	C 7	H 14				0
2	D	1	Total 24	C 8	H 16				0
2	D	1	Total 27	C 9	H 18				0
2	D	1	Total 18	C 6	H 12				0
2	D	1	Total 12	C 4	H 8				0
2	D	1	Total 24	C 8	H 16				0
2	D	1	Total 36	C 12	H 24				0
2	D	1	Total 18	C 6	H 12				0
2	D	1	Total 21	C 7	H 14				0
2	D	1	Total 27	C 9	H 18				0
2	D	1	Total 67	C 21	H 37	O 8	P 1		0
2	D	1	Total 39	C 13	H 26				0
2	D	1	Total 36	C 12	H 24				0

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Mol	Chain	Residues	Atoms						AltConf
2	D	1	Total	C	H				0
			36	12	24				
2	D	1	Total	C	H				0
			30	10	20				
2	D	1	Total	C	H				0
			36	12	24				
2	D	1	Total	C	H				0
			39	13	26				
2	D	1	Total	C	H				0
			30	10	20				
2	D	1	Total	C	H				0
			33	11	22				
2	D	1	Total	C	H				0
			18	6	12				
2	D	1	Total	C	H				0
			24	8	16				
2	D	1	Total	C	H				0
			21	7	14				
2	D	1	Total	C	H				0
			18	6	12				
2	D	1	Total	C	H				0
			21	7	14				
2	D	1	Total	C	H				0
			15	5	10				
2	D	1	Total	C	H	N	O	P	0
			62	18	34	1	8	1	
2	E	1	Total	C	H	O	P		0
			76	24	43	8	1		
2	E	1	Total	C	H				0
			39	13	26				
2	E	1	Total	C	H				0
			39	13	26				
2	E	1	Total	C	H				0
			36	12	24				
2	E	1	Total	C	H				0
			36	12	24				
2	E	1	Total	C	H				0
			36	12	24				
2	E	1	Total	C	H				0
			27	9	18				
2	E	1	Total	C	H				0
			21	7	14				

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Mol	Chain	Residues	Atoms					AltConf
2	E	1	Total	C	H			0
			24	8	16			
2	E	1	Total	C	H			0
			27	9	18			
2	E	1	Total	C	H			0
			18	6	12			
2	E	1	Total	C	H			0
			12	4	8			
2	E	1	Total	C	H			0
			24	8	16			
2	E	1	Total	C	H			0
			36	12	24			
2	E	1	Total	C	H			0
			18	6	12			
2	E	1	Total	C	H			0
			21	7	14			
2	E	1	Total	C	H			0
			27	9	18			
2	E	1	Total	C	H	O	P	0
			67	21	37	8	1	
2	E	1	Total	C	H			0
			39	13	26			
2	E	1	Total	C	H			0
			36	12	24			
2	E	1	Total	C	H			0
			36	12	24			
2	E	1	Total	C	H			0
			30	10	20			
2	E	1	Total	C	H			0
			36	12	24			
2	E	1	Total	C	H			0
			39	13	26			
2	E	1	Total	C	H			0
			30	10	20			
2	E	1	Total	C	H			0
			33	11	22			
2	E	1	Total	C	H			0
			18	6	12			
2	E	1	Total	C	H			0
			24	8	16			
2	E	1	Total	C	H			0
			21	7	14			

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Mol	Chain	Residues	Atoms						AltConf
2	E	1	Total	C	H				0
			18	6	12				
2	E	1	Total	C	H				0
			21	7	14				
2	E	1	Total	C	H				0
			15	5	10				
2	E	1	Total	C	H	N	O	P	0
			62	18	34	1	8	1	
2	F	1	Total	C	H				0
			39	13	26				
2	F	1	Total	C	H				0
			36	12	24				
2	F	1	Total	C	H				0
			36	12	24				
2	F	1	Total	C	H				0
			30	10	20				
2	F	1	Total	C	H				0
			36	12	24				
2	F	1	Total	C	H				0
			39	13	26				
2	F	1	Total	C	H				0
			30	10	20				
2	F	1	Total	C	H				0
			33	11	22				
2	F	1	Total	C	H				0
			18	6	12				
2	F	1	Total	C	H				0
			24	8	16				
2	F	1	Total	C	H				0
			21	7	14				
2	F	1	Total	C	H				0
			18	6	12				
2	F	1	Total	C	H				0
			21	7	14				
2	F	1	Total	C	H				0
			15	5	10				
2	F	1	Total	C	H	N	O	P	0
			62	18	34	1	8	1	
2	F	1	Total	C	H	O	P		0
			76	24	43	8	1		
2	F	1	Total	C	H				0
			39	13	26				

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Mol	Chain	Residues	Atoms					AltConf
2	F	1	Total	C	H			0
			39	13	26			
2	F	1	Total	C	H			0
			36	12	24			
2	F	1	Total	C	H			0
			36	12	24			
2	F	1	Total	C	H			0
			36	12	24			
2	F	1	Total	C	H			0
			27	9	18			
2	F	1	Total	C	H			0
			21	7	14			
2	F	1	Total	C	H			0
			24	8	16			
2	F	1	Total	C	H			0
			27	9	18			
2	F	1	Total	C	H			0
			18	6	12			
2	F	1	Total	C	H			0
			12	4	8			
2	F	1	Total	C	H			0
			24	8	16			
2	F	1	Total	C	H			0
			36	12	24			
2	F	1	Total	C	H			0
			18	6	12			
2	F	1	Total	C	H			0
			21	7	14			
2	F	1	Total	C	H			0
			27	9	18			
2	F	1	Total	C	H	O	P	0
			67	21	37	8	1	
2	G	1	Total	C	H	O	P	0
			76	24	43	8	1	
2	G	1	Total	C	H			0
			39	13	26			
2	G	1	Total	C	H			0
			39	13	26			
2	G	1	Total	C	H			0
			36	12	24			
2	G	1	Total	C	H			0
			36	12	24			

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Mol	Chain	Residues	Atoms					AltConf
2	G	1	Total	C	H			0
			36	12	24			
2	G	1	Total	C	H			0
			27	9	18			
2	G	1	Total	C	H			0
			21	7	14			
2	G	1	Total	C	H			0
			24	8	16			
2	G	1	Total	C	H			0
			27	9	18			
2	G	1	Total	C	H			0
			18	6	12			
2	G	1	Total	C	H			0
			12	4	8			
2	G	1	Total	C	H			0
			24	8	16			
2	G	1	Total	C	H			0
			36	12	24			
2	G	1	Total	C	H			0
			18	6	12			
2	G	1	Total	C	H			0
			21	7	14			
2	G	1	Total	C	H			0
			27	9	18			
2	G	1	Total	C	H	O	P	0
			67	21	37	8	1	
2	G	1	Total	C	H			0
			39	13	26			
2	G	1	Total	C	H			0
			36	12	24			
2	G	1	Total	C	H			0
			36	12	24			
2	G	1	Total	C	H			0
			30	10	20			
2	G	1	Total	C	H			0
			36	12	24			
2	G	1	Total	C	H			0
			39	13	26			
2	G	1	Total	C	H			0
			30	10	20			
2	G	1	Total	C	H			0
			33	11	22			

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Mol	Chain	Residues	Atoms						AltConf
2	G	1	Total	C	H				0
			18	6	12				
2	G	1	Total	C	H				0
			24	8	16				
2	G	1	Total	C	H				0
			21	7	14				
2	G	1	Total	C	H				0
			18	6	12				
2	G	1	Total	C	H				0
			21	7	14				
2	G	1	Total	C	H				0
			15	5	10				
2	G	1	Total	C	H	N	O	P	0
			62	18	34	1	8	1	
2	H	1	Total	C	H	O	P		0
			76	24	43	8	1		
2	H	1	Total	C	H				0
			39	13	26				
2	H	1	Total	C	H				0
			39	13	26				
2	H	1	Total	C	H				0
			36	12	24				
2	H	1	Total	C	H				0
			36	12	24				
2	H	1	Total	C	H				0
			36	12	24				
2	H	1	Total	C	H				0
			27	9	18				
2	H	1	Total	C	H				0
			21	7	14				
2	H	1	Total	C	H				0
			24	8	16				
2	H	1	Total	C	H				0
			27	9	18				
2	H	1	Total	C	H				0
			18	6	12				
2	H	1	Total	C	H				0
			12	4	8				
2	H	1	Total	C	H				0
			24	8	16				
2	H	1	Total	C	H				0
			36	12	24				

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Mol	Chain	Residues	Atoms					AltConf
2	H	1	Total	C	H			0
			18	6	12			
2	H	1	Total	C	H			0
			21	7	14			
2	H	1	Total	C	H			0
			27	9	18			
2	H	1	Total	C	H	O	P	0
			67	21	37	8	1	
2	H	1	Total	C	H			0
			39	13	26			
2	H	1	Total	C	H			0
			36	12	24			
2	H	1	Total	C	H			0
			36	12	24			
2	H	1	Total	C	H			0
			30	10	20			
2	H	1	Total	C	H			0
			36	12	24			
2	H	1	Total	C	H			0
			39	13	26			
2	H	1	Total	C	H			0
			30	10	20			
2	H	1	Total	C	H			0
			33	11	22			
2	H	1	Total	C	H			0
			18	6	12			
2	H	1	Total	C	H			0
			24	8	16			
2	H	1	Total	C	H			0
			21	7	14			
2	H	1	Total	C	H			0
			18	6	12			
2	H	1	Total	C	H			0
			21	7	14			
2	H	1	Total	C	H			0
			15	5	10			
2	H	1	Total	C	H	N	O	P
			62	18	34	1	8	1
2	I	1	Total	C	H	O	P	0
			76	24	43	8	1	
2	I	1	Total	C	H			0
			39	13	26			

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Mol	Chain	Residues	Atoms					AltConf
2	I	1	Total	C	H			0
			39	13	26			
2	I	1	Total	C	H			0
			36	12	24			
2	I	1	Total	C	H			0
			36	12	24			
2	I	1	Total	C	H			0
			36	12	24			
2	I	1	Total	C	H			0
			27	9	18			
2	I	1	Total	C	H			0
			21	7	14			
2	I	1	Total	C	H			0
			24	8	16			
2	I	1	Total	C	H			0
			27	9	18			
2	I	1	Total	C	H			0
			18	6	12			
2	I	1	Total	C	H			0
			12	4	8			
2	I	1	Total	C	H			0
			24	8	16			
2	I	1	Total	C	H			0
			36	12	24			
2	I	1	Total	C	H			0
			18	6	12			
2	I	1	Total	C	H			0
			21	7	14			
2	I	1	Total	C	H			0
			27	9	18			
2	I	1	Total	C	H	O	P	0
			67	21	37	8	1	
2	I	1	Total	C	H			0
			39	13	26			
2	I	1	Total	C	H			0
			36	12	24			
2	I	1	Total	C	H			0
			36	12	24			
2	I	1	Total	C	H			0
			30	10	20			
2	I	1	Total	C	H			0
			36	12	24			

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Mol	Chain	Residues	Atoms						AltConf
2	I	1	Total	C	H				0
			39	13	26				
2	I	1	Total	C	H				0
			30	10	20				
2	I	1	Total	C	H				0
			33	11	22				
2	I	1	Total	C	H				0
			18	6	12				
2	I	1	Total	C	H				0
			24	8	16				
2	I	1	Total	C	H				0
			21	7	14				
2	I	1	Total	C	H				0
			18	6	12				
2	I	1	Total	C	H				0
			21	7	14				
2	I	1	Total	C	H				0
			15	5	10				
2	I	1	Total	C	H	N	O	P	0
			62	18	34	1	8	1	
2	J	1	Total	C	H	O	P		0
			76	24	43	8	1		
2	J	1	Total	C	H				0
			39	13	26				
2	J	1	Total	C	H				0
			39	13	26				
2	J	1	Total	C	H				0
			36	12	24				
2	J	1	Total	C	H				0
			36	12	24				
2	J	1	Total	C	H				0
			36	12	24				
2	J	1	Total	C	H				0
			27	9	18				
2	J	1	Total	C	H				0
			21	7	14				
2	J	1	Total	C	H				0
			24	8	16				
2	J	1	Total	C	H				0
			27	9	18				
2	J	1	Total	C	H				0
			18	6	12				

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Mol	Chain	Residues	Atoms					AltConf
2	J	1	Total	C	H			0
			12	4	8			
2	J	1	Total	C	H			0
			24	8	16			
2	J	1	Total	C	H			0
			36	12	24			
2	J	1	Total	C	H			0
			18	6	12			
2	J	1	Total	C	H			0
			21	7	14			
2	J	1	Total	C	H			0
			27	9	18			
2	J	1	Total	C	H	O	P	0
			67	21	37	8	1	
2	J	1	Total	C	H			0
			39	13	26			
2	J	1	Total	C	H			0
			36	12	24			
2	J	1	Total	C	H			0
			36	12	24			
2	J	1	Total	C	H			0
			30	10	20			
2	J	1	Total	C	H			0
			36	12	24			
2	J	1	Total	C	H			0
			39	13	26			
2	J	1	Total	C	H			0
			30	10	20			
2	J	1	Total	C	H			0
			33	11	22			
2	J	1	Total	C	H			0
			18	6	12			
2	J	1	Total	C	H			0
			24	8	16			
2	J	1	Total	C	H			0
			21	7	14			
2	J	1	Total	C	H			0
			18	6	12			
2	J	1	Total	C	H			0
			21	7	14			
2	J	1	Total	C	H			0
			15	5	10			

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Mol	Chain	Residues	Atoms					AltConf	
2	J	1	Total 62	C 18	H 34	N 1	O 8	P 1	0
2	K	1	Total 76	C 24	H 43	O 8	P 1		0
2	K	1	Total 39	C 13	H 26				0
2	K	1	Total 39	C 13	H 26				0
2	K	1	Total 36	C 12	H 24				0
2	K	1	Total 36	C 12	H 24				0
2	K	1	Total 36	C 12	H 24				0
2	K	1	Total 27	C 9	H 18				0
2	K	1	Total 21	C 7	H 14				0
2	K	1	Total 24	C 8	H 16				0
2	K	1	Total 27	C 9	H 18				0
2	K	1	Total 18	C 6	H 12				0
2	K	1	Total 12	C 4	H 8				0
2	K	1	Total 24	C 8	H 16				0
2	K	1	Total 36	C 12	H 24				0
2	K	1	Total 18	C 6	H 12				0
2	K	1	Total 21	C 7	H 14				0
2	K	1	Total 27	C 9	H 18				0
2	K	1	Total 67	C 21	H 37	O 8	P 1		0
2	K	1	Total 39	C 13	H 26				0
2	K	1	Total 36	C 12	H 24				0

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Mol	Chain	Residues	Atoms						AltConf
2	K	1	Total	C	H				0
			36	12	24				
2	K	1	Total	C	H				0
			30	10	20				
2	K	1	Total	C	H				0
			36	12	24				
2	K	1	Total	C	H				0
			39	13	26				
2	K	1	Total	C	H				0
			30	10	20				
2	K	1	Total	C	H				0
			33	11	22				
2	K	1	Total	C	H				0
			18	6	12				
2	K	1	Total	C	H				0
			24	8	16				
2	K	1	Total	C	H				0
			21	7	14				
2	K	1	Total	C	H				0
			18	6	12				
2	K	1	Total	C	H				0
			21	7	14				
2	K	1	Total	C	H				0
			15	5	10				
2	K	1	Total	C	H	N	O	P	0
			62	18	34	1	8	1	
2	L	1	Total	C	H				0
			39	13	26				
2	L	1	Total	C	H				0
			36	12	24				
2	L	1	Total	C	H				0
			36	12	24				
2	L	1	Total	C	H				0
			30	10	20				
2	L	1	Total	C	H				0
			36	12	24				
2	L	1	Total	C	H				0
			39	13	26				
2	L	1	Total	C	H				0
			30	10	20				
2	L	1	Total	C	H				0
			33	11	22				

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Mol	Chain	Residues	Atoms						AltConf
2	L	1	Total	C	H				0
			18	6	12				
2	L	1	Total	C	H				0
			24	8	16				
2	L	1	Total	C	H				0
			21	7	14				
2	L	1	Total	C	H				0
			18	6	12				
2	L	1	Total	C	H				0
			21	7	14				
2	L	1	Total	C	H				0
			15	5	10				
2	L	1	Total	C	H	N	O	P	0
			62	18	34	1	8	1	
2	L	1	Total	C	H	O	P		0
			76	24	43	8	1		
2	L	1	Total	C	H				0
			39	13	26				
2	L	1	Total	C	H				0
			39	13	26				
2	L	1	Total	C	H				0
			36	12	24				
2	L	1	Total	C	H				0
			36	12	24				
2	L	1	Total	C	H				0
			36	12	24				
2	L	1	Total	C	H				0
			27	9	18				
2	L	1	Total	C	H				0
			21	7	14				
2	L	1	Total	C	H				0
			24	8	16				
2	L	1	Total	C	H				0
			27	9	18				
2	L	1	Total	C	H				0
			18	6	12				
2	L	1	Total	C	H				0
			12	4	8				
2	L	1	Total	C	H				0
			24	8	16				
2	L	1	Total	C	H				0
			36	12	24				

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Mol	Chain	Residues	Atoms					AltConf
2	L	1	Total	C	H			0
			18	6	12			
2	L	1	Total	C	H			0
			21	7	14			
2	L	1	Total	C	H			0
			27	9	18			
2	L	1	Total	C	H	O	P	0
			67	21	37	8	1	

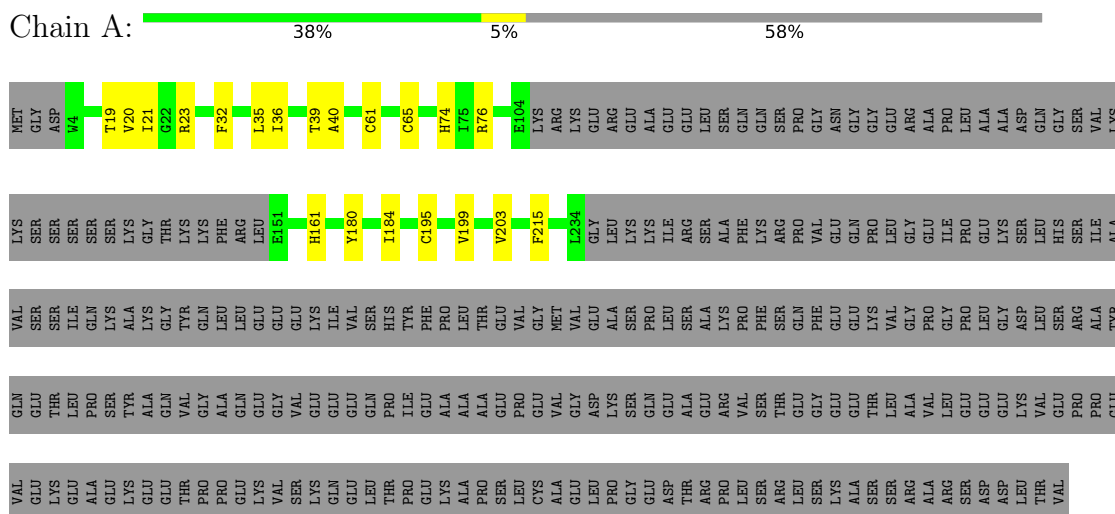
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	75	Total	O	0
			75	75	
3	B	75	Total	O	0
			75	75	
3	C	75	Total	O	0
			75	75	
3	D	75	Total	O	0
			75	75	
3	E	75	Total	O	0
			75	75	
3	F	75	Total	O	0
			75	75	
3	G	75	Total	O	0
			75	75	
3	H	75	Total	O	0
			75	75	
3	I	75	Total	O	0
			75	75	
3	J	75	Total	O	0
			75	75	
3	K	75	Total	O	0
			75	75	
3	L	75	Total	O	0
			75	75	

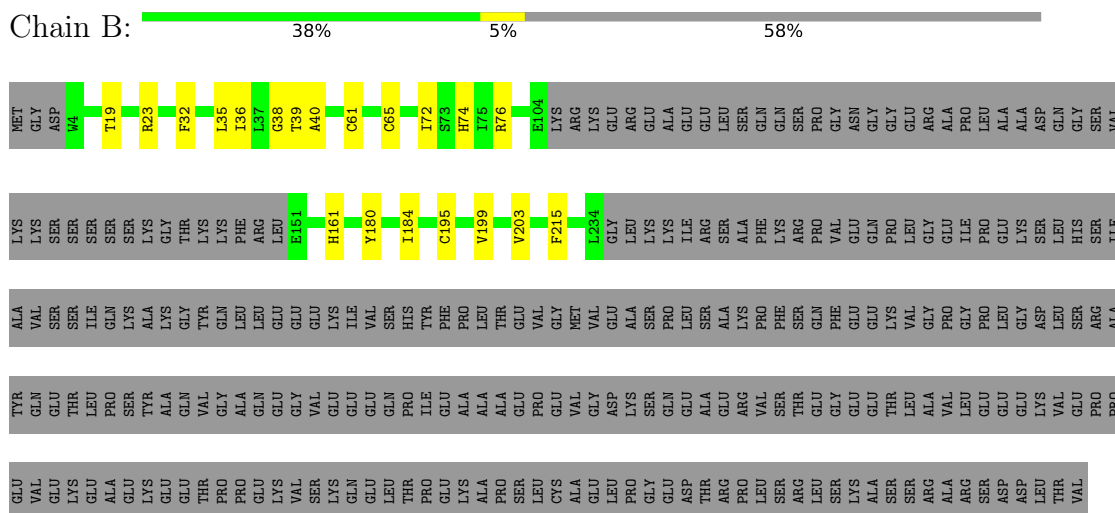
3 Residue-property plots

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. 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. 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.

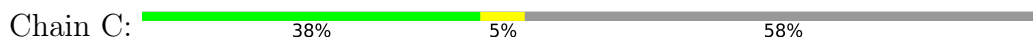
- Molecule 1: Gap junction alpha-8 protein



- Molecule 1: Gap junction alpha-8 protein



- Molecule 1: Gap junction alpha-8 protein



58%

- Molecule 1: Gap junction alpha-8 protein

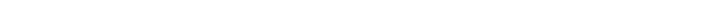
58%

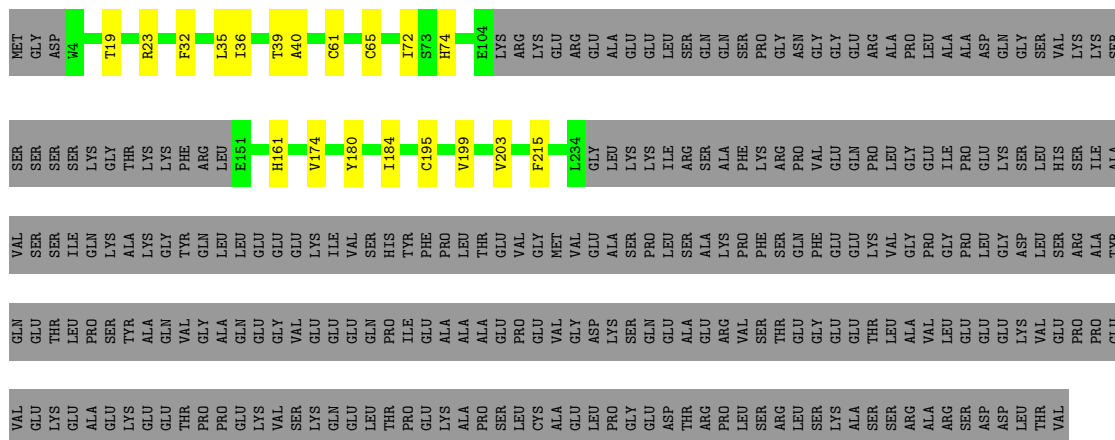
- Molecule 1: Gap junction alpha-8 protein

58%



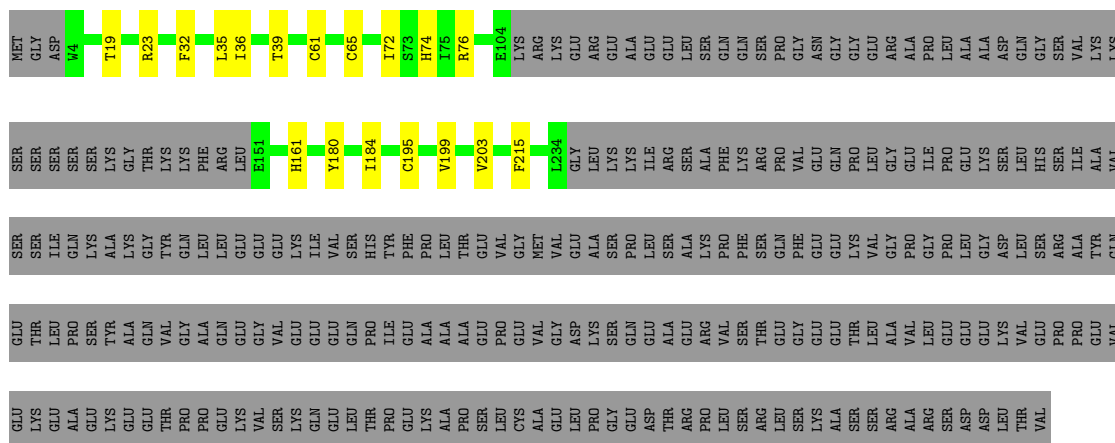
- Molecule 1: Gap junction alpha-8 protein

Chain I:  38% . 58%



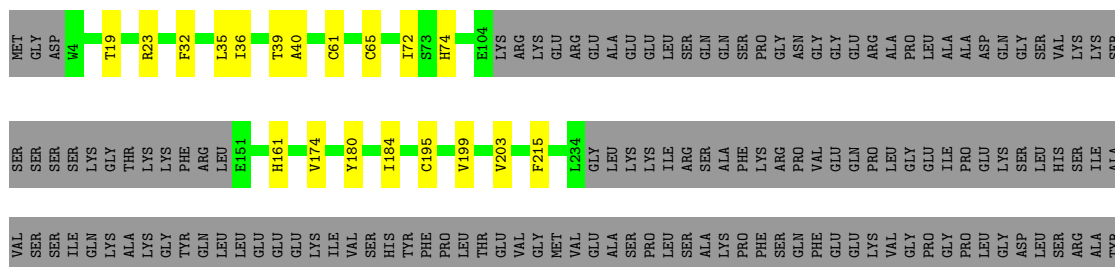
- Molecule 1: Gap junction alpha-8 protein

Chain J: 38% . 58%



- Molecule 1: Gap junction alpha-8 protein

Chain K: 38% . 58%



VAL	GLU	LYS	GLU	ALA	GLY	LYS	GLU	GLU	THR	PRO	PRO	GLU	LYS	VAL	SER	LYS	GLN	GLU	LEU	THR	PRO	GLU	LYS	ALA	GLU	LEU	PRO	SER	SER	CYS	ALA	ALA	GLU	LEU	PRO	GLY	GLU	ASP	THR	ARG	PRO	LEU	SER	ARG	ARG	LEU	SER	LYS	ALA	SER	SER	SER	ASP	ASP	LEU	THR	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain L: 37% 5% 58%

VAL	GLU	PRO	PRO	GLU	VAL	GLU	LYS	GLU	LYS	GLU	THR	THR	LEU	GLY	LYS	ALA	PRO	SER	CYS	ASP	THR	ARG	PRO	LEU	SER	LYS	ALA	ALA	SER	ARG	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

THR	VAL
-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	106741	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.00	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.825	Depositor
Minimum map value	-0.247	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	Unknown	
Map size ($\text{\AA}$)	378.88, 378.88, 378.88	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.96, 2.96, 2.96	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MC3

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	0.55	0/1481	0.49	0/2024
1	B	0.55	0/1481	0.49	0/2024
1	C	0.55	0/1481	0.49	0/2024
1	D	0.55	0/1481	0.49	0/2024
1	E	0.55	0/1481	0.49	0/2024
1	F	0.55	0/1481	0.49	0/2024
1	G	0.55	0/1481	0.49	0/2024
1	H	0.55	0/1481	0.49	0/2024
1	I	0.55	0/1481	0.49	0/2024
1	J	0.55	0/1481	0.49	0/2024
1	K	0.55	0/1481	0.49	0/2024
1	L	0.55	0/1481	0.49	0/2024
All	All	0.55	0/17772	0.49	0/24288

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

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	1439	1384	1375	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1439	1384	1375	15	0
1	C	1439	1384	1375	15	0
1	D	1439	1384	1375	15	0
1	E	1439	1384	1375	15	0
1	F	1439	1384	1375	16	0
1	G	1439	1384	1375	15	0
1	H	1439	1384	1375	14	0
1	I	1439	1384	1375	14	0
1	J	1439	1384	1375	13	0
1	K	1439	1384	1375	14	0
1	L	1439	1384	1375	17	0
2	A	370	672	567	2	0
2	B	370	672	567	1	0
2	C	370	672	567	1	0
2	D	370	672	567	3	0
2	E	370	672	567	3	0
2	F	370	672	567	3	0
2	G	370	672	567	1	0
2	H	370	672	567	1	0
2	I	370	672	567	1	0
2	J	370	672	567	1	0
2	K	370	672	567	4	0
2	L	370	672	567	5	0
3	A	75	0	0	0	0
3	B	75	0	0	0	0
3	C	75	0	0	0	0
3	D	75	0	0	0	0
3	E	75	0	0	0	0
3	F	75	0	0	0	0
3	G	75	0	0	0	0
3	H	75	0	0	0	0
3	I	75	0	0	0	0
3	J	75	0	0	0	0
3	K	75	0	0	0	0
3	L	75	0	0	0	0
All	All	22608	24672	23304	174	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 4.

The worst 5 of 174 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:B:32:PHE:HA	1:B:36:ILE:HD12	1.69	0.75
1:H:32:PHE:HA	1:H:36:ILE:HD12	1.69	0.75
1:A:32:PHE:HA	1:A:36:ILE:HD12	1.69	0.74
1:C:32:PHE:HA	1:C:36:ILE:HD12	1.69	0.74
1:I:32:PHE:HA	1:I:36:ILE:HD12	1.69	0.74

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	181/440 (41%)	181 (100%)	0	0	100	100
1	B	181/440 (41%)	181 (100%)	0	0	100	100
1	C	181/440 (41%)	181 (100%)	0	0	100	100
1	D	181/440 (41%)	181 (100%)	0	0	100	100
1	E	181/440 (41%)	181 (100%)	0	0	100	100
1	F	181/440 (41%)	181 (100%)	0	0	100	100
1	G	181/440 (41%)	181 (100%)	0	0	100	100
1	H	181/440 (41%)	181 (100%)	0	0	100	100
1	I	181/440 (41%)	181 (100%)	0	0	100	100
1	J	181/440 (41%)	181 (100%)	0	0	100	100
1	K	181/440 (41%)	181 (100%)	0	0	100	100
1	L	181/440 (41%)	181 (100%)	0	0	100	100
All	All	2172/5280 (41%)	2172 (100%)	0	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	151/385 (39%)	150 (99%)	1 (1%)	76	87
1	B	151/385 (39%)	150 (99%)	1 (1%)	76	87
1	C	151/385 (39%)	150 (99%)	1 (1%)	76	87
1	D	151/385 (39%)	150 (99%)	1 (1%)	76	87
1	E	151/385 (39%)	150 (99%)	1 (1%)	76	87
1	F	151/385 (39%)	150 (99%)	1 (1%)	76	87
1	G	151/385 (39%)	150 (99%)	1 (1%)	76	87
1	H	151/385 (39%)	150 (99%)	1 (1%)	76	87
1	I	151/385 (39%)	150 (99%)	1 (1%)	76	87
1	J	151/385 (39%)	150 (99%)	1 (1%)	76	87
1	K	151/385 (39%)	150 (99%)	1 (1%)	76	87
1	L	151/385 (39%)	150 (99%)	1 (1%)	76	87
All	All	1812/4620 (39%)	1800 (99%)	12 (1%)	73	87

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	161	HIS
1	I	161	HIS
1	L	161	HIS
1	J	161	HIS
1	D	161	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	95	HIS
1	I	74	HIS
1	L	57	GLN
1	H	49	GLN

Continued on next page...

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Mol	Chain	Res	Type
1	H	81	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

396 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	$\# Z > 2$
2	MC3	H	504	-	11,11,45	0.16	0	10,10,53	0.24	0
2	MC3	D	533	-	27,27,45	0.42	0	33,35,53	0.56	0
2	MC3	G	529	-	6,6,45	0.22	0	5,5,53	0.24	0
2	MC3	G	501	-	32,32,45	0.73	1 (3%)	35,37,53	1.13	2 (5%)
2	MC3	G	510	-	8,8,45	0.22	0	7,7,53	0.20	0
2	MC3	H	521	-	11,11,45	0.16	0	10,10,53	0.21	0
2	MC3	J	501	-	32,32,45	0.73	1 (3%)	35,37,53	1.13	2 (5%)
2	MC3	B	503	-	12,12,45	0.14	0	11,11,53	0.22	0
2	MC3	E	525	-	9,9,45	0.22	0	8,8,53	0.22	0
2	MC3	I	529	-	6,6,45	0.22	0	5,5,53	0.24	0
2	MC3	K	531	-	6,6,45	0.23	0	5,5,53	0.24	0
2	MC3	I	508	-	6,6,45	0.25	0	5,5,53	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	G	507	-	8,8,45	0.21	0	7,7,53	0.18	0
2	MC3	G	514	-	11,11,45	0.20	0	10,10,53	0.22	0
2	MC3	D	526	-	10,10,45	0.21	0	9,9,53	0.27	0
2	MC3	B	505	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	I	511	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	G	512	-	3,3,45	0.33	0	2,2,53	0.56	0
2	MC3	B	519	-	12,12,45	0.13	0	11,11,53	0.21	0
2	MC3	L	520	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	A	521	-	11,11,45	0.16	0	10,10,53	0.21	0
2	MC3	E	510	-	8,8,45	0.22	0	7,7,53	0.20	0
2	MC3	E	514	-	11,11,45	0.20	0	10,10,53	0.22	0
2	MC3	K	514	-	11,11,45	0.20	0	10,10,53	0.22	0
2	MC3	I	519	-	12,12,45	0.13	0	11,11,53	0.21	0
2	MC3	F	507	-	9,9,45	0.22	0	8,8,53	0.22	0
2	MC3	F	514	-	4,4,45	0.27	0	3,3,53	0.21	0
2	MC3	F	512	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	H	513	-	7,7,45	0.23	0	6,6,53	0.22	0
2	MC3	J	531	-	6,6,45	0.23	0	5,5,53	0.24	0
2	MC3	L	516	-	32,32,45	0.73	1 (3%)	35,37,53	1.13	2 (5%)
2	MC3	A	511	-	5,5,45	0.25	0	4,4,53	0.15	0
2	MC3	B	523	-	11,11,45	0.18	0	10,10,53	0.23	0
2	MC3	D	527	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	J	524	-	12,12,45	0.16	0	11,11,53	0.25	0
2	MC3	H	527	-	5,5,45	0.25	0	4,4,53	0.17	0
2	MC3	I	523	-	11,11,45	0.18	0	10,10,53	0.22	0
2	MC3	I	526	-	10,10,45	0.21	0	9,9,53	0.27	0
2	MC3	G	523	-	11,11,45	0.18	0	10,10,53	0.23	0
2	MC3	A	525	-	9,9,45	0.22	0	8,8,53	0.22	0
2	MC3	B	531	-	6,6,45	0.23	0	5,5,53	0.24	0
2	MC3	H	524	-	12,12,45	0.16	0	11,11,53	0.24	0
2	MC3	G	508	-	6,6,45	0.25	0	5,5,53	0.20	0
2	MC3	L	515	-	27,27,45	0.42	0	33,35,53	0.56	0
2	MC3	L	510	-	7,7,45	0.23	0	6,6,53	0.20	0
2	MC3	G	517	-	8,8,45	0.18	0	7,7,53	0.18	0
2	MC3	C	512	-	3,3,45	0.33	0	2,2,53	0.55	0
2	MC3	L	513	-	6,6,45	0.22	0	5,5,53	0.24	0
2	MC3	D	528	-	7,7,45	0.23	0	6,6,53	0.20	0
2	MC3	F	533	-	29,29,45	0.46	0	32,34,53	0.58	1 (3%)
2	MC3	A	508	-	6,6,45	0.24	0	5,5,53	0.19	0
2	MC3	L	522	-	8,8,45	0.21	0	7,7,53	0.18	0
2	MC3	J	502	-	12,12,45	0.14	0	11,11,53	0.15	0
2	MC3	H	509	-	7,7,45	0.24	0	6,6,53	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	B	517	-	8,8,45	0.18	0	7,7,53	0.18	0
2	MC3	L	506	-	12,12,45	0.16	0	11,11,53	0.24	0
2	MC3	D	516	-	6,6,45	0.21	0	5,5,53	0.17	0
2	MC3	C	528	-	7,7,45	0.23	0	6,6,53	0.20	0
2	MC3	D	525	-	9,9,45	0.22	0	8,8,53	0.22	0
2	MC3	H	533	-	27,27,45	0.42	0	33,35,53	0.56	0
2	MC3	D	524	-	12,12,45	0.16	0	11,11,53	0.24	0
2	MC3	B	509	-	7,7,45	0.24	0	6,6,53	0.19	0
2	MC3	L	533	-	29,29,45	0.45	0	32,34,53	0.57	1 (3%)
2	MC3	J	527	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	K	533	-	27,27,45	0.42	0	33,35,53	0.56	0
2	MC3	L	529	-	11,11,45	0.20	0	10,10,53	0.22	0
2	MC3	A	531	-	6,6,45	0.22	0	5,5,53	0.24	0
2	MC3	F	528	-	7,7,45	0.23	0	6,6,53	0.23	0
2	MC3	C	506	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	H	510	-	8,8,45	0.22	0	7,7,53	0.20	0
2	MC3	K	526	-	10,10,45	0.21	0	9,9,53	0.27	0
2	MC3	B	529	-	6,6,45	0.23	0	5,5,53	0.24	0
2	MC3	D	515	-	5,5,45	0.25	0	4,4,53	0.17	0
2	MC3	I	505	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	A	522	-	9,9,45	0.22	0	8,8,53	0.20	0
2	MC3	L	511	-	6,6,45	0.22	0	5,5,53	0.24	0
2	MC3	C	510	-	8,8,45	0.22	0	7,7,53	0.20	0
2	MC3	G	515	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	A	520	-	11,11,45	0.17	0	10,10,53	0.40	0
2	MC3	A	528	-	7,7,45	0.23	0	6,6,53	0.20	0
2	MC3	J	509	-	7,7,45	0.24	0	6,6,53	0.19	0
2	MC3	B	533	-	27,27,45	0.41	0	33,35,53	0.55	0
2	MC3	I	514	-	11,11,45	0.20	0	10,10,53	0.22	0
2	MC3	H	512	-	3,3,45	0.33	0	2,2,53	0.56	0
2	MC3	F	529	-	11,11,45	0.20	0	10,10,53	0.22	0
2	MC3	D	521	-	11,11,45	0.17	0	10,10,53	0.21	0
2	MC3	A	532	-	4,4,45	0.27	0	3,3,53	0.21	0
2	MC3	I	533	-	27,27,45	0.42	0	33,35,53	0.55	0
2	MC3	B	526	-	10,10,45	0.21	0	9,9,53	0.27	0
2	MC3	D	530	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	L	507	-	9,9,45	0.22	0	8,8,53	0.22	0
2	MC3	L	509	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	C	531	-	6,6,45	0.22	0	5,5,53	0.23	0
2	MC3	F	522	-	8,8,45	0.21	0	7,7,53	0.18	0
2	MC3	G	531	-	6,6,45	0.23	0	5,5,53	0.24	0
2	MC3	H	528	-	7,7,45	0.23	0	6,6,53	0.20	0
2	MC3	H	508	-	6,6,45	0.24	0	5,5,53	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	I	521	-	11,11,45	0.17	0	10,10,53	0.21	0
2	MC3	C	517	-	8,8,45	0.18	0	7,7,53	0.18	0
2	MC3	F	506	-	12,12,45	0.16	0	11,11,53	0.24	0
2	MC3	J	518	-	29,29,45	0.46	0	32,34,53	0.58	1 (3%)
2	MC3	H	506	-	11,11,45	0.19	0	10,10,53	0.20	0
2	MC3	A	518	-	29,29,45	0.45	0	32,34,53	0.58	1 (3%)
2	MC3	C	522	-	9,9,45	0.22	0	8,8,53	0.20	0
2	MC3	A	513	-	7,7,45	0.23	0	6,6,53	0.22	0
2	MC3	G	522	-	9,9,45	0.22	0	8,8,53	0.20	0
2	MC3	C	520	-	11,11,45	0.17	0	10,10,53	0.40	0
2	MC3	C	511	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	C	513	-	7,7,45	0.23	0	6,6,53	0.22	0
2	MC3	G	528	-	7,7,45	0.23	0	6,6,53	0.20	0
2	MC3	F	510	-	7,7,45	0.23	0	6,6,53	0.20	0
2	MC3	K	521	-	11,11,45	0.16	0	10,10,53	0.21	0
2	MC3	E	513	-	7,7,45	0.23	0	6,6,53	0.23	0
2	MC3	E	532	-	4,4,45	0.27	0	3,3,53	0.21	0
2	MC3	K	532	-	4,4,45	0.27	0	3,3,53	0.21	0
2	MC3	F	519	-	11,11,45	0.17	0	10,10,53	0.24	0
2	MC3	G	518	-	29,29,45	0.45	0	32,34,53	0.58	1 (3%)
2	MC3	C	503	-	12,12,45	0.14	0	11,11,53	0.21	0
2	MC3	K	520	-	11,11,45	0.17	0	10,10,53	0.40	0
2	MC3	E	505	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	F	501	-	12,12,45	0.13	0	11,11,53	0.21	0
2	MC3	I	502	-	12,12,45	0.14	0	11,11,53	0.16	0
2	MC3	I	531	-	6,6,45	0.23	0	5,5,53	0.24	0
2	MC3	B	530	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	K	515	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	E	508	-	6,6,45	0.24	0	5,5,53	0.19	0
2	MC3	C	526	-	10,10,45	0.21	0	9,9,53	0.27	0
2	MC3	A	523	-	11,11,45	0.18	0	10,10,53	0.22	0
2	MC3	D	502	-	12,12,45	0.14	0	11,11,53	0.15	0
2	MC3	K	516	-	6,6,45	0.22	0	5,5,53	0.18	0
2	MC3	K	504	-	11,11,45	0.16	0	10,10,53	0.24	0
2	MC3	F	509	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	K	525	-	9,9,45	0.22	0	8,8,53	0.22	0
2	MC3	B	516	-	6,6,45	0.22	0	5,5,53	0.18	0
2	MC3	J	520	-	11,11,45	0.17	0	10,10,53	0.40	0
2	MC3	A	504	-	11,11,45	0.16	0	10,10,53	0.24	0
2	MC3	A	509	-	7,7,45	0.24	0	6,6,53	0.19	0
2	MC3	C	508	-	6,6,45	0.24	0	5,5,53	0.19	0
2	MC3	H	531	-	6,6,45	0.23	0	5,5,53	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	C	523	-	11,11,45	0.18	0	10,10,53	0.23	0
2	MC3	E	507	-	8,8,45	0.21	0	7,7,53	0.18	0
2	MC3	L	532	-	8,8,45	0.18	0	7,7,53	0.18	0
2	MC3	I	525	-	9,9,45	0.21	0	8,8,53	0.22	0
2	MC3	G	511	-	5,5,45	0.24	0	4,4,53	0.15	0
2	MC3	C	507	-	8,8,45	0.21	0	7,7,53	0.18	0
2	MC3	K	505	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	B	520	-	11,11,45	0.17	0	10,10,53	0.40	0
2	MC3	H	507	-	8,8,45	0.21	0	7,7,53	0.18	0
2	MC3	B	515	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	L	514	-	4,4,45	0.27	0	3,3,53	0.21	0
2	MC3	D	520	-	11,11,45	0.17	0	10,10,53	0.40	0
2	MC3	E	515	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	H	529	-	6,6,45	0.22	0	5,5,53	0.24	0
2	MC3	B	504	-	11,11,45	0.16	0	10,10,53	0.24	0
2	MC3	K	530	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	H	511	-	5,5,45	0.25	0	4,4,53	0.15	0
2	MC3	K	502	-	12,12,45	0.14	0	11,11,53	0.15	0
2	MC3	D	504	-	11,11,45	0.16	0	10,10,53	0.24	0
2	MC3	L	518	-	12,12,45	0.14	0	11,11,53	0.22	0
2	MC3	A	507	-	8,8,45	0.21	0	7,7,53	0.18	0
2	MC3	F	517	-	12,12,45	0.14	0	11,11,53	0.15	0
2	MC3	A	512	-	3,3,45	0.33	0	2,2,53	0.56	0
2	MC3	J	529	-	6,6,45	0.22	0	5,5,53	0.24	0
2	MC3	A	527	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	J	526	-	10,10,45	0.21	0	9,9,53	0.27	0
2	MC3	H	532	-	4,4,45	0.27	0	3,3,53	0.21	0
2	MC3	H	503	-	12,12,45	0.15	0	11,11,53	0.22	0
2	MC3	I	530	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	J	507	-	8,8,45	0.21	0	7,7,53	0.18	0
2	MC3	I	512	-	3,3,45	0.33	0	2,2,53	0.56	0
2	MC3	F	515	-	27,27,45	0.42	0	33,35,53	0.56	0
2	MC3	F	523	-	6,6,45	0.24	0	5,5,53	0.19	0
2	MC3	A	529	-	6,6,45	0.22	0	5,5,53	0.24	0
2	MC3	C	509	-	7,7,45	0.24	0	6,6,53	0.19	0
2	MC3	G	503	-	12,12,45	0.14	0	11,11,53	0.21	0
2	MC3	G	504	-	11,11,45	0.16	0	10,10,53	0.24	0
2	MC3	L	501	-	12,12,45	0.13	0	11,11,53	0.21	0
2	MC3	J	532	-	4,4,45	0.27	0	3,3,53	0.21	0
2	MC3	D	512	-	3,3,45	0.33	0	2,2,53	0.55	0
2	MC3	L	508	-	10,10,45	0.21	0	9,9,53	0.27	0
2	MC3	A	501	-	32,32,45	0.73	1 (3%)	35,37,53	1.13	2 (5%)
2	MC3	H	523	-	11,11,45	0.18	0	10,10,53	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	B	514	-	11,11,45	0.19	0	10,10,53	0.22	0
2	MC3	C	532	-	4,4,45	0.27	0	3,3,53	0.21	0
2	MC3	B	521	-	11,11,45	0.17	0	10,10,53	0.21	0
2	MC3	D	513	-	7,7,45	0.22	0	6,6,53	0.22	0
2	MC3	K	528	-	7,7,45	0.23	0	6,6,53	0.20	0
2	MC3	L	531	-	6,6,45	0.21	0	5,5,53	0.17	0
2	MC3	K	522	-	9,9,45	0.22	0	8,8,53	0.20	0
2	MC3	B	502	-	12,12,45	0.14	0	11,11,53	0.15	0
2	MC3	J	521	-	11,11,45	0.17	0	10,10,53	0.21	0
2	MC3	E	506	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	L	517	-	12,12,45	0.14	0	11,11,53	0.15	0
2	MC3	E	530	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	J	525	-	9,9,45	0.22	0	8,8,53	0.22	0
2	MC3	L	524	-	7,7,45	0.24	0	6,6,53	0.19	0
2	MC3	A	533	-	27,27,45	0.42	0	33,35,53	0.55	0
2	MC3	D	506	-	11,11,45	0.19	0	10,10,53	0.20	0
2	MC3	G	530	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	L	503	-	11,11,45	0.17	0	10,10,53	0.21	0
2	MC3	K	517	-	8,8,45	0.18	0	7,7,53	0.18	0
2	MC3	A	526	-	10,10,45	0.21	0	9,9,53	0.27	0
2	MC3	I	516	-	6,6,45	0.22	0	5,5,53	0.18	0
2	MC3	G	527	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	L	523	-	6,6,45	0.24	0	5,5,53	0.20	0
2	MC3	J	530	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	K	507	-	8,8,45	0.21	0	7,7,53	0.18	0
2	MC3	J	514	-	11,11,45	0.20	0	10,10,53	0.22	0
2	MC3	H	530	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	B	528	-	7,7,45	0.23	0	6,6,53	0.20	0
2	MC3	I	517	-	8,8,45	0.18	0	7,7,53	0.18	0
2	MC3	J	512	-	3,3,45	0.33	0	2,2,53	0.56	0
2	MC3	B	525	-	9,9,45	0.22	0	8,8,53	0.22	0
2	MC3	L	525	-	8,8,45	0.22	0	7,7,53	0.19	0
2	MC3	E	520	-	11,11,45	0.17	0	10,10,53	0.40	0
2	MC3	C	501	-	32,32,45	0.73	1 (3%)	35,37,53	1.13	2 (5%)
2	MC3	D	509	-	7,7,45	0.24	0	6,6,53	0.19	0
2	MC3	B	518	-	29,29,45	0.46	0	32,34,53	0.58	1 (3%)
2	MC3	G	520	-	11,11,45	0.17	0	10,10,53	0.40	0
2	MC3	I	515	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	E	504	-	11,11,45	0.16	0	10,10,53	0.24	0
2	MC3	F	531	-	6,6,45	0.21	0	5,5,53	0.17	0
2	MC3	L	527	-	3,3,45	0.33	0	2,2,53	0.56	0
2	MC3	F	532	-	8,8,45	0.18	0	7,7,53	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	I	518	-	29,29,45	0.45	0	32,34,53	0.58	1 (3%)
2	MC3	I	504	-	11,11,45	0.17	0	10,10,53	0.24	0
2	MC3	F	505	-	11,11,45	0.18	0	10,10,53	0.22	0
2	MC3	G	509	-	7,7,45	0.24	0	6,6,53	0.19	0
2	MC3	D	510	-	8,8,45	0.23	0	7,7,53	0.20	0
2	MC3	J	528	-	7,7,45	0.23	0	6,6,53	0.20	0
2	MC3	G	524	-	12,12,45	0.16	0	11,11,53	0.25	0
2	MC3	H	505	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	D	507	-	8,8,45	0.21	0	7,7,53	0.18	0
2	MC3	F	502	-	11,11,45	0.17	0	10,10,53	0.40	0
2	MC3	F	503	-	11,11,45	0.16	0	10,10,53	0.21	0
2	MC3	E	512	-	3,3,45	0.33	0	2,2,53	0.56	0
2	MC3	A	516	-	6,6,45	0.21	0	5,5,53	0.17	0
2	MC3	I	520	-	11,11,45	0.17	0	10,10,53	0.40	0
2	MC3	I	513	-	7,7,45	0.23	0	6,6,53	0.22	0
2	MC3	B	512	-	3,3,45	0.33	0	2,2,53	0.56	0
2	MC3	D	519	-	12,12,45	0.13	0	11,11,53	0.21	0
2	MC3	A	506	-	11,11,45	0.18	0	10,10,53	0.20	0
2	MC3	E	517	-	8,8,45	0.18	0	7,7,53	0.18	0
2	MC3	I	522	-	9,9,45	0.22	0	8,8,53	0.20	0
2	MC3	C	530	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	E	511	-	5,5,45	0.25	0	4,4,53	0.15	0
2	MC3	A	515	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	C	502	-	12,12,45	0.14	0	11,11,53	0.15	0
2	MC3	E	522	-	9,9,45	0.22	0	8,8,53	0.20	0
2	MC3	D	508	-	6,6,45	0.25	0	5,5,53	0.20	0
2	MC3	E	523	-	11,11,45	0.18	0	10,10,53	0.23	0
2	MC3	J	516	-	6,6,45	0.21	0	5,5,53	0.17	0
2	MC3	G	502	-	12,12,45	0.14	0	11,11,53	0.15	0
2	MC3	B	522	-	9,9,45	0.22	0	8,8,53	0.20	0
2	MC3	K	506	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	K	513	-	7,7,45	0.23	0	6,6,53	0.22	0
2	MC3	A	510	-	8,8,45	0.22	0	7,7,53	0.20	0
2	MC3	D	511	-	5,5,45	0.24	0	4,4,53	0.15	0
2	MC3	K	518	-	29,29,45	0.46	0	32,34,53	0.58	1 (3%)
2	MC3	B	506	-	11,11,45	0.18	0	10,10,53	0.20	0
2	MC3	H	514	-	11,11,45	0.20	0	10,10,53	0.22	0
2	MC3	C	529	-	6,6,45	0.22	0	5,5,53	0.24	0
2	MC3	E	527	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	K	527	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	E	503	-	12,12,45	0.14	0	11,11,53	0.21	0
2	MC3	H	517	-	8,8,45	0.18	0	7,7,53	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	L	519	-	11,11,45	0.16	0	10,10,53	0.24	0
2	MC3	E	533	-	27,27,45	0.42	0	33,35,53	0.56	0
2	MC3	I	507	-	8,8,45	0.21	0	7,7,53	0.18	0
2	MC3	E	529	-	6,6,45	0.22	0	5,5,53	0.24	0
2	MC3	E	519	-	12,12,45	0.13	0	11,11,53	0.21	0
2	MC3	L	505	-	11,11,45	0.18	0	10,10,53	0.22	0
2	MC3	A	503	-	12,12,45	0.14	0	11,11,53	0.22	0
2	MC3	E	526	-	10,10,45	0.21	0	9,9,53	0.27	0
2	MC3	I	527	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	J	513	-	7,7,45	0.23	0	6,6,53	0.22	0
2	MC3	K	519	-	12,12,45	0.13	0	11,11,53	0.21	0
2	MC3	K	501	-	32,32,45	0.73	1 (3%)	35,37,53	1.13	2 (5%)
2	MC3	C	533	-	27,27,45	0.42	0	33,35,53	0.55	0
2	MC3	G	521	-	11,11,45	0.17	0	10,10,53	0.21	0
2	MC3	F	525	-	8,8,45	0.22	0	7,7,53	0.20	0
2	MC3	I	510	-	8,8,45	0.22	0	7,7,53	0.20	0
2	MC3	J	522	-	9,9,45	0.22	0	8,8,53	0.20	0
2	MC3	J	506	-	11,11,45	0.18	0	10,10,53	0.21	0
2	MC3	G	532	-	4,4,45	0.27	0	3,3,53	0.21	0
2	MC3	K	509	-	7,7,45	0.24	0	6,6,53	0.19	0
2	MC3	H	516	-	6,6,45	0.21	0	5,5,53	0.17	0
2	MC3	B	527	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	H	525	-	9,9,45	0.22	0	8,8,53	0.22	0
2	MC3	H	519	-	12,12,45	0.13	0	11,11,53	0.21	0
2	MC3	J	503	-	12,12,45	0.14	0	11,11,53	0.21	0
2	MC3	H	526	-	10,10,45	0.21	0	9,9,53	0.27	0
2	MC3	J	505	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	B	510	-	8,8,45	0.23	0	7,7,53	0.20	0
2	MC3	I	509	-	7,7,45	0.24	0	6,6,53	0.19	0
2	MC3	L	521	-	11,11,45	0.19	0	10,10,53	0.20	0
2	MC3	J	519	-	12,12,45	0.13	0	11,11,53	0.21	0
2	MC3	H	502	-	12,12,45	0.14	0	11,11,53	0.15	0
2	MC3	G	525	-	9,9,45	0.22	0	8,8,53	0.22	0
2	MC3	J	508	-	6,6,45	0.24	0	5,5,53	0.19	0
2	MC3	J	510	-	8,8,45	0.22	0	7,7,53	0.20	0
2	MC3	A	517	-	8,8,45	0.18	0	7,7,53	0.18	0
2	MC3	J	533	-	27,27,45	0.42	0	33,35,53	0.55	0
2	MC3	B	501	-	32,32,45	0.72	1 (3%)	35,37,53	1.13	2 (5%)
2	MC3	C	519	-	12,12,45	0.13	0	11,11,53	0.21	0
2	MC3	L	530	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	K	510	-	8,8,45	0.22	0	7,7,53	0.20	0
2	MC3	D	501	-	32,32,45	0.73	1 (3%)	35,37,53	1.13	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	C	505	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	F	530	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	J	511	-	5,5,45	0.25	0	4,4,53	0.15	0
2	MC3	D	522	-	9,9,45	0.22	0	8,8,53	0.20	0
2	MC3	J	523	-	11,11,45	0.18	0	10,10,53	0.23	0
2	MC3	B	511	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	B	513	-	7,7,45	0.23	0	6,6,53	0.22	0
2	MC3	K	508	-	6,6,45	0.24	0	5,5,53	0.19	0
2	MC3	L	504	-	9,9,45	0.22	0	8,8,53	0.20	0
2	MC3	I	528	-	7,7,45	0.23	0	6,6,53	0.20	0
2	MC3	E	509	-	7,7,45	0.24	0	6,6,53	0.19	0
2	MC3	E	516	-	6,6,45	0.21	0	5,5,53	0.17	0
2	MC3	F	516	-	32,32,45	0.73	1 (3%)	35,37,53	1.13	2 (5%)
2	MC3	C	518	-	29,29,45	0.46	0	32,34,53	0.58	1 (3%)
2	MC3	K	524	-	12,12,45	0.16	0	11,11,53	0.25	0
2	MC3	G	533	-	27,27,45	0.42	0	33,35,53	0.56	0
2	MC3	D	505	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	D	532	-	4,4,45	0.27	0	3,3,53	0.21	0
2	MC3	I	506	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	L	526	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	C	516	-	6,6,45	0.22	0	5,5,53	0.18	0
2	MC3	F	520	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	E	528	-	7,7,45	0.23	0	6,6,53	0.20	0
2	MC3	K	529	-	6,6,45	0.22	0	5,5,53	0.24	0
2	MC3	H	522	-	9,9,45	0.22	0	8,8,53	0.20	0
2	MC3	D	514	-	11,11,45	0.20	0	10,10,53	0.22	0
2	MC3	D	523	-	11,11,45	0.18	0	10,10,53	0.23	0
2	MC3	K	511	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	B	508	-	6,6,45	0.24	0	5,5,53	0.19	0
2	MC3	A	530	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	L	502	-	11,11,45	0.16	0	10,10,53	0.40	0
2	MC3	D	518	-	29,29,45	0.45	0	32,34,53	0.58	1 (3%)
2	MC3	E	518	-	29,29,45	0.46	0	32,34,53	0.58	1 (3%)
2	MC3	F	524	-	7,7,45	0.24	0	6,6,53	0.19	0
2	MC3	C	515	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	J	504	-	11,11,45	0.16	0	10,10,53	0.24	0
2	MC3	B	524	-	12,12,45	0.16	0	11,11,53	0.24	0
2	MC3	I	501	-	32,32,45	0.73	1 (3%)	35,37,53	1.13	2 (5%)
2	MC3	F	527	-	3,3,45	0.33	0	2,2,53	0.56	0
2	MC3	E	524	-	12,12,45	0.16	0	11,11,53	0.25	0
2	MC3	C	504	-	11,11,45	0.16	0	10,10,53	0.24	0
2	MC3	C	514	-	11,11,45	0.20	0	10,10,53	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	C	521	-	11,11,45	0.17	0	10,10,53	0.21	0
2	MC3	F	508	-	10,10,45	0.21	0	9,9,53	0.27	0
2	MC3	F	518	-	12,12,45	0.14	0	11,11,53	0.22	0
2	MC3	F	511	-	6,6,45	0.22	0	5,5,53	0.24	0
2	MC3	A	519	-	12,12,45	0.13	0	11,11,53	0.21	0
2	MC3	F	513	-	6,6,45	0.23	0	5,5,53	0.24	0
2	MC3	J	517	-	8,8,45	0.18	0	7,7,53	0.18	0
2	MC3	G	506	-	11,11,45	0.18	0	10,10,53	0.20	0
2	MC3	B	507	-	8,8,45	0.21	0	7,7,53	0.18	0
2	MC3	E	501	-	32,32,45	0.73	1 (3%)	35,37,53	1.13	2 (5%)
2	MC3	G	526	-	10,10,45	0.21	0	9,9,53	0.27	0
2	MC3	L	512	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	H	518	-	29,29,45	0.45	0	32,34,53	0.58	1 (3%)
2	MC3	E	531	-	6,6,45	0.23	0	5,5,53	0.24	0
2	MC3	A	514	-	11,11,45	0.20	0	10,10,53	0.22	0
2	MC3	J	515	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	G	505	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	D	531	-	6,6,45	0.22	0	5,5,53	0.23	0
2	MC3	E	521	-	11,11,45	0.16	0	10,10,53	0.21	0
2	MC3	D	503	-	12,12,45	0.14	0	11,11,53	0.22	0
2	MC3	G	513	-	7,7,45	0.23	0	6,6,53	0.22	0
2	MC3	K	503	-	12,12,45	0.14	0	11,11,53	0.21	0
2	MC3	A	502	-	12,12,45	0.14	0	11,11,53	0.15	0
2	MC3	D	517	-	8,8,45	0.18	0	7,7,53	0.18	0
2	MC3	K	512	-	3,3,45	0.33	0	2,2,53	0.56	0
2	MC3	G	516	-	6,6,45	0.22	0	5,5,53	0.17	0
2	MC3	B	532	-	4,4,45	0.27	0	3,3,53	0.21	0
2	MC3	A	524	-	12,12,45	0.16	0	11,11,53	0.24	0
2	MC3	C	527	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	D	529	-	6,6,45	0.22	0	5,5,53	0.24	0
2	MC3	L	528	-	7,7,45	0.23	0	6,6,53	0.22	0
2	MC3	F	526	-	5,5,45	0.25	0	4,4,53	0.16	0
2	MC3	C	525	-	9,9,45	0.22	0	8,8,53	0.22	0
2	MC3	I	532	-	4,4,45	0.27	0	3,3,53	0.21	0
2	MC3	I	503	-	12,12,45	0.14	0	11,11,53	0.22	0
2	MC3	H	501	-	32,32,45	0.73	1 (3%)	35,37,53	1.13	2 (5%)
2	MC3	A	505	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	H	520	-	11,11,45	0.17	0	10,10,53	0.40	0
2	MC3	C	524	-	12,12,45	0.16	0	11,11,53	0.25	0
2	MC3	I	524	-	12,12,45	0.16	0	11,11,53	0.25	0
2	MC3	F	504	-	9,9,45	0.22	0	8,8,53	0.20	0
2	MC3	H	515	-	5,5,45	0.25	0	4,4,53	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	F	521	-	11,11,45	0.19	0	10,10,53	0.21	0
2	MC3	K	523	-	11,11,45	0.18	0	10,10,53	0.22	0
2	MC3	G	519	-	12,12,45	0.13	0	11,11,53	0.21	0
2	MC3	E	502	-	12,12,45	0.14	0	11,11,53	0.16	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
2	MC3	H	504	-	-	0/9/9/49	-
2	MC3	D	533	-	-	17/31/31/49	-
2	MC3	G	529	-	-	0/4/4/49	-
2	MC3	G	501	-	-	8/34/34/49	-
2	MC3	G	510	-	-	0/6/6/49	-
2	MC3	H	521	-	-	0/9/9/49	-
2	MC3	J	501	-	-	8/34/34/49	-
2	MC3	B	503	-	-	0/10/10/49	-
2	MC3	E	525	-	-	0/7/7/49	-
2	MC3	I	529	-	-	0/4/4/49	-
2	MC3	K	531	-	-	0/4/4/49	-
2	MC3	I	508	-	-	0/4/4/49	-
2	MC3	G	507	-	-	0/6/6/49	-
2	MC3	G	514	-	-	3/9/9/49	-
2	MC3	D	526	-	-	0/8/8/49	-
2	MC3	B	505	-	-	0/9/9/49	-
2	MC3	I	511	-	-	0/3/3/49	-
2	MC3	G	512	-	-	1/1/1/49	-
2	MC3	B	519	-	-	0/10/10/49	-
2	MC3	L	520	-	-	0/9/9/49	-
2	MC3	A	521	-	-	0/9/9/49	-
2	MC3	E	510	-	-	0/6/6/49	-
2	MC3	E	514	-	-	3/9/9/49	-
2	MC3	K	514	-	-	3/9/9/49	-
2	MC3	I	519	-	-	0/10/10/49	-
2	MC3	F	507	-	-	0/7/7/49	-
2	MC3	F	514	-	-	0/2/2/49	-
2	MC3	F	512	-	-	1/3/3/49	-
2	MC3	H	513	-	-	0/5/5/49	-
2	MC3	J	531	-	-	0/4/4/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	L	516	-	-	8/34/34/49	-
2	MC3	A	511	-	-	0/3/3/49	-
2	MC3	B	523	-	-	0/9/9/49	-
2	MC3	D	527	-	-	0/3/3/49	-
2	MC3	J	524	-	-	0/10/10/49	-
2	MC3	H	527	-	-	0/3/3/49	-
2	MC3	I	523	-	-	0/9/9/49	-
2	MC3	I	526	-	-	0/8/8/49	-
2	MC3	G	523	-	-	0/9/9/49	-
2	MC3	A	525	-	-	0/7/7/49	-
2	MC3	B	531	-	-	0/4/4/49	-
2	MC3	H	524	-	-	0/10/10/49	-
2	MC3	G	508	-	-	0/4/4/49	-
2	MC3	L	515	-	-	17/31/31/49	-
2	MC3	L	510	-	-	0/5/5/49	-
2	MC3	G	517	-	-	1/6/6/49	-
2	MC3	C	512	-	-	1/1/1/49	-
2	MC3	L	513	-	-	0/4/4/49	-
2	MC3	D	528	-	-	0/5/5/49	-
2	MC3	F	533	-	-	11/31/31/49	-
2	MC3	A	508	-	-	0/4/4/49	-
2	MC3	L	522	-	-	0/6/6/49	-
2	MC3	J	502	-	-	0/10/10/49	-
2	MC3	H	509	-	-	0/5/5/49	-
2	MC3	B	517	-	-	1/6/6/49	-
2	MC3	L	506	-	-	0/10/10/49	-
2	MC3	D	516	-	-	1/4/4/49	-
2	MC3	C	528	-	-	0/5/5/49	-
2	MC3	D	525	-	-	0/7/7/49	-
2	MC3	H	533	-	-	17/31/31/49	-
2	MC3	D	524	-	-	0/10/10/49	-
2	MC3	B	509	-	-	0/5/5/49	-
2	MC3	L	533	-	-	11/31/31/49	-
2	MC3	J	527	-	-	0/3/3/49	-
2	MC3	K	533	-	-	17/31/31/49	-
2	MC3	L	529	-	-	3/9/9/49	-
2	MC3	A	531	-	-	0/4/4/49	-
2	MC3	F	528	-	-	0/5/5/49	-
2	MC3	C	506	-	-	0/9/9/49	-
2	MC3	H	510	-	-	0/6/6/49	-
2	MC3	K	526	-	-	0/8/8/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	B	529	-	-	0/4/4/49	-
2	MC3	D	515	-	-	0/3/3/49	-
2	MC3	I	505	-	-	0/9/9/49	-
2	MC3	A	522	-	-	0/7/7/49	-
2	MC3	L	511	-	-	0/4/4/49	-
2	MC3	C	510	-	-	0/6/6/49	-
2	MC3	G	515	-	-	0/3/3/49	-
2	MC3	A	520	-	-	0/9/9/49	-
2	MC3	A	528	-	-	0/5/5/49	-
2	MC3	J	509	-	-	0/5/5/49	-
2	MC3	B	533	-	-	17/31/31/49	-
2	MC3	I	514	-	-	3/9/9/49	-
2	MC3	H	512	-	-	1/1/1/49	-
2	MC3	F	529	-	-	3/9/9/49	-
2	MC3	D	521	-	-	0/9/9/49	-
2	MC3	A	532	-	-	0/2/2/49	-
2	MC3	I	533	-	-	17/31/31/49	-
2	MC3	B	526	-	-	0/8/8/49	-
2	MC3	D	530	-	-	1/3/3/49	-
2	MC3	L	507	-	-	0/7/7/49	-
2	MC3	L	509	-	-	0/3/3/49	-
2	MC3	C	531	-	-	0/4/4/49	-
2	MC3	F	522	-	-	0/6/6/49	-
2	MC3	G	531	-	-	0/4/4/49	-
2	MC3	H	528	-	-	0/5/5/49	-
2	MC3	H	508	-	-	0/4/4/49	-
2	MC3	I	521	-	-	0/9/9/49	-
2	MC3	C	517	-	-	1/6/6/49	-
2	MC3	F	506	-	-	0/10/10/49	-
2	MC3	J	518	-	-	11/31/31/49	-
2	MC3	H	506	-	-	0/9/9/49	-
2	MC3	A	518	-	-	11/31/31/49	-
2	MC3	C	522	-	-	0/7/7/49	-
2	MC3	A	513	-	-	0/5/5/49	-
2	MC3	G	522	-	-	0/7/7/49	-
2	MC3	C	520	-	-	0/9/9/49	-
2	MC3	C	511	-	-	0/3/3/49	-
2	MC3	C	513	-	-	0/5/5/49	-
2	MC3	G	528	-	-	0/5/5/49	-
2	MC3	F	510	-	-	0/5/5/49	-
2	MC3	K	521	-	-	0/9/9/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	E	513	-	-	0/5/5/49	-
2	MC3	E	532	-	-	0/2/2/49	-
2	MC3	K	532	-	-	0/2/2/49	-
2	MC3	F	519	-	-	0/9/9/49	-
2	MC3	G	518	-	-	11/31/31/49	-
2	MC3	C	503	-	-	0/10/10/49	-
2	MC3	K	520	-	-	0/9/9/49	-
2	MC3	E	505	-	-	0/9/9/49	-
2	MC3	F	501	-	-	0/10/10/49	-
2	MC3	I	502	-	-	0/10/10/49	-
2	MC3	I	531	-	-	0/4/4/49	-
2	MC3	B	530	-	-	1/3/3/49	-
2	MC3	K	515	-	-	0/3/3/49	-
2	MC3	E	508	-	-	0/4/4/49	-
2	MC3	C	526	-	-	0/8/8/49	-
2	MC3	A	523	-	-	0/9/9/49	-
2	MC3	D	502	-	-	0/10/10/49	-
2	MC3	K	516	-	-	1/4/4/49	-
2	MC3	K	504	-	-	0/9/9/49	-
2	MC3	F	509	-	-	0/3/3/49	-
2	MC3	K	525	-	-	0/7/7/49	-
2	MC3	B	516	-	-	1/4/4/49	-
2	MC3	J	520	-	-	0/9/9/49	-
2	MC3	A	504	-	-	0/9/9/49	-
2	MC3	A	509	-	-	0/5/5/49	-
2	MC3	C	508	-	-	0/4/4/49	-
2	MC3	H	531	-	-	0/4/4/49	-
2	MC3	C	523	-	-	0/9/9/49	-
2	MC3	E	507	-	-	0/6/6/49	-
2	MC3	L	532	-	-	1/6/6/49	-
2	MC3	I	525	-	-	0/7/7/49	-
2	MC3	G	511	-	-	0/3/3/49	-
2	MC3	C	507	-	-	0/6/6/49	-
2	MC3	K	505	-	-	0/9/9/49	-
2	MC3	B	520	-	-	0/9/9/49	-
2	MC3	H	507	-	-	0/6/6/49	-
2	MC3	B	515	-	-	0/3/3/49	-
2	MC3	L	514	-	-	0/2/2/49	-
2	MC3	D	520	-	-	0/9/9/49	-
2	MC3	E	515	-	-	0/3/3/49	-
2	MC3	H	529	-	-	0/4/4/49	-
2	MC3	B	504	-	-	0/9/9/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	K	530	-	-	1/3/3/49	-
2	MC3	H	511	-	-	0/3/3/49	-
2	MC3	K	502	-	-	0/10/10/49	-
2	MC3	D	504	-	-	0/9/9/49	-
2	MC3	L	518	-	-	0/10/10/49	-
2	MC3	A	507	-	-	0/6/6/49	-
2	MC3	F	517	-	-	0/10/10/49	-
2	MC3	A	512	-	-	1/1/1/49	-
2	MC3	J	529	-	-	0/4/4/49	-
2	MC3	A	527	-	-	0/3/3/49	-
2	MC3	J	526	-	-	0/8/8/49	-
2	MC3	H	532	-	-	0/2/2/49	-
2	MC3	H	503	-	-	0/10/10/49	-
2	MC3	I	530	-	-	1/3/3/49	-
2	MC3	J	507	-	-	0/6/6/49	-
2	MC3	I	512	-	-	1/1/1/49	-
2	MC3	F	515	-	-	17/31/31/49	-
2	MC3	F	523	-	-	0/4/4/49	-
2	MC3	A	529	-	-	0/4/4/49	-
2	MC3	C	509	-	-	0/5/5/49	-
2	MC3	G	503	-	-	0/10/10/49	-
2	MC3	G	504	-	-	0/9/9/49	-
2	MC3	L	501	-	-	0/10/10/49	-
2	MC3	J	532	-	-	0/2/2/49	-
2	MC3	D	512	-	-	1/1/1/49	-
2	MC3	L	508	-	-	0/8/8/49	-
2	MC3	A	501	-	-	8/34/34/49	-
2	MC3	H	523	-	-	0/9/9/49	-
2	MC3	B	514	-	-	3/9/9/49	-
2	MC3	C	532	-	-	0/2/2/49	-
2	MC3	B	521	-	-	0/9/9/49	-
2	MC3	D	513	-	-	0/5/5/49	-
2	MC3	K	528	-	-	0/5/5/49	-
2	MC3	L	531	-	-	1/4/4/49	-
2	MC3	K	522	-	-	0/7/7/49	-
2	MC3	B	502	-	-	0/10/10/49	-
2	MC3	J	521	-	-	0/9/9/49	-
2	MC3	E	506	-	-	0/9/9/49	-
2	MC3	L	517	-	-	0/10/10/49	-
2	MC3	E	530	-	-	1/3/3/49	-
2	MC3	J	525	-	-	0/7/7/49	-
2	MC3	L	524	-	-	0/5/5/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	A	533	-	-	17/31/31/49	-
2	MC3	D	506	-	-	0/9/9/49	-
2	MC3	G	530	-	-	1/3/3/49	-
2	MC3	L	503	-	-	0/9/9/49	-
2	MC3	K	517	-	-	1/6/6/49	-
2	MC3	A	526	-	-	0/8/8/49	-
2	MC3	I	516	-	-	1/4/4/49	-
2	MC3	G	527	-	-	0/3/3/49	-
2	MC3	L	523	-	-	0/4/4/49	-
2	MC3	J	530	-	-	1/3/3/49	-
2	MC3	K	507	-	-	0/6/6/49	-
2	MC3	J	514	-	-	3/9/9/49	-
2	MC3	H	530	-	-	1/3/3/49	-
2	MC3	B	528	-	-	0/5/5/49	-
2	MC3	I	517	-	-	1/6/6/49	-
2	MC3	J	512	-	-	1/1/1/49	-
2	MC3	B	525	-	-	0/7/7/49	-
2	MC3	L	525	-	-	0/6/6/49	-
2	MC3	E	520	-	-	0/9/9/49	-
2	MC3	C	501	-	-	8/34/34/49	-
2	MC3	D	509	-	-	0/5/5/49	-
2	MC3	B	518	-	-	11/31/31/49	-
2	MC3	G	520	-	-	0/9/9/49	-
2	MC3	I	515	-	-	0/3/3/49	-
2	MC3	E	504	-	-	0/9/9/49	-
2	MC3	F	531	-	-	1/4/4/49	-
2	MC3	L	527	-	-	1/1/1/49	-
2	MC3	F	532	-	-	1/6/6/49	-
2	MC3	I	518	-	-	11/31/31/49	-
2	MC3	I	504	-	-	0/9/9/49	-
2	MC3	F	505	-	-	0/9/9/49	-
2	MC3	G	509	-	-	0/5/5/49	-
2	MC3	D	510	-	-	0/6/6/49	-
2	MC3	J	528	-	-	0/5/5/49	-
2	MC3	G	524	-	-	0/10/10/49	-
2	MC3	H	505	-	-	0/9/9/49	-
2	MC3	D	507	-	-	0/6/6/49	-
2	MC3	F	502	-	-	0/9/9/49	-
2	MC3	F	503	-	-	0/9/9/49	-
2	MC3	E	512	-	-	1/1/1/49	-
2	MC3	A	516	-	-	1/4/4/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	I	520	-	-	0/9/9/49	-
2	MC3	I	513	-	-	0/5/5/49	-
2	MC3	B	512	-	-	1/1/1/49	-
2	MC3	D	519	-	-	0/10/10/49	-
2	MC3	A	506	-	-	0/9/9/49	-
2	MC3	E	517	-	-	1/6/6/49	-
2	MC3	I	522	-	-	0/7/7/49	-
2	MC3	C	530	-	-	1/3/3/49	-
2	MC3	E	511	-	-	0/3/3/49	-
2	MC3	A	515	-	-	0/3/3/49	-
2	MC3	C	502	-	-	0/10/10/49	-
2	MC3	E	522	-	-	0/7/7/49	-
2	MC3	D	508	-	-	0/4/4/49	-
2	MC3	E	523	-	-	0/9/9/49	-
2	MC3	J	516	-	-	1/4/4/49	-
2	MC3	G	502	-	-	0/10/10/49	-
2	MC3	B	522	-	-	0/7/7/49	-
2	MC3	K	506	-	-	0/9/9/49	-
2	MC3	K	513	-	-	0/5/5/49	-
2	MC3	A	510	-	-	0/6/6/49	-
2	MC3	D	511	-	-	0/3/3/49	-
2	MC3	K	518	-	-	11/31/31/49	-
2	MC3	B	506	-	-	0/9/9/49	-
2	MC3	H	514	-	-	3/9/9/49	-
2	MC3	C	529	-	-	0/4/4/49	-
2	MC3	E	527	-	-	0/3/3/49	-
2	MC3	K	527	-	-	0/3/3/49	-
2	MC3	E	503	-	-	0/10/10/49	-
2	MC3	H	517	-	-	1/6/6/49	-
2	MC3	L	519	-	-	0/9/9/49	-
2	MC3	E	533	-	-	17/31/31/49	-
2	MC3	I	507	-	-	0/6/6/49	-
2	MC3	E	529	-	-	0/4/4/49	-
2	MC3	E	519	-	-	0/10/10/49	-
2	MC3	L	505	-	-	0/9/9/49	-
2	MC3	A	503	-	-	0/10/10/49	-
2	MC3	E	526	-	-	0/8/8/49	-
2	MC3	I	527	-	-	0/3/3/49	-
2	MC3	J	513	-	-	0/5/5/49	-
2	MC3	K	519	-	-	0/10/10/49	-
2	MC3	K	501	-	-	8/34/34/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	C	533	-	-	17/31/31/49	-
2	MC3	G	521	-	-	0/9/9/49	-
2	MC3	F	525	-	-	0/6/6/49	-
2	MC3	I	510	-	-	0/6/6/49	-
2	MC3	J	522	-	-	0/7/7/49	-
2	MC3	J	506	-	-	0/9/9/49	-
2	MC3	G	532	-	-	0/2/2/49	-
2	MC3	K	509	-	-	0/5/5/49	-
2	MC3	H	516	-	-	1/4/4/49	-
2	MC3	B	527	-	-	0/3/3/49	-
2	MC3	H	525	-	-	0/7/7/49	-
2	MC3	H	519	-	-	0/10/10/49	-
2	MC3	J	503	-	-	0/10/10/49	-
2	MC3	H	526	-	-	0/8/8/49	-
2	MC3	J	505	-	-	0/9/9/49	-
2	MC3	B	510	-	-	0/6/6/49	-
2	MC3	I	509	-	-	0/5/5/49	-
2	MC3	L	521	-	-	0/9/9/49	-
2	MC3	J	519	-	-	0/10/10/49	-
2	MC3	H	502	-	-	0/10/10/49	-
2	MC3	G	525	-	-	0/7/7/49	-
2	MC3	J	508	-	-	0/4/4/49	-
2	MC3	J	510	-	-	0/6/6/49	-
2	MC3	A	517	-	-	1/6/6/49	-
2	MC3	J	533	-	-	17/31/31/49	-
2	MC3	B	501	-	-	8/34/34/49	-
2	MC3	C	519	-	-	0/10/10/49	-
2	MC3	L	530	-	-	0/3/3/49	-
2	MC3	K	510	-	-	0/6/6/49	-
2	MC3	D	501	-	-	8/34/34/49	-
2	MC3	C	505	-	-	0/9/9/49	-
2	MC3	F	530	-	-	0/3/3/49	-
2	MC3	J	511	-	-	0/3/3/49	-
2	MC3	D	522	-	-	0/7/7/49	-
2	MC3	J	523	-	-	0/9/9/49	-
2	MC3	B	511	-	-	0/3/3/49	-
2	MC3	B	513	-	-	0/5/5/49	-
2	MC3	K	508	-	-	0/4/4/49	-
2	MC3	L	504	-	-	0/7/7/49	-
2	MC3	I	528	-	-	0/5/5/49	-
2	MC3	E	509	-	-	0/5/5/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	E	516	-	-	1/4/4/49	-
2	MC3	F	516	-	-	8/34/34/49	-
2	MC3	C	518	-	-	11/31/31/49	-
2	MC3	K	524	-	-	0/10/10/49	-
2	MC3	G	533	-	-	17/31/31/49	-
2	MC3	D	505	-	-	0/9/9/49	-
2	MC3	D	532	-	-	0/2/2/49	-
2	MC3	I	506	-	-	0/9/9/49	-
2	MC3	L	526	-	-	0/3/3/49	-
2	MC3	C	516	-	-	1/4/4/49	-
2	MC3	F	520	-	-	0/9/9/49	-
2	MC3	E	528	-	-	0/5/5/49	-
2	MC3	K	529	-	-	0/4/4/49	-
2	MC3	H	522	-	-	0/7/7/49	-
2	MC3	D	514	-	-	3/9/9/49	-
2	MC3	D	523	-	-	0/9/9/49	-
2	MC3	K	511	-	-	0/3/3/49	-
2	MC3	B	508	-	-	0/4/4/49	-
2	MC3	A	530	-	-	1/3/3/49	-
2	MC3	L	502	-	-	0/9/9/49	-
2	MC3	D	518	-	-	11/31/31/49	-
2	MC3	E	518	-	-	11/31/31/49	-
2	MC3	F	524	-	-	0/5/5/49	-
2	MC3	C	515	-	-	0/3/3/49	-
2	MC3	J	504	-	-	0/9/9/49	-
2	MC3	B	524	-	-	0/10/10/49	-
2	MC3	I	501	-	-	8/34/34/49	-
2	MC3	F	527	-	-	1/1/1/49	-
2	MC3	E	524	-	-	0/10/10/49	-
2	MC3	C	504	-	-	0/9/9/49	-
2	MC3	C	514	-	-	3/9/9/49	-
2	MC3	C	521	-	-	0/9/9/49	-
2	MC3	F	508	-	-	0/8/8/49	-
2	MC3	F	518	-	-	0/10/10/49	-
2	MC3	F	511	-	-	0/4/4/49	-
2	MC3	A	519	-	-	0/10/10/49	-
2	MC3	F	513	-	-	0/4/4/49	-
2	MC3	J	517	-	-	1/6/6/49	-
2	MC3	G	506	-	-	0/9/9/49	-
2	MC3	B	507	-	-	0/6/6/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	E	501	-	-	8/34/34/49	-
2	MC3	G	526	-	-	0/8/8/49	-
2	MC3	L	512	-	-	1/3/3/49	-
2	MC3	H	518	-	-	11/31/31/49	-
2	MC3	E	531	-	-	0/4/4/49	-
2	MC3	A	514	-	-	3/9/9/49	-
2	MC3	J	515	-	-	0/3/3/49	-
2	MC3	G	505	-	-	0/9/9/49	-
2	MC3	D	531	-	-	0/4/4/49	-
2	MC3	E	521	-	-	0/9/9/49	-
2	MC3	D	503	-	-	0/10/10/49	-
2	MC3	G	513	-	-	0/5/5/49	-
2	MC3	K	503	-	-	0/10/10/49	-
2	MC3	A	502	-	-	0/10/10/49	-
2	MC3	D	517	-	-	1/6/6/49	-
2	MC3	K	512	-	-	1/1/1/49	-
2	MC3	G	516	-	-	1/4/4/49	-
2	MC3	B	532	-	-	0/2/2/49	-
2	MC3	A	524	-	-	0/10/10/49	-
2	MC3	C	527	-	-	0/3/3/49	-
2	MC3	D	529	-	-	0/4/4/49	-
2	MC3	L	528	-	-	0/5/5/49	-
2	MC3	F	526	-	-	0/3/3/49	-
2	MC3	C	525	-	-	0/7/7/49	-
2	MC3	I	532	-	-	0/2/2/49	-
2	MC3	I	503	-	-	0/10/10/49	-
2	MC3	H	501	-	-	8/34/34/49	-
2	MC3	A	505	-	-	0/9/9/49	-
2	MC3	H	520	-	-	0/9/9/49	-
2	MC3	C	524	-	-	0/10/10/49	-
2	MC3	I	524	-	-	0/10/10/49	-
2	MC3	F	504	-	-	0/7/7/49	-
2	MC3	H	515	-	-	0/3/3/49	-
2	MC3	F	521	-	-	0/9/9/49	-
2	MC3	K	523	-	-	0/9/9/49	-
2	MC3	G	519	-	-	0/10/10/49	-
2	MC3	E	502	-	-	0/10/10/49	-

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	516	MC3	P-O4P	2.85	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	MC3	P-O4P	2.85	1.65	1.54
2	E	501	MC3	P-O4P	2.85	1.65	1.54
2	G	501	MC3	P-O4P	2.85	1.65	1.54
2	D	501	MC3	P-O4P	2.84	1.65	1.54

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	MC3	O4P-P-O3P	-5.17	93.20	106.67
2	F	516	MC3	O4P-P-O3P	-5.16	93.21	106.67
2	J	501	MC3	O4P-P-O3P	-5.15	93.23	106.67
2	L	516	MC3	O4P-P-O3P	-5.15	93.24	106.67
2	G	501	MC3	O4P-P-O3P	-5.15	93.24	106.67

There are no chirality outliers.

5 of 516 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	512	MC3	C32-C33-C34-C35
2	A	518	MC3	C32-C31-O2-C2
2	A	533	MC3	C1-O3P-P-O2P
2	A	533	MC3	C1-O3P-P-O4P
2	A	533	MC3	C4-O4P-P-O1P

There are no ring outliers.

17 monomers are involved in 19 short contacts:

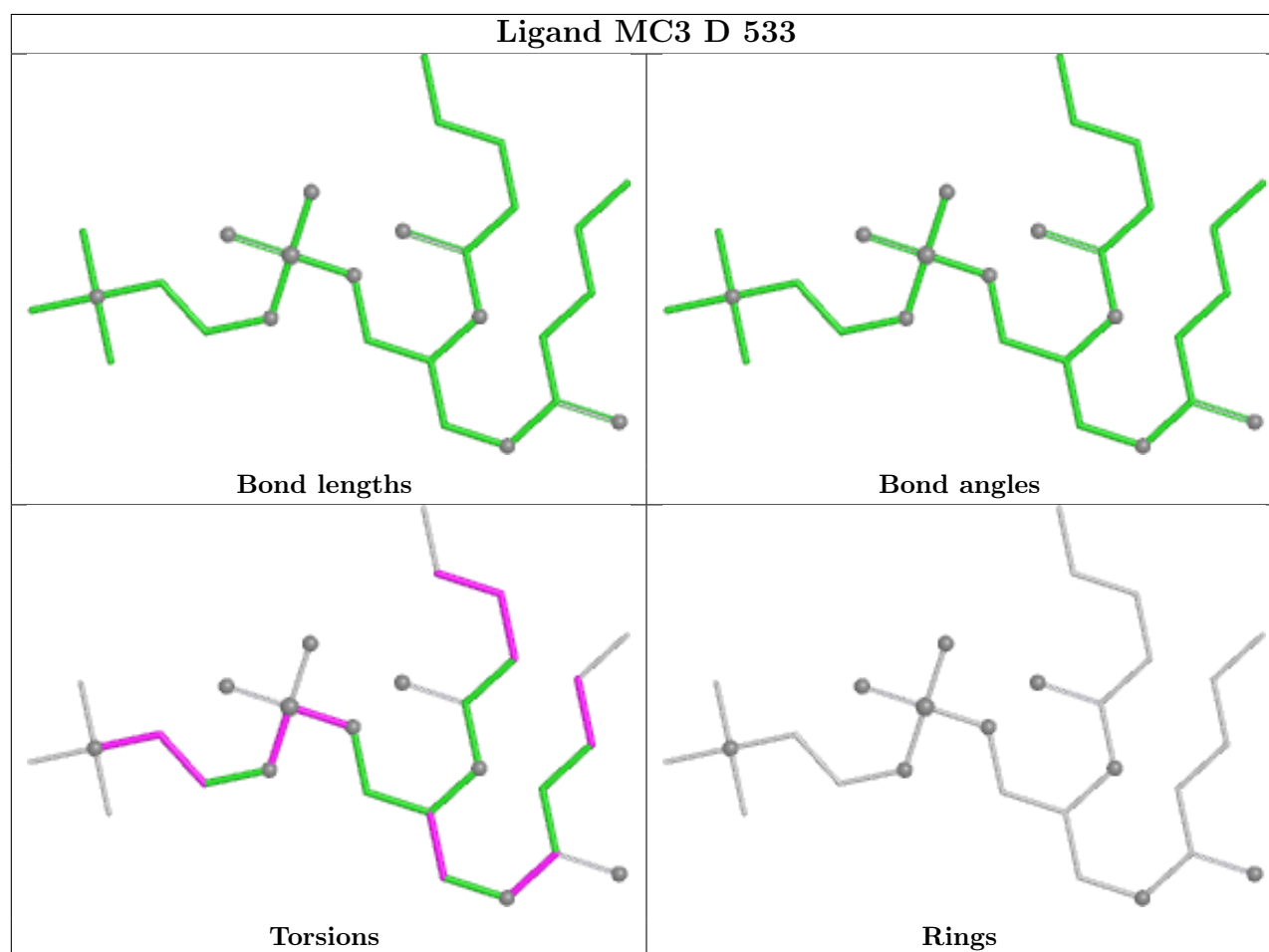
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	533	MC3	2	0
2	G	514	MC3	1	0
2	E	514	MC3	1	0
2	K	514	MC3	1	0
2	L	515	MC3	4	0
2	H	533	MC3	1	0
2	K	533	MC3	3	0
2	L	529	MC3	1	0
2	B	533	MC3	1	0
2	I	514	MC3	1	0
2	F	529	MC3	1	0
2	F	515	MC3	2	0
2	A	533	MC3	2	0

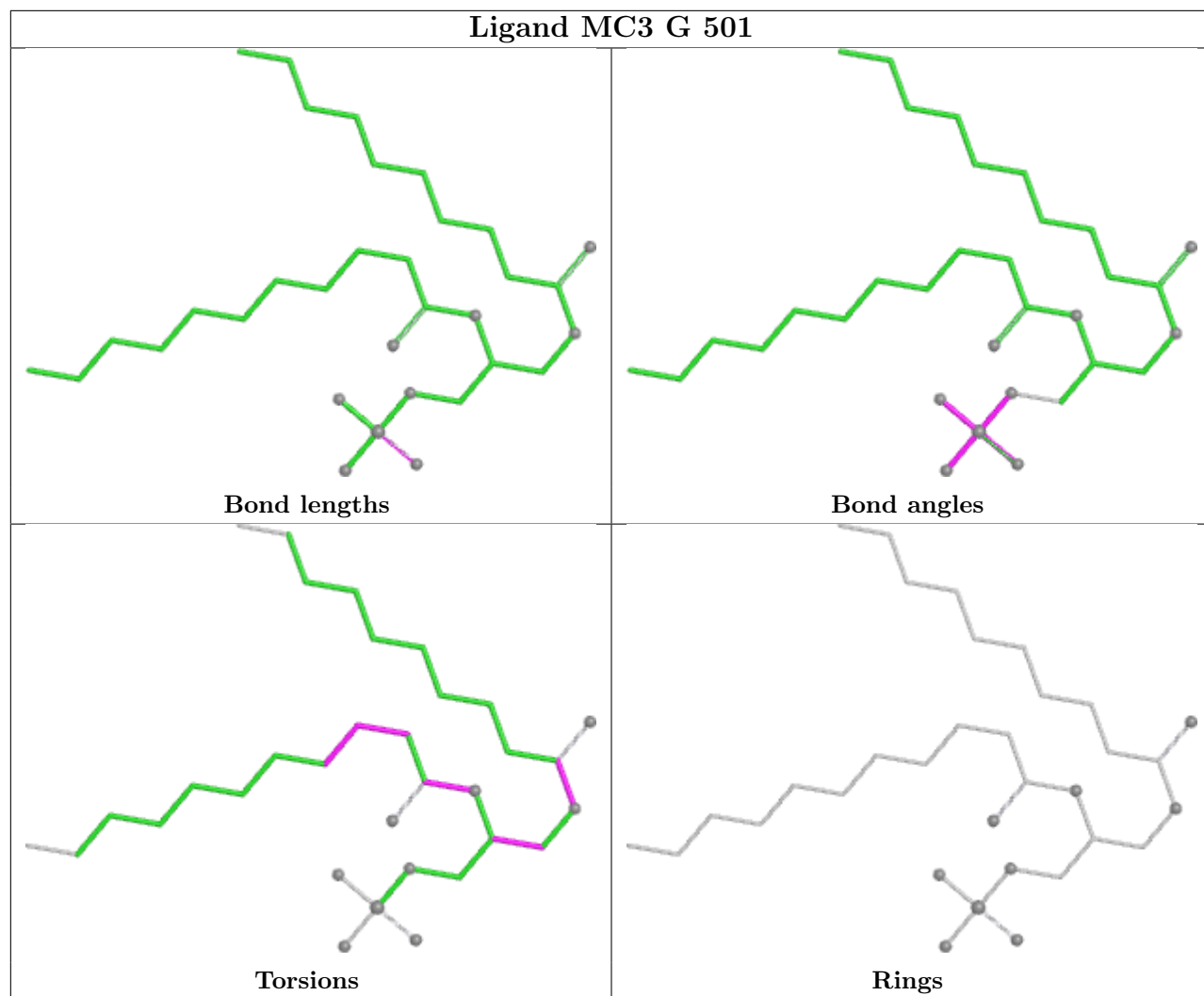
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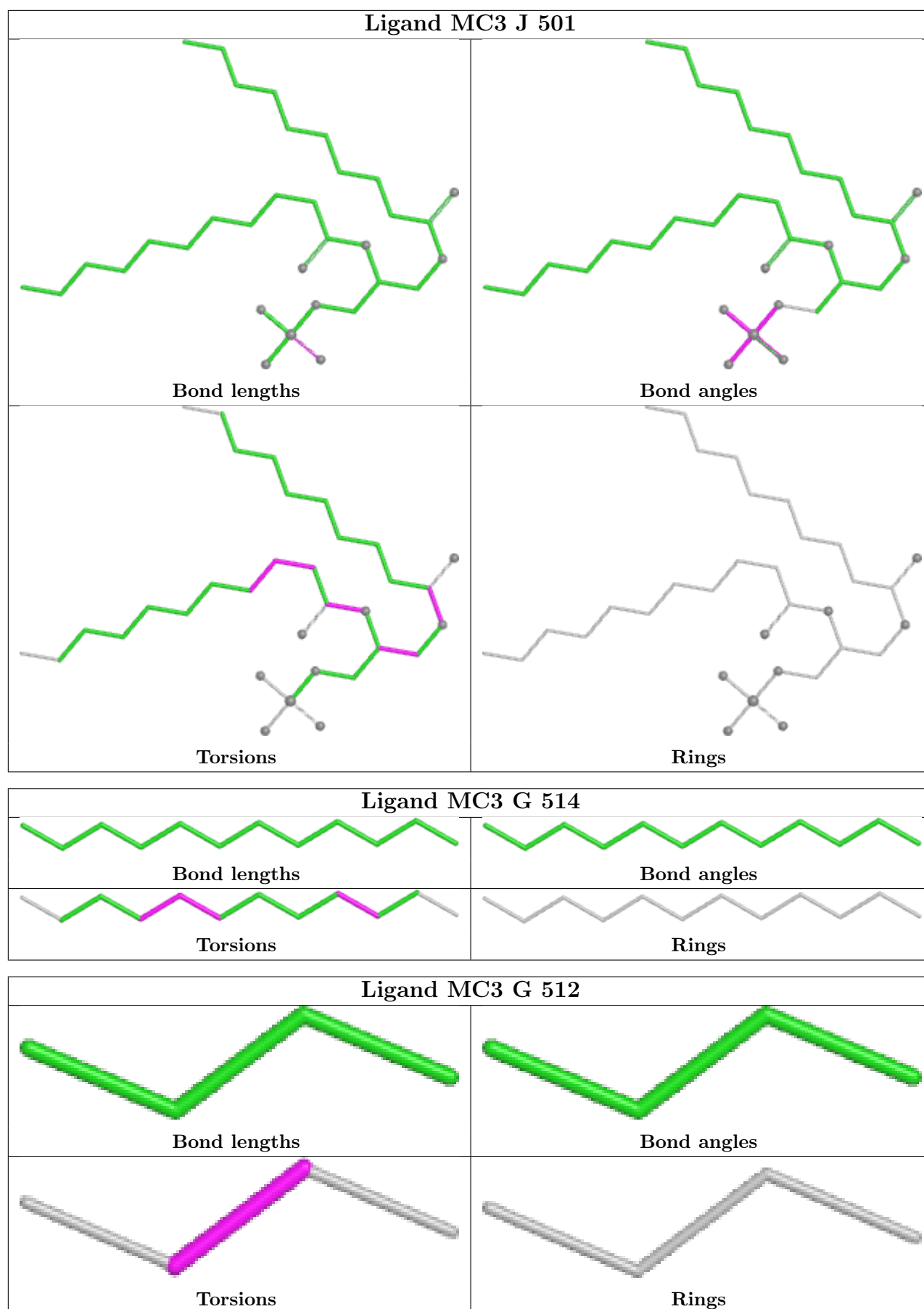
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	533	MC3	2	0
2	J	533	MC3	1	0
2	D	514	MC3	1	0
2	C	514	MC3	1	0

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.



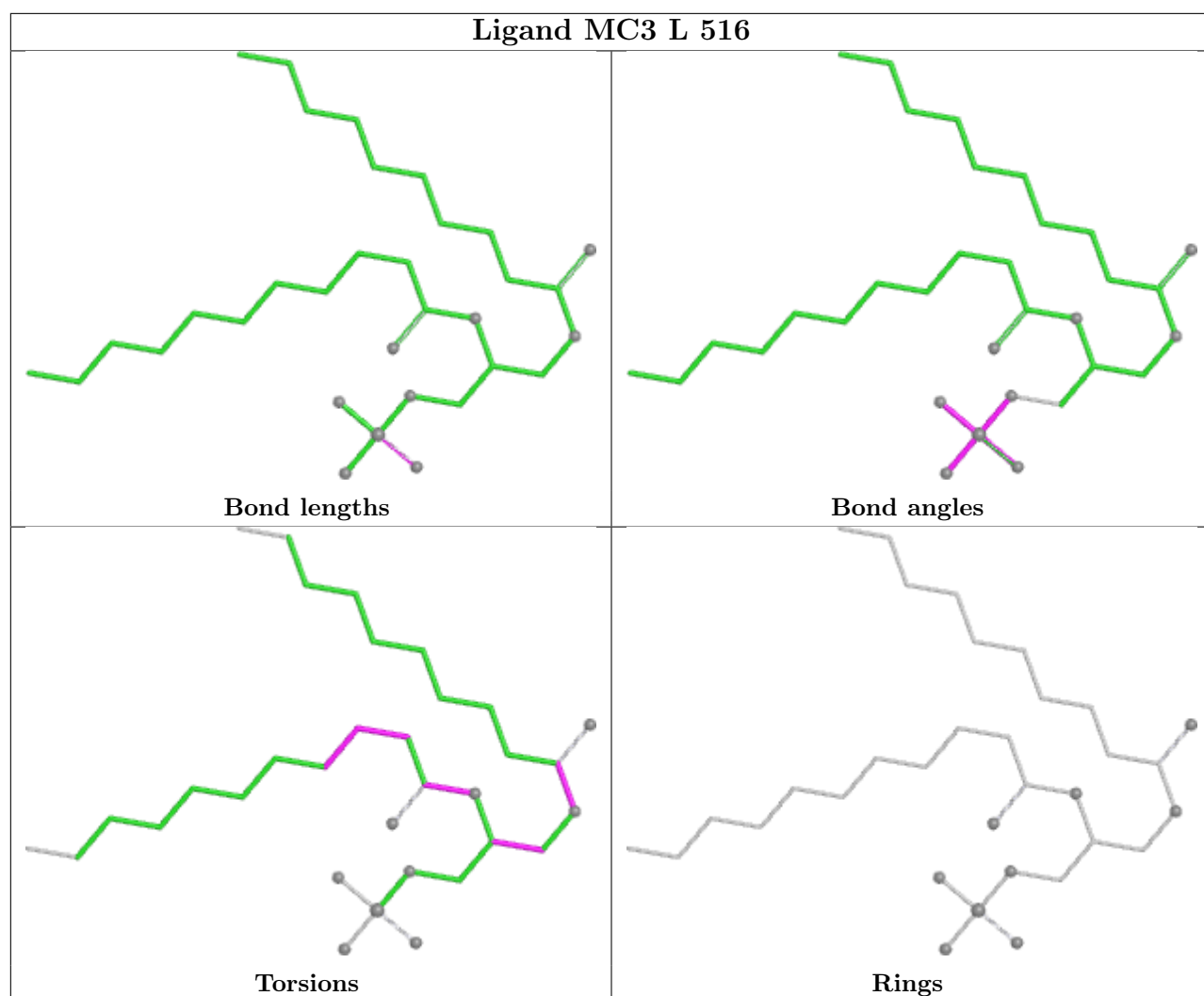


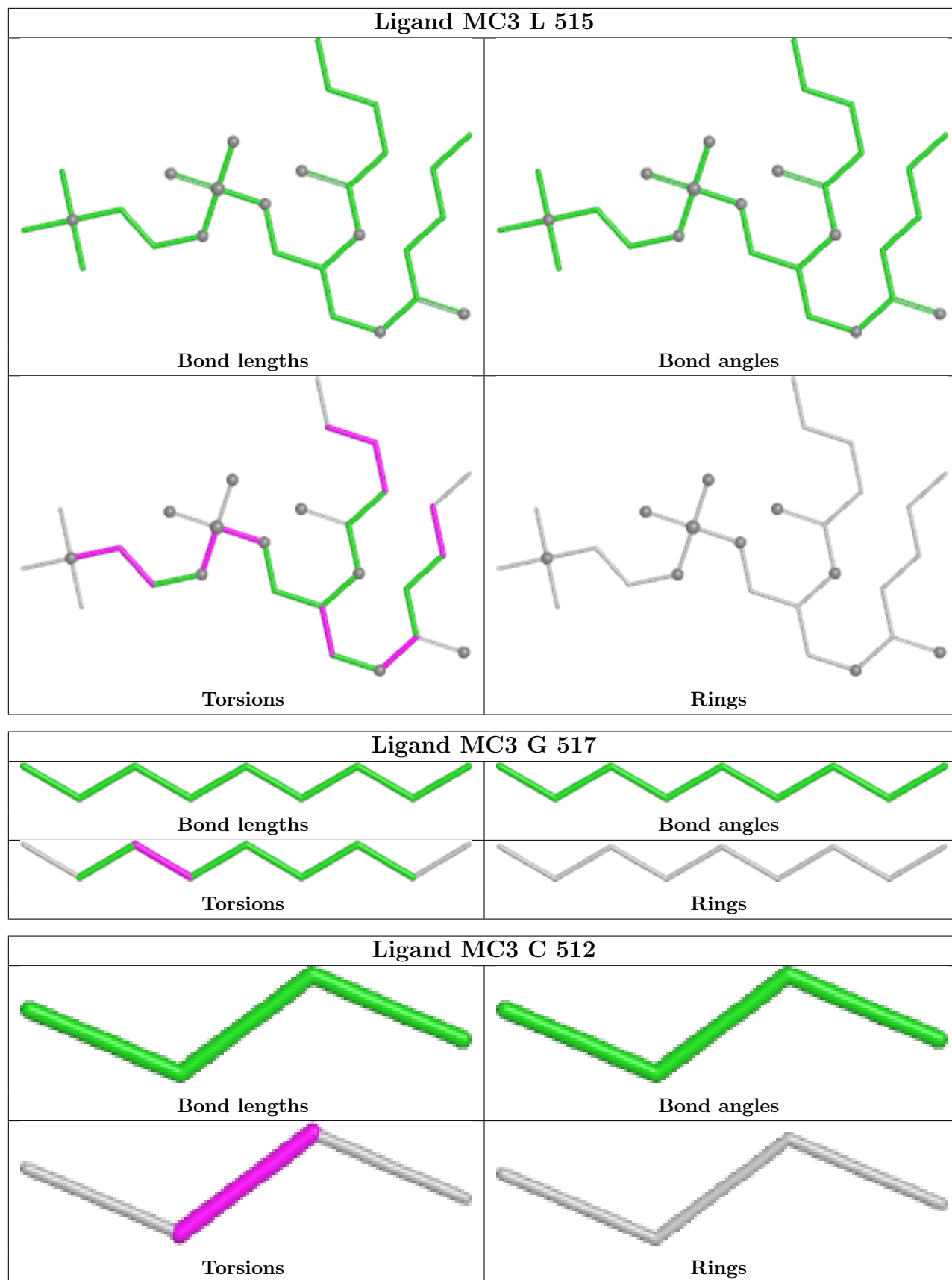


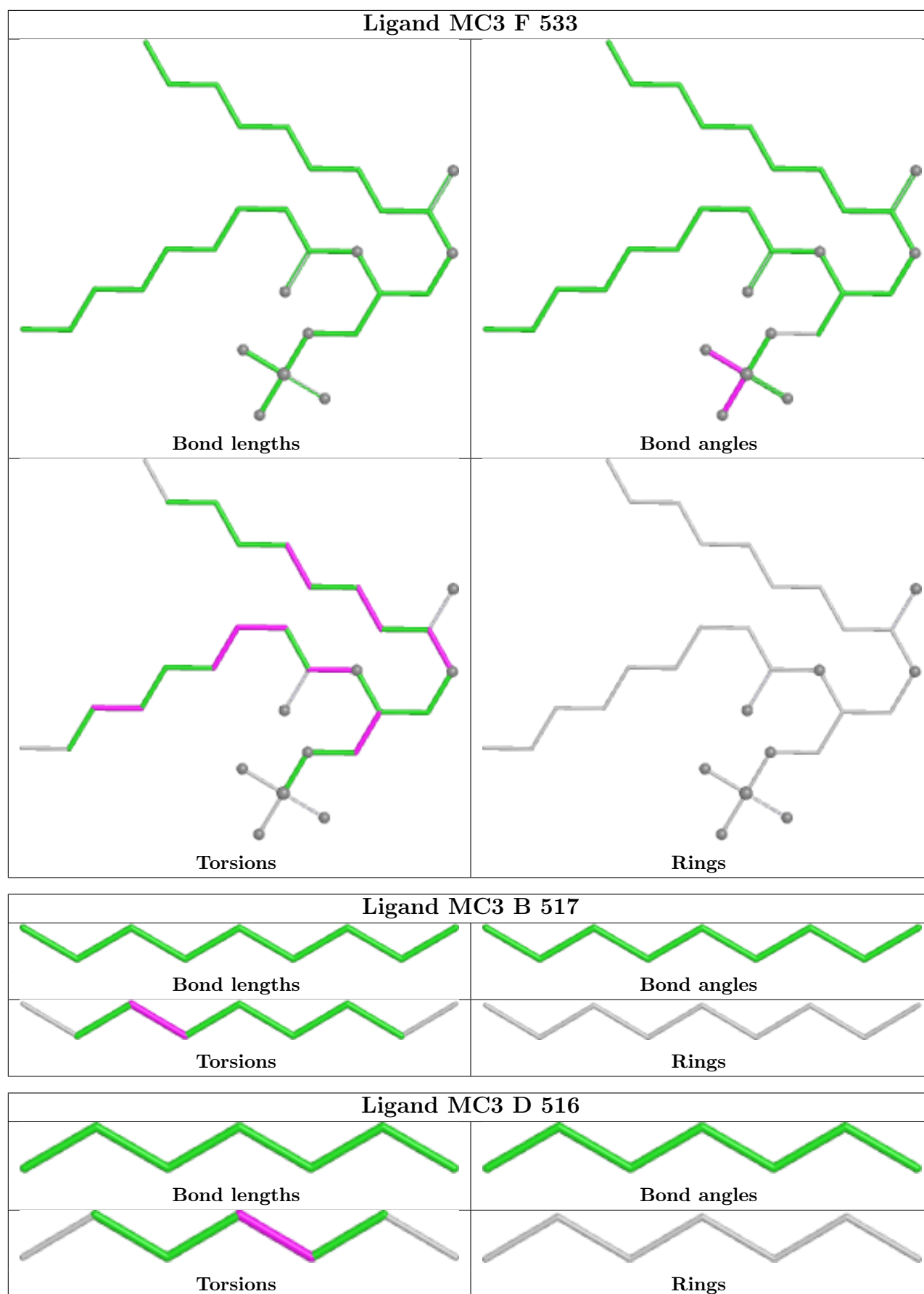
Ligand MC3 E 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

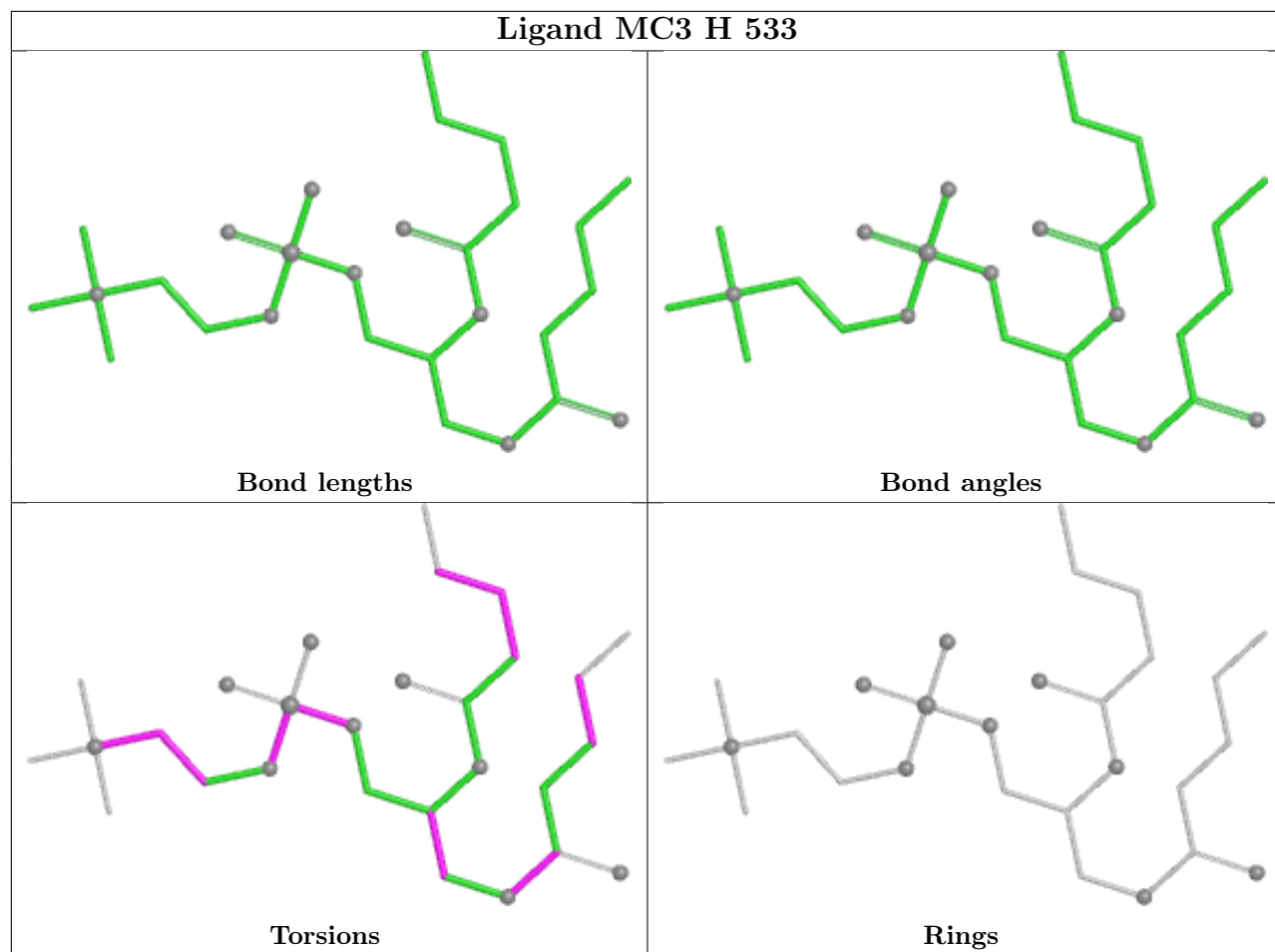
Ligand MC3 K 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

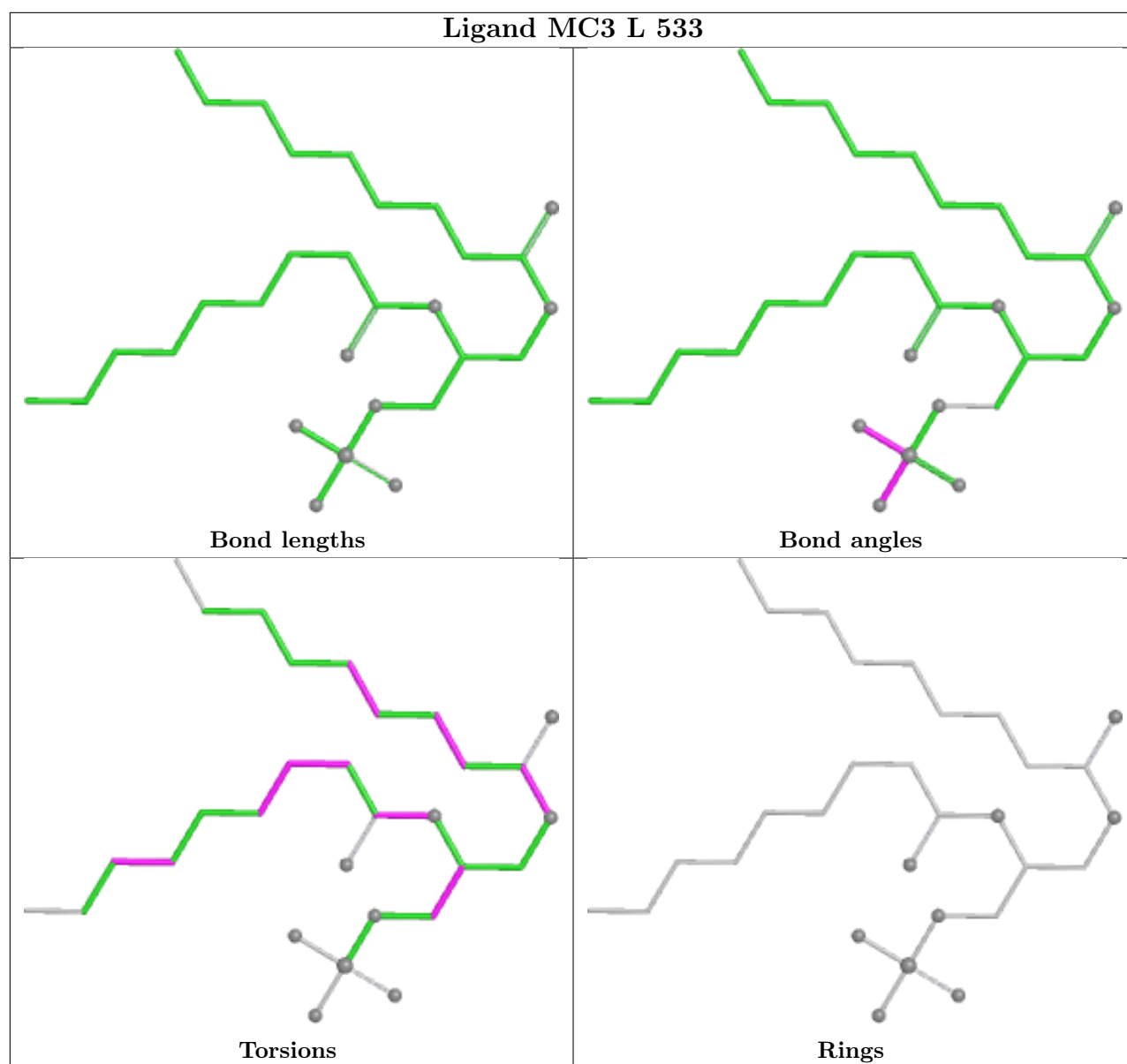
Ligand MC3 F 512	
 Bond lengths	 Bond angles
 Torsions	 Rings

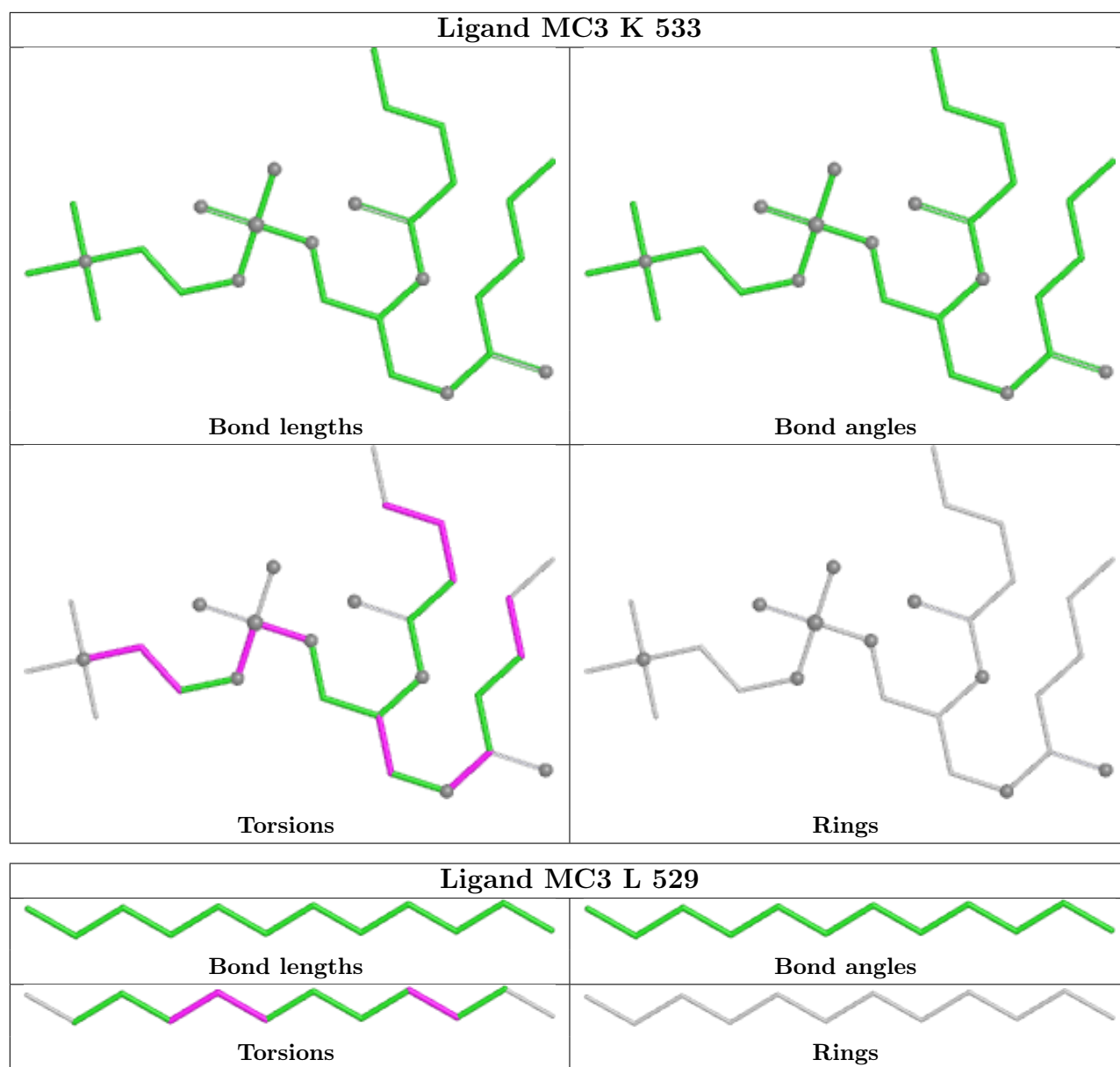


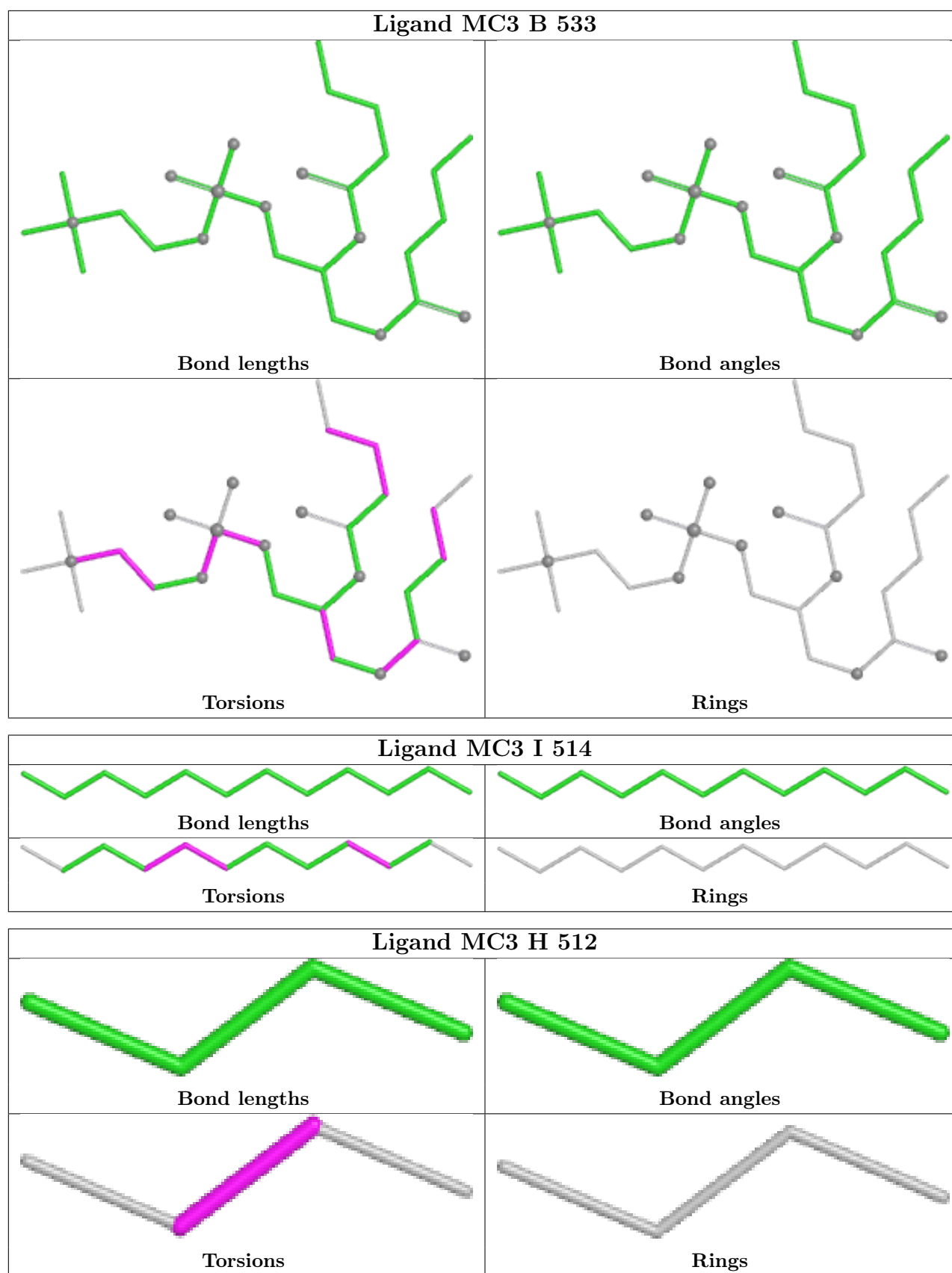


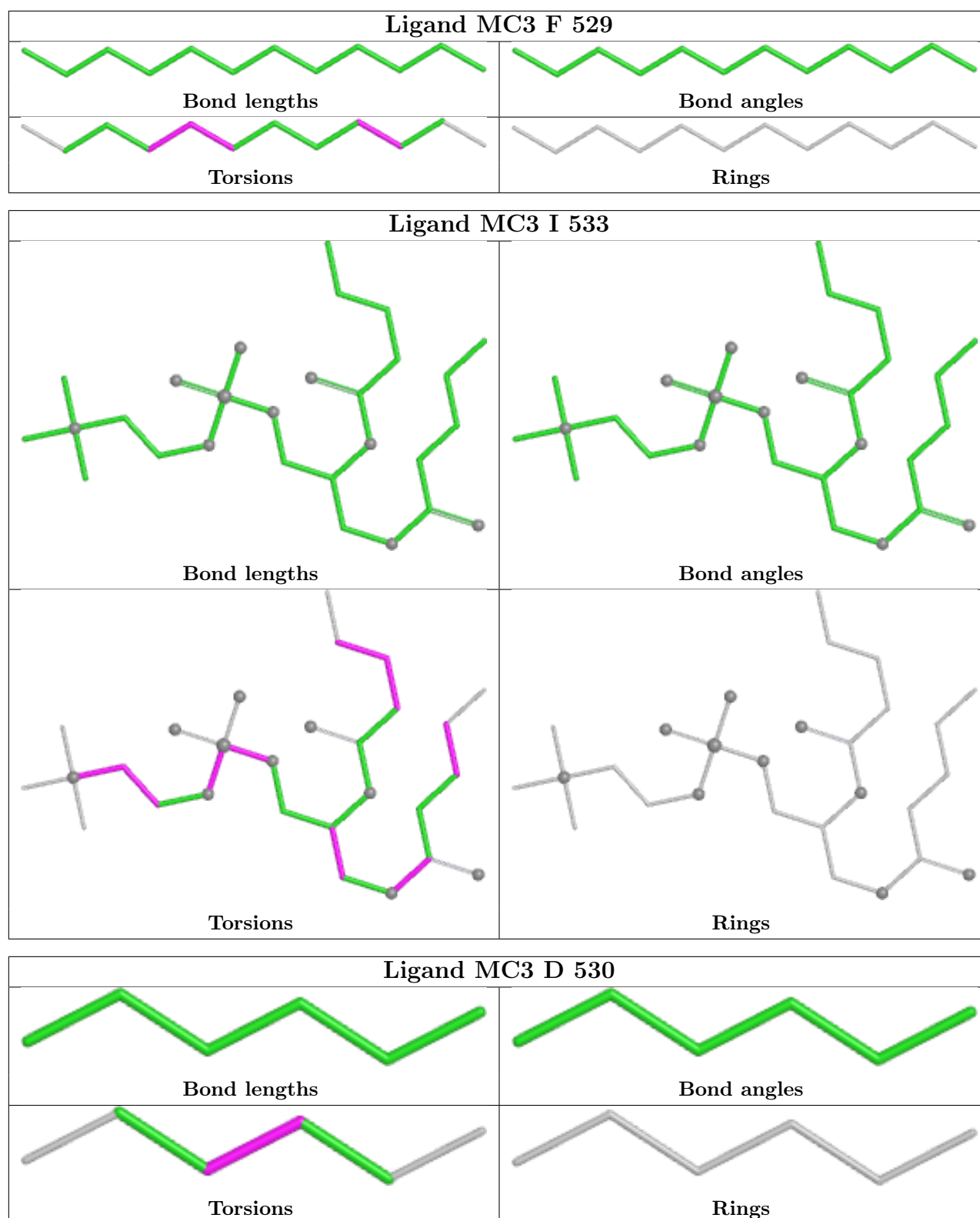


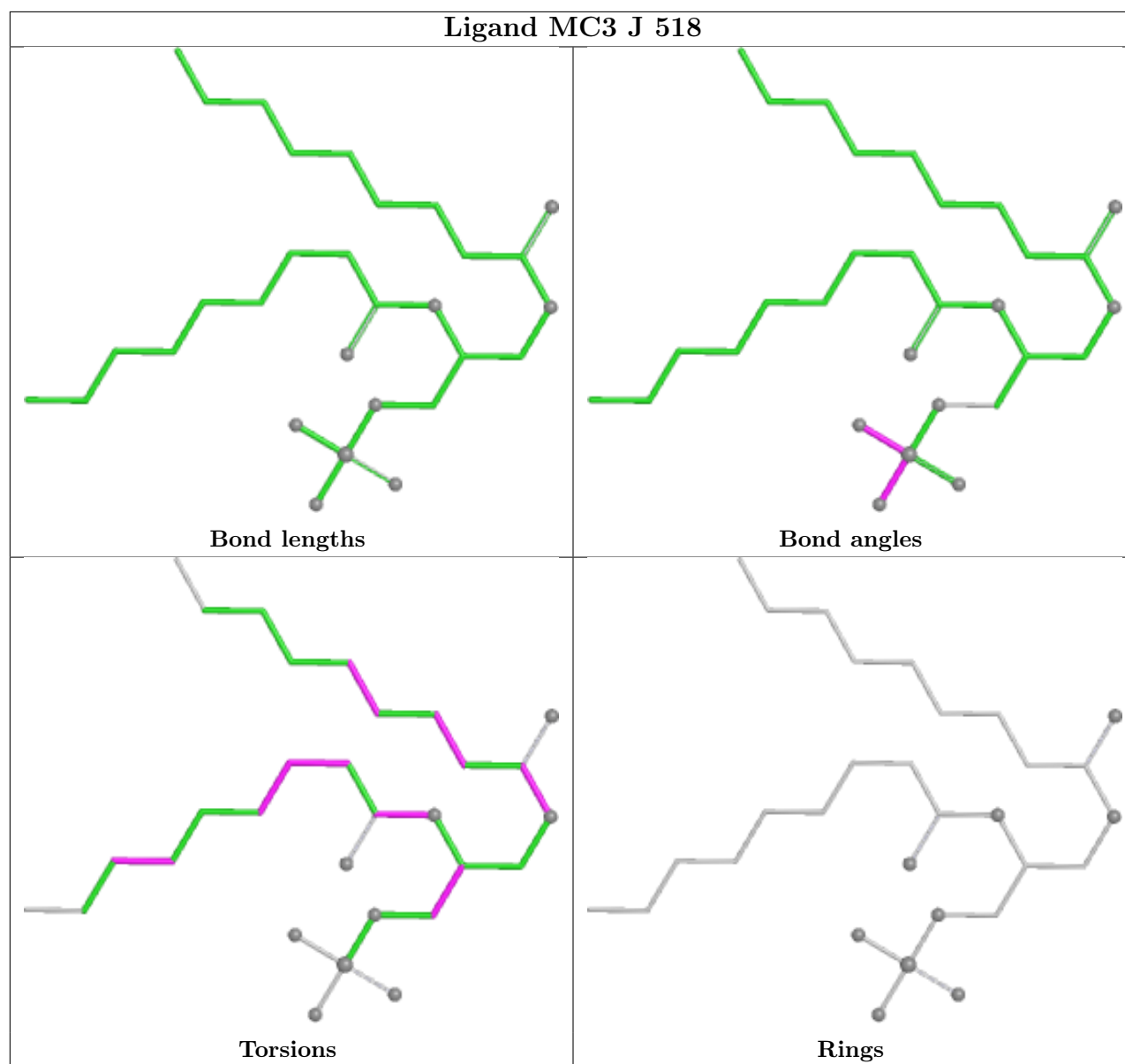
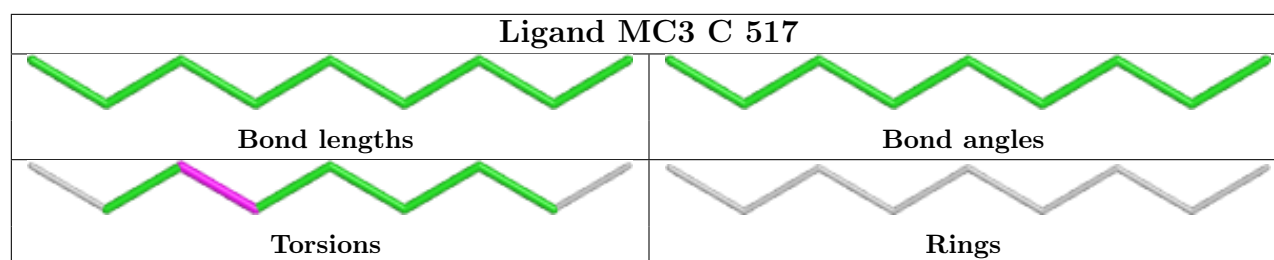


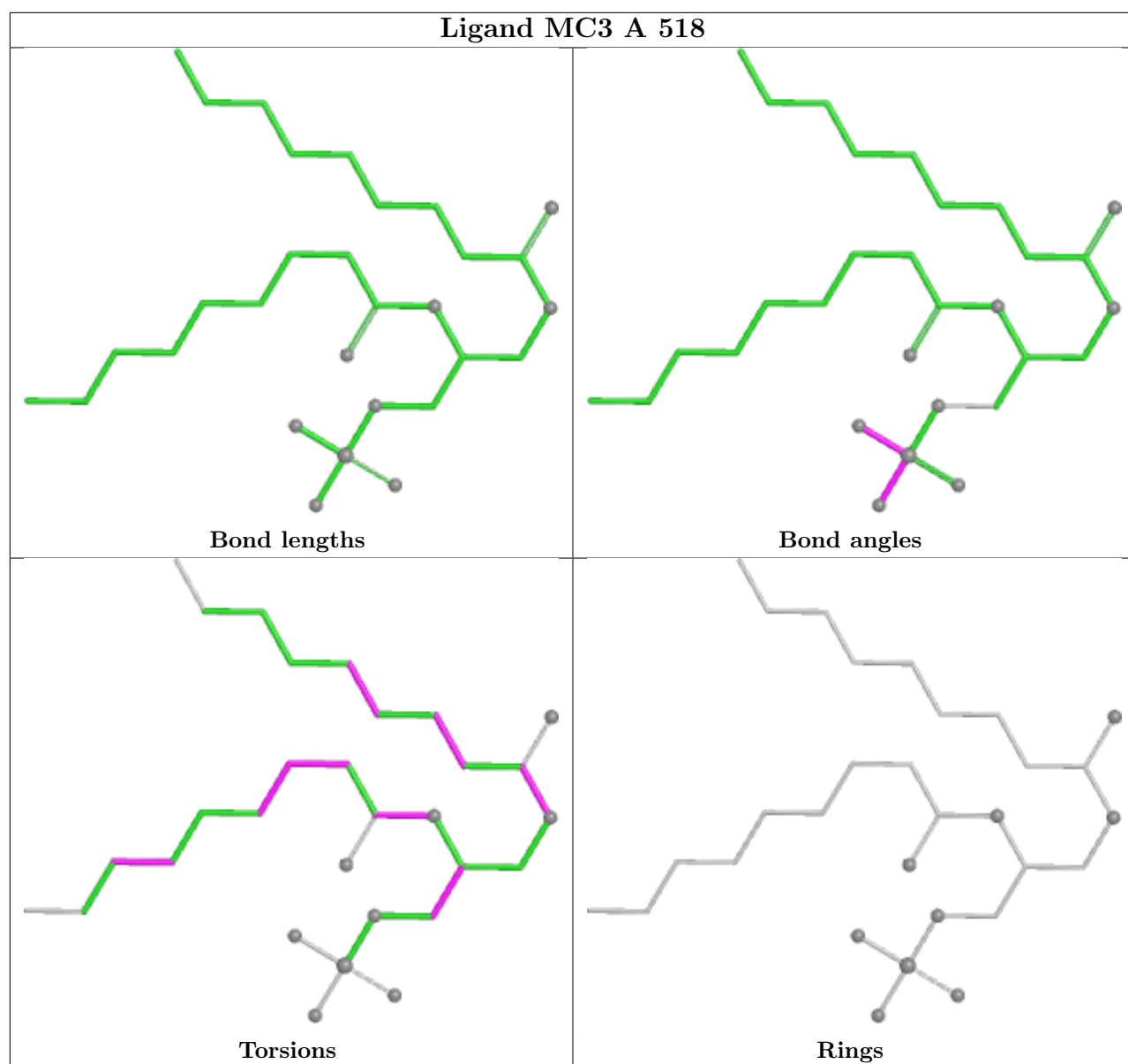


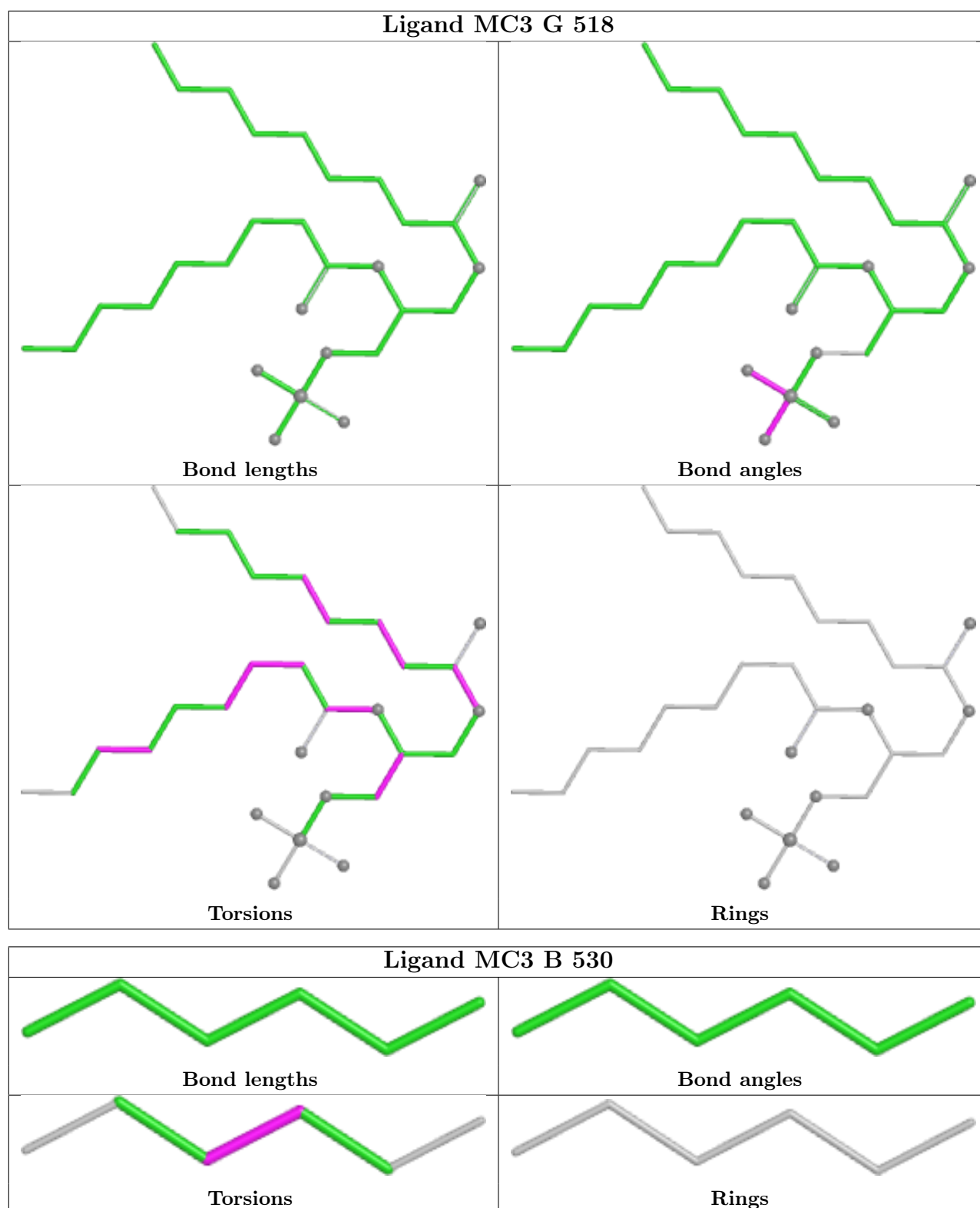


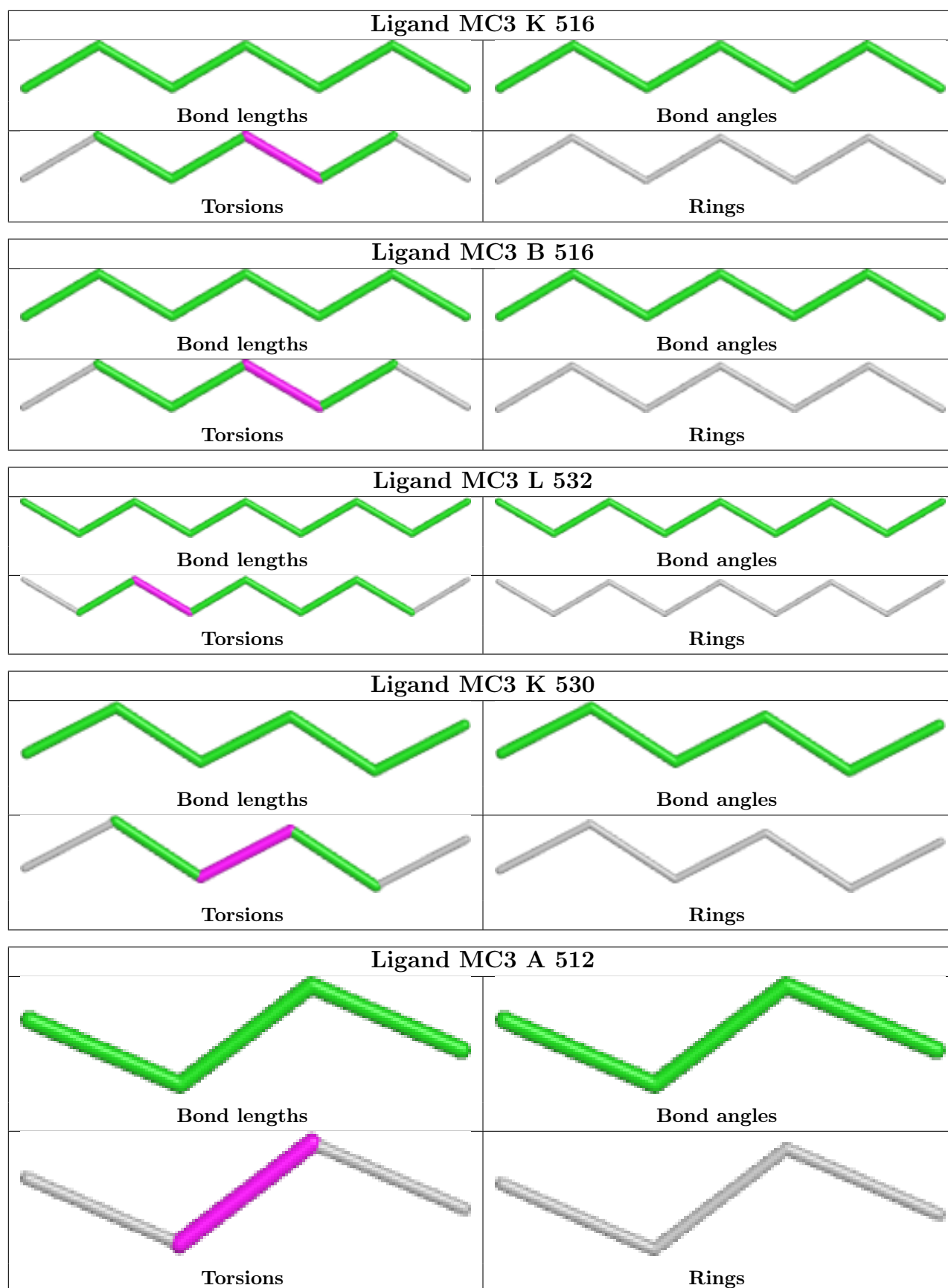


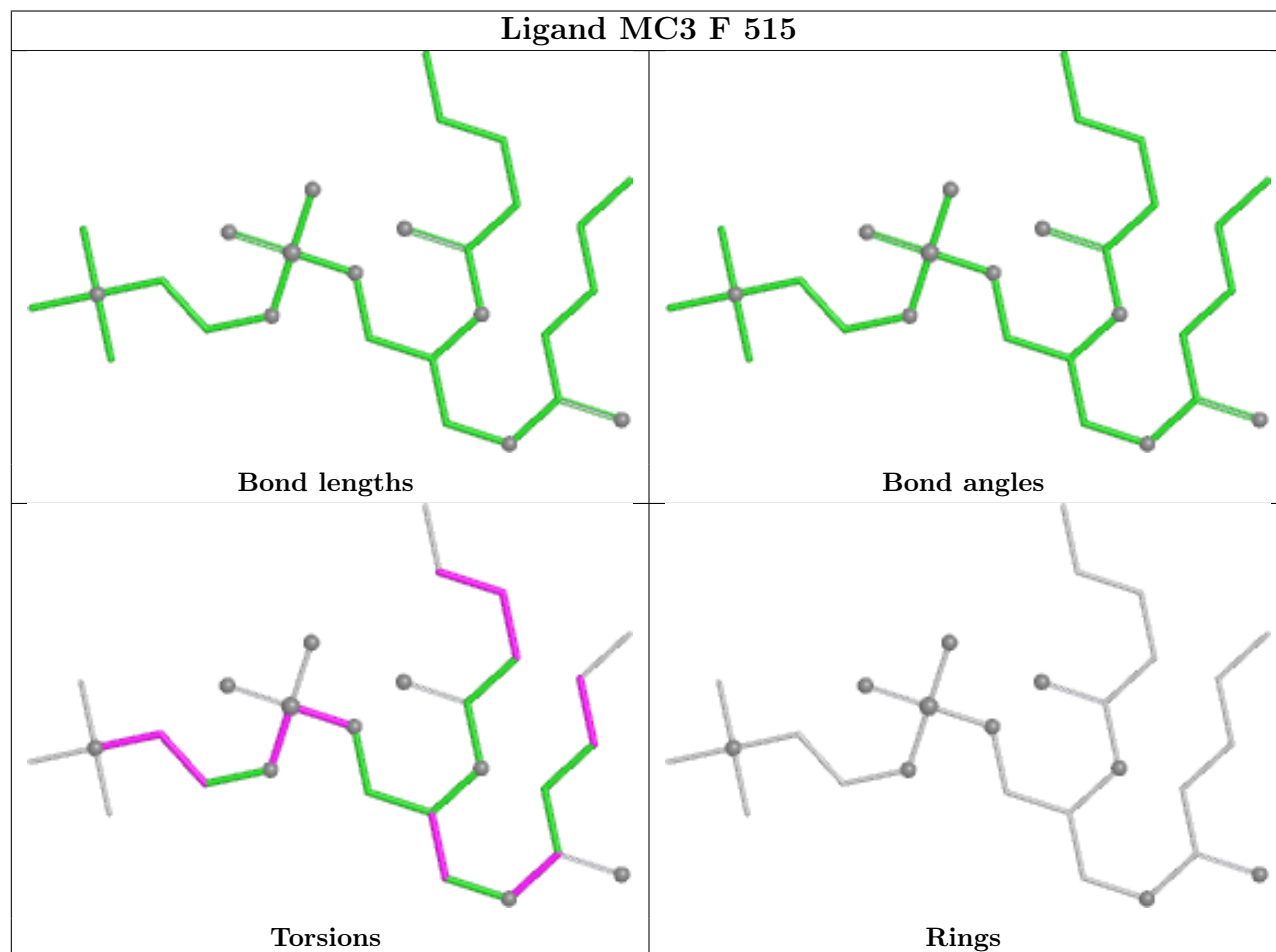
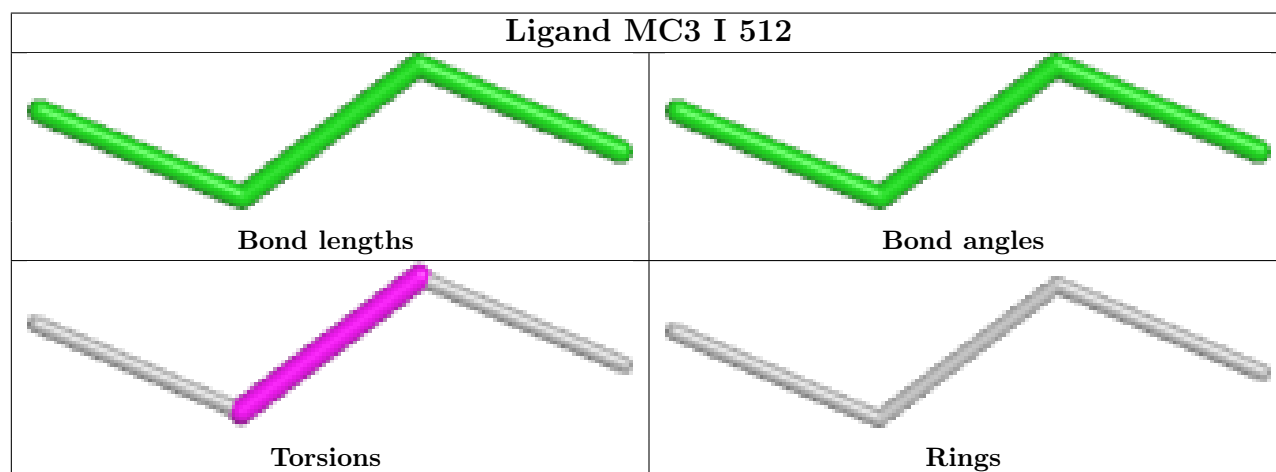
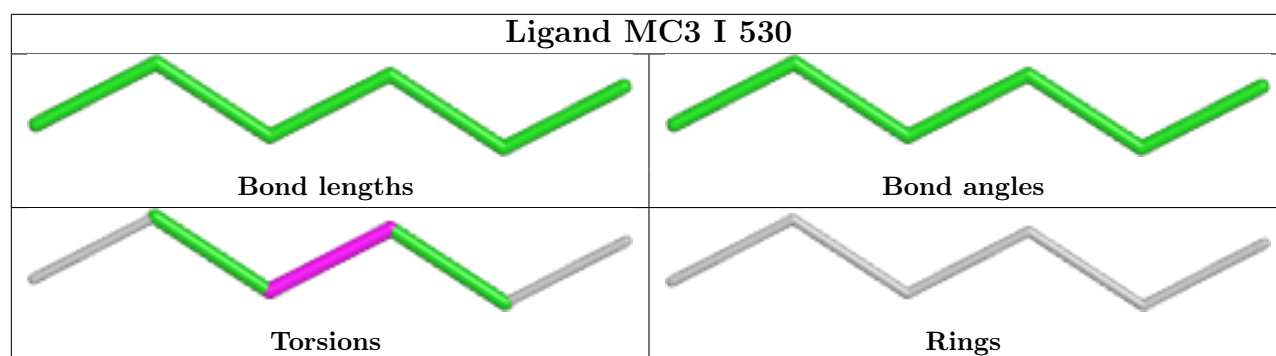


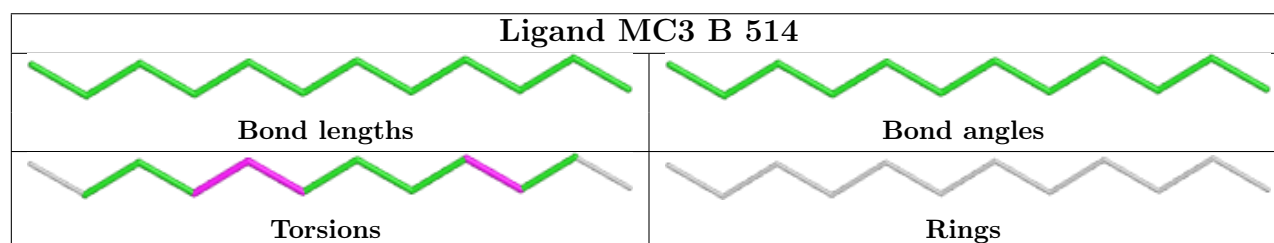
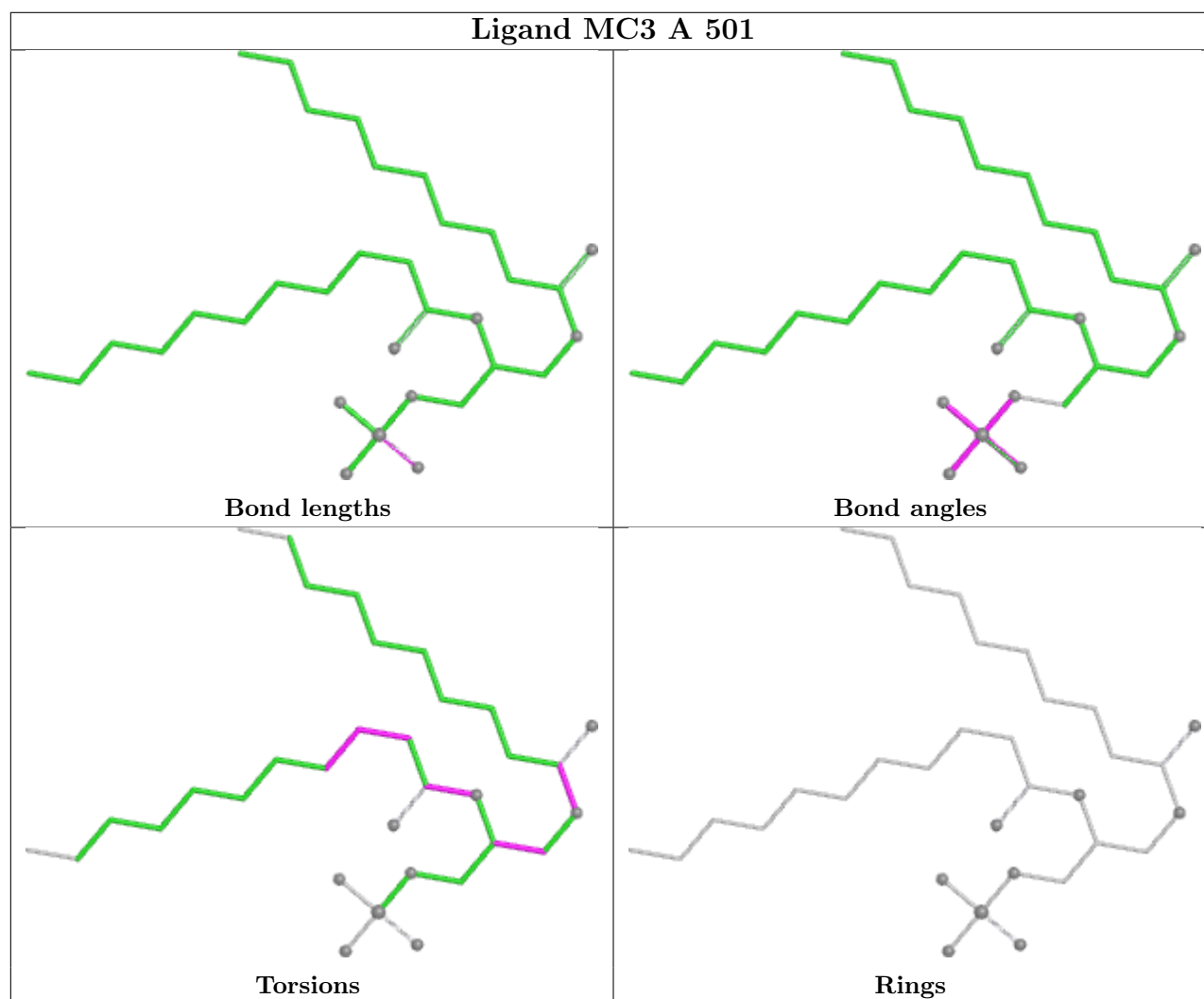
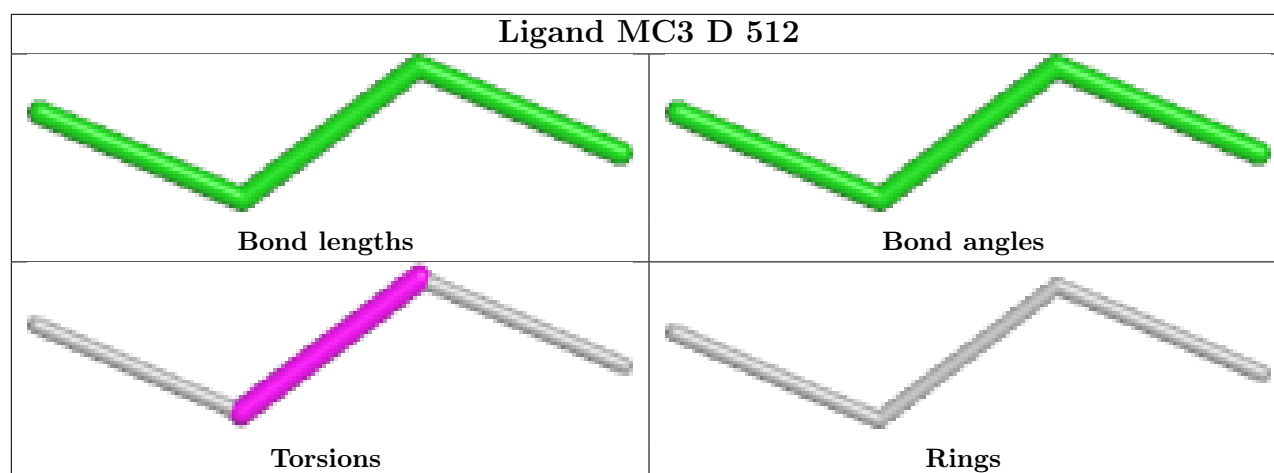


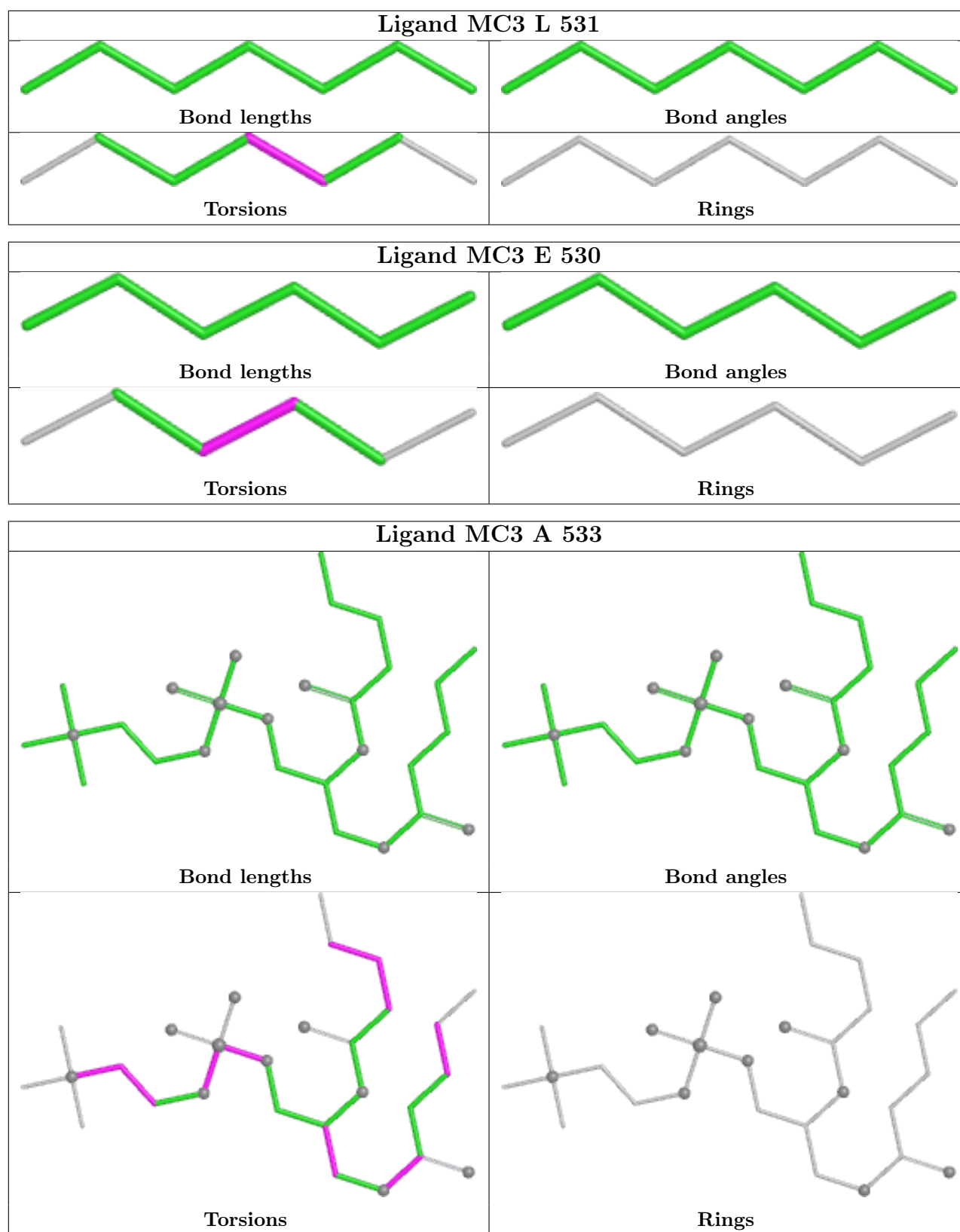


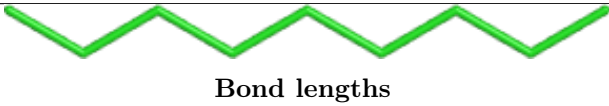
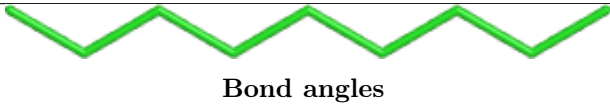
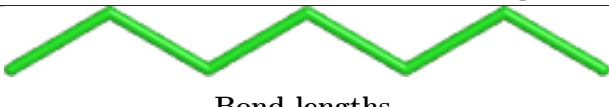
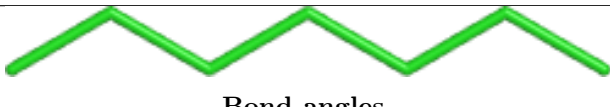
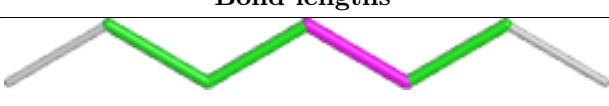
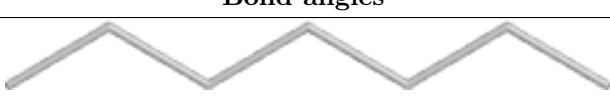
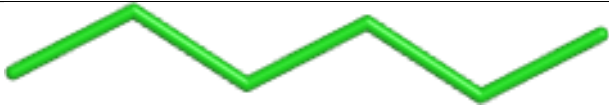
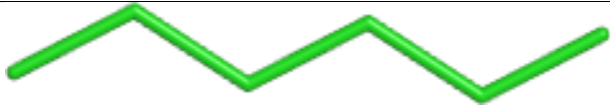
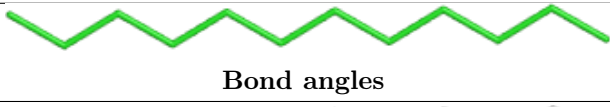


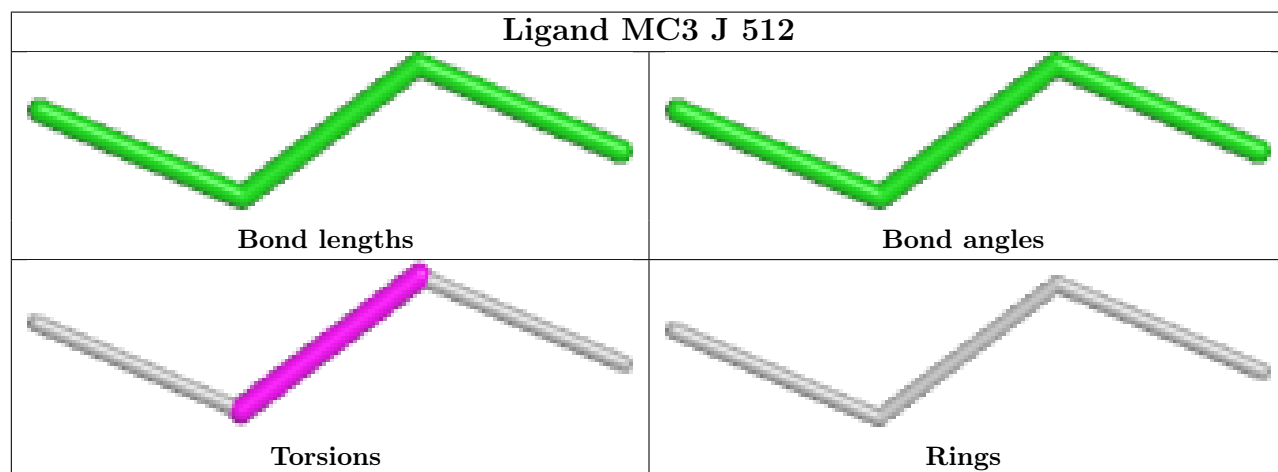
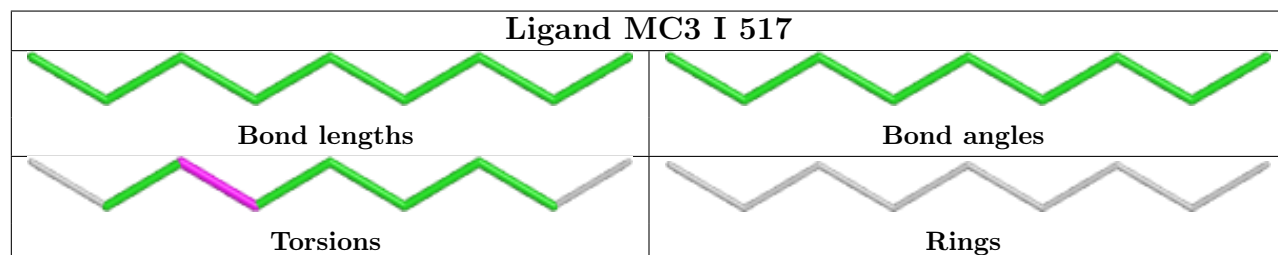
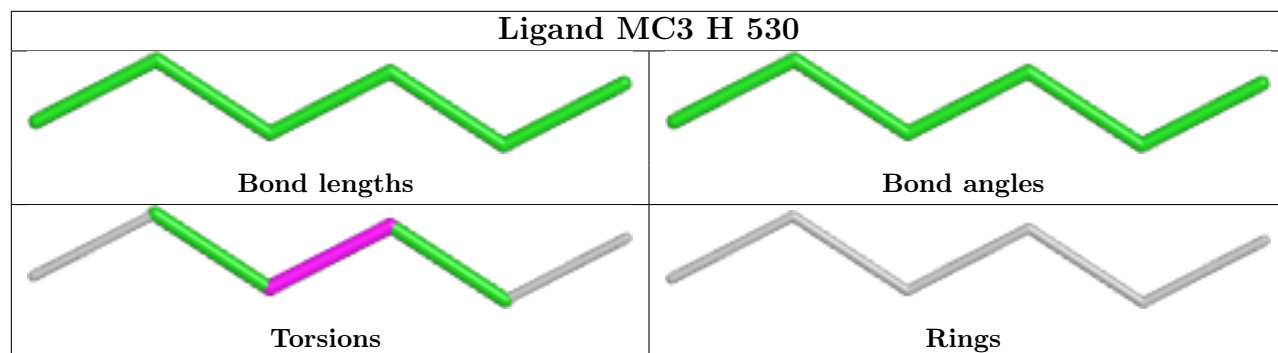


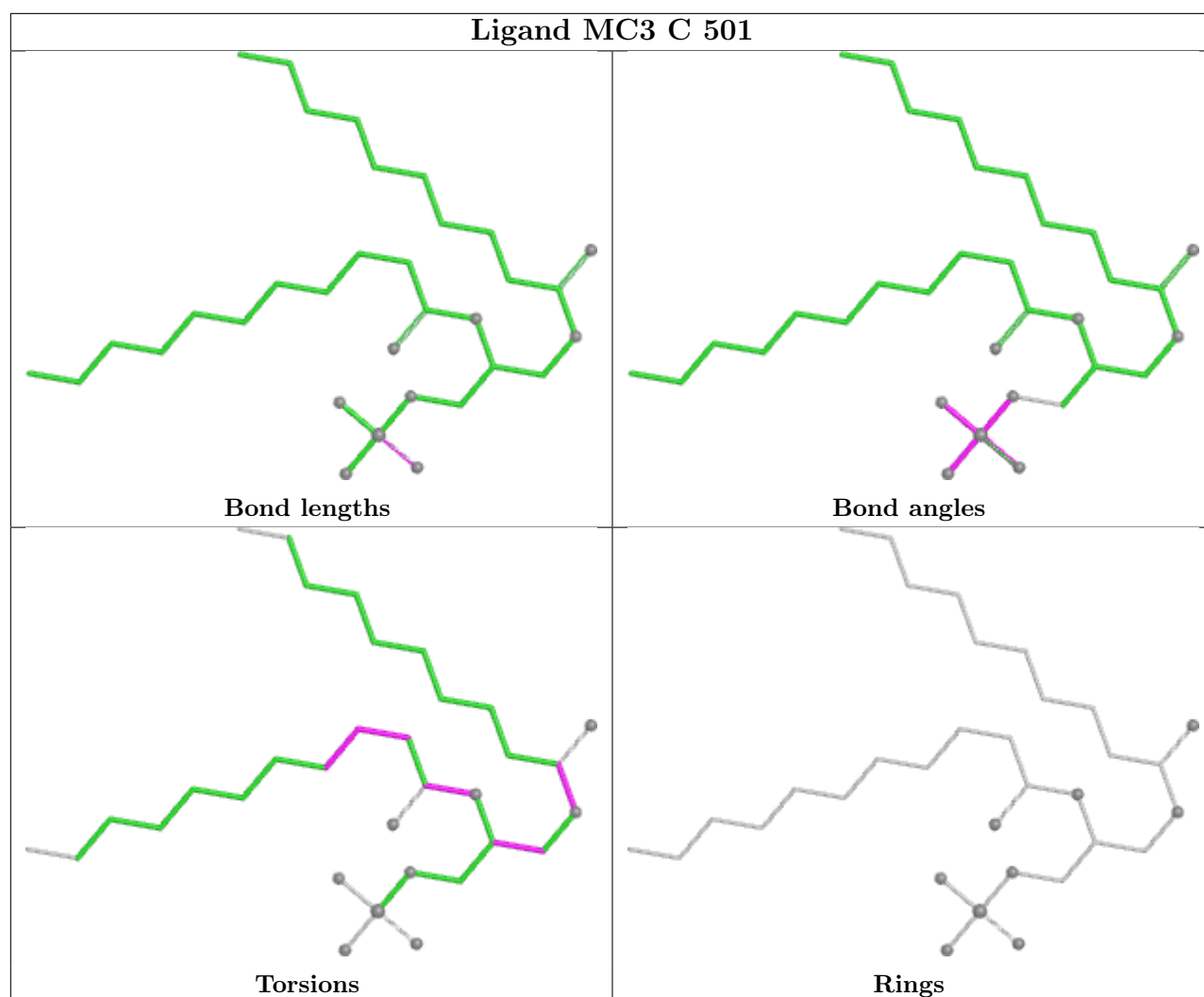


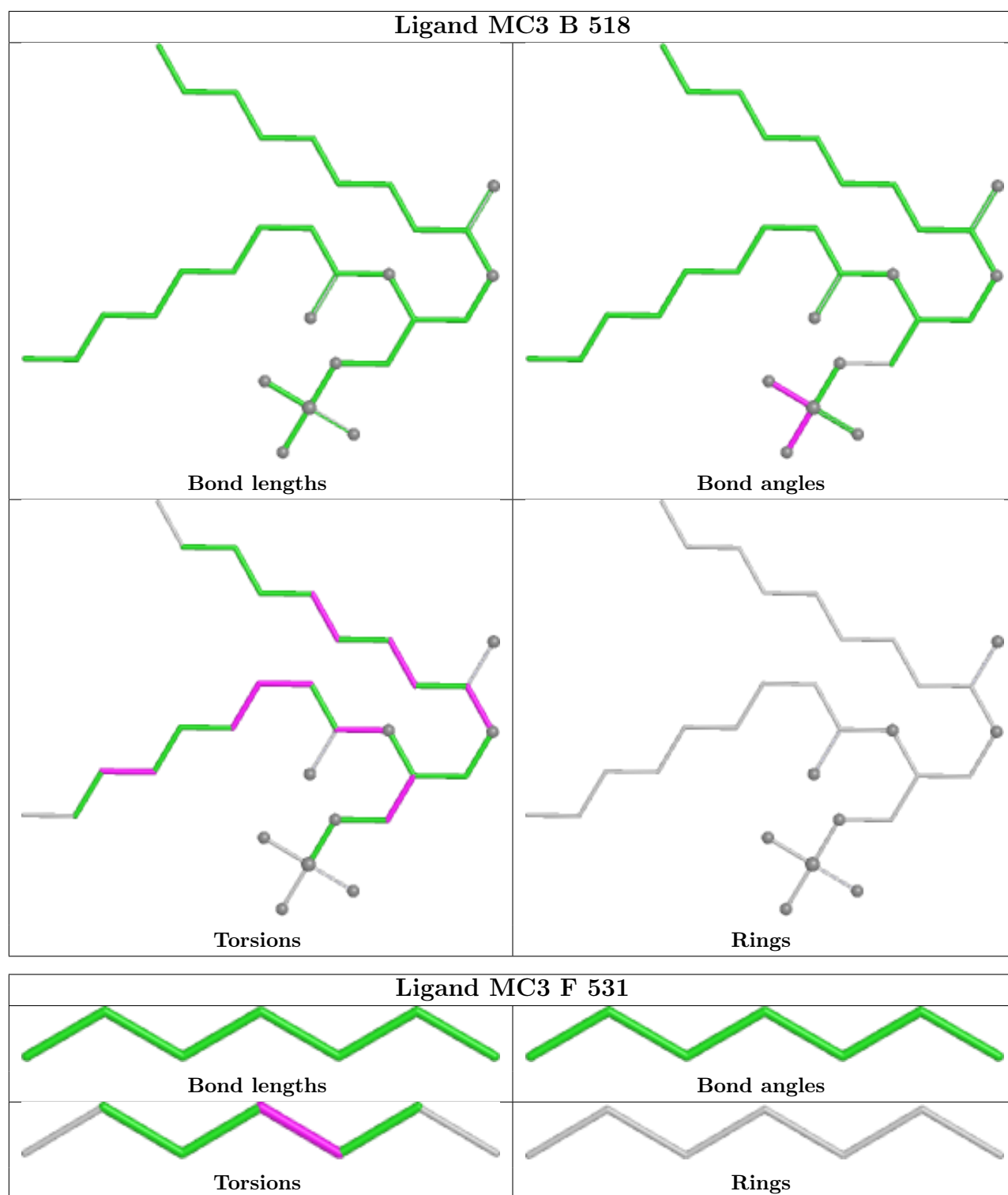


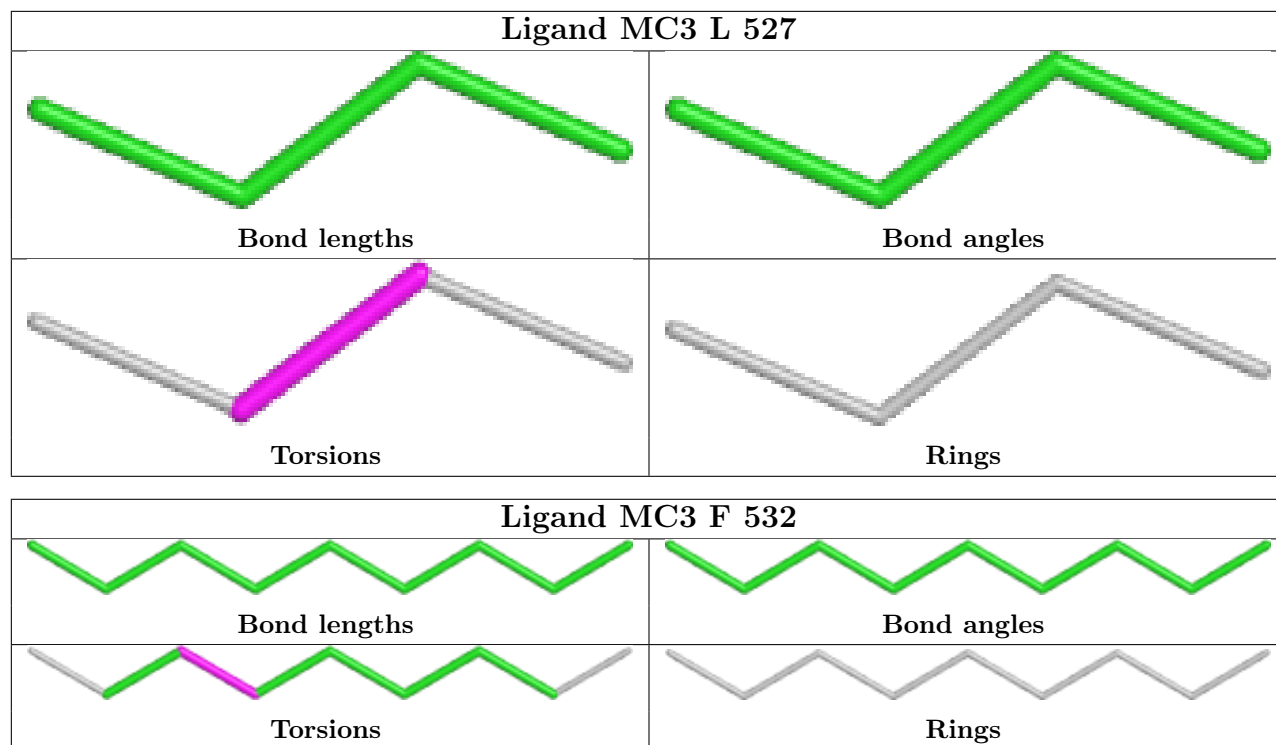


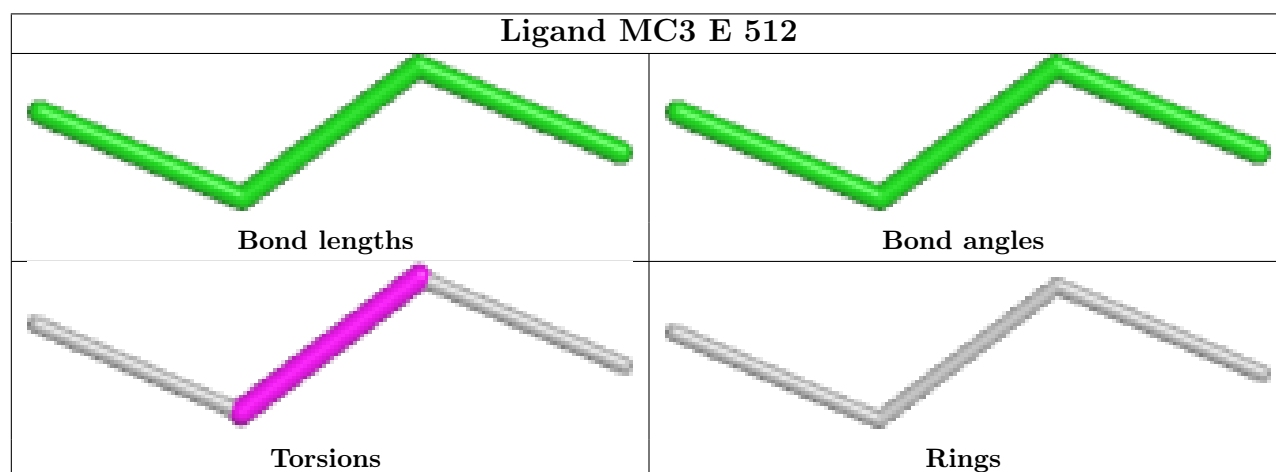
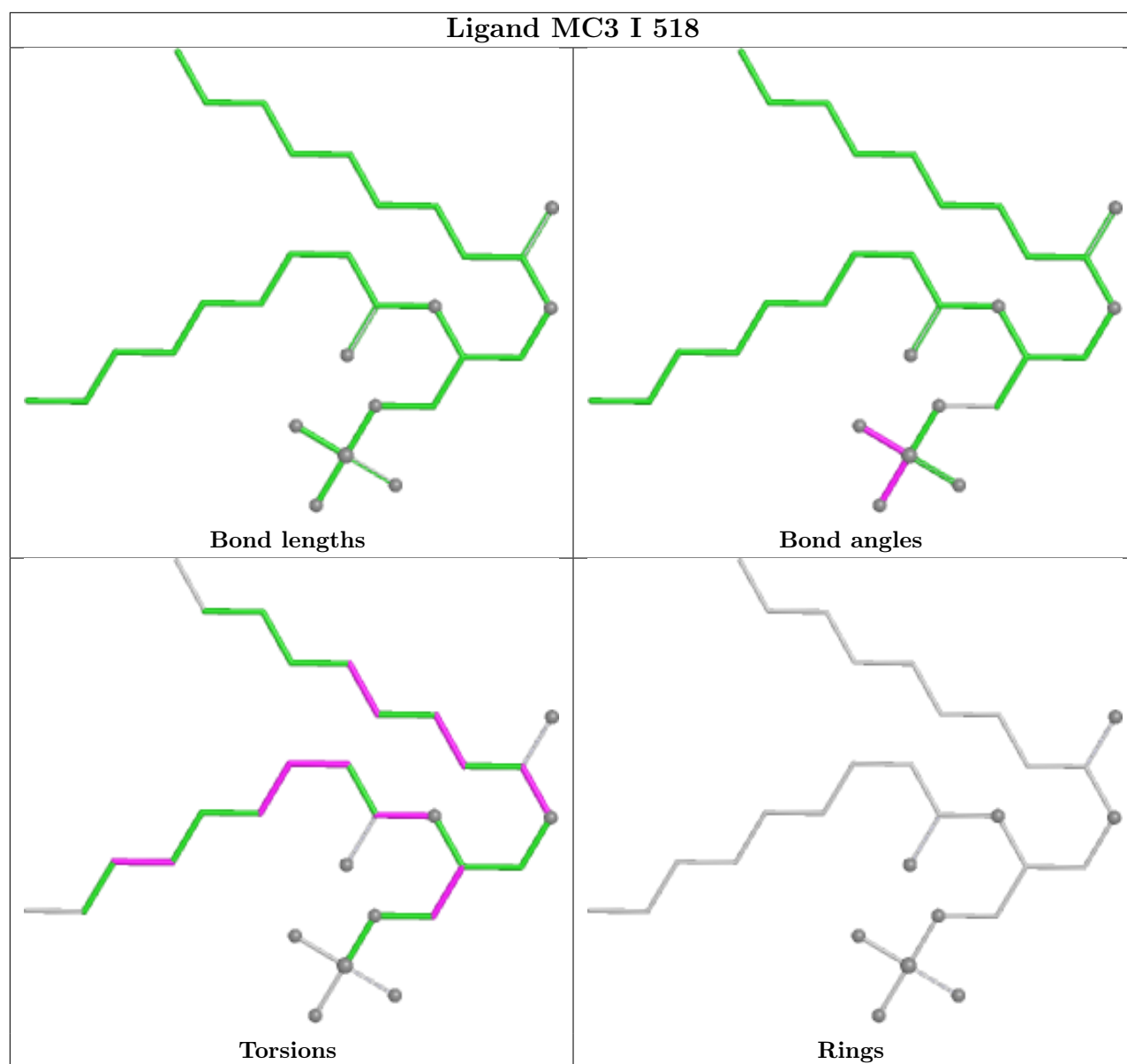
Ligand MC3 G 530	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand MC3 K 517	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand MC3 I 516	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand MC3 J 530	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand MC3 J 514	
 Bond lengths	 Bond angles
 Torsions	 Rings

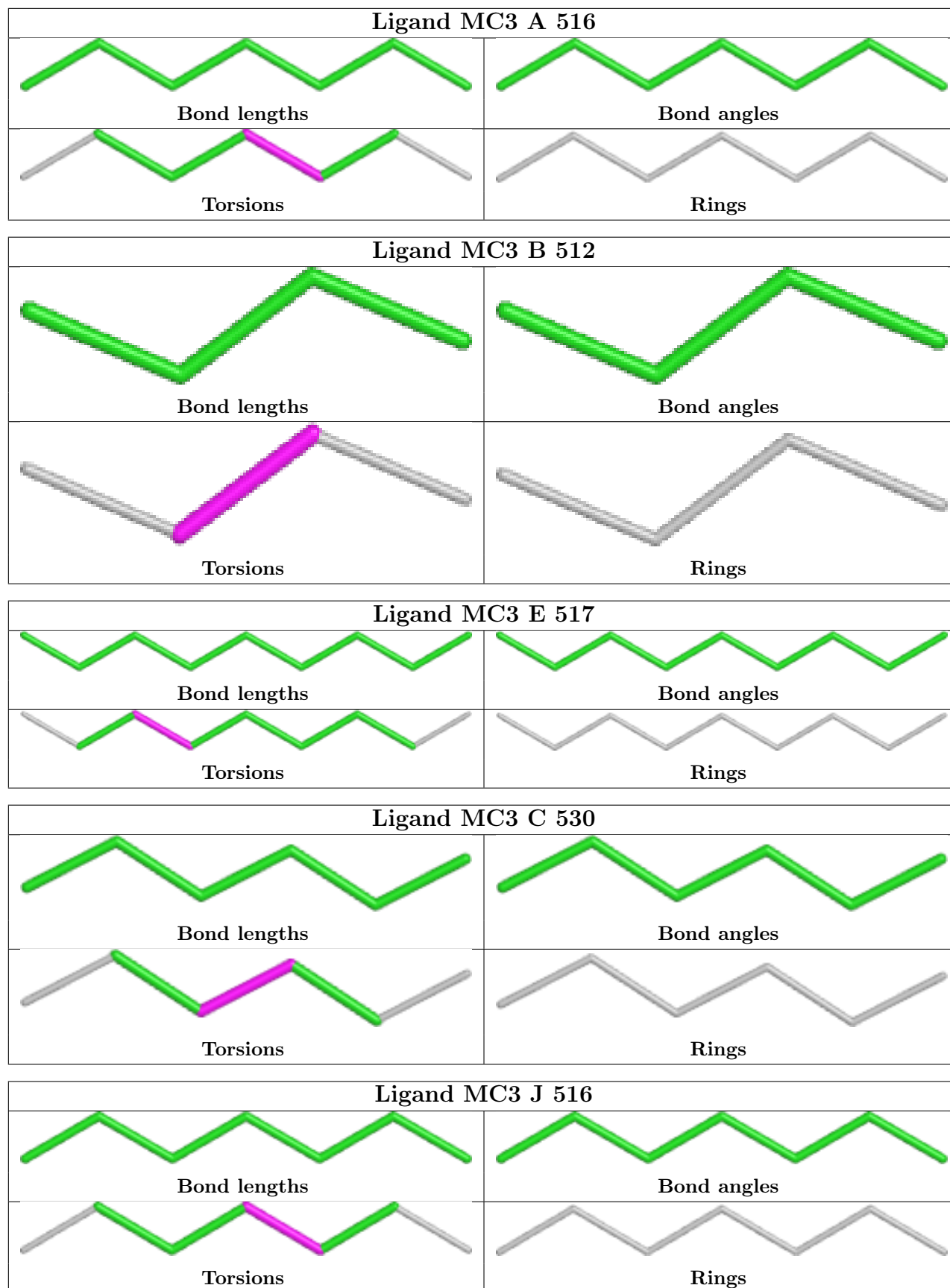


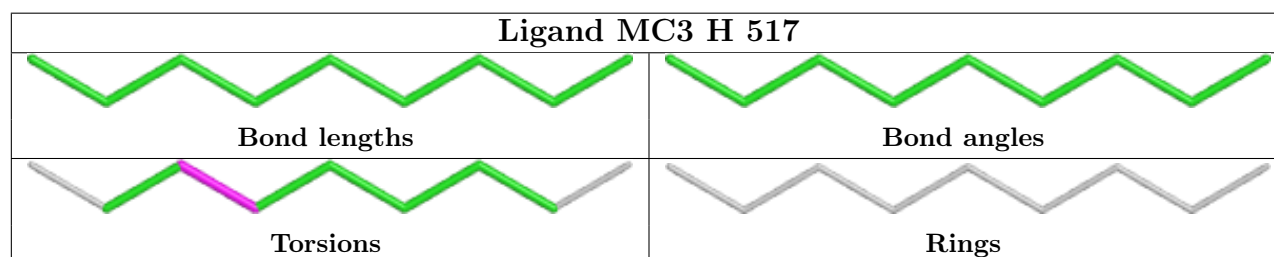
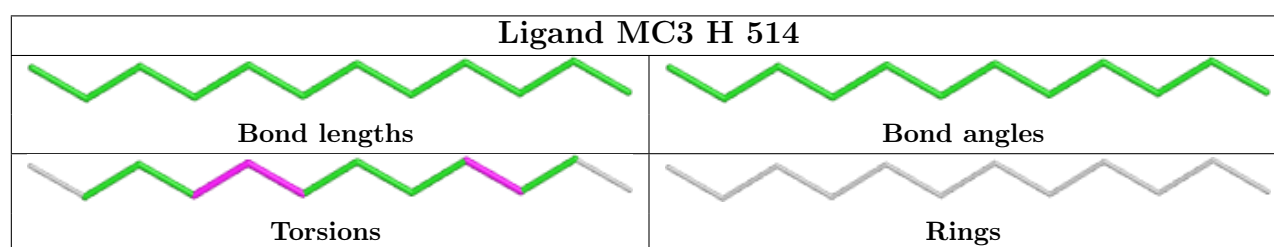
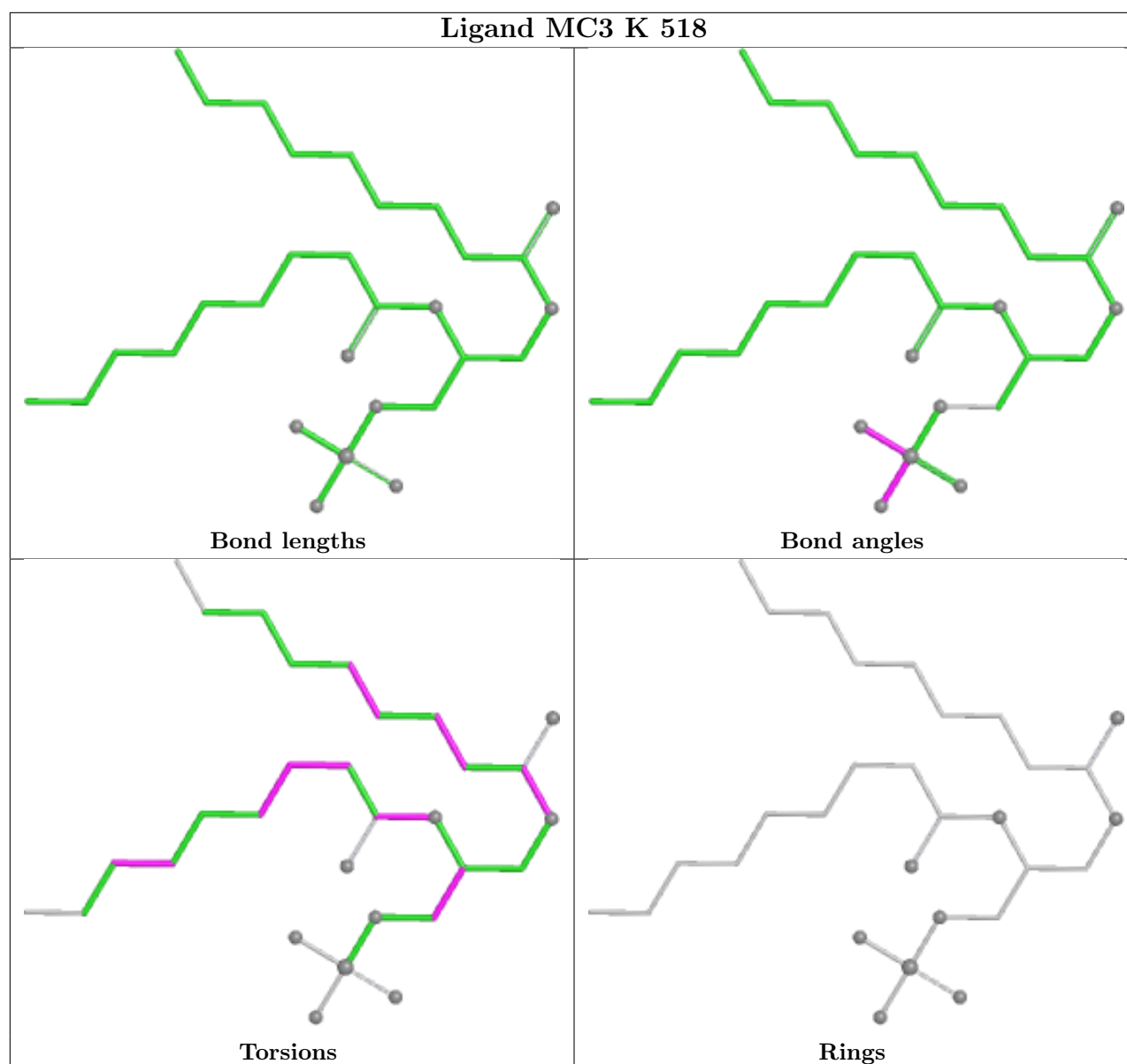


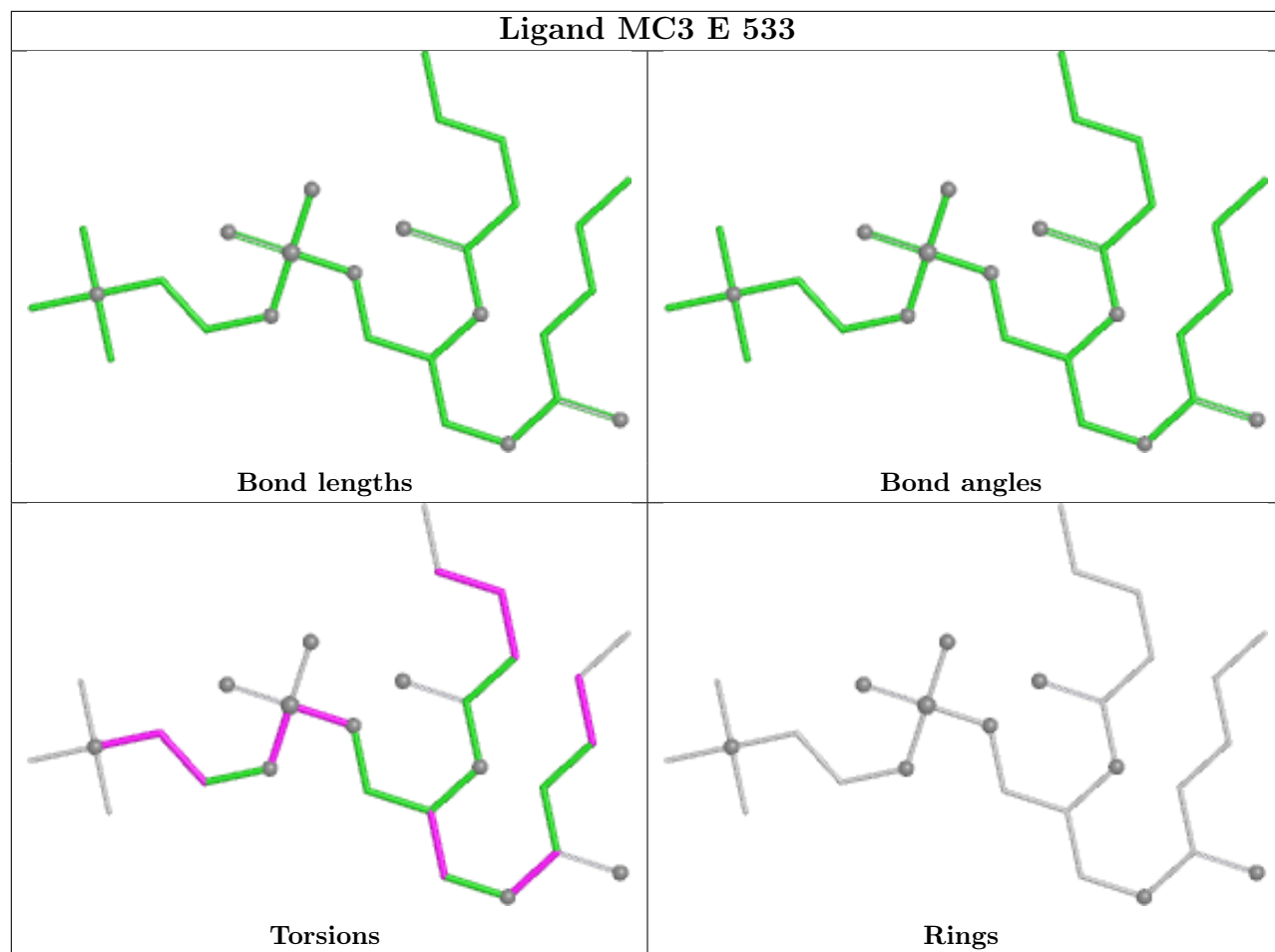


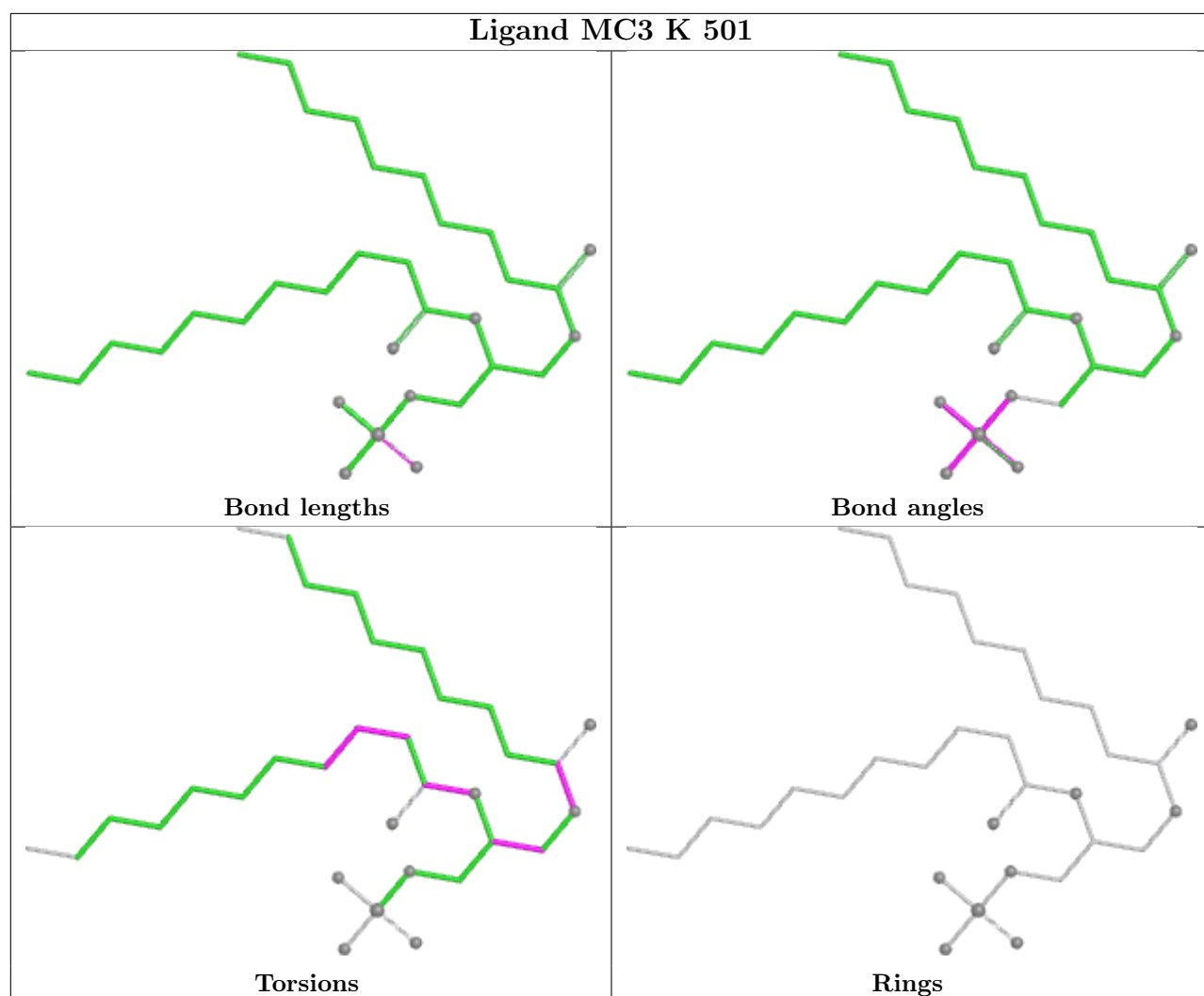


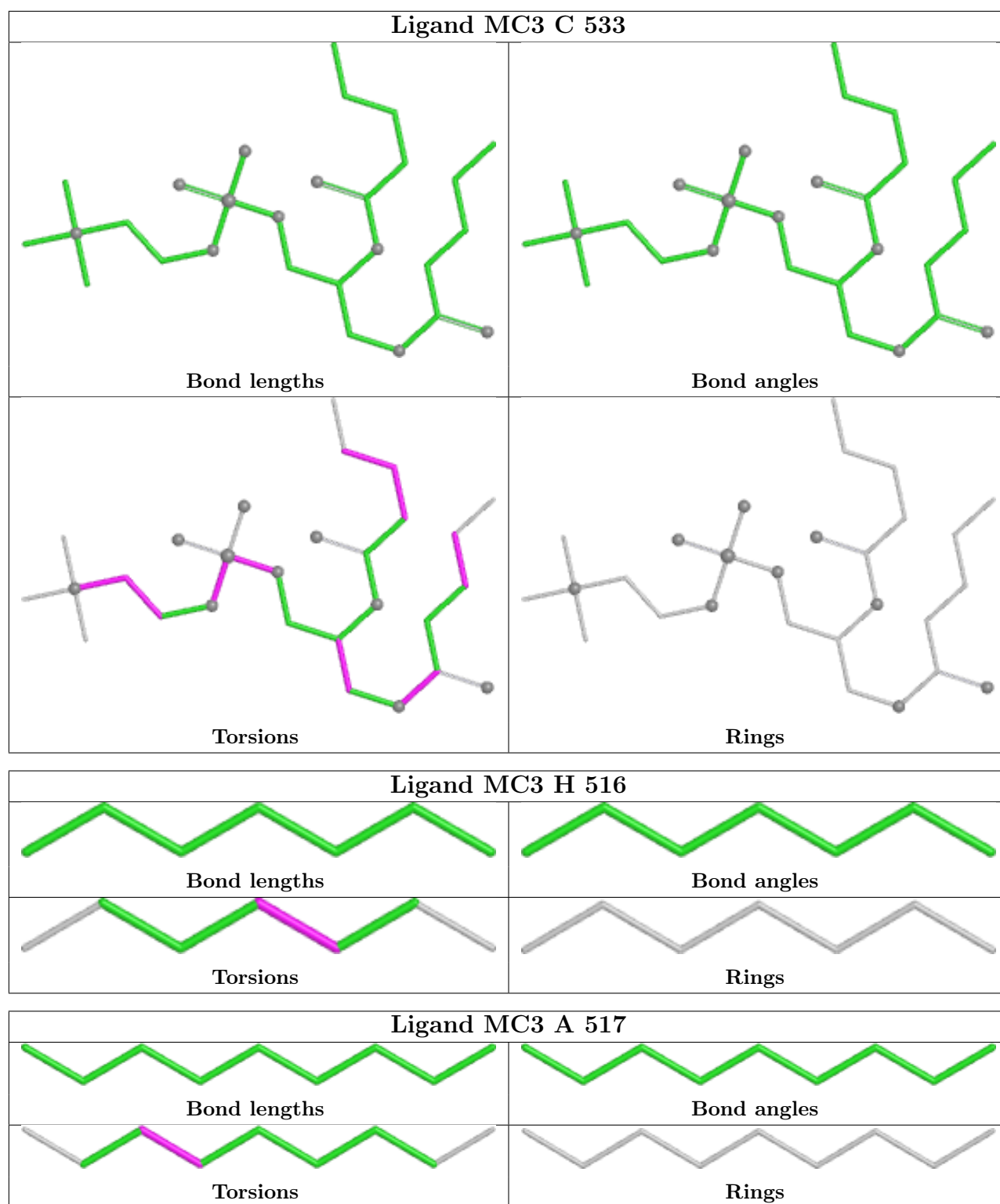


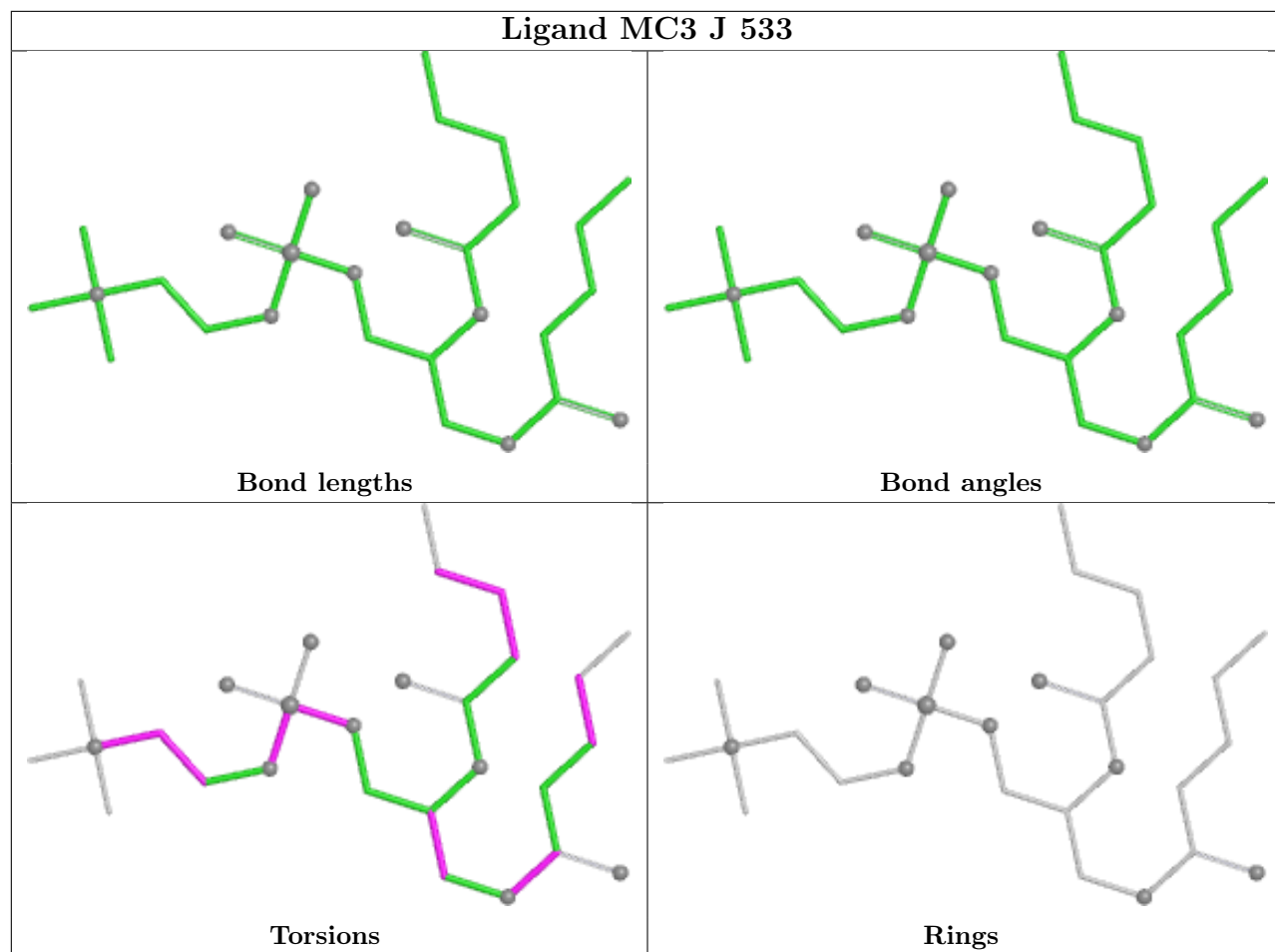


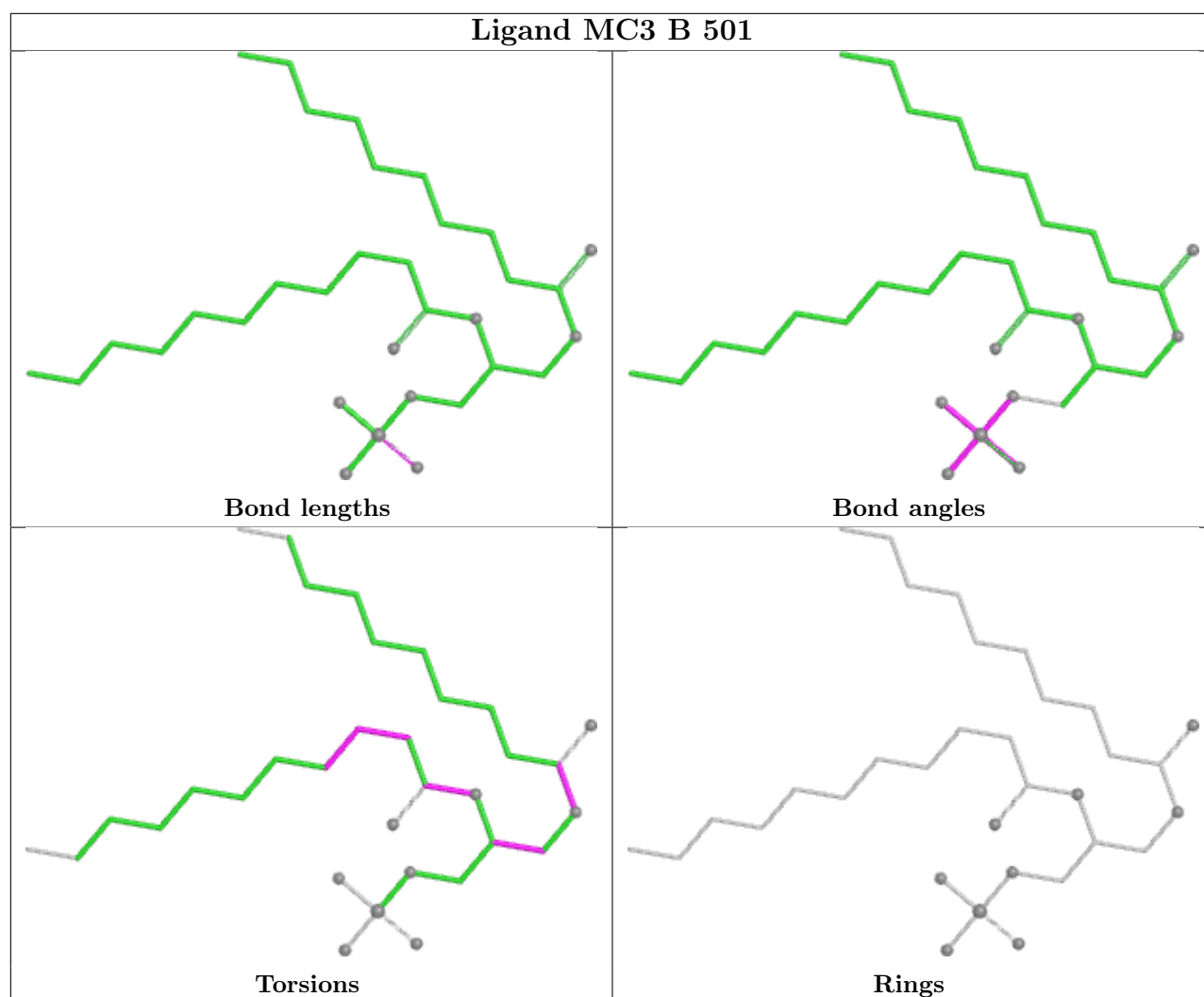


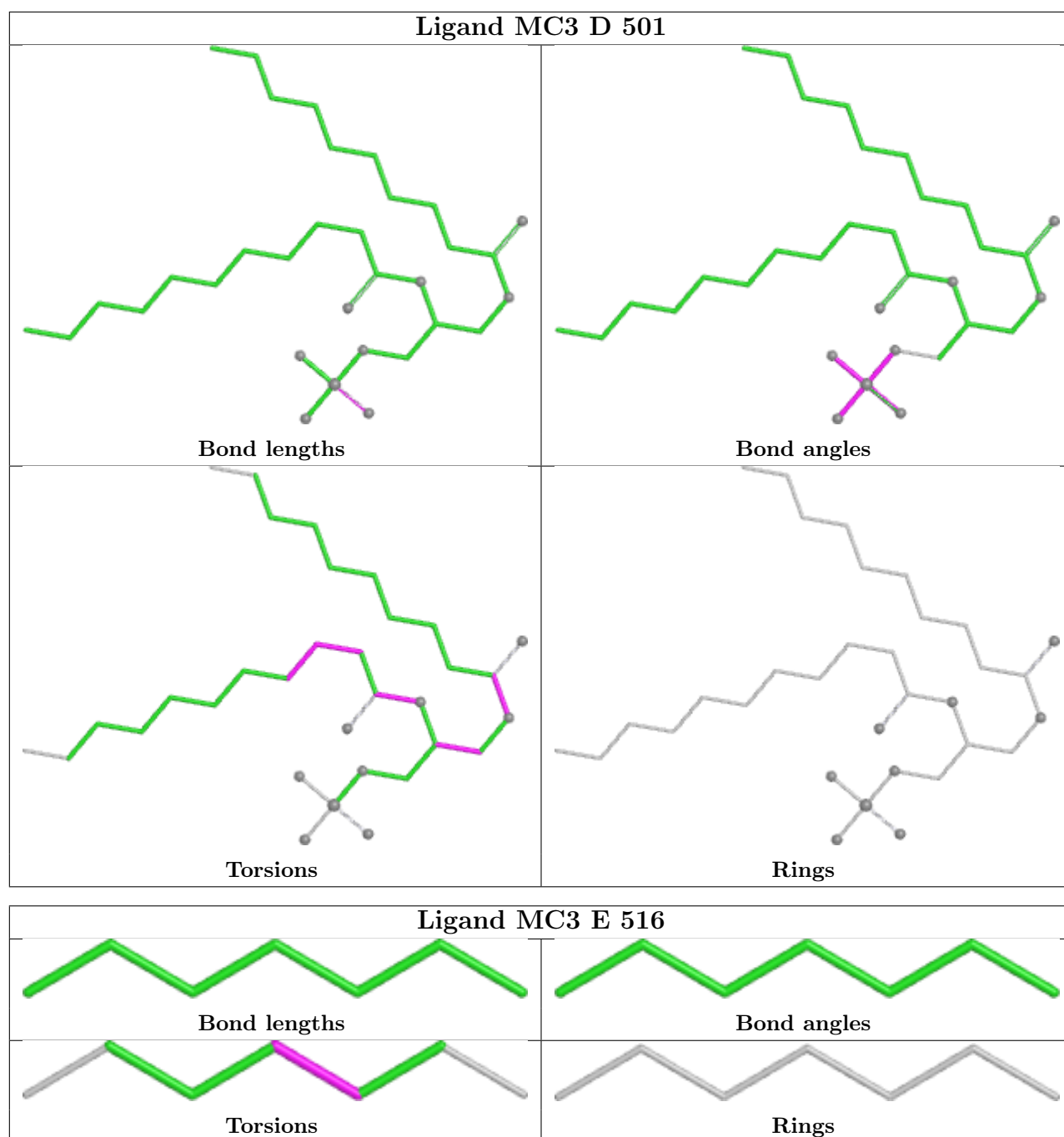


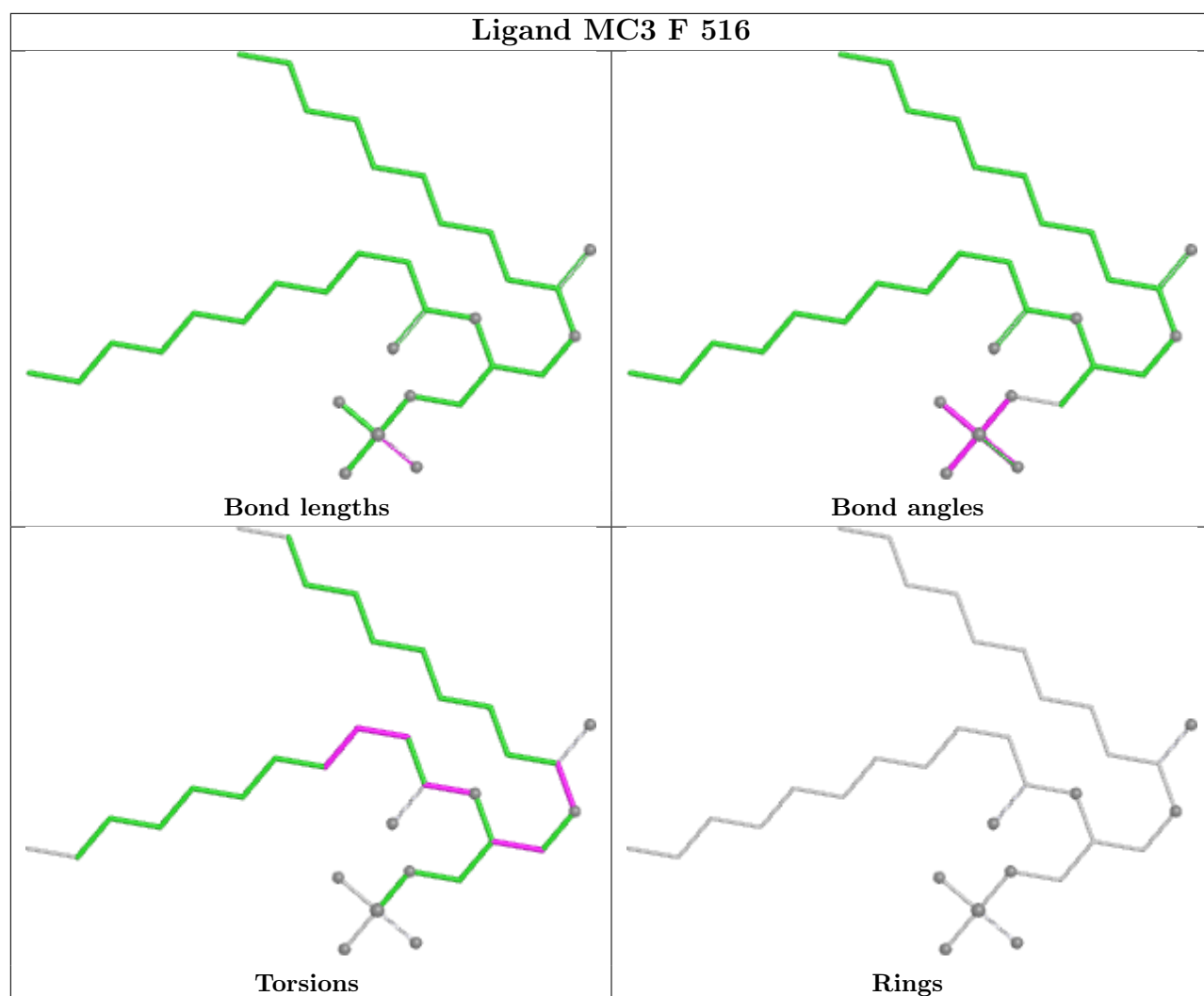


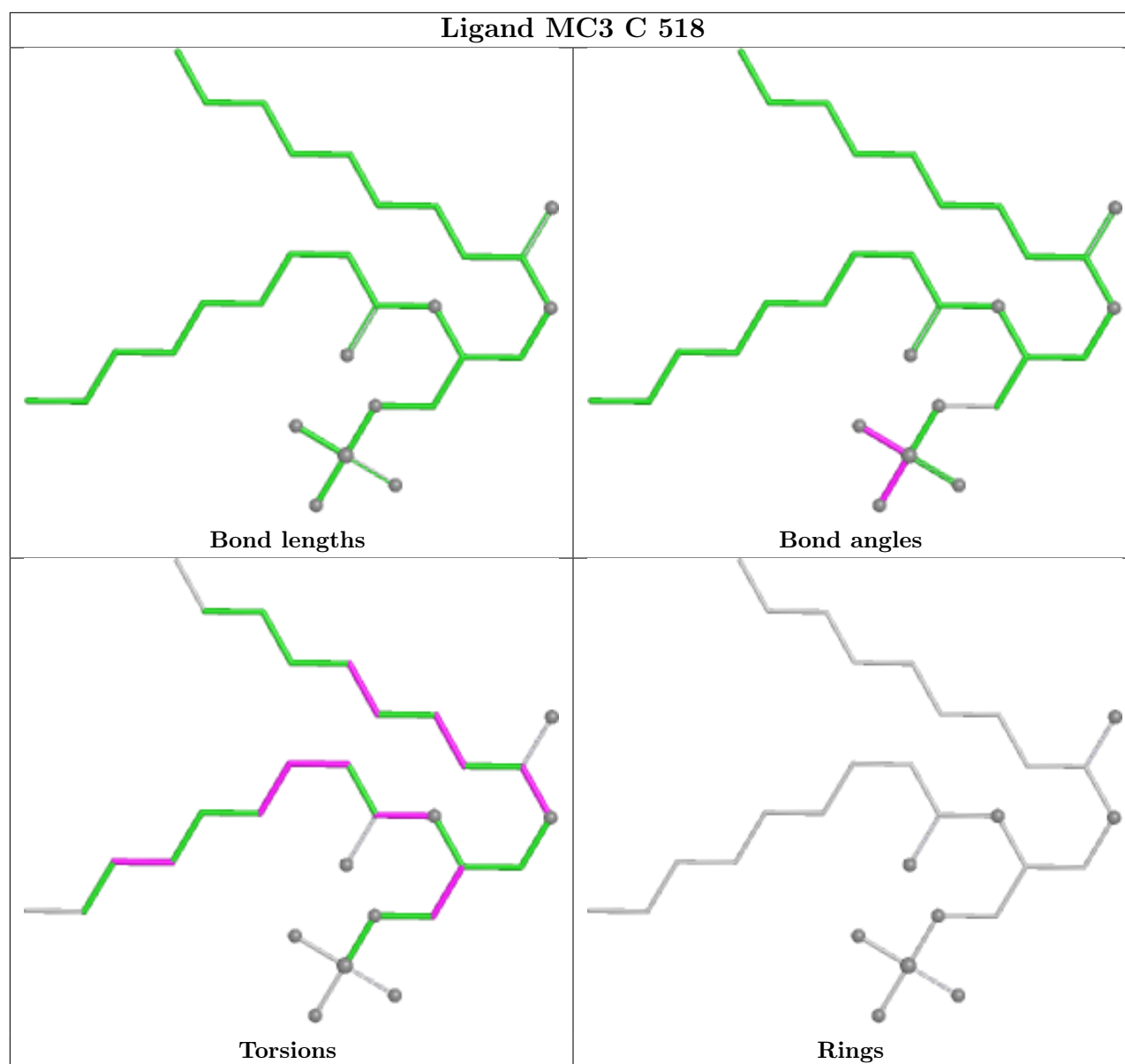


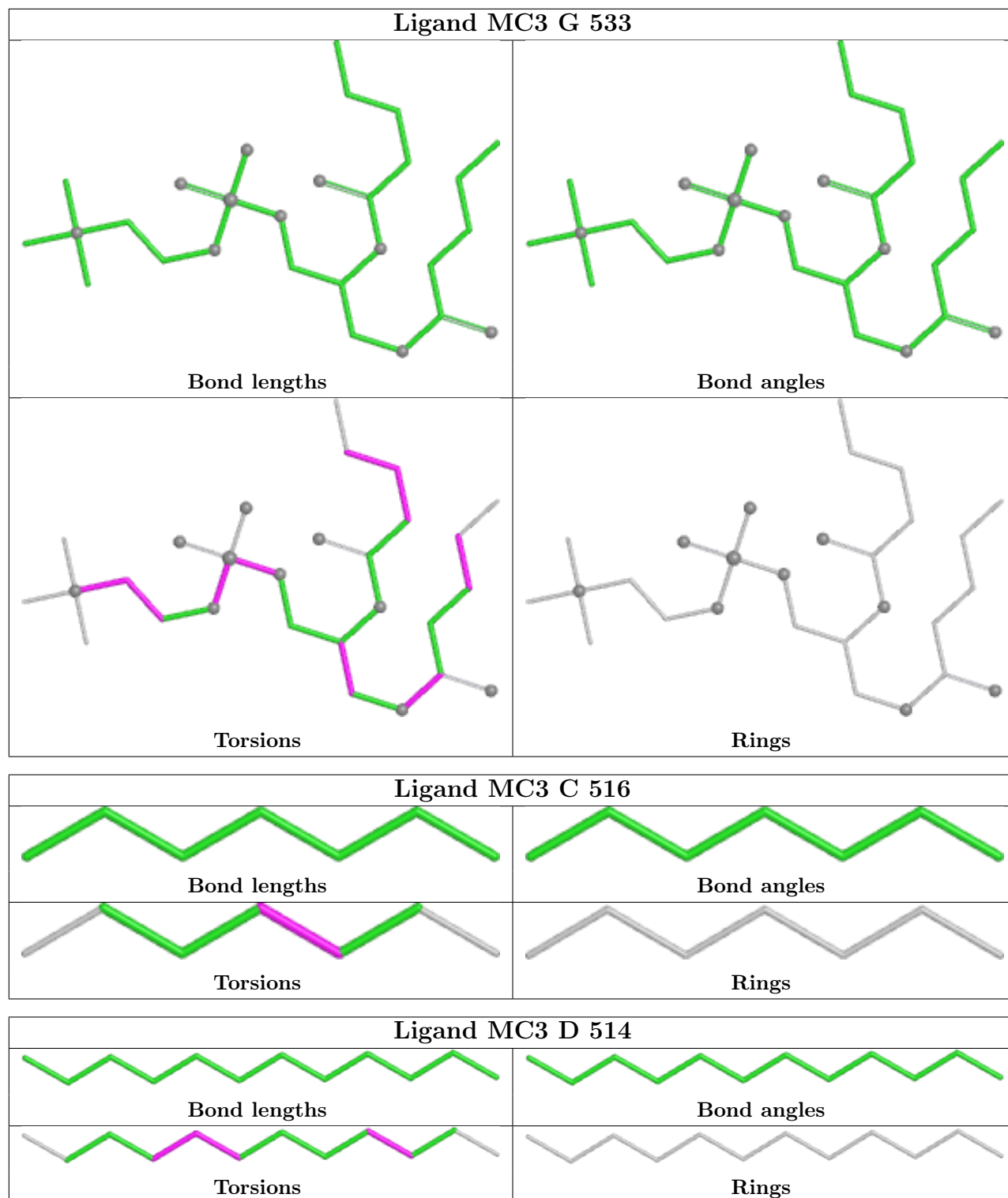


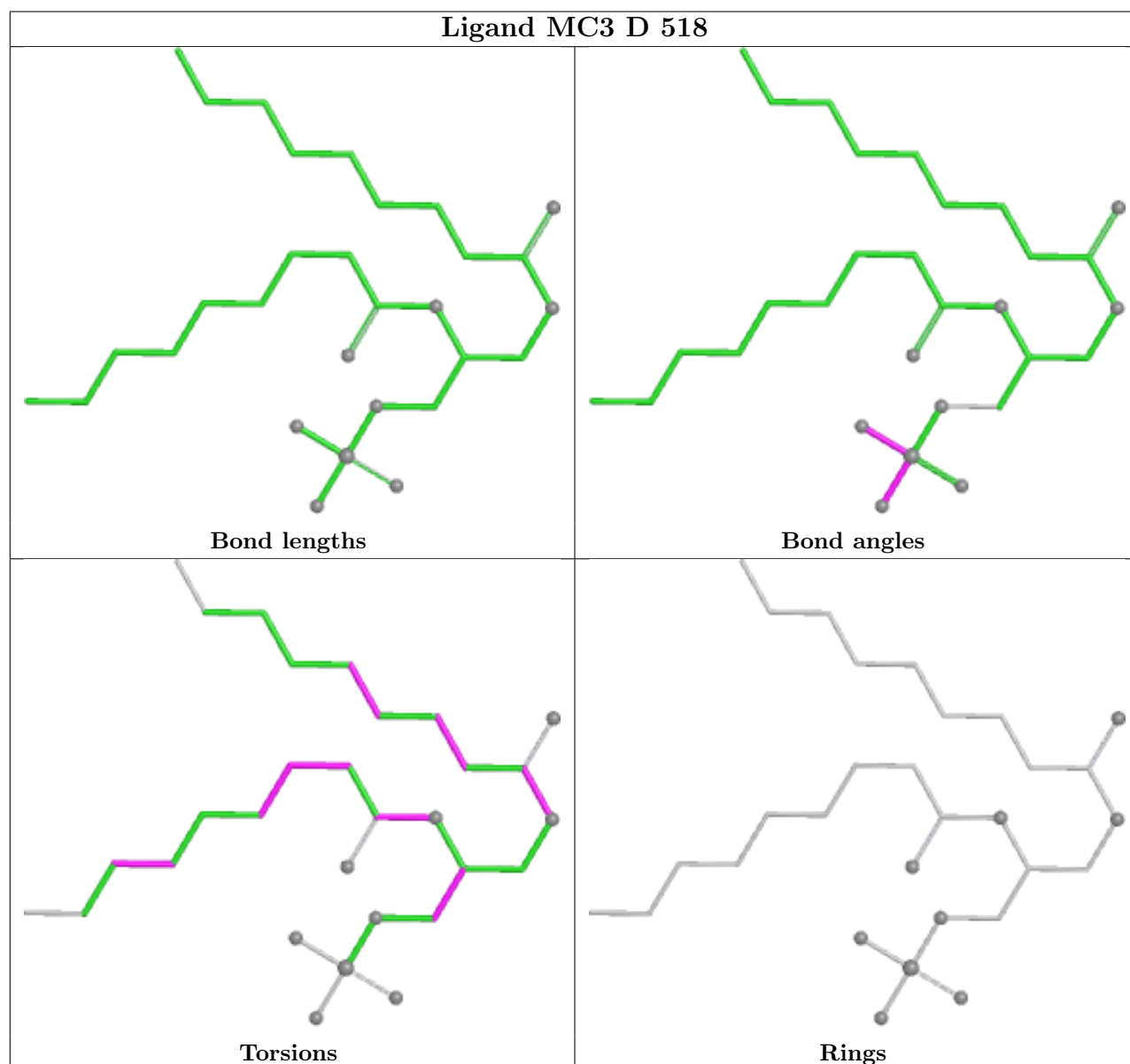
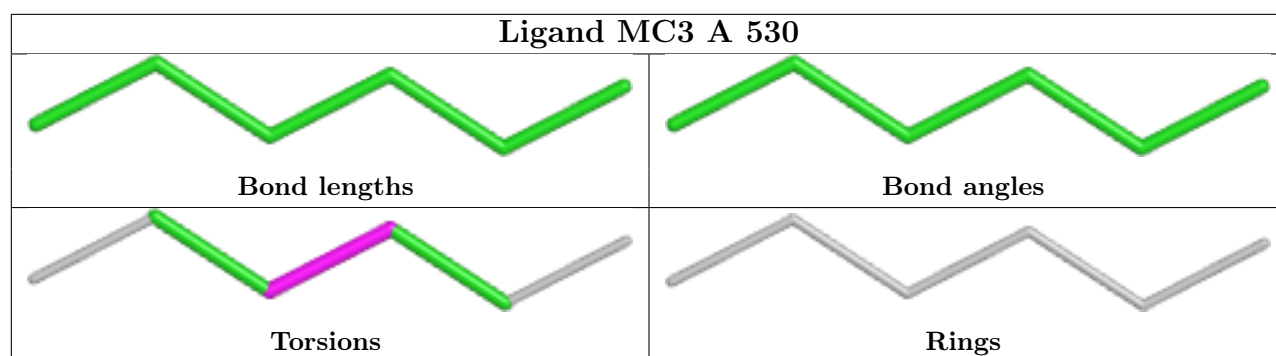


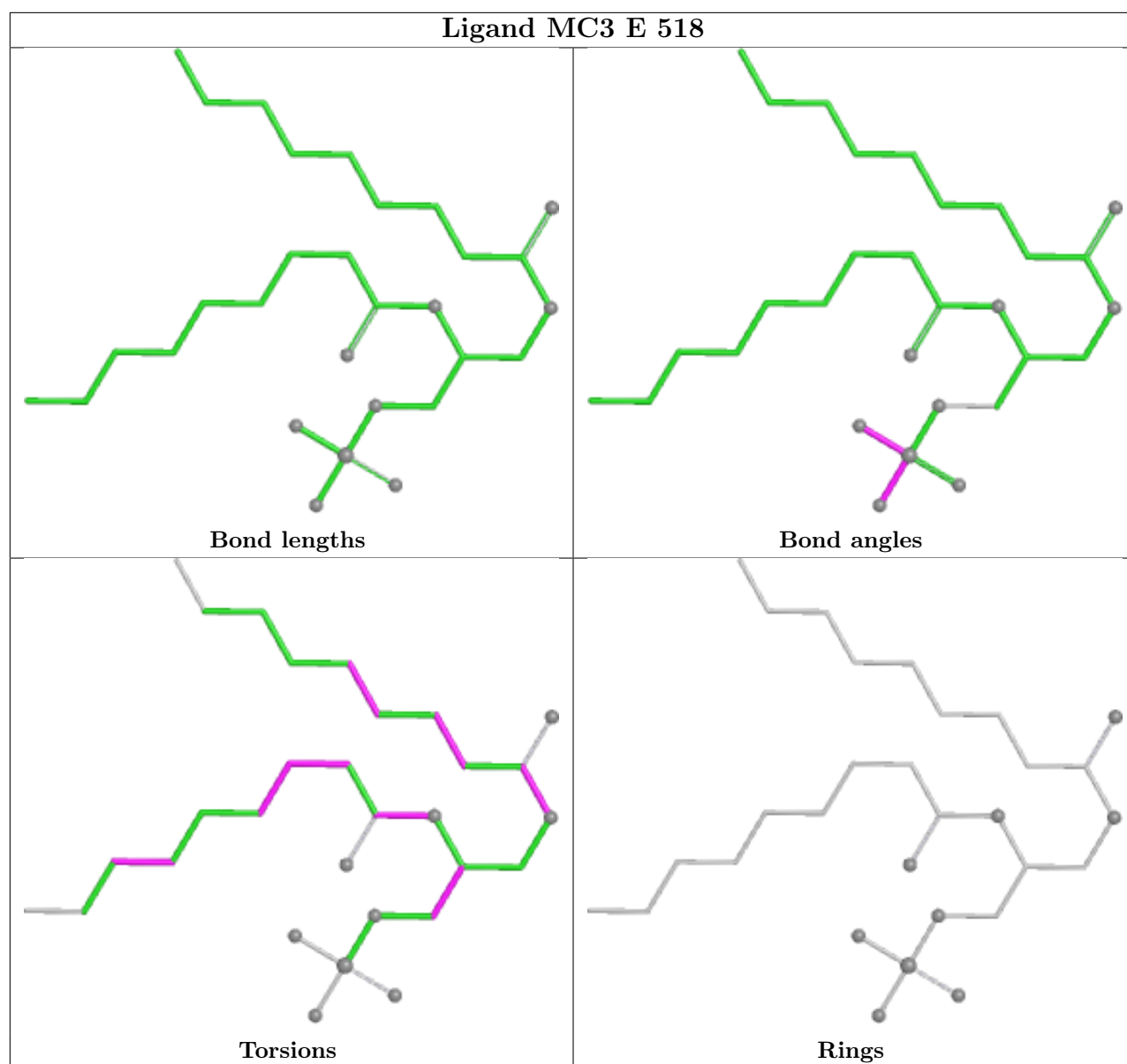


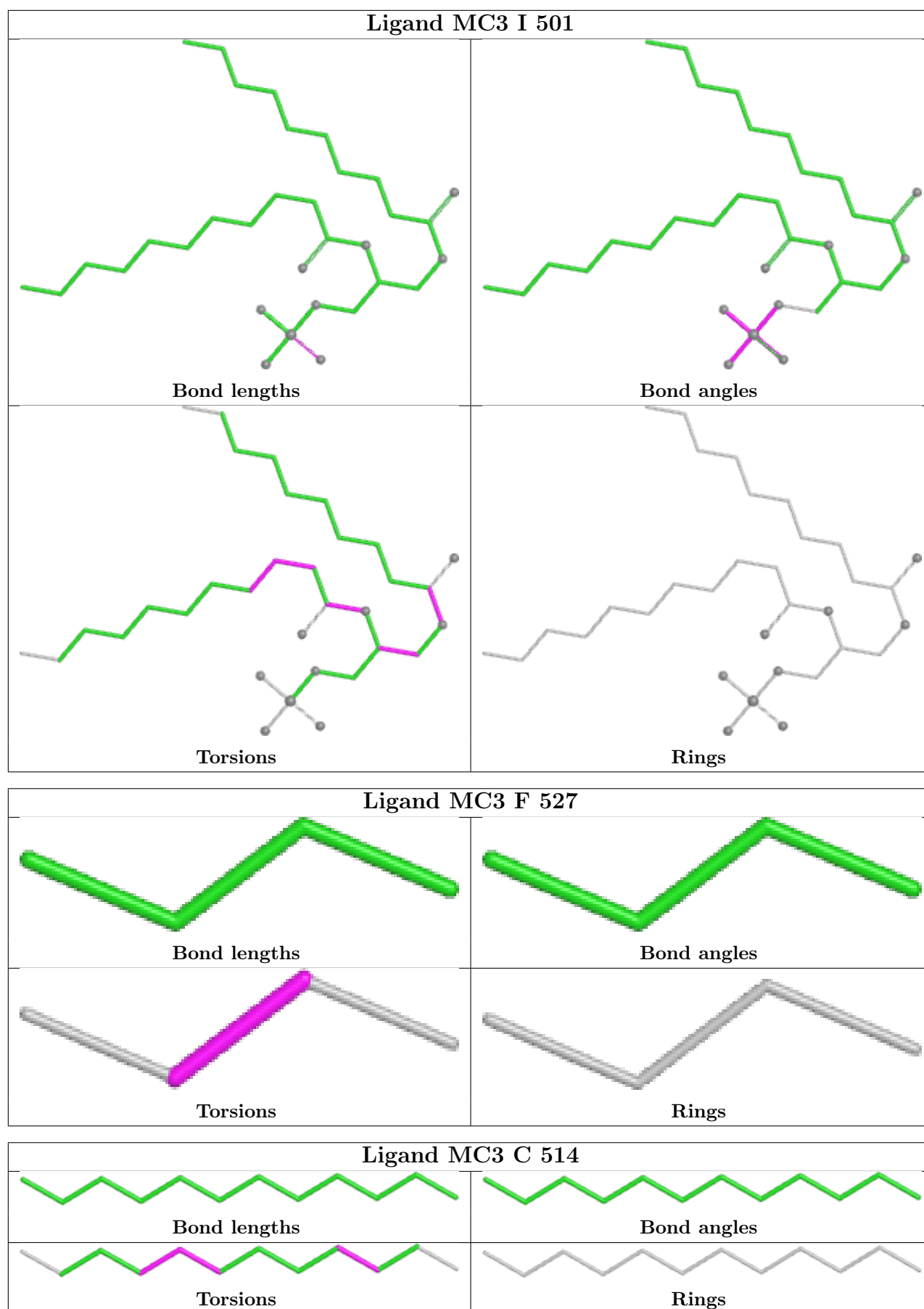


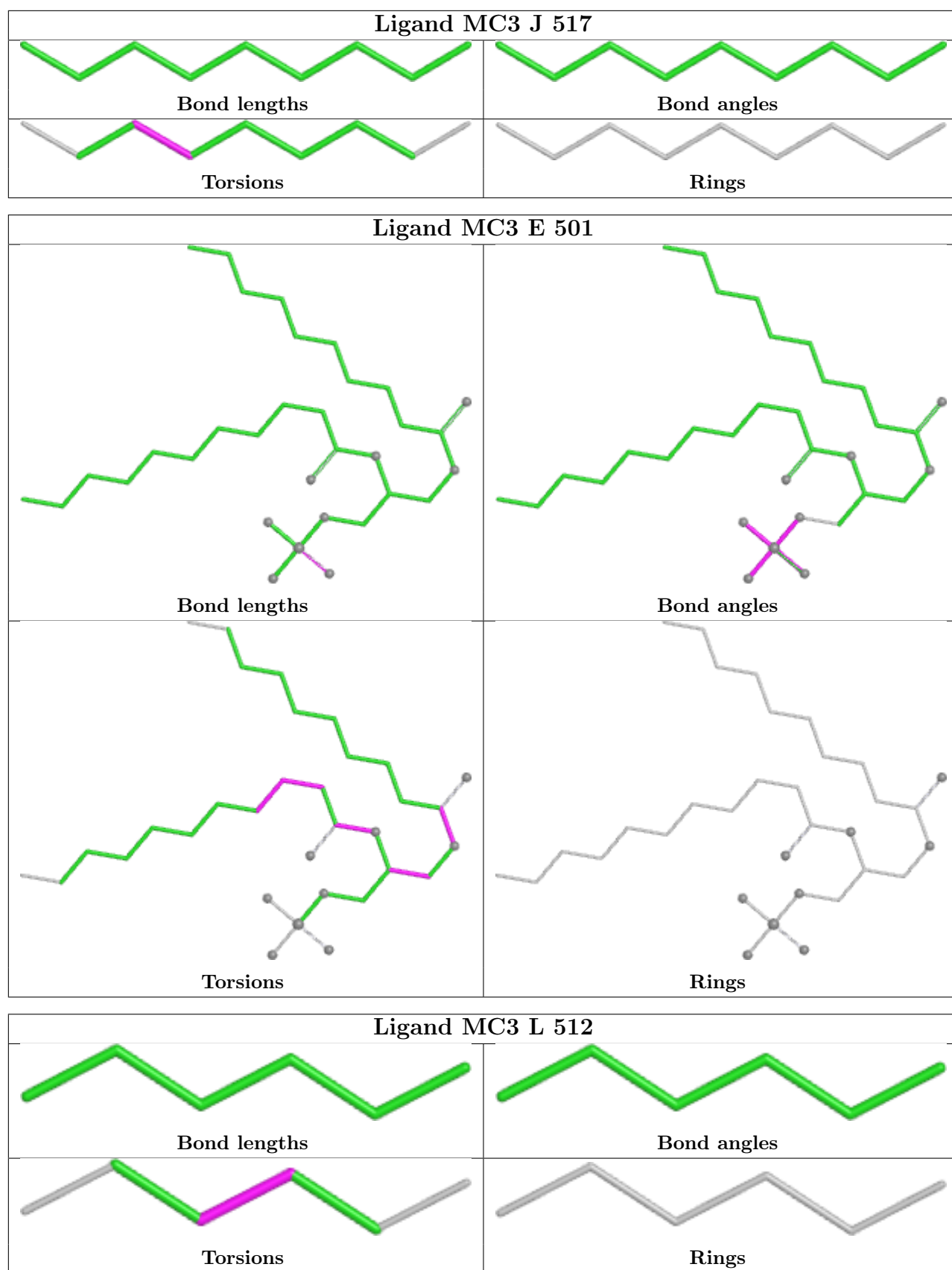


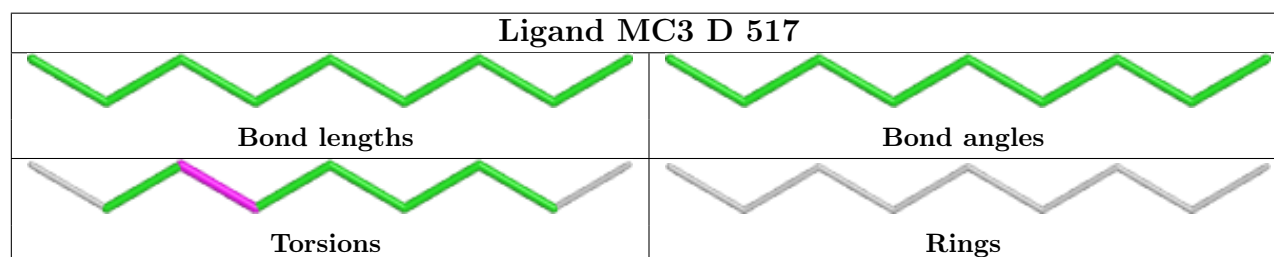
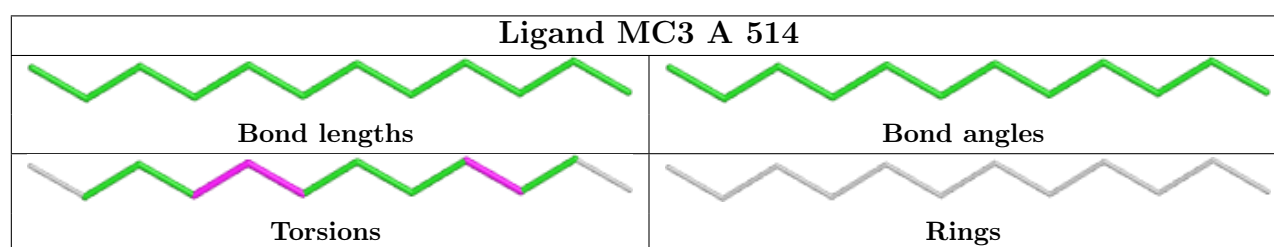
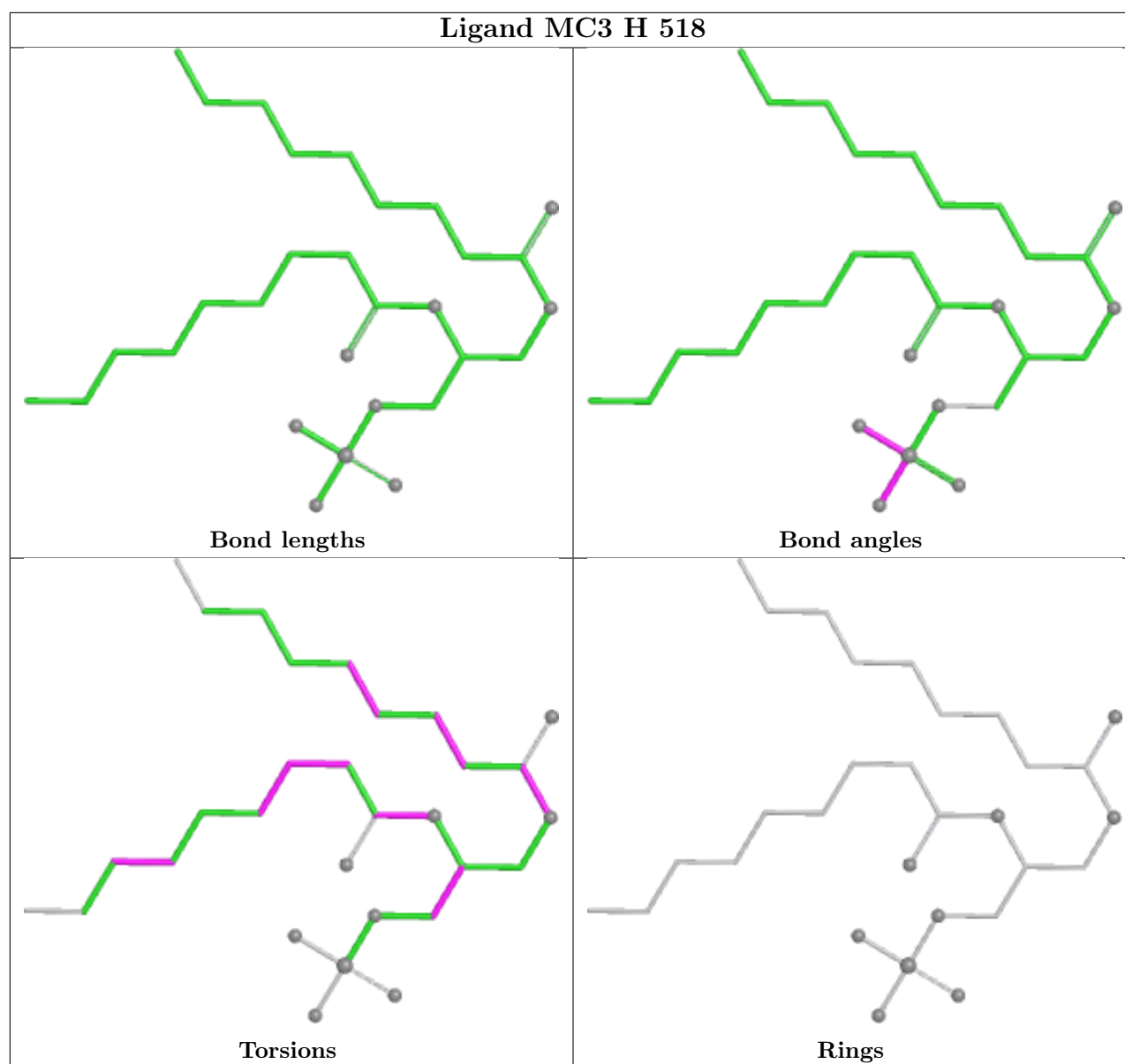


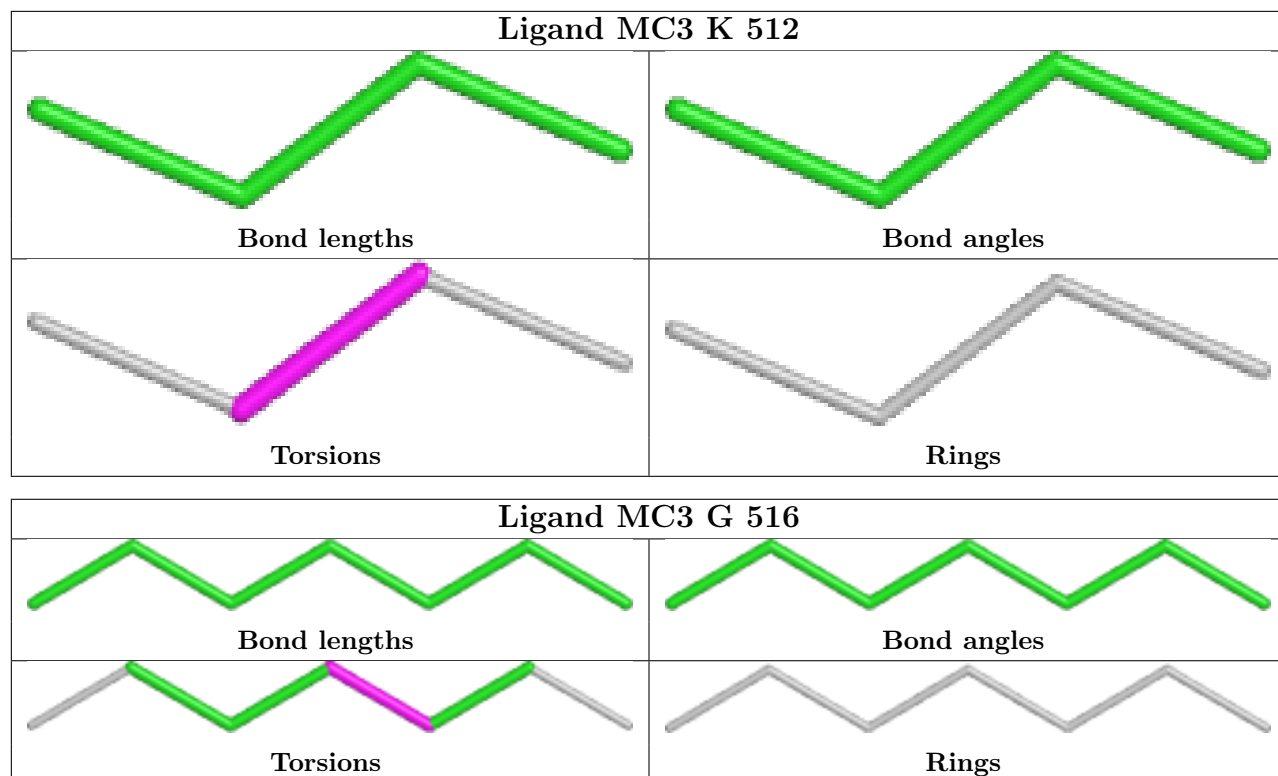


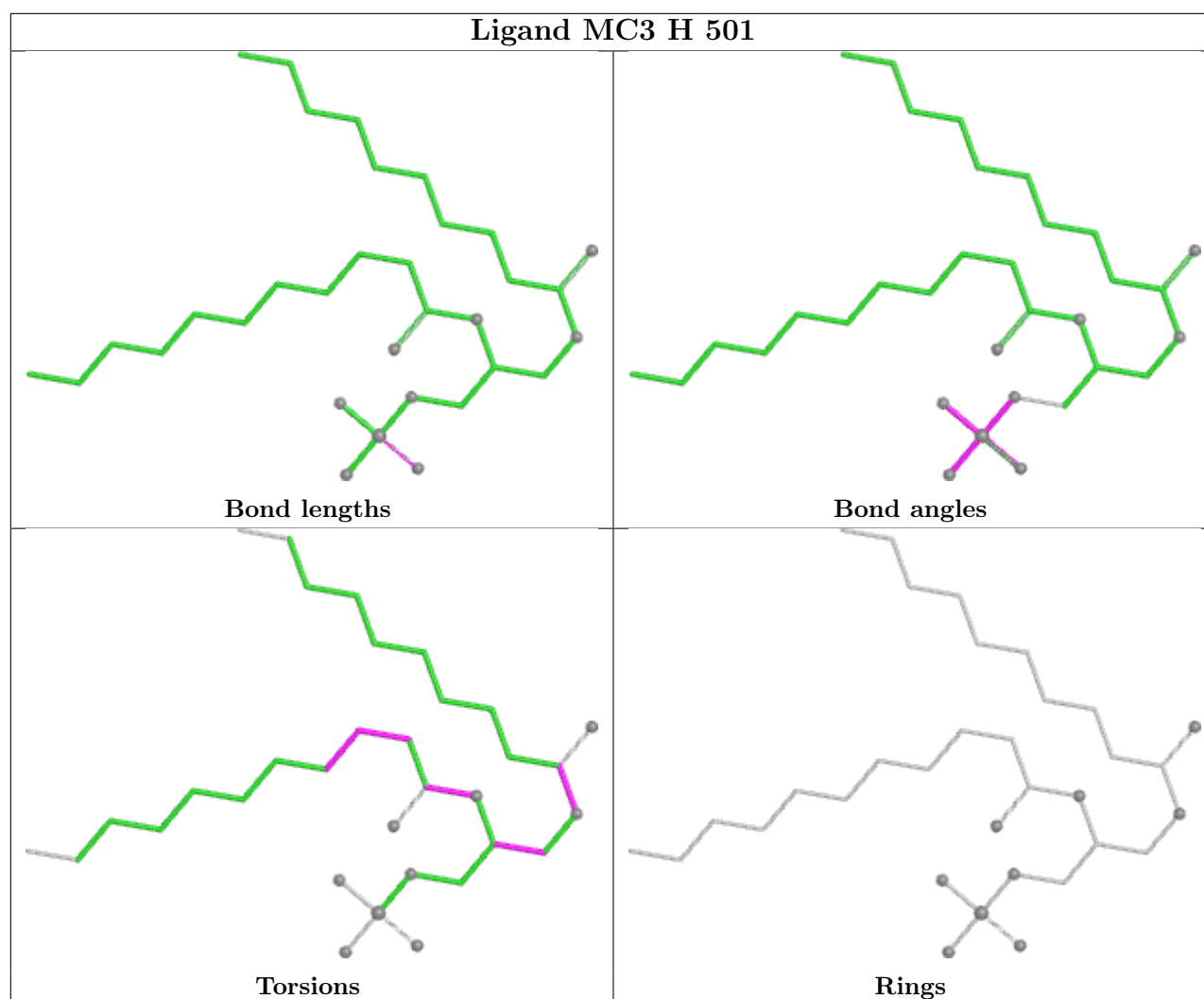












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

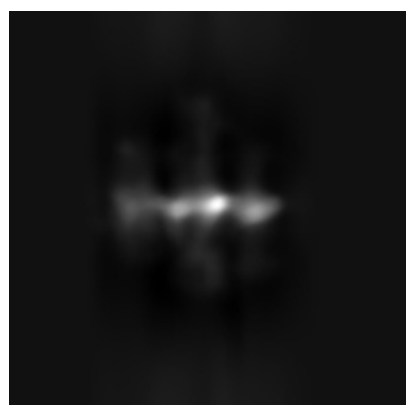
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7396. These allow visual inspection of the internal detail of the map and identification of artifacts.

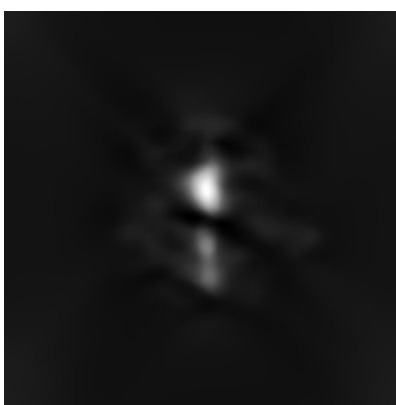
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y



Z

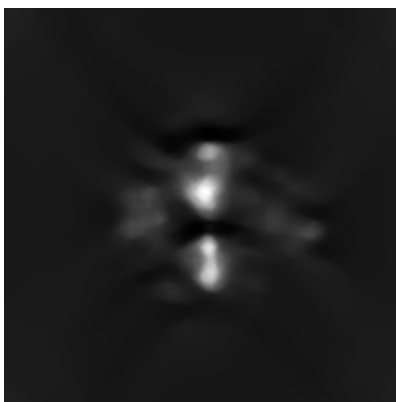
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 64



Y Index: 64



Z Index: 64

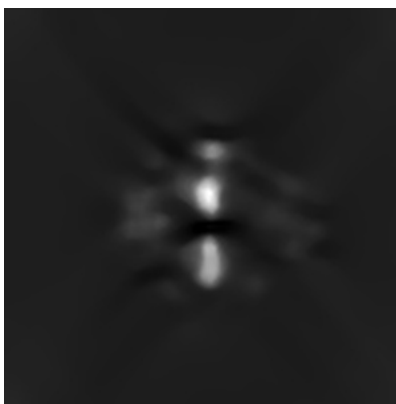
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 71



Y Index: 66

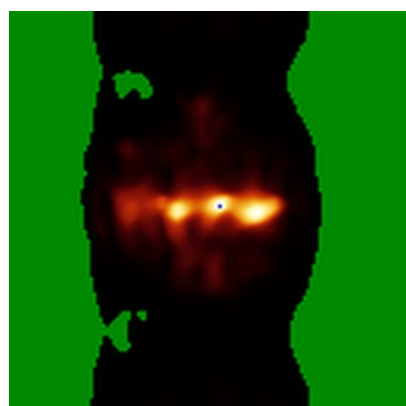


Z Index: 65

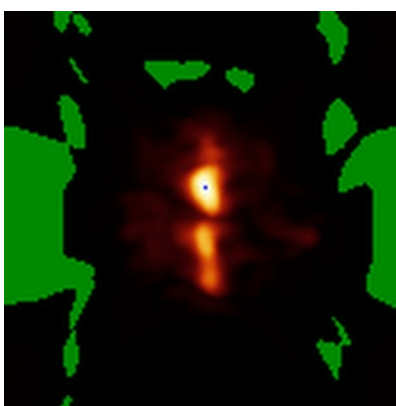
The images above show the largest variance slices of the map in three orthogonal directions.

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

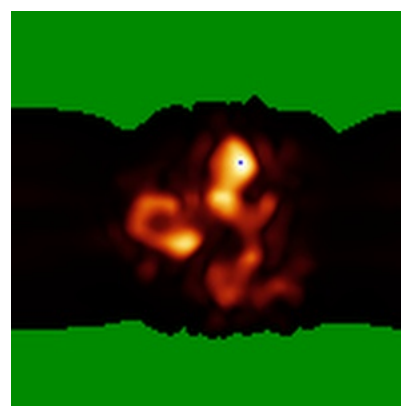
6.4.1 Primary map



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

This section was not generated.

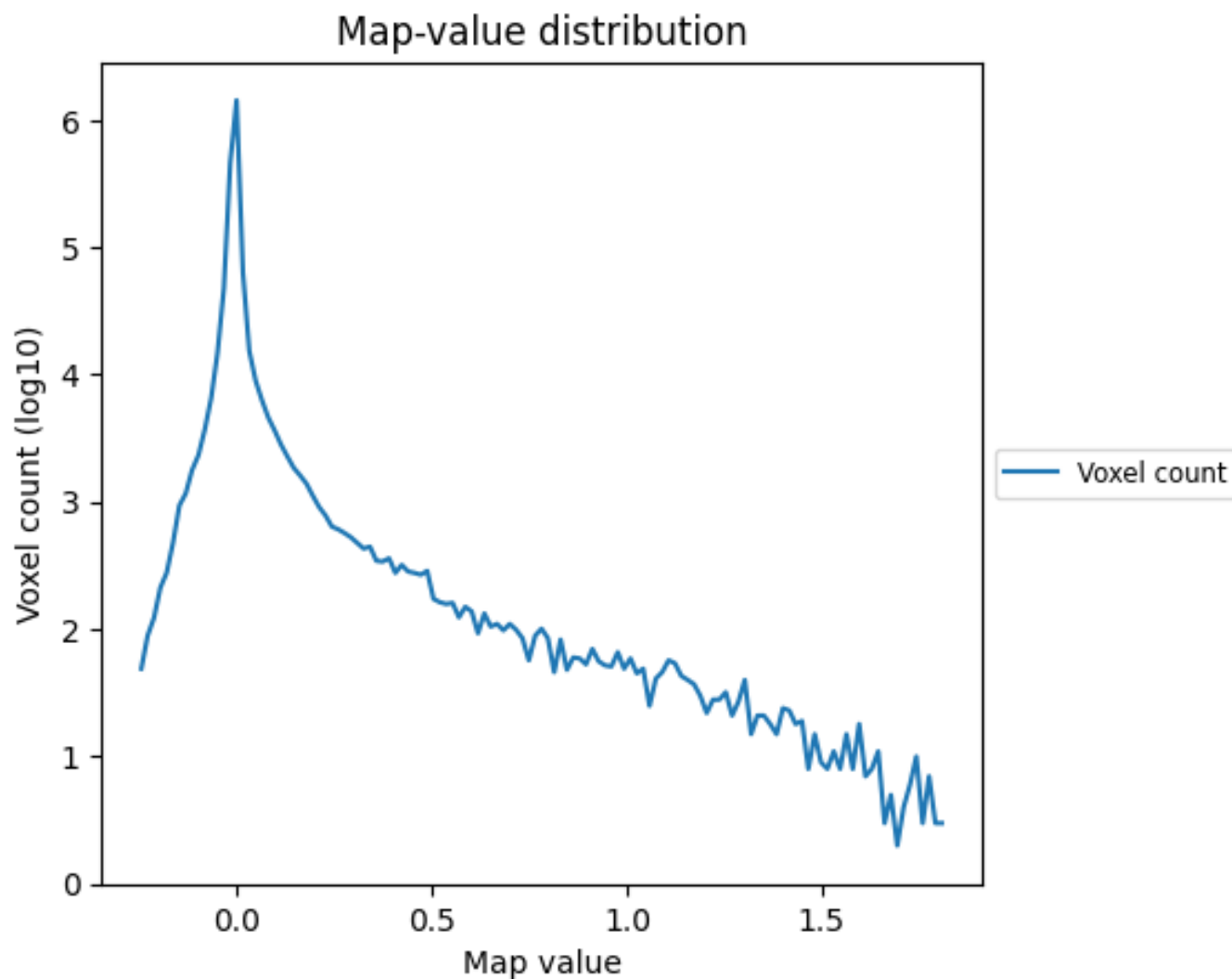
6.6 Mask visualisation

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

7 Map analysis [i](#)

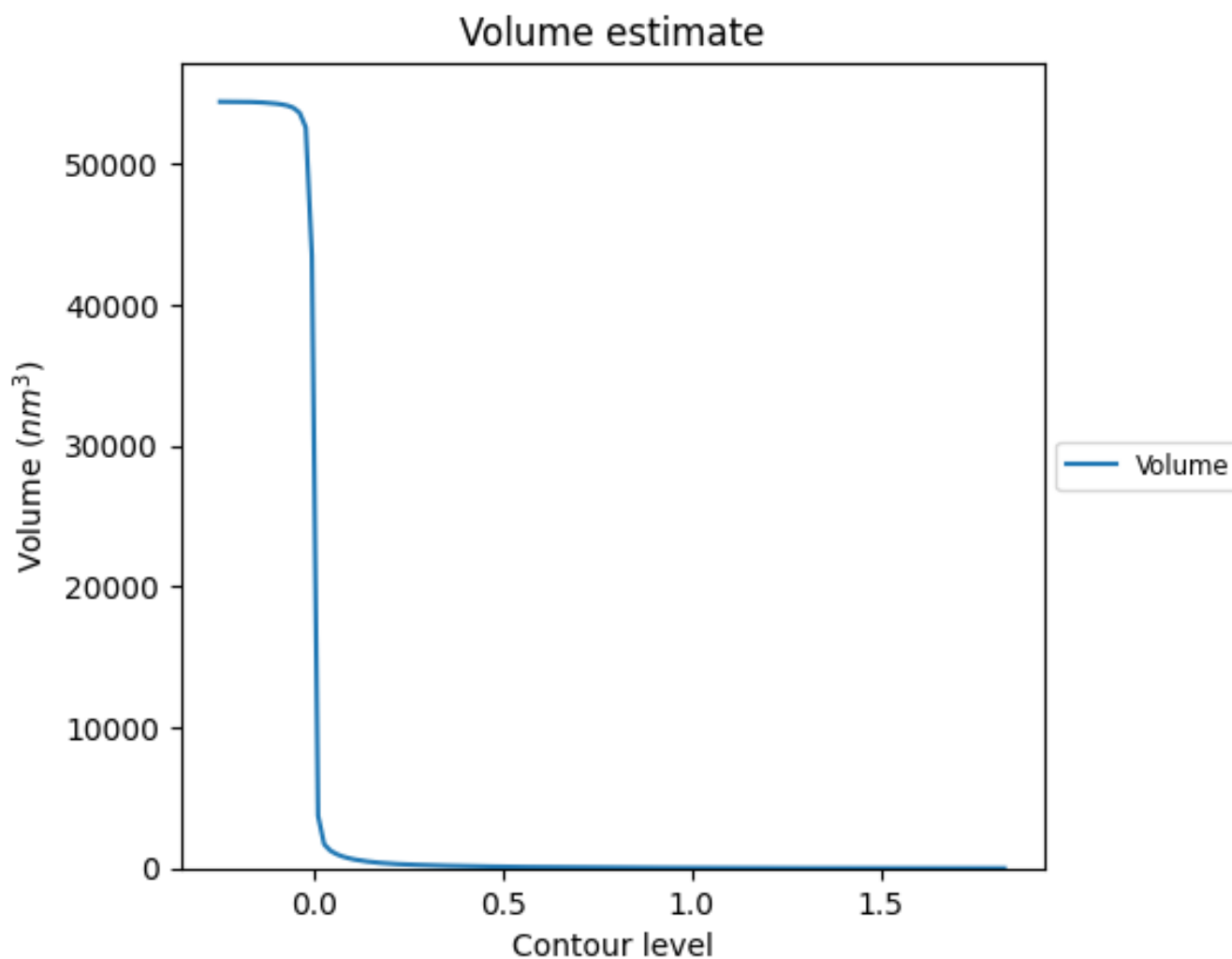
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



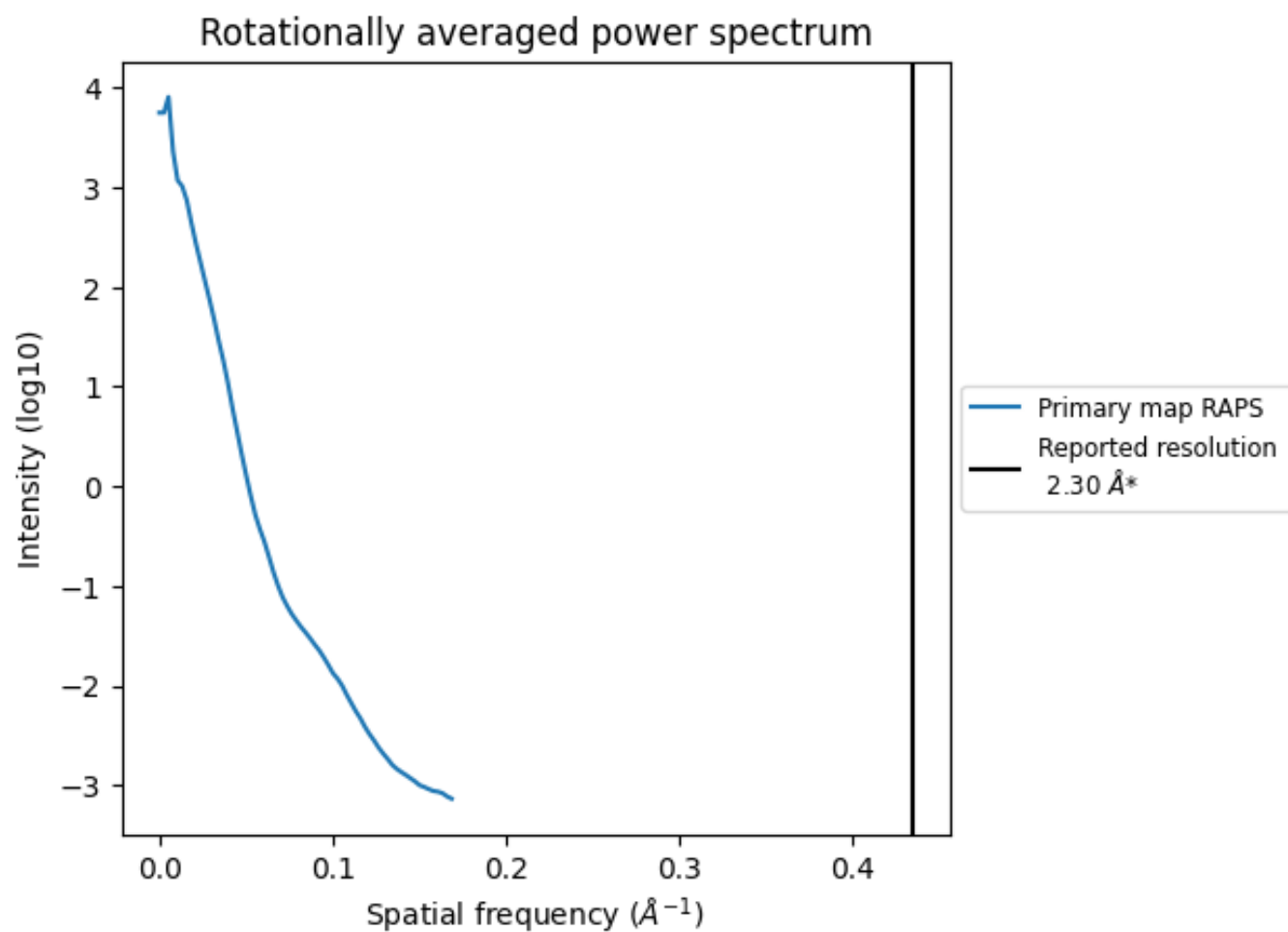
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume 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 ⓘ

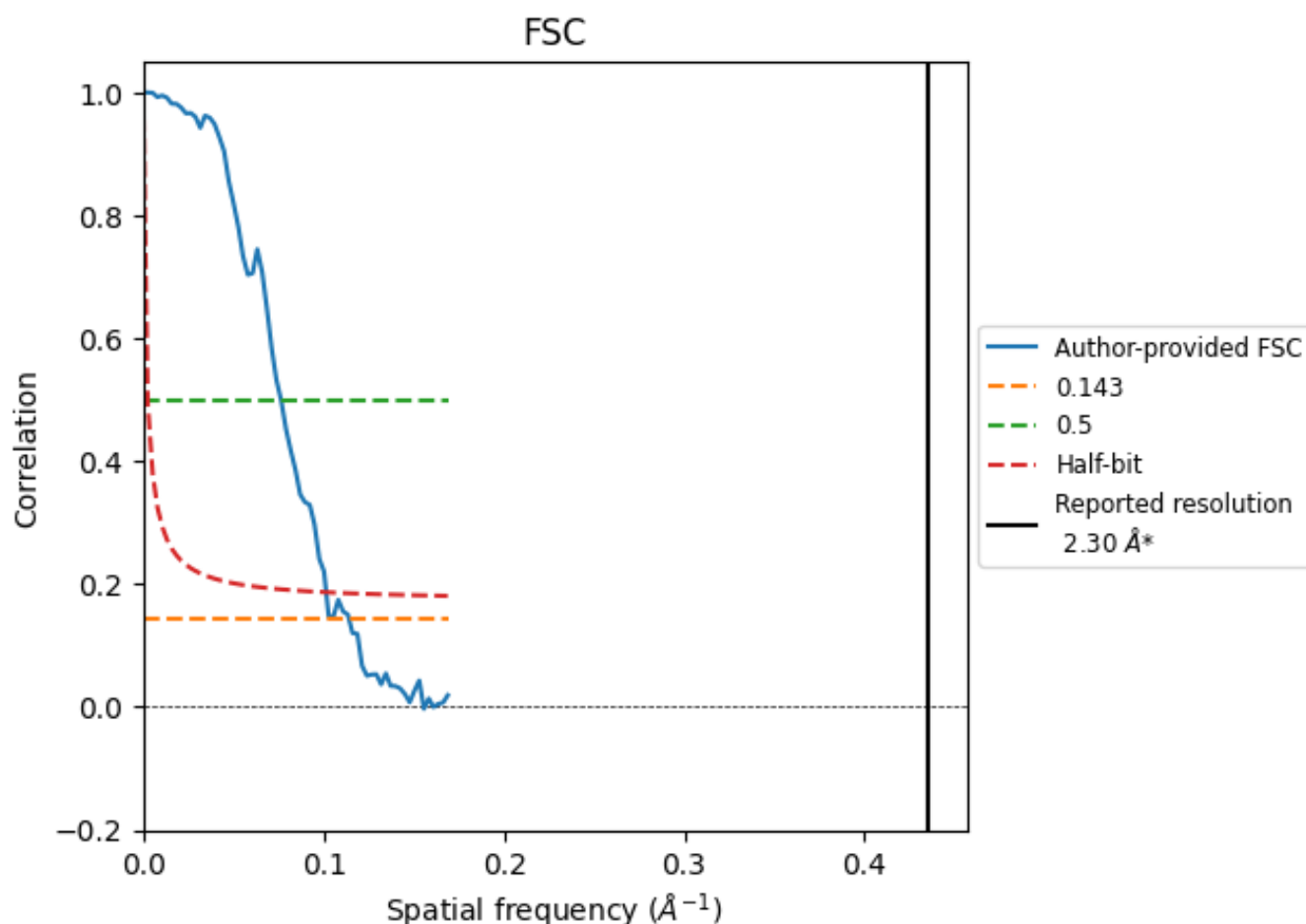


*Reported resolution corresponds to spatial frequency of 0.435 Å⁻¹

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 0.435 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	8.76	13.07	9.85
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 8.76 differs from the reported value 2.3 by more than 10 %

9 Map-model fit

This section was not generated.