



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 02:08 AM UTC

PDB ID : 9Z9X / pdb_00009z9x
EMDB ID : EMD-73962
Title : Gated state sheep connexin-46 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 : 7jkc

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

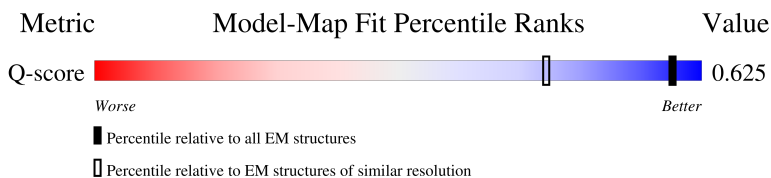
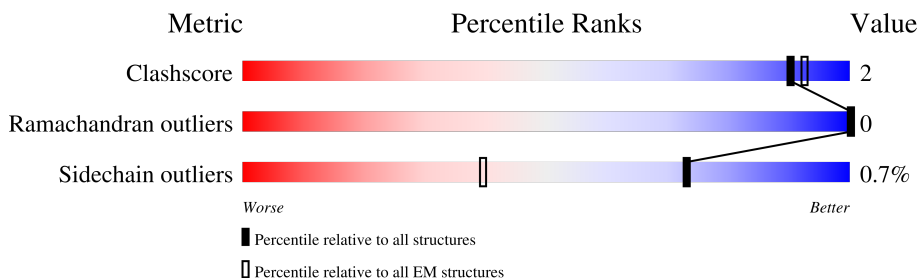
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.30 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4254 (1.80 - 2.80)

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	413	
1	B	413	
1	C	413	
1	D	413	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	413	 43% . 55%
1	F	413	 44% . 55%
1	G	413	 44% . 55%
1	H	413	 43% . 55%
1	I	413	 43% . 55%
1	J	413	 43% . 55%
1	K	413	 43% . 55%
1	L	413	 44% . 55%

2 Entry composition [i](#)

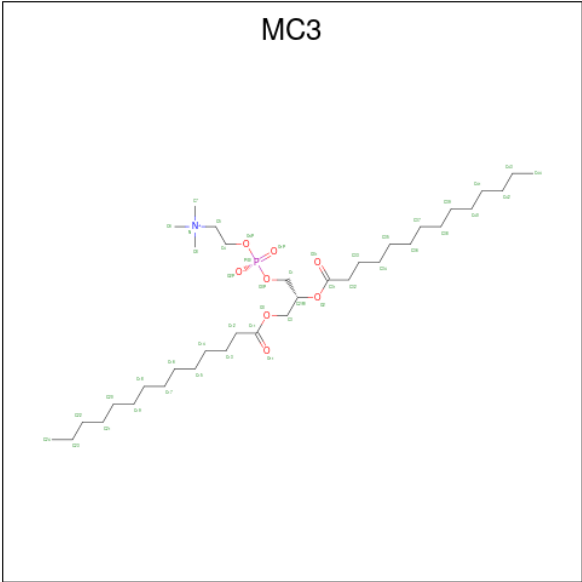
There are 3 unique types of molecules in this entry. The entry contains 47508 atoms, of which 24852 are hydrogens and 0 are deuteriums.

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-3 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	185	Total	C	H	N	O	S	0	0
			2842	959	1399	232	244	8		
1	B	185	Total	C	H	N	O	S	0	0
			2842	959	1399	232	244	8		
1	C	185	Total	C	H	N	O	S	0	0
			2842	959	1399	232	244	8		
1	D	185	Total	C	H	N	O	S	0	0
			2842	959	1399	232	244	8		
1	E	185	Total	C	H	N	O	S	0	0
			2842	959	1399	232	244	8		
1	F	185	Total	C	H	N	O	S	0	0
			2842	959	1399	232	244	8		
1	G	185	Total	C	H	N	O	S	0	0
			2842	959	1399	232	244	8		
1	H	185	Total	C	H	N	O	S	0	0
			2842	959	1399	232	244	8		
1	I	185	Total	C	H	N	O	S	0	0
			2842	959	1399	232	244	8		
1	J	185	Total	C	H	N	O	S	0	0
			2842	959	1399	232	244	8		
1	K	185	Total	C	H	N	O	S	0	0
			2842	959	1399	232	244	8		
1	L	185	Total	C	H	N	O	S	0	0
			2842	959	1399	232	244	8		

- 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			0
			27	9	18			
2	A	1	Total	C	H	O	P	0
			67	21	37	8	1	
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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
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
			36	12	24				
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	N	O	P	0
			62	18	34	1	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
			15	5	10				
2	A	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	H	O	P	0
			76	24	43	8	1	
2	B	1	Total	C	H			0
			39	13	26			
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
			18	6	12			
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	N	O	P
			62	18	34	1	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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	H			0
			30	10	20			
2	B	1	Total	C	H			0
			36	12	24			
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
			15	5	10			
2	B	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	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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
2	C	1	Total	C	H				0
			27	9	18				
2	C	1	Total	C	H				0
			18	6	12				
2	C	1	Total	C	H				0
			12	4	8				
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
			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	N	O	P	0
			62	18	34	1	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
			15	5	10				

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	H			0
			39	13	26			
2	D	1	Total	C	H			0
			36	12	24			
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
			15	5	10			
2	D	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	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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
2	E	1	Total	C	H				0
			27	9	18				
2	E	1	Total	C	H				0
			21	7	14				
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
			18	6	12				
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	N	O	P	0
			62	18	34	1	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				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
2	E	1	Total	C	H				0
			24	8	16				
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				0
			21	7	14				
2	F	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
			15	5	10				
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	F	1	Total	C	H	O	P		0
			76	24	43	8	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	
2	F	1	Total	C	H		0	
			39	13	26			
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	
			18	6	12			
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	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	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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
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
			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
			18	6	12				
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	N	O	P	0
			62	18	34	1	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				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	G	1	Total	C	H			0
			30	10	20			
2	G	1	Total	C	H			0
			33	11	22			
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
			15	5	10			
2	G	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	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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
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
			36	12	24				
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	N	O	P	0
			62	18	34	1	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
			15	5	10				
2	H	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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	I	1	Total	C	H	O	P	0
			76	24	43	8	1	
2	I	1	Total	C	H			0
			39	13	26			
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
			18	6	12			
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	N	O	P
			62	18	34	1	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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	I	1	Total	C	H			0
			30	10	20			
2	I	1	Total	C	H			0
			36	12	24			
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
			15	5	10			
2	I	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	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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
2	J	1	Total	C	H				0
			27	9	18				
2	J	1	Total	C	H				0
			18	6	12				
2	J	1	Total	C	H				0
			12	4	8				
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
			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	N	O	P	0
			62	18	34	1	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
			15	5	10				

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						AltConf
2	K	1	Total	C	H				0
			39	13	26				
2	K	1	Total	C	H				0
			36	12	24				
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
			15	5	10				
2	K	1	Total	C	H				0
			21	7	14				
2	L	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				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	L	1	Total	C	H			0
			33	11	22			
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
			15	5	10			
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	
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
			18	6	12			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
2	L	1	Total	C	H	0
			24	8	16	
2	L	1	Total	C	H	0
			36	12	24	
2	L	1	Total	C	H	0
			18	6	12	
2	L	1	Total	C	H	0
			21	7	14	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	76	Total	O	0
			76	76	
3	B	75	Total	O	0
			75	75	
3	C	75	Total	O	0
			75	75	
3	D	76	Total	O	0
			76	76	
3	E	74	Total	O	0
			74	74	
3	F	75	Total	O	0
			75	75	
3	G	74	Total	O	0
			74	74	
3	H	76	Total	O	0
			76	76	
3	I	73	Total	O	0
			73	73	
3	J	75	Total	O	0
			75	75	
3	K	75	Total	O	0
			75	75	
3	L	76	Total	O	0
			76	76	

ALA ASP LEU ALA ILE	PRO ALA ALA ALA GLY GLY GLN PHE LEU PRO GLY GLY GLY ALA ALA GLY SER SER ASP SER ASP GLY GLY GLY ALA VAL THR ALA VAL GLU LEU HIS ALA PRO GLU PRO PRO ALA ASP GLY ARG SER SER LYS SER GLY GLY ARG ALA ALA	THR PRO GLU PRO PRO LEU PRO ALA LEU PRO GLY THR PRO GLY THR PRO GLY GLY THR GLY GLY GLY ASN GLN GLY LEU ARG ALA PRO ALA GLN CYS ASN ASN ARG GLU ALA GLU PRO GLN THR GLY SER SER LYS SER SER PRO PRO ALA ALA THR PRO THR	GLN GLY MET SER PRO PHE ARG PRO ASP THR PRO GLY GLY SER ARG ALA GLY SER ALA LYS PRO MET GLY GLY SER PRO LEU LEU PRO ASN PRO PRO ASN SER SER PRO PRO ALA VAL THR ILE GLY PHE PRO PRO TYR TYR ALA PRO SER SER LEU GLY GLN ALA SER SER ALA GLY GLN ALA SER ALA PRO GLY
---------------------------------	--	--	---

- Molecule 1: Gap junction alpha-3 protein

Chain D:  43% . 55%

[illegible]

- Molecule 1: Gap junction alpha-3 protein

Chain E: 43% . 55%

[illegible]

- Molecule 1: Gap junction alpha-3 protein

Chain F:  44% . 55%

NET	GLY	ASP	W4	G38	E104	LYS	ARG	LYS	GLU	GLU	GLU	GLU	PRO	PRO	LYS	ALA	ALA	GLY	GLN	ASP	PRO	PRO	VAL	ARG	ASP	ASP	ARG	GLY	LYS	VAL	ARG	ILE	A139	N149	I150	Q164	E218	L272	TRP	LYS	LYS	LEU	LYS	GLN	GLY
-----	-----	-----	----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----

[illegible]

- Molecule 1: Gap junction alpha-3 protein



ILE	ALA	PRO	SER	MET
	GLY	LEU	PRO	GLY
ILE	GLY	PRO	PHE	ASP
	PRO	ALA	ARG	W4
ILE	GLN	ALA	PRO	E104
	GLN	LEU	ASP	E104
ILE	PHE	PRO	THR	LYS
	LEU	GLY	PRO	ARG
ILE	PRO	THR	GLY	LYS
	GLY	PRO	SER	GLU
ILE	GLY	GLY	ARG	GLU
	ALA	THR	ALA	GLU
ILE	ALA	PRO	GLY	GLU
	GLY	THR	SER	GLU
ILE	SER	THR	ALA	PRO
	SER	PRO	LYS	PRO
ILE	GLY	GLY	PRO	LYS
	ASP	THR	MET	ALA
ILE	SER	LEU	GLY	ALA
	ASP	GLY	GLY	GLY
ILE	GLY	GLY	SER	PRO
	GLU	GLY	PRO	ALA
ILE	GLY	GLY	LEU	GLU
	ALA	GLY	LEU	GLU
ILE	VAL	ASN	LEU	HIS
	THR	GLN	LEU	PRO
ILE	ALA	GLY	PRO	ASP
	VAL	LEU	ASN	PRO
ILE	GLY	LEU	SER	ALA
	LEU	ALA	ALA	PRO
ILE	HIS	PRO	PRO	VAL
	ALA	ALA	PRO	ARG
ILE	PRO	GLN	ALA	ASP
	PRO	ASN	VAL	ASP
ILE	GLY	CYS	THR	ARG
	PRO	ALA	ILE	GLY
ILE	PRO	ASN	GLY	LYS
	ALA	ARG	PHE	VAL
ILE	ASP	GLU	PRO	ARG
	PRO	ALA	PRO	ILE
ILE	GLY	GLU	TYR	A139
	ARG	PRO	TYR	A139
ILE	ARG	GLN	ALA	N149
	SER	THR	PRO	N150
ILE	SER	SER	SER	Q164
	ALA	ALA	ALA	Q164
ILE	SER	ARG	SER	E218
	LYS	LYS	SER	E218
ILE	SER	ALA	LEU	L222
	SER	SER	GLY	L222
ILE	GLY	PRO	GLN	GLY
	GLY	PRO	ALA	TRP
ILE	ARG	ALA	SER	LYS
	ALA	SER	ALA	LYS
ILE	ARG	THR	PRO	LEU
	ALA	PRO	GLY	LEU
ILE	ALA	PRO	TYR	GLN
	ASP	ALA	PRO	GLY
ILE	LEU	ALA	GLU	MET
	ALA	PRO	PRO	THR

- Molecule 1: Gap junction alpha-3 protein

[illegible]

- Molecule 1: Gap junction alpha-3 protein



NET	GLY	ASP	W4	G38	E104	LYS	ARG	LYS	GLU	GLU	GLU	PRO	PRO	LYS	ALA	ALA	GLY	GLN	ASP	PRO	ALA	PRO	VAL	ASP	ASP	ARG	GLY	LYS	VAL	ARG	ILE	A139	N149	I150	Q164	I191	E218	L222	GLY	TRP	LYS	LYS	LEU	LEU
-----	-----	-----	----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----

ALA ASP LEU ILE	PRO ALA ALA ALA GLY GLY Gln PHE LEU PRO GLY GLY GLY GLY ALA ALA GLY SER SER ASP SER ASP GLY GLY GLY ALA VAL THR ALA VAL GLU LEU HIS ALA PRO GLU PRO PRO ALA ASP GLY ARG SER SER LYS SER SER GLY GLY ARG ALA ALA ALA	THR PRO GLU PRO PRO LEU PRO ALA LEU PRO GLY THR PRO GLY THR PRO GLY GLY GLY ASN GLN GLY LEU ARG ALA PRO ALA GLN CYS ASN ASN ARG GLU ALA GLU PRO GLN THR VAL GLU HIS ALA ASP SER SER LYS SER SER GLY GLY ARG ALA ALA ALA	Gln GLY MET SER PRO PHE ARG PRO ASP THR PRO GLY GLY SER ARG ALA GLY SER ALA LYS PRO MET GLY GLY SER LEU GLY PRO GLY THR GLY THR GLY GLY ASN GLN LEU SER ALA PRO ASN SER ALA PRO ALA VAL THR ILE GLY PHE PRO PRO TYR TYR ALA PRO SER SER SER LEU GLY GLN ALA SER SER ALA GLY PRO THR
--------------------------	---	--	---

- Molecule 1: Gap junction alpha-3 protein

Chain J:  43% . 55%

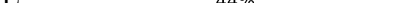
[illegible]

- Molecule 1: Gap junction alpha-3 protein

Chain K: 43% . 55%

[illegible]

- Molecule 1: Gap junction alpha-3 protein

Chain L:  44% . 55%

NET	GLY	ASP	W4	G38	E104	LYS	ARG	LYS	GLU	GLU	GLU	GLU	PRO	PRO	LYS	ALA	ALA	GLY	GLN	ASP	PRO	ALA	VAL	ARG	ASP	ASP	ARG	GLY	LYS	VAL	ARG	ILE	A139	N149	I150	Q164	E218	L272	TRP	LYS	LEU	LYS	GLN
-----	-----	-----	----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	-----	-----	-----	-----	-----

GLU	MET
PRO	THR
PRO	SER
LEU	PRO
PRO	PHE
ALA	ARG
ALA	PRO
LEU	ASP
PRO	THR
GLY	PRO
THR	GLY
PRO	SER
GLY	ARG
THR	ALA
PRO	GLY
GLY	SER
THR	ALA
SER	LYS
PRO	GLY
GLY	PRO
THR	MET
LEU	GLY
GLY	GLY
GLY	SER
PRO	PRO
GLY	GLY
GLY	LEU
GLY	LEU
ASN	LEU
GLN	PRO
GLY	PRO
LEU	ASN
ARG	SER
ALA	ALA
PRO	PRO
ALA	PRO
GLN	ALA
ASN	VAL
CYS	THR
ALA	THR
ASN	GLY
ARG	PHE
GLU	PRO
ALA	PRO
GLY	ALA
PRO	TYR
ARG	TYR
SER	ALA
LYS	PRO
SER	ALA
GLY	SER
GLN	GLY
PRO	ALA
ALA	ALA
SER	SER
THR	ALA
PRO	PRO
ALA	TYR
ASP	ALA
ALA	PRO
GLY	GLY
GLN	THR
PRO	PRO
ASP	GLY
GLY	THR
ARG	ALA
SER	ARG
LYS	ALA
SER	ALA
GLY	ALA
GLY	ARG
ARG	ALA
SER	ALA
LYS	ASP

LEU
ALA
ILE

ALA
PRO
ALA
GLY
PRO
GLN
GLN
PHE
LEU
PRO
GLY
GLY
ALA
ALA
GLY
SER
SER
GLY
ASP
SER
ASP
GLY
GLU
GLY
ALA
VAL
THR
ALA
VAL
GLU
LEU
HIS
ALA
PRO
PRO
GLU
PRO
PRO
ALA
ASP
PRO
GLY
ARG
SER
SER
LYS
ALA
SER
LYS
SER
SER
GLY
GLY
ARG
ALA
ARG
ALA
ALA
ASP

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	1.226	Depositor
Minimum map value	-0.684	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	307.8144, 307.8144, 307.8144	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8016, 0.8016, 0.8016	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: 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	0.21	0/1483	0.40	0/2027
1	B	0.21	0/1483	0.40	0/2027
1	C	0.21	0/1483	0.40	0/2027
1	D	0.21	0/1483	0.40	0/2027
1	E	0.21	0/1483	0.40	0/2027
1	F	0.21	0/1483	0.40	0/2027
1	G	0.21	0/1483	0.40	0/2027
1	H	0.21	0/1483	0.40	0/2027
1	I	0.21	0/1483	0.40	0/2027
1	J	0.21	0/1483	0.40	0/2027
1	K	0.21	0/1483	0.40	0/2027
1	L	0.21	0/1483	0.40	0/2027
All	All	0.21	0/17796	0.40	0/24324

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	1443	1399	1396	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1443	1399	1396	5	0
1	C	1443	1399	1396	4	0
1	D	1443	1399	1396	4	0
1	E	1443	1399	1396	4	0
1	F	1443	1399	1396	4	0
1	G	1443	1399	1396	2	0
1	H	1443	1399	1396	5	0
1	I	1443	1399	1396	5	0
1	J	1443	1399	1396	4	0
1	K	1443	1399	1396	4	0
1	L	1443	1399	1396	3	0
2	A	370	672	567	6	0
2	B	370	672	567	8	0
2	C	370	672	567	7	0
2	D	370	672	567	7	0
2	E	370	672	567	6	0
2	F	370	672	567	7	0
2	G	370	672	567	6	0
2	H	370	672	567	7	0
2	I	370	672	567	7	0
2	J	370	672	567	7	0
2	K	370	672	567	7	0
2	L	370	672	567	7	0
3	A	76	0	0	1	0
3	B	75	0	0	1	0
3	C	75	0	0	1	0
3	D	76	0	0	1	0
3	E	74	0	0	1	0
3	F	75	0	0	1	0
3	G	74	0	0	1	0
3	H	76	0	0	1	0
3	I	73	0	0	1	0
3	J	75	0	0	1	0
3	K	75	0	0	1	0
3	L	76	0	0	1	0
All	All	22656	24852	23556	79	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 2.

All (79) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:520:MC3:P	2:H:520:MC3:H61	2.36	0.66
2:A:520:MC3:H61	2:F:501:MC3:P	2.40	0.61
2:C:520:MC3:P	2:D:520:MC3:H61	2.41	0.60
2:K:520:MC3:P	2:L:501:MC3:H61	2.41	0.60
2:A:520:MC3:P	2:B:520:MC3:H61	2.43	0.58
2:D:520:MC3:P	2:E:520:MC3:H61	2.44	0.58
2:J:520:MC3:P	2:K:520:MC3:H61	2.44	0.58
2:I:520:MC3:P	2:J:520:MC3:H61	2.45	0.56
2:B:520:MC3:P	2:C:520:MC3:H61	2.45	0.56
2:G:520:MC3:O2P	2:H:520:MC3:H61	2.05	0.56
2:G:520:MC3:H61	2:L:501:MC3:P	2.46	0.55
1:E:164:GLN:HG2	3:E:622:HOH:O	2.07	0.55
1:K:164:GLN:HG2	3:K:622:HOH:O	2.07	0.55
1:D:164:GLN:HG2	3:D:622:HOH:O	2.07	0.55
1:L:164:GLN:HG2	3:L:622:HOH:O	2.07	0.55
1:F:164:GLN:HG2	3:F:622:HOH:O	2.07	0.55
1:J:164:GLN:HG2	3:J:622:HOH:O	2.07	0.55
1:C:164:GLN:HG2	3:C:622:HOH:O	2.07	0.54
1:I:164:GLN:HG2	3:I:621:HOH:O	2.07	0.54
1:G:164:GLN:HG2	3:G:622:HOH:O	2.07	0.54
1:A:164:GLN:HG2	3:A:622:HOH:O	2.07	0.54
2:H:520:MC3:P	2:I:520:MC3:H61	2.49	0.53
1:B:164:GLN:HG2	3:B:621:HOH:O	2.07	0.52
1:H:164:GLN:HG2	3:H:622:HOH:O	2.07	0.52
2:E:520:MC3:P	2:F:501:MC3:H61	2.49	0.52
2:K:520:MC3:O2P	2:L:501:MC3:H61	2.10	0.51
2:C:520:MC3:O2P	2:D:520:MC3:H61	2.11	0.50
2:A:520:MC3:O2P	2:B:520:MC3:H61	2.12	0.50
2:A:520:MC3:H61	2:F:501:MC3:O2P	2.11	0.49
2:D:520:MC3:O2P	2:E:520:MC3:H61	2.13	0.49
1:I:38:GLY:HA2	2:I:520:MC3:H83	1.95	0.48
2:J:520:MC3:O2P	2:K:520:MC3:H61	2.15	0.47
2:I:520:MC3:O2P	2:J:520:MC3:H61	2.15	0.47
2:B:520:MC3:O2P	2:C:520:MC3:H61	2.16	0.46
2:A:520:MC3:H61	2:F:501:MC3:O1P	2.15	0.46
2:H:520:MC3:O2P	2:I:520:MC3:H61	2.16	0.45
1:I:38:GLY:CA	2:I:520:MC3:H83	2.46	0.45
1:H:38:GLY:HA2	2:H:520:MC3:H83	1.97	0.45
2:G:520:MC3:H61	2:L:501:MC3:O2P	2.16	0.45
1:B:38:GLY:HA2	2:B:520:MC3:H83	1.98	0.44
1:L:38:GLY:HA2	2:L:501:MC3:H83	2.00	0.44
2:G:520:MC3:O1P	2:H:520:MC3:H61	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:GLY:HA2	2:D:520:MC3:H83	2.00	0.43
1:E:38:GLY:HA2	2:E:520:MC3:H83	2.00	0.43
1:J:38:GLY:HA2	2:J:520:MC3:H83	2.00	0.43
2:C:520:MC3:O1P	2:D:520:MC3:H61	2.19	0.43
2:J:520:MC3:O1P	2:K:520:MC3:H61	2.19	0.43
2:K:520:MC3:O1P	2:L:501:MC3:H61	2.19	0.43
1:F:38:GLY:HA2	2:F:501:MC3:H83	2.02	0.42
1:H:38:GLY:CA	2:H:520:MC3:H83	2.50	0.42
1:J:191:ILE:HD12	1:J:191:ILE:N	2.36	0.41
1:C:191:ILE:N	1:C:191:ILE:HD12	2.35	0.41
2:G:520:MC3:H61	2:L:501:MC3:O1P	2.20	0.41
1:B:38:GLY:CA	2:B:520:MC3:H83	2.50	0.41
2:D:520:MC3:O1P	2:E:520:MC3:H61	2.21	0.41
1:D:191:ILE:HD12	1:D:191:ILE:N	2.36	0.41
1:I:191:ILE:HD12	1:I:191:ILE:N	2.36	0.41
2:B:520:MC3:O1P	2:C:520:MC3:H61	2.20	0.41
1:E:191:ILE:HD12	1:E:191:ILE:N	2.36	0.41
1:K:38:GLY:HA2	2:K:520:MC3:H83	2.02	0.41
1:K:191:ILE:N	1:K:191:ILE:HD12	2.36	0.41
2:A:520:MC3:O1P	2:B:520:MC3:H61	2.21	0.41
1:B:150:ILE:HD11	1:B:218:GLU:OE1	2.21	0.41
1:C:150:ILE:HD11	1:C:218:GLU:OE1	2.21	0.41
1:E:150:ILE:HD11	1:E:218:GLU:OE1	2.21	0.41
2:E:520:MC3:O1P	2:F:501:MC3:H61	2.21	0.41
1:F:150:ILE:HD11	1:F:218:GLU:OE1	2.21	0.41
1:H:150:ILE:HD11	1:H:218:GLU:OE1	2.21	0.41
1:I:150:ILE:HD11	1:I:218:GLU:OE1	2.21	0.41
1:K:150:ILE:HD11	1:K:218:GLU:OE1	2.21	0.41
1:C:38:GLY:HA2	2:C:520:MC3:H83	2.02	0.41
1:D:150:ILE:HD11	1:D:218:GLU:OE1	2.21	0.41
1:J:150:ILE:HD11	1:J:218:GLU:OE1	2.21	0.41
1:L:150:ILE:HD11	1:L:218:GLU:OE1	2.21	0.41
1:H:191:ILE:HD12	1:H:191:ILE:N	2.36	0.40
1:B:191:ILE:HD12	1:B:191:ILE:N	2.36	0.40
2:I:520:MC3:O1P	2:J:520:MC3:H61	2.21	0.40
1:G:150:ILE:HD11	1:G:218:GLU:OE1	2.21	0.40
1:F:38:GLY:CA	2:F:501:MC3:H83	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
1	B	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
1	C	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
1	D	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
1	E	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
1	F	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
1	G	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
1	H	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
1	I	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
1	J	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
1	K	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
1	L	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
All	All	2172/4956 (44%)	2160 (99%)	12 (1%)	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	149/325 (46%)	148 (99%)	1 (1%)	76	87
1	B	149/325 (46%)	148 (99%)	1 (1%)	76	87

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	149/325 (46%)	148 (99%)	1 (1%)	76	87
1	D	149/325 (46%)	148 (99%)	1 (1%)	76	87
1	E	149/325 (46%)	148 (99%)	1 (1%)	76	87
1	F	149/325 (46%)	148 (99%)	1 (1%)	76	87
1	G	149/325 (46%)	148 (99%)	1 (1%)	76	87
1	H	149/325 (46%)	148 (99%)	1 (1%)	76	87
1	I	149/325 (46%)	148 (99%)	1 (1%)	76	87
1	J	149/325 (46%)	148 (99%)	1 (1%)	76	87
1	K	149/325 (46%)	148 (99%)	1 (1%)	76	87
1	L	149/325 (46%)	148 (99%)	1 (1%)	76	87
All	All	1788/3900 (46%)	1776 (99%)	12 (1%)	73	87

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ASN
1	B	149	ASN
1	C	149	ASN
1	D	149	ASN
1	E	149	ASN
1	F	149	ASN
1	G	149	ASN
1	H	149	ASN
1	I	149	ASN
1	J	149	ASN
1	K	149	ASN
1	L	149	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	58	GLN
1	B	49	GLN
1	B	57	GLN
1	B	58	GLN
1	C	49	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	58	GLN
1	D	49	GLN
1	D	58	GLN
1	E	49	GLN
1	E	58	GLN
1	F	49	GLN
1	F	57	GLN
1	F	58	GLN
1	G	49	GLN
1	G	58	GLN
1	H	49	GLN
1	H	57	GLN
1	H	58	GLN
1	I	49	GLN
1	I	57	GLN
1	I	58	GLN
1	J	49	GLN
1	J	58	GLN
1	K	49	GLN
1	K	57	GLN
1	K	58	GLN
1	L	49	GLN
1	L	57	GLN
1	L	58	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	J	507	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	B	524	-	9,9,45	0.24	0	8,8,53	0.20	0
2	MC3	E	513	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	E	515	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	A	505	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	L	522	-	11,11,45	0.24	0	10,10,53	0.20	0
2	MC3	I	525	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	L	509	-	10,10,45	0.24	0	9,9,53	0.21	0
2	MC3	I	506	-	11,11,45	0.24	0	10,10,53	0.21	0
2	MC3	I	527	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	C	504	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	C	519	-	6,6,45	0.25	0	5,5,53	0.17	0
2	MC3	G	532	-	4,4,45	0.28	0	3,3,53	0.23	0
2	MC3	J	529	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	J	509	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	E	509	-	8,8,45	0.25	0	7,7,53	0.20	0
2	MC3	H	503	-	32,32,45	0.73	1 (3%)	35,37,53	1.14	2 (5%)
2	MC3	C	520	-	27,27,45	0.50	0	33,35,53	0.69	0
2	MC3	B	503	-	32,32,45	0.73	1 (3%)	35,37,53	1.14	2 (5%)
2	MC3	F	505	-	9,9,45	0.24	0	8,8,53	0.20	0
2	MC3	L	520	-	11,11,45	0.24	0	10,10,53	0.21	0
2	MC3	K	507	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	F	512	-	6,6,45	0.24	0	5,5,53	0.23	0
2	MC3	C	512	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	F	530	-	7,7,45	0.24	0	6,6,53	0.23	0
2	MC3	G	530	-	7,7,45	0.25	0	6,6,53	0.19	0
2	MC3	C	515	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	D	514	-	3,3,45	0.34	0	2,2,53	0.56	0
2	MC3	E	530	-	7,7,45	0.25	0	6,6,53	0.19	0
2	MC3	B	525	-	11,11,45	0.24	0	10,10,53	0.20	0
2	MC3	K	525	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	L	508	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	C	532	-	4,4,45	0.28	0	3,3,53	0.23	0
2	MC3	H	513	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	F	521	-	11,11,45	0.24	0	10,10,53	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	F	527	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	C	507	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	J	520	-	27,27,45	0.50	0	33,35,53	0.69	0
2	MC3	E	508	-	11,11,45	0.24	0	10,10,53	0.20	0
2	MC3	K	503	-	32,32,45	0.72	1 (3%)	35,37,53	1.14	2 (5%)
2	MC3	B	504	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	G	527	-	9,9,45	0.24	0	8,8,53	0.20	0
2	MC3	I	522	-	11,11,45	0.23	0	10,10,53	0.26	0
2	MC3	E	521	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	I	516	-	7,7,45	0.23	0	6,6,53	0.23	0
2	MC3	B	529	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	B	531	-	6,6,45	0.24	0	5,5,53	0.23	0
2	MC3	H	520	-	27,27,45	0.49	0	33,35,53	0.69	0
2	MC3	K	531	-	6,6,45	0.25	0	5,5,53	0.23	0
2	MC3	D	506	-	11,11,45	0.24	0	10,10,53	0.22	0
2	MC3	L	530	-	7,7,45	0.24	0	6,6,53	0.23	0
2	MC3	A	514	-	3,3,45	0.34	0	2,2,53	0.56	0
2	MC3	L	501	-	27,27,45	0.50	0	33,35,53	0.69	0
2	MC3	G	529	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	H	528	-	10,10,45	0.24	0	9,9,53	0.21	0
2	MC3	E	505	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	B	532	-	4,4,45	0.28	0	3,3,53	0.23	0
2	MC3	B	513	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	B	520	-	27,27,45	0.49	0	33,35,53	0.70	0
2	MC3	F	523	-	8,8,45	0.25	0	7,7,53	0.20	0
2	MC3	J	530	-	7,7,45	0.25	0	6,6,53	0.19	0
2	MC3	B	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	B	528	-	10,10,45	0.24	0	9,9,53	0.21	0
2	MC3	D	511	-	7,7,45	0.25	0	6,6,53	0.18	0
2	MC3	F	524	-	6,6,45	0.25	0	5,5,53	0.18	0
2	MC3	C	518	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	A	522	-	11,11,45	0.23	0	10,10,53	0.25	0
2	MC3	G	515	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	L	516	-	29,29,45	0.77	1 (3%)	32,34,53	1.15	2 (6%)
2	MC3	E	510	-	6,6,45	0.25	0	5,5,53	0.19	0
2	MC3	E	503	-	32,32,45	0.73	1 (3%)	35,37,53	1.14	2 (5%)
2	MC3	C	527	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	A	528	-	10,10,45	0.24	0	9,9,53	0.21	0
2	MC3	I	502	-	29,29,45	0.77	1 (3%)	32,34,53	1.15	2 (6%)
2	MC3	C	509	-	8,8,45	0.25	0	7,7,53	0.20	0
2	MC3	E	512	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	D	517	-	11,11,45	0.23	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	533	-	6,6,45	0.24	0	5,5,53	0.24	0
2	MC3	F	504	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	I	515	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	E	511	-	7,7,45	0.25	0	6,6,53	0.18	0
2	MC3	I	514	-	3,3,45	0.34	0	2,2,53	0.56	0
2	MC3	I	505	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	L	503	-	11,11,45	0.23	0	10,10,53	0.26	0
2	MC3	G	503	-	32,32,45	0.73	1 (3%)	35,37,53	1.14	2 (5%)
2	MC3	K	526	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	J	503	-	32,32,45	0.73	1 (3%)	35,37,53	1.14	2 (5%)
2	MC3	H	531	-	6,6,45	0.24	0	5,5,53	0.23	0
2	MC3	E	522	-	11,11,45	0.22	0	10,10,53	0.25	0
2	MC3	K	529	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	K	518	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	F	509	-	10,10,45	0.24	0	9,9,53	0.21	0
2	MC3	H	518	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	F	525	-	7,7,45	0.25	0	6,6,53	0.18	0
2	MC3	C	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	A	517	-	11,11,45	0.23	0	10,10,53	0.22	0
2	MC3	E	517	-	11,11,45	0.23	0	10,10,53	0.22	0
2	MC3	J	515	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	L	506	-	11,11,45	0.24	0	10,10,53	0.21	0
2	MC3	F	526	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	H	510	-	6,6,45	0.25	0	5,5,53	0.18	0
2	MC3	L	514	-	6,6,45	0.25	0	5,5,53	0.24	0
2	MC3	L	517	-	32,32,45	0.73	1 (3%)	35,37,53	1.14	2 (5%)
2	MC3	G	526	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	F	508	-	9,9,45	0.24	0	8,8,53	0.20	0
2	MC3	K	505	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	H	505	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	H	509	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	I	519	-	6,6,45	0.25	0	5,5,53	0.17	0
2	MC3	G	507	-	11,11,45	0.24	0	10,10,53	0.20	0
2	MC3	K	512	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	E	523	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	C	522	-	11,11,45	0.23	0	10,10,53	0.26	0
2	MC3	L	526	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	B	505	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	E	504	-	12,12,45	0.21	0	11,11,53	0.21	0
2	MC3	F	529	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	C	516	-	7,7,45	0.24	0	6,6,53	0.23	0
2	MC3	G	533	-	6,6,45	0.24	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	F	502	-	12,12,45	0.21	0	11,11,53	0.23	0
2	MC3	L	510	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	E	526	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	F	515	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	G	505	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	K	510	-	6,6,45	0.25	0	5,5,53	0.19	0
2	MC3	E	525	-	11,11,45	0.24	0	10,10,53	0.21	0
2	MC3	G	509	-	8,8,45	0.25	0	7,7,53	0.20	0
2	MC3	I	507	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	F	514	-	6,6,45	0.24	0	5,5,53	0.24	0
2	MC3	D	532	-	4,4,45	0.29	0	3,3,53	0.23	0
2	MC3	B	510	-	6,6,45	0.25	0	5,5,53	0.19	0
2	MC3	D	530	-	7,7,45	0.25	0	6,6,53	0.19	0
2	MC3	D	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	I	528	-	10,10,45	0.24	0	9,9,53	0.21	0
2	MC3	K	517	-	11,11,45	0.22	0	10,10,53	0.22	0
2	MC3	K	532	-	4,4,45	0.28	0	3,3,53	0.23	0
2	MC3	F	531	-	11,11,45	0.23	0	10,10,53	0.22	0
2	MC3	C	510	-	6,6,45	0.25	0	5,5,53	0.19	0
2	MC3	F	532	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	H	530	-	7,7,45	0.25	0	6,6,53	0.19	0
2	MC3	I	524	-	9,9,45	0.25	0	8,8,53	0.20	0
2	MC3	J	526	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	G	510	-	6,6,45	0.25	0	5,5,53	0.19	0
2	MC3	I	509	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	L	524	-	6,6,45	0.26	0	5,5,53	0.19	0
2	MC3	G	521	-	12,12,45	0.21	0	11,11,53	0.23	0
2	MC3	K	523	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	J	510	-	6,6,45	0.26	0	5,5,53	0.19	0
2	MC3	L	529	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	L	531	-	11,11,45	0.23	0	10,10,53	0.22	0
2	MC3	E	532	-	4,4,45	0.28	0	3,3,53	0.23	0
2	MC3	H	527	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	A	532	-	4,4,45	0.28	0	3,3,53	0.23	0
2	MC3	J	521	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	D	516	-	7,7,45	0.23	0	6,6,53	0.23	0
2	MC3	D	520	-	27,27,45	0.49	0	33,35,53	0.70	0
2	MC3	G	517	-	11,11,45	0.23	0	10,10,53	0.22	0
2	MC3	H	507	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	C	514	-	3,3,45	0.34	0	2,2,53	0.56	0
2	MC3	G	511	-	7,7,45	0.25	0	6,6,53	0.18	0
2	MC3	E	531	-	6,6,45	0.24	0	5,5,53	0.23	0
2	MC3	F	517	-	32,32,45	0.73	1 (3%)	35,37,53	1.14	2 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	L	512	-	6,6,45	0.25	0	5,5,53	0.24	0
2	MC3	L	502	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	B	527	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	H	521	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	A	506	-	11,11,45	0.24	0	10,10,53	0.21	0
2	MC3	B	507	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	G	508	-	11,11,45	0.24	0	10,10,53	0.20	0
2	MC3	J	505	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	K	527	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	J	508	-	11,11,45	0.24	0	10,10,53	0.20	0
2	MC3	D	503	-	32,32,45	0.72	1 (3%)	35,37,53	1.14	2 (5%)
2	MC3	I	511	-	7,7,45	0.25	0	6,6,53	0.18	0
2	MC3	A	518	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	F	516	-	29,29,45	0.77	1 (3%)	32,34,53	1.15	2 (6%)
2	MC3	K	504	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	A	516	-	7,7,45	0.23	0	6,6,53	0.23	0
2	MC3	F	501	-	27,27,45	0.49	0	33,35,53	0.69	0
2	MC3	J	531	-	6,6,45	0.24	0	5,5,53	0.23	0
2	MC3	J	532	-	4,4,45	0.29	0	3,3,53	0.23	0
2	MC3	A	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	G	512	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	G	514	-	3,3,45	0.34	0	2,2,53	0.56	0
2	MC3	G	525	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	C	523	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	E	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	E	519	-	6,6,45	0.25	0	5,5,53	0.17	0
2	MC3	J	512	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	E	514	-	3,3,45	0.34	0	2,2,53	0.56	0
2	MC3	E	527	-	9,9,45	0.24	0	8,8,53	0.20	0
2	MC3	J	517	-	11,11,45	0.23	0	10,10,53	0.22	0
2	MC3	D	513	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	F	503	-	11,11,45	0.23	0	10,10,53	0.25	0
2	MC3	A	511	-	7,7,45	0.25	0	6,6,53	0.18	0
2	MC3	J	511	-	7,7,45	0.24	0	6,6,53	0.18	0
2	MC3	A	503	-	32,32,45	0.73	1 (3%)	35,37,53	1.14	2 (5%)
2	MC3	D	528	-	10,10,45	0.24	0	9,9,53	0.21	0
2	MC3	H	515	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	G	523	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	I	531	-	6,6,45	0.24	0	5,5,53	0.23	0
2	MC3	A	520	-	27,27,45	0.49	0	33,35,53	0.69	0
2	MC3	D	518	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	H	526	-	12,12,45	0.22	0	11,11,53	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	G	522	-	11,11,45	0.23	0	10,10,53	0.26	0
2	MC3	B	515	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	G	520	-	27,27,45	0.49	0	33,35,53	0.69	0
2	MC3	J	523	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	K	524	-	9,9,45	0.25	0	8,8,53	0.20	0
2	MC3	H	508	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	I	504	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	I	533	-	6,6,45	0.25	0	5,5,53	0.24	0
2	MC3	J	522	-	11,11,45	0.23	0	10,10,53	0.26	0
2	MC3	D	510	-	6,6,45	0.26	0	5,5,53	0.19	0
2	MC3	E	533	-	6,6,45	0.24	0	5,5,53	0.24	0
2	MC3	I	510	-	6,6,45	0.25	0	5,5,53	0.19	0
2	MC3	L	525	-	7,7,45	0.24	0	6,6,53	0.18	0
2	MC3	L	527	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	C	513	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	K	516	-	7,7,45	0.23	0	6,6,53	0.23	0
2	MC3	I	520	-	27,27,45	0.49	0	33,35,53	0.70	0
2	MC3	H	525	-	11,11,45	0.24	0	10,10,53	0.21	0
2	MC3	C	524	-	9,9,45	0.24	0	8,8,53	0.20	0
2	MC3	J	514	-	3,3,45	0.34	0	2,2,53	0.56	0
2	MC3	A	530	-	7,7,45	0.25	0	6,6,53	0.19	0
2	MC3	J	525	-	11,11,45	0.24	0	10,10,53	0.21	0
2	MC3	J	527	-	9,9,45	0.24	0	8,8,53	0.20	0
2	MC3	K	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	E	506	-	11,11,45	0.23	0	10,10,53	0.21	0
2	MC3	L	519	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	L	513	-	4,4,45	0.29	0	3,3,53	0.23	0
2	MC3	G	504	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	K	519	-	6,6,45	0.25	0	5,5,53	0.17	0
2	MC3	K	514	-	3,3,45	0.34	0	2,2,53	0.56	0
2	MC3	J	504	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	E	518	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	B	526	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	C	531	-	6,6,45	0.24	0	5,5,53	0.23	0
2	MC3	D	521	-	12,12,45	0.21	0	11,11,53	0.23	0
2	MC3	H	533	-	6,6,45	0.24	0	5,5,53	0.24	0
2	MC3	G	506	-	11,11,45	0.23	0	10,10,53	0.21	0
2	MC3	K	522	-	11,11,45	0.22	0	10,10,53	0.25	0
2	MC3	C	528	-	10,10,45	0.24	0	9,9,53	0.21	0
2	MC3	C	508	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	J	506	-	11,11,45	0.24	0	10,10,53	0.21	0
2	MC3	D	512	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	C	511	-	7,7,45	0.25	0	6,6,53	0.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	F	506	-	11,11,45	0.23	0	10,10,53	0.21	0
2	MC3	D	508	-	11,11,45	0.24	0	10,10,53	0.20	0
2	MC3	I	530	-	7,7,45	0.25	0	6,6,53	0.19	0
2	MC3	K	515	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	A	510	-	6,6,45	0.25	0	5,5,53	0.19	0
2	MC3	A	521	-	12,12,45	0.21	0	11,11,53	0.23	0
2	MC3	F	520	-	11,11,45	0.24	0	10,10,53	0.21	0
2	MC3	L	533	-	6,6,45	0.25	0	5,5,53	0.17	0
2	MC3	I	518	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	G	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	I	503	-	32,32,45	0.73	1 (3%)	35,37,53	1.14	2 (5%)
2	MC3	I	521	-	12,12,45	0.21	0	11,11,53	0.23	0
2	MC3	H	529	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	A	512	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	J	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	J	533	-	6,6,45	0.24	0	5,5,53	0.24	0
2	MC3	E	520	-	27,27,45	0.49	0	33,35,53	0.69	0
2	MC3	E	502	-	29,29,45	0.77	1 (3%)	32,34,53	1.16	2 (6%)
2	MC3	H	532	-	4,4,45	0.28	0	3,3,53	0.23	0
2	MC3	H	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	C	529	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	K	506	-	11,11,45	0.24	0	10,10,53	0.21	0
2	MC3	K	528	-	10,10,45	0.24	0	9,9,53	0.21	0
2	MC3	H	506	-	11,11,45	0.24	0	10,10,53	0.21	0
2	MC3	L	504	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	C	533	-	6,6,45	0.24	0	5,5,53	0.24	0
2	MC3	D	523	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	B	517	-	11,11,45	0.23	0	10,10,53	0.22	0
2	MC3	K	511	-	7,7,45	0.25	0	6,6,53	0.18	0
2	MC3	I	513	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	B	506	-	11,11,45	0.23	0	10,10,53	0.21	0
2	MC3	D	524	-	9,9,45	0.24	0	8,8,53	0.20	0
2	MC3	G	502	-	29,29,45	0.77	1 (3%)	32,34,53	1.15	2 (6%)
2	MC3	H	511	-	7,7,45	0.25	0	6,6,53	0.18	0
2	MC3	K	530	-	7,7,45	0.25	0	6,6,53	0.19	0
2	MC3	L	523	-	8,8,45	0.25	0	7,7,53	0.20	0
2	MC3	J	502	-	29,29,45	0.77	1 (3%)	32,34,53	1.15	2 (6%)
2	MC3	B	511	-	7,7,45	0.25	0	6,6,53	0.18	0
2	MC3	G	519	-	6,6,45	0.25	0	5,5,53	0.17	0
2	MC3	B	518	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	L	515	-	8,8,45	0.24	0	7,7,53	0.18	0
2	MC3	E	516	-	7,7,45	0.23	0	6,6,53	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	D	525	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	D	527	-	9,9,45	0.24	0	8,8,53	0.20	0
2	MC3	C	505	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	L	505	-	9,9,45	0.25	0	8,8,53	0.20	0
2	MC3	J	519	-	6,6,45	0.25	0	5,5,53	0.17	0
2	MC3	A	523	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	G	518	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	G	531	-	6,6,45	0.24	0	5,5,53	0.23	0
2	MC3	H	517	-	11,11,45	0.23	0	10,10,53	0.22	0
2	MC3	D	504	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	B	509	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	I	517	-	11,11,45	0.23	0	10,10,53	0.22	0
2	MC3	I	508	-	11,11,45	0.24	0	10,10,53	0.20	0
2	MC3	B	514	-	3,3,45	0.34	0	2,2,53	0.56	0
2	MC3	G	516	-	7,7,45	0.23	0	6,6,53	0.23	0
2	MC3	I	526	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	J	516	-	7,7,45	0.24	0	6,6,53	0.23	0
2	MC3	H	523	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	A	525	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	A	527	-	9,9,45	0.24	0	8,8,53	0.20	0
2	MC3	H	504	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	C	530	-	7,7,45	0.25	0	6,6,53	0.19	0
2	MC3	H	524	-	9,9,45	0.25	0	8,8,53	0.20	0
2	MC3	A	507	-	11,11,45	0.24	0	10,10,53	0.20	0
2	MC3	D	515	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	B	523	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	K	521	-	12,12,45	0.21	0	11,11,53	0.23	0
2	MC3	L	532	-	5,5,45	0.26	0	4,4,53	0.16	0
2	MC3	K	502	-	29,29,45	0.77	1 (3%)	32,34,53	1.15	2 (6%)
2	MC3	B	522	-	11,11,45	0.23	0	10,10,53	0.25	0
2	MC3	K	513	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	A	504	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	A	524	-	9,9,45	0.24	0	8,8,53	0.20	0
2	MC3	H	514	-	3,3,45	0.34	0	2,2,53	0.56	0
2	MC3	E	524	-	9,9,45	0.24	0	8,8,53	0.20	0
2	MC3	C	503	-	32,32,45	0.72	1 (3%)	35,37,53	1.14	2 (5%)
2	MC3	J	518	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	B	530	-	7,7,45	0.25	0	6,6,53	0.19	0
2	MC3	C	502	-	29,29,45	0.77	1 (3%)	32,34,53	1.15	2 (6%)
2	MC3	B	508	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	D	522	-	11,11,45	0.23	0	10,10,53	0.26	0
2	MC3	K	508	-	11,11,45	0.24	0	10,10,53	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	F	507	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	F	513	-	4,4,45	0.28	0	3,3,53	0.23	0
2	MC3	A	513	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	I	529	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	A	515	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	D	502	-	29,29,45	0.77	1 (3%)	32,34,53	1.15	2 (6%)
2	MC3	K	533	-	6,6,45	0.24	0	5,5,53	0.24	0
2	MC3	G	513	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	H	522	-	11,11,45	0.23	0	10,10,53	0.25	0
2	MC3	G	524	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	C	525	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	H	516	-	7,7,45	0.23	0	6,6,53	0.23	0
2	MC3	C	506	-	11,11,45	0.23	0	10,10,53	0.21	0
2	MC3	J	513	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	D	519	-	6,6,45	0.25	0	5,5,53	0.17	0
2	MC3	J	528	-	10,10,45	0.24	0	9,9,53	0.21	0
2	MC3	E	528	-	10,10,45	0.24	0	9,9,53	0.20	0
2	MC3	J	524	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	I	512	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	B	516	-	7,7,45	0.23	0	6,6,53	0.23	0
2	MC3	A	508	-	11,11,45	0.24	0	10,10,53	0.20	0
2	MC3	K	509	-	8,8,45	0.25	0	7,7,53	0.20	0
2	MC3	G	528	-	10,10,45	0.24	0	9,9,53	0.21	0
2	MC3	D	526	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	D	529	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	D	531	-	6,6,45	0.24	0	5,5,53	0.23	0
2	MC3	F	528	-	3,3,45	0.34	0	2,2,53	0.56	0
2	MC3	D	507	-	11,11,45	0.24	0	10,10,53	0.20	0
2	MC3	L	521	-	11,11,45	0.24	0	10,10,53	0.20	0
2	MC3	I	532	-	4,4,45	0.29	0	3,3,53	0.23	0
2	MC3	D	533	-	6,6,45	0.24	0	5,5,53	0.24	0
2	MC3	B	521	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	I	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	A	519	-	6,6,45	0.25	0	5,5,53	0.17	0
2	MC3	E	507	-	11,11,45	0.23	0	10,10,53	0.20	0
2	MC3	L	528	-	3,3,45	0.34	0	2,2,53	0.56	0
2	MC3	A	509	-	8,8,45	0.25	0	7,7,53	0.20	0
2	MC3	C	517	-	11,11,45	0.23	0	10,10,53	0.22	0
2	MC3	H	512	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	H	502	-	29,29,45	0.77	1 (3%)	32,34,53	1.15	2 (6%)
2	MC3	D	505	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	F	511	-	7,7,45	0.25	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	L	511	-	7,7,45	0.25	0	6,6,53	0.19	0
2	MC3	D	509	-	8,8,45	0.25	0	7,7,53	0.20	0
2	MC3	F	518	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	K	520	-	27,27,45	0.49	0	33,35,53	0.69	0
2	MC3	C	526	-	12,12,45	0.22	0	11,11,53	0.23	0
2	MC3	A	526	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	B	512	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	A	529	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	A	531	-	6,6,45	0.24	0	5,5,53	0.23	0
2	MC3	B	502	-	29,29,45	0.77	1 (3%)	32,34,53	1.15	2 (6%)
2	MC3	F	533	-	6,6,45	0.25	0	5,5,53	0.18	0
2	MC3	H	519	-	6,6,45	0.25	0	5,5,53	0.17	0
2	MC3	A	502	-	29,29,45	0.77	1 (3%)	32,34,53	1.15	2 (6%)
2	MC3	F	510	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	L	507	-	12,12,45	0.23	0	11,11,53	0.23	0
2	MC3	E	529	-	5,5,45	0.27	0	4,4,53	0.16	0
2	MC3	L	518	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	C	521	-	12,12,45	0.21	0	11,11,53	0.23	0
2	MC3	F	522	-	11,11,45	0.24	0	10,10,53	0.20	0
2	MC3	B	519	-	6,6,45	0.25	0	5,5,53	0.17	0
2	MC3	F	519	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	I	523	-	11,11,45	0.23	0	10,10,53	0.19	0
2	MC3	A	533	-	6,6,45	0.24	0	5,5,53	0.24	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	J	507	-	-	0/9/9/49	-
2	MC3	B	524	-	-	0/7/7/49	-
2	MC3	E	513	-	-	0/3/3/49	-
2	MC3	E	515	-	-	0/3/3/49	-
2	MC3	A	505	-	-	0/10/10/49	-
2	MC3	L	522	-	-	0/9/9/49	-
2	MC3	I	525	-	-	0/9/9/49	-
2	MC3	L	509	-	-	0/8/8/49	-
2	MC3	I	506	-	-	0/9/9/49	-
2	MC3	I	527	-	-	0/7/7/49	-
2	MC3	C	504	-	-	0/10/10/49	-
2	MC3	C	519	-	-	0/4/4/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	G	532	-	-	0/2/2/49	-
2	MC3	J	529	-	-	0/3/3/49	-
2	MC3	J	509	-	-	0/6/6/49	-
2	MC3	E	509	-	-	0/6/6/49	-
2	MC3	H	503	-	-	7/34/34/49	-
2	MC3	C	520	-	-	20/31/31/49	-
2	MC3	B	503	-	-	7/34/34/49	-
2	MC3	F	505	-	-	0/7/7/49	-
2	MC3	L	520	-	-	0/9/9/49	-
2	MC3	K	507	-	-	0/9/9/49	-
2	MC3	F	512	-	-	0/4/4/49	-
2	MC3	C	512	-	-	0/6/6/49	-
2	MC3	F	530	-	-	0/5/5/49	-
2	MC3	G	530	-	-	0/5/5/49	-
2	MC3	C	515	-	-	0/3/3/49	-
2	MC3	D	514	-	-	1/1/1/49	-
2	MC3	E	530	-	-	0/5/5/49	-
2	MC3	B	525	-	-	0/9/9/49	-
2	MC3	K	525	-	-	0/9/9/49	-
2	MC3	L	508	-	-	0/7/7/49	-
2	MC3	C	532	-	-	0/2/2/49	-
2	MC3	H	513	-	-	0/3/3/49	-
2	MC3	F	521	-	-	0/9/9/49	-
2	MC3	F	527	-	-	0/3/3/49	-
2	MC3	C	507	-	-	0/9/9/49	-
2	MC3	J	520	-	-	20/31/31/49	-
2	MC3	E	508	-	-	0/9/9/49	-
2	MC3	K	503	-	-	7/34/34/49	-
2	MC3	B	504	-	-	0/10/10/49	-
2	MC3	G	527	-	-	0/7/7/49	-
2	MC3	I	522	-	-	0/9/9/49	-
2	MC3	E	521	-	-	0/10/10/49	-
2	MC3	I	516	-	-	0/5/5/49	-
2	MC3	B	529	-	-	0/3/3/49	-
2	MC3	B	531	-	-	0/4/4/49	-
2	MC3	H	520	-	-	20/31/31/49	-
2	MC3	K	531	-	-	0/4/4/49	-
2	MC3	D	506	-	-	0/9/9/49	-
2	MC3	L	530	-	-	0/5/5/49	-
2	MC3	A	514	-	-	1/1/1/49	-
2	MC3	L	501	-	-	20/31/31/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	G	529	-	-	0/3/3/49	-
2	MC3	H	528	-	-	0/8/8/49	-
2	MC3	E	505	-	-	0/10/10/49	-
2	MC3	B	532	-	-	0/2/2/49	-
2	MC3	B	513	-	-	0/3/3/49	-
2	MC3	B	520	-	-	20/31/31/49	-
2	MC3	F	523	-	-	0/6/6/49	-
2	MC3	J	530	-	-	0/5/5/49	-
2	MC3	B	501	-	-	1/6/6/49	-
2	MC3	B	528	-	-	0/8/8/49	-
2	MC3	D	511	-	-	0/5/5/49	-
2	MC3	F	524	-	-	0/4/4/49	-
2	MC3	C	518	-	-	0/3/3/49	-
2	MC3	A	522	-	-	0/9/9/49	-
2	MC3	G	515	-	-	0/3/3/49	-
2	MC3	L	516	-	-	13/31/31/49	-
2	MC3	E	510	-	-	0/4/4/49	-
2	MC3	E	503	-	-	7/34/34/49	-
2	MC3	C	527	-	-	0/7/7/49	-
2	MC3	A	528	-	-	0/8/8/49	-
2	MC3	I	502	-	-	13/31/31/49	-
2	MC3	C	509	-	-	0/6/6/49	-
2	MC3	E	512	-	-	0/6/6/49	-
2	MC3	D	517	-	-	2/9/9/49	-
2	MC3	B	533	-	-	0/4/4/49	-
2	MC3	F	504	-	-	0/9/9/49	-
2	MC3	I	515	-	-	0/3/3/49	-
2	MC3	E	511	-	-	0/5/5/49	-
2	MC3	I	514	-	-	1/1/1/49	-
2	MC3	I	505	-	-	0/10/10/49	-
2	MC3	L	503	-	-	0/9/9/49	-
2	MC3	G	503	-	-	7/34/34/49	-
2	MC3	K	526	-	-	0/10/10/49	-
2	MC3	J	503	-	-	7/34/34/49	-
2	MC3	H	531	-	-	0/4/4/49	-
2	MC3	E	522	-	-	0/9/9/49	-
2	MC3	K	529	-	-	0/3/3/49	-
2	MC3	K	518	-	-	0/3/3/49	-
2	MC3	F	509	-	-	0/8/8/49	-
2	MC3	H	518	-	-	0/3/3/49	-
2	MC3	F	525	-	-	0/5/5/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	C	501	-	-	1/6/6/49	-
2	MC3	A	517	-	-	2/9/9/49	-
2	MC3	E	517	-	-	2/9/9/49	-
2	MC3	J	515	-	-	0/3/3/49	-
2	MC3	L	506	-	-	0/9/9/49	-
2	MC3	F	526	-	-	0/6/6/49	-
2	MC3	H	510	-	-	0/4/4/49	-
2	MC3	L	514	-	-	0/4/4/49	-
2	MC3	L	517	-	-	7/34/34/49	-
2	MC3	G	526	-	-	0/10/10/49	-
2	MC3	F	508	-	-	0/7/7/49	-
2	MC3	K	505	-	-	0/10/10/49	-
2	MC3	H	505	-	-	0/10/10/49	-
2	MC3	H	509	-	-	0/6/6/49	-
2	MC3	I	519	-	-	0/4/4/49	-
2	MC3	G	507	-	-	0/9/9/49	-
2	MC3	K	512	-	-	0/6/6/49	-
2	MC3	E	523	-	-	0/9/9/49	-
2	MC3	C	522	-	-	0/9/9/49	-
2	MC3	L	526	-	-	0/6/6/49	-
2	MC3	B	505	-	-	0/10/10/49	-
2	MC3	E	504	-	-	0/10/10/49	-
2	MC3	F	529	-	-	0/3/3/49	-
2	MC3	C	516	-	-	0/5/5/49	-
2	MC3	G	533	-	-	0/4/4/49	-
2	MC3	F	502	-	-	0/10/10/49	-
2	MC3	L	510	-	-	0/3/3/49	-
2	MC3	E	526	-	-	0/10/10/49	-
2	MC3	F	515	-	-	1/6/6/49	-
2	MC3	G	505	-	-	0/10/10/49	-
2	MC3	K	510	-	-	0/4/4/49	-
2	MC3	E	525	-	-	0/9/9/49	-
2	MC3	G	509	-	-	0/6/6/49	-
2	MC3	I	507	-	-	0/9/9/49	-
2	MC3	F	514	-	-	0/4/4/49	-
2	MC3	D	532	-	-	0/2/2/49	-
2	MC3	B	510	-	-	0/4/4/49	-
2	MC3	D	530	-	-	0/5/5/49	-
2	MC3	D	501	-	-	1/6/6/49	-
2	MC3	I	528	-	-	0/8/8/49	-
2	MC3	K	517	-	-	2/9/9/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	K	532	-	-	0/2/2/49	-
2	MC3	F	531	-	-	2/9/9/49	-
2	MC3	C	510	-	-	0/4/4/49	-
2	MC3	F	532	-	-	0/3/3/49	-
2	MC3	H	530	-	-	0/5/5/49	-
2	MC3	I	524	-	-	0/7/7/49	-
2	MC3	J	526	-	-	0/10/10/49	-
2	MC3	G	510	-	-	0/4/4/49	-
2	MC3	I	509	-	-	0/6/6/49	-
2	MC3	L	524	-	-	0/4/4/49	-
2	MC3	G	521	-	-	0/10/10/49	-
2	MC3	K	523	-	-	0/9/9/49	-
2	MC3	J	510	-	-	0/4/4/49	-
2	MC3	L	529	-	-	0/3/3/49	-
2	MC3	L	531	-	-	2/9/9/49	-
2	MC3	E	532	-	-	0/2/2/49	-
2	MC3	H	527	-	-	0/7/7/49	-
2	MC3	A	532	-	-	0/2/2/49	-
2	MC3	J	521	-	-	0/10/10/49	-
2	MC3	D	516	-	-	0/5/5/49	-
2	MC3	D	520	-	-	20/31/31/49	-
2	MC3	G	517	-	-	2/9/9/49	-
2	MC3	H	507	-	-	0/9/9/49	-
2	MC3	C	514	-	-	1/1/1/49	-
2	MC3	G	511	-	-	0/5/5/49	-
2	MC3	E	531	-	-	0/4/4/49	-
2	MC3	F	517	-	-	7/34/34/49	-
2	MC3	L	512	-	-	0/4/4/49	-
2	MC3	L	502	-	-	0/10/10/49	-
2	MC3	B	527	-	-	0/7/7/49	-
2	MC3	H	521	-	-	0/10/10/49	-
2	MC3	A	506	-	-	0/9/9/49	-
2	MC3	B	507	-	-	0/9/9/49	-
2	MC3	G	508	-	-	0/9/9/49	-
2	MC3	J	505	-	-	0/10/10/49	-
2	MC3	K	527	-	-	0/7/7/49	-
2	MC3	J	508	-	-	0/9/9/49	-
2	MC3	D	503	-	-	7/34/34/49	-
2	MC3	I	511	-	-	0/5/5/49	-
2	MC3	A	518	-	-	0/3/3/49	-
2	MC3	F	516	-	-	13/31/31/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	K	504	-	-	0/10/10/49	-
2	MC3	A	516	-	-	0/5/5/49	-
2	MC3	F	501	-	-	20/31/31/49	-
2	MC3	J	531	-	-	0/4/4/49	-
2	MC3	J	532	-	-	0/2/2/49	-
2	MC3	A	501	-	-	1/6/6/49	-
2	MC3	G	512	-	-	0/6/6/49	-
2	MC3	G	514	-	-	1/1/1/49	-
2	MC3	G	525	-	-	0/9/9/49	-
2	MC3	C	523	-	-	0/9/9/49	-
2	MC3	E	501	-	-	1/6/6/49	-
2	MC3	E	519	-	-	0/4/4/49	-
2	MC3	J	512	-	-	0/6/6/49	-
2	MC3	E	514	-	-	1/1/1/49	-
2	MC3	E	527	-	-	0/7/7/49	-
2	MC3	J	517	-	-	2/9/9/49	-
2	MC3	D	513	-	-	0/3/3/49	-
2	MC3	F	503	-	-	0/9/9/49	-
2	MC3	A	511	-	-	0/5/5/49	-
2	MC3	J	511	-	-	0/5/5/49	-
2	MC3	A	503	-	-	7/34/34/49	-
2	MC3	D	528	-	-	0/8/8/49	-
2	MC3	H	515	-	-	0/3/3/49	-
2	MC3	G	523	-	-	0/9/9/49	-
2	MC3	I	531	-	-	0/4/4/49	-
2	MC3	A	520	-	-	20/31/31/49	-
2	MC3	D	518	-	-	0/3/3/49	-
2	MC3	H	526	-	-	0/10/10/49	-
2	MC3	G	522	-	-	0/9/9/49	-
2	MC3	B	515	-	-	0/3/3/49	-
2	MC3	G	520	-	-	20/31/31/49	-
2	MC3	J	523	-	-	0/9/9/49	-
2	MC3	K	524	-	-	0/7/7/49	-
2	MC3	H	508	-	-	0/9/9/49	-
2	MC3	I	504	-	-	0/10/10/49	-
2	MC3	I	533	-	-	0/4/4/49	-
2	MC3	J	522	-	-	0/9/9/49	-
2	MC3	D	510	-	-	0/4/4/49	-
2	MC3	E	533	-	-	0/4/4/49	-
2	MC3	I	510	-	-	0/4/4/49	-
2	MC3	L	525	-	-	0/5/5/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	L	527	-	-	0/3/3/49	-
2	MC3	C	513	-	-	0/3/3/49	-
2	MC3	K	516	-	-	0/5/5/49	-
2	MC3	I	520	-	-	20/31/31/49	-
2	MC3	H	525	-	-	0/9/9/49	-
2	MC3	C	524	-	-	0/7/7/49	-
2	MC3	J	514	-	-	1/1/1/49	-
2	MC3	A	530	-	-	0/5/5/49	-
2	MC3	J	525	-	-	0/9/9/49	-
2	MC3	J	527	-	-	0/7/7/49	-
2	MC3	K	501	-	-	1/6/6/49	-
2	MC3	E	506	-	-	0/9/9/49	-
2	MC3	L	519	-	-	0/10/10/49	-
2	MC3	L	513	-	-	0/2/2/49	-
2	MC3	G	504	-	-	0/10/10/49	-
2	MC3	K	519	-	-	0/4/4/49	-
2	MC3	K	514	-	-	1/1/1/49	-
2	MC3	J	504	-	-	0/10/10/49	-
2	MC3	E	518	-	-	0/3/3/49	-
2	MC3	B	526	-	-	0/10/10/49	-
2	MC3	C	531	-	-	0/4/4/49	-
2	MC3	D	521	-	-	0/10/10/49	-
2	MC3	H	533	-	-	0/4/4/49	-
2	MC3	G	506	-	-	0/9/9/49	-
2	MC3	K	522	-	-	0/9/9/49	-
2	MC3	C	528	-	-	0/8/8/49	-
2	MC3	C	508	-	-	0/9/9/49	-
2	MC3	J	506	-	-	0/9/9/49	-
2	MC3	D	512	-	-	0/6/6/49	-
2	MC3	C	511	-	-	0/5/5/49	-
2	MC3	F	506	-	-	0/9/9/49	-
2	MC3	D	508	-	-	0/9/9/49	-
2	MC3	I	530	-	-	0/5/5/49	-
2	MC3	K	515	-	-	0/3/3/49	-
2	MC3	A	510	-	-	0/4/4/49	-
2	MC3	A	521	-	-	0/10/10/49	-
2	MC3	F	520	-	-	0/9/9/49	-
2	MC3	L	533	-	-	0/4/4/49	-
2	MC3	I	518	-	-	0/3/3/49	-
2	MC3	G	501	-	-	1/6/6/49	-
2	MC3	I	503	-	-	7/34/34/49	-
2	MC3	I	521	-	-	0/10/10/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	H	529	-	-	0/3/3/49	-
2	MC3	A	512	-	-	0/6/6/49	-
2	MC3	J	501	-	-	1/6/6/49	-
2	MC3	J	533	-	-	0/4/4/49	-
2	MC3	E	520	-	-	20/31/31/49	-
2	MC3	E	502	-	-	13/31/31/49	-
2	MC3	H	532	-	-	0/2/2/49	-
2	MC3	H	501	-	-	1/6/6/49	-
2	MC3	C	529	-	-	0/3/3/49	-
2	MC3	K	506	-	-	0/9/9/49	-
2	MC3	K	528	-	-	0/8/8/49	-
2	MC3	H	506	-	-	0/9/9/49	-
2	MC3	L	504	-	-	0/9/9/49	-
2	MC3	C	533	-	-	0/4/4/49	-
2	MC3	D	523	-	-	0/9/9/49	-
2	MC3	B	517	-	-	2/9/9/49	-
2	MC3	K	511	-	-	0/5/5/49	-
2	MC3	I	513	-	-	0/3/3/49	-
2	MC3	B	506	-	-	0/9/9/49	-
2	MC3	D	524	-	-	0/7/7/49	-
2	MC3	G	502	-	-	13/31/31/49	-
2	MC3	H	511	-	-	0/5/5/49	-
2	MC3	K	530	-	-	0/5/5/49	-
2	MC3	L	523	-	-	0/6/6/49	-
2	MC3	J	502	-	-	13/31/31/49	-
2	MC3	B	511	-	-	0/5/5/49	-
2	MC3	G	519	-	-	0/4/4/49	-
2	MC3	B	518	-	-	0/3/3/49	-
2	MC3	L	515	-	-	1/6/6/49	-
2	MC3	E	516	-	-	0/5/5/49	-
2	MC3	D	525	-	-	0/9/9/49	-
2	MC3	D	527	-	-	0/7/7/49	-
2	MC3	C	505	-	-	0/10/10/49	-
2	MC3	L	505	-	-	0/7/7/49	-
2	MC3	J	519	-	-	0/4/4/49	-
2	MC3	A	523	-	-	0/9/9/49	-
2	MC3	G	518	-	-	0/3/3/49	-
2	MC3	G	531	-	-	0/4/4/49	-
2	MC3	H	517	-	-	2/9/9/49	-
2	MC3	D	504	-	-	0/10/10/49	-
2	MC3	B	509	-	-	0/6/6/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	I	517	-	-	2/9/9/49	-
2	MC3	I	508	-	-	0/9/9/49	-
2	MC3	B	514	-	-	1/1/1/49	-
2	MC3	G	516	-	-	0/5/5/49	-
2	MC3	I	526	-	-	0/10/10/49	-
2	MC3	J	516	-	-	0/5/5/49	-
2	MC3	H	523	-	-	0/9/9/49	-
2	MC3	A	525	-	-	0/9/9/49	-
2	MC3	A	527	-	-	0/7/7/49	-
2	MC3	H	504	-	-	0/10/10/49	-
2	MC3	C	530	-	-	0/5/5/49	-
2	MC3	H	524	-	-	0/7/7/49	-
2	MC3	A	507	-	-	0/9/9/49	-
2	MC3	D	515	-	-	0/3/3/49	-
2	MC3	B	523	-	-	0/9/9/49	-
2	MC3	K	521	-	-	0/10/10/49	-
2	MC3	L	532	-	-	0/3/3/49	-
2	MC3	K	502	-	-	13/31/31/49	-
2	MC3	B	522	-	-	0/9/9/49	-
2	MC3	K	513	-	-	0/3/3/49	-
2	MC3	A	504	-	-	0/10/10/49	-
2	MC3	A	524	-	-	0/7/7/49	-
2	MC3	H	514	-	-	1/1/1/49	-
2	MC3	E	524	-	-	0/7/7/49	-
2	MC3	C	503	-	-	7/34/34/49	-
2	MC3	J	518	-	-	0/3/3/49	-
2	MC3	B	530	-	-	0/5/5/49	-
2	MC3	C	502	-	-	13/31/31/49	-
2	MC3	B	508	-	-	0/9/9/49	-
2	MC3	D	522	-	-	0/9/9/49	-
2	MC3	K	508	-	-	0/9/9/49	-
2	MC3	F	507	-	-	0/10/10/49	-
2	MC3	F	513	-	-	0/2/2/49	-
2	MC3	A	513	-	-	0/3/3/49	-
2	MC3	I	529	-	-	0/3/3/49	-
2	MC3	A	515	-	-	0/3/3/49	-
2	MC3	D	502	-	-	13/31/31/49	-
2	MC3	K	533	-	-	0/4/4/49	-
2	MC3	G	513	-	-	0/3/3/49	-
2	MC3	H	522	-	-	0/9/9/49	-
2	MC3	G	524	-	-	0/7/7/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	C	525	-	-	0/9/9/49	-
2	MC3	H	516	-	-	0/5/5/49	-
2	MC3	C	506	-	-	0/9/9/49	-
2	MC3	J	513	-	-	0/3/3/49	-
2	MC3	D	519	-	-	0/4/4/49	-
2	MC3	J	528	-	-	0/8/8/49	-
2	MC3	E	528	-	-	0/8/8/49	-
2	MC3	J	524	-	-	0/7/7/49	-
2	MC3	I	512	-	-	0/6/6/49	-
2	MC3	B	516	-	-	0/5/5/49	-
2	MC3	A	508	-	-	0/9/9/49	-
2	MC3	K	509	-	-	0/6/6/49	-
2	MC3	G	528	-	-	0/8/8/49	-
2	MC3	D	526	-	-	0/10/10/49	-
2	MC3	D	529	-	-	0/3/3/49	-
2	MC3	D	531	-	-	0/4/4/49	-
2	MC3	F	528	-	-	1/1/1/49	-
2	MC3	D	507	-	-	0/9/9/49	-
2	MC3	L	521	-	-	0/9/9/49	-
2	MC3	I	532	-	-	0/2/2/49	-
2	MC3	D	533	-	-	0/4/4/49	-
2	MC3	B	521	-	-	0/10/10/49	-
2	MC3	I	501	-	-	1/6/6/49	-
2	MC3	A	519	-	-	0/4/4/49	-
2	MC3	E	507	-	-	0/9/9/49	-
2	MC3	L	528	-	-	1/1/1/49	-
2	MC3	A	509	-	-	0/6/6/49	-
2	MC3	C	517	-	-	2/9/9/49	-
2	MC3	H	512	-	-	0/6/6/49	-
2	MC3	H	502	-	-	13/31/31/49	-
2	MC3	D	505	-	-	0/10/10/49	-
2	MC3	F	511	-	-	0/5/5/49	-
2	MC3	L	511	-	-	0/5/5/49	-
2	MC3	D	509	-	-	0/6/6/49	-
2	MC3	F	518	-	-	0/10/10/49	-
2	MC3	K	520	-	-	20/31/31/49	-
2	MC3	C	526	-	-	0/10/10/49	-
2	MC3	A	526	-	-	0/10/10/49	-
2	MC3	B	512	-	-	0/6/6/49	-
2	MC3	A	529	-	-	0/3/3/49	-
2	MC3	A	531	-	-	0/4/4/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	B	502	-	-	13/31/31/49	-
2	MC3	F	533	-	-	0/4/4/49	-
2	MC3	H	519	-	-	0/4/4/49	-
2	MC3	A	502	-	-	13/31/31/49	-
2	MC3	F	510	-	-	0/3/3/49	-
2	MC3	L	507	-	-	0/10/10/49	-
2	MC3	E	529	-	-	0/3/3/49	-
2	MC3	L	518	-	-	0/10/10/49	-
2	MC3	C	521	-	-	0/10/10/49	-
2	MC3	F	522	-	-	0/9/9/49	-
2	MC3	B	519	-	-	0/4/4/49	-
2	MC3	F	519	-	-	0/10/10/49	-
2	MC3	I	523	-	-	0/9/9/49	-
2	MC3	A	533	-	-	0/4/4/49	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	502	MC3	P-O4P	2.88	1.65	1.54
2	E	502	MC3	P-O4P	2.88	1.65	1.54
2	G	502	MC3	P-O4P	2.87	1.65	1.54
2	F	516	MC3	P-O4P	2.87	1.65	1.54
2	A	502	MC3	P-O4P	2.86	1.65	1.54
2	B	502	MC3	P-O4P	2.86	1.65	1.54
2	K	502	MC3	P-O4P	2.86	1.65	1.54
2	H	502	MC3	P-O4P	2.86	1.65	1.54
2	J	502	MC3	P-O4P	2.85	1.65	1.54
2	B	503	MC3	P-O4P	2.85	1.65	1.54
2	L	516	MC3	P-O4P	2.85	1.65	1.54
2	C	502	MC3	P-O4P	2.85	1.65	1.54
2	D	502	MC3	P-O4P	2.85	1.65	1.54
2	H	503	MC3	P-O4P	2.84	1.65	1.54
2	G	503	MC3	P-O4P	2.84	1.65	1.54
2	E	503	MC3	P-O4P	2.83	1.65	1.54
2	A	503	MC3	P-O4P	2.83	1.65	1.54
2	C	503	MC3	P-O4P	2.83	1.65	1.54
2	K	503	MC3	P-O4P	2.82	1.65	1.54
2	F	517	MC3	P-O4P	2.82	1.65	1.54
2	L	517	MC3	P-O4P	2.82	1.65	1.54
2	I	503	MC3	P-O4P	2.82	1.65	1.54
2	D	503	MC3	P-O4P	2.81	1.65	1.54
2	J	503	MC3	P-O4P	2.81	1.65	1.54

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	503	MC3	O4P-P-O3P	-5.34	92.76	106.67
2	K	503	MC3	O4P-P-O3P	-5.33	92.77	106.67
2	B	503	MC3	O4P-P-O3P	-5.33	92.78	106.67
2	I	503	MC3	O4P-P-O3P	-5.33	92.78	106.67
2	A	503	MC3	O4P-P-O3P	-5.33	92.78	106.67
2	L	517	MC3	O4P-P-O3P	-5.33	92.78	106.67
2	E	503	MC3	O4P-P-O3P	-5.33	92.78	106.67
2	H	503	MC3	O4P-P-O3P	-5.32	92.79	106.67
2	J	503	MC3	O4P-P-O3P	-5.32	92.80	106.67
2	D	503	MC3	O4P-P-O3P	-5.32	92.80	106.67
2	F	517	MC3	O4P-P-O3P	-5.32	92.81	106.67
2	C	503	MC3	O4P-P-O3P	-5.31	92.81	106.67
2	E	502	MC3	O4P-P-O3P	-5.18	93.16	106.67
2	B	502	MC3	O4P-P-O3P	-5.17	93.18	106.67
2	D	502	MC3	O4P-P-O3P	-5.17	93.18	106.67
2	F	516	MC3	O4P-P-O3P	-5.17	93.19	106.67
2	A	502	MC3	O4P-P-O3P	-5.17	93.19	106.67
2	K	502	MC3	O4P-P-O3P	-5.17	93.20	106.67
2	H	502	MC3	O4P-P-O3P	-5.17	93.20	106.67
2	I	502	MC3	O4P-P-O3P	-5.17	93.20	106.67
2	G	502	MC3	O4P-P-O3P	-5.16	93.20	106.67
2	L	516	MC3	O4P-P-O3P	-5.16	93.21	106.67
2	C	502	MC3	O4P-P-O3P	-5.16	93.22	106.67
2	J	502	MC3	O4P-P-O3P	-5.15	93.23	106.67
2	E	503	MC3	O2P-P-O1P	2.30	119.80	110.83
2	H	503	MC3	O2P-P-O1P	2.30	119.79	110.83
2	B	503	MC3	O2P-P-O1P	2.30	119.78	110.83
2	G	503	MC3	O2P-P-O1P	2.30	119.78	110.83
2	J	503	MC3	O2P-P-O1P	2.30	119.78	110.83
2	A	503	MC3	O2P-P-O1P	2.29	119.76	110.83
2	F	517	MC3	O2P-P-O1P	2.29	119.75	110.83
2	L	517	MC3	O2P-P-O1P	2.29	119.75	110.83
2	I	503	MC3	O2P-P-O1P	2.29	119.75	110.83
2	K	503	MC3	O2P-P-O1P	2.29	119.74	110.83
2	C	503	MC3	O2P-P-O1P	2.28	119.72	110.83
2	D	503	MC3	O2P-P-O1P	2.27	119.70	110.83
2	H	502	MC3	O2P-P-O1P	2.26	119.65	110.83
2	I	502	MC3	O2P-P-O1P	2.26	119.65	110.83
2	D	502	MC3	O2P-P-O1P	2.26	119.65	110.83
2	F	516	MC3	O2P-P-O1P	2.26	119.64	110.83
2	E	502	MC3	O2P-P-O1P	2.26	119.64	110.83
2	A	502	MC3	O2P-P-O1P	2.26	119.64	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	516	MC3	O2P-P-O1P	2.26	119.64	110.83
2	B	502	MC3	O2P-P-O1P	2.26	119.64	110.83
2	G	502	MC3	O2P-P-O1P	2.26	119.63	110.83
2	K	502	MC3	O2P-P-O1P	2.25	119.62	110.83
2	C	502	MC3	O2P-P-O1P	2.25	119.60	110.83
2	J	502	MC3	O2P-P-O1P	2.24	119.58	110.83

There are no chirality outliers.

All (528) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	MC3	C32-C31-O2-C2
2	A	502	MC3	C1-O3P-P-O1P
2	A	502	MC3	C1-O3P-P-O2P
2	A	502	MC3	C1-O3P-P-O4P
2	A	503	MC3	C1-O3P-P-O2P
2	A	503	MC3	C1-O3P-P-O4P
2	A	520	MC3	O4P-C4-C5-N
2	A	520	MC3	C1-O3P-P-O1P
2	A	520	MC3	C1-O3P-P-O4P
2	A	520	MC3	C4-O4P-P-O1P
2	A	520	MC3	C4-O4P-P-O2P
2	A	520	MC3	C4-O4P-P-O3P
2	B	502	MC3	C32-C31-O2-C2
2	B	502	MC3	C1-O3P-P-O1P
2	B	502	MC3	C1-O3P-P-O2P
2	B	502	MC3	C1-O3P-P-O4P
2	B	503	MC3	C1-O3P-P-O2P
2	B	503	MC3	C1-O3P-P-O4P
2	B	520	MC3	O4P-C4-C5-N
2	B	520	MC3	C1-O3P-P-O1P
2	B	520	MC3	C1-O3P-P-O4P
2	B	520	MC3	C4-O4P-P-O1P
2	B	520	MC3	C4-O4P-P-O2P
2	B	520	MC3	C4-O4P-P-O3P
2	C	502	MC3	C32-C31-O2-C2
2	C	502	MC3	C1-O3P-P-O1P
2	C	502	MC3	C1-O3P-P-O2P
2	C	502	MC3	C1-O3P-P-O4P
2	C	503	MC3	C1-O3P-P-O2P
2	C	503	MC3	C1-O3P-P-O4P
2	C	520	MC3	O4P-C4-C5-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	520	MC3	C1-O3P-P-O1P
2	C	520	MC3	C1-O3P-P-O4P
2	C	520	MC3	C4-O4P-P-O1P
2	C	520	MC3	C4-O4P-P-O2P
2	C	520	MC3	C4-O4P-P-O3P
2	D	502	MC3	C32-C31-O2-C2
2	D	502	MC3	C1-O3P-P-O1P
2	D	502	MC3	C1-O3P-P-O2P
2	D	502	MC3	C1-O3P-P-O4P
2	D	503	MC3	C1-O3P-P-O2P
2	D	503	MC3	C1-O3P-P-O4P
2	D	520	MC3	O4P-C4-C5-N
2	D	520	MC3	C1-O3P-P-O1P
2	D	520	MC3	C1-O3P-P-O4P
2	D	520	MC3	C4-O4P-P-O1P
2	D	520	MC3	C4-O4P-P-O2P
2	D	520	MC3	C4-O4P-P-O3P
2	E	502	MC3	C32-C31-O2-C2
2	E	502	MC3	C1-O3P-P-O1P
2	E	502	MC3	C1-O3P-P-O2P
2	E	502	MC3	C1-O3P-P-O4P
2	E	503	MC3	C1-O3P-P-O2P
2	E	503	MC3	C1-O3P-P-O4P
2	E	520	MC3	O4P-C4-C5-N
2	E	520	MC3	C1-O3P-P-O1P
2	E	520	MC3	C1-O3P-P-O4P
2	E	520	MC3	C4-O4P-P-O1P
2	E	520	MC3	C4-O4P-P-O2P
2	E	520	MC3	C4-O4P-P-O3P
2	F	501	MC3	O4P-C4-C5-N
2	F	501	MC3	C1-O3P-P-O1P
2	F	501	MC3	C1-O3P-P-O4P
2	F	501	MC3	C4-O4P-P-O1P
2	F	501	MC3	C4-O4P-P-O2P
2	F	501	MC3	C4-O4P-P-O3P
2	F	516	MC3	C32-C31-O2-C2
2	F	516	MC3	C1-O3P-P-O1P
2	F	516	MC3	C1-O3P-P-O2P
2	F	516	MC3	C1-O3P-P-O4P
2	F	517	MC3	C1-O3P-P-O2P
2	F	517	MC3	C1-O3P-P-O4P
2	G	502	MC3	C32-C31-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	G	502	MC3	C1-O3P-P-O1P
2	G	502	MC3	C1-O3P-P-O2P
2	G	502	MC3	C1-O3P-P-O4P
2	G	503	MC3	C1-O3P-P-O2P
2	G	503	MC3	C1-O3P-P-O4P
2	G	520	MC3	O4P-C4-C5-N
2	G	520	MC3	C1-O3P-P-O1P
2	G	520	MC3	C1-O3P-P-O4P
2	G	520	MC3	C4-O4P-P-O1P
2	G	520	MC3	C4-O4P-P-O2P
2	G	520	MC3	C4-O4P-P-O3P
2	H	502	MC3	C32-C31-O2-C2
2	H	502	MC3	C1-O3P-P-O1P
2	H	502	MC3	C1-O3P-P-O2P
2	H	502	MC3	C1-O3P-P-O4P
2	H	503	MC3	C1-O3P-P-O2P
2	H	503	MC3	C1-O3P-P-O4P
2	H	520	MC3	O4P-C4-C5-N
2	H	520	MC3	C1-O3P-P-O1P
2	H	520	MC3	C1-O3P-P-O4P
2	H	520	MC3	C4-O4P-P-O1P
2	H	520	MC3	C4-O4P-P-O2P
2	H	520	MC3	C4-O4P-P-O3P
2	I	502	MC3	C32-C31-O2-C2
2	I	502	MC3	C1-O3P-P-O1P
2	I	502	MC3	C1-O3P-P-O2P
2	I	502	MC3	C1-O3P-P-O4P
2	I	503	MC3	C1-O3P-P-O2P
2	I	503	MC3	C1-O3P-P-O4P
2	I	520	MC3	O4P-C4-C5-N
2	I	520	MC3	C1-O3P-P-O1P
2	I	520	MC3	C1-O3P-P-O4P
2	I	520	MC3	C4-O4P-P-O1P
2	I	520	MC3	C4-O4P-P-O2P
2	I	520	MC3	C4-O4P-P-O3P
2	J	502	MC3	C32-C31-O2-C2
2	J	502	MC3	C1-O3P-P-O1P
2	J	502	MC3	C1-O3P-P-O2P
2	J	502	MC3	C1-O3P-P-O4P
2	J	503	MC3	C1-O3P-P-O2P
2	J	503	MC3	C1-O3P-P-O4P
2	J	520	MC3	O4P-C4-C5-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	J	520	MC3	C1-O3P-P-O1P
2	J	520	MC3	C1-O3P-P-O4P
2	J	520	MC3	C4-O4P-P-O1P
2	J	520	MC3	C4-O4P-P-O2P
2	J	520	MC3	C4-O4P-P-O3P
2	K	502	MC3	C32-C31-O2-C2
2	K	502	MC3	C1-O3P-P-O1P
2	K	502	MC3	C1-O3P-P-O2P
2	K	502	MC3	C1-O3P-P-O4P
2	K	503	MC3	C1-O3P-P-O2P
2	K	503	MC3	C1-O3P-P-O4P
2	K	520	MC3	O4P-C4-C5-N
2	K	520	MC3	C1-O3P-P-O1P
2	K	520	MC3	C1-O3P-P-O4P
2	K	520	MC3	C4-O4P-P-O1P
2	K	520	MC3	C4-O4P-P-O2P
2	K	520	MC3	C4-O4P-P-O3P
2	L	501	MC3	O4P-C4-C5-N
2	L	501	MC3	C1-O3P-P-O1P
2	L	501	MC3	C1-O3P-P-O4P
2	L	501	MC3	C4-O4P-P-O1P
2	L	501	MC3	C4-O4P-P-O2P
2	L	501	MC3	C4-O4P-P-O3P
2	L	516	MC3	C32-C31-O2-C2
2	L	516	MC3	C1-O3P-P-O1P
2	L	516	MC3	C1-O3P-P-O2P
2	L	516	MC3	C1-O3P-P-O4P
2	L	517	MC3	C1-O3P-P-O2P
2	L	517	MC3	C1-O3P-P-O4P
2	A	520	MC3	O11-C11-O3-C3
2	B	520	MC3	O11-C11-O3-C3
2	C	520	MC3	O11-C11-O3-C3
2	D	520	MC3	O11-C11-O3-C3
2	E	520	MC3	O11-C11-O3-C3
2	F	501	MC3	O11-C11-O3-C3
2	G	520	MC3	O11-C11-O3-C3
2	H	520	MC3	O11-C11-O3-C3
2	I	520	MC3	O11-C11-O3-C3
2	J	520	MC3	O11-C11-O3-C3
2	K	520	MC3	O11-C11-O3-C3
2	L	501	MC3	O11-C11-O3-C3
2	A	520	MC3	C12-C11-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	520	MC3	C12-C11-O3-C3
2	C	520	MC3	C12-C11-O3-C3
2	D	520	MC3	C12-C11-O3-C3
2	E	520	MC3	C12-C11-O3-C3
2	F	501	MC3	C12-C11-O3-C3
2	G	520	MC3	C12-C11-O3-C3
2	H	520	MC3	C12-C11-O3-C3
2	I	520	MC3	C12-C11-O3-C3
2	J	520	MC3	C12-C11-O3-C3
2	K	520	MC3	C12-C11-O3-C3
2	L	501	MC3	C12-C11-O3-C3
2	A	502	MC3	O31-C31-O2-C2
2	B	502	MC3	O31-C31-O2-C2
2	C	502	MC3	O31-C31-O2-C2
2	D	502	MC3	O31-C31-O2-C2
2	E	502	MC3	O31-C31-O2-C2
2	F	516	MC3	O31-C31-O2-C2
2	G	502	MC3	O31-C31-O2-C2
2	H	502	MC3	O31-C31-O2-C2
2	I	502	MC3	O31-C31-O2-C2
2	J	502	MC3	O31-C31-O2-C2
2	K	502	MC3	O31-C31-O2-C2
2	L	516	MC3	O31-C31-O2-C2
2	A	503	MC3	C12-C11-O3-C3
2	B	503	MC3	C12-C11-O3-C3
2	C	503	MC3	C12-C11-O3-C3
2	D	503	MC3	C12-C11-O3-C3
2	E	503	MC3	C12-C11-O3-C3
2	F	517	MC3	C12-C11-O3-C3
2	G	503	MC3	C12-C11-O3-C3
2	H	503	MC3	C12-C11-O3-C3
2	I	503	MC3	C12-C11-O3-C3
2	J	503	MC3	C12-C11-O3-C3
2	K	503	MC3	C12-C11-O3-C3
2	L	517	MC3	C12-C11-O3-C3
2	A	503	MC3	C31-C32-C33-C34
2	B	503	MC3	C31-C32-C33-C34
2	C	503	MC3	C31-C32-C33-C34
2	D	503	MC3	C31-C32-C33-C34
2	E	503	MC3	C31-C32-C33-C34
2	F	517	MC3	C31-C32-C33-C34
2	G	503	MC3	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	503	MC3	C31-C32-C33-C34
2	I	503	MC3	C31-C32-C33-C34
2	J	503	MC3	C31-C32-C33-C34
2	K	503	MC3	C31-C32-C33-C34
2	L	517	MC3	C31-C32-C33-C34
2	A	503	MC3	O11-C11-O3-C3
2	B	503	MC3	O11-C11-O3-C3
2	C	503	MC3	O11-C11-O3-C3
2	D	503	MC3	O11-C11-O3-C3
2	E	503	MC3	O11-C11-O3-C3
2	F	517	MC3	O11-C11-O3-C3
2	G	503	MC3	O11-C11-O3-C3
2	H	503	MC3	O11-C11-O3-C3
2	I	503	MC3	O11-C11-O3-C3
2	J	503	MC3	O11-C11-O3-C3
2	K	503	MC3	O11-C11-O3-C3
2	L	517	MC3	O11-C11-O3-C3
2	A	502	MC3	C12-C11-O3-C3
2	B	502	MC3	C12-C11-O3-C3
2	C	502	MC3	C12-C11-O3-C3
2	D	502	MC3	C12-C11-O3-C3
2	E	502	MC3	C12-C11-O3-C3
2	F	516	MC3	C12-C11-O3-C3
2	G	502	MC3	C12-C11-O3-C3
2	H	502	MC3	C12-C11-O3-C3
2	I	502	MC3	C12-C11-O3-C3
2	J	502	MC3	C12-C11-O3-C3
2	K	502	MC3	C12-C11-O3-C3
2	L	516	MC3	C12-C11-O3-C3
2	A	520	MC3	C31-C32-C33-C34
2	B	520	MC3	C31-C32-C33-C34
2	C	520	MC3	C31-C32-C33-C34
2	D	520	MC3	C31-C32-C33-C34
2	E	520	MC3	C31-C32-C33-C34
2	F	501	MC3	C31-C32-C33-C34
2	G	520	MC3	C31-C32-C33-C34
2	H	520	MC3	C31-C32-C33-C34
2	I	520	MC3	C31-C32-C33-C34
2	J	520	MC3	C31-C32-C33-C34
2	K	520	MC3	C31-C32-C33-C34
2	L	501	MC3	C31-C32-C33-C34
2	A	502	MC3	O11-C11-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	502	MC3	O11-C11-O3-C3
2	C	502	MC3	O11-C11-O3-C3
2	D	502	MC3	O11-C11-O3-C3
2	E	502	MC3	O11-C11-O3-C3
2	F	516	MC3	O11-C11-O3-C3
2	G	502	MC3	O11-C11-O3-C3
2	H	502	MC3	O11-C11-O3-C3
2	I	502	MC3	O11-C11-O3-C3
2	J	502	MC3	O11-C11-O3-C3
2	K	502	MC3	O11-C11-O3-C3
2	L	516	MC3	O11-C11-O3-C3
2	A	517	MC3	C37-C38-C39-C40
2	B	517	MC3	C37-C38-C39-C40
2	C	517	MC3	C37-C38-C39-C40
2	D	517	MC3	C37-C38-C39-C40
2	E	517	MC3	C37-C38-C39-C40
2	F	531	MC3	C37-C38-C39-C40
2	G	517	MC3	C37-C38-C39-C40
2	H	517	MC3	C37-C38-C39-C40
2	I	517	MC3	C37-C38-C39-C40
2	J	517	MC3	C37-C38-C39-C40
2	K	517	MC3	C37-C38-C39-C40
2	L	531	MC3	C37-C38-C39-C40
2	A	501	MC3	C15-C16-C17-C18
2	D	501	MC3	C15-C16-C17-C18
2	G	501	MC3	C15-C16-C17-C18
2	H	501	MC3	C15-C16-C17-C18
2	K	501	MC3	C15-C16-C17-C18
2	L	515	MC3	C15-C16-C17-C18
2	C	501	MC3	C15-C16-C17-C18
2	F	515	MC3	C15-C16-C17-C18
2	I	501	MC3	C15-C16-C17-C18
2	J	501	MC3	C15-C16-C17-C18
2	B	501	MC3	C15-C16-C17-C18
2	E	501	MC3	C15-C16-C17-C18
2	A	520	MC3	C32-C31-O2-C2
2	B	520	MC3	C32-C31-O2-C2
2	C	520	MC3	C32-C31-O2-C2
2	D	520	MC3	C32-C31-O2-C2
2	E	520	MC3	C32-C31-O2-C2
2	F	501	MC3	C32-C31-O2-C2
2	G	520	MC3	C32-C31-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	520	MC3	C32-C31-O2-C2
2	I	520	MC3	C32-C31-O2-C2
2	J	520	MC3	C32-C31-O2-C2
2	K	520	MC3	C32-C31-O2-C2
2	L	501	MC3	C32-C31-O2-C2
2	B	502	MC3	C31-C32-C33-C34
2	E	502	MC3	C31-C32-C33-C34
2	J	502	MC3	C31-C32-C33-C34
2	L	516	MC3	C31-C32-C33-C34
2	A	502	MC3	C31-C32-C33-C34
2	C	502	MC3	C31-C32-C33-C34
2	D	502	MC3	C31-C32-C33-C34
2	F	516	MC3	C31-C32-C33-C34
2	G	502	MC3	C31-C32-C33-C34
2	H	502	MC3	C31-C32-C33-C34
2	I	502	MC3	C31-C32-C33-C34
2	K	502	MC3	C31-C32-C33-C34
2	J	502	MC3	C35-C36-C37-C38
2	A	502	MC3	C35-C36-C37-C38
2	D	502	MC3	C35-C36-C37-C38
2	E	502	MC3	C35-C36-C37-C38
2	F	516	MC3	C35-C36-C37-C38
2	G	502	MC3	C35-C36-C37-C38
2	H	502	MC3	C35-C36-C37-C38
2	L	516	MC3	C35-C36-C37-C38
2	B	502	MC3	C35-C36-C37-C38
2	C	502	MC3	C35-C36-C37-C38
2	I	502	MC3	C35-C36-C37-C38
2	K	502	MC3	C35-C36-C37-C38
2	A	520	MC3	O31-C31-O2-C2
2	B	520	MC3	O31-C31-O2-C2
2	C	520	MC3	O31-C31-O2-C2
2	D	520	MC3	O31-C31-O2-C2
2	F	501	MC3	O31-C31-O2-C2
2	G	520	MC3	O31-C31-O2-C2
2	H	520	MC3	O31-C31-O2-C2
2	I	520	MC3	O31-C31-O2-C2
2	J	520	MC3	O31-C31-O2-C2
2	K	520	MC3	O31-C31-O2-C2
2	L	501	MC3	O31-C31-O2-C2
2	E	520	MC3	O31-C31-O2-C2
2	A	502	MC3	O3P-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	502	MC3	O3P-C1-C2-C3
2	C	502	MC3	O3P-C1-C2-C3
2	D	502	MC3	O3P-C1-C2-C3
2	E	502	MC3	O3P-C1-C2-C3
2	F	516	MC3	O3P-C1-C2-C3
2	G	502	MC3	O3P-C1-C2-C3
2	H	502	MC3	O3P-C1-C2-C3
2	I	502	MC3	O3P-C1-C2-C3
2	J	502	MC3	O3P-C1-C2-C3
2	K	502	MC3	O3P-C1-C2-C3
2	L	516	MC3	O3P-C1-C2-C3
2	I	520	MC3	C12-C13-C14-C15
2	D	520	MC3	C12-C13-C14-C15
2	E	520	MC3	C12-C13-C14-C15
2	F	501	MC3	C12-C13-C14-C15
2	G	520	MC3	C12-C13-C14-C15
2	H	520	MC3	C12-C13-C14-C15
2	J	520	MC3	C12-C13-C14-C15
2	K	520	MC3	C12-C13-C14-C15
2	L	501	MC3	C12-C13-C14-C15
2	A	520	MC3	C12-C13-C14-C15
2	B	520	MC3	C12-C13-C14-C15
2	C	520	MC3	C12-C13-C14-C15
2	A	520	MC3	C1-C2-C3-O3
2	B	520	MC3	C1-C2-C3-O3
2	C	520	MC3	C1-C2-C3-O3
2	D	520	MC3	C1-C2-C3-O3
2	E	520	MC3	C1-C2-C3-O3
2	F	501	MC3	C1-C2-C3-O3
2	G	520	MC3	C1-C2-C3-O3
2	H	520	MC3	C1-C2-C3-O3
2	I	520	MC3	C1-C2-C3-O3
2	J	520	MC3	C1-C2-C3-O3
2	K	520	MC3	C1-C2-C3-O3
2	L	501	MC3	C1-C2-C3-O3
2	A	502	MC3	O3P-C1-C2-O2
2	B	502	MC3	O3P-C1-C2-O2
2	C	502	MC3	O3P-C1-C2-O2
2	D	502	MC3	O3P-C1-C2-O2
2	E	502	MC3	O3P-C1-C2-O2
2	F	516	MC3	O3P-C1-C2-O2
2	G	502	MC3	O3P-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	H	502	MC3	O3P-C1-C2-O2
2	I	502	MC3	O3P-C1-C2-O2
2	J	502	MC3	O3P-C1-C2-O2
2	K	502	MC3	O3P-C1-C2-O2
2	L	516	MC3	O3P-C1-C2-O2
2	D	517	MC3	C33-C34-C35-C36
2	H	517	MC3	C33-C34-C35-C36
2	J	517	MC3	C33-C34-C35-C36
2	B	517	MC3	C33-C34-C35-C36
2	C	517	MC3	C33-C34-C35-C36
2	F	531	MC3	C33-C34-C35-C36
2	G	517	MC3	C33-C34-C35-C36
2	I	517	MC3	C33-C34-C35-C36
2	K	517	MC3	C33-C34-C35-C36
2	L	531	MC3	C33-C34-C35-C36
2	A	517	MC3	C33-C34-C35-C36
2	E	517	MC3	C33-C34-C35-C36
2	A	520	MC3	O3P-C1-C2-O2
2	B	520	MC3	O3P-C1-C2-O2
2	C	520	MC3	O3P-C1-C2-O2
2	D	520	MC3	O3P-C1-C2-O2
2	E	520	MC3	O3P-C1-C2-O2
2	F	501	MC3	O3P-C1-C2-O2
2	G	520	MC3	O3P-C1-C2-O2
2	H	520	MC3	O3P-C1-C2-O2
2	I	520	MC3	O3P-C1-C2-O2
2	J	520	MC3	O3P-C1-C2-O2
2	K	520	MC3	O3P-C1-C2-O2
2	L	501	MC3	O3P-C1-C2-O2
2	A	520	MC3	O2-C2-C3-O3
2	B	520	MC3	O2-C2-C3-O3
2	C	520	MC3	O2-C2-C3-O3
2	D	520	MC3	O2-C2-C3-O3
2	E	520	MC3	O2-C2-C3-O3
2	F	501	MC3	O2-C2-C3-O3
2	G	520	MC3	O2-C2-C3-O3
2	H	520	MC3	O2-C2-C3-O3
2	I	520	MC3	O2-C2-C3-O3
2	J	520	MC3	O2-C2-C3-O3
2	K	520	MC3	O2-C2-C3-O3
2	L	501	MC3	O2-C2-C3-O3
2	C	502	MC3	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	502	MC3	C32-C33-C34-C35
2	G	502	MC3	C32-C33-C34-C35
2	A	502	MC3	C32-C33-C34-C35
2	B	502	MC3	C32-C33-C34-C35
2	E	502	MC3	C32-C33-C34-C35
2	F	516	MC3	C32-C33-C34-C35
2	J	502	MC3	C32-C33-C34-C35
2	K	502	MC3	C32-C33-C34-C35
2	L	516	MC3	C32-C33-C34-C35
2	H	502	MC3	C32-C33-C34-C35
2	I	502	MC3	C32-C33-C34-C35
2	A	520	MC3	O3P-C1-C2-C3
2	B	520	MC3	O3P-C1-C2-C3
2	C	520	MC3	O3P-C1-C2-C3
2	D	520	MC3	O3P-C1-C2-C3
2	E	520	MC3	O3P-C1-C2-C3
2	F	501	MC3	O3P-C1-C2-C3
2	G	520	MC3	O3P-C1-C2-C3
2	H	520	MC3	O3P-C1-C2-C3
2	I	520	MC3	O3P-C1-C2-C3
2	J	520	MC3	O3P-C1-C2-C3
2	K	520	MC3	O3P-C1-C2-C3
2	L	501	MC3	O3P-C1-C2-C3
2	A	520	MC3	C4-C5-N-C7
2	A	520	MC3	C1-O3P-P-O2P
2	B	520	MC3	C4-C5-N-C7
2	B	520	MC3	C1-O3P-P-O2P
2	C	520	MC3	C4-C5-N-C7
2	C	520	MC3	C1-O3P-P-O2P
2	D	520	MC3	C4-C5-N-C7
2	D	520	MC3	C1-O3P-P-O2P
2	E	520	MC3	C4-C5-N-C7
2	E	520	MC3	C1-O3P-P-O2P
2	F	501	MC3	C4-C5-N-C7
2	F	501	MC3	C1-O3P-P-O2P
2	G	520	MC3	C4-C5-N-C7
2	G	520	MC3	C1-O3P-P-O2P
2	H	520	MC3	C4-C5-N-C7
2	H	520	MC3	C1-O3P-P-O2P
2	I	520	MC3	C4-C5-N-C7
2	I	520	MC3	C1-O3P-P-O2P
2	J	520	MC3	C4-C5-N-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	J	520	MC3	C1-O3P-P-O2P
2	K	520	MC3	C4-C5-N-C7
2	K	520	MC3	C1-O3P-P-O2P
2	L	501	MC3	C4-C5-N-C7
2	L	501	MC3	C1-O3P-P-O2P
2	A	503	MC3	C1-O3P-P-O1P
2	B	503	MC3	C1-O3P-P-O1P
2	C	503	MC3	C1-O3P-P-O1P
2	D	503	MC3	C1-O3P-P-O1P
2	E	503	MC3	C1-O3P-P-O1P
2	F	517	MC3	C1-O3P-P-O1P
2	G	503	MC3	C1-O3P-P-O1P
2	H	503	MC3	C1-O3P-P-O1P
2	I	503	MC3	C1-O3P-P-O1P
2	J	503	MC3	C1-O3P-P-O1P
2	K	503	MC3	C1-O3P-P-O1P
2	L	517	MC3	C1-O3P-P-O1P
2	C	520	MC3	C32-C33-C34-C35
2	G	520	MC3	C32-C33-C34-C35
2	B	520	MC3	C32-C33-C34-C35
2	D	520	MC3	C32-C33-C34-C35
2	E	520	MC3	C32-C33-C34-C35
2	F	501	MC3	C32-C33-C34-C35
2	H	520	MC3	C32-C33-C34-C35
2	I	520	MC3	C32-C33-C34-C35
2	K	520	MC3	C32-C33-C34-C35
2	L	501	MC3	C32-C33-C34-C35
2	A	520	MC3	C32-C33-C34-C35
2	J	520	MC3	C32-C33-C34-C35
2	A	503	MC3	C1-C2-C3-O3
2	B	503	MC3	C1-C2-C3-O3
2	C	503	MC3	C1-C2-C3-O3
2	D	503	MC3	C1-C2-C3-O3
2	E	503	MC3	C1-C2-C3-O3
2	F	517	MC3	C1-C2-C3-O3
2	G	503	MC3	C1-C2-C3-O3
2	H	503	MC3	C1-C2-C3-O3
2	I	503	MC3	C1-C2-C3-O3
2	J	503	MC3	C1-C2-C3-O3
2	K	503	MC3	C1-C2-C3-O3
2	L	517	MC3	C1-C2-C3-O3
2	C	502	MC3	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	J	502	MC3	C13-C14-C15-C16
2	D	502	MC3	C13-C14-C15-C16
2	E	502	MC3	C13-C14-C15-C16
2	G	502	MC3	C13-C14-C15-C16
2	H	502	MC3	C13-C14-C15-C16
2	A	502	MC3	C13-C14-C15-C16
2	L	516	MC3	C13-C14-C15-C16
2	B	502	MC3	C13-C14-C15-C16
2	F	516	MC3	C13-C14-C15-C16
2	I	502	MC3	C13-C14-C15-C16
2	K	502	MC3	C13-C14-C15-C16
2	A	514	MC3	C32-C33-C34-C35
2	B	514	MC3	C32-C33-C34-C35
2	C	514	MC3	C32-C33-C34-C35
2	D	514	MC3	C32-C33-C34-C35
2	E	514	MC3	C32-C33-C34-C35
2	F	528	MC3	C32-C33-C34-C35
2	G	514	MC3	C32-C33-C34-C35
2	H	514	MC3	C32-C33-C34-C35
2	I	514	MC3	C32-C33-C34-C35
2	J	514	MC3	C32-C33-C34-C35
2	K	514	MC3	C32-C33-C34-C35
2	L	528	MC3	C32-C33-C34-C35
2	A	520	MC3	C4-C5-N-C6
2	B	520	MC3	C4-C5-N-C6
2	C	520	MC3	C4-C5-N-C6
2	D	520	MC3	C4-C5-N-C6
2	E	520	MC3	C4-C5-N-C6
2	F	501	MC3	C4-C5-N-C6
2	G	520	MC3	C4-C5-N-C6
2	H	520	MC3	C4-C5-N-C6
2	I	520	MC3	C4-C5-N-C6
2	J	520	MC3	C4-C5-N-C6
2	K	520	MC3	C4-C5-N-C6
2	L	501	MC3	C4-C5-N-C6

There are no ring outliers.

12 monomers are involved in 48 short contacts:

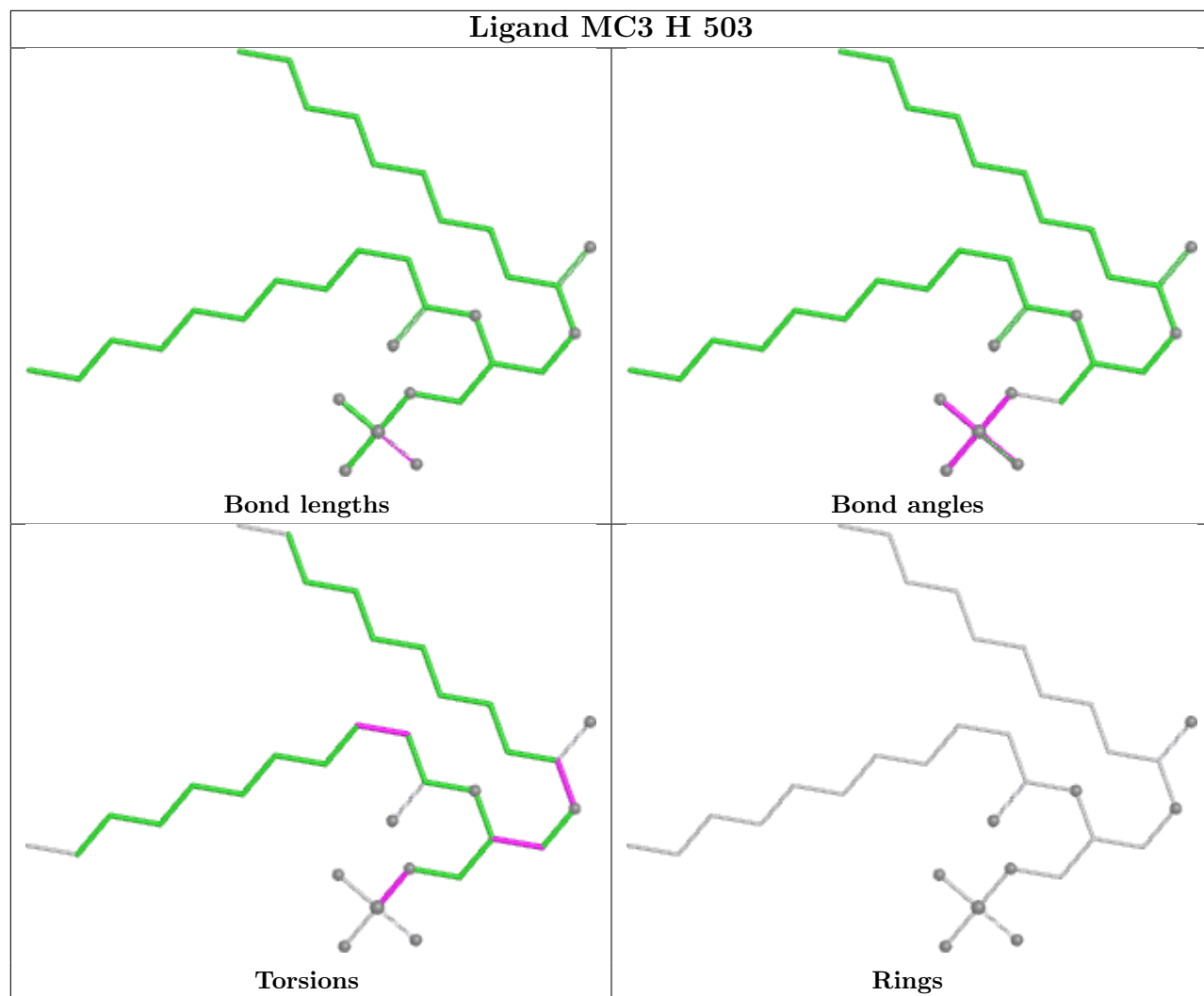
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	520	MC3	7	0
2	J	520	MC3	7	0

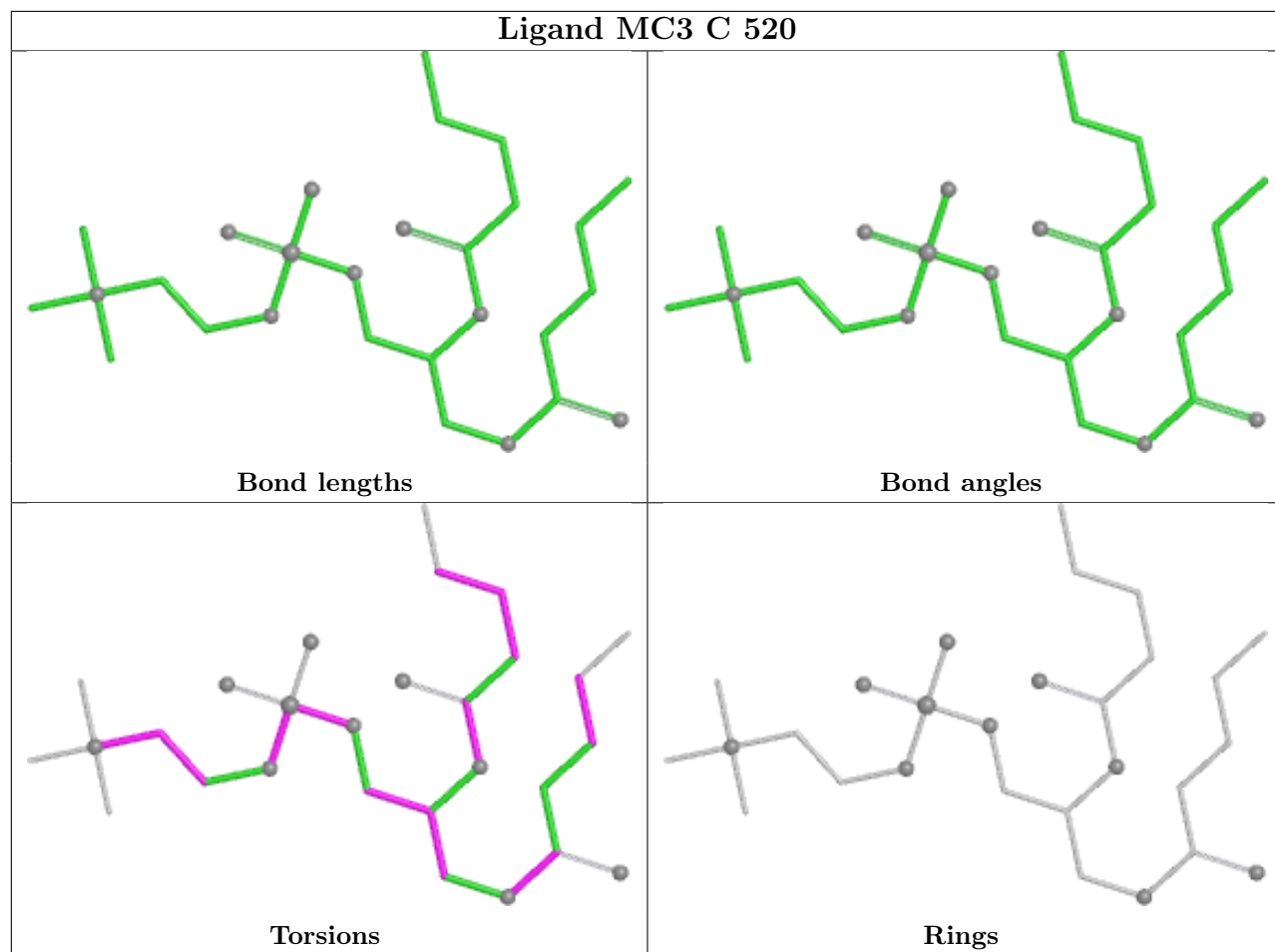
Continued on next page...

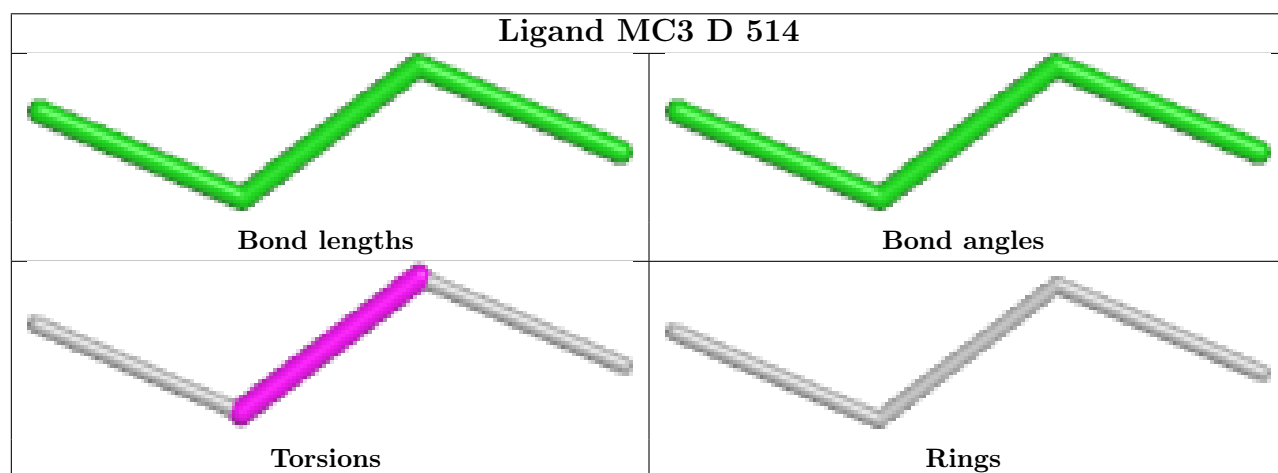
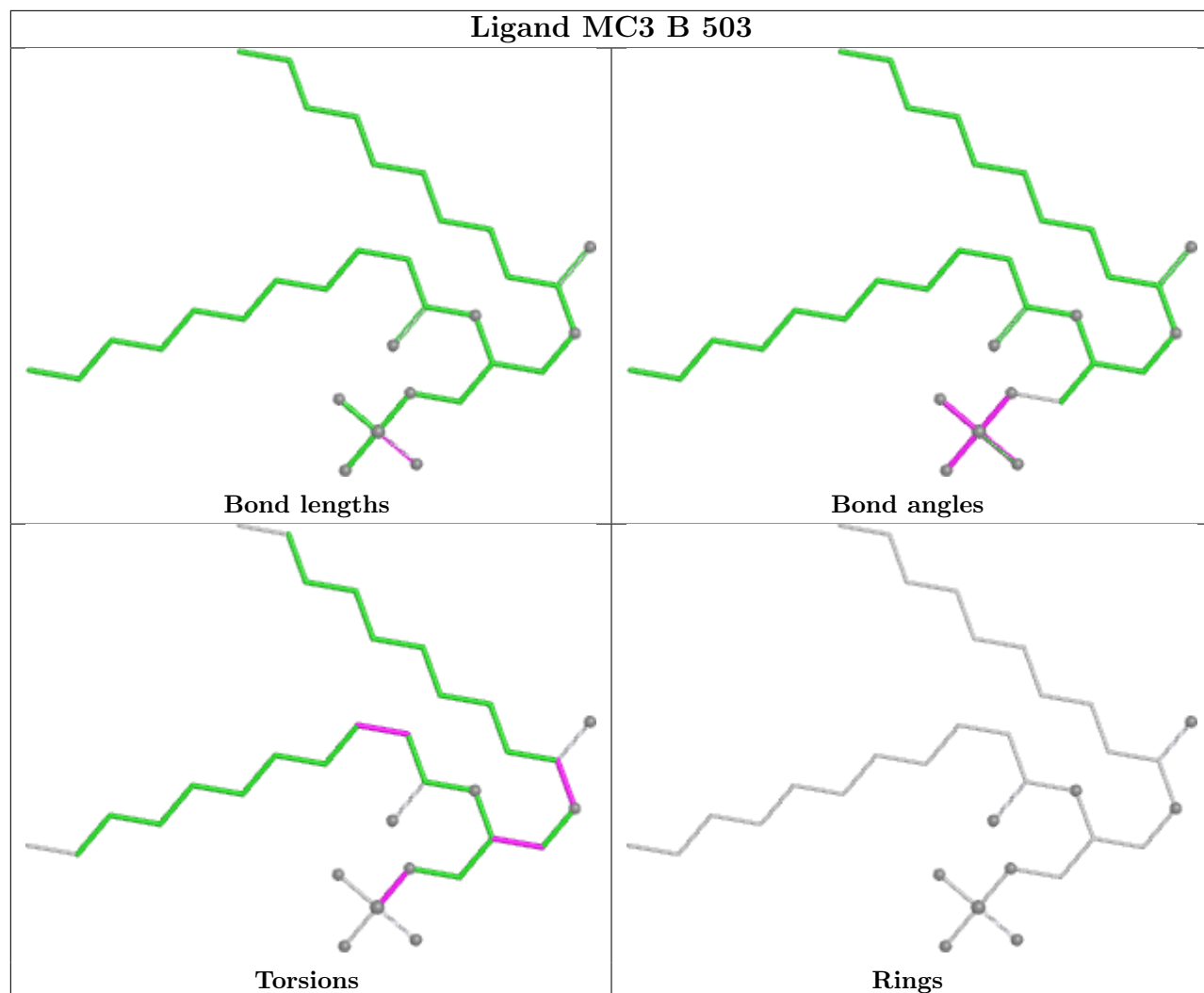
Continued from previous page...

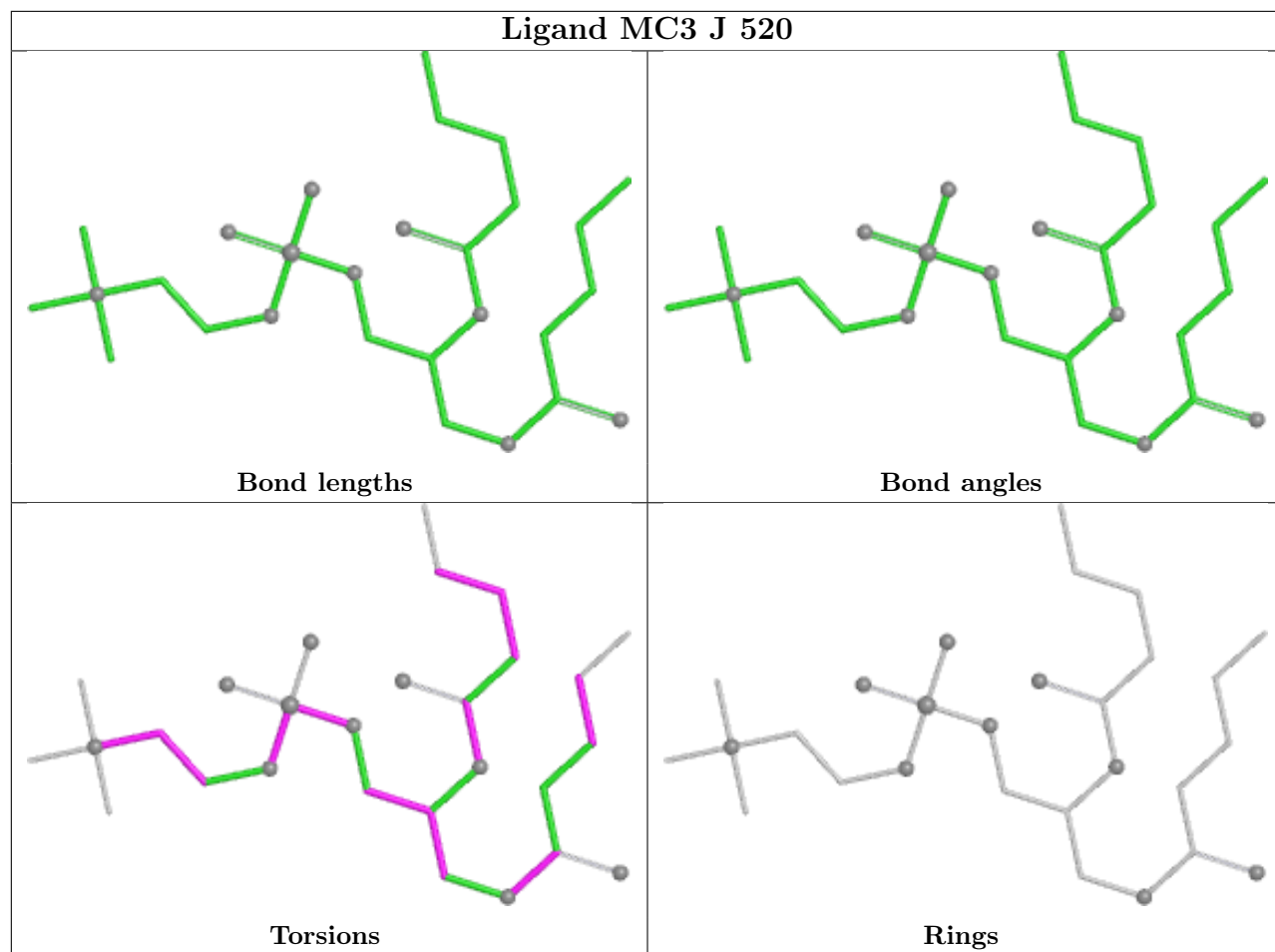
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	520	MC3	7	0
2	L	501	MC3	7	0
2	B	520	MC3	8	0
2	D	520	MC3	7	0
2	F	501	MC3	7	0
2	A	520	MC3	6	0
2	G	520	MC3	6	0
2	I	520	MC3	7	0
2	E	520	MC3	6	0
2	K	520	MC3	7	0

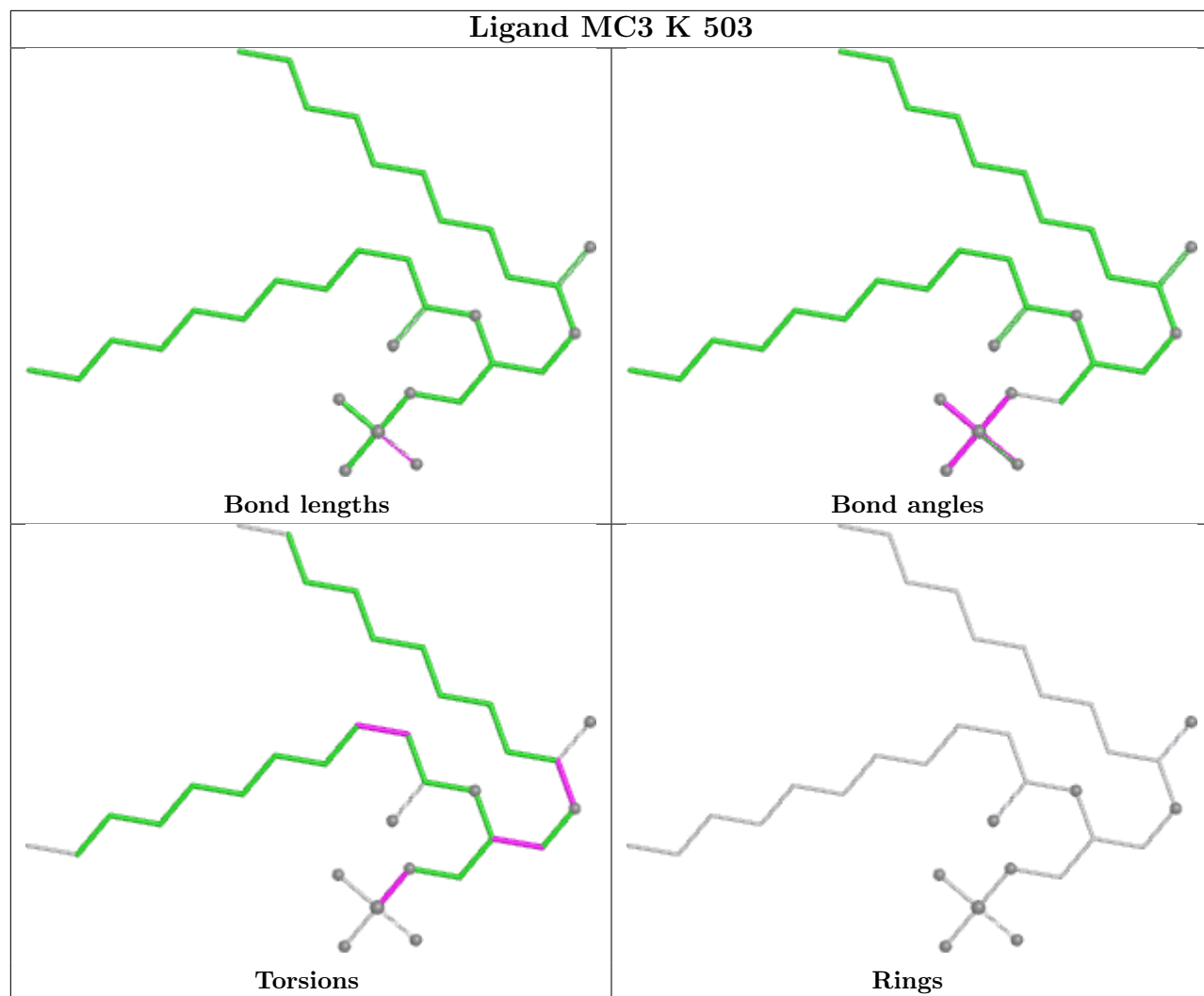
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

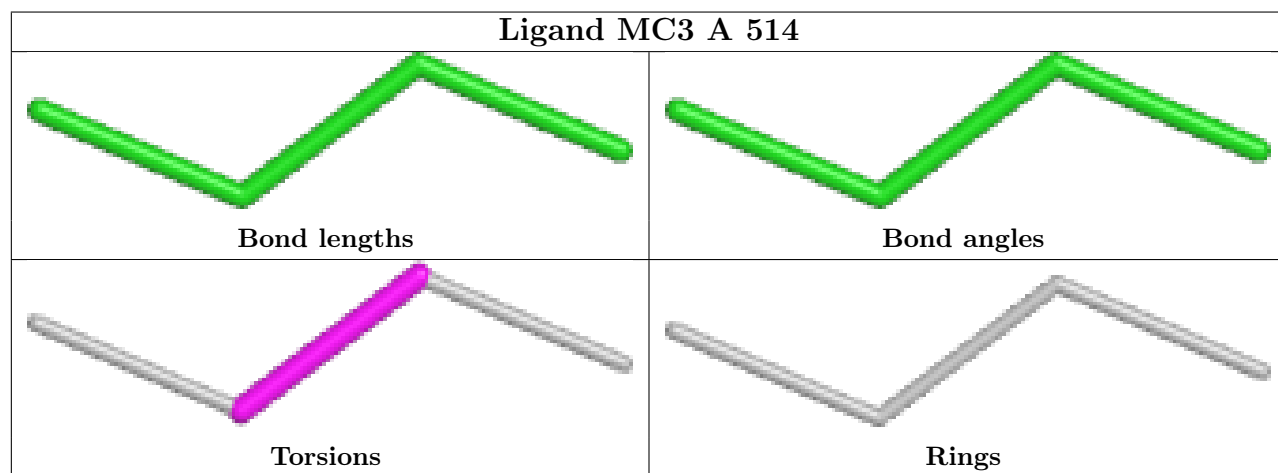
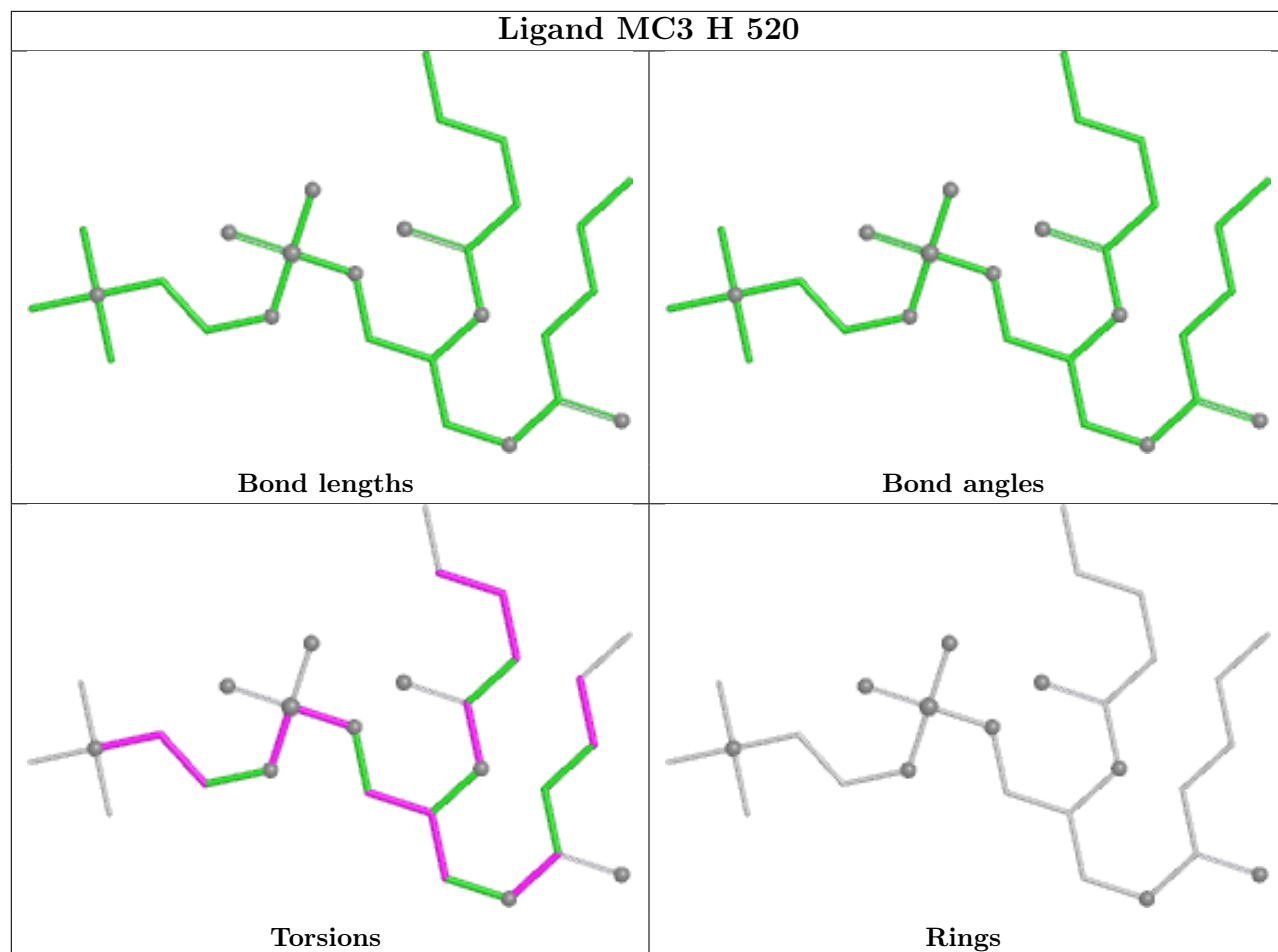


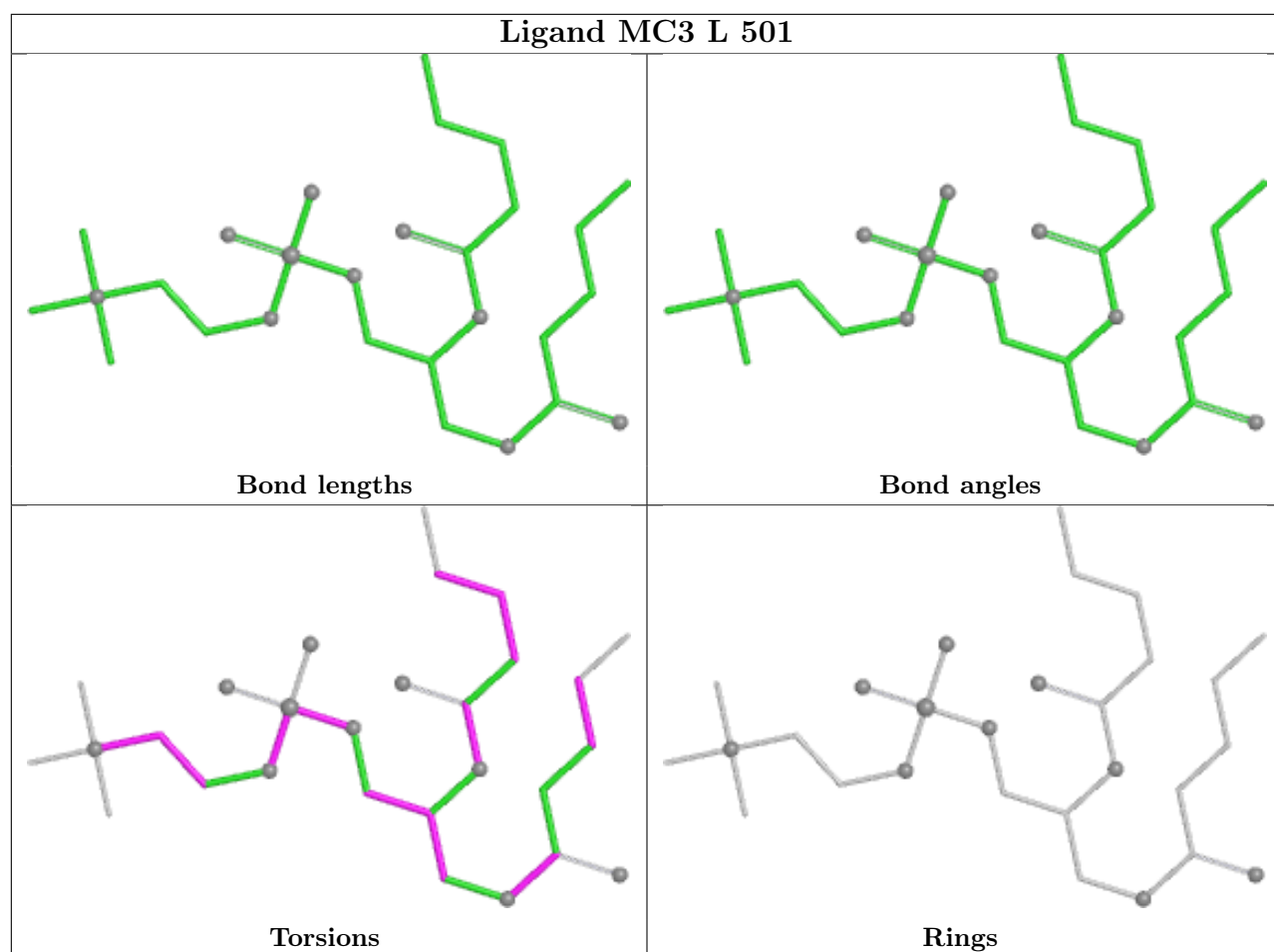


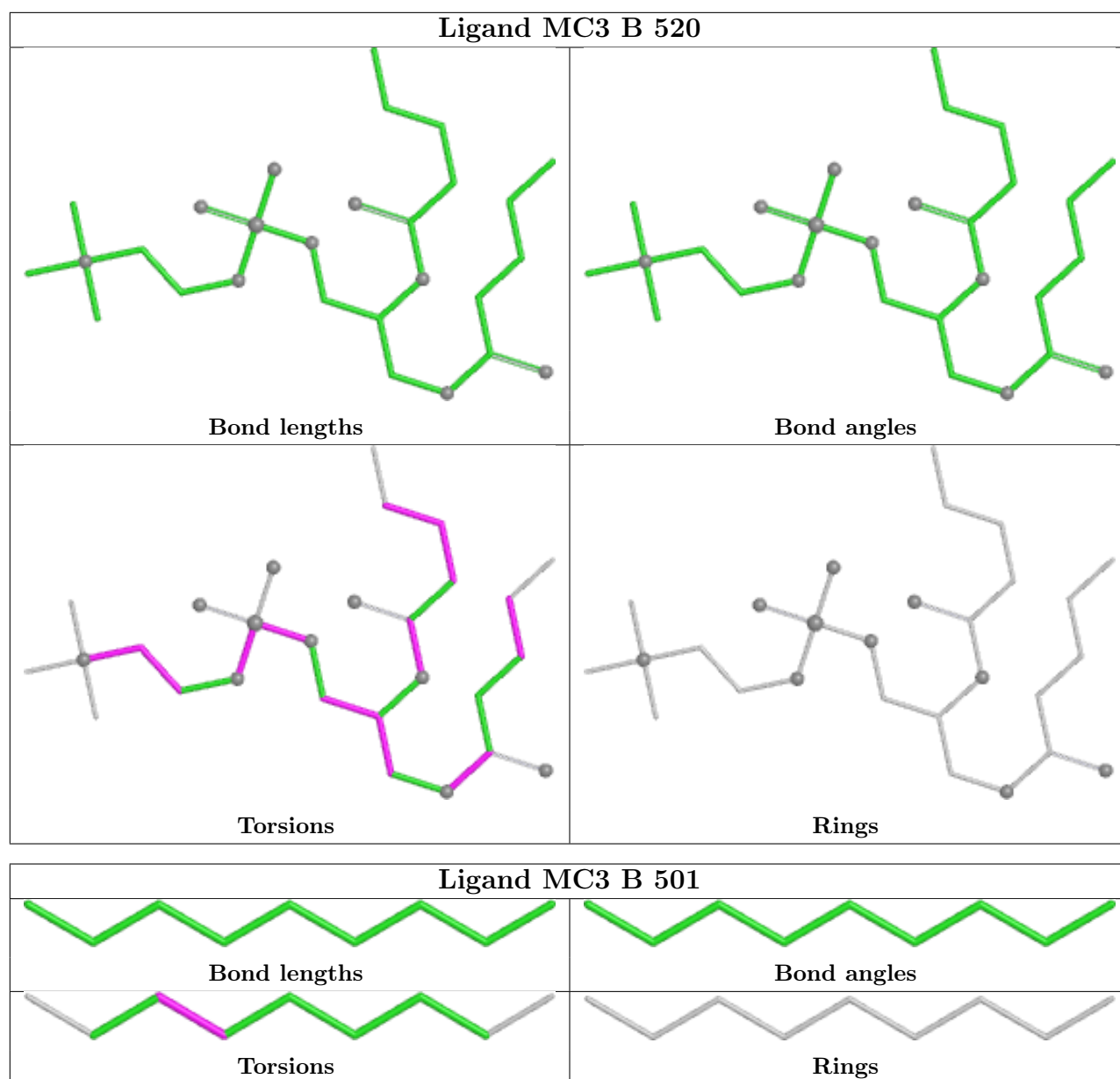


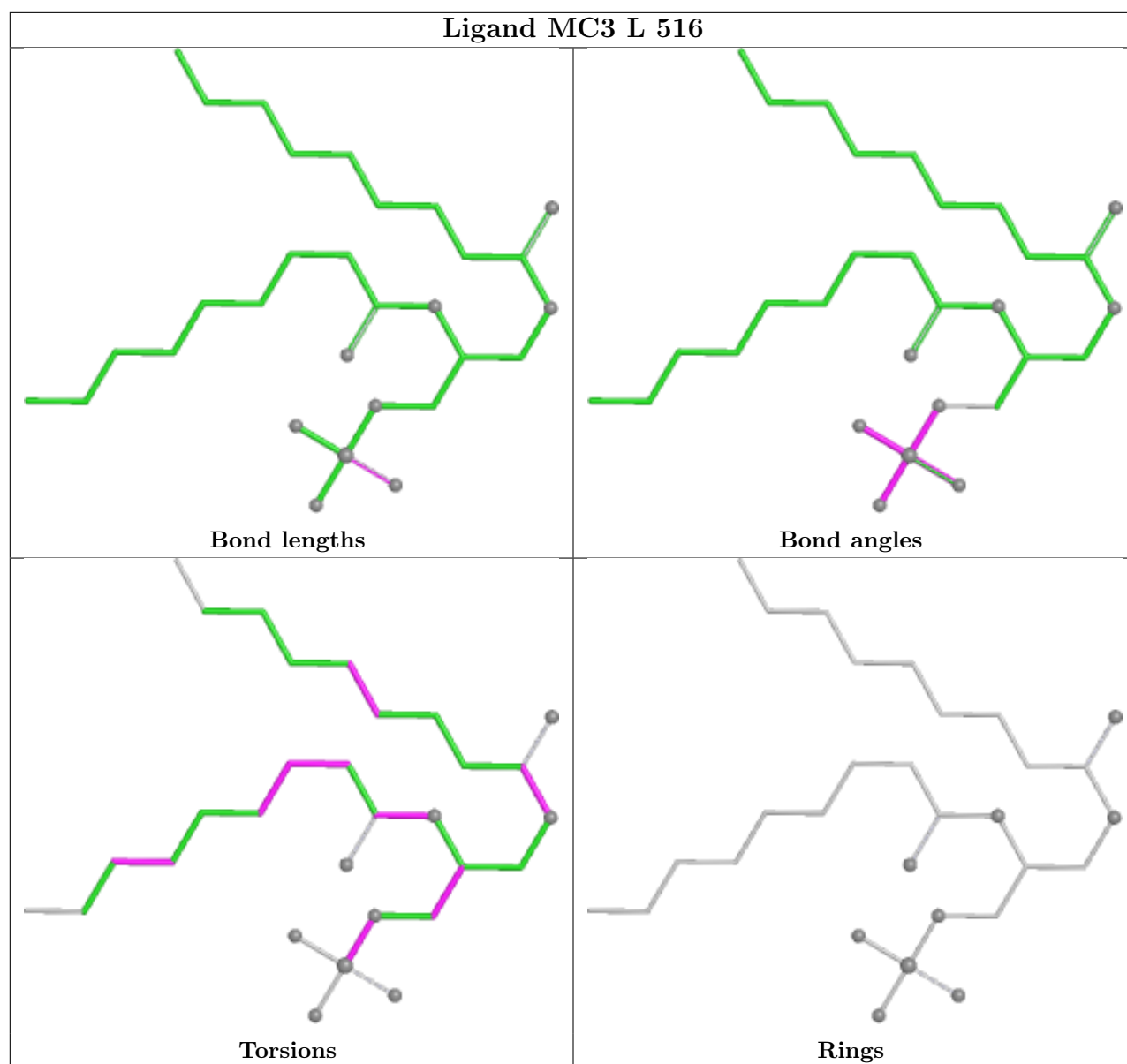


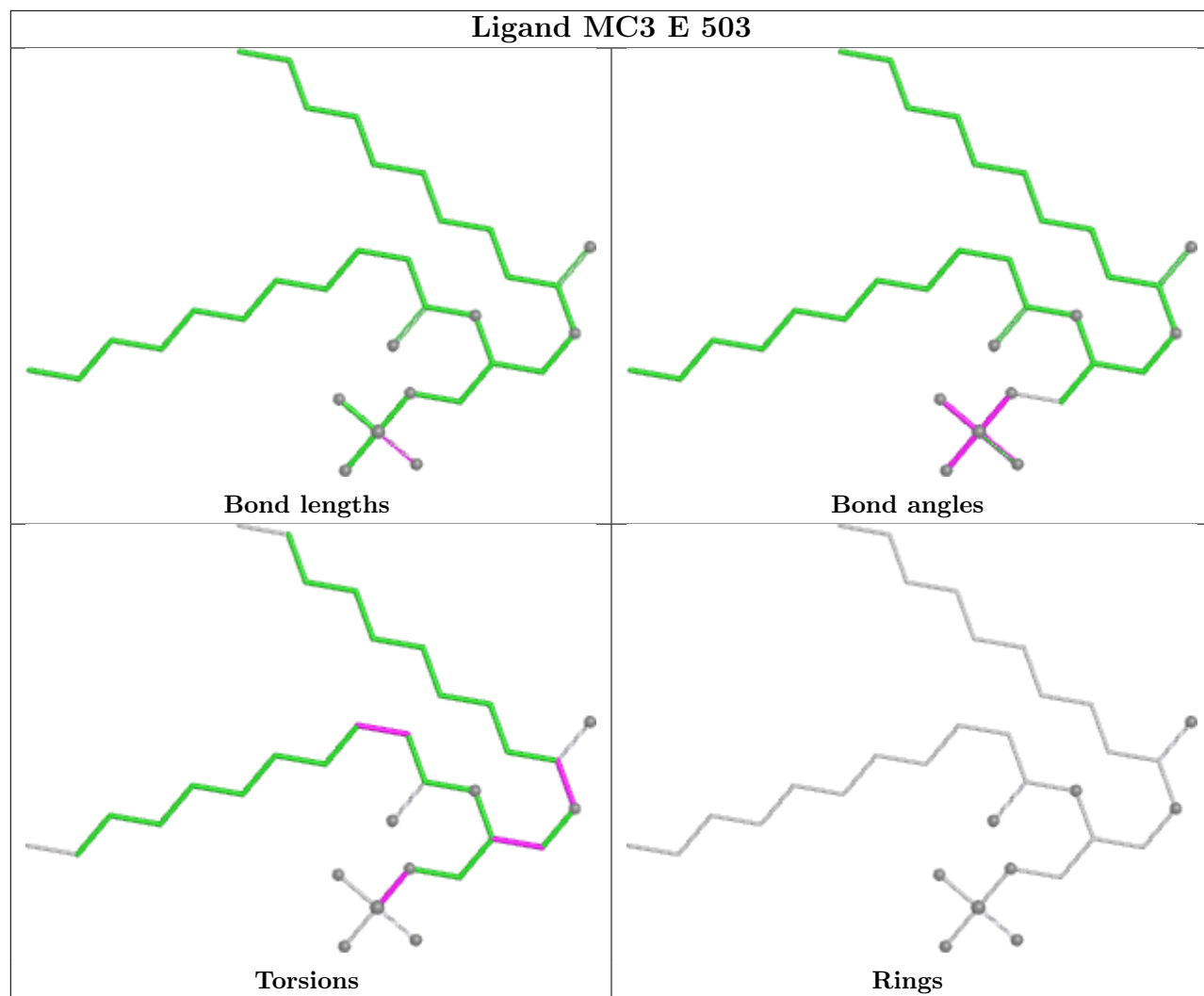


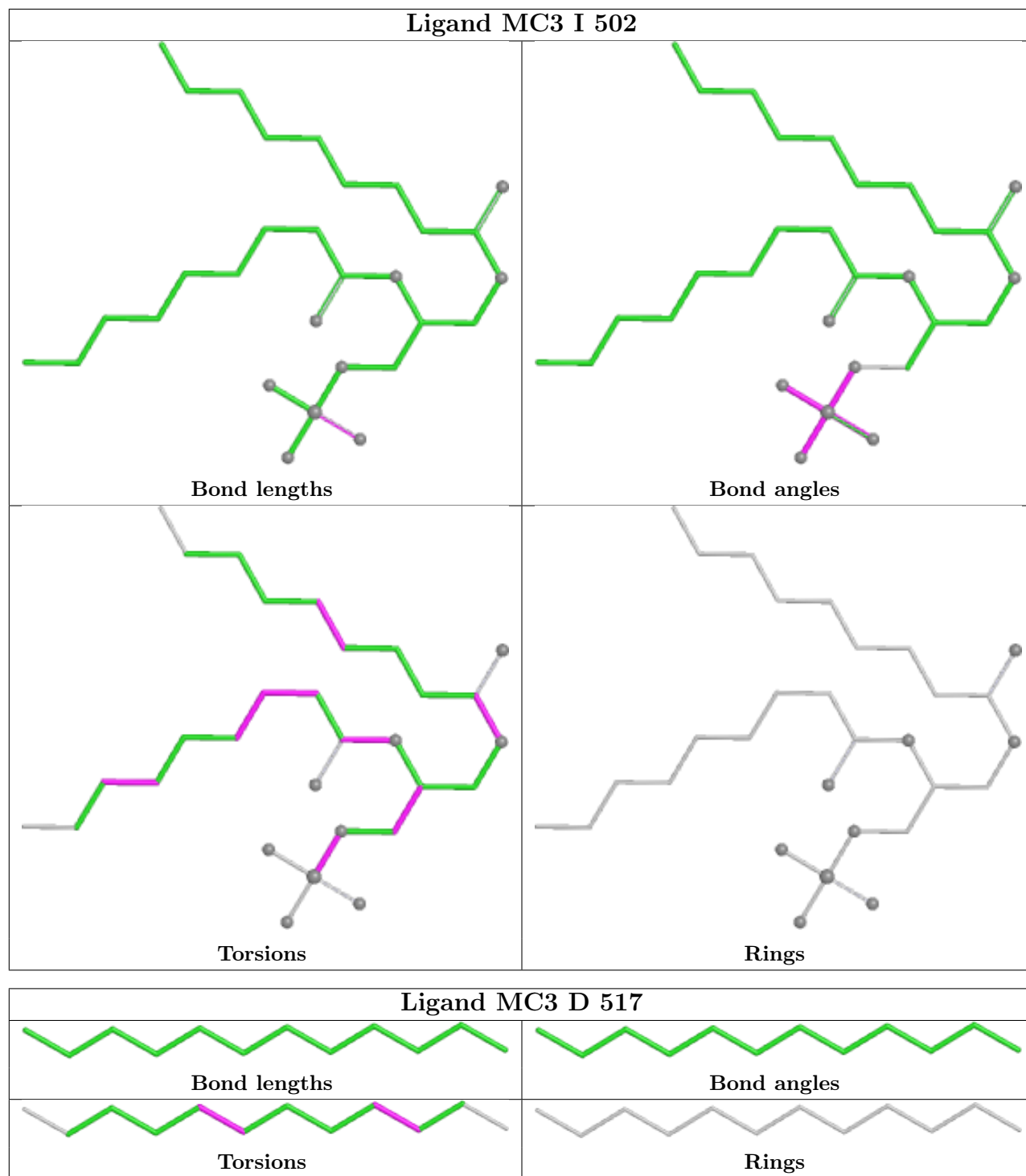


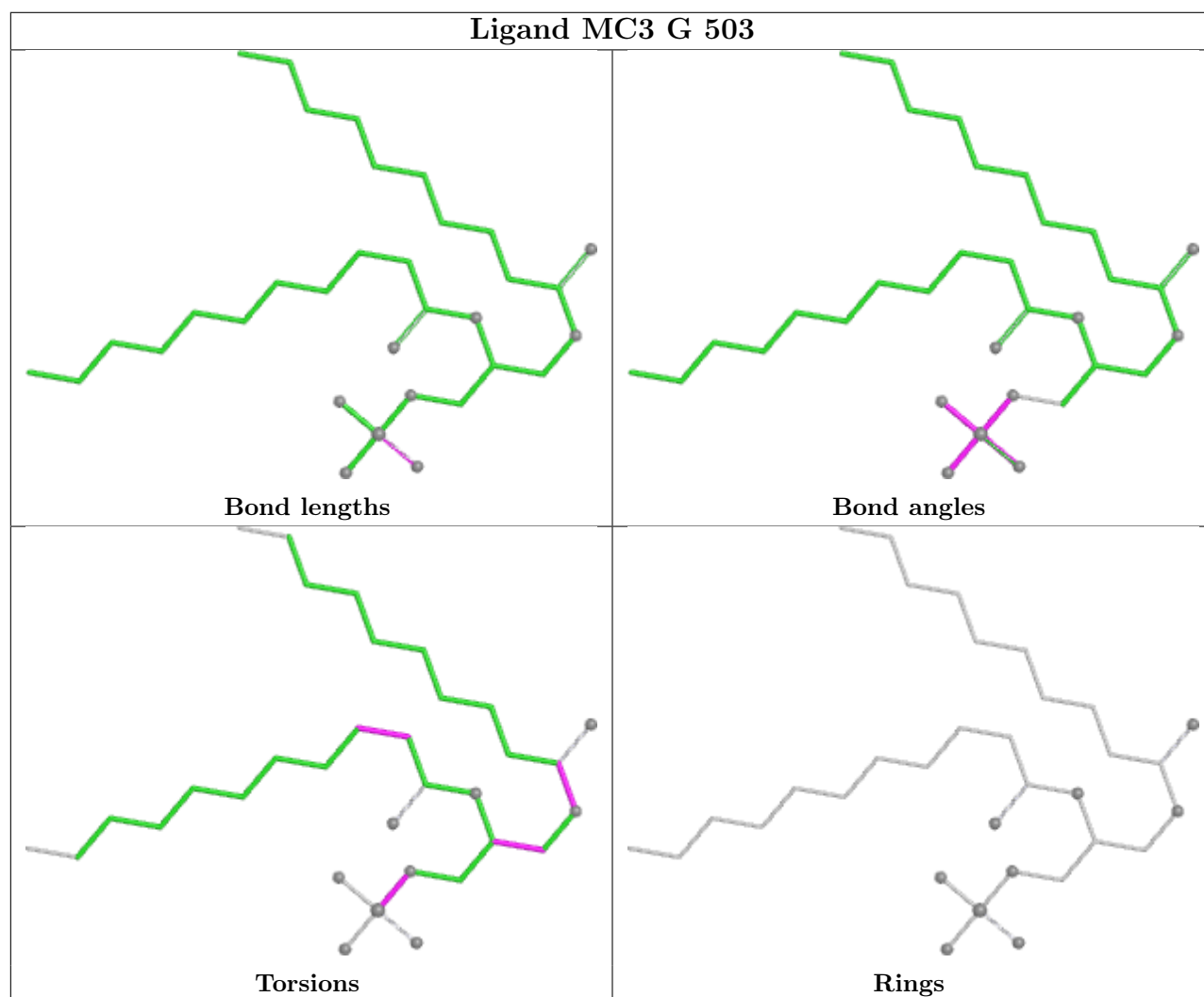
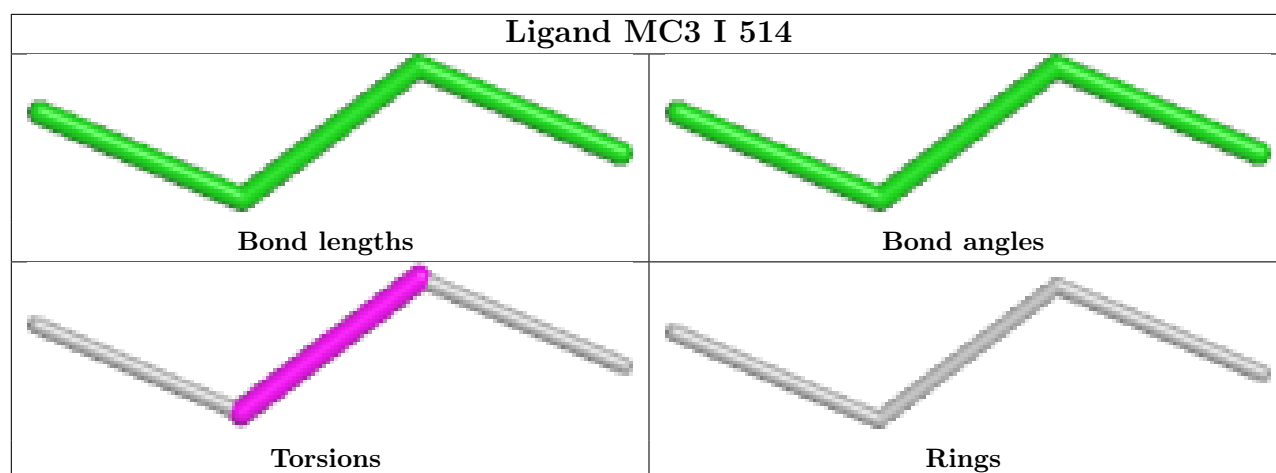


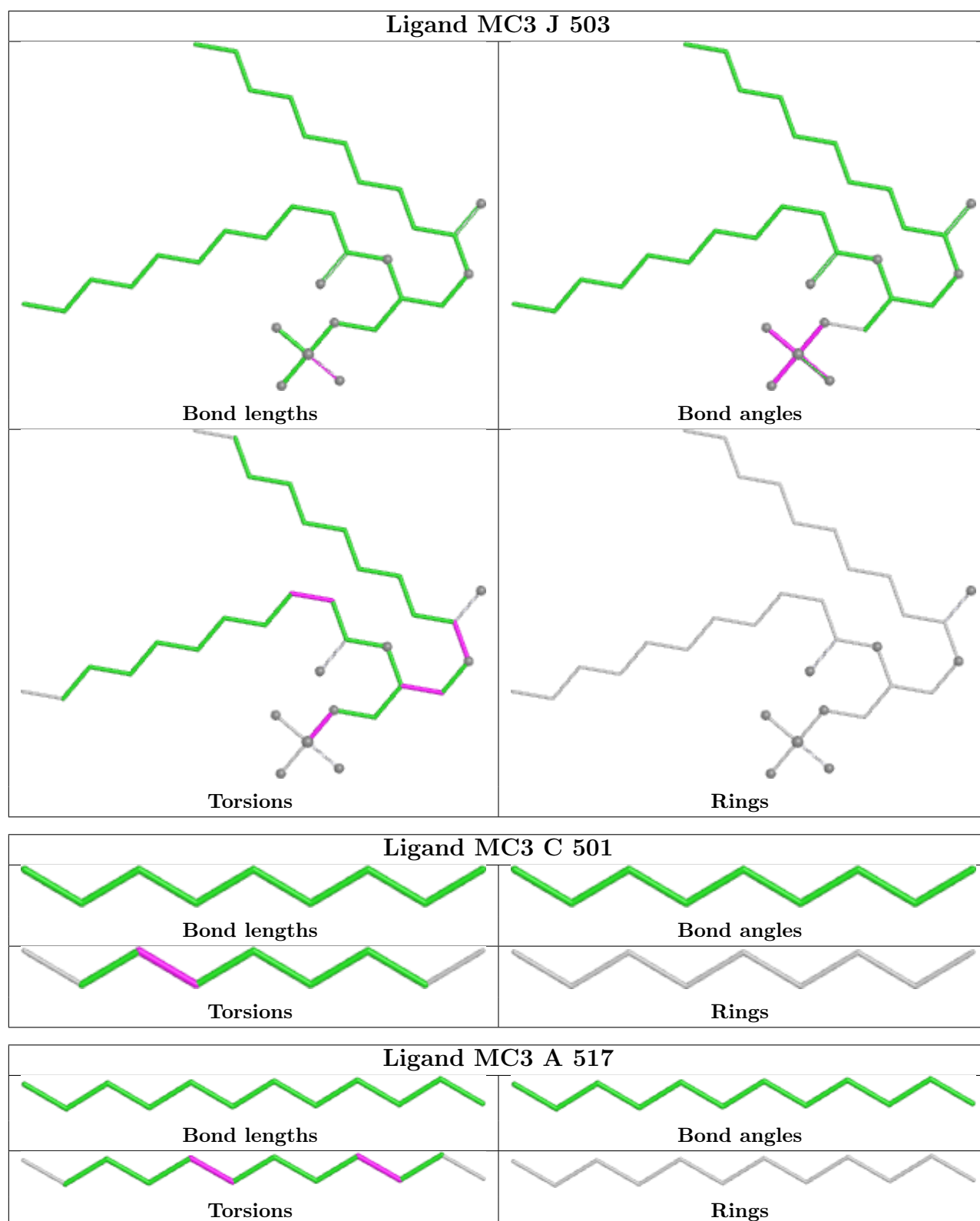


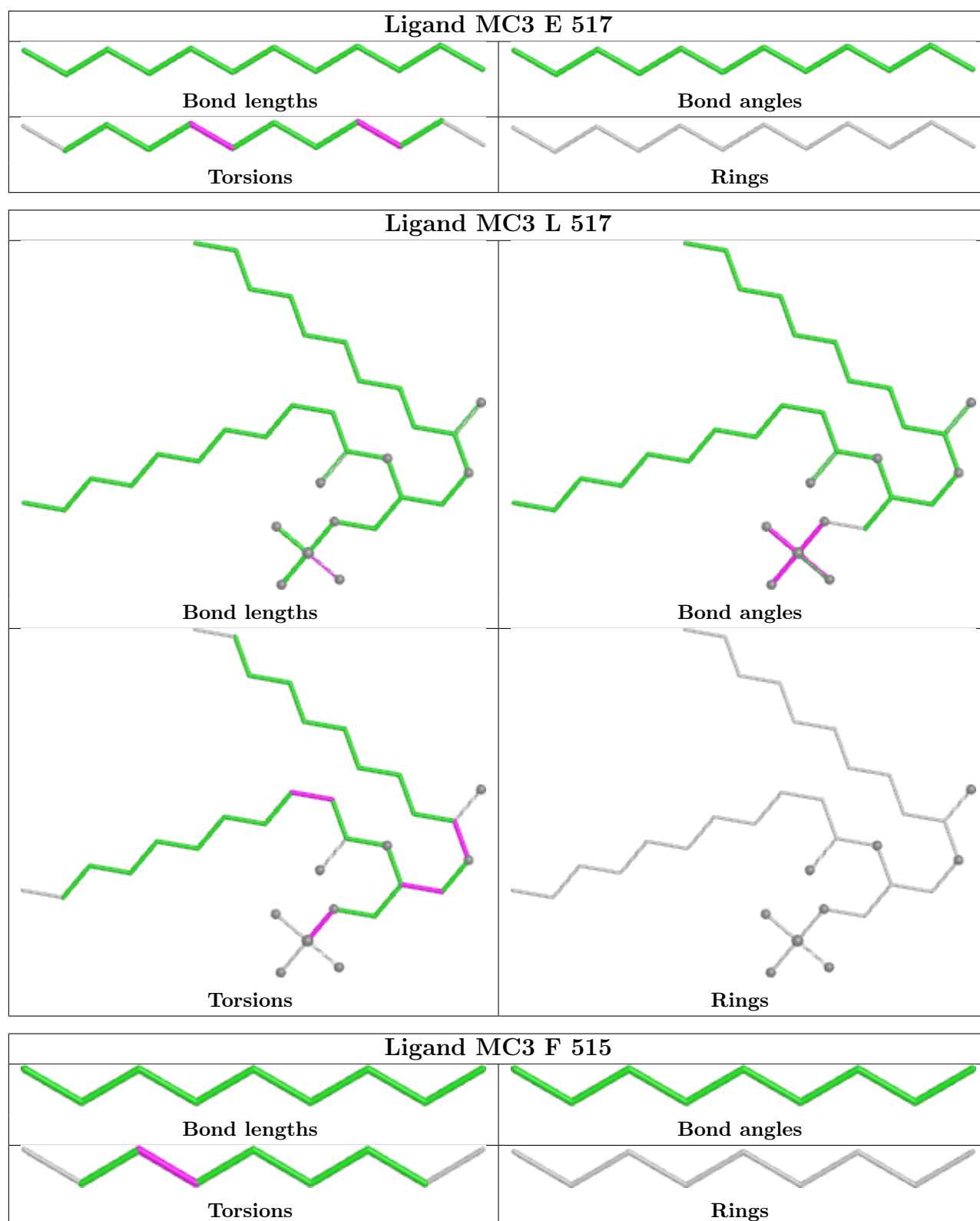


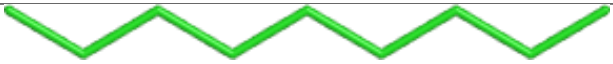
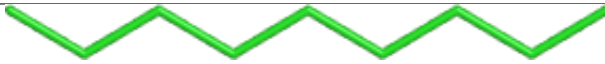
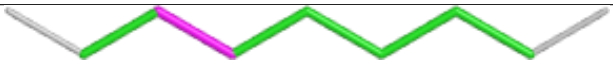








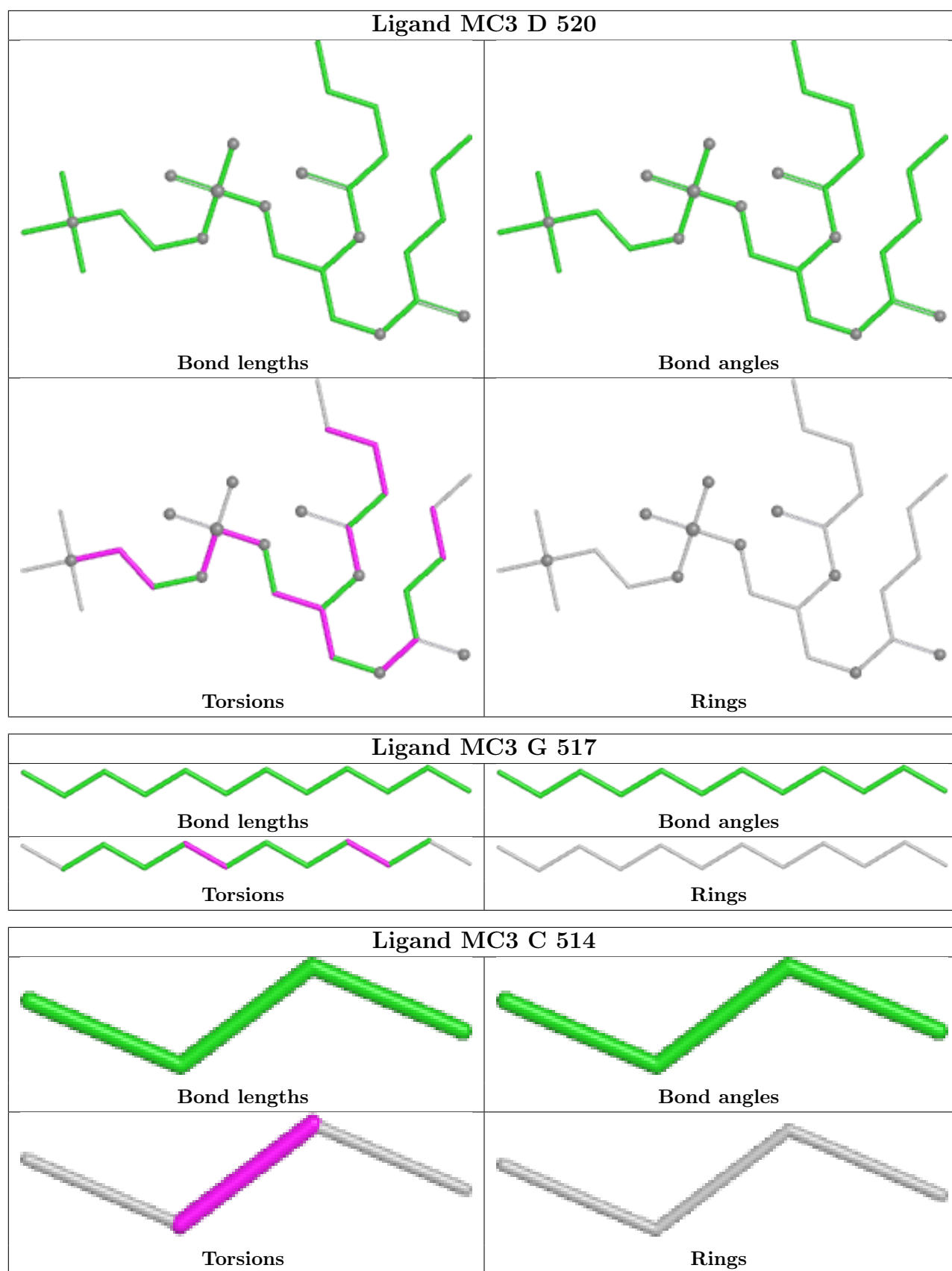


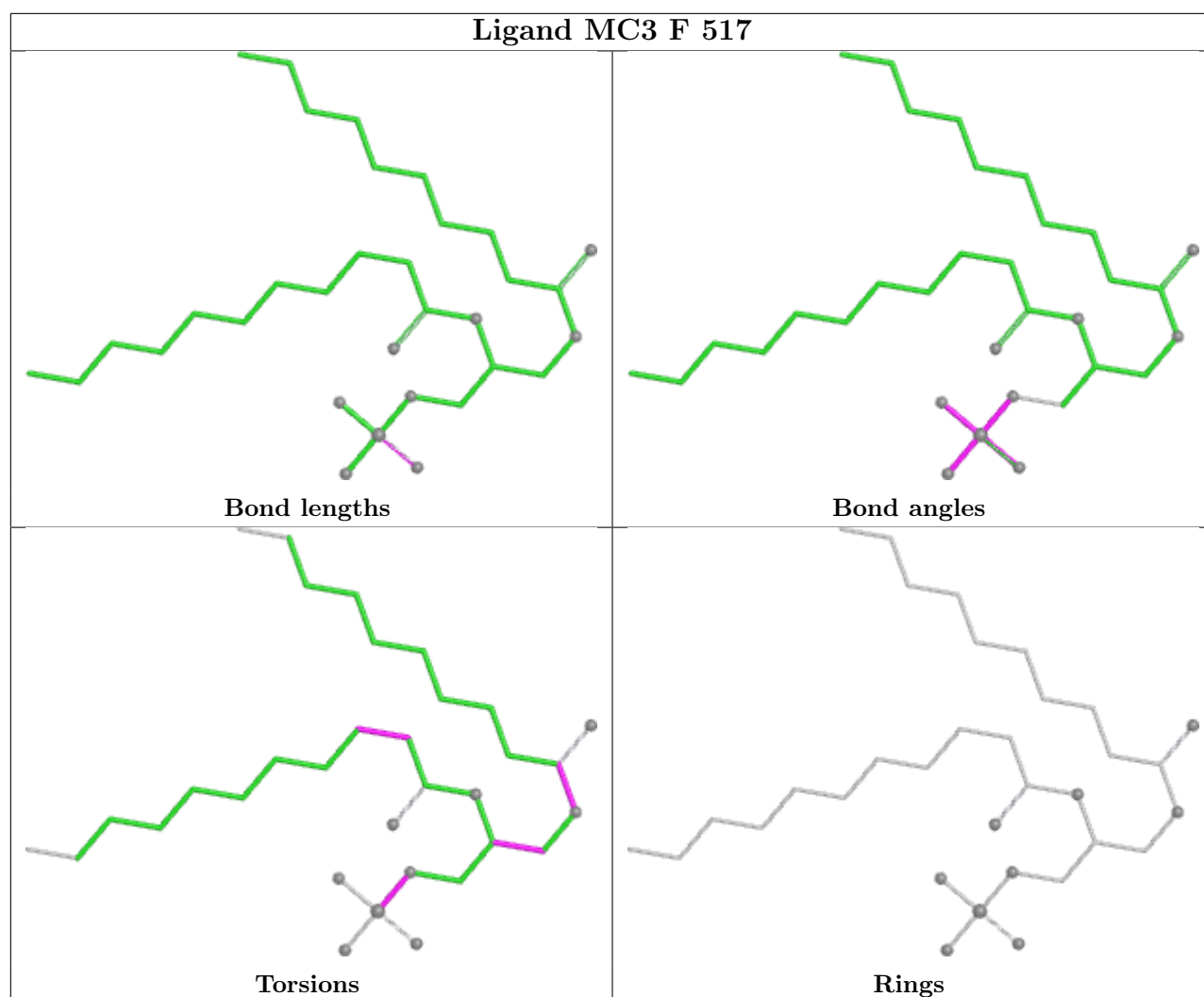
Ligand MC3 D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

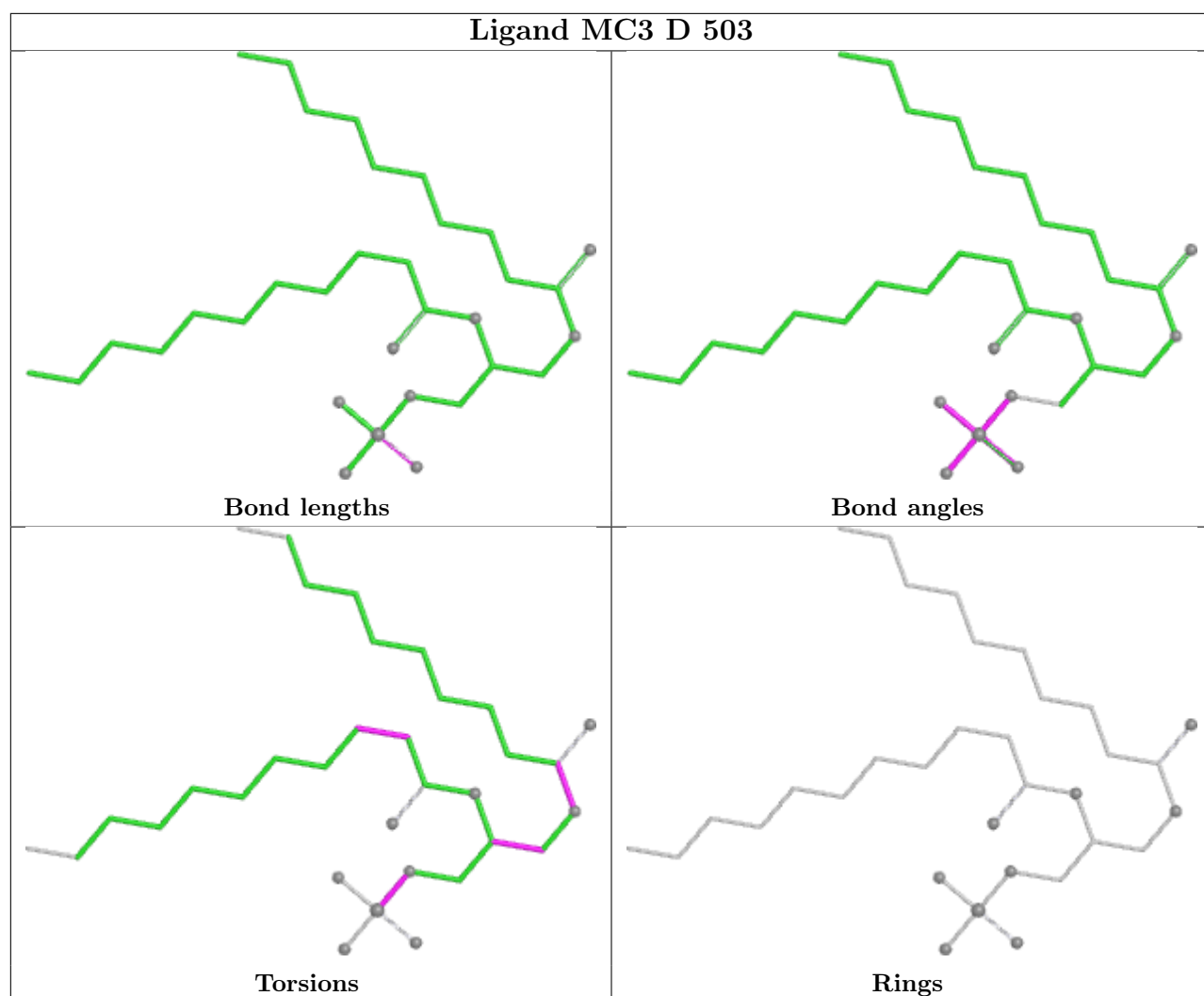
Ligand MC3 K 517	
 Bond lengths	 Bond angles
 Torsions	 Rings

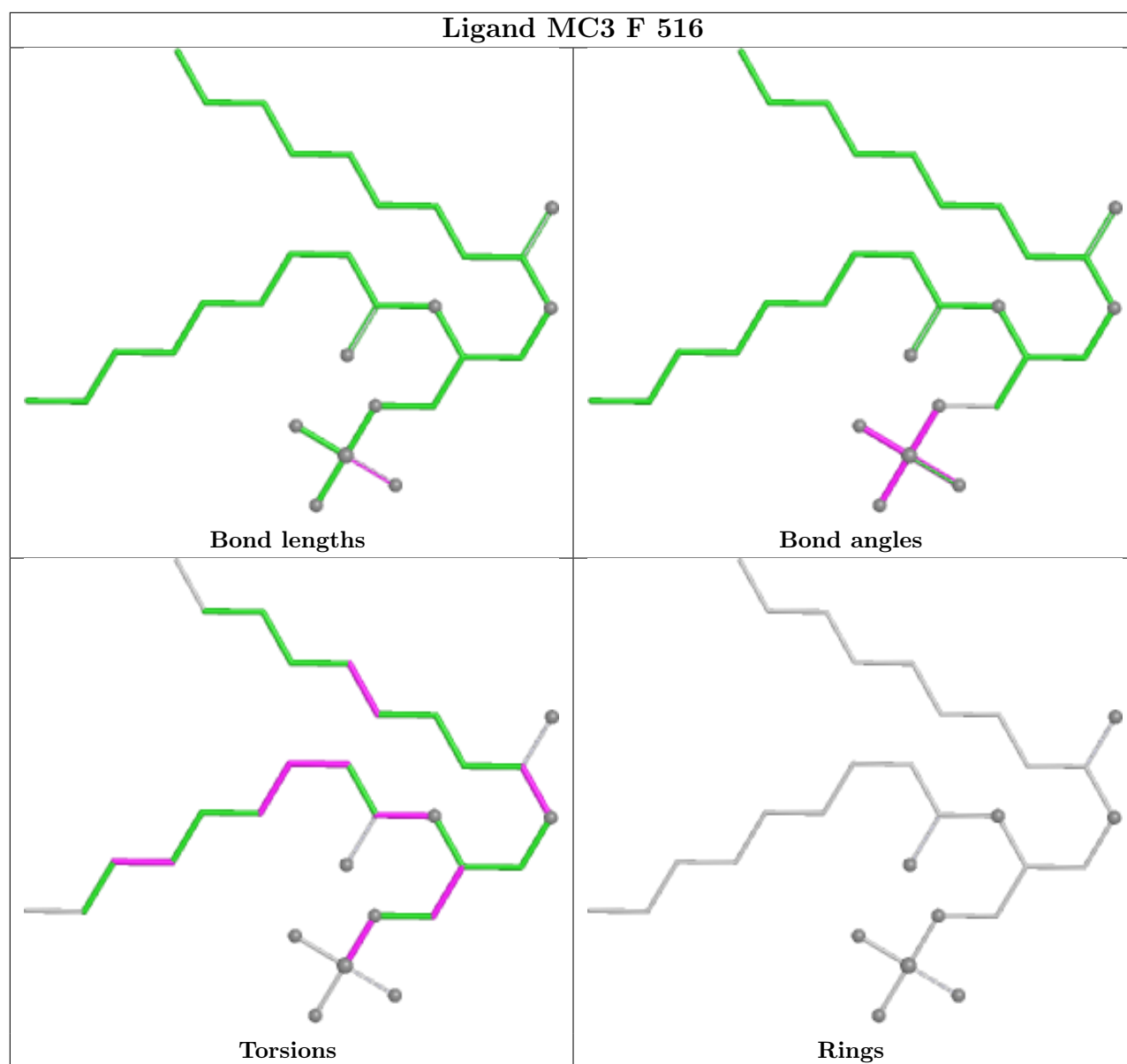
Ligand MC3 F 531	
 Bond lengths	 Bond angles
 Torsions	 Rings

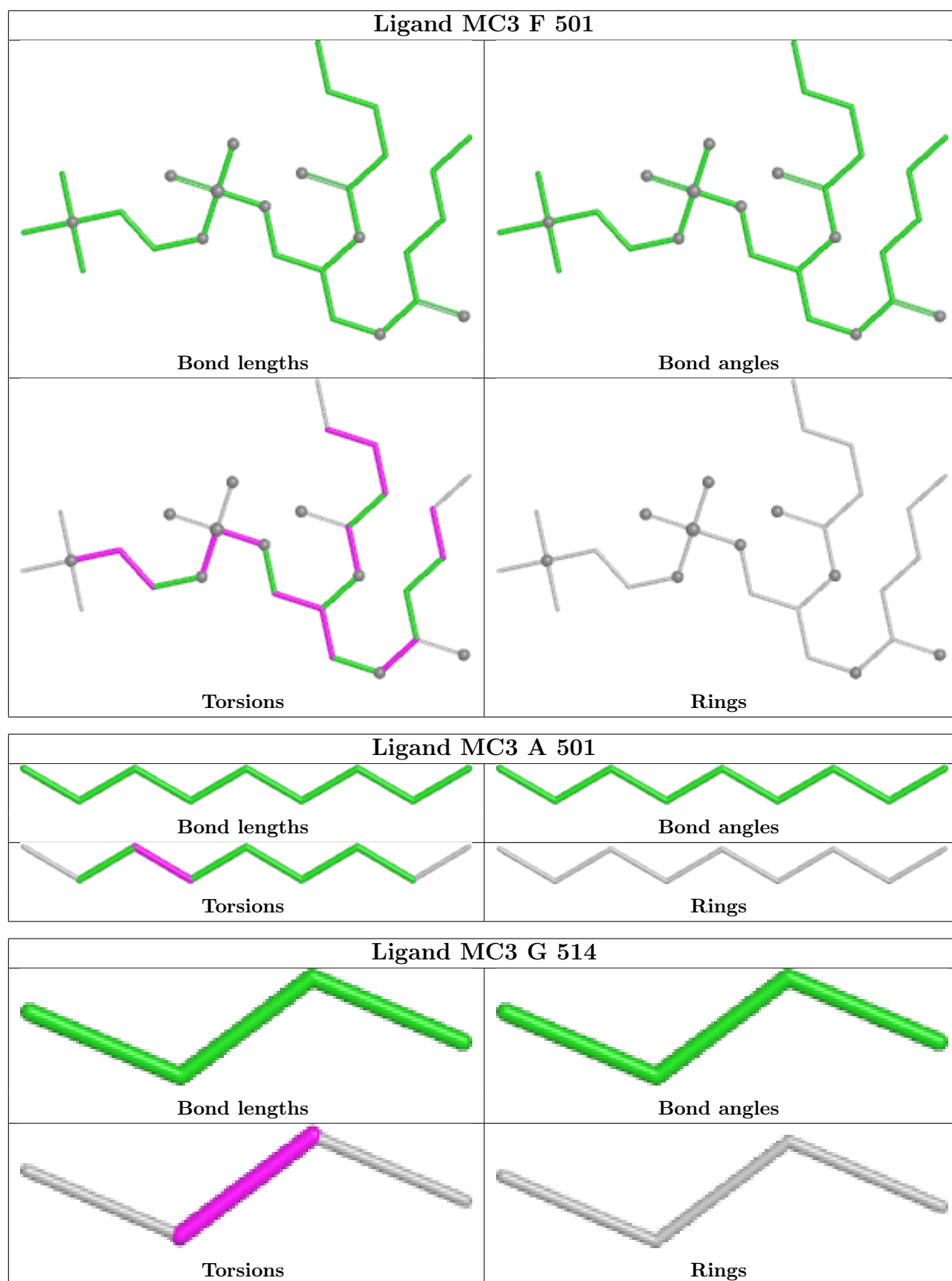
Ligand MC3 L 531	
 Bond lengths	 Bond angles
 Torsions	 Rings

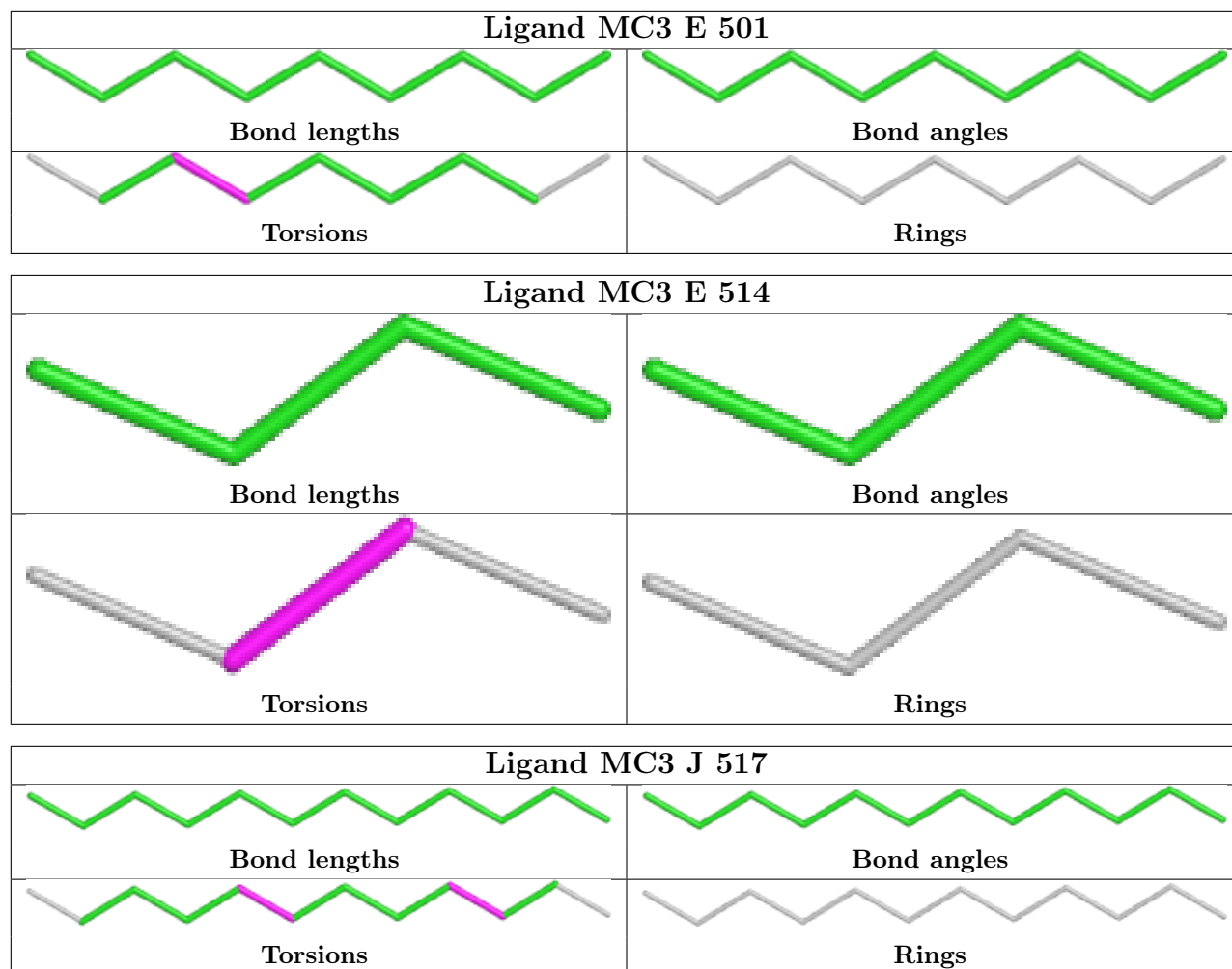


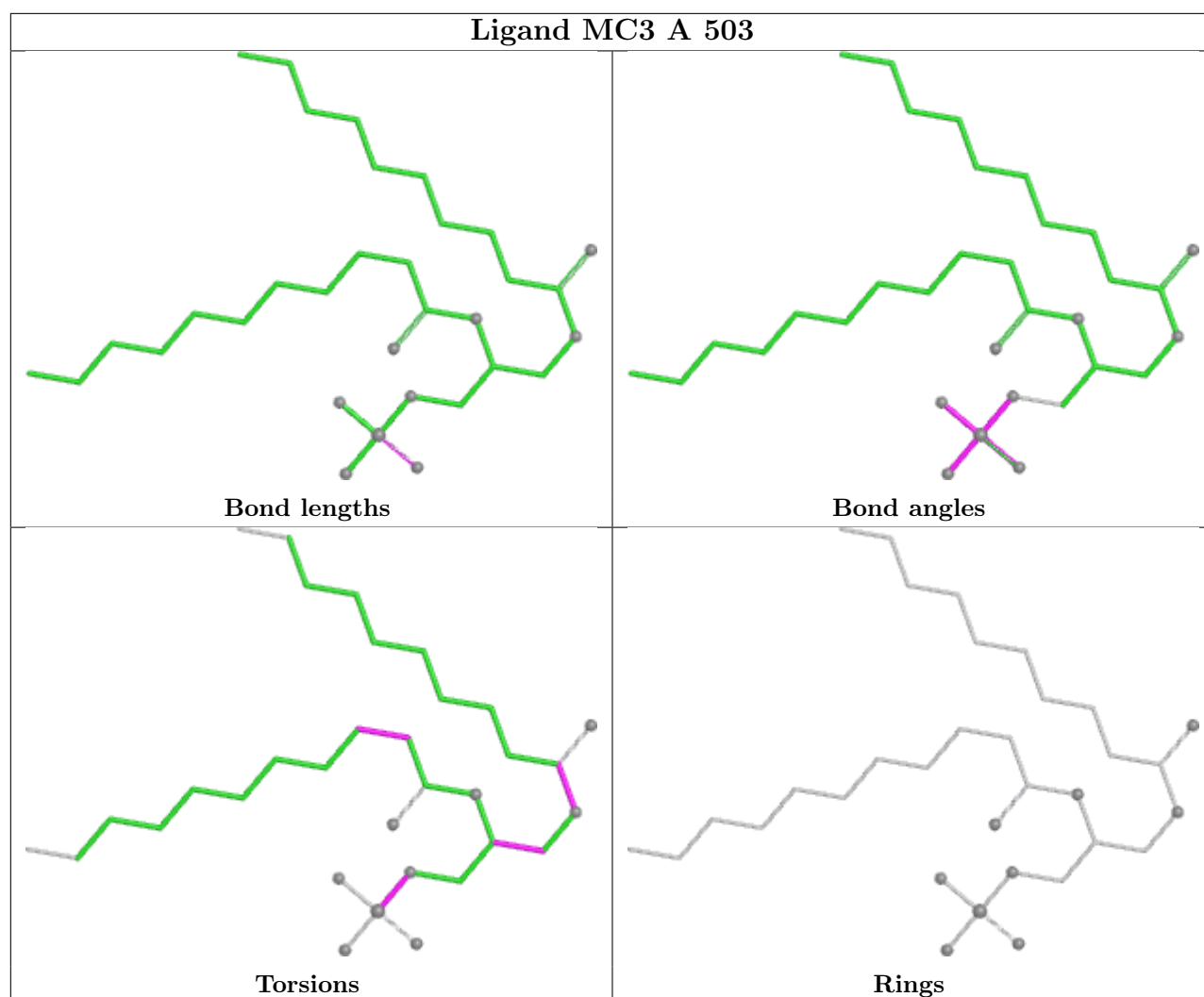


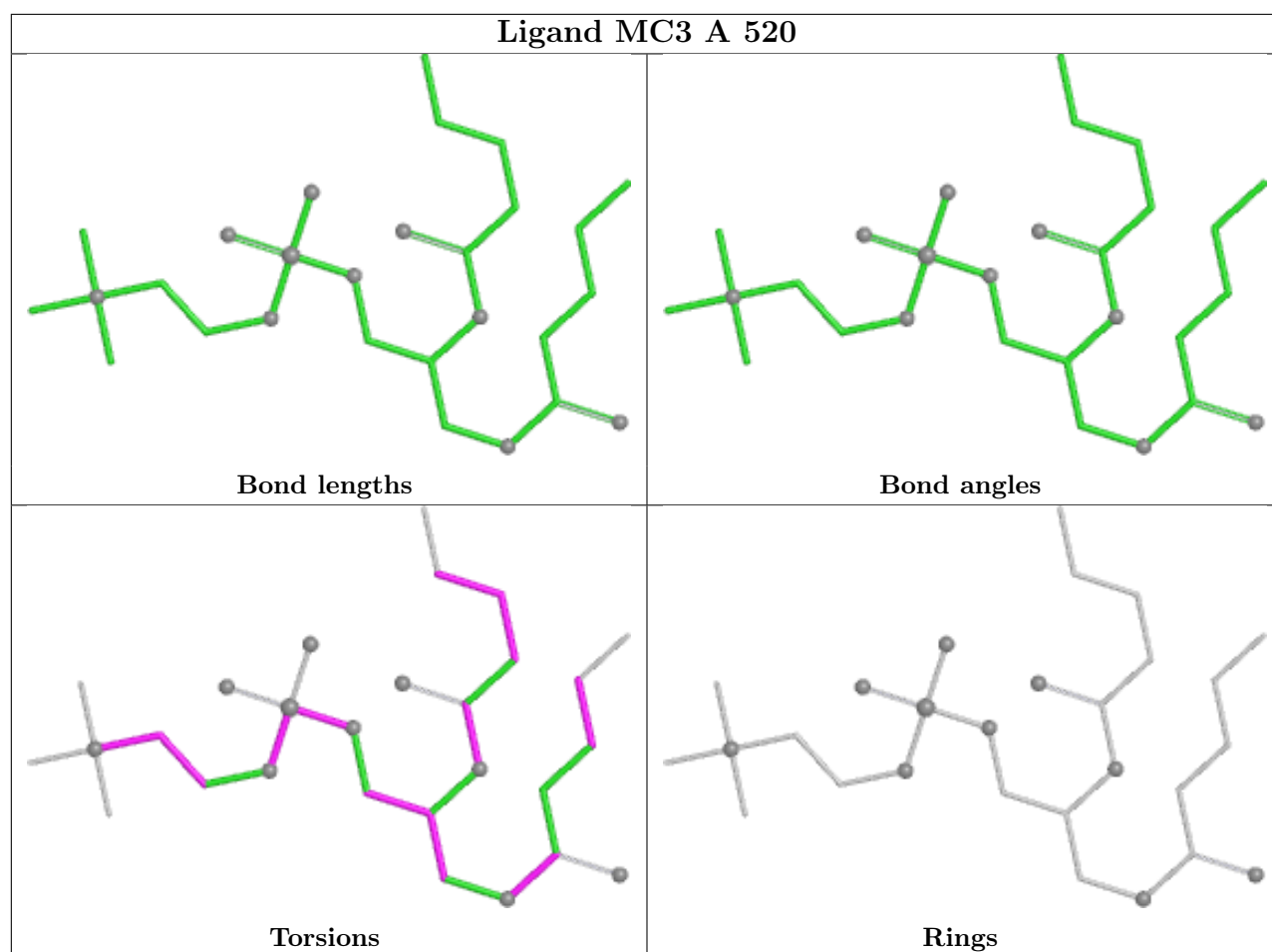


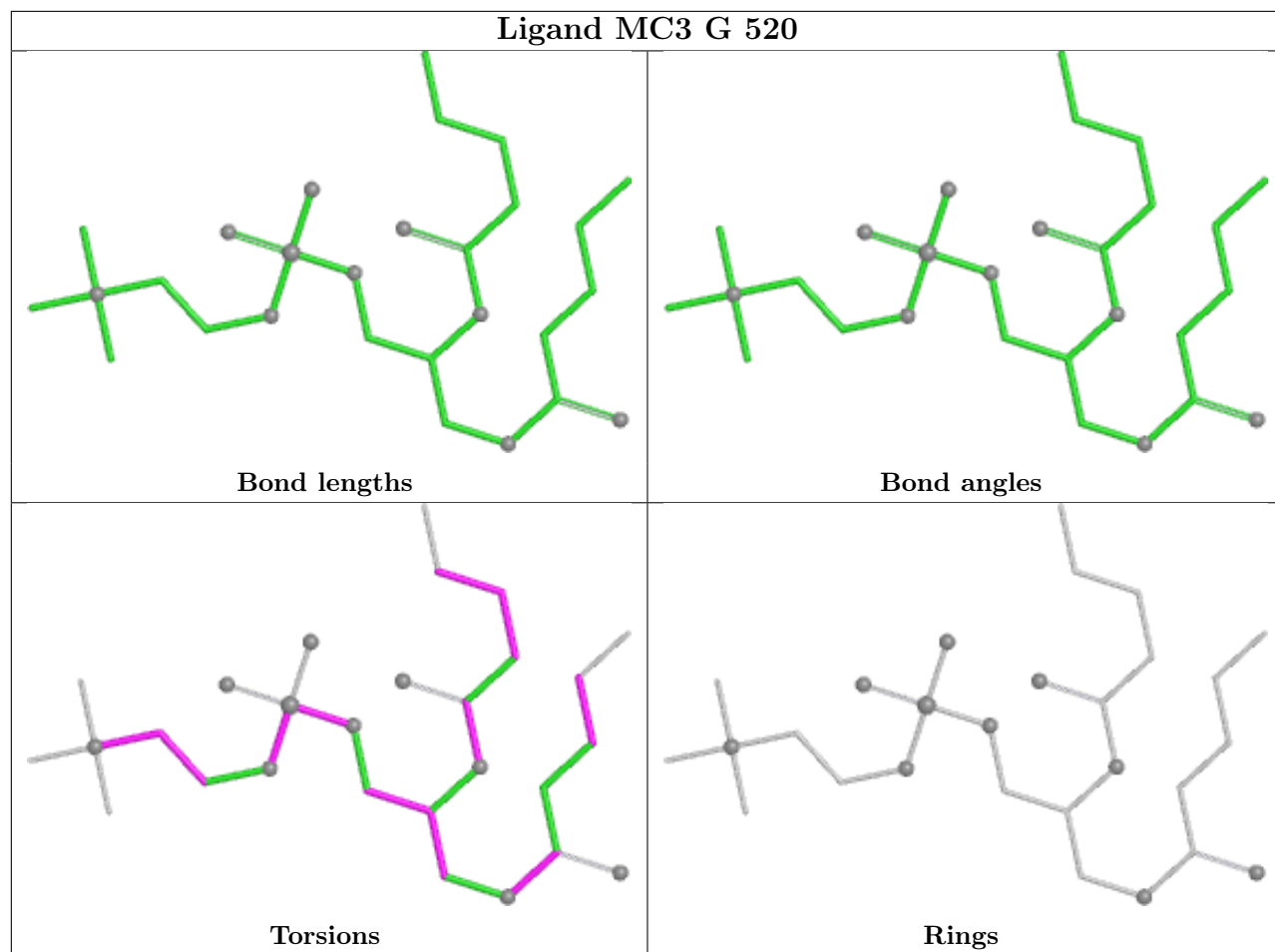


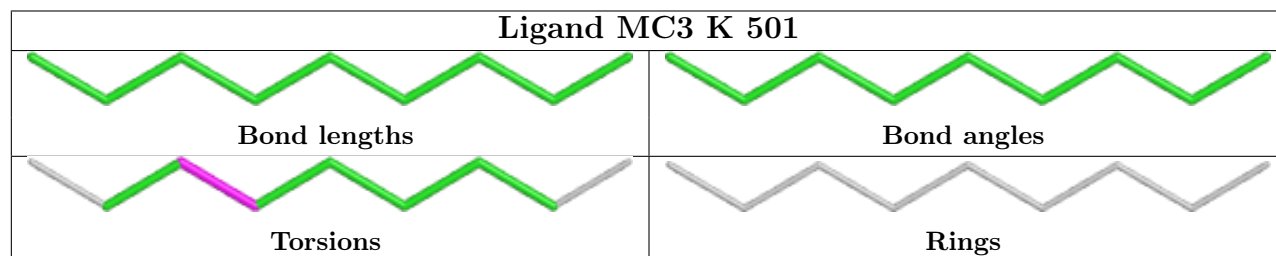
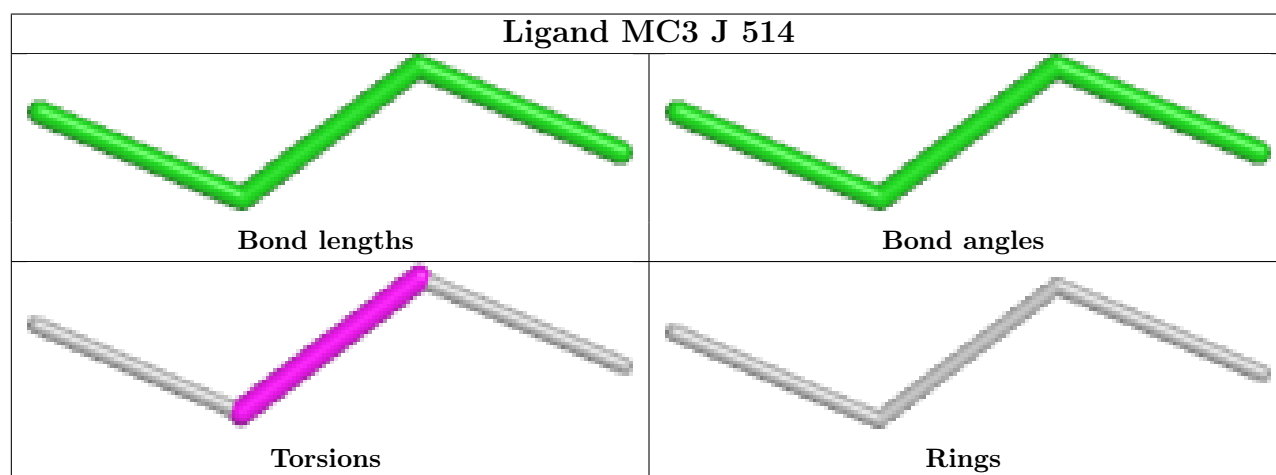
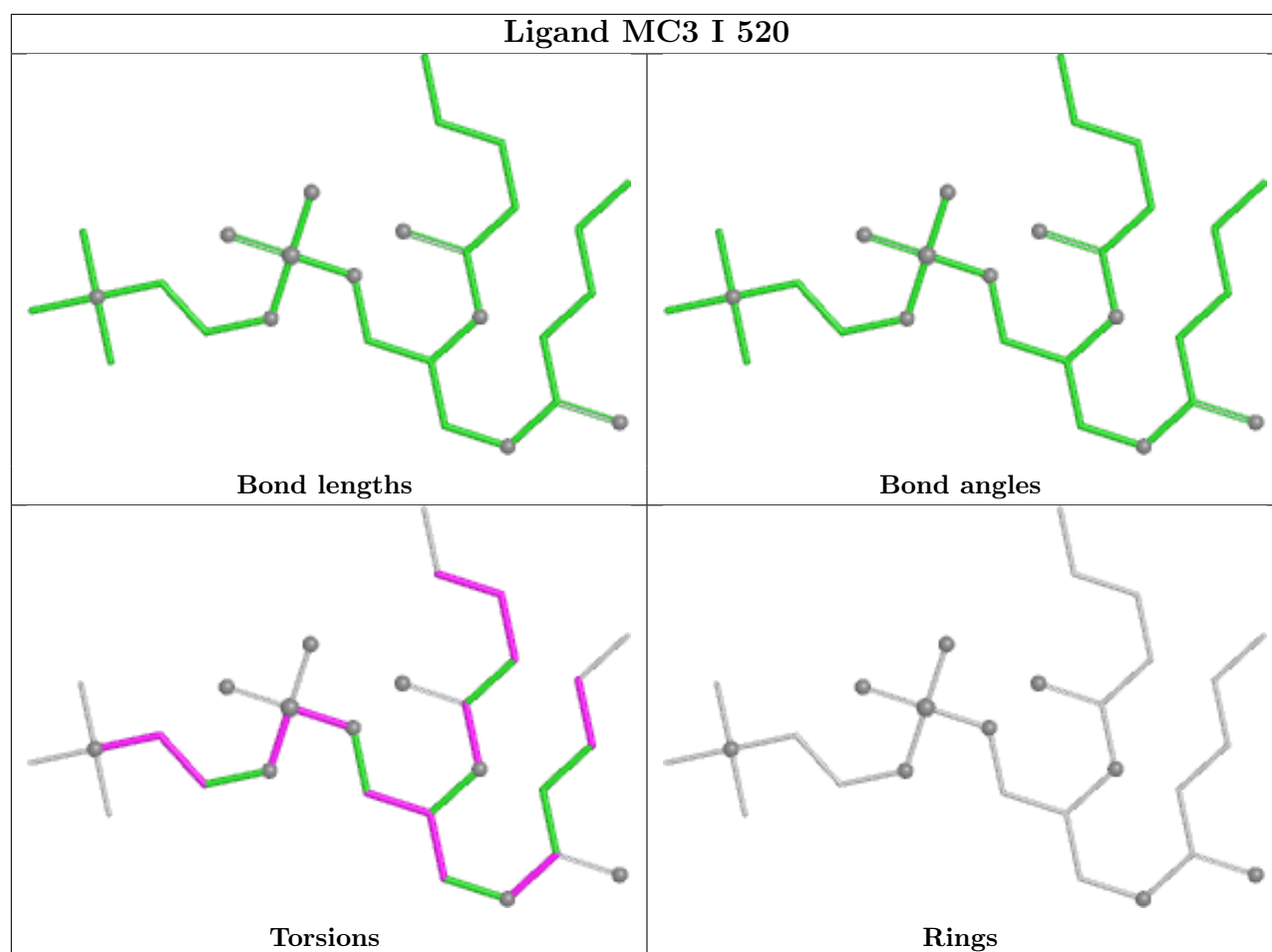


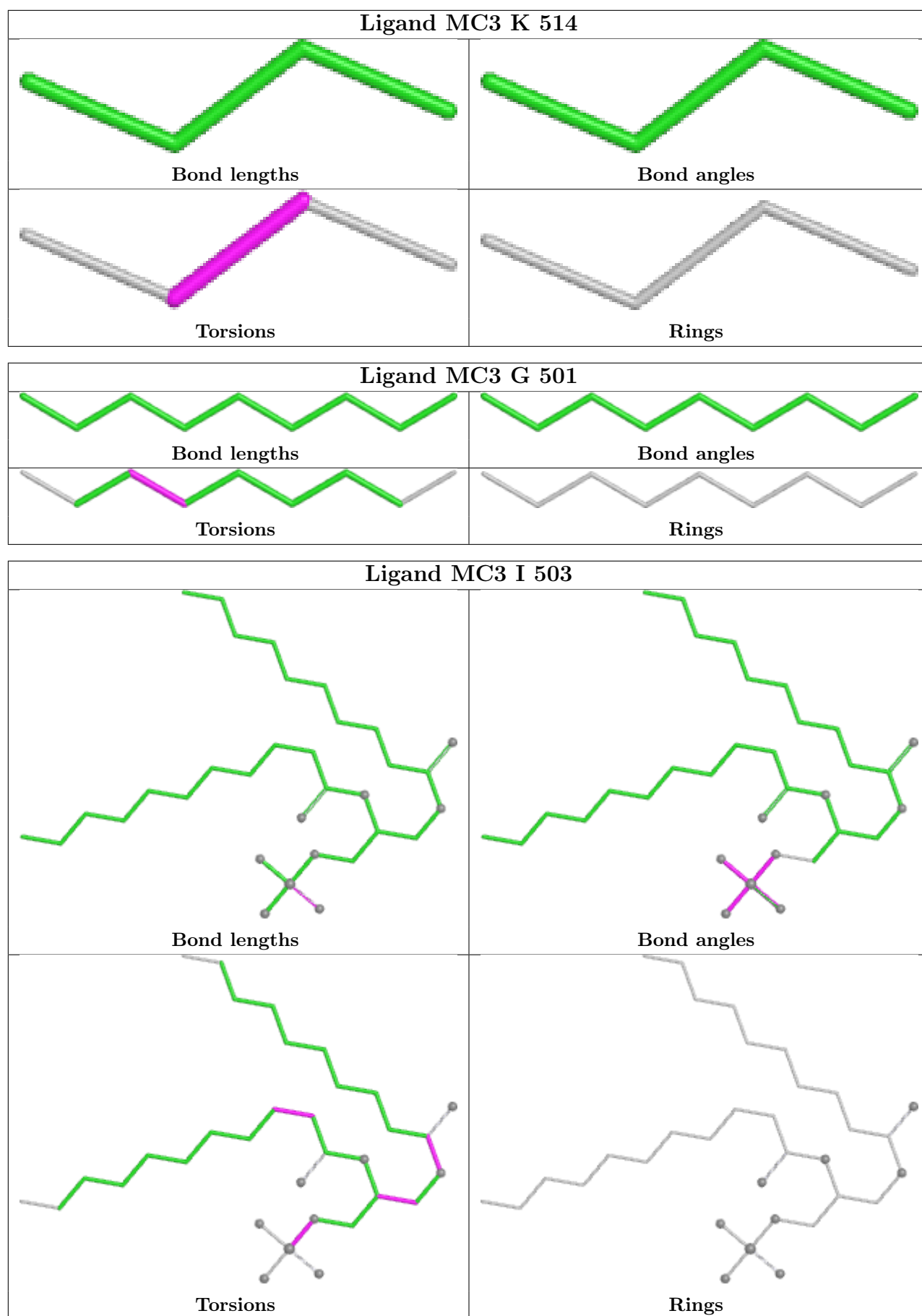


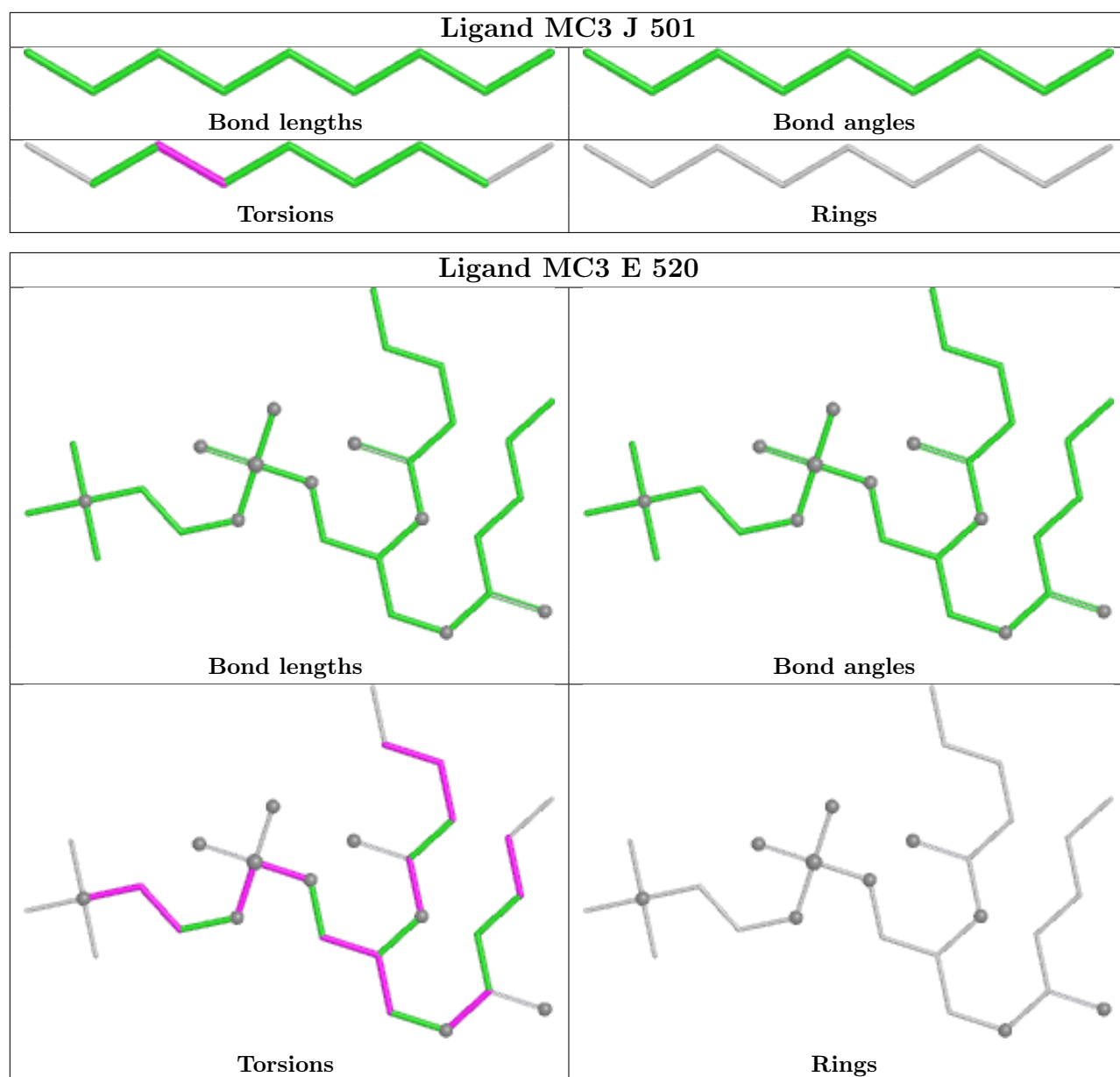


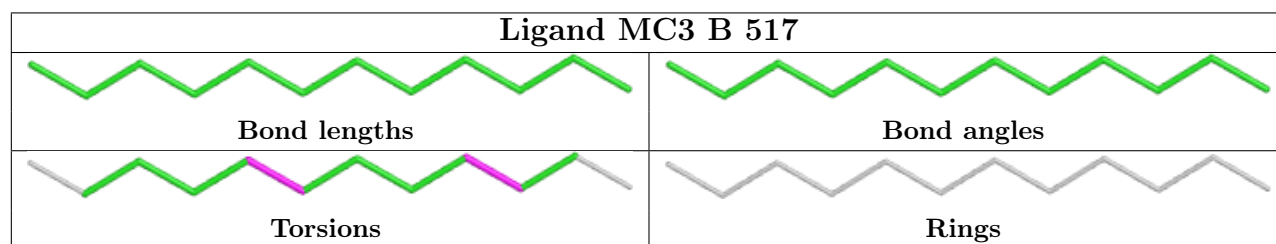
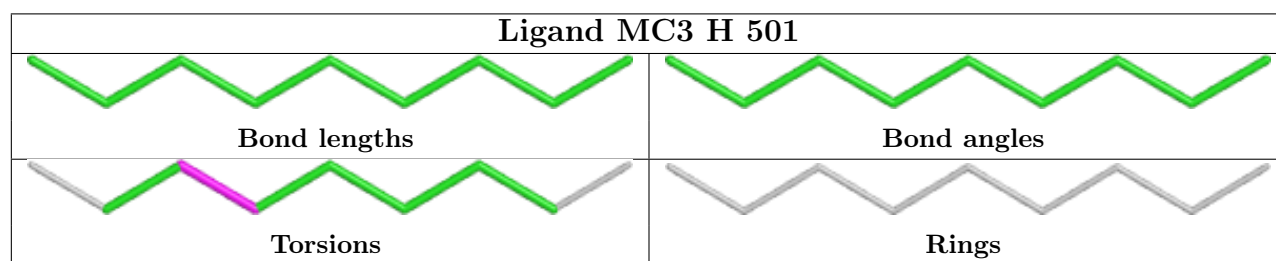
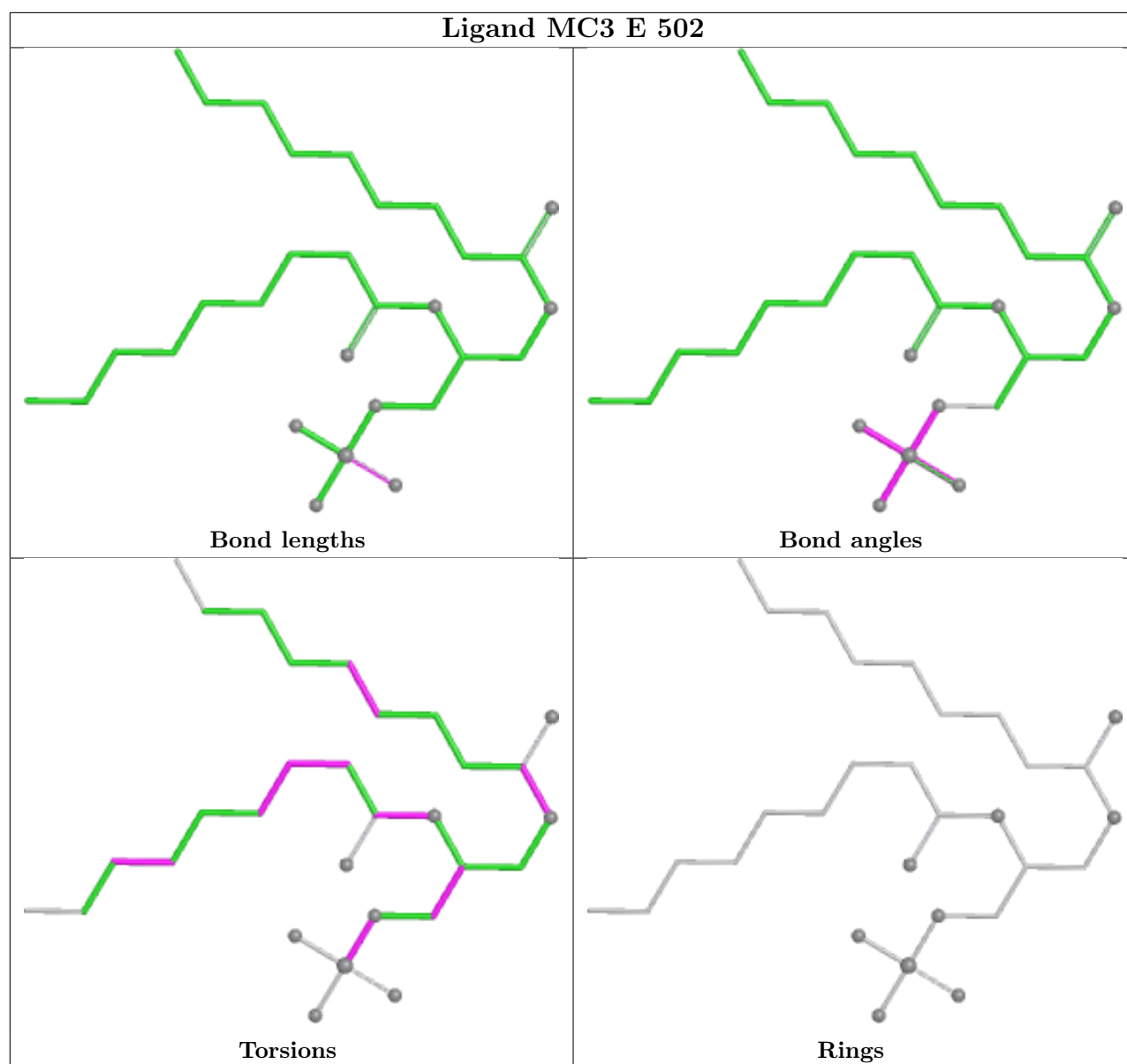


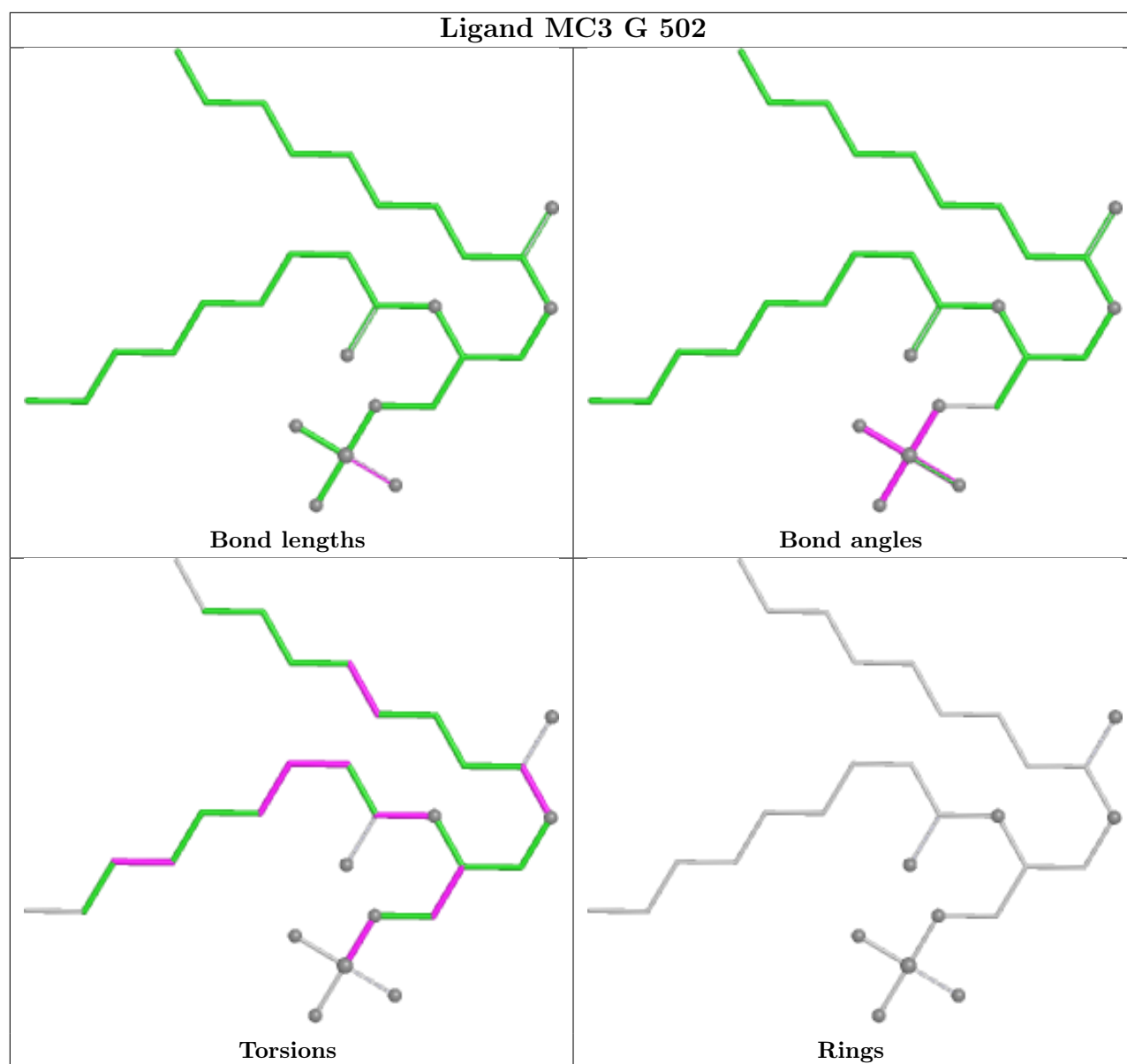


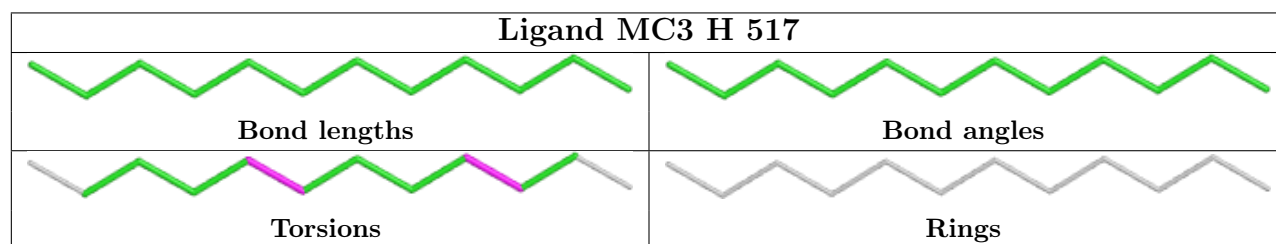
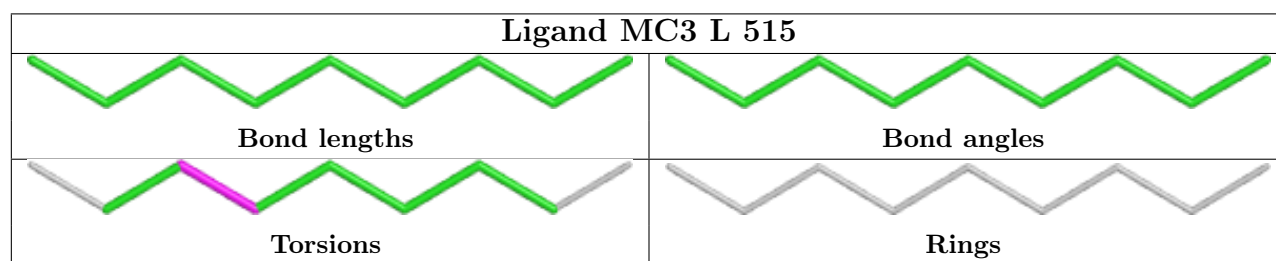
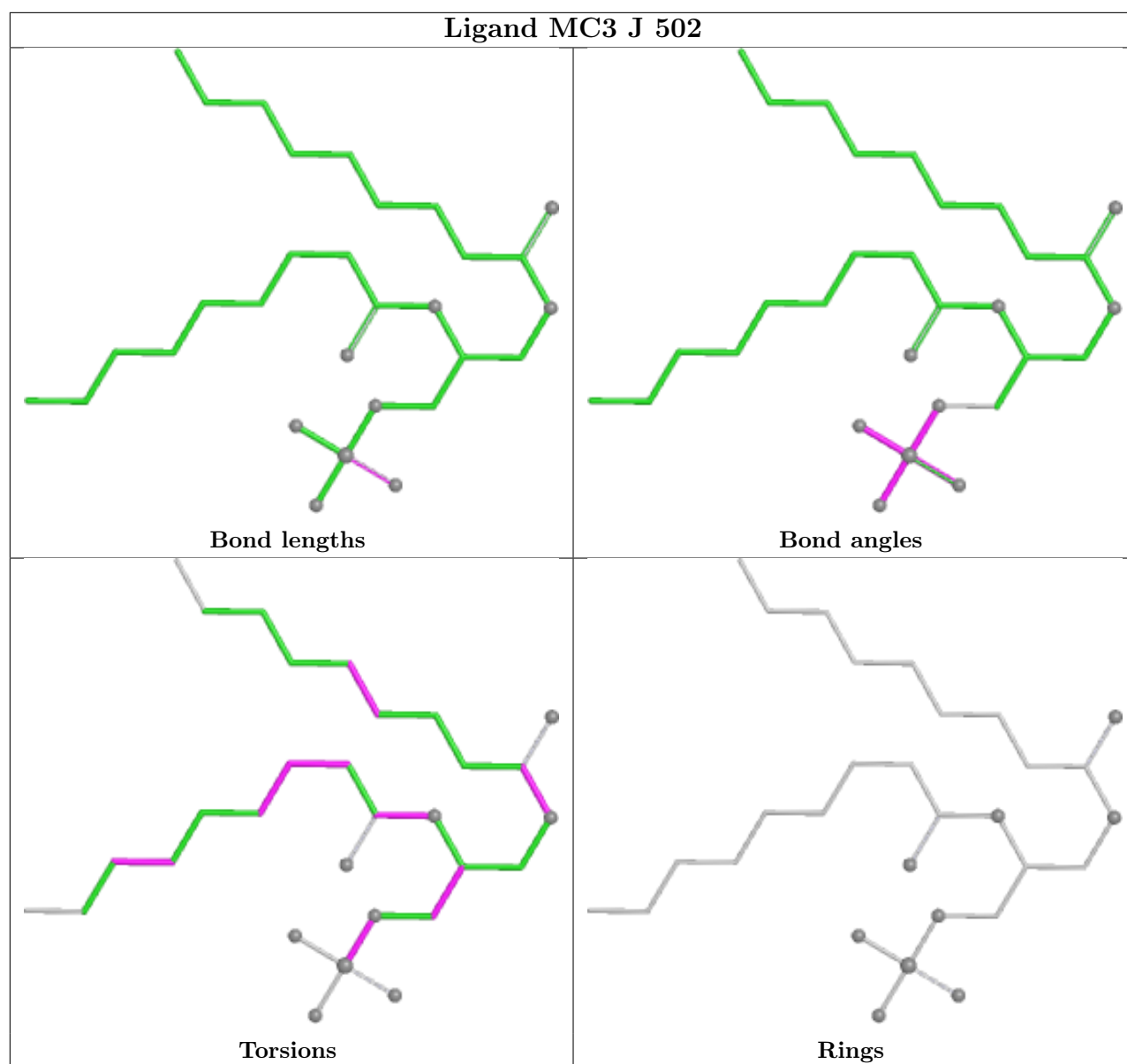


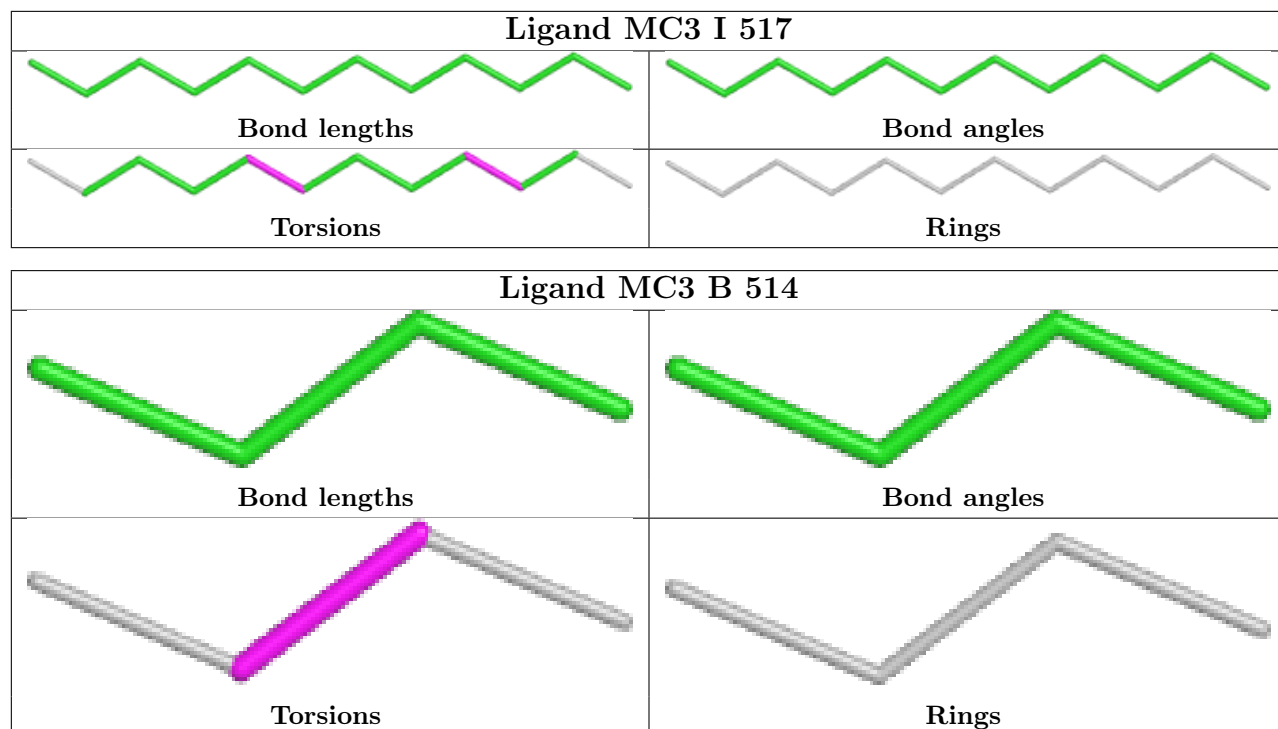


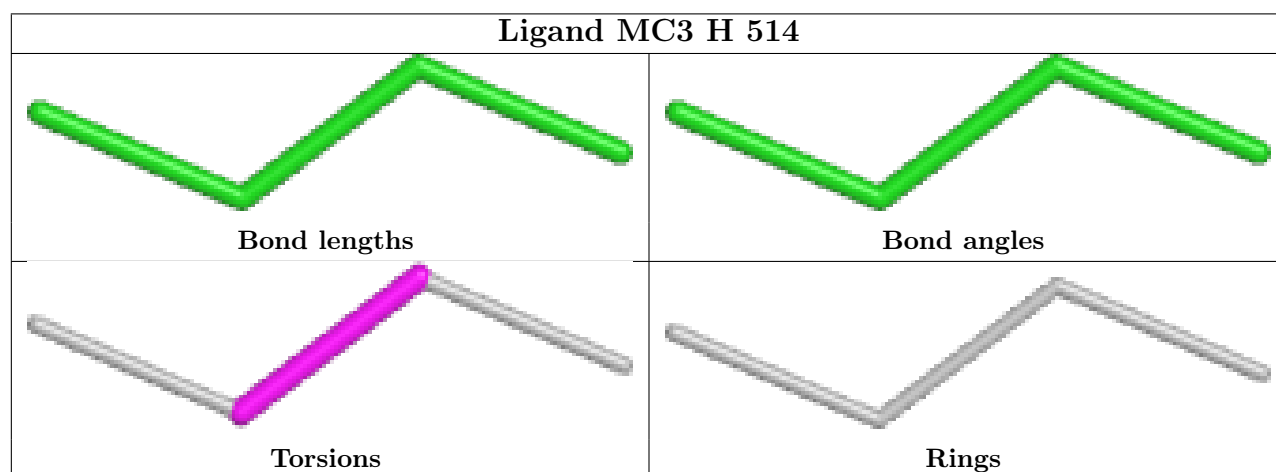
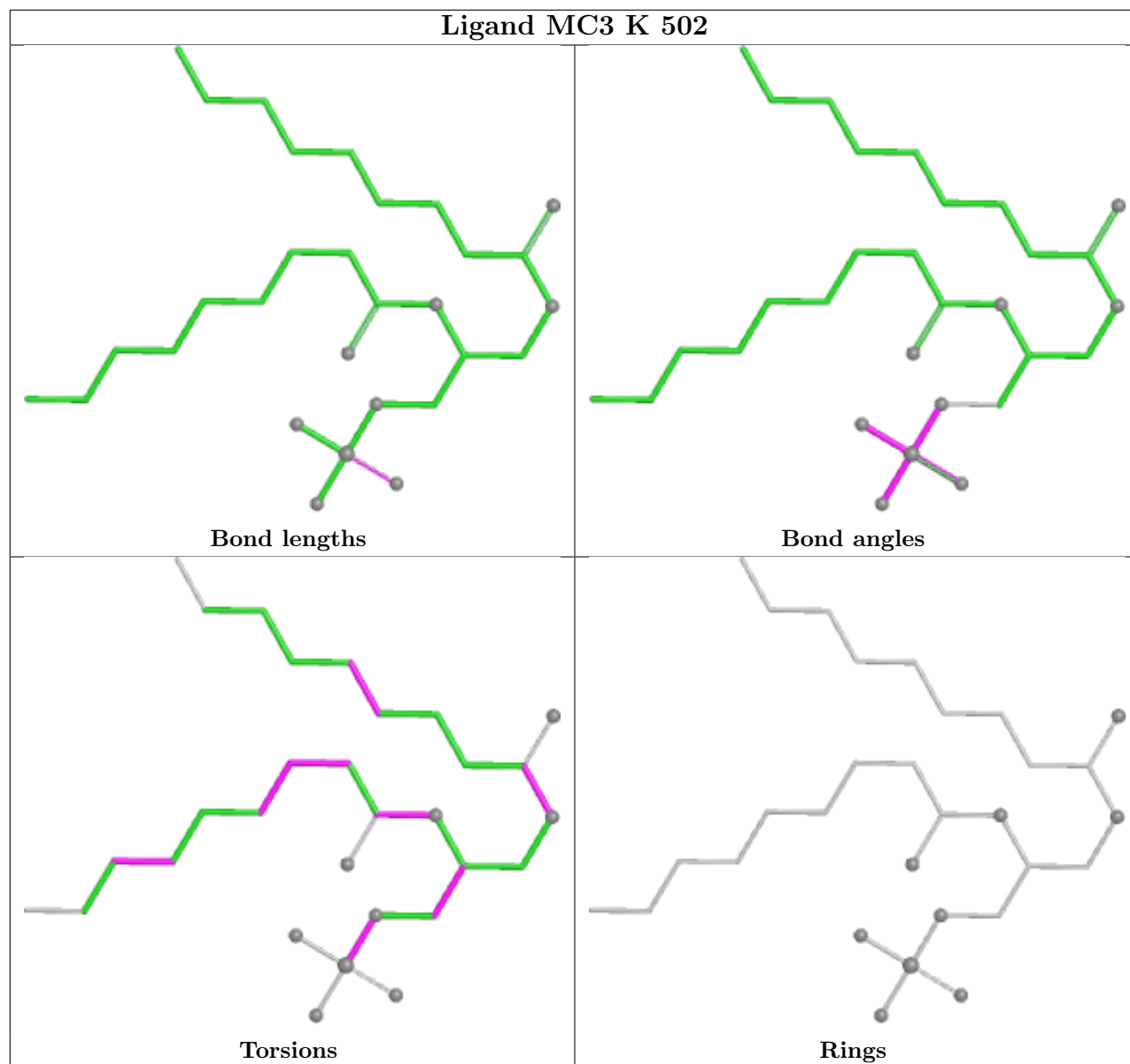


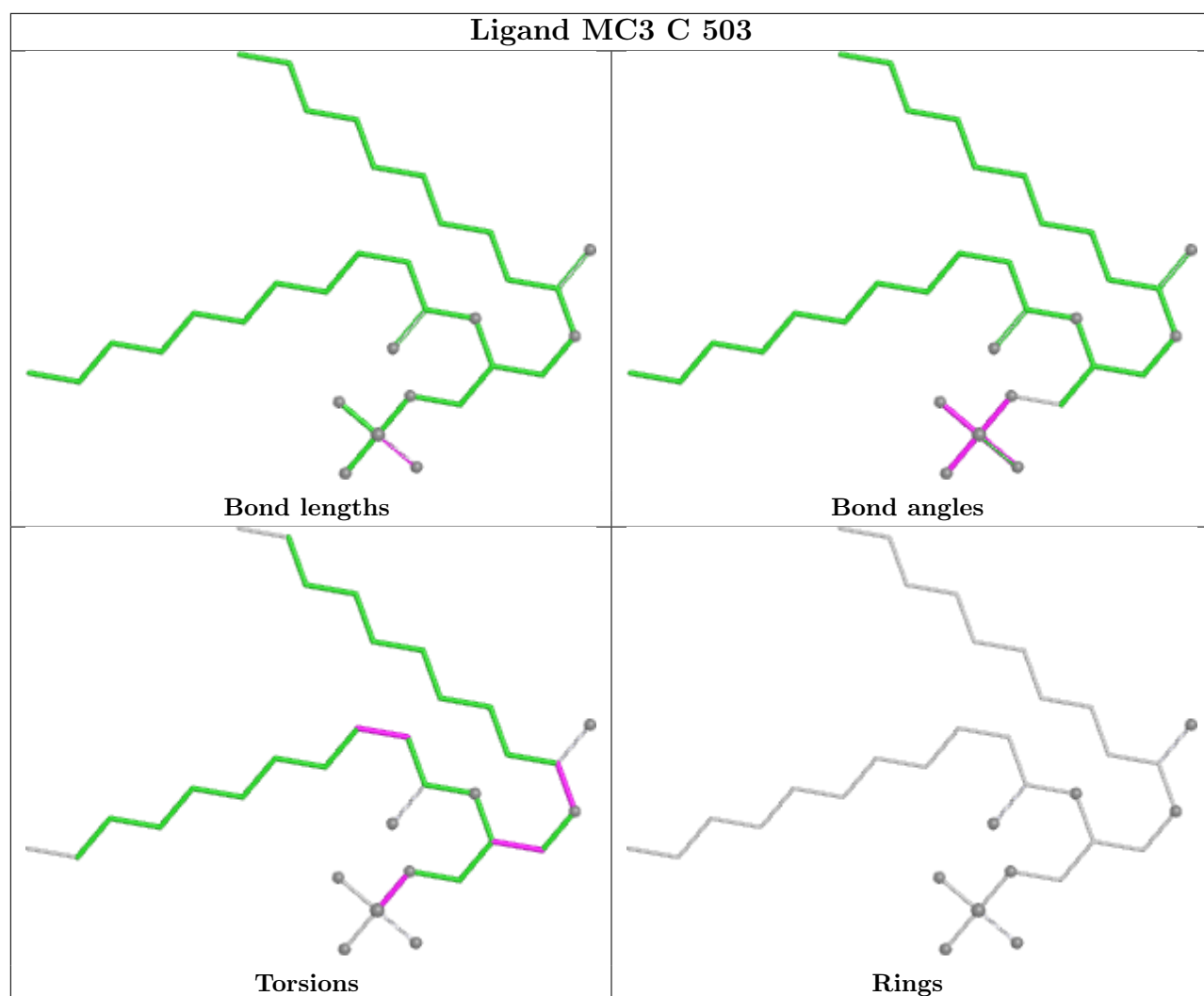


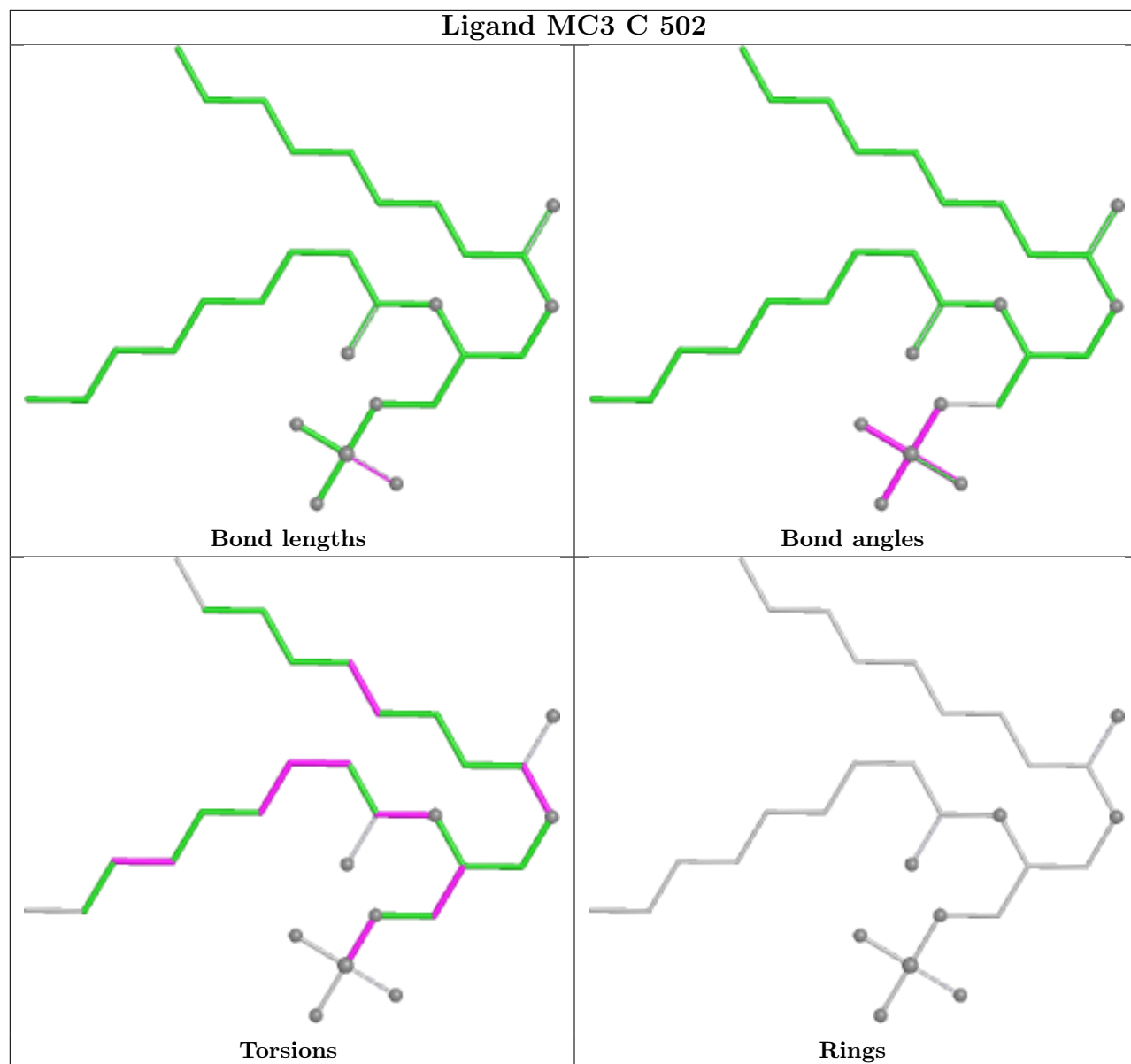


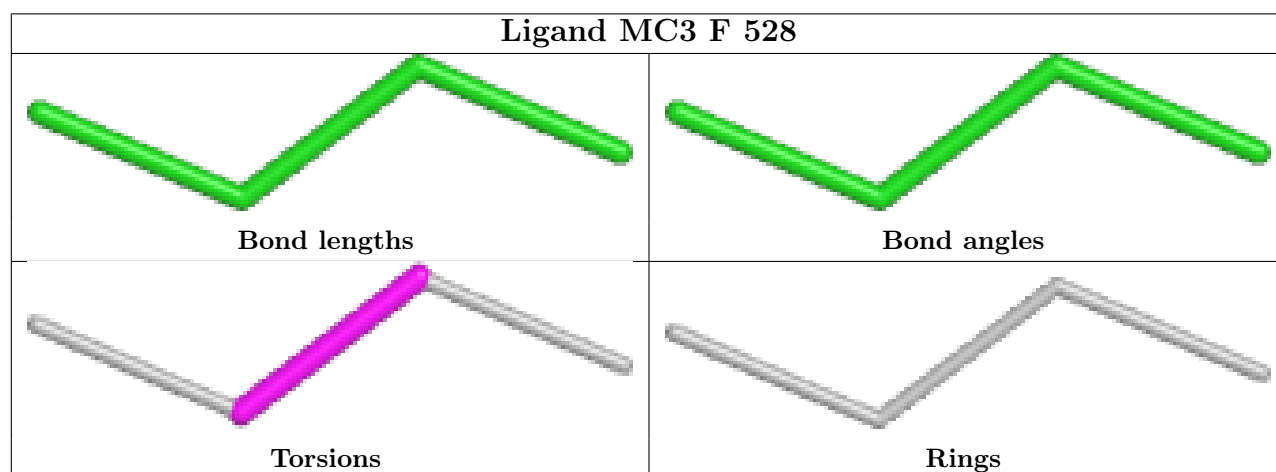
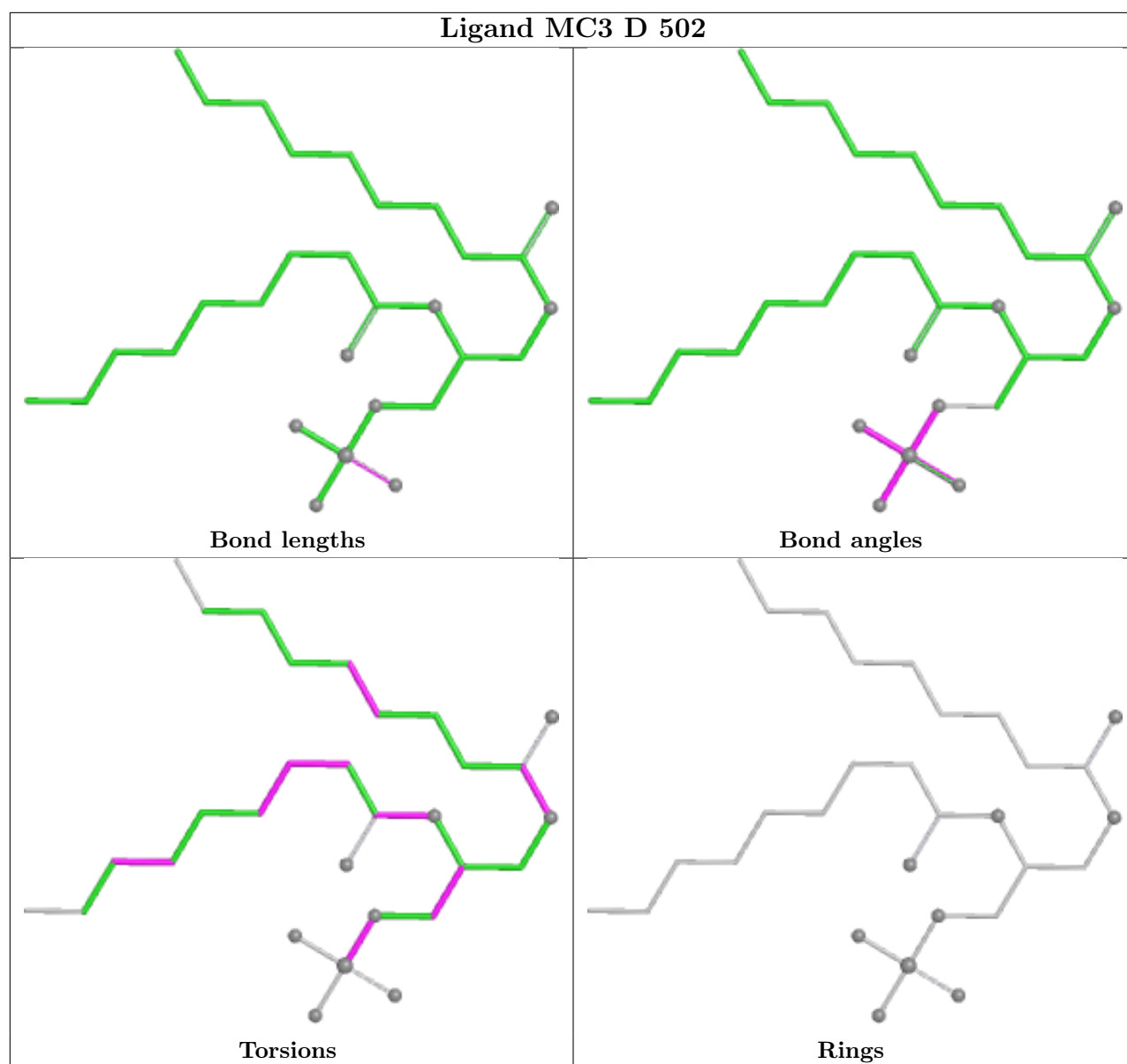


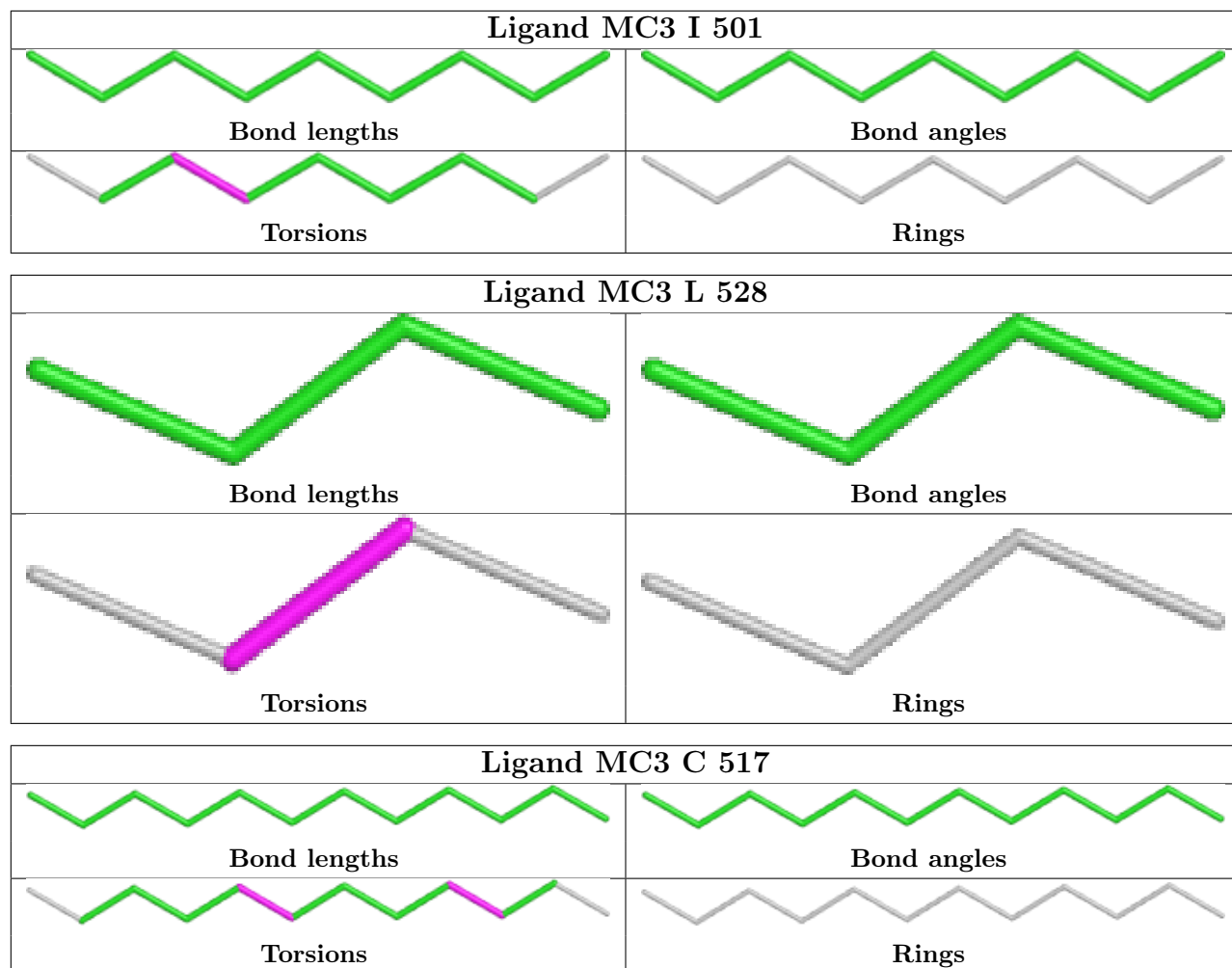


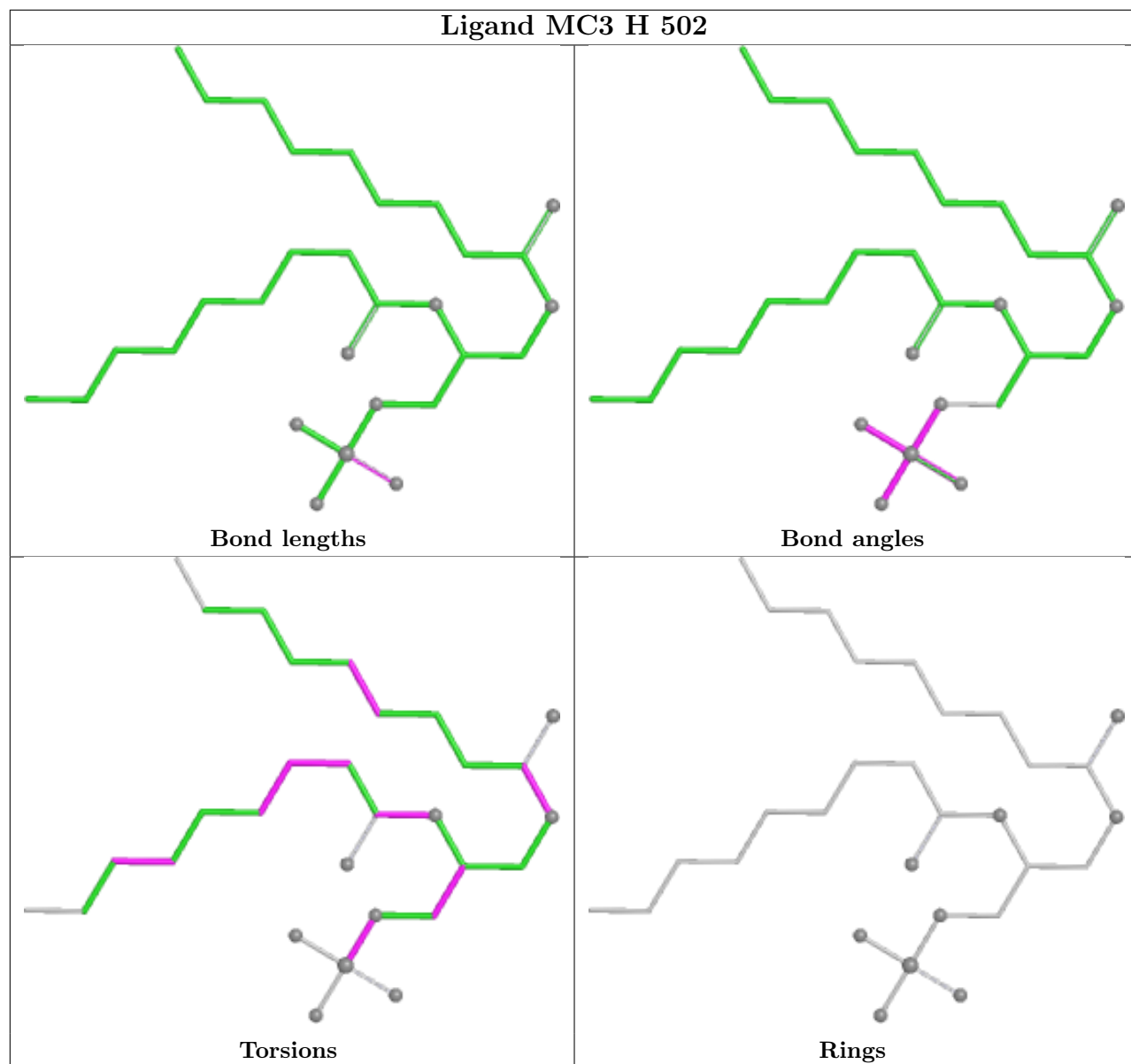


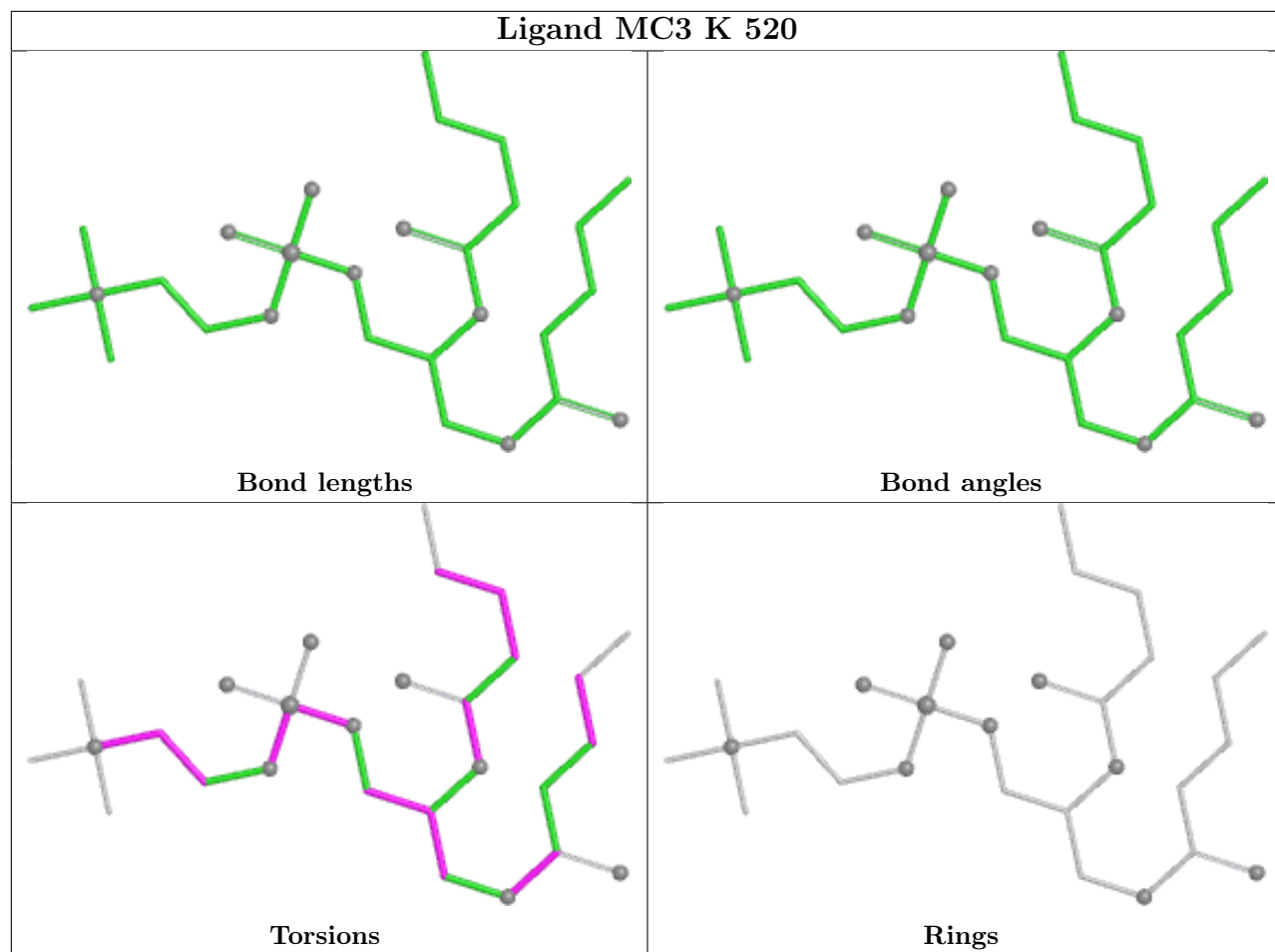


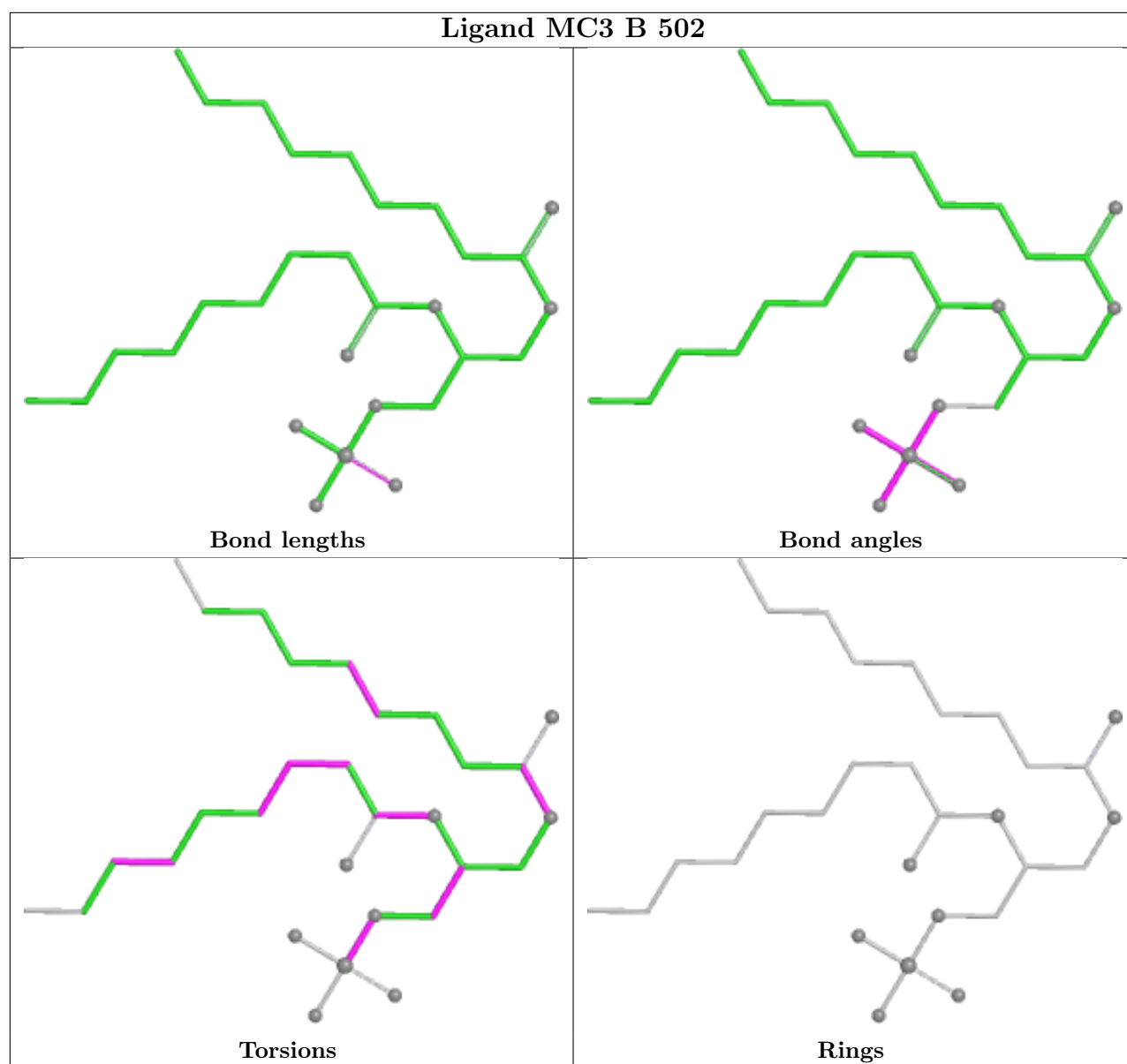


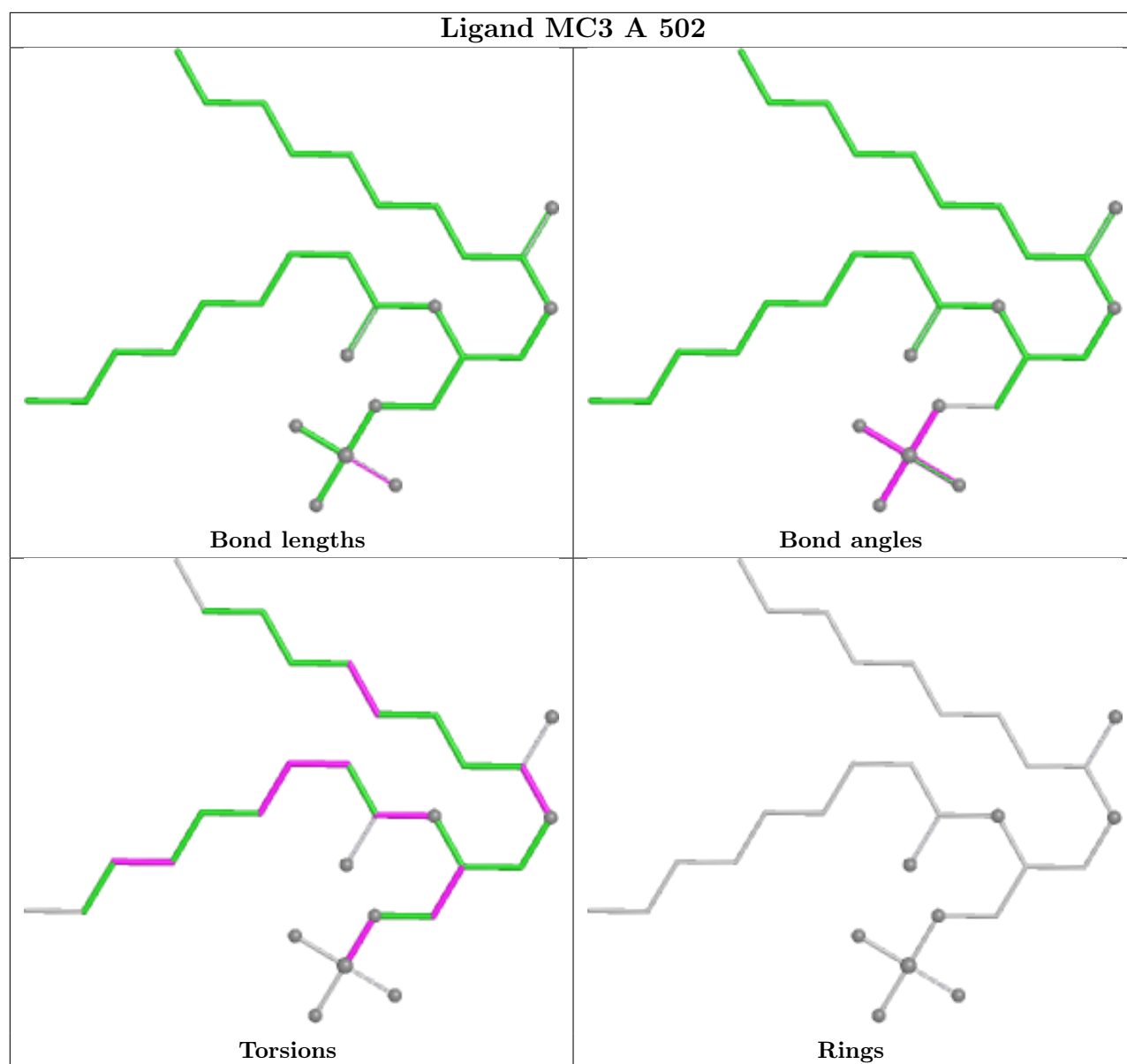












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

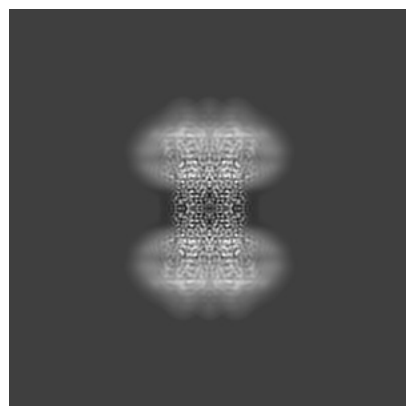
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73962. These allow visual inspection of the internal detail of the map and identification of artifacts.

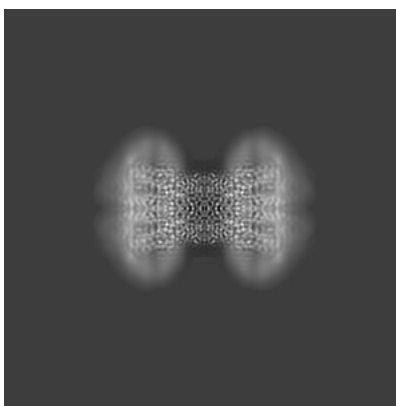
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

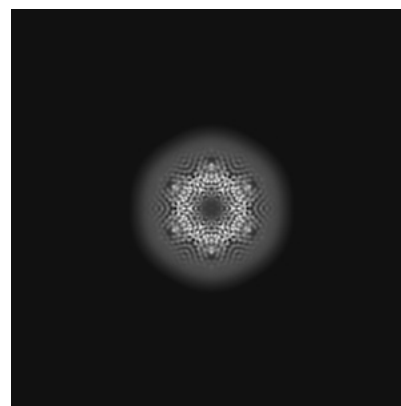
6.1.1 Primary map



X

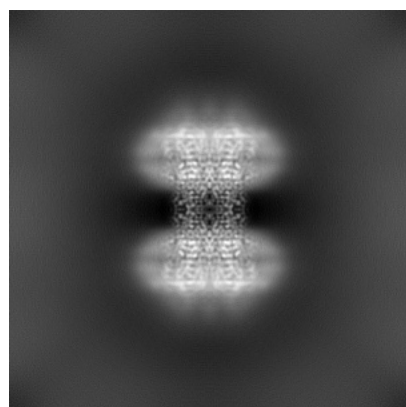


Y

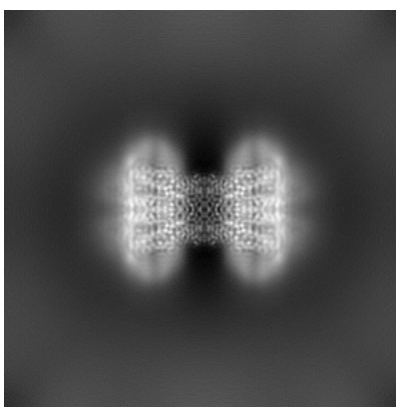


Z

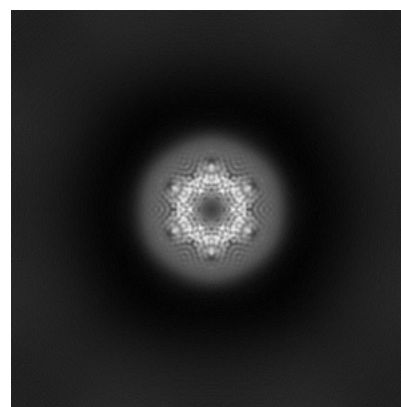
6.1.2 Raw map



X



Y

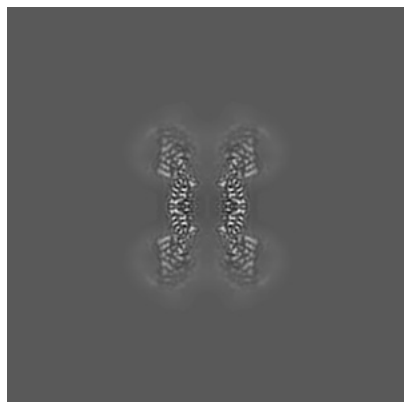


Z

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

6.2 Central slices [i](#)

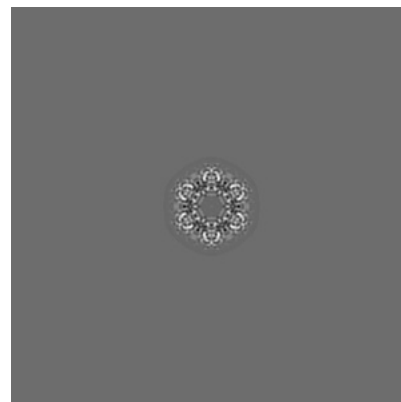
6.2.1 Primary map



X Index: 192

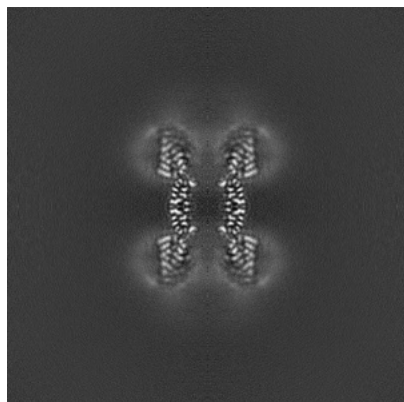


Y Index: 192

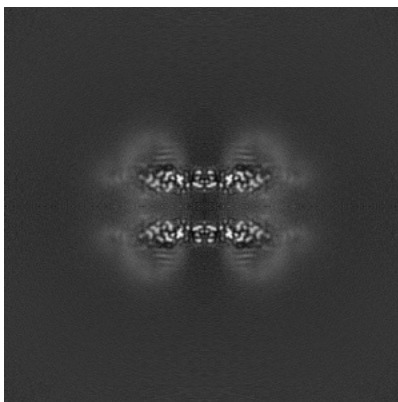


Z Index: 192

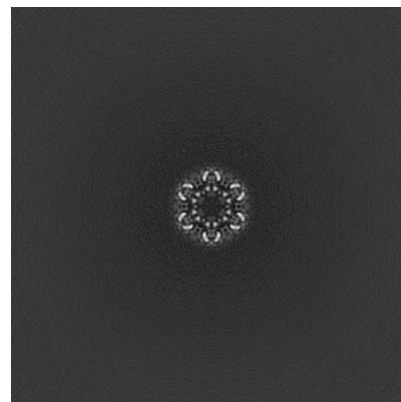
6.2.2 Raw map



X Index: 192



Y Index: 192



Z Index: 192

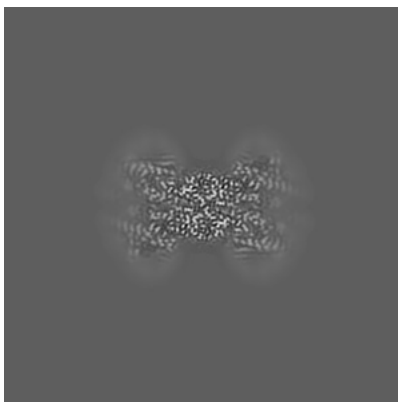
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

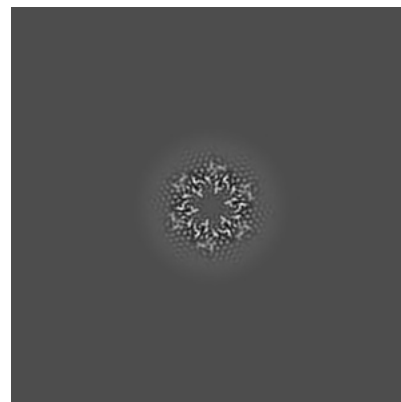
6.3.1 Primary map



X Index: 171

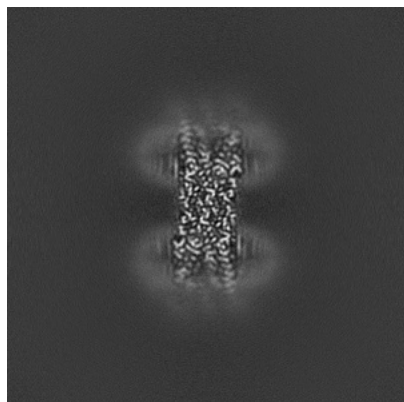


Y Index: 174

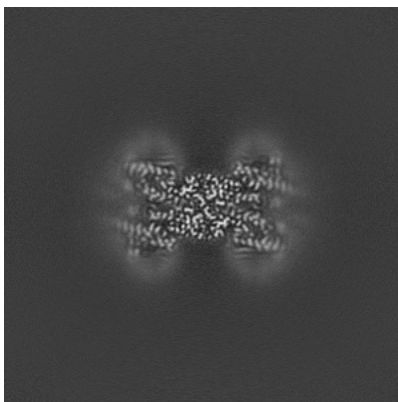


Z Index: 161

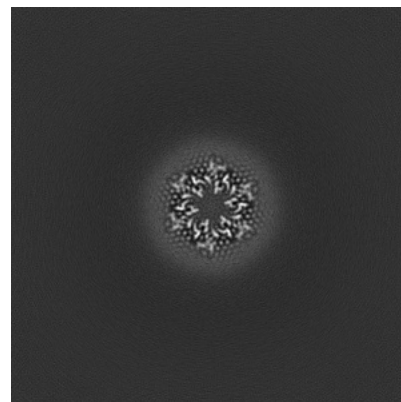
6.3.2 Raw map



X Index: 213



Y Index: 174

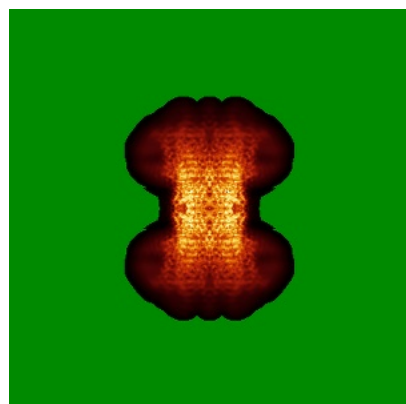


Z Index: 161

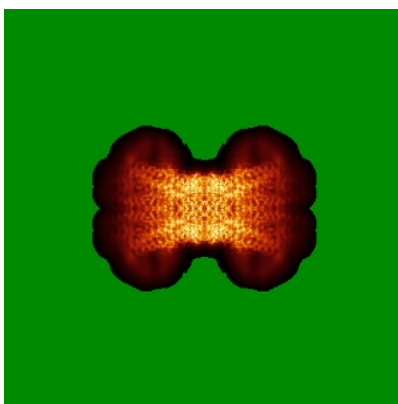
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

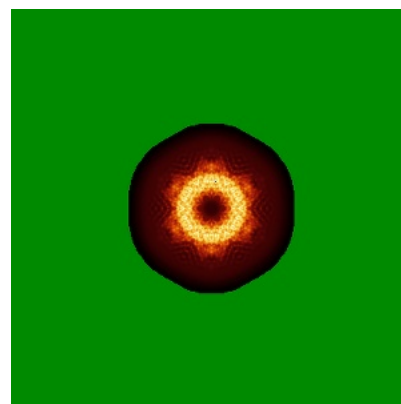
6.4.1 Primary map



X

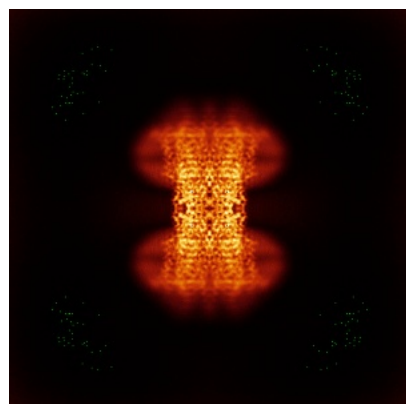


Y

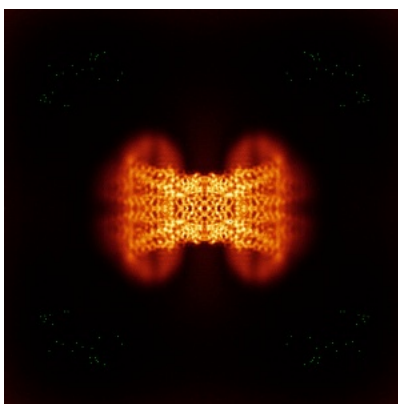


Z

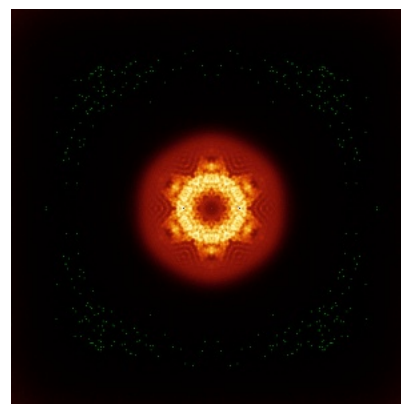
6.4.2 Raw map



X



Y

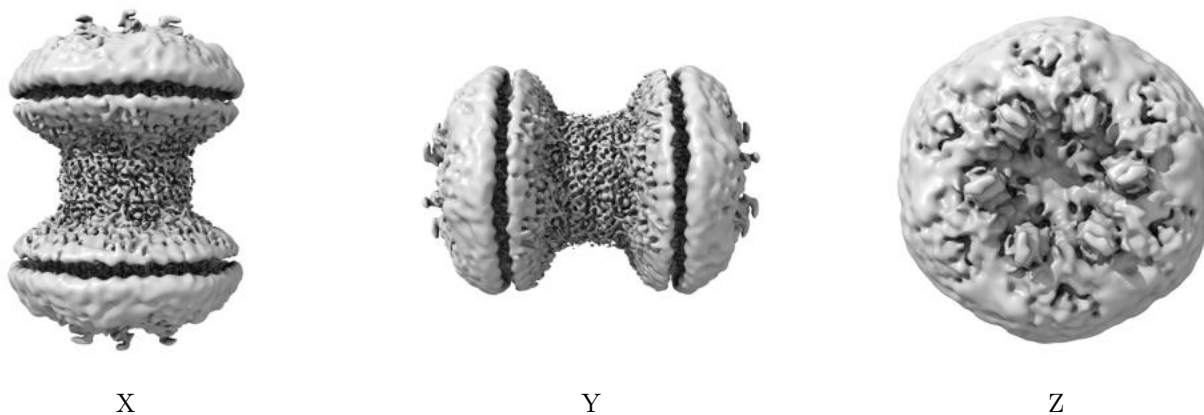


Z

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

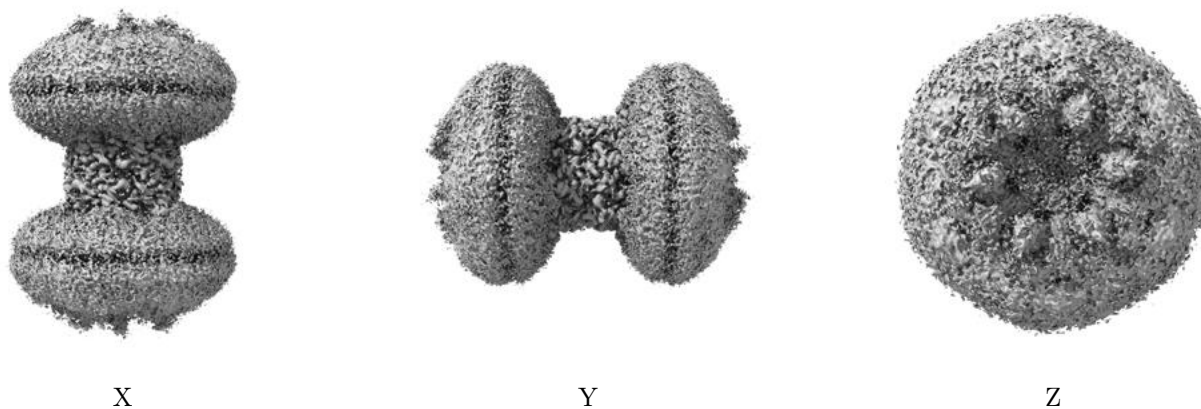
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

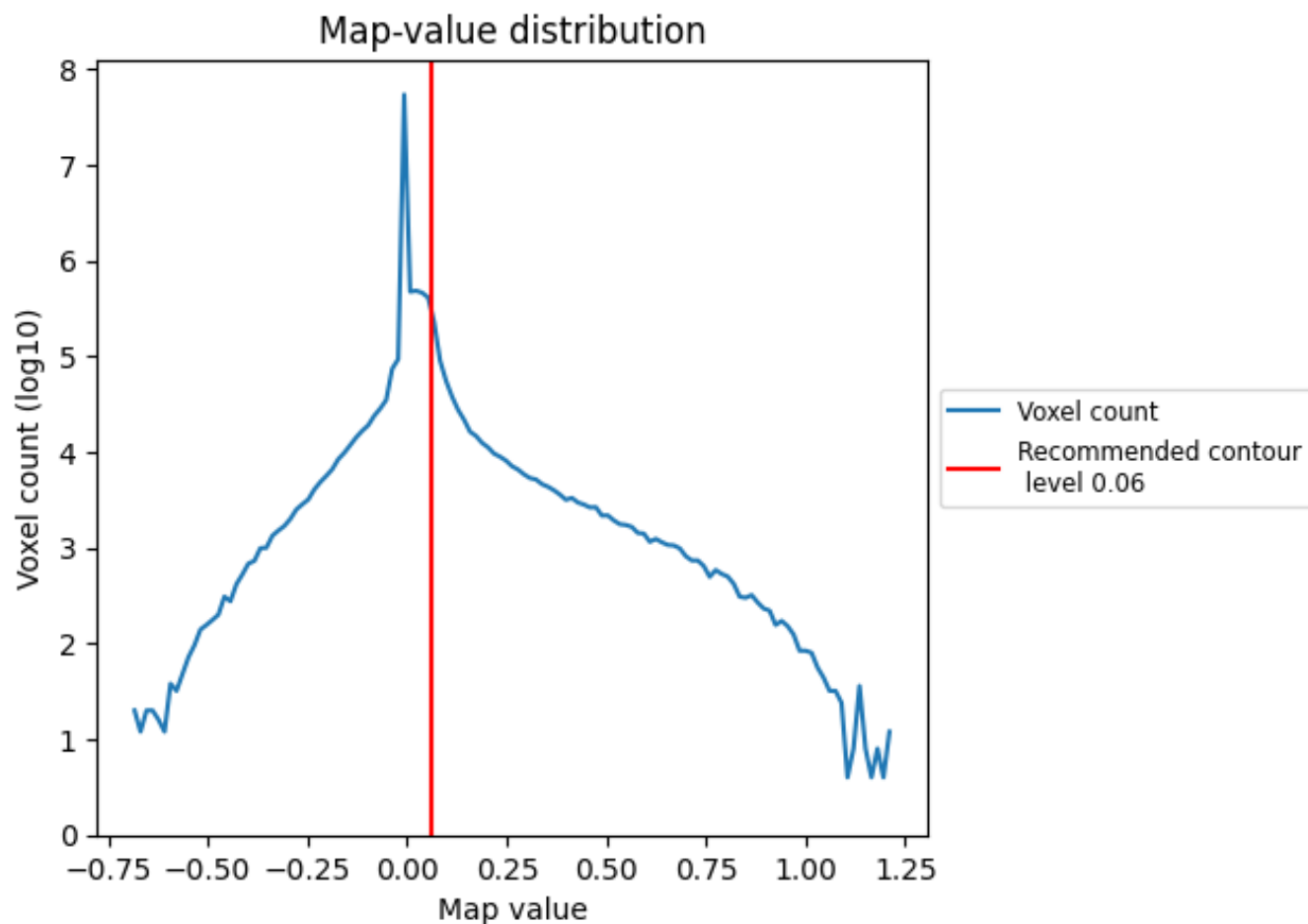
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

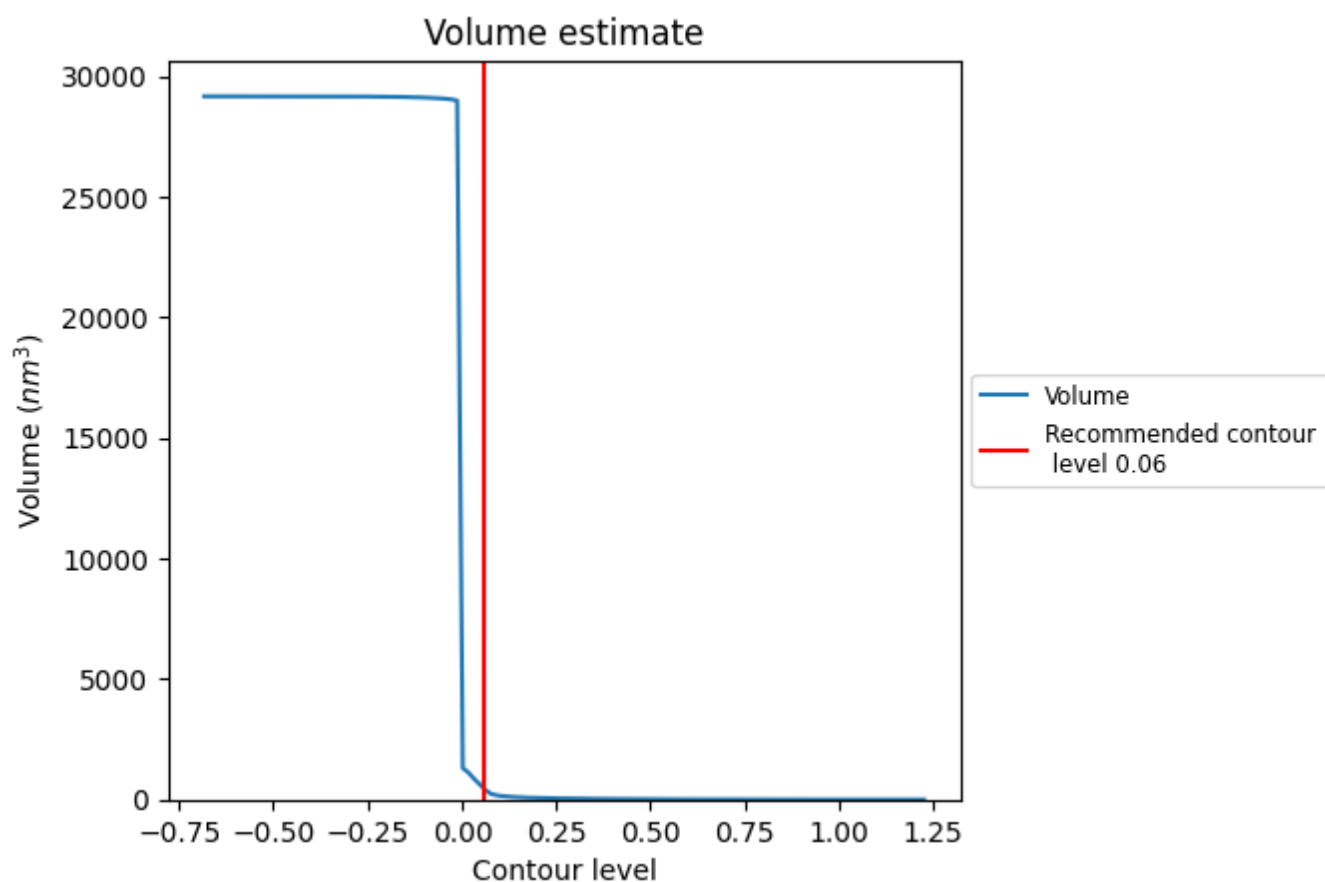
This section contains the results of statistical analysis of the map.

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.

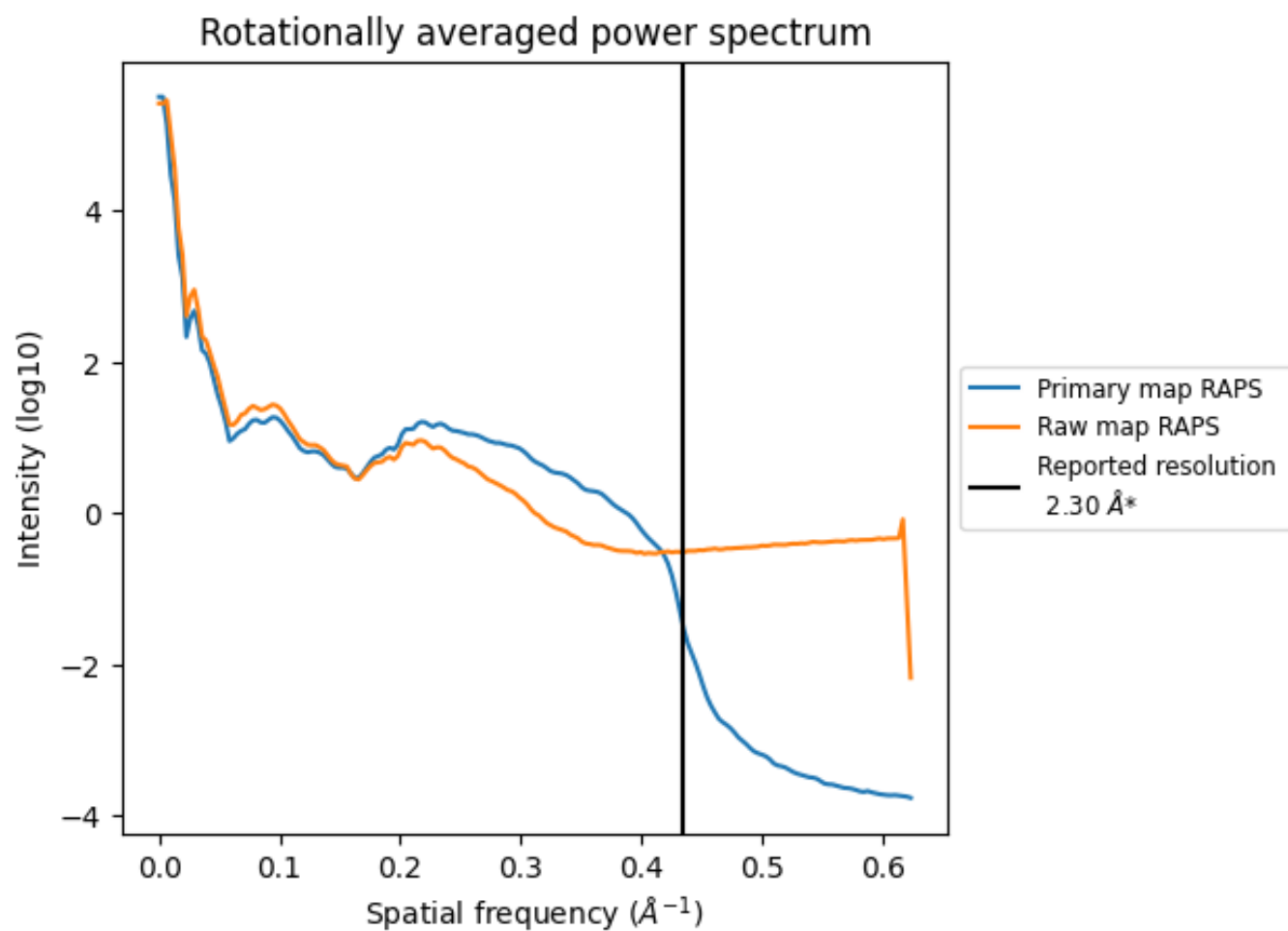
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 436 nm³; this corresponds to an approximate mass of 393 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 ⓘ

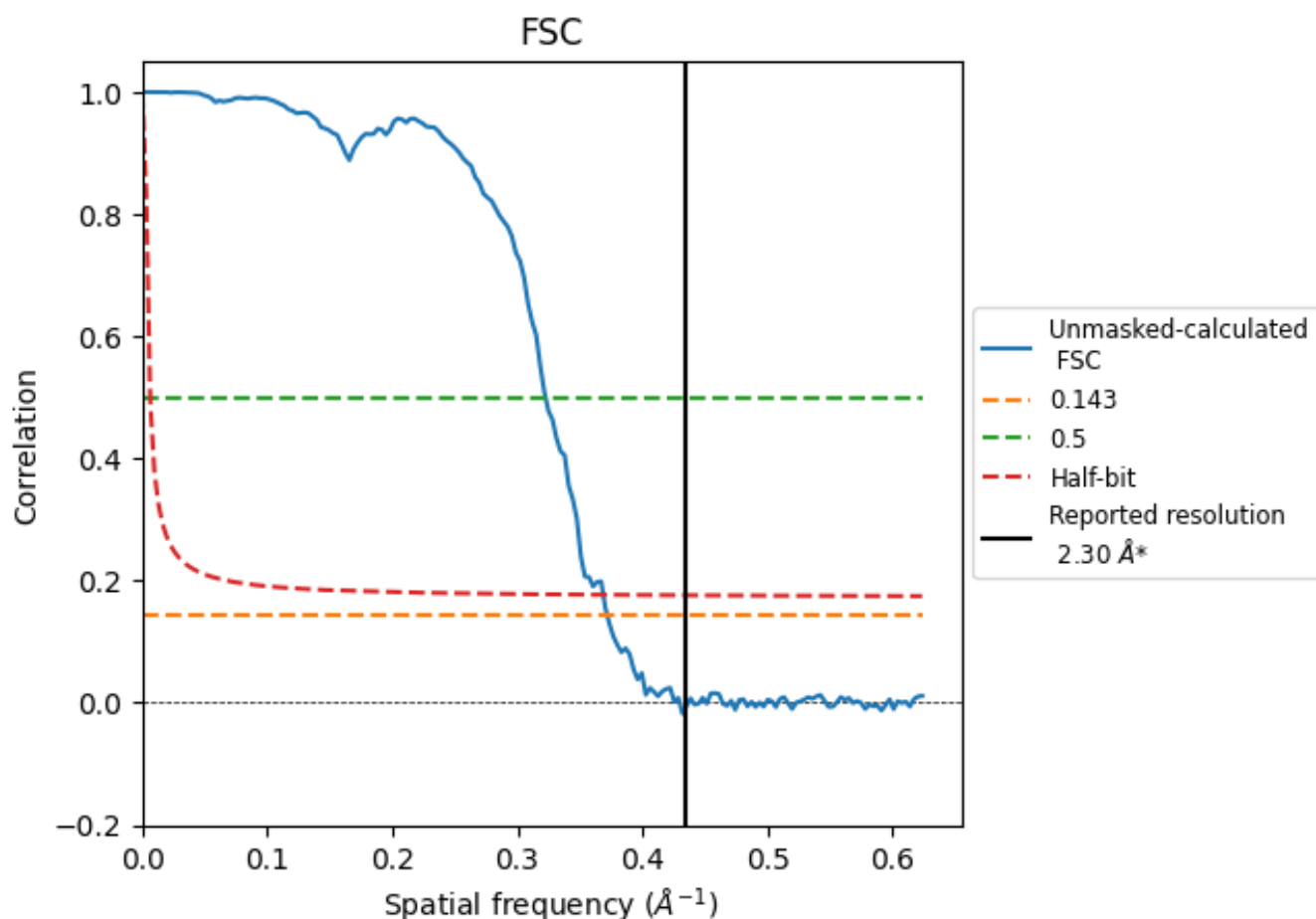


*Reported resolution corresponds to spatial frequency of $0.435 \text{ \AA}^{-1}$

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 $0.435 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

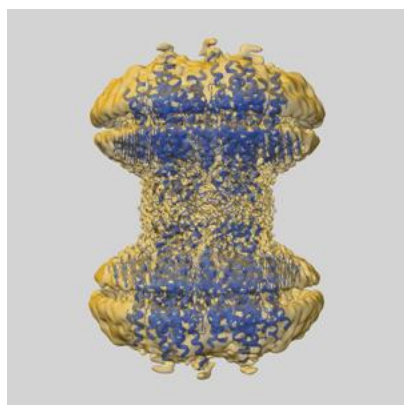
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.69	3.10	2.71

*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 2.69 differs from the reported value 2.3 by more than 10 %

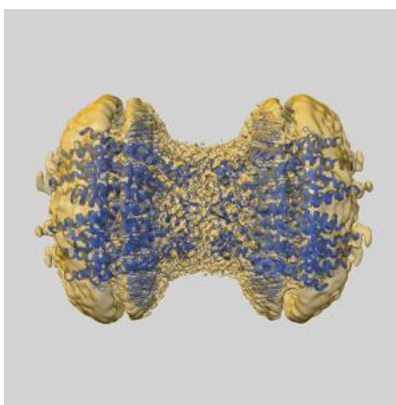
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73962 and PDB model 9Z9X. Per-residue inclusion information can be found in section [3](#) on page [25](#).

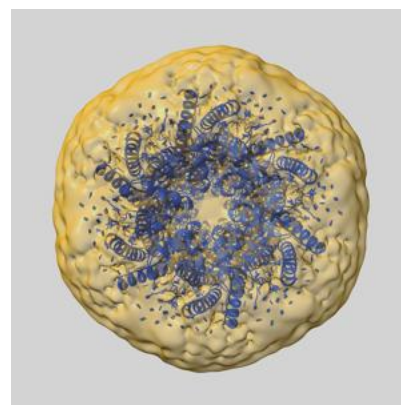
9.1 Map-model overlay [i](#)



X



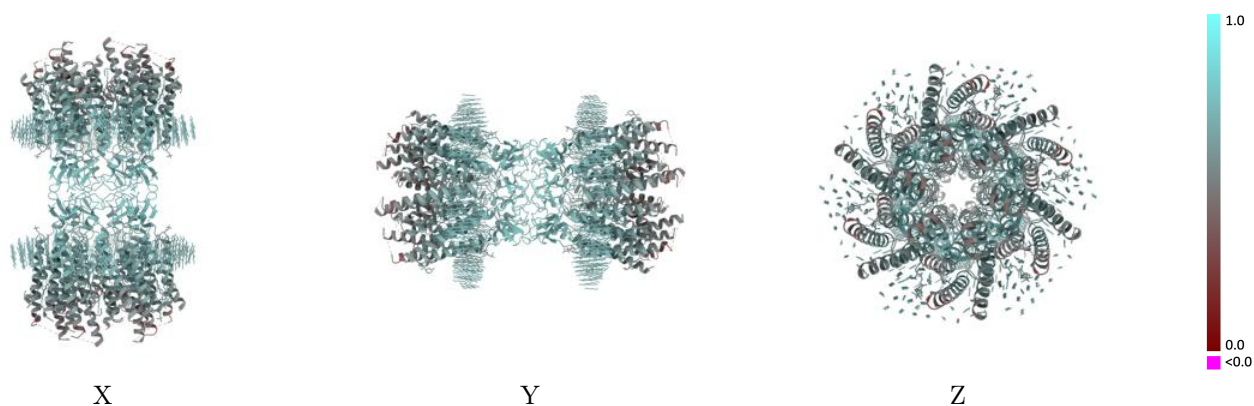
Y



Z

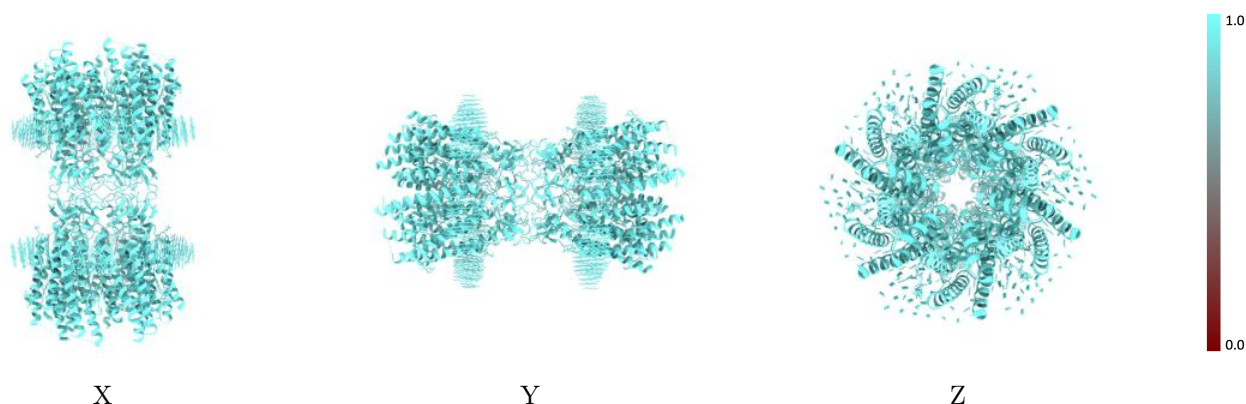
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



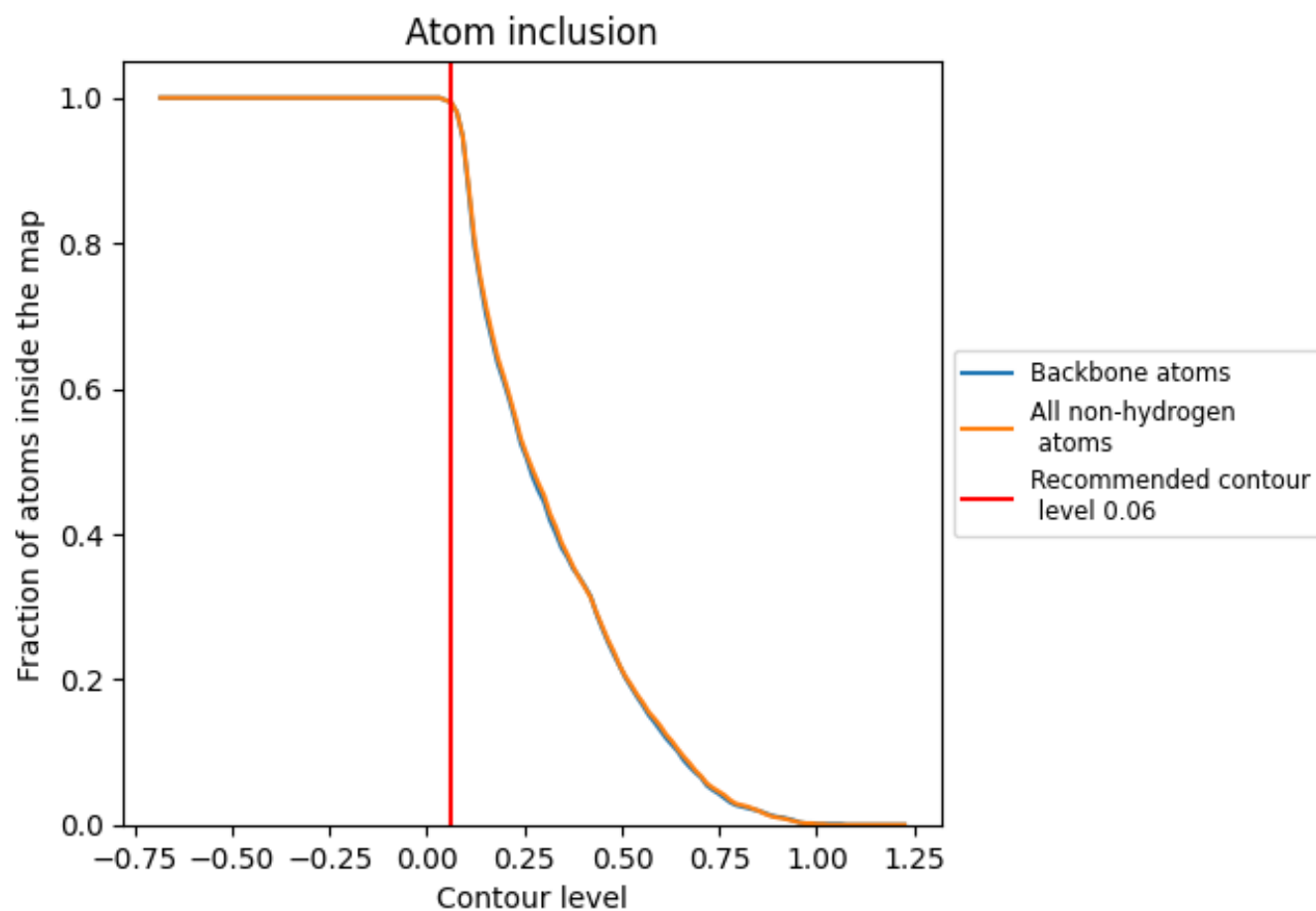
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9940	0.6250
A	0.9930	0.6240
B	0.9930	0.6260
C	0.9940	0.6250
D	0.9940	0.6260
E	0.9940	0.6250
F	0.9940	0.6230
G	0.9940	0.6260
H	0.9930	0.6260
I	0.9950	0.6230
J	0.9940	0.6230
K	0.9930	0.6240
L	0.9940	0.6230

1.0

0.0

<0.0