



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:03 AM UTC

PDB ID : 9Z8M / pdb_00009z8m
EMDB ID : EMD-73900
Title : Gated state sheep connexin-46 in DMPC nanodiscs at neutral pH
Authors : Jarodsky, J.M.; Myers, J.B.; Reichow, S.L.
Deposited on : 2025-11-18
Resolution : 2.70 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 EMD 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

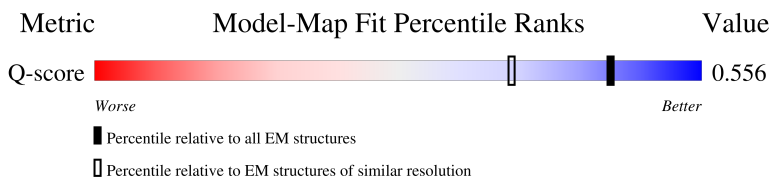
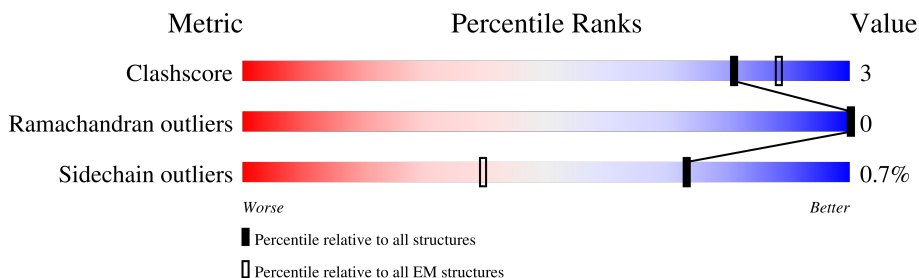
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	

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Mol	Chain	Length	Quality of chain
1	E	413	 41% . 55%
1	F	413	 41% . 55%
1	G	413	 41% . 55%
1	H	413	 41% . 55%
1	I	413	 41% . 55%
1	J	413	 41% . 55%
1	K	413	 41% . 55%
1	L	413	 41% . 55%

2 Entry composition

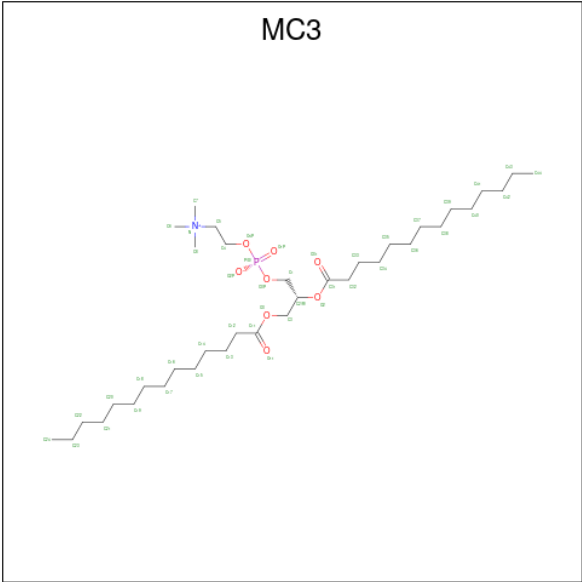
There are 2 unique types of molecules in this entry. The entry contains 40740 atoms, of which 21024 are hydrogens and 0 are deuteriums.

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	184	Total	C	H	N	O	S	0	0
			2844	959	1400	234	243	8		
1	B	184	Total	C	H	N	O	S	0	0
			2844	959	1400	234	243	8		
1	C	184	Total	C	H	N	O	S	0	0
			2844	959	1400	234	243	8		
1	D	184	Total	C	H	N	O	S	0	0
			2844	959	1400	234	243	8		
1	E	184	Total	C	H	N	O	S	0	0
			2844	959	1400	234	243	8		
1	F	184	Total	C	H	N	O	S	0	0
			2844	959	1400	234	243	8		
1	G	184	Total	C	H	N	O	S	0	0
			2844	959	1400	234	243	8		
1	H	184	Total	C	H	N	O	S	0	0
			2844	959	1400	234	243	8		
1	I	184	Total	C	H	N	O	S	0	0
			2844	959	1400	234	243	8		
1	J	184	Total	C	H	N	O	S	0	0
			2844	959	1400	234	243	8		
1	K	184	Total	C	H	N	O	S	0	0
			2844	959	1400	234	243	8		
1	L	184	Total	C	H	N	O	S	0	0
			2844	959	1400	234	243	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
			36	12	24	
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
			30	10	20	
2	A	1	Total	C	H	0
			39	13	26	
2	A	1	Total	C	H	0
			18	6	12	
2	A	1	Total	C	H	0
			27	9	18	
2	A	1	Total	C	H	0
			33	11	22	
2	A	1	Total	C	H	0
			24	8	16	
2	A	1	Total	C	H	0
			39	13	26	
2	A	1	Total	C	H	0
			33	11	22	
2	A	1	Total	C	H	0
			36	12	24	
2	A	1	Total	C	H	0
			24	8	16	
2	A	1	Total	C	H	0
			30	10	20	

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Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	H	O	P	0
			61	19	33	8	1	
2	A	1	Total	C	H	O	P	0
			43	13	21	8	1	
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
			39	13	26			
2	B	1	Total	C	H			0
			30	10	20			
2	B	1	Total	C	H			0
			39	13	26			
2	B	1	Total	C	H			0
			18	6	12			
2	B	1	Total	C	H			0
			27	9	18			
2	B	1	Total	C	H			0
			33	11	22			
2	B	1	Total	C	H			0
			24	8	16			
2	B	1	Total	C	H			0
			39	13	26			
2	B	1	Total	C	H			0
			33	11	22			
2	B	1	Total	C	H			0
			36	12	24			
2	B	1	Total	C	H			0
			24	8	16			
2	B	1	Total	C	H			0
			30	10	20			
2	B	1	Total	C	H	O	P	0
			61	19	33	8	1	
2	B	1	Total	C	H	O	P	0
			43	13	21	8	1	
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
			39	13	26			

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Mol	Chain	Residues	Atoms					AltConf	
2	C	1	Total 30	C 10	H 20				0
2	C	1	Total 39	C 13	H 26				0
2	C	1	Total 18	C 6	H 12				0
2	C	1	Total 27	C 9	H 18				0
2	C	1	Total 33	C 11	H 22				0
2	C	1	Total 24	C 8	H 16				0
2	C	1	Total 39	C 13	H 26				0
2	C	1	Total 33	C 11	H 22				0
2	C	1	Total 36	C 12	H 24				0
2	C	1	Total 24	C 8	H 16				0
2	C	1	Total 30	C 10	H 20				0
2	C	1	Total 61	C 19	H 33	O 8	P 1		0
2	C	1	Total 43	C 13	H 21	O 8	P 1		0
2	D	1	Total 36	C 12	H 24				0
2	D	1	Total 39	C 13	H 26				0
2	D	1	Total 39	C 13	H 26				0
2	D	1	Total 30	C 10	H 20				0
2	D	1	Total 39	C 13	H 26				0
2	D	1	Total 18	C 6	H 12				0
2	D	1	Total 27	C 9	H 18				0
2	D	1	Total 33	C 11	H 22				0

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Mol	Chain	Residues	Atoms					AltConf
2	D	1	Total	C	H			0
			24	8	16			
2	D	1	Total	C	H			0
			39	13	26			
2	D	1	Total	C	H			0
			33	11	22			
2	D	1	Total	C	H			0
			36	12	24			
2	D	1	Total	C	H			0
			24	8	16			
2	D	1	Total	C	H			0
			30	10	20			
2	D	1	Total	C	H	O	P	0
			61	19	33	8	1	
2	D	1	Total	C	H	O	P	0
			43	13	21	8	1	
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
			39	13	26			
2	E	1	Total	C	H			0
			30	10	20			
2	E	1	Total	C	H			0
			39	13	26			
2	E	1	Total	C	H			0
			18	6	12			
2	E	1	Total	C	H			0
			27	9	18			
2	E	1	Total	C	H			0
			33	11	22			
2	E	1	Total	C	H			0
			24	8	16			
2	E	1	Total	C	H			0
			39	13	26			
2	E	1	Total	C	H			0
			33	11	22			
2	E	1	Total	C	H			0
			36	12	24			
2	E	1	Total	C	H			0
			24	8	16			

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Mol	Chain	Residues	Atoms					AltConf
2	E	1	Total	C	H			0
			30	10	20			
2	E	1	Total	C	H	O	P	0
			61	19	33	8	1	
2	E	1	Total	C	H	O	P	0
			43	13	21	8	1	
2	F	1	Total	C	H			0
			39	13	26			
2	F	1	Total	C	H			0
			33	11	22			
2	F	1	Total	C	H			0
			36	12	24			
2	F	1	Total	C	H			0
			24	8	16			
2	F	1	Total	C	H			0
			30	10	20			
2	F	1	Total	C	H	O	P	0
			61	19	33	8	1	
2	F	1	Total	C	H	O	P	0
			43	13	21	8	1	
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
			39	13	26			
2	F	1	Total	C	H			0
			30	10	20			
2	F	1	Total	C	H			0
			39	13	26			
2	F	1	Total	C	H			0
			18	6	12			
2	F	1	Total	C	H			0
			27	9	18			
2	F	1	Total	C	H			0
			33	11	22			
2	F	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
			39	13	26			

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Mol	Chain	Residues	Atoms					AltConf
2	G	1	Total	C	H			0
			39	13	26			
2	G	1	Total	C	H			0
			30	10	20			
2	G	1	Total	C	H			0
			39	13	26			
2	G	1	Total	C	H			0
			18	6	12			
2	G	1	Total	C	H			0
			27	9	18			
2	G	1	Total	C	H			0
			33	11	22			
2	G	1	Total	C	H			0
			24	8	16			
2	G	1	Total	C	H			0
			39	13	26			
2	G	1	Total	C	H			0
			33	11	22			
2	G	1	Total	C	H			0
			36	12	24			
2	G	1	Total	C	H			0
			24	8	16			
2	G	1	Total	C	H			0
			30	10	20			
2	G	1	Total	C	H	O	P	0
			61	19	33	8	1	
2	G	1	Total	C	H	O	P	0
			43	13	21	8	1	
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
			39	13	26			
2	H	1	Total	C	H			0
			30	10	20			
2	H	1	Total	C	H			0
			39	13	26			
2	H	1	Total	C	H			0
			18	6	12			
2	H	1	Total	C	H			0
			27	9	18			

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Mol	Chain	Residues	Atoms					AltConf
2	H	1	Total 33	C 11	H 22			0
2	H	1	Total 24	C 8	H 16			0
2	H	1	Total 39	C 13	H 26			0
2	H	1	Total 33	C 11	H 22			0
2	H	1	Total 36	C 12	H 24			0
2	H	1	Total 24	C 8	H 16			0
2	H	1	Total 30	C 10	H 20			0
2	H	1	Total 61	C 19	H 33	O 8	P 1	0
2	H	1	Total 43	C 13	H 21	O 8	P 1	0
2	I	1	Total 36	C 12	H 24			0
2	I	1	Total 39	C 13	H 26			0
2	I	1	Total 39	C 13	H 26			0
2	I	1	Total 30	C 10	H 20			0
2	I	1	Total 39	C 13	H 26			0
2	I	1	Total 18	C 6	H 12			0
2	I	1	Total 27	C 9	H 18			0
2	I	1	Total 33	C 11	H 22			0
2	I	1	Total 24	C 8	H 16			0
2	I	1	Total 39	C 13	H 26			0
2	I	1	Total 33	C 11	H 22			0
2	I	1	Total 36	C 12	H 24			0

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Mol	Chain	Residues	Atoms					AltConf
2	I	1	Total	C	H			0
			24	8	16			
2	I	1	Total	C	H			0
			30	10	20			
2	I	1	Total	C	H	O	P	0
			61	19	33	8	1	
2	I	1	Total	C	H	O	P	0
			43	13	21	8	1	
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
			39	13	26			
2	J	1	Total	C	H			0
			30	10	20			
2	J	1	Total	C	H			0
			39	13	26			
2	J	1	Total	C	H			0
			18	6	12			
2	J	1	Total	C	H			0
			27	9	18			
2	J	1	Total	C	H			0
			33	11	22			
2	J	1	Total	C	H			0
			24	8	16			
2	J	1	Total	C	H			0
			39	13	26			
2	J	1	Total	C	H			0
			33	11	22			
2	J	1	Total	C	H			0
			36	12	24			
2	J	1	Total	C	H			0
			24	8	16			
2	J	1	Total	C	H			0
			30	10	20			
2	J	1	Total	C	H	O	P	0
			61	19	33	8	1	
2	J	1	Total	C	H	O	P	0
			43	13	21	8	1	
2	K	1	Total	C	H			0
			36	12	24			

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Mol	Chain	Residues	Atoms					AltConf
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
			30	10	20			
2	K	1	Total	C	H			0
			39	13	26			
2	K	1	Total	C	H			0
			18	6	12			
2	K	1	Total	C	H			0
			27	9	18			
2	K	1	Total	C	H			0
			33	11	22			
2	K	1	Total	C	H			0
			24	8	16			
2	K	1	Total	C	H			0
			39	13	26			
2	K	1	Total	C	H			0
			33	11	22			
2	K	1	Total	C	H			0
			36	12	24			
2	K	1	Total	C	H			0
			24	8	16			
2	K	1	Total	C	H			0
			30	10	20			
2	K	1	Total	C	H	O	P	0
			61	19	33	8	1	
2	K	1	Total	C	H	O	P	0
			43	13	21	8	1	
2	L	1	Total	C	H			0
			39	13	26			
2	L	1	Total	C	H			0
			33	11	22			
2	L	1	Total	C	H			0
			36	12	24			
2	L	1	Total	C	H			0
			24	8	16			
2	L	1	Total	C	H			0
			30	10	20			
2	L	1	Total	C	H	O	P	0
			61	19	33	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	L	1	Total 43	C 13	H 21	O 8	P 1	0
2	L	1	Total 36	C 12	H 24			0
2	L	1	Total 39	C 13	H 26			0
2	L	1	Total 39	C 13	H 26			0
2	L	1	Total 30	C 10	H 20			0
2	L	1	Total 39	C 13	H 26			0
2	L	1	Total 18	C 6	H 12			0
2	L	1	Total 27	C 9	H 18			0
2	L	1	Total 33	C 11	H 22			0
2	L	1	Total 24	C 8	H 16			0

SER	THR	PRO	L142	MET
LYS	SER	SER	T145	GLY
ALA	ALA	ALA		W4
SER	ARG	SER		
LYS	LYS	SER	Y220	Y24
SER	ALA	LEU	H221	
SER	PRO	GLY	L222	L37
GLY	PRO	GLN		
GLY	ALA	ALA	TRP	E42
ARG	ALA	SER	LYS	
ALA	SER	ALA	LYS	Q81
ARG	THR	PRO	LEU	
ALA	THR	GLY	LYS	W85
ALA	PRO	TYR	GLN	
ASP	ALA	PRO	GLY	S86
LEU	ALA	GLU	MET	T87
ALA	ALA	PRO	THR	
ILE	ALA	PRO	SER	Y92
	GLY	LEU	PRO	
	GLY	PRO	PHE	Y96
	PRO	ALA	ARG	L97
	PRO	ALA	PRO	
	GLN	LEU	ASP	E103
	GLN	PRO	THR	
	PHE	PRO	ARG	LYS
	LEU	GLY	GLY	ARG
	PRO	THR	SER	GLY
	GLY	PRO	GLY	GLU
	GLY	GLY	ARG	ARG
	ALA	THR	ALA	GLU
	ALA	PRO	GLY	GLU
	GLY	GLY	SER	GLU
	SER	THR	MET	LYS
	ASP	LEU	GLY	ALA
	ASP	GLY	GLY	ALA
	GLY	GLY	SER	PRO
	GLY	GLY	PRO	ALA
	GLY	GLY	LEU	GLU
	ALA	GLY	LEU	GLU
	VAL	ASN	LEU	HIS
	THR	GLN	LEU	GLN
	ALA	GLY	PRO	ASP
	VAL	LEU	PRO	PRO
	GLU	ARG	ASN	ALA
	LEU	ALA	SER	ALA
	HIS	PRO	ALA	PRO
	ALA	ALA	PRO	VAL
	PRO	GLN	ALA	ARG
	PRO	ASN	VAL	ASP
	GLU	CYS	THR	ASP
	PRO	ALA	ILE	ARG
	PRO	ASN	GLY	GLY
	ALA	ARG	PHE	LYS
	ASP	GLU	PRO	VAL
	PRO	ALA	PRO	ARG
	GLY	GLU	TTR	ILE
	ARG	PRO	TTR	ALA
	SER	CYS	ALA	Y143
				G140

SER	GLN	ALA		A141	MET
SER	THR	PRO		L142	GLY
LYS	SER	ALA		T145	ASP
ALA	ARG	ALA			V4
SER	LYS	SER		Y220	V24
SER	ALA	LEU		H221	
SER	SER	GLY		L222	L37
GLY	PRO	GLN		GLY	E42
GLY	PRO	ALA		TRP	
ARG	ALA	SER		LYS	Q61
ALA	SER	ALA		LYS	
ARG	THR	PRO		LEU	V85
ALA	PRO	TYR		LYS	S86
ALA	PRO	GLN		GLN	T57
ASP	ALA	PRO		GLY	
LEU	ALA	GLU		MET	I91
ALA	PRO	PRO		THR	Y92
ILE	ALA	PRO		SER	V96
	GLY	LEU		PHE	L97
	GLY	PRO		ALA	
	PRO	ALA		ARG	F104
	GLN	ALA		PRO	LYS
	GLN	LEU		ASP	ARG
	PHE	PRO		THR	LYS
	LEU	GLY		PRO	LYS
	PRO	THR		GLY	GLU
	GLY	PRO		SER	ARG
	GLY	GLY		ARG	GLU
	ALA	THR		ALA	GLU
	ALA	PRO		GLY	GLU
	GLY	THR		ALA	PRO
	SER	THR		ALA	PRO
	SER	THR		LYS	LYS
	GLY	THR		PRO	ALA
	ASP	THR		MET	ALA
	SER	LEU		GLY	GLY
	ASP	GLY		SER	PRO
	GLY	GLY		SER	ALA
	GLU	GLY		PRO	GLU
	GLY	GLY		LEU	GLU
	ALA	GLY		LEU	GLU
	VAL	ASN		LEU	HIS
	THR	GLN		PRO	GLN
	ALA	GLY		PRO	ASP
	VAL	LEU		ASN	PRO
	GLU	ARG		SER	ALA
	LEU	ALA		ALA	PRO
	HIS	PRO		PRO	VAL
	ALA	GLN		PRO	ASP
	PRO	GLN		ALA	ASP
	PRO	ASN		VAL	ARG
	GLU	CYS		THR	GLY
	PRO	ALA		ILE	GLY
	PRO	ASN		PHE	LYS
	ALA	ARG		THR	VAL
	ASP	GLU		PRO	ILE
	PRO	ALA		ALA	ALA
	GLY	GLU		THR	GLA
	ARG	PRO		TVR	G104

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D6	Depositor
Number of particles used	15342	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	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.294	Depositor
Minimum map value	-0.962	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	315.648, 315.648, 315.648	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.822, 0.822, 0.822	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	0.12	0/1484	0.25	0/2027
1	B	0.13	0/1484	0.25	0/2027
1	C	0.12	0/1484	0.25	0/2027
1	D	0.13	0/1484	0.25	0/2027
1	E	0.13	0/1484	0.25	0/2027
1	F	0.13	0/1484	0.25	0/2027
1	G	0.13	0/1484	0.25	0/2027
1	H	0.13	0/1484	0.25	0/2027
1	I	0.13	0/1484	0.25	0/2027
1	J	0.13	0/1484	0.25	0/2027
1	K	0.12	0/1484	0.25	0/2027
1	L	0.13	0/1484	0.25	0/2027
All	All	0.13	0/17808	0.25	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	1444	1400	1402	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1444	1400	1402	9	0
1	C	1444	1400	1402	7	0
1	D	1444	1400	1402	8	0
1	E	1444	1400	1402	9	0
1	F	1444	1400	1402	9	0
1	G	1444	1400	1402	9	0
1	H	1444	1400	1402	10	0
1	I	1444	1400	1402	9	0
1	J	1444	1400	1402	9	0
1	K	1444	1400	1402	8	0
1	L	1444	1400	1402	9	0
2	A	199	352	309	2	0
2	B	199	352	309	1	0
2	C	199	352	309	2	0
2	D	199	352	309	2	0
2	E	199	352	309	2	0
2	F	199	352	309	2	0
2	G	199	352	309	2	0
2	H	199	352	309	2	0
2	I	199	352	309	2	0
2	J	199	352	309	2	0
2	K	199	352	309	2	0
2	L	199	352	309	2	0
All	All	19716	21024	20532	106	0

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

All (106) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:37:LEU:O	1:E:42:GLU:HG2	1.94	0.68
1:L:37:LEU:O	1:L:42:GLU:HG2	1.94	0.68
1:J:37:LEU:O	1:J:42:GLU:HG2	1.94	0.68
1:C:37:LEU:O	1:C:42:GLU:HG2	1.94	0.68
1:G:37:LEU:O	1:G:42:GLU:HG2	1.93	0.67
1:K:37:LEU:O	1:K:42:GLU:HG2	1.94	0.67
1:B:37:LEU:O	1:B:42:GLU:HG2	1.94	0.67
1:I:37:LEU:O	1:I:42:GLU:HG2	1.94	0.67
1:D:37:LEU:O	1:D:42:GLU:HG2	1.94	0.67
1:F:37:LEU:O	1:F:42:GLU:HG2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:LEU:O	1:H:42:GLU:HG2	1.93	0.67
1:A:37:LEU:O	1:A:42:GLU:HG2	1.94	0.67
1:C:96:VAL:HG22	1:C:142:LEU:HD11	1.91	0.53
1:J:96:VAL:HG22	1:J:142:LEU:HD11	1.91	0.53
1:B:96:VAL:HG22	1:B:142:LEU:HD11	1.91	0.53
1:D:96:VAL:HG22	1:D:142:LEU:HD11	1.91	0.53
1:I:96:VAL:HG22	1:I:142:LEU:HD11	1.91	0.53
1:K:96:VAL:HG22	1:K:142:LEU:HD11	1.91	0.53
1:F:24:VAL:HG13	2:F:506:MC3:H131	1.90	0.52
1:L:24:VAL:HG13	2:L:506:MC3:H131	1.90	0.52
1:E:96:VAL:HG22	1:E:142:LEU:HD11	1.91	0.52
1:H:96:VAL:HG22	1:H:142:LEU:HD11	1.91	0.52
1:L:96:VAL:HG22	1:L:142:LEU:HD11	1.91	0.52
1:A:96:VAL:HG22	1:A:142:LEU:HD11	1.91	0.52
1:L:97:LEU:C	1:L:97:LEU:HD13	2.35	0.52
1:E:97:LEU:C	1:E:97:LEU:HD13	2.35	0.52
1:G:96:VAL:HG22	1:G:142:LEU:HD11	1.91	0.52
1:F:96:VAL:HG22	1:F:142:LEU:HD11	1.91	0.52
1:F:97:LEU:HD13	1:F:97:LEU:C	2.35	0.51
1:G:97:LEU:C	1:G:97:LEU:HD13	2.35	0.51
1:E:24:VAL:HG13	2:E:515:MC3:H131	1.91	0.51
1:K:97:LEU:C	1:K:97:LEU:HD13	2.35	0.51
1:D:97:LEU:C	1:D:97:LEU:HD13	2.35	0.51
1:H:24:VAL:HG13	2:H:515:MC3:H131	1.92	0.51
1:A:97:LEU:C	1:A:97:LEU:HD13	2.35	0.51
1:C:97:LEU:C	1:C:97:LEU:HD13	2.35	0.51
1:I:97:LEU:C	1:I:97:LEU:HD13	2.35	0.51
1:H:97:LEU:C	1:H:97:LEU:HD13	2.35	0.50
1:J:97:LEU:C	1:J:97:LEU:HD13	2.35	0.50
1:B:97:LEU:C	1:B:97:LEU:HD13	2.35	0.50
1:I:24:VAL:HG13	2:I:515:MC3:H131	1.92	0.50
1:B:24:VAL:HG13	2:B:515:MC3:H131	1.92	0.50
1:K:24:VAL:HG13	2:K:515:MC3:H131	1.93	0.50
1:C:24:VAL:HG13	2:C:515:MC3:H131	1.94	0.48
1:A:92:TYR:HD2	1:A:145:THR:HG22	1.79	0.48
1:F:92:TYR:HD2	1:F:145:THR:HG22	1.79	0.48
1:G:92:TYR:HD2	1:G:145:THR:HG22	1.79	0.48
1:D:24:VAL:HG13	2:D:515:MC3:H131	1.95	0.48
1:H:92:TYR:HD2	1:H:145:THR:HG22	1.79	0.48
1:I:92:TYR:HD2	1:I:145:THR:HG22	1.79	0.47
1:B:92:TYR:HD2	1:B:145:THR:HG22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:TYR:HD2	1:E:145:THR:HG22	1.79	0.47
1:L:92:TYR:HD2	1:L:145:THR:HG22	1.79	0.47
1:K:92:TYR:HD2	1:K:145:THR:HG22	1.79	0.46
1:J:92:TYR:HD2	1:J:145:THR:HG22	1.79	0.46
1:D:92:TYR:HD2	1:D:145:THR:HG22	1.79	0.46
1:C:92:TYR:HD2	1:C:145:THR:HG22	1.79	0.46
1:G:24:VAL:HG13	2:G:515:MC3:H131	1.99	0.44
1:A:24:VAL:HG13	2:A:515:MC3:H131	1.99	0.44
1:F:81:GLN:O	1:F:85:VAL:HG22	2.18	0.44
1:G:81:GLN:O	1:G:85:VAL:HG22	2.18	0.44
1:L:81:GLN:O	1:L:85:VAL:HG22	2.18	0.44
1:E:81:GLN:O	1:E:85:VAL:HG22	2.18	0.44
1:E:220:TYR:C	1:E:220:TYR:CD2	2.96	0.44
1:L:220:TYR:CD2	1:L:220:TYR:C	2.96	0.44
1:D:220:TYR:C	1:D:220:TYR:CD2	2.96	0.43
1:F:220:TYR:C	1:F:220:TYR:CD2	2.96	0.43
1:G:220:TYR:CD2	1:G:220:TYR:C	2.96	0.43
1:H:81:GLN:O	1:H:85:VAL:HG22	2.18	0.43
1:A:81:GLN:O	1:A:85:VAL:HG22	2.18	0.43
1:C:220:TYR:C	1:C:220:TYR:CD2	2.96	0.43
1:K:220:TYR:C	1:K:220:TYR:CD2	2.96	0.43
1:J:220:TYR:CD2	1:J:220:TYR:C	2.96	0.43
1:J:24:VAL:HG13	2:J:515:MC3:H131	2.00	0.43
1:D:81:GLN:O	1:D:85:VAL:HG22	2.18	0.43
1:H:220:TYR:CD2	1:H:220:TYR:C	2.96	0.43
1:K:81:GLN:O	1:K:85:VAL:HG22	2.18	0.43
1:A:220:TYR:CD2	1:A:220:TYR:C	2.96	0.43
1:B:81:GLN:O	1:B:85:VAL:HG22	2.18	0.43
1:I:81:GLN:O	1:I:85:VAL:HG22	2.18	0.43
1:I:220:TYR:CD2	1:I:220:TYR:C	2.96	0.43
1:C:81:GLN:O	1:C:85:VAL:HG22	2.18	0.43
1:B:220:TYR:CD2	1:B:220:TYR:C	2.96	0.43
1:J:81:GLN:O	1:J:85:VAL:HG22	2.18	0.43
2:C:515:MC3:H351	1:D:91:ILE:HG13	2.02	0.42
2:D:515:MC3:H351	1:E:91:ILE:HG13	2.02	0.42
2:J:515:MC3:H351	1:K:91:ILE:HG13	2.02	0.42
2:K:515:MC3:H351	1:L:91:ILE:HG13	2.02	0.42
1:G:91:ILE:HG13	2:L:506:MC3:H351	2.02	0.41
2:E:515:MC3:H351	1:F:91:ILE:HG13	2.02	0.41
2:H:515:MC3:H351	1:I:91:ILE:HG13	2.02	0.41
2:A:515:MC3:H351	1:B:91:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:GLU:OE2	1:F:218:GLU:HA	2.21	0.41
1:G:218:GLU:OE2	1:G:218:GLU:HA	2.21	0.41
1:A:91:ILE:HG13	2:F:506:MC3:H351	2.02	0.41
1:L:218:GLU:OE2	1:L:218:GLU:HA	2.21	0.41
1:A:33:ARG:HG2	1:A:207:VAL:HG11	2.03	0.41
1:E:218:GLU:OE2	1:E:218:GLU:HA	2.21	0.41
2:G:515:MC3:H351	1:H:91:ILE:HG13	2.02	0.40
1:I:33:ARG:HG2	1:I:207:VAL:HG11	2.03	0.40
1:A:218:GLU:OE2	1:A:218:GLU:HA	2.21	0.40
1:B:33:ARG:HG2	1:B:207:VAL:HG11	2.03	0.40
1:H:33:ARG:HG2	1:H:207:VAL:HG11	2.03	0.40
1:H:218:GLU:OE2	1:H:218:GLU:HA	2.21	0.40
1:J:218:GLU:HA	1:J:218:GLU:OE2	2.21	0.40
2:I:515:MC3:H351	1:J:91:ILE:HG13	2.02	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	180/413 (44%)	177 (98%)	3 (2%)	0	100	100
1	B	180/413 (44%)	177 (98%)	3 (2%)	0	100	100
1	C	180/413 (44%)	177 (98%)	3 (2%)	0	100	100
1	D	180/413 (44%)	177 (98%)	3 (2%)	0	100	100
1	E	180/413 (44%)	177 (98%)	3 (2%)	0	100	100
1	F	180/413 (44%)	177 (98%)	3 (2%)	0	100	100
1	G	180/413 (44%)	177 (98%)	3 (2%)	0	100	100
1	H	180/413 (44%)	177 (98%)	3 (2%)	0	100	100
1	I	180/413 (44%)	177 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	180/413 (44%)	177 (98%)	3 (2%)	0	100	100
1	K	180/413 (44%)	177 (98%)	3 (2%)	0	100	100
1	L	180/413 (44%)	177 (98%)	3 (2%)	0	100	100
All	All	2160/4956 (44%)	2124 (98%)	36 (2%)	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	150/325 (46%)	149 (99%)	1 (1%)	76	90
1	B	150/325 (46%)	149 (99%)	1 (1%)	76	90
1	C	150/325 (46%)	149 (99%)	1 (1%)	76	90
1	D	150/325 (46%)	149 (99%)	1 (1%)	76	90
1	E	150/325 (46%)	149 (99%)	1 (1%)	76	90
1	F	150/325 (46%)	149 (99%)	1 (1%)	76	90
1	G	150/325 (46%)	149 (99%)	1 (1%)	76	90
1	H	150/325 (46%)	149 (99%)	1 (1%)	76	90
1	I	150/325 (46%)	149 (99%)	1 (1%)	76	90
1	J	150/325 (46%)	149 (99%)	1 (1%)	76	90
1	K	150/325 (46%)	149 (99%)	1 (1%)	76	90
1	L	150/325 (46%)	149 (99%)	1 (1%)	76	90
All	All	1800/3900 (46%)	1788 (99%)	12 (1%)	73	90

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

Mol	Chain	Res	Type
1	A	87	THR
1	B	87	THR

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Mol	Chain	Res	Type
1	C	87	THR
1	D	87	THR
1	E	87	THR
1	F	87	THR
1	G	87	THR
1	H	87	THR
1	I	87	THR
1	J	87	THR
1	K	87	THR
1	L	87	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	81	GLN
1	B	57	GLN
1	B	81	GLN
1	C	57	GLN
1	C	81	GLN
1	D	81	GLN
1	E	57	GLN
1	E	81	GLN
1	F	57	GLN
1	F	81	GLN
1	G	57	GLN
1	G	81	GLN
1	H	57	GLN
1	H	81	GLN
1	I	81	GLN
1	J	81	GLN
1	K	57	GLN
1	K	81	GLN
1	L	57	GLN
1	L	81	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

192 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	K	506	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	A	505	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	H	510	-	12,12,45	0.21	0	11,11,53	0.21	0
2	MC3	E	502	-	12,12,45	0.23	0	11,11,53	0.22	0
2	MC3	G	503	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	B	511	-	10,10,45	0.24	0	9,9,53	0.18	0
2	MC3	L	515	-	10,10,45	0.23	0	9,9,53	0.22	0
2	MC3	D	513	-	7,7,45	0.26	0	6,6,53	0.18	0
2	MC3	E	507	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	K	514	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	D	516	-	21,21,45	0.58	0	24,26,53	0.61	1 (4%)
2	MC3	I	502	-	12,12,45	0.23	0	11,11,53	0.21	0
2	MC3	K	502	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	C	513	-	7,7,45	0.26	0	6,6,53	0.19	0
2	MC3	F	505	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	E	503	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	F	510	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	B	507	-	8,8,45	0.25	0	7,7,53	0.18	0
2	MC3	B	510	-	12,12,45	0.21	0	11,11,53	0.21	0
2	MC3	B	516	-	21,21,45	0.58	0	24,26,53	0.62	1 (4%)
2	MC3	K	508	-	10,10,45	0.23	0	9,9,53	0.22	0
2	MC3	A	515	-	27,27,45	0.50	0	30,32,53	0.65	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	C	510	-	12,12,45	0.21	0	11,11,53	0.21	0
2	MC3	G	513	-	7,7,45	0.26	0	6,6,53	0.18	0
2	MC3	I	514	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	A	509	-	7,7,45	0.55	0	6,6,53	0.38	0
2	MC3	J	505	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	D	503	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	F	511	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	A	510	-	12,12,45	0.21	0	11,11,53	0.21	0
2	MC3	G	516	-	21,21,45	0.58	0	24,26,53	0.61	1 (4%)
2	MC3	L	511	-	9,9,45	0.23	0	8,8,53	0.19	0
2	MC3	B	515	-	27,27,45	0.49	0	30,32,53	0.65	1 (3%)
2	MC3	E	505	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	E	511	-	10,10,45	0.24	0	9,9,53	0.18	0
2	MC3	J	513	-	7,7,45	0.26	0	6,6,53	0.18	0
2	MC3	C	509	-	7,7,45	0.55	0	6,6,53	0.38	0
2	MC3	D	512	-	11,11,45	0.24	0	10,10,53	0.18	0
2	MC3	J	514	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	F	513	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	D	505	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	B	504	-	9,9,45	0.23	0	8,8,53	0.19	0
2	MC3	L	516	-	7,7,45	0.55	0	6,6,53	0.39	0
2	MC3	B	505	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	C	512	-	11,11,45	0.24	0	10,10,53	0.18	0
2	MC3	A	508	-	10,10,45	0.23	0	9,9,53	0.22	0
2	MC3	D	501	-	11,11,45	0.23	0	10,10,53	0.19	0
2	MC3	G	506	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	D	506	-	5,5,45	0.26	0	4,4,53	0.18	0
2	MC3	J	511	-	10,10,45	0.24	0	9,9,53	0.18	0
2	MC3	D	514	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	I	515	-	27,27,45	0.50	0	30,32,53	0.65	1 (3%)
2	MC3	K	504	-	9,9,45	0.23	0	8,8,53	0.19	0
2	MC3	F	501	-	12,12,45	0.21	0	11,11,53	0.21	0
2	MC3	K	511	-	10,10,45	0.23	0	9,9,53	0.18	0
2	MC3	F	503	-	11,11,45	0.24	0	10,10,53	0.18	0
2	MC3	C	506	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	F	506	-	27,27,45	0.49	0	30,32,53	0.65	1 (3%)
2	MC3	B	506	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	L	503	-	11,11,45	0.24	0	10,10,53	0.18	0
2	MC3	H	501	-	11,11,45	0.22	0	10,10,53	0.19	0
2	MC3	H	509	-	7,7,45	0.55	0	6,6,53	0.39	0
2	MC3	A	504	-	9,9,45	0.23	0	8,8,53	0.19	0
2	MC3	D	509	-	7,7,45	0.55	0	6,6,53	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	F	512	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	G	502	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	F	514	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	H	511	-	10,10,45	0.24	0	9,9,53	0.18	0
2	MC3	I	516	-	21,21,45	0.58	0	24,26,53	0.61	1 (4%)
2	MC3	K	512	-	11,11,45	0.24	0	10,10,53	0.18	0
2	MC3	K	513	-	7,7,45	0.25	0	6,6,53	0.18	0
2	MC3	A	507	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	E	501	-	11,11,45	0.22	0	10,10,53	0.19	0
2	MC3	E	513	-	7,7,45	0.26	0	6,6,53	0.19	0
2	MC3	B	502	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	H	506	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	I	508	-	10,10,45	0.23	0	9,9,53	0.22	0
2	MC3	H	502	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	C	505	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	H	504	-	9,9,45	0.23	0	8,8,53	0.19	0
2	MC3	J	507	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	L	506	-	27,27,45	0.49	0	30,32,53	0.65	1 (3%)
2	MC3	A	513	-	7,7,45	0.25	0	6,6,53	0.18	0
2	MC3	I	503	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	E	504	-	9,9,45	0.23	0	8,8,53	0.19	0
2	MC3	K	503	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	G	510	-	12,12,45	0.20	0	11,11,53	0.21	0
2	MC3	J	512	-	11,11,45	0.24	0	10,10,53	0.18	0
2	MC3	A	512	-	11,11,45	0.24	0	10,10,53	0.18	0
2	MC3	C	503	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	G	504	-	9,9,45	0.23	0	8,8,53	0.19	0
2	MC3	I	504	-	9,9,45	0.23	0	8,8,53	0.19	0
2	MC3	L	502	-	10,10,45	0.23	0	9,9,53	0.18	0
2	MC3	L	514	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	J	503	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	I	507	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	E	512	-	11,11,45	0.24	0	10,10,53	0.18	0
2	MC3	E	514	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	L	508	-	11,11,45	0.22	0	10,10,53	0.19	0
2	MC3	C	501	-	11,11,45	0.22	0	10,10,53	0.19	0
2	MC3	I	506	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	J	508	-	10,10,45	0.23	0	9,9,53	0.22	0
2	MC3	G	512	-	11,11,45	0.24	0	10,10,53	0.18	0
2	MC3	H	513	-	7,7,45	0.25	0	6,6,53	0.18	0
2	MC3	J	501	-	11,11,45	0.22	0	10,10,53	0.19	0
2	MC3	F	515	-	10,10,45	0.23	0	9,9,53	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	H	505	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	I	513	-	7,7,45	0.26	0	6,6,53	0.18	0
2	MC3	I	510	-	12,12,45	0.21	0	11,11,53	0.21	0
2	MC3	G	511	-	10,10,45	0.24	0	9,9,53	0.18	0
2	MC3	H	508	-	10,10,45	0.23	0	9,9,53	0.22	0
2	MC3	B	509	-	7,7,45	0.55	0	6,6,53	0.39	0
2	MC3	H	515	-	27,27,45	0.49	0	30,32,53	0.65	1 (3%)
2	MC3	K	510	-	12,12,45	0.21	0	11,11,53	0.21	0
2	MC3	L	504	-	7,7,45	0.26	0	6,6,53	0.19	0
2	MC3	A	511	-	10,10,45	0.24	0	9,9,53	0.18	0
2	MC3	A	502	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	L	505	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	K	507	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	C	504	-	9,9,45	0.23	0	8,8,53	0.19	0
2	MC3	C	511	-	10,10,45	0.24	0	9,9,53	0.18	0
2	MC3	H	512	-	11,11,45	0.24	0	10,10,53	0.18	0
2	MC3	C	507	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	F	508	-	11,11,45	0.23	0	10,10,53	0.19	0
2	MC3	G	514	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	F	509	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	C	508	-	10,10,45	0.23	0	9,9,53	0.22	0
2	MC3	G	509	-	7,7,45	0.55	0	6,6,53	0.39	0
2	MC3	K	515	-	27,27,45	0.49	0	30,32,53	0.65	1 (3%)
2	MC3	J	510	-	12,12,45	0.21	0	11,11,53	0.21	0
2	MC3	D	510	-	12,12,45	0.21	0	11,11,53	0.21	0
2	MC3	F	516	-	7,7,45	0.55	0	6,6,53	0.38	0
2	MC3	B	501	-	11,11,45	0.22	0	10,10,53	0.19	0
2	MC3	B	503	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	D	511	-	10,10,45	0.23	0	9,9,53	0.18	0
2	MC3	C	516	-	21,21,45	0.58	0	24,26,53	0.62	1 (4%)
2	MC3	L	513	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	L	512	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	J	516	-	21,21,45	0.58	0	24,26,53	0.62	1 (4%)
2	MC3	D	504	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	I	501	-	11,11,45	0.22	0	10,10,53	0.19	0
2	MC3	A	501	-	11,11,45	0.22	0	10,10,53	0.19	0
2	MC3	I	511	-	10,10,45	0.24	0	9,9,53	0.18	0
2	MC3	A	503	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	D	507	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	C	515	-	27,27,45	0.49	0	30,32,53	0.65	1 (3%)
2	MC3	E	510	-	12,12,45	0.21	0	11,11,53	0.21	0
2	MC3	E	516	-	21,21,45	0.58	0	24,26,53	0.61	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	H	514	-	9,9,45	0.23	0	8,8,53	0.18	0
2	MC3	J	515	-	27,27,45	0.49	0	30,32,53	0.65	1 (3%)
2	MC3	H	507	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	H	516	-	21,21,45	0.58	0	24,26,53	0.61	1 (4%)
2	MC3	L	507	-	21,21,45	0.59	0	24,26,53	0.62	1 (4%)
2	MC3	I	509	-	7,7,45	0.56	0	6,6,53	0.38	0
2	MC3	K	509	-	7,7,45	0.55	0	6,6,53	0.38	0
2	MC3	G	505	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	L	509	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	G	507	-	8,8,45	0.25	0	7,7,53	0.19	0
2	MC3	E	508	-	10,10,45	0.23	0	9,9,53	0.22	0
2	MC3	B	512	-	11,11,45	0.24	0	10,10,53	0.18	0
2	MC3	E	515	-	27,27,45	0.49	0	30,32,53	0.65	1 (3%)
2	MC3	B	513	-	7,7,45	0.26	0	6,6,53	0.19	0
2	MC3	B	514	-	9,9,45	0.24	0	8,8,53	0.19	0
2	MC3	C	502	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	K	516	-	21,21,45	0.58	0	24,26,53	0.61	1 (4%)
2	MC3	D	508	-	10,10,45	0.23	0	9,9,53	0.22	0
2	MC3	G	515	-	27,27,45	0.49	0	30,32,53	0.65	1 (3%)
2	MC3	D	515	-	27,27,45	0.50	0	30,32,53	0.65	1 (3%)
2	MC3	G	501	-	11,11,45	0.22	0	10,10,53	0.19	0
2	MC3	F	504	-	7,7,45	0.26	0	6,6,53	0.19	0
2	MC3	L	501	-	12,12,45	0.20	0	11,11,53	0.21	0
2	MC3	B	508	-	10,10,45	0.23	0	9,9,53	0.22	0
2	MC3	H	503	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	F	507	-	21,21,45	0.58	0	24,26,53	0.61	1 (4%)
2	MC3	A	516	-	21,21,45	0.58	0	24,26,53	0.62	1 (4%)
2	MC3	J	506	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	A	514	-	9,9,45	0.23	0	8,8,53	0.19	0
2	MC3	J	509	-	7,7,45	0.56	0	6,6,53	0.38	0
2	MC3	I	512	-	11,11,45	0.24	0	10,10,53	0.18	0
2	MC3	F	502	-	10,10,45	0.24	0	9,9,53	0.18	0
2	MC3	I	505	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	E	506	-	5,5,45	0.26	0	4,4,53	0.17	0
2	MC3	K	505	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	L	510	-	12,12,45	0.22	0	11,11,53	0.22	0
2	MC3	A	506	-	5,5,45	0.27	0	4,4,53	0.17	0
2	MC3	E	509	-	7,7,45	0.55	0	6,6,53	0.38	0
2	MC3	C	514	-	9,9,45	0.23	0	8,8,53	0.18	0
2	MC3	D	502	-	12,12,45	0.23	0	11,11,53	0.22	0
2	MC3	G	508	-	10,10,45	0.23	0	9,9,53	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	J	502	-	12,12,45	0.22	0	11,11,53	0.21	0
2	MC3	J	504	-	9,9,45	0.23	0	8,8,53	0.19	0
2	MC3	K	501	-	11,11,45	0.22	0	10,10,53	0.19	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	K	506	-	-	0/3/3/49	-
2	MC3	A	505	-	-	0/10/10/49	-
2	MC3	H	510	-	-	0/10/10/49	-
2	MC3	E	502	-	-	0/10/10/49	-
2	MC3	G	503	-	-	0/10/10/49	-
2	MC3	B	511	-	-	0/8/8/49	-
2	MC3	L	515	-	-	0/8/8/49	-
2	MC3	D	513	-	-	0/5/5/49	-
2	MC3	E	507	-	-	0/6/6/49	-
2	MC3	K	514	-	-	0/7/7/49	-
2	MC3	D	516	-	-	8/23/23/49	-
2	MC3	I	502	-	-	0/10/10/49	-
2	MC3	K	502	-	-	0/10/10/49	-
2	MC3	C	513	-	-	0/5/5/49	-
2	MC3	F	505	-	-	0/7/7/49	-
2	MC3	E	503	-	-	0/10/10/49	-
2	MC3	F	510	-	-	0/10/10/49	-
2	MC3	B	507	-	-	0/6/6/49	-
2	MC3	B	510	-	-	0/10/10/49	-
2	MC3	B	516	-	-	8/23/23/49	-
2	MC3	K	508	-	-	0/8/8/49	-
2	MC3	A	515	-	-	15/29/29/49	-
2	MC3	C	510	-	-	0/10/10/49	-
2	MC3	G	513	-	-	0/5/5/49	-
2	MC3	I	514	-	-	0/7/7/49	-
2	MC3	A	509	-	-	1/5/5/49	-
2	MC3	J	505	-	-	0/10/10/49	-
2	MC3	D	503	-	-	0/10/10/49	-
2	MC3	F	511	-	-	0/7/7/49	-
2	MC3	A	510	-	-	0/10/10/49	-
2	MC3	G	516	-	-	8/23/23/49	-
2	MC3	L	511	-	-	0/7/7/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	B	515	-	-	15/29/29/49	-
2	MC3	E	505	-	-	0/10/10/49	-
2	MC3	E	511	-	-	0/8/8/49	-
2	MC3	J	513	-	-	0/5/5/49	-
2	MC3	C	509	-	-	1/5/5/49	-
2	MC3	D	512	-	-	0/9/9/49	-
2	MC3	J	514	-	-	0/7/7/49	-
2	MC3	F	513	-	-	0/3/3/49	-
2	MC3	D	505	-	-	0/10/10/49	-
2	MC3	B	504	-	-	0/7/7/49	-
2	MC3	L	516	-	-	1/5/5/49	-
2	MC3	B	505	-	-	0/10/10/49	-
2	MC3	C	512	-	-	0/9/9/49	-
2	MC3	A	508	-	-	0/8/8/49	-
2	MC3	D	501	-	-	0/9/9/49	-
2	MC3	G	506	-	-	0/3/3/49	-
2	MC3	D	506	-	-	0/3/3/49	-
2	MC3	J	511	-	-	0/8/8/49	-
2	MC3	D	514	-	-	0/7/7/49	-
2	MC3	I	515	-	-	15/29/29/49	-
2	MC3	K	504	-	-	0/7/7/49	-
2	MC3	F	501	-	-	0/10/10/49	-
2	MC3	K	511	-	-	0/8/8/49	-
2	MC3	F	503	-	-	0/9/9/49	-
2	MC3	C	506	-	-	0/3/3/49	-
2	MC3	F	506	-	-	15/29/29/49	-
2	MC3	B	506	-	-	0/3/3/49	-
2	MC3	L	503	-	-	0/9/9/49	-
2	MC3	H	501	-	-	0/9/9/49	-
2	MC3	H	509	-	-	1/5/5/49	-
2	MC3	A	504	-	-	0/7/7/49	-
2	MC3	D	509	-	-	1/5/5/49	-
2	MC3	F	512	-	-	0/10/10/49	-
2	MC3	G	502	-	-	0/10/10/49	-
2	MC3	F	514	-	-	0/6/6/49	-
2	MC3	H	511	-	-	0/8/8/49	-
2	MC3	I	516	-	-	8/23/23/49	-
2	MC3	K	512	-	-	0/9/9/49	-
2	MC3	K	513	-	-	0/5/5/49	-
2	MC3	A	507	-	-	0/6/6/49	-
2	MC3	E	501	-	-	0/9/9/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	E	513	-	-	0/5/5/49	-
2	MC3	B	502	-	-	0/10/10/49	-
2	MC3	H	506	-	-	0/3/3/49	-
2	MC3	I	508	-	-	0/8/8/49	-
2	MC3	H	502	-	-	0/10/10/49	-
2	MC3	C	505	-	-	0/10/10/49	-
2	MC3	H	504	-	-	0/7/7/49	-
2	MC3	J	507	-	-	0/6/6/49	-
2	MC3	L	506	-	-	15/29/29/49	-
2	MC3	A	513	-	-	0/5/5/49	-
2	MC3	I	503	-	-	0/10/10/49	-
2	MC3	E	504	-	-	0/7/7/49	-
2	MC3	K	503	-	-	0/10/10/49	-
2	MC3	G	510	-	-	0/10/10/49	-
2	MC3	J	512	-	-	0/9/9/49	-
2	MC3	A	512	-	-	0/9/9/49	-
2	MC3	C	503	-	-	0/10/10/49	-
2	MC3	G	504	-	-	0/7/7/49	-
2	MC3	I	504	-	-	0/7/7/49	-
2	MC3	L	502	-	-	0/8/8/49	-
2	MC3	L	514	-	-	0/6/6/49	-
2	MC3	J	503	-	-	0/10/10/49	-
2	MC3	I	507	-	-	0/6/6/49	-
2	MC3	E	512	-	-	0/9/9/49	-
2	MC3	E	514	-	-	0/7/7/49	-
2	MC3	L	508	-	-	0/9/9/49	-
2	MC3	C	501	-	-	0/9/9/49	-
2	MC3	I	506	-	-	0/3/3/49	-
2	MC3	J	508	-	-	0/8/8/49	-
2	MC3	G	512	-	-	0/9/9/49	-
2	MC3	H	513	-	-	0/5/5/49	-
2	MC3	J	501	-	-	0/9/9/49	-
2	MC3	F	515	-	-	0/8/8/49	-
2	MC3	H	505	-	-	0/10/10/49	-
2	MC3	I	513	-	-	0/5/5/49	-
2	MC3	I	510	-	-	0/10/10/49	-
2	MC3	G	511	-	-	0/8/8/49	-
2	MC3	H	508	-	-	0/8/8/49	-
2	MC3	B	509	-	-	1/5/5/49	-
2	MC3	H	515	-	-	15/29/29/49	-
2	MC3	K	510	-	-	0/10/10/49	-
2	MC3	L	504	-	-	0/5/5/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	A	511	-	-	0/8/8/49	-
2	MC3	A	502	-	-	0/10/10/49	-
2	MC3	L	505	-	-	0/7/7/49	-
2	MC3	K	507	-	-	0/6/6/49	-
2	MC3	C	504	-	-	0/7/7/49	-
2	MC3	C	511	-	-	0/8/8/49	-
2	MC3	H	512	-	-	0/9/9/49	-
2	MC3	C	507	-	-	0/6/6/49	-
2	MC3	F	508	-	-	0/9/9/49	-
2	MC3	G	514	-	-	0/7/7/49	-
2	MC3	F	509	-	-	0/10/10/49	-
2	MC3	C	508	-	-	0/8/8/49	-
2	MC3	G	509	-	-	1/5/5/49	-
2	MC3	K	515	-	-	15/29/29/49	-
2	MC3	J	510	-	-	0/10/10/49	-
2	MC3	D	510	-	-	0/10/10/49	-
2	MC3	F	516	-	-	1/5/5/49	-
2	MC3	B	501	-	-	0/9/9/49	-
2	MC3	B	503	-	-	0/10/10/49	-
2	MC3	D	511	-	-	0/8/8/49	-
2	MC3	C	516	-	-	7/23/23/49	-
2	MC3	L	513	-	-	0/3/3/49	-
2	MC3	L	512	-	-	0/10/10/49	-
2	MC3	J	516	-	-	7/23/23/49	-
2	MC3	D	504	-	-	0/7/7/49	-
2	MC3	I	501	-	-	0/9/9/49	-
2	MC3	A	501	-	-	0/9/9/49	-
2	MC3	I	511	-	-	0/8/8/49	-
2	MC3	A	503	-	-	0/10/10/49	-
2	MC3	D	507	-	-	0/6/6/49	-
2	MC3	C	515	-	-	15/29/29/49	-
2	MC3	E	510	-	-	0/10/10/49	-
2	MC3	E	516	-	-	8/23/23/49	-
2	MC3	H	514	-	-	0/7/7/49	-
2	MC3	J	515	-	-	15/29/29/49	-
2	MC3	H	507	-	-	0/6/6/49	-
2	MC3	H	516	-	-	7/23/23/49	-
2	MC3	L	507	-	-	8/23/23/49	-
2	MC3	I	509	-	-	1/5/5/49	-
2	MC3	K	509	-	-	1/5/5/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	G	505	-	-	0/10/10/49	-
2	MC3	L	509	-	-	0/10/10/49	-
2	MC3	G	507	-	-	0/6/6/49	-
2	MC3	E	508	-	-	0/8/8/49	-
2	MC3	B	512	-	-	0/9/9/49	-
2	MC3	E	515	-	-	15/29/29/49	-
2	MC3	B	513	-	-	0/5/5/49	-
2	MC3	B	514	-	-	0/7/7/49	-
2	MC3	C	502	-	-	0/10/10/49	-
2	MC3	K	516	-	-	7/23/23/49	-
2	MC3	D	508	-	-	0/8/8/49	-
2	MC3	G	515	-	-	15/29/29/49	-
2	MC3	D	515	-	-	15/29/29/49	-
2	MC3	G	501	-	-	0/9/9/49	-
2	MC3	F	504	-	-	0/5/5/49	-
2	MC3	L	501	-	-	0/10/10/49	-
2	MC3	B	508	-	-	0/8/8/49	-
2	MC3	H	503	-	-	0/10/10/49	-
2	MC3	F	507	-	-	8/23/23/49	-
2	MC3	A	516	-	-	7/23/23/49	-
2	MC3	J	506	-	-	0/3/3/49	-
2	MC3	A	514	-	-	0/7/7/49	-
2	MC3	J	509	-	-	1/5/5/49	-
2	MC3	I	512	-	-	0/9/9/49	-
2	MC3	F	502	-	-	0/8/8/49	-
2	MC3	I	505	-	-	0/10/10/49	-
2	MC3	E	506	-	-	0/3/3/49	-
2	MC3	K	505	-	-	0/10/10/49	-
2	MC3	L	510	-	-	0/10/10/49	-
2	MC3	A	506	-	-	0/3/3/49	-
2	MC3	E	509	-	-	1/5/5/49	-
2	MC3	C	514	-	-	0/7/7/49	-
2	MC3	D	502	-	-	0/10/10/49	-
2	MC3	G	508	-	-	0/8/8/49	-
2	MC3	J	502	-	-	0/10/10/49	-
2	MC3	J	504	-	-	0/7/7/49	-
2	MC3	K	501	-	-	0/9/9/49	-

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	515	MC3	O2P-P-O1P	2.28	119.72	110.83
2	D	515	MC3	O2P-P-O1P	2.28	119.70	110.83
2	L	507	MC3	O2P-P-O1P	2.27	119.70	110.83
2	A	516	MC3	O2P-P-O1P	2.27	119.69	110.83
2	B	515	MC3	O2P-P-O1P	2.27	119.69	110.83
2	E	515	MC3	O2P-P-O1P	2.27	119.69	110.83
2	C	516	MC3	O2P-P-O1P	2.27	119.69	110.83
2	I	515	MC3	O2P-P-O1P	2.27	119.68	110.83
2	G	515	MC3	O2P-P-O1P	2.27	119.68	110.83
2	J	516	MC3	O2P-P-O1P	2.27	119.68	110.83
2	B	516	MC3	O2P-P-O1P	2.27	119.67	110.83
2	H	515	MC3	O2P-P-O1P	2.27	119.66	110.83
2	L	506	MC3	O2P-P-O1P	2.26	119.66	110.83
2	C	515	MC3	O2P-P-O1P	2.26	119.64	110.83
2	D	516	MC3	O2P-P-O1P	2.26	119.64	110.83
2	H	516	MC3	O2P-P-O1P	2.26	119.64	110.83
2	J	515	MC3	O2P-P-O1P	2.26	119.64	110.83
2	F	506	MC3	O2P-P-O1P	2.26	119.64	110.83
2	F	507	MC3	O2P-P-O1P	2.26	119.64	110.83
2	K	515	MC3	O2P-P-O1P	2.26	119.64	110.83
2	E	516	MC3	O2P-P-O1P	2.26	119.63	110.83
2	K	516	MC3	O2P-P-O1P	2.25	119.61	110.83
2	G	516	MC3	O2P-P-O1P	2.25	119.59	110.83
2	I	516	MC3	O2P-P-O1P	2.24	119.58	110.83

There are no chirality outliers.

All (283) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	515	MC3	C1-C2-O2-C31
2	A	515	MC3	C32-C31-O2-C2
2	A	515	MC3	C1-O3P-P-O2P
2	A	515	MC3	C1-O3P-P-O4P
2	B	515	MC3	C1-C2-O2-C31
2	B	515	MC3	C32-C31-O2-C2
2	B	515	MC3	C1-O3P-P-O2P
2	B	515	MC3	C1-O3P-P-O4P
2	C	515	MC3	C1-C2-O2-C31
2	C	515	MC3	C32-C31-O2-C2
2	C	515	MC3	C1-O3P-P-O2P
2	C	515	MC3	C1-O3P-P-O4P
2	D	515	MC3	C1-C2-O2-C31
2	D	515	MC3	C32-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
2	D	515	MC3	C1-O3P-P-O2P
2	D	515	MC3	C1-O3P-P-O4P
2	E	515	MC3	C1-C2-O2-C31
2	E	515	MC3	C32-C31-O2-C2
2	E	515	MC3	C1-O3P-P-O2P
2	E	515	MC3	C1-O3P-P-O4P
2	F	506	MC3	C1-C2-O2-C31
2	F	506	MC3	C32-C31-O2-C2
2	F	506	MC3	C1-O3P-P-O2P
2	F	506	MC3	C1-O3P-P-O4P
2	G	515	MC3	C1-C2-O2-C31
2	G	515	MC3	C32-C31-O2-C2
2	G	515	MC3	C1-O3P-P-O2P
2	G	515	MC3	C1-O3P-P-O4P
2	H	515	MC3	C1-C2-O2-C31
2	H	515	MC3	C32-C31-O2-C2
2	H	515	MC3	C1-O3P-P-O2P
2	H	515	MC3	C1-O3P-P-O4P
2	I	515	MC3	C1-C2-O2-C31
2	I	515	MC3	C32-C31-O2-C2
2	I	515	MC3	C1-O3P-P-O2P
2	I	515	MC3	C1-O3P-P-O4P
2	J	515	MC3	C1-C2-O2-C31
2	J	515	MC3	C32-C31-O2-C2
2	J	515	MC3	C1-O3P-P-O2P
2	J	515	MC3	C1-O3P-P-O4P
2	K	515	MC3	C1-C2-O2-C31
2	K	515	MC3	C32-C31-O2-C2
2	K	515	MC3	C1-O3P-P-O2P
2	K	515	MC3	C1-O3P-P-O4P
2	L	506	MC3	C1-C2-O2-C31
2	L	506	MC3	C32-C31-O2-C2
2	L	506	MC3	C1-O3P-P-O2P
2	L	506	MC3	C1-O3P-P-O4P
2	A	515	MC3	O31-C31-O2-C2
2	B	515	MC3	O31-C31-O2-C2
2	E	515	MC3	O31-C31-O2-C2
2	H	515	MC3	O31-C31-O2-C2
2	I	515	MC3	O31-C31-O2-C2
2	L	506	MC3	O31-C31-O2-C2
2	A	516	MC3	C12-C11-O3-C3
2	B	516	MC3	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
2	D	516	MC3	C12-C11-O3-C3
2	F	507	MC3	C12-C11-O3-C3
2	H	516	MC3	C12-C11-O3-C3
2	J	516	MC3	C12-C11-O3-C3
2	K	516	MC3	C12-C11-O3-C3
2	C	515	MC3	O31-C31-O2-C2
2	D	515	MC3	O31-C31-O2-C2
2	F	506	MC3	O31-C31-O2-C2
2	G	515	MC3	O31-C31-O2-C2
2	J	515	MC3	O31-C31-O2-C2
2	K	515	MC3	O31-C31-O2-C2
2	C	516	MC3	C12-C11-O3-C3
2	E	516	MC3	C12-C11-O3-C3
2	G	516	MC3	C12-C11-O3-C3
2	I	516	MC3	C12-C11-O3-C3
2	L	507	MC3	C12-C11-O3-C3
2	A	516	MC3	O11-C11-O3-C3
2	B	516	MC3	O11-C11-O3-C3
2	C	516	MC3	O11-C11-O3-C3
2	D	516	MC3	O11-C11-O3-C3
2	E	516	MC3	O11-C11-O3-C3
2	F	507	MC3	O11-C11-O3-C3
2	G	516	MC3	O11-C11-O3-C3
2	H	516	MC3	O11-C11-O3-C3
2	I	516	MC3	O11-C11-O3-C3
2	J	516	MC3	O11-C11-O3-C3
2	K	516	MC3	O11-C11-O3-C3
2	L	507	MC3	O11-C11-O3-C3
2	A	515	MC3	C14-C15-C16-C17
2	D	515	MC3	C14-C15-C16-C17
2	E	515	MC3	C14-C15-C16-C17
2	F	506	MC3	C14-C15-C16-C17
2	H	515	MC3	C14-C15-C16-C17
2	I	515	MC3	C14-C15-C16-C17
2	J	515	MC3	C14-C15-C16-C17
2	L	506	MC3	C14-C15-C16-C17
2	A	515	MC3	C12-C11-O3-C3
2	B	515	MC3	C12-C11-O3-C3
2	C	515	MC3	C12-C11-O3-C3
2	D	515	MC3	C12-C11-O3-C3
2	E	515	MC3	C12-C11-O3-C3
2	F	506	MC3	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
2	G	515	MC3	C12-C11-O3-C3
2	H	515	MC3	C12-C11-O3-C3
2	I	515	MC3	C12-C11-O3-C3
2	J	515	MC3	C12-C11-O3-C3
2	K	515	MC3	C12-C11-O3-C3
2	L	506	MC3	C12-C11-O3-C3
2	B	515	MC3	C14-C15-C16-C17
2	C	515	MC3	C14-C15-C16-C17
2	G	515	MC3	C14-C15-C16-C17
2	K	515	MC3	C14-C15-C16-C17
2	F	506	MC3	C13-C14-C15-C16
2	H	515	MC3	C13-C14-C15-C16
2	I	515	MC3	C13-C14-C15-C16
2	A	515	MC3	C13-C14-C15-C16
2	B	515	MC3	C13-C14-C15-C16
2	C	515	MC3	C13-C14-C15-C16
2	D	515	MC3	C13-C14-C15-C16
2	E	515	MC3	C13-C14-C15-C16
2	G	515	MC3	C13-C14-C15-C16
2	J	515	MC3	C13-C14-C15-C16
2	K	515	MC3	C13-C14-C15-C16
2	L	506	MC3	C13-C14-C15-C16
2	C	515	MC3	O11-C11-O3-C3
2	B	515	MC3	O11-C11-O3-C3
2	D	515	MC3	O11-C11-O3-C3
2	E	515	MC3	O11-C11-O3-C3
2	F	506	MC3	O11-C11-O3-C3
2	G	515	MC3	O11-C11-O3-C3
2	H	515	MC3	O11-C11-O3-C3
2	I	515	MC3	O11-C11-O3-C3
2	J	515	MC3	O11-C11-O3-C3
2	K	515	MC3	O11-C11-O3-C3
2	L	506	MC3	O11-C11-O3-C3
2	A	515	MC3	O11-C11-O3-C3
2	A	515	MC3	C31-C32-C33-C34
2	B	515	MC3	C31-C32-C33-C34
2	C	515	MC3	C31-C32-C33-C34
2	D	515	MC3	C31-C32-C33-C34
2	E	515	MC3	C31-C32-C33-C34
2	F	506	MC3	C31-C32-C33-C34
2	G	515	MC3	C31-C32-C33-C34
2	H	515	MC3	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	I	515	MC3	C31-C32-C33-C34
2	J	515	MC3	C31-C32-C33-C34
2	K	515	MC3	C31-C32-C33-C34
2	L	506	MC3	C31-C32-C33-C34
2	A	516	MC3	C32-C31-O2-C2
2	C	516	MC3	C32-C31-O2-C2
2	D	516	MC3	C32-C31-O2-C2
2	E	516	MC3	C32-C31-O2-C2
2	F	507	MC3	C32-C31-O2-C2
2	G	516	MC3	C32-C31-O2-C2
2	I	516	MC3	C32-C31-O2-C2
2	J	516	MC3	C32-C31-O2-C2
2	K	516	MC3	C32-C31-O2-C2
2	L	507	MC3	C32-C31-O2-C2
2	B	516	MC3	C32-C31-O2-C2
2	H	516	MC3	C32-C31-O2-C2
2	K	516	MC3	O31-C31-O2-C2
2	A	515	MC3	C16-C17-C18-C19
2	C	515	MC3	C16-C17-C18-C19
2	D	515	MC3	C16-C17-C18-C19
2	F	506	MC3	C16-C17-C18-C19
2	G	515	MC3	C16-C17-C18-C19
2	H	515	MC3	C16-C17-C18-C19
2	K	515	MC3	C16-C17-C18-C19
2	L	506	MC3	C16-C17-C18-C19
2	B	515	MC3	C16-C17-C18-C19
2	E	515	MC3	C16-C17-C18-C19
2	I	515	MC3	C16-C17-C18-C19
2	J	515	MC3	C16-C17-C18-C19
2	A	515	MC3	C15-C16-C17-C18
2	B	515	MC3	C15-C16-C17-C18
2	C	515	MC3	C15-C16-C17-C18
2	D	515	MC3	C15-C16-C17-C18
2	E	515	MC3	C15-C16-C17-C18
2	F	506	MC3	C15-C16-C17-C18
2	G	515	MC3	C15-C16-C17-C18
2	I	515	MC3	C15-C16-C17-C18
2	J	515	MC3	C15-C16-C17-C18
2	K	515	MC3	C15-C16-C17-C18
2	L	506	MC3	C15-C16-C17-C18
2	H	515	MC3	C15-C16-C17-C18
2	A	516	MC3	O31-C31-O2-C2

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Mol	Chain	Res	Type	Atoms
2	B	516	MC3	O31-C31-O2-C2
2	C	516	MC3	O31-C31-O2-C2
2	D	516	MC3	O31-C31-O2-C2
2	E	516	MC3	O31-C31-O2-C2
2	F	507	MC3	O31-C31-O2-C2
2	G	516	MC3	O31-C31-O2-C2
2	H	516	MC3	O31-C31-O2-C2
2	I	516	MC3	O31-C31-O2-C2
2	J	516	MC3	O31-C31-O2-C2
2	L	507	MC3	O31-C31-O2-C2
2	B	516	MC3	C32-C33-C34-C35
2	C	516	MC3	C32-C33-C34-C35
2	F	507	MC3	C32-C33-C34-C35
2	G	516	MC3	C32-C33-C34-C35
2	H	516	MC3	C32-C33-C34-C35
2	J	516	MC3	C32-C33-C34-C35
2	A	516	MC3	C32-C33-C34-C35
2	D	516	MC3	C32-C33-C34-C35
2	E	516	MC3	C32-C33-C34-C35
2	I	516	MC3	C32-C33-C34-C35
2	K	516	MC3	C32-C33-C34-C35
2	L	507	MC3	C32-C33-C34-C35
2	A	515	MC3	C33-C34-C35-C36
2	E	515	MC3	C33-C34-C35-C36
2	F	506	MC3	C33-C34-C35-C36
2	G	515	MC3	C33-C34-C35-C36
2	H	515	MC3	C33-C34-C35-C36
2	I	515	MC3	C33-C34-C35-C36
2	B	515	MC3	C33-C34-C35-C36
2	C	515	MC3	C33-C34-C35-C36
2	D	515	MC3	C33-C34-C35-C36
2	J	515	MC3	C33-C34-C35-C36
2	K	515	MC3	C33-C34-C35-C36
2	L	506	MC3	C33-C34-C35-C36
2	A	516	MC3	O3P-C1-C2-O2
2	B	516	MC3	O3P-C1-C2-O2
2	C	516	MC3	O3P-C1-C2-O2
2	D	516	MC3	O3P-C1-C2-O2
2	E	516	MC3	O3P-C1-C2-O2
2	F	507	MC3	O3P-C1-C2-O2
2	G	516	MC3	O3P-C1-C2-O2
2	H	516	MC3	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	I	516	MC3	O3P-C1-C2-O2
2	J	516	MC3	O3P-C1-C2-O2
2	K	516	MC3	O3P-C1-C2-O2
2	L	507	MC3	O3P-C1-C2-O2
2	J	509	MC3	C16-C17-C18-C19
2	C	509	MC3	C16-C17-C18-C19
2	I	509	MC3	C16-C17-C18-C19
2	A	509	MC3	C16-C17-C18-C19
2	B	509	MC3	C16-C17-C18-C19
2	E	509	MC3	C16-C17-C18-C19
2	F	516	MC3	C16-C17-C18-C19
2	G	509	MC3	C16-C17-C18-C19
2	K	509	MC3	C16-C17-C18-C19
2	D	509	MC3	C16-C17-C18-C19
2	L	516	MC3	C16-C17-C18-C19
2	H	509	MC3	C16-C17-C18-C19
2	A	515	MC3	O3-C11-C12-C13
2	E	515	MC3	O3-C11-C12-C13
2	H	515	MC3	O3-C11-C12-C13
2	I	515	MC3	O3-C11-C12-C13
2	B	515	MC3	O3-C11-C12-C13
2	F	506	MC3	O3-C11-C12-C13
2	G	515	MC3	O3-C11-C12-C13
2	J	515	MC3	O3-C11-C12-C13
2	K	515	MC3	O3-C11-C12-C13
2	L	506	MC3	O3-C11-C12-C13
2	C	515	MC3	O3-C11-C12-C13
2	D	515	MC3	O3-C11-C12-C13
2	A	516	MC3	O3P-C1-C2-C3
2	B	516	MC3	O3P-C1-C2-C3
2	C	516	MC3	O3P-C1-C2-C3
2	D	516	MC3	O3P-C1-C2-C3
2	E	516	MC3	O3P-C1-C2-C3
2	F	507	MC3	O3P-C1-C2-C3
2	G	516	MC3	O3P-C1-C2-C3
2	H	516	MC3	O3P-C1-C2-C3
2	I	516	MC3	O3P-C1-C2-C3
2	J	516	MC3	O3P-C1-C2-C3
2	K	516	MC3	O3P-C1-C2-C3
2	L	507	MC3	O3P-C1-C2-C3
2	F	506	MC3	O11-C11-C12-C13
2	J	515	MC3	O11-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
2	A	515	MC3	O11-C11-C12-C13
2	B	515	MC3	O11-C11-C12-C13
2	C	515	MC3	O11-C11-C12-C13
2	E	515	MC3	O11-C11-C12-C13
2	G	515	MC3	O11-C11-C12-C13
2	I	515	MC3	O11-C11-C12-C13
2	K	515	MC3	O11-C11-C12-C13
2	L	506	MC3	O11-C11-C12-C13
2	D	515	MC3	O11-C11-C12-C13
2	H	515	MC3	O11-C11-C12-C13
2	B	516	MC3	O3-C11-C12-C13
2	D	516	MC3	O3-C11-C12-C13
2	G	516	MC3	O3-C11-C12-C13
2	I	516	MC3	O3-C11-C12-C13
2	L	507	MC3	O3-C11-C12-C13
2	E	516	MC3	O3-C11-C12-C13
2	F	507	MC3	O3-C11-C12-C13

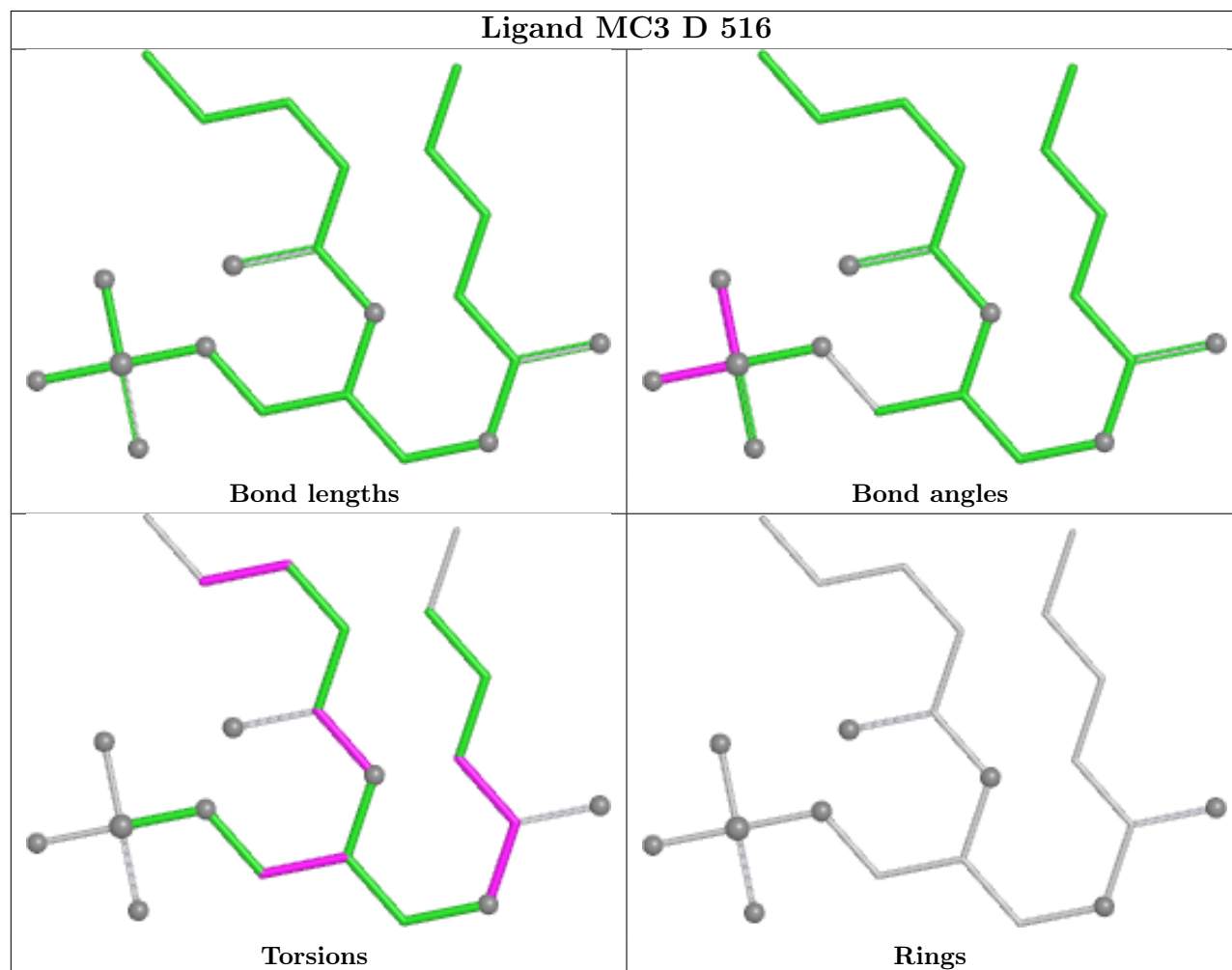
There are no ring outliers.

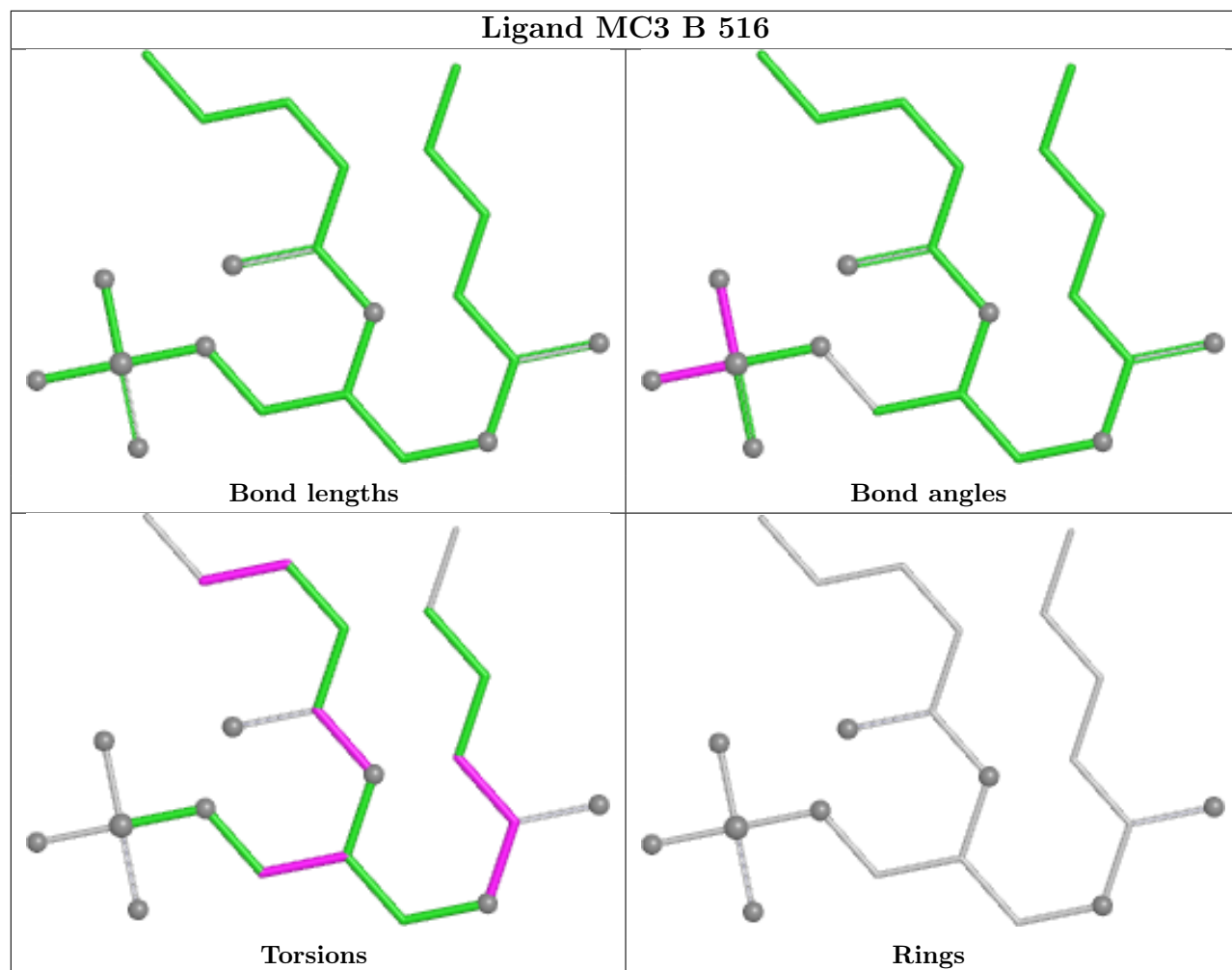
12 monomers are involved in 23 short contacts:

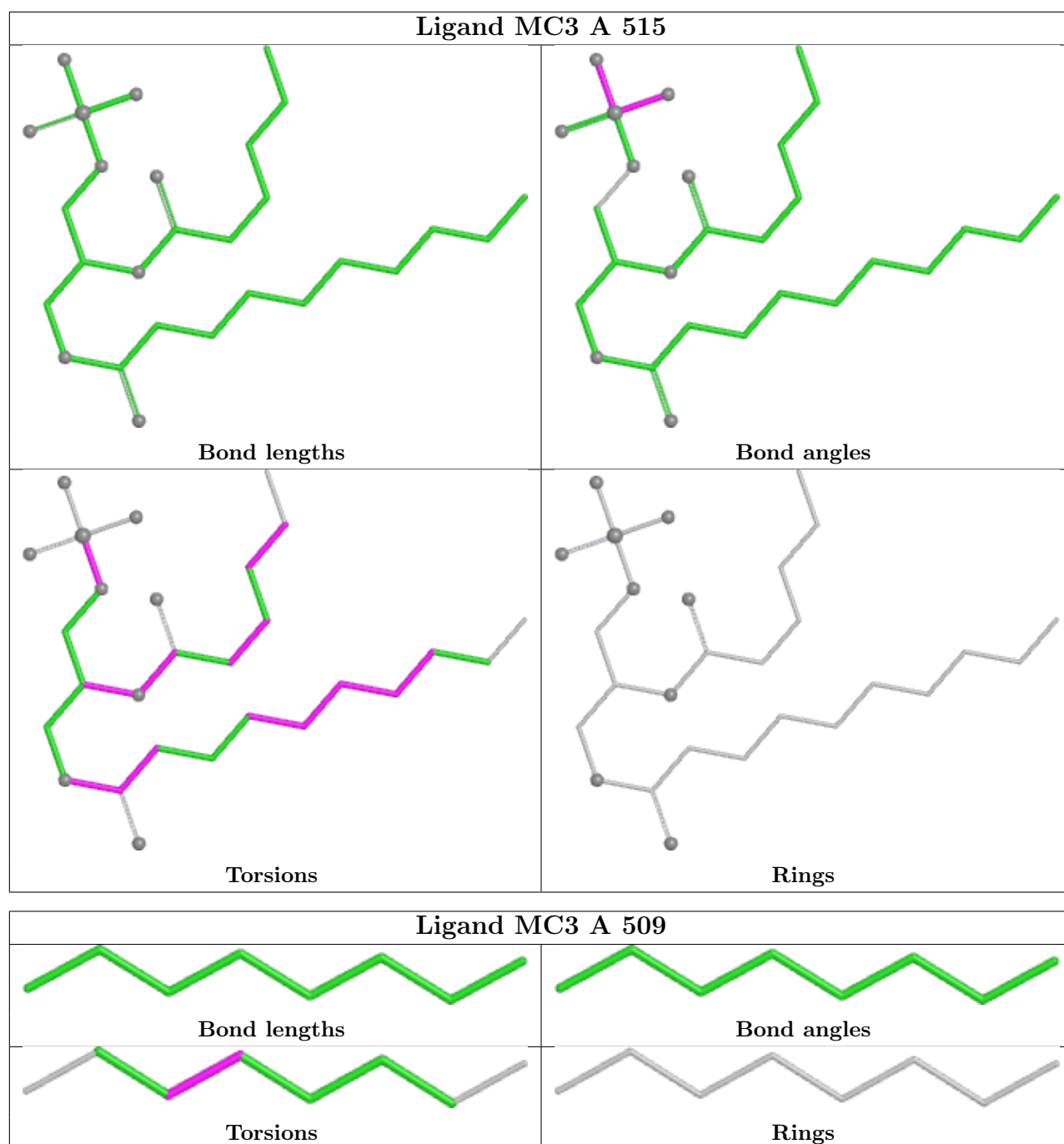
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	515	MC3	2	0
2	B	515	MC3	1	0
2	I	515	MC3	2	0
2	F	506	MC3	2	0
2	L	506	MC3	2	0
2	H	515	MC3	2	0
2	K	515	MC3	2	0
2	C	515	MC3	2	0
2	J	515	MC3	2	0
2	E	515	MC3	2	0
2	G	515	MC3	2	0
2	D	515	MC3	2	0

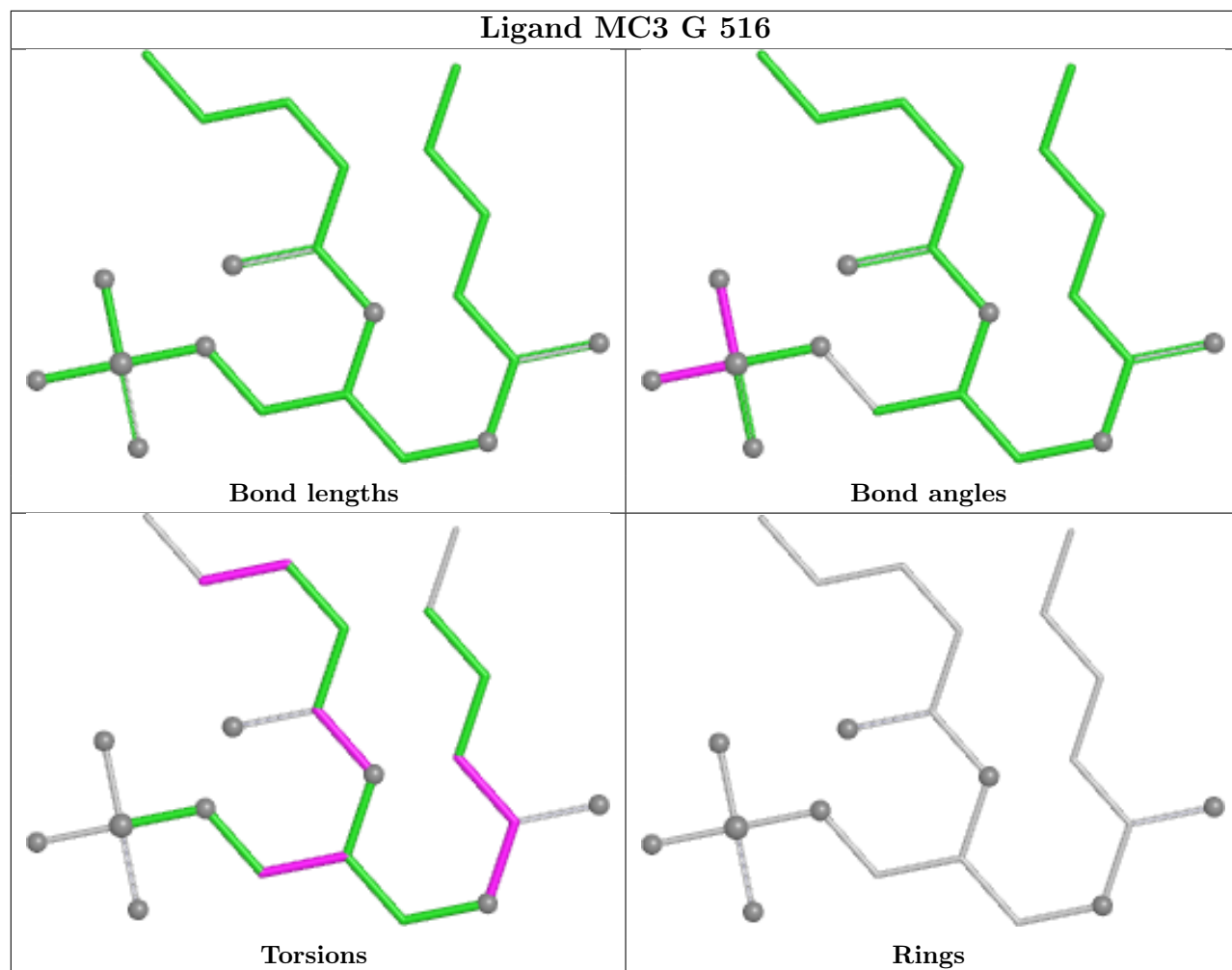
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

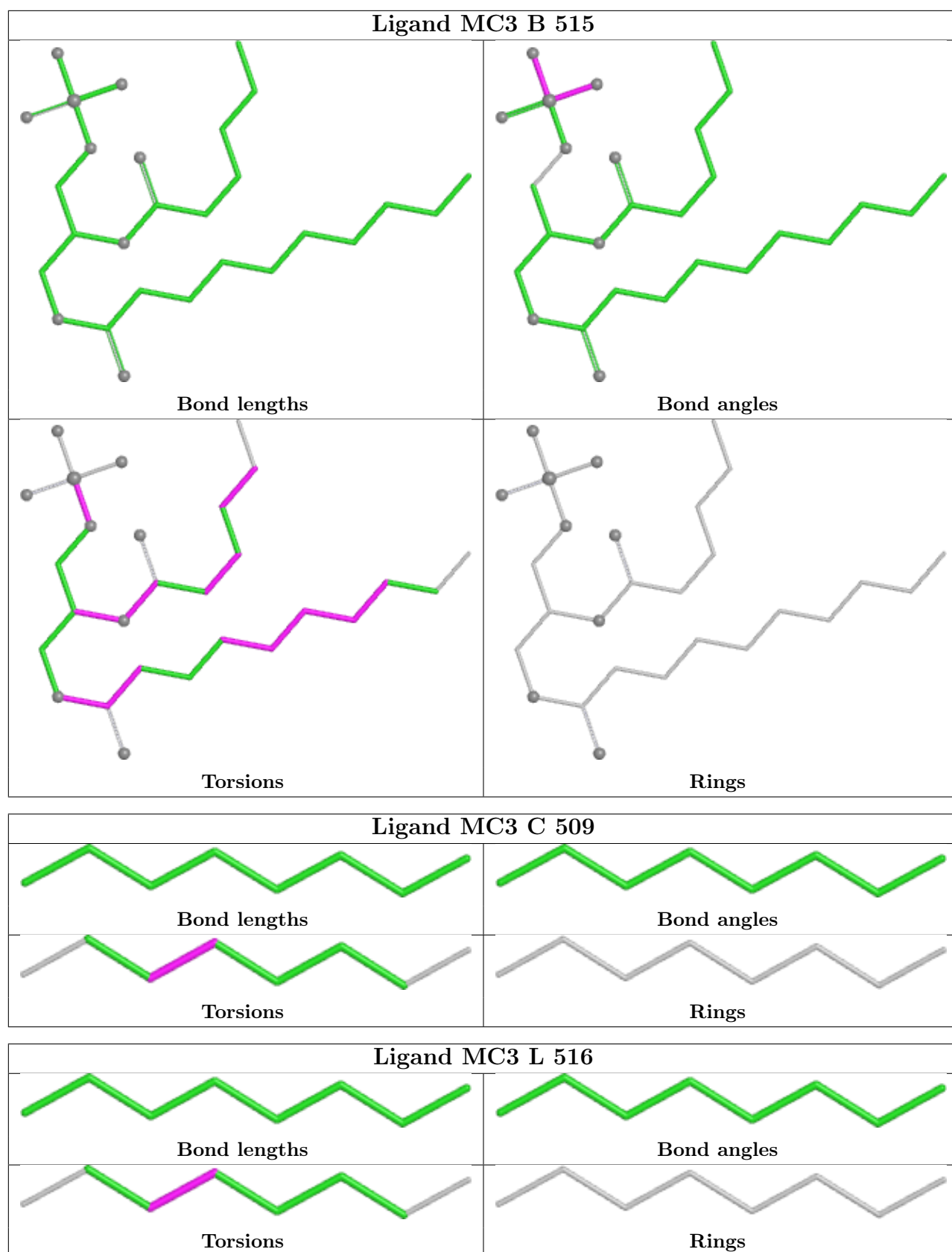
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

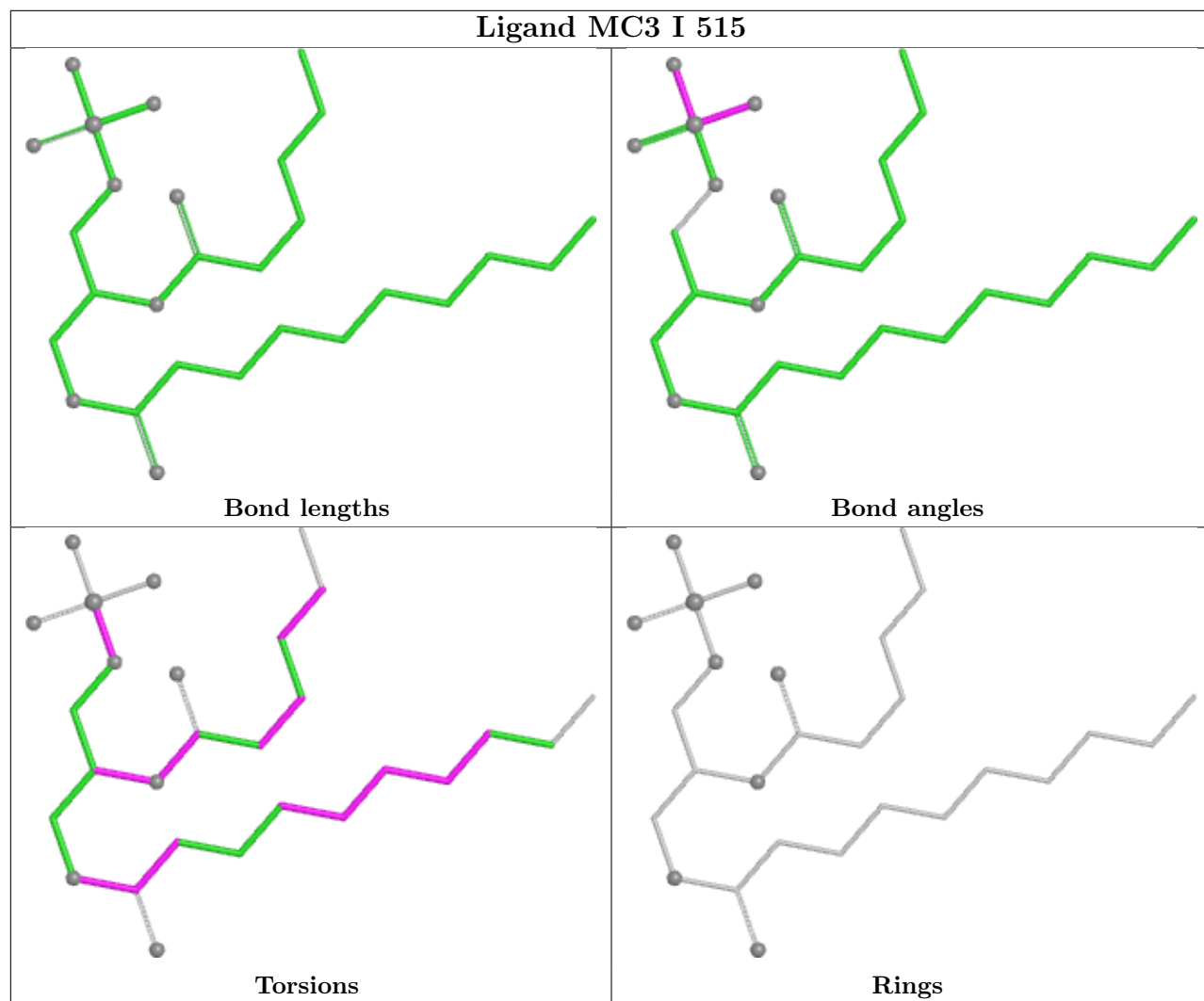


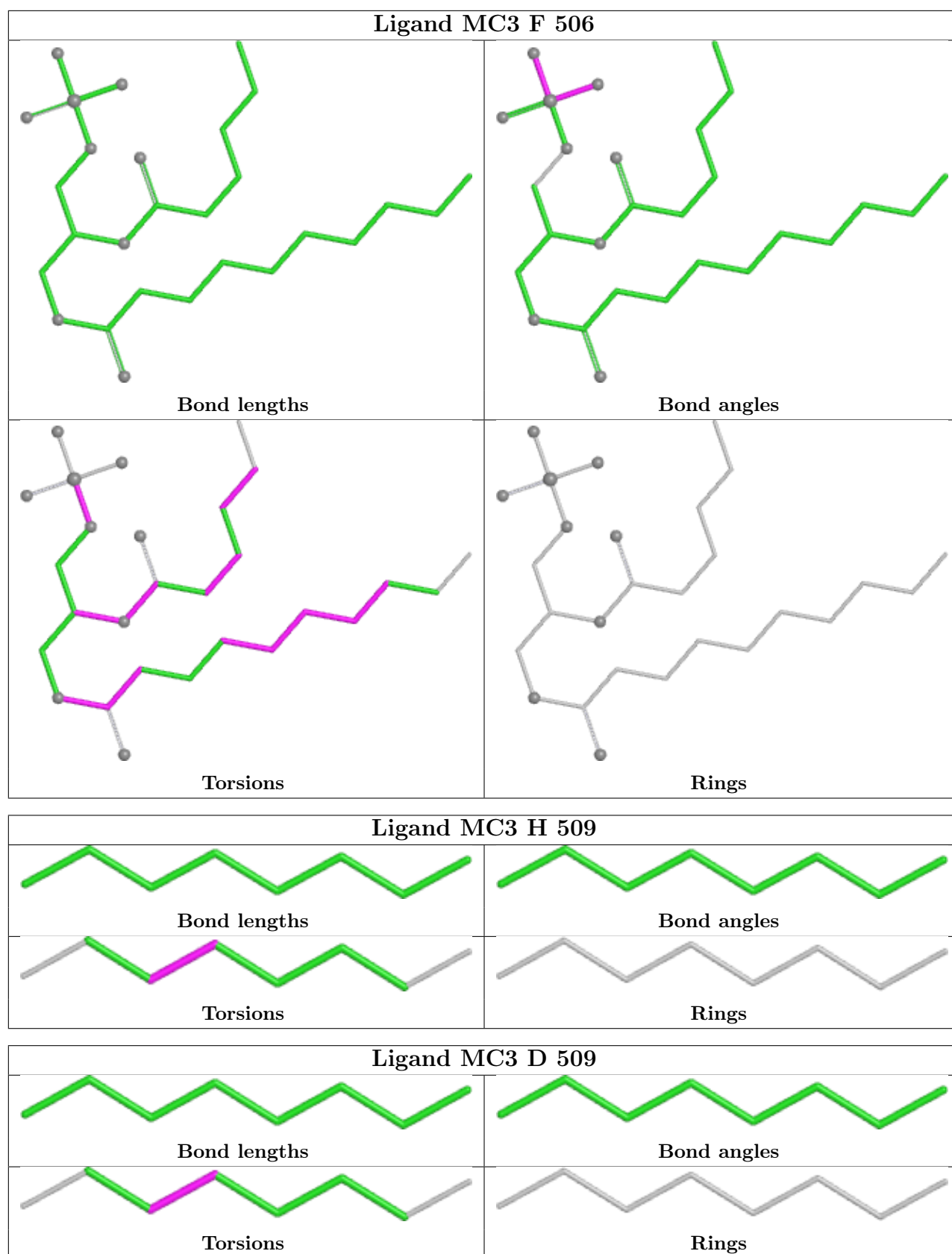


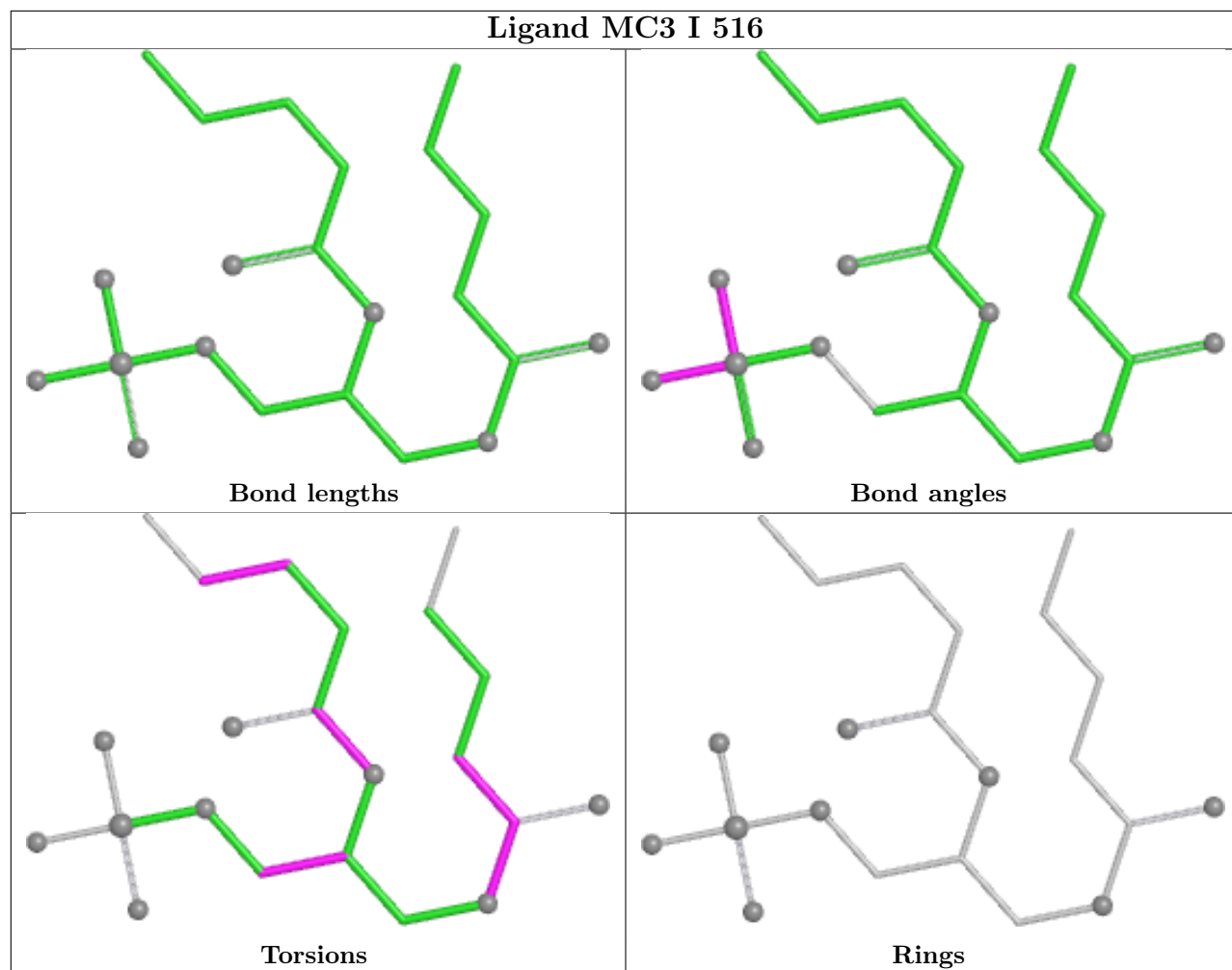


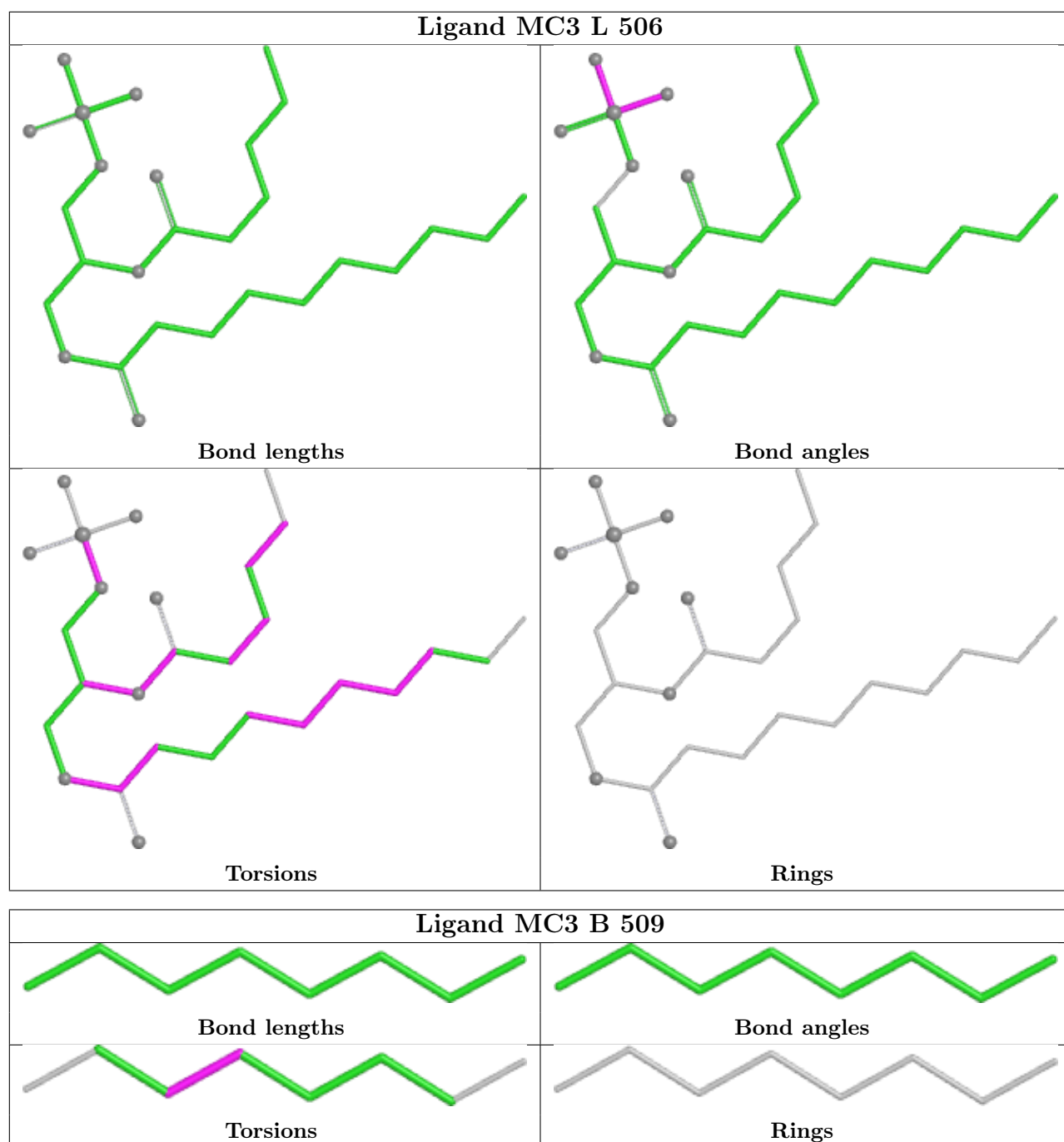


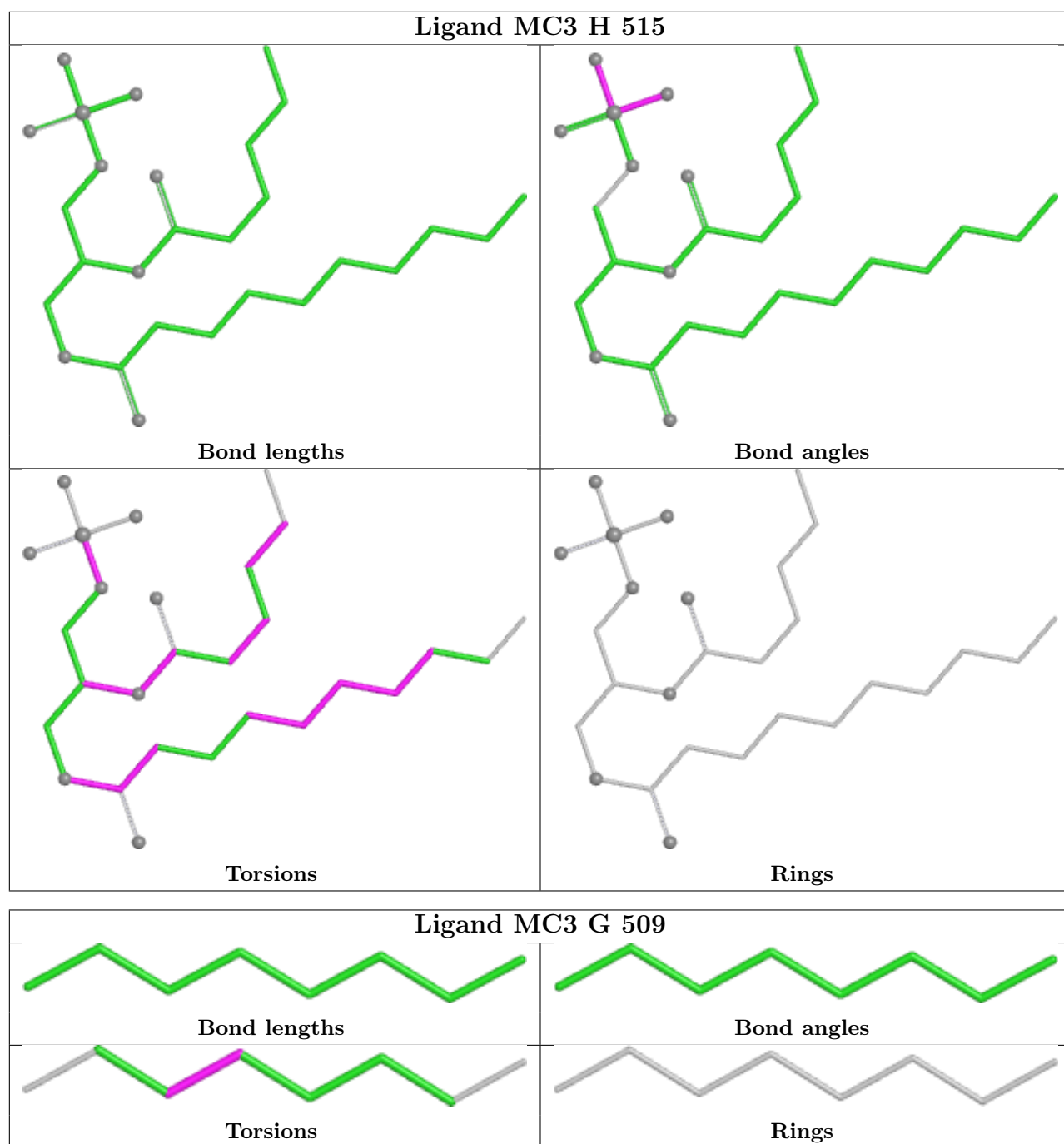


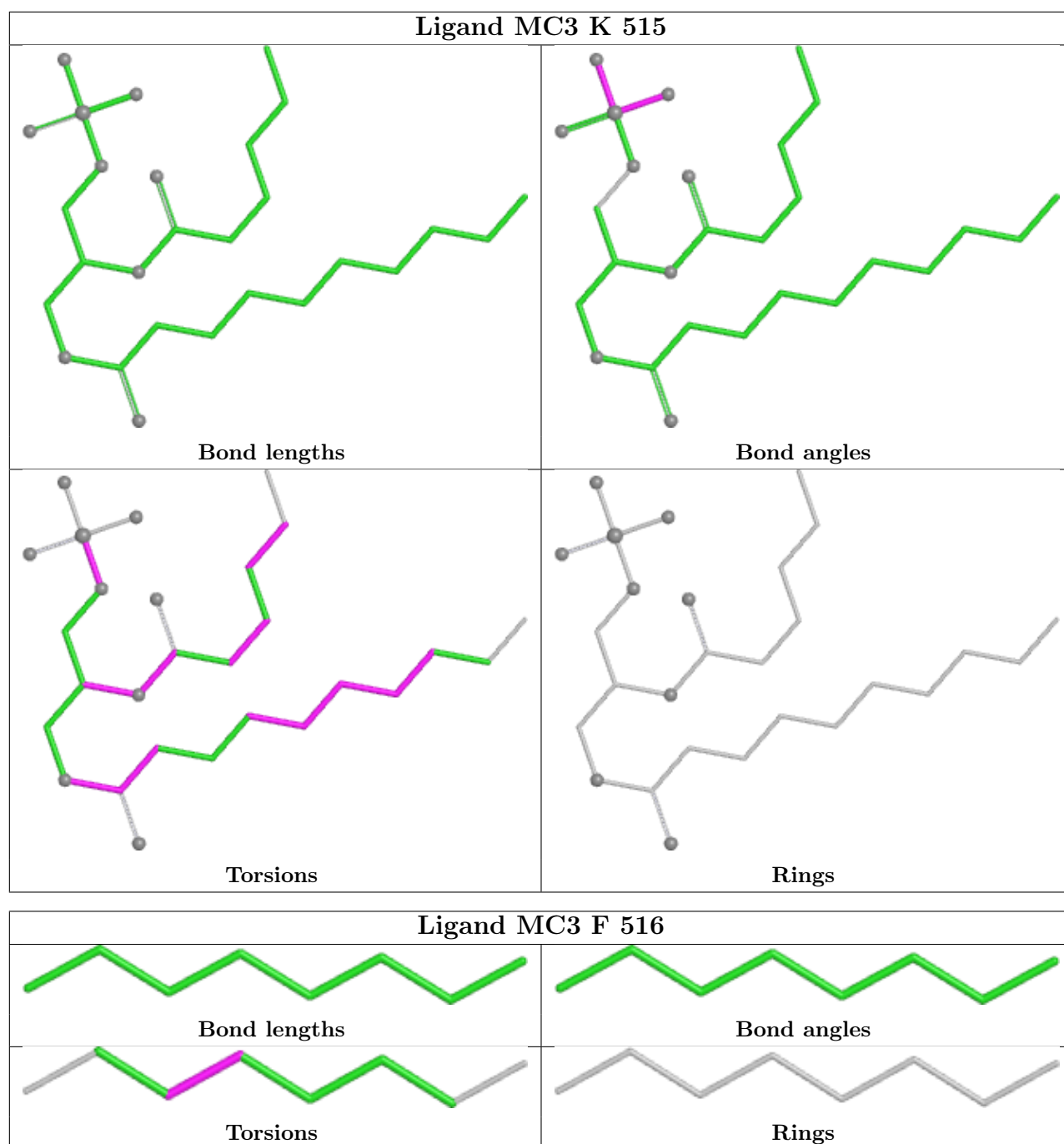


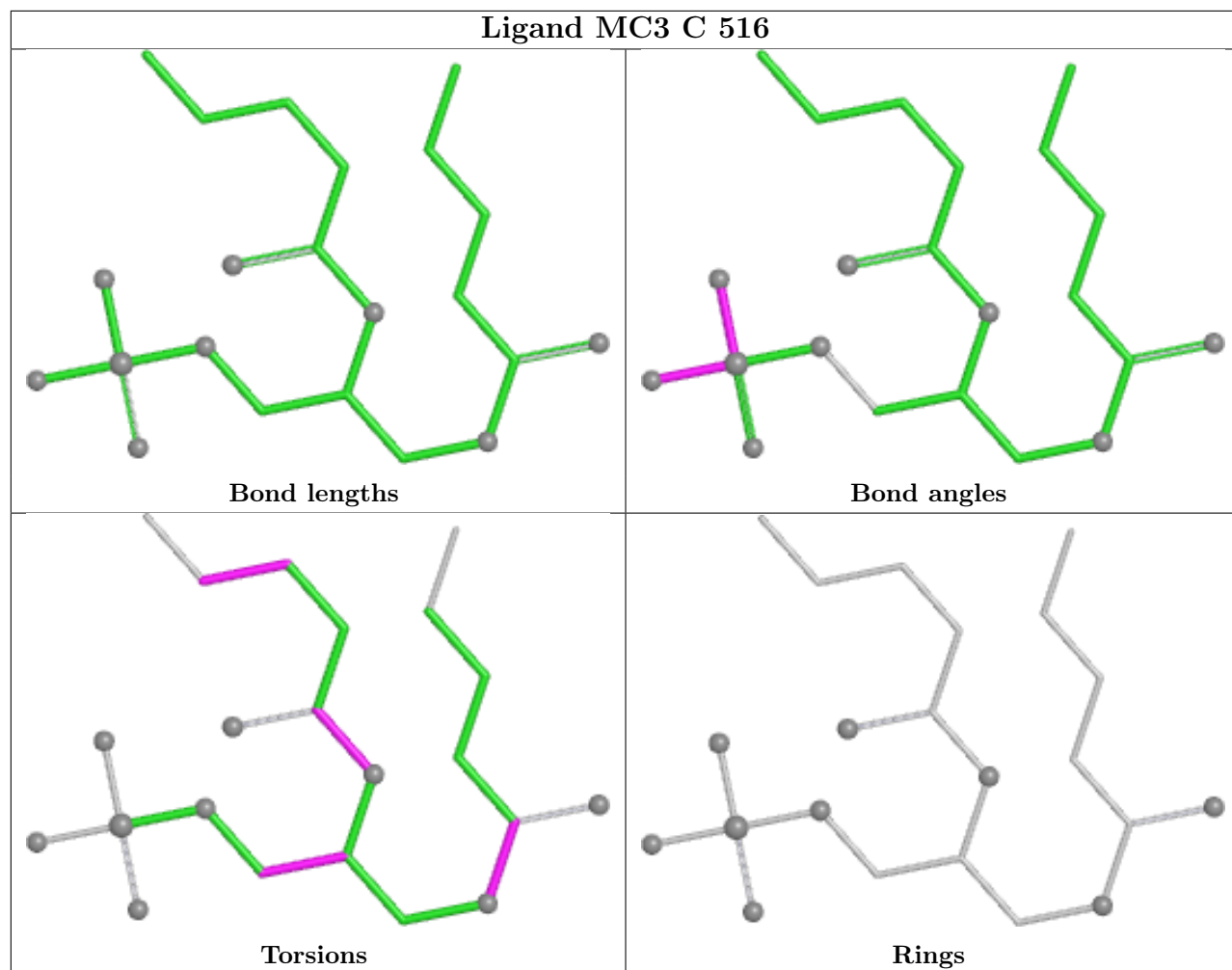


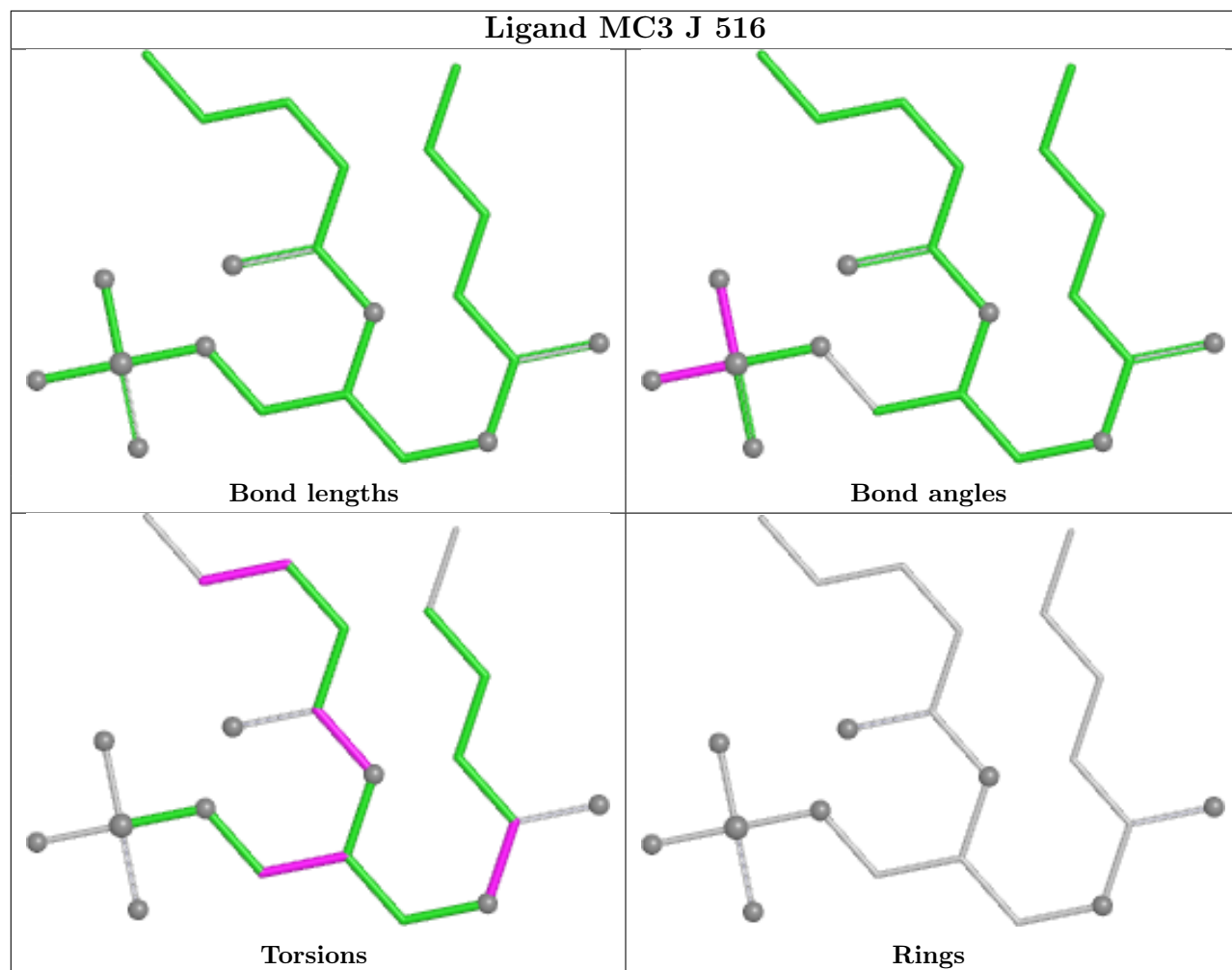


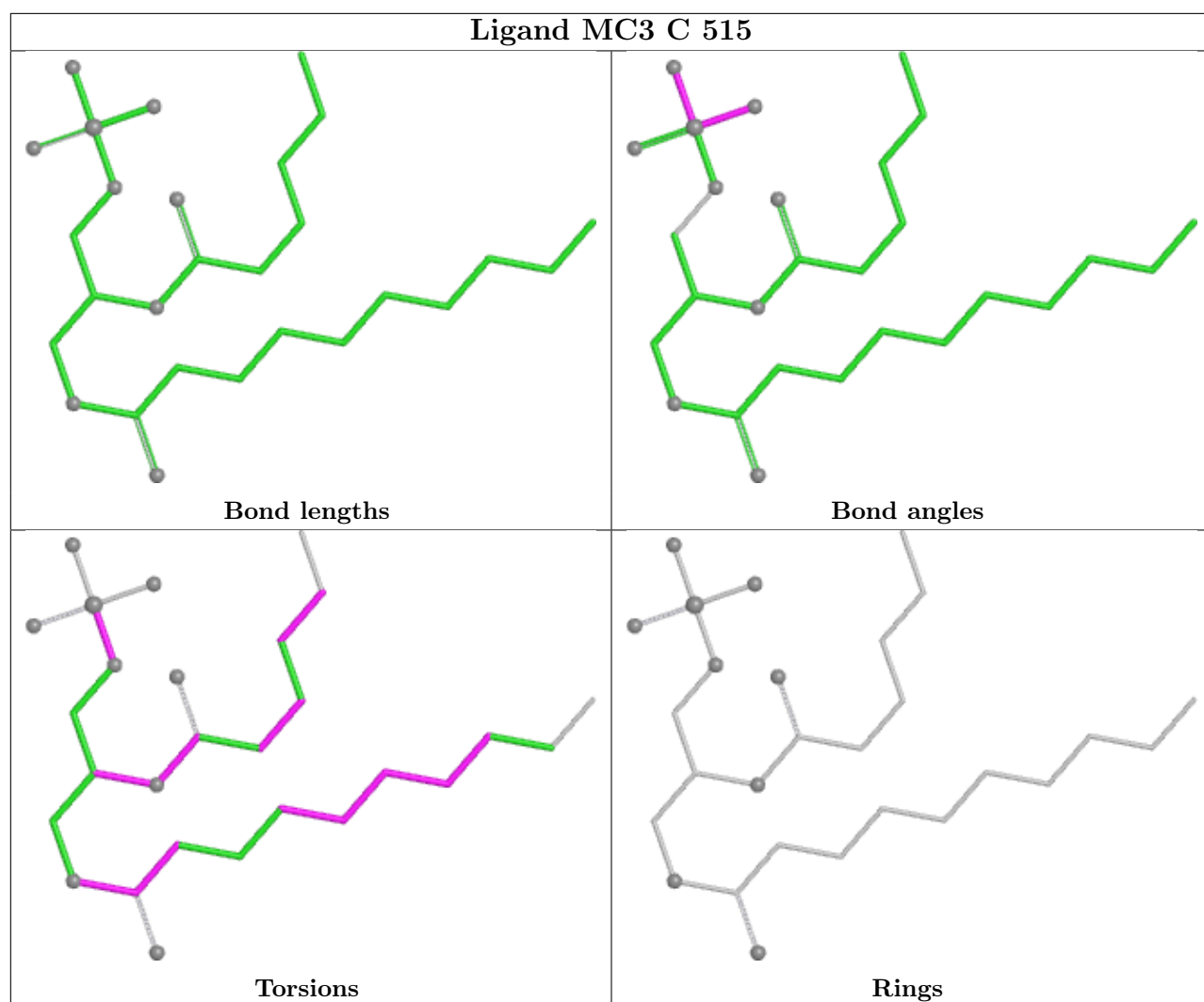


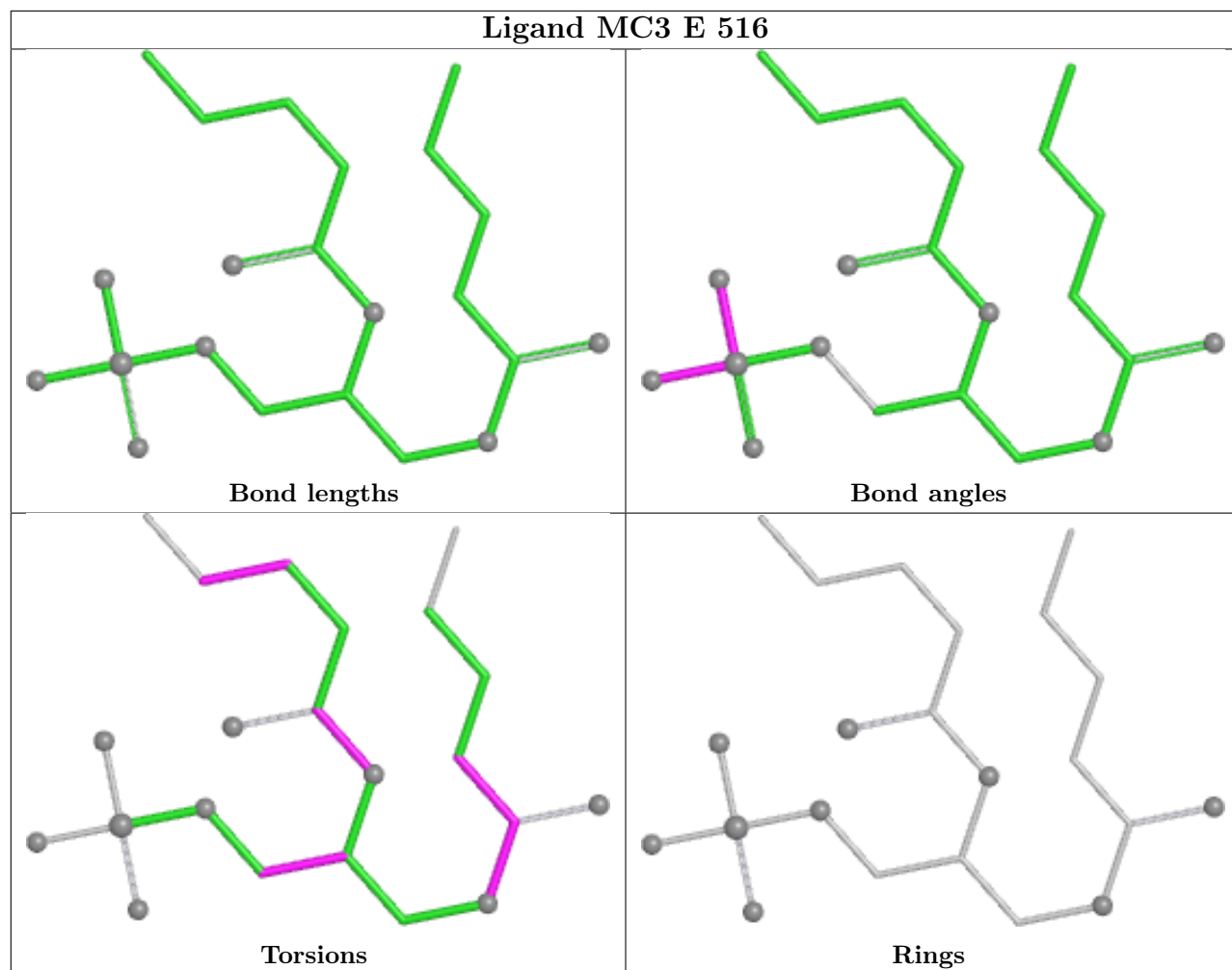


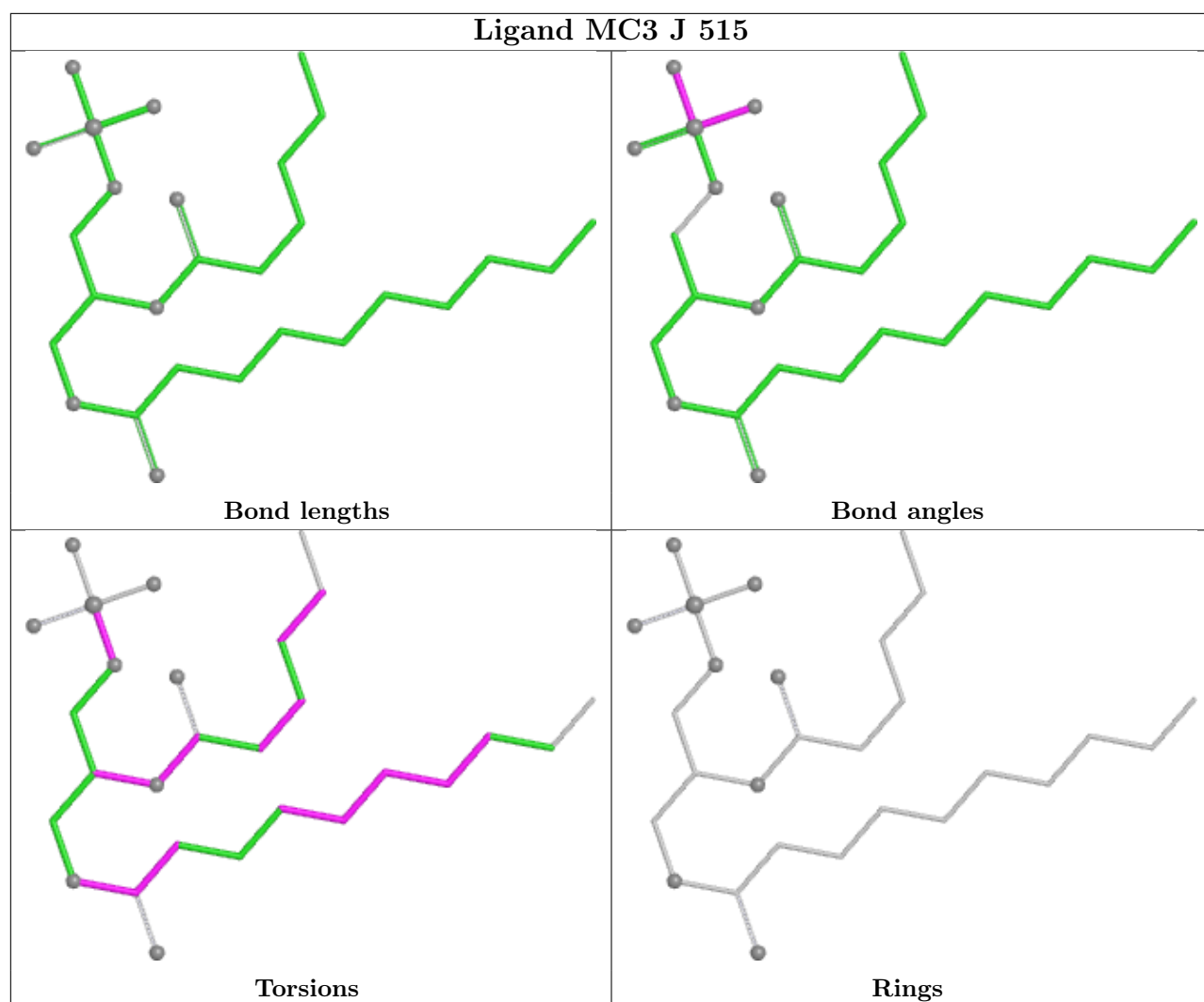


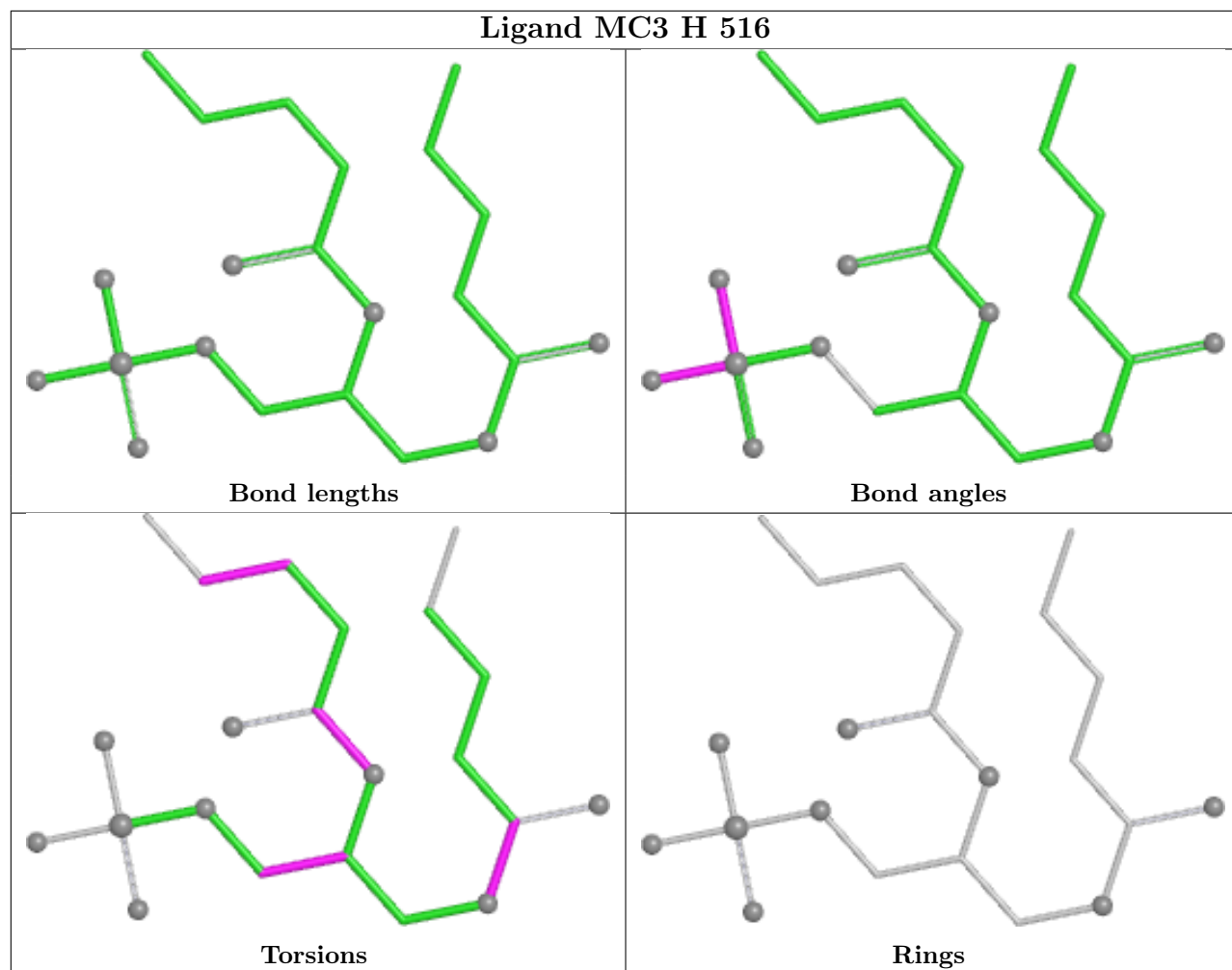


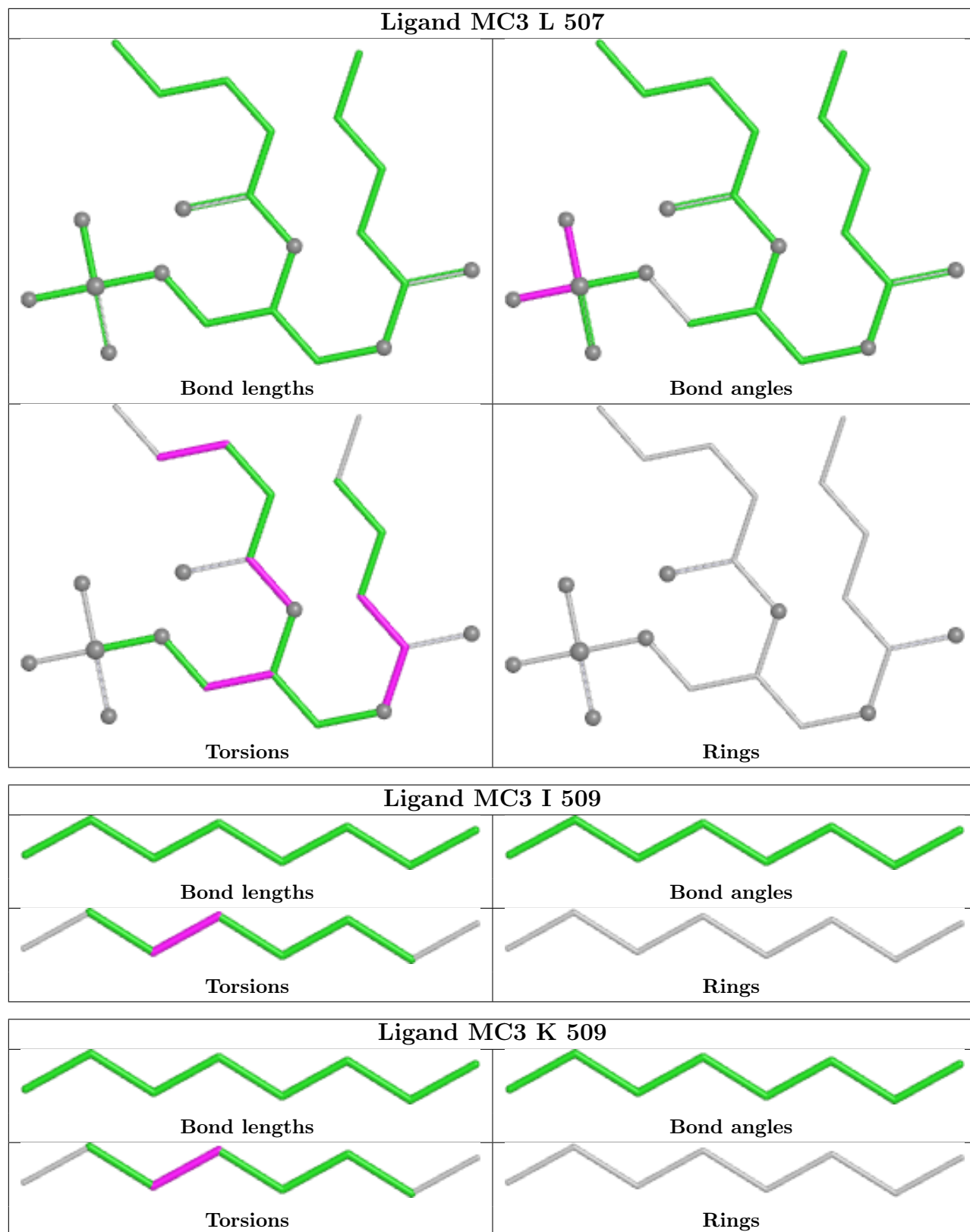


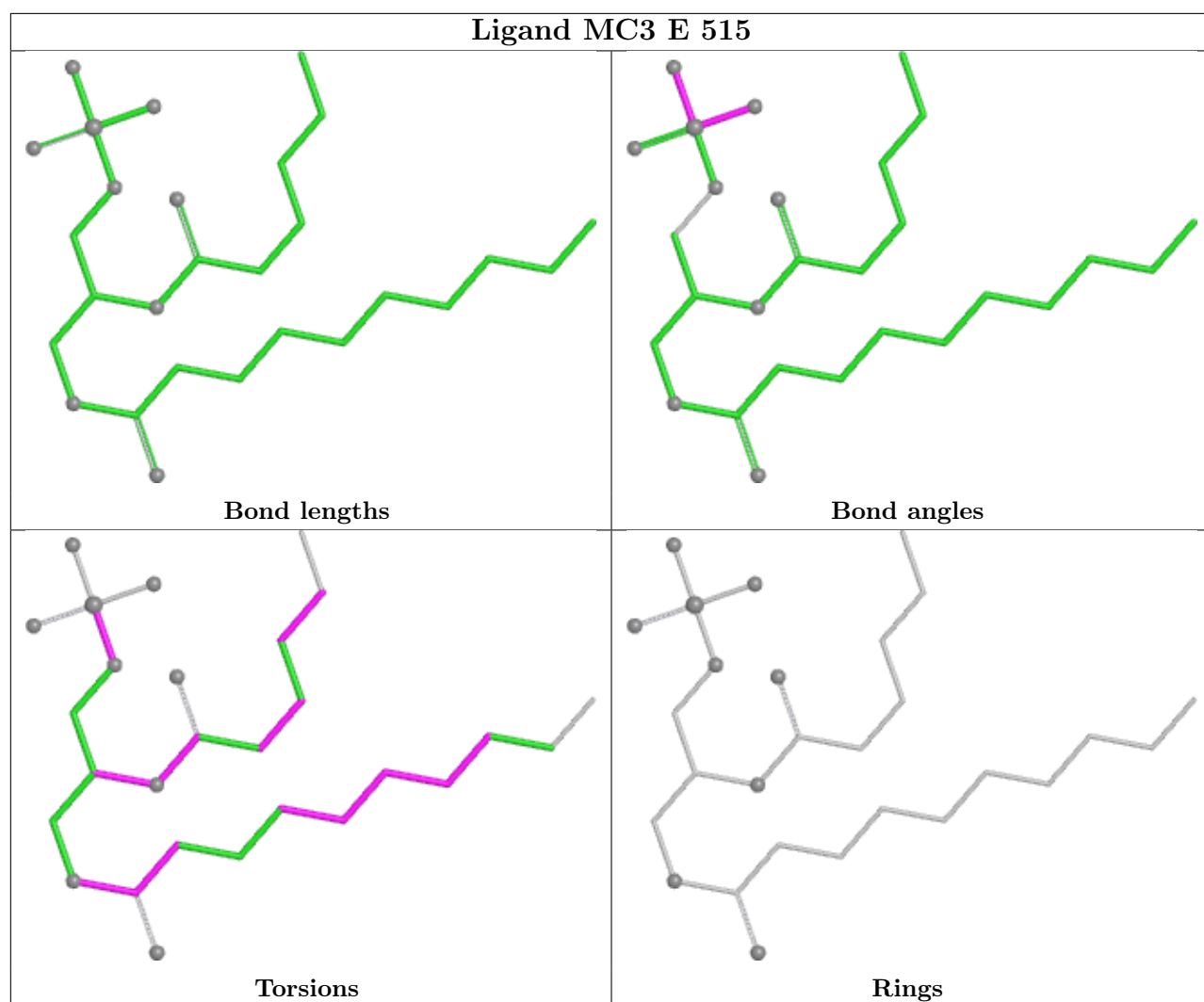


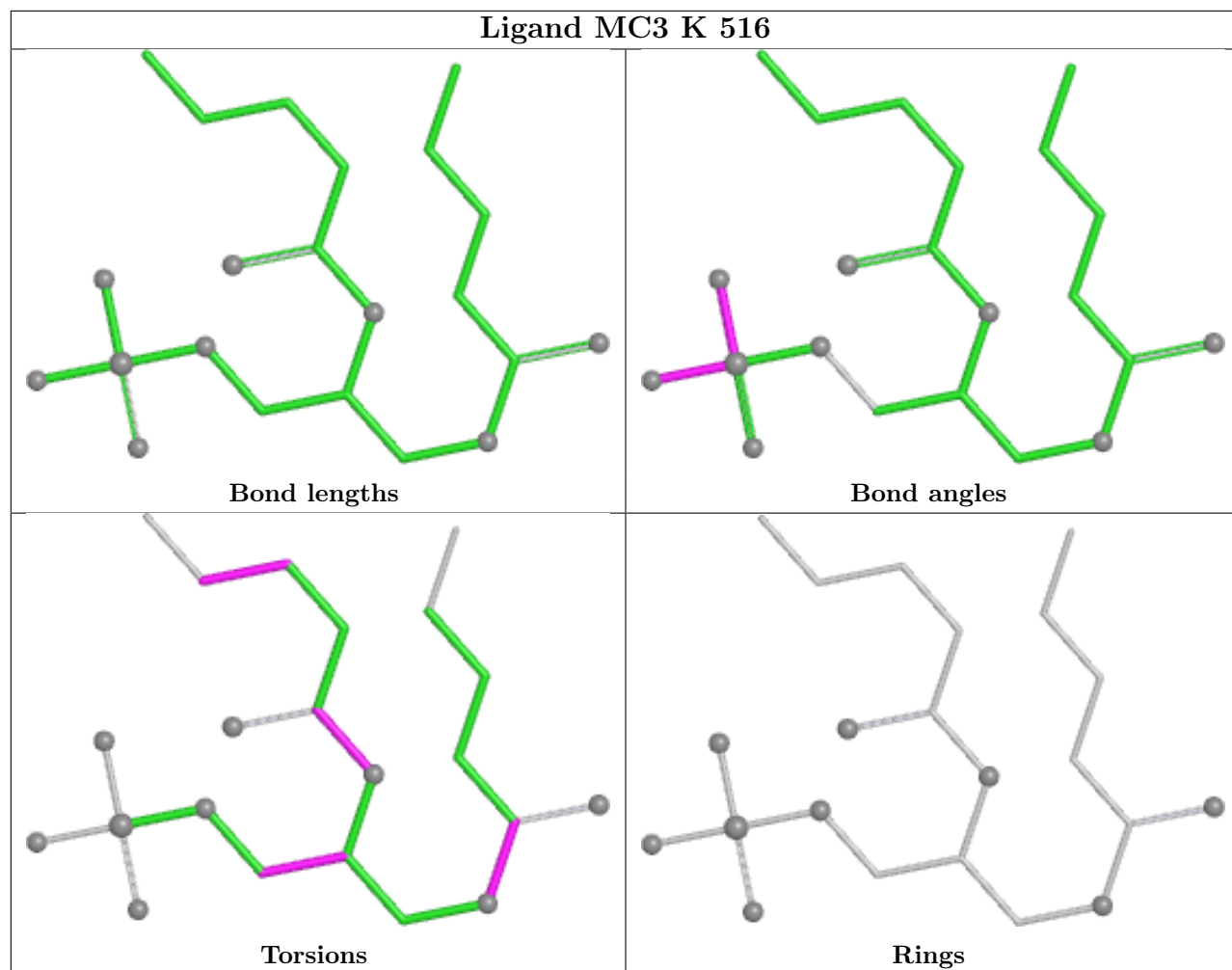


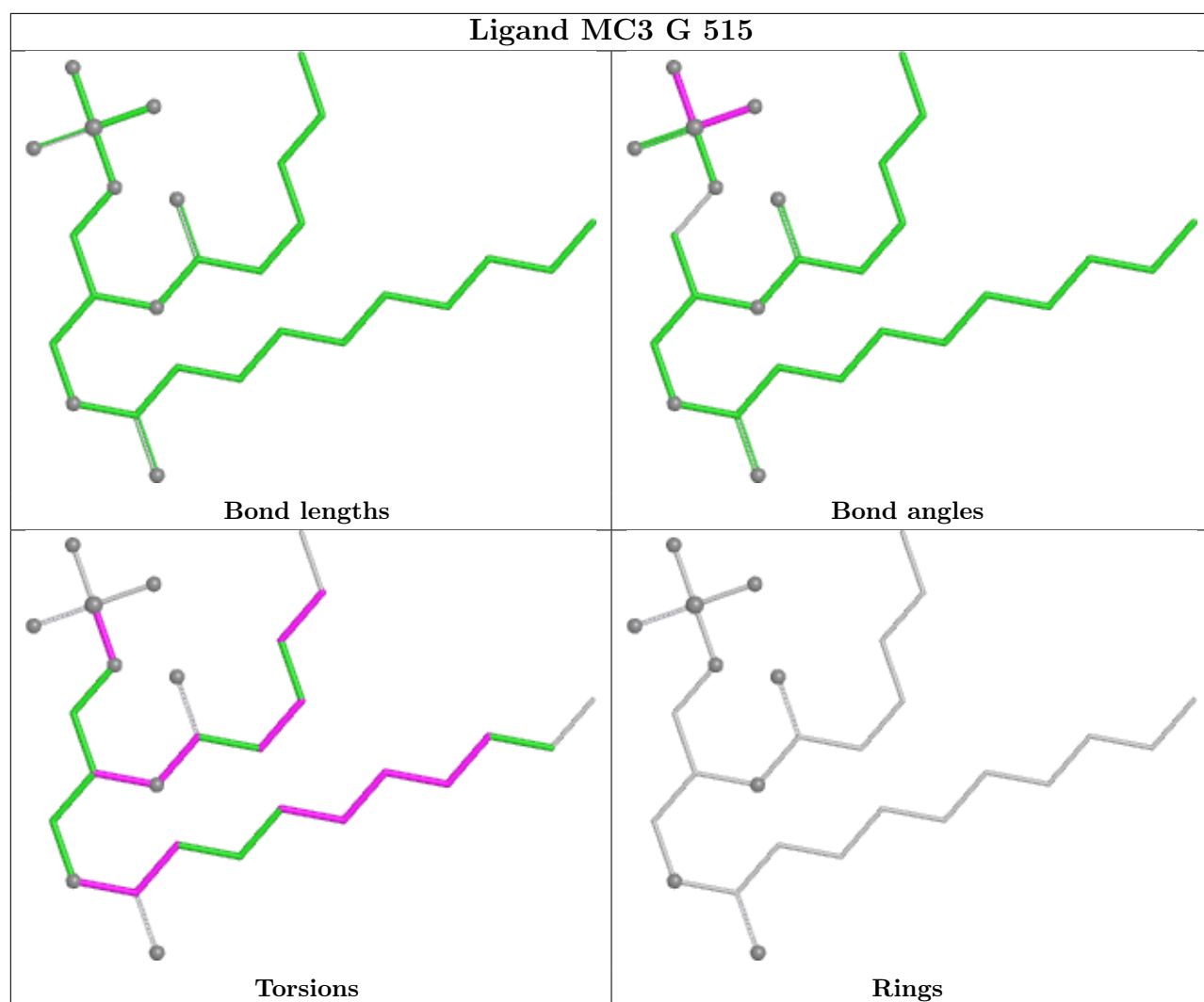


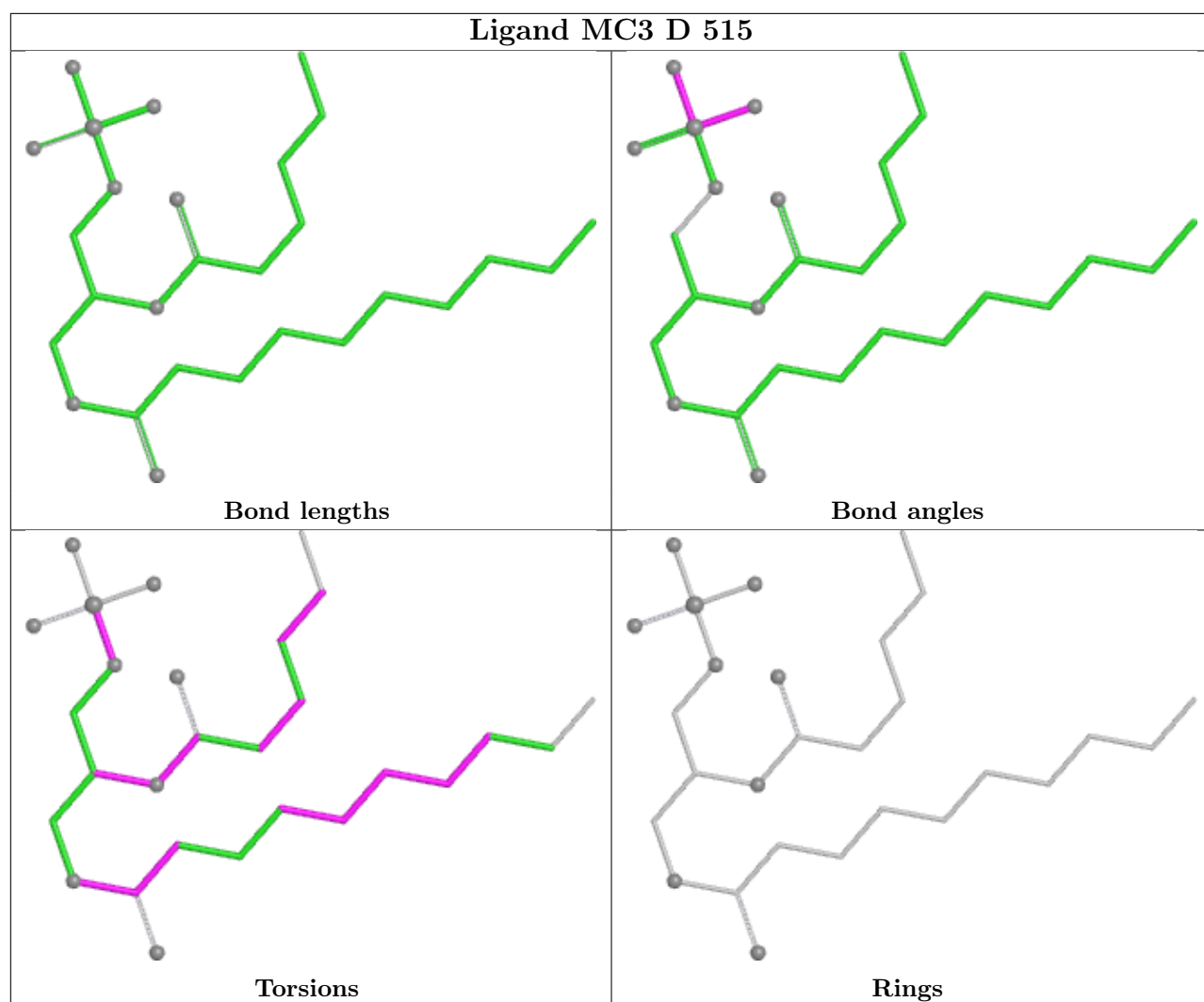


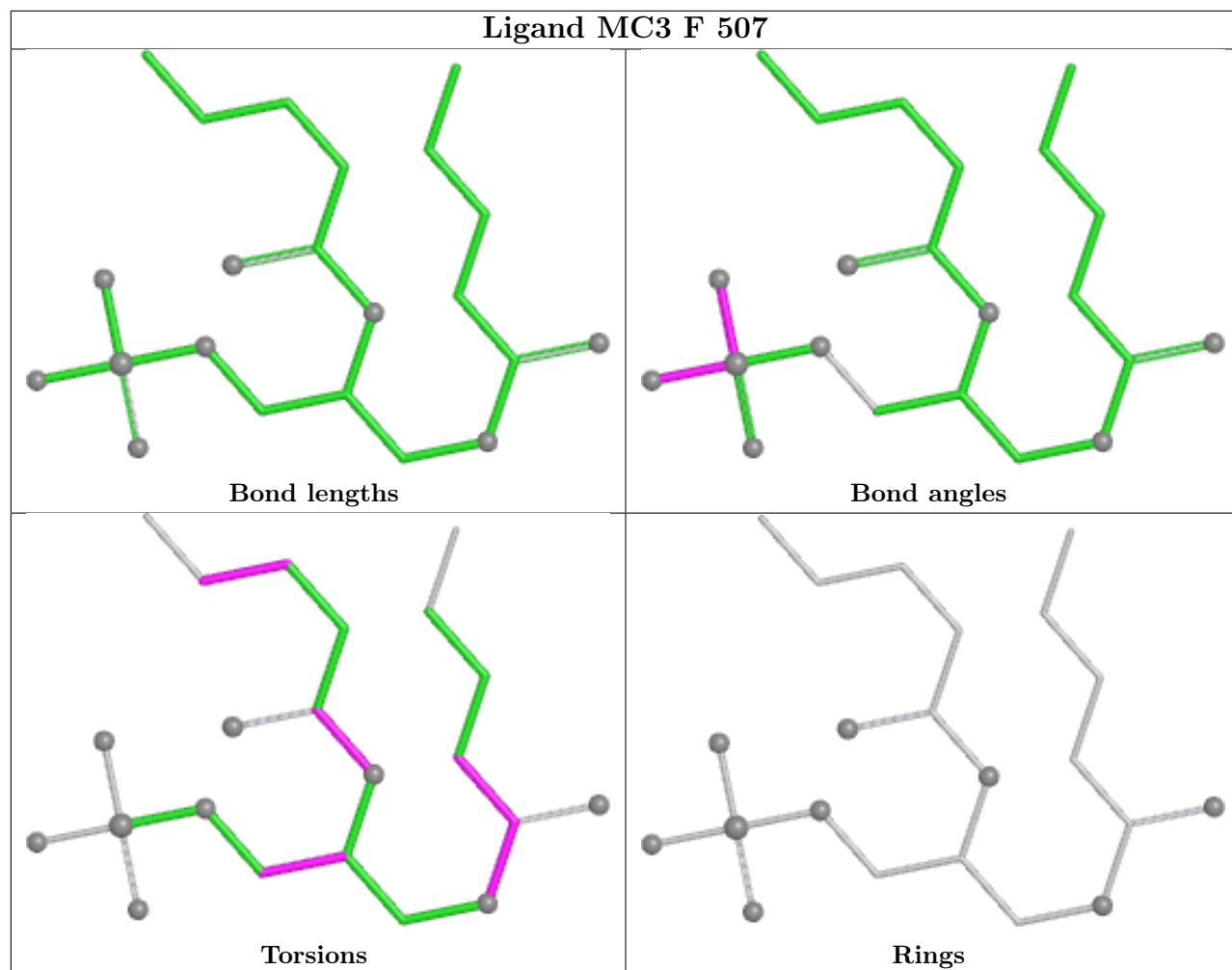


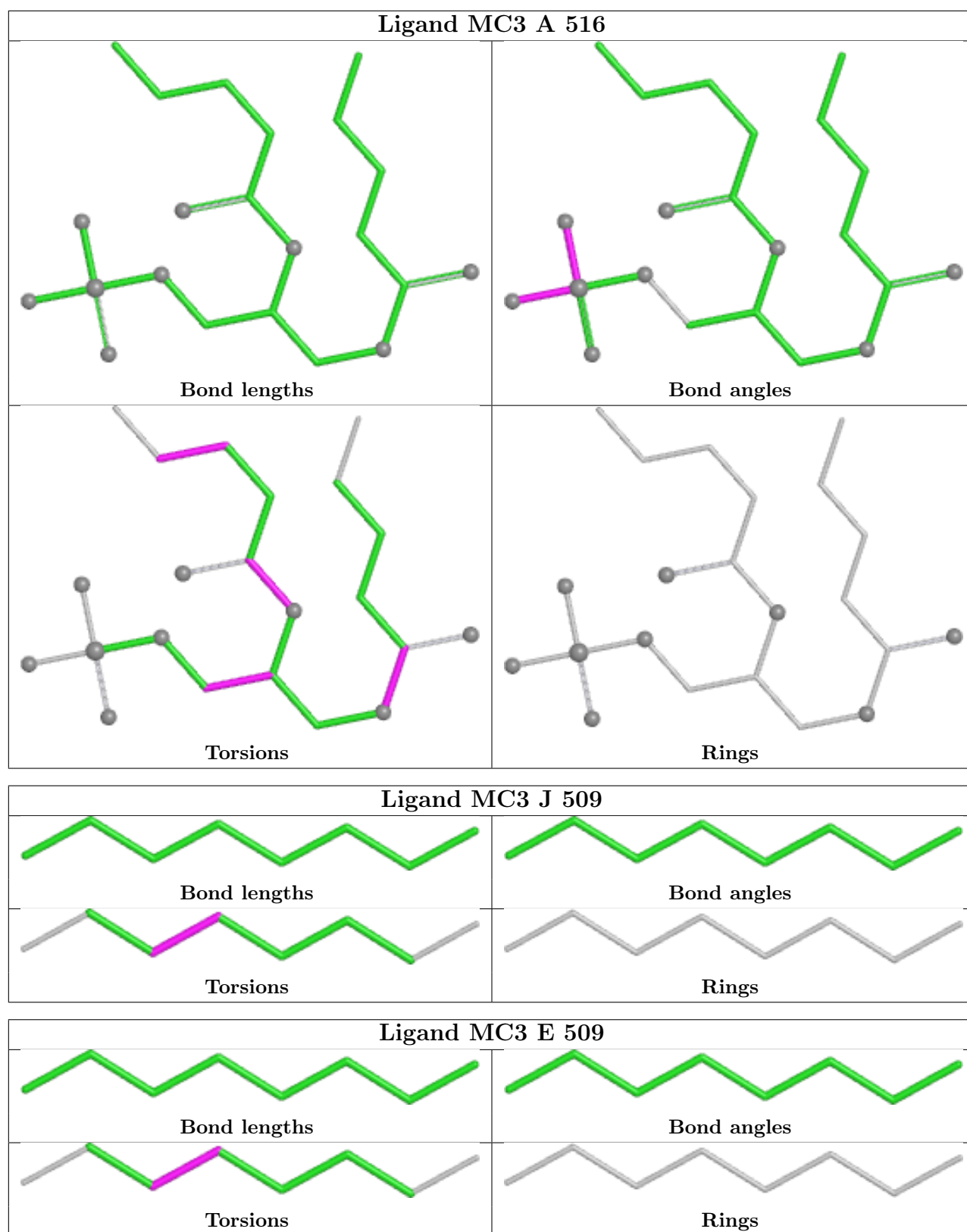












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

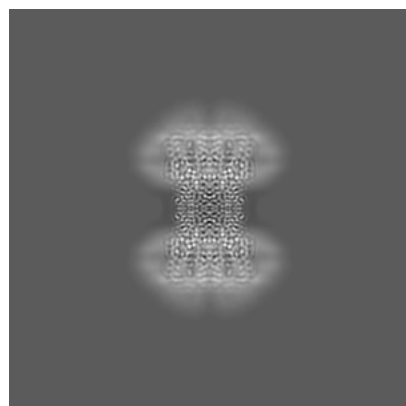
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73900. These allow visual inspection of the internal detail of the map and identification of artifacts.

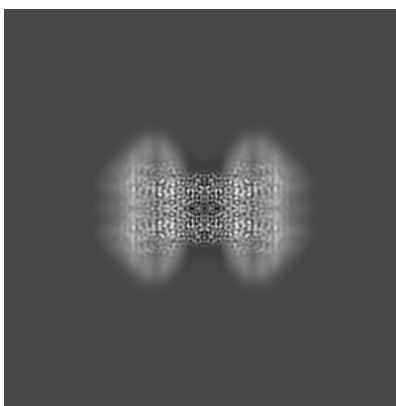
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

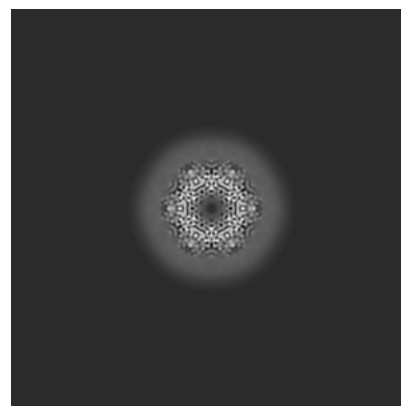
6.1.1 Primary map



X

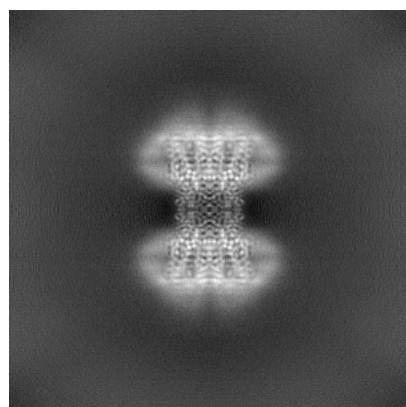


Y

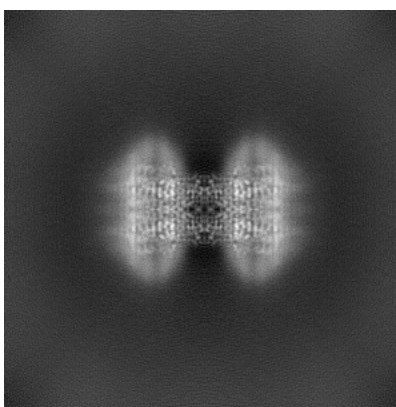


Z

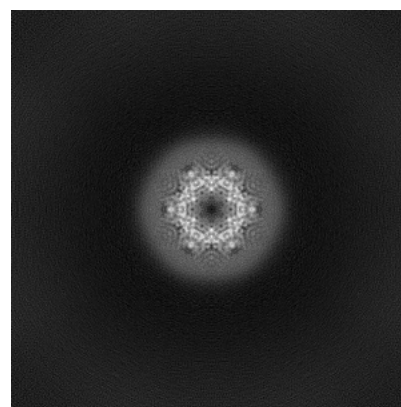
6.1.2 Raw map



X



Y

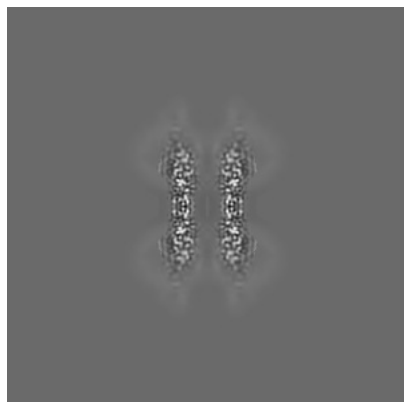


Z

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

6.2 Central slices [i](#)

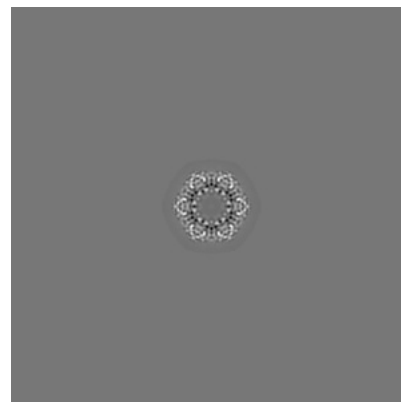
6.2.1 Primary map



X Index: 192

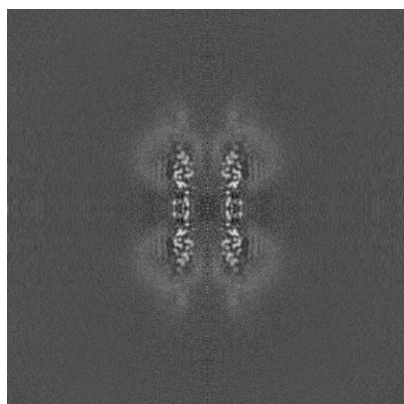


Y Index: 192

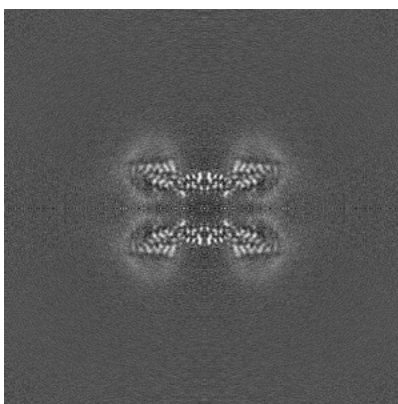


Z Index: 192

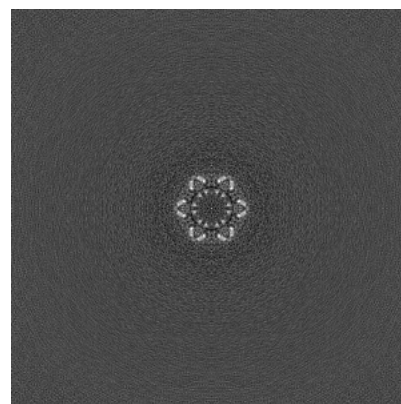
6.2.2 Raw map



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](#)

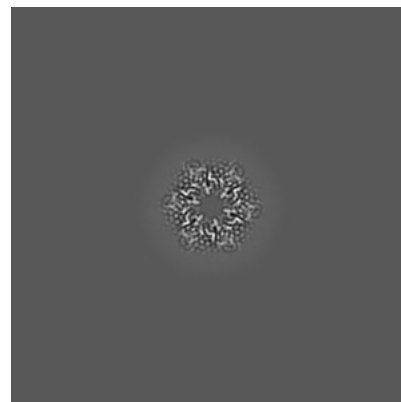
6.3.1 Primary map



X Index: 175

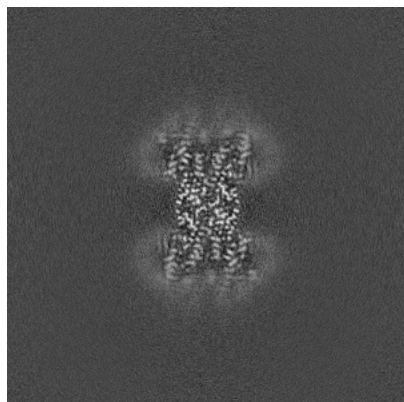


Y Index: 172

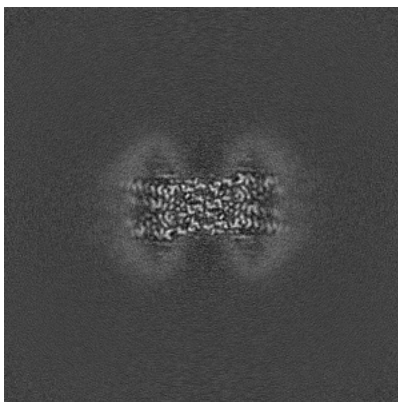


Z Index: 162

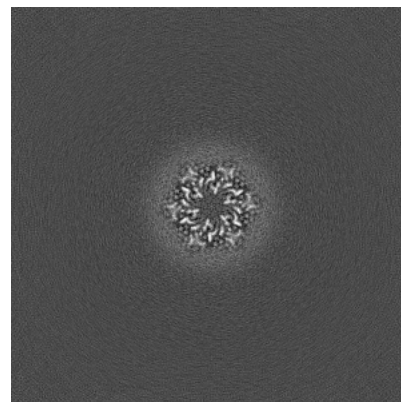
6.3.2 Raw map



X Index: 175



Y Index: 172

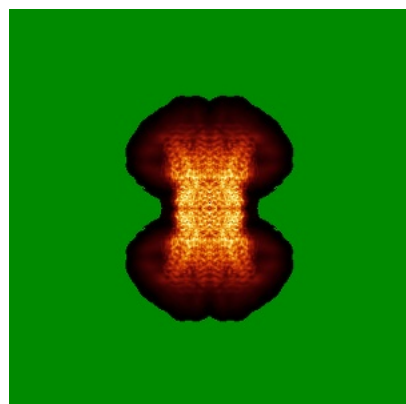


Z Index: 222

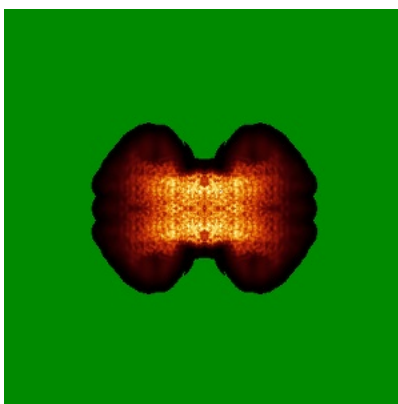
The images above show the largest variance slices of the map in three orthogonal directions.

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

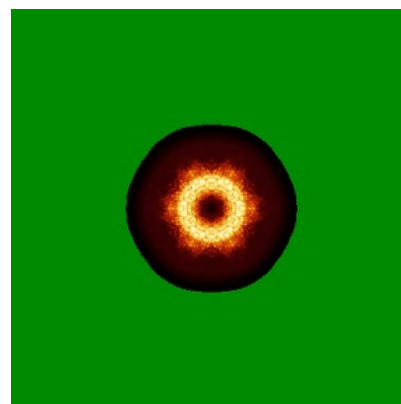
6.4.1 Primary map



X

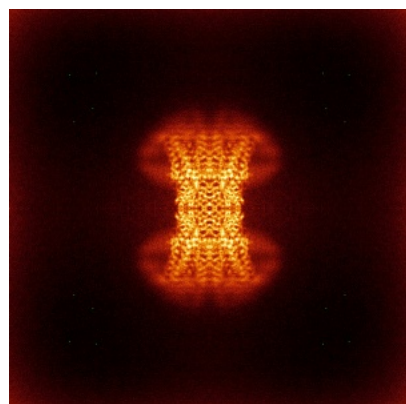


Y

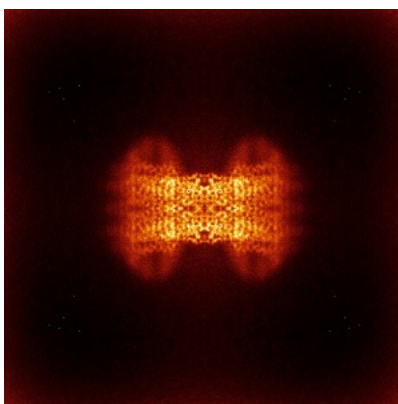


Z

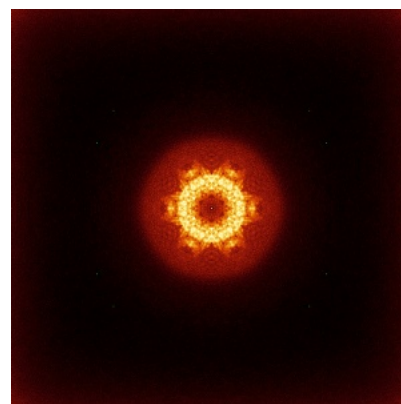
6.4.2 Raw map



X



Y



Z

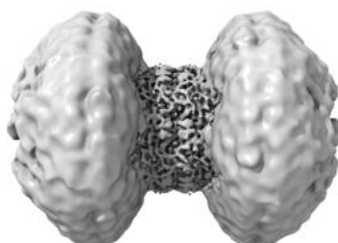
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

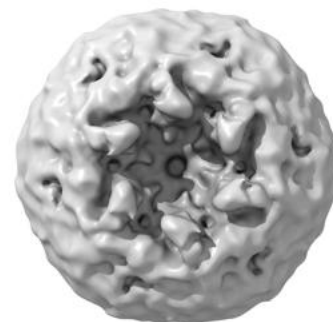
6.5.1 Primary map



X



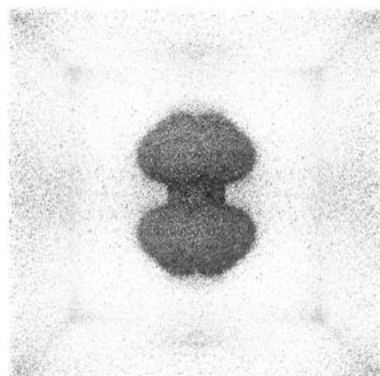
Y



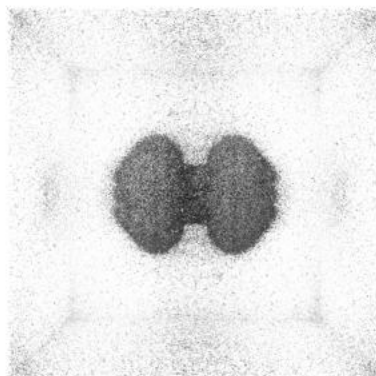
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

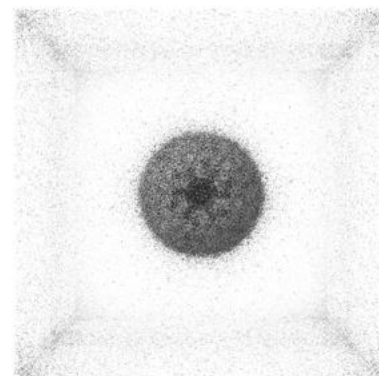
6.5.2 Raw map



X



Y



Z

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.

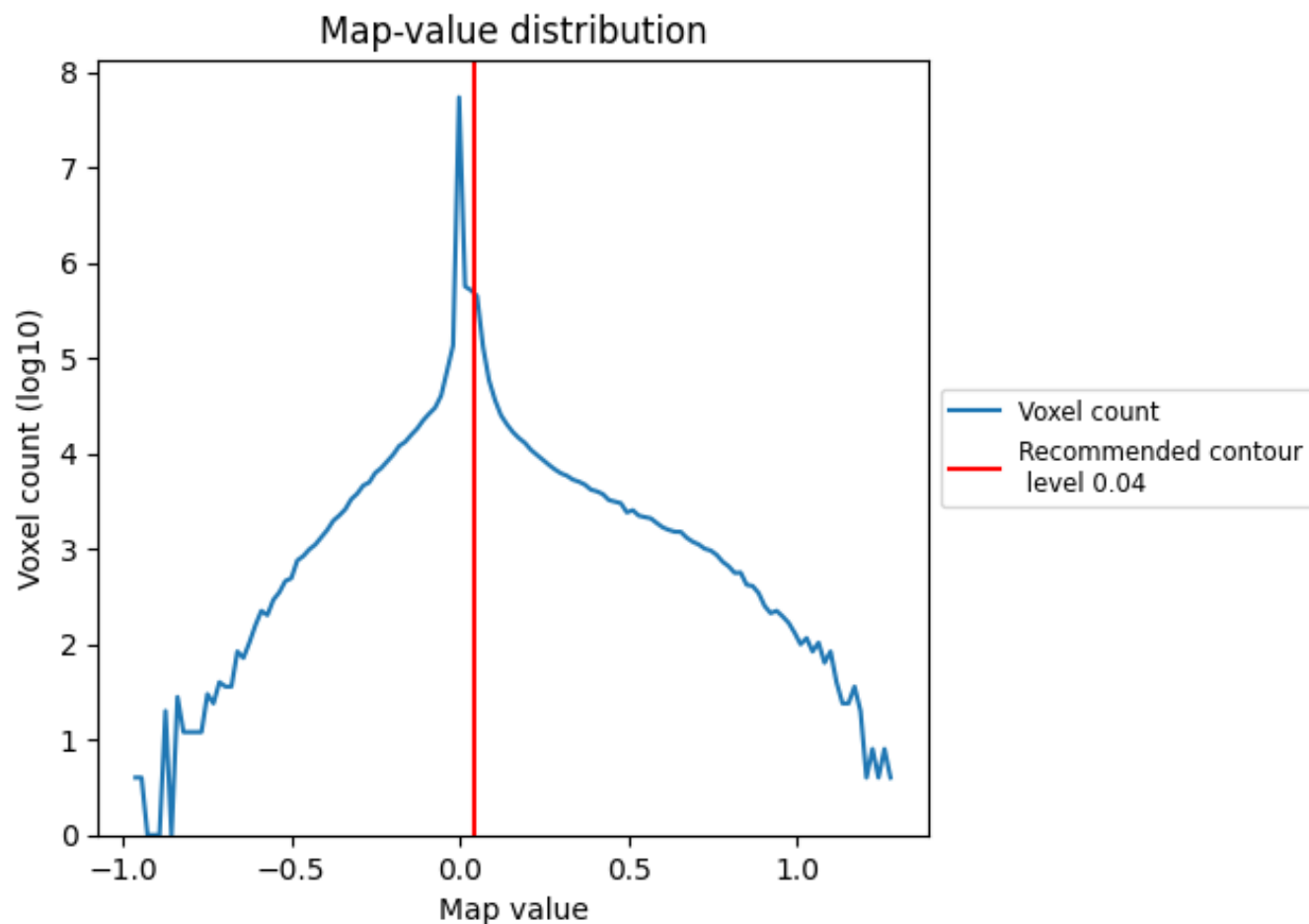
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

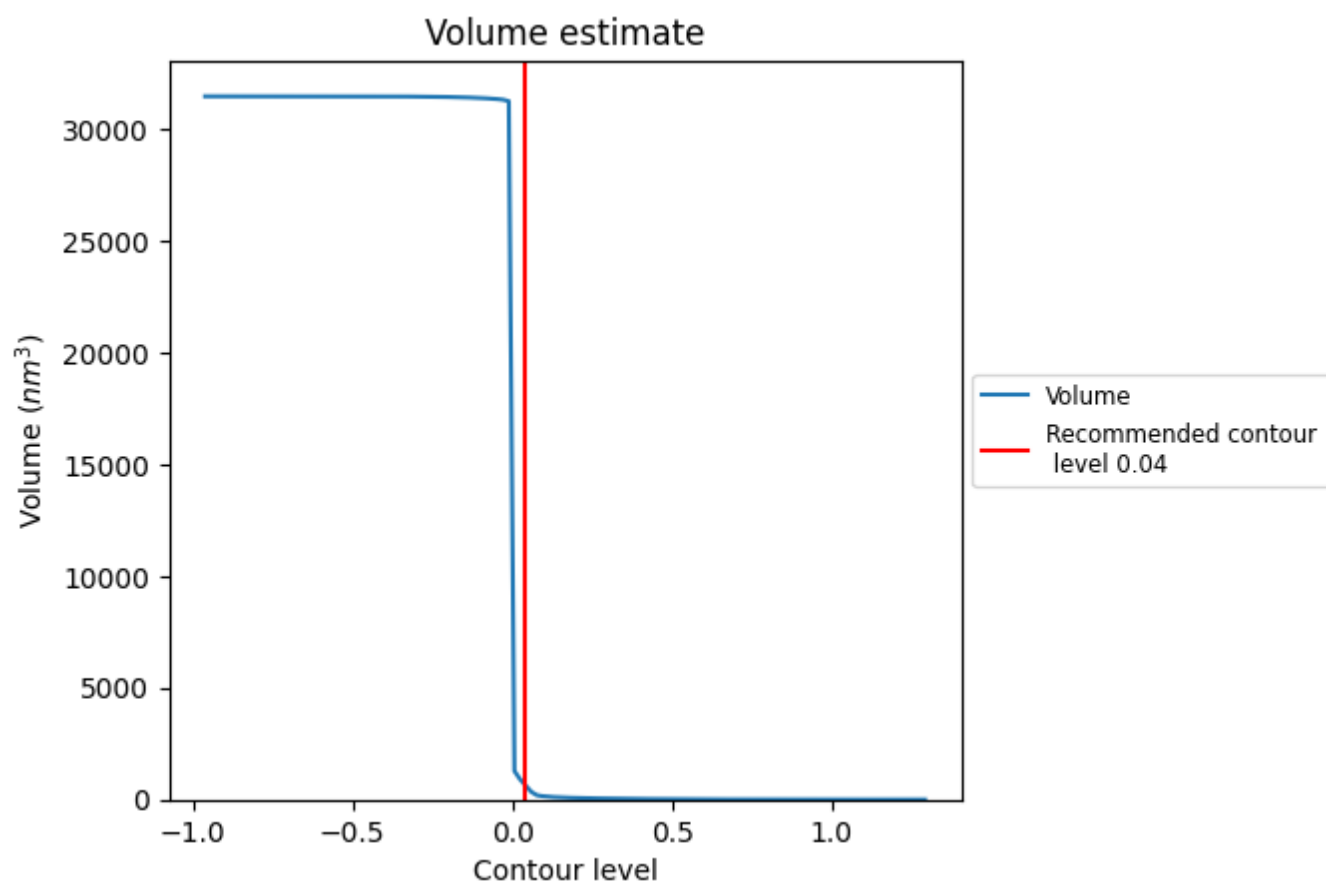
This section contains the results of statistical analysis of the map.

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.

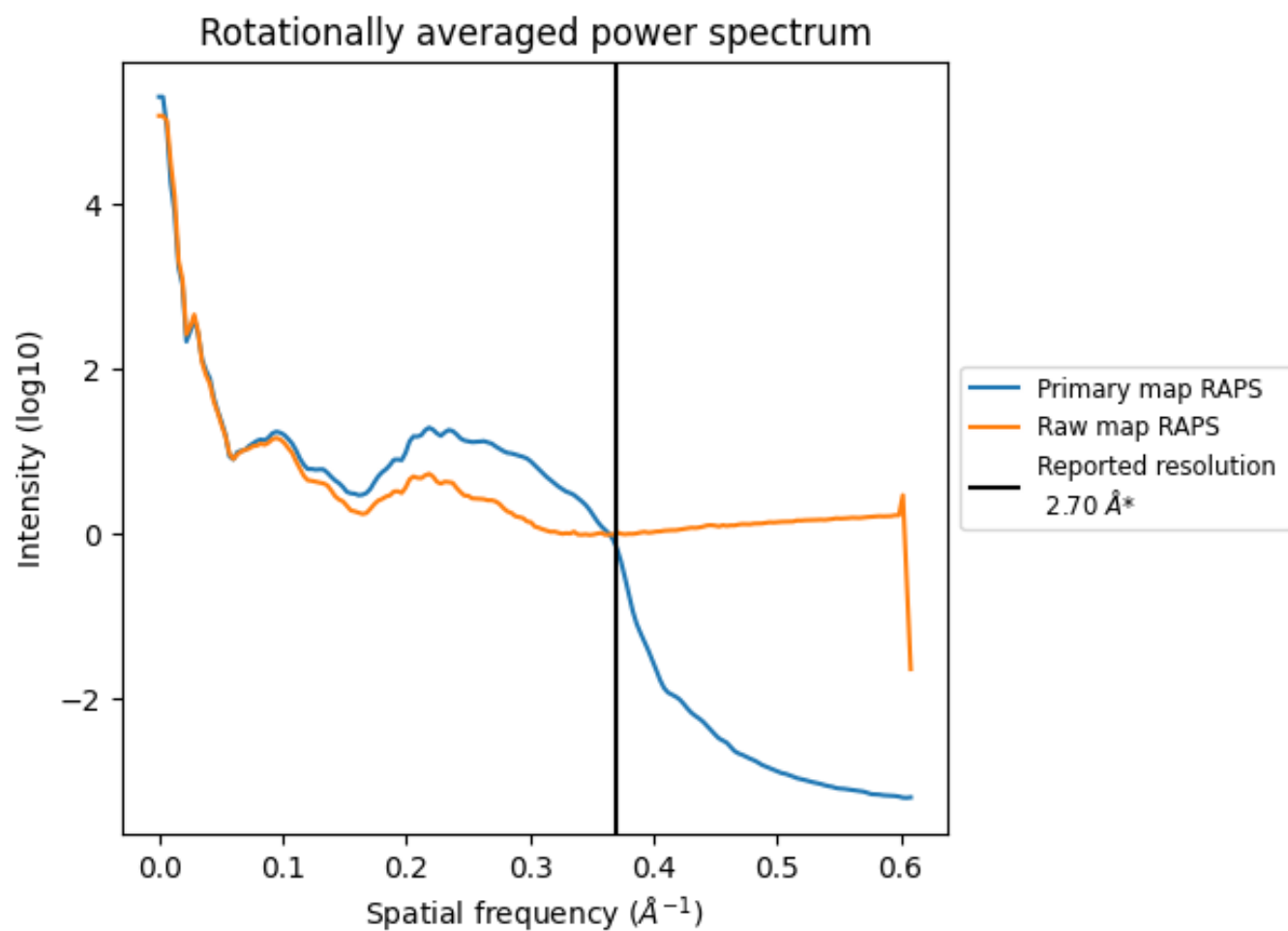
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 665 nm³; this corresponds to an approximate mass of 601 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 ⓘ

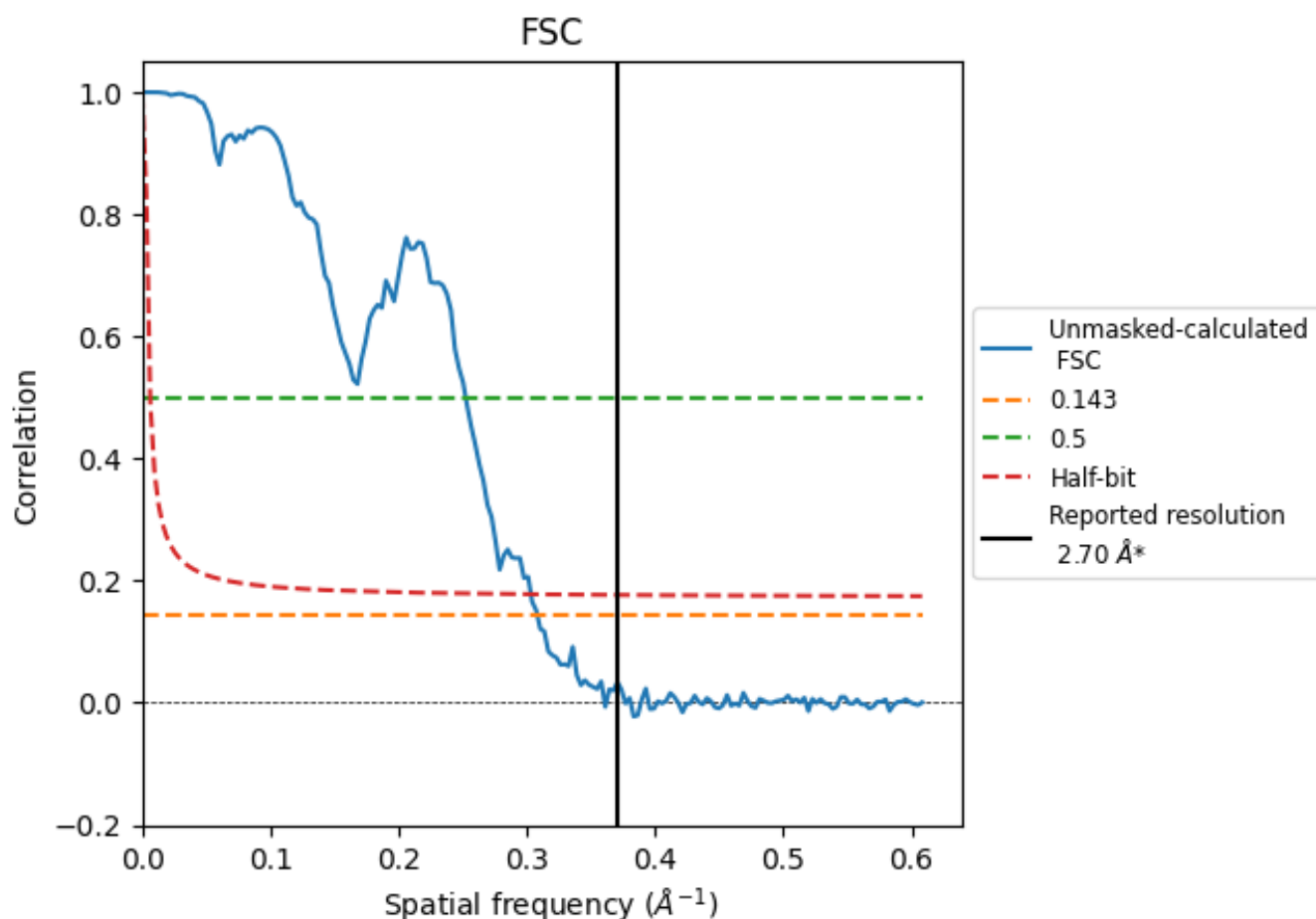


*Reported resolution corresponds to spatial frequency of $0.370 \text{ \AA}^{-1}$

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 $0.370 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.24	3.96	3.30

*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 3.24 differs from the reported value 2.7 by more than 10 %

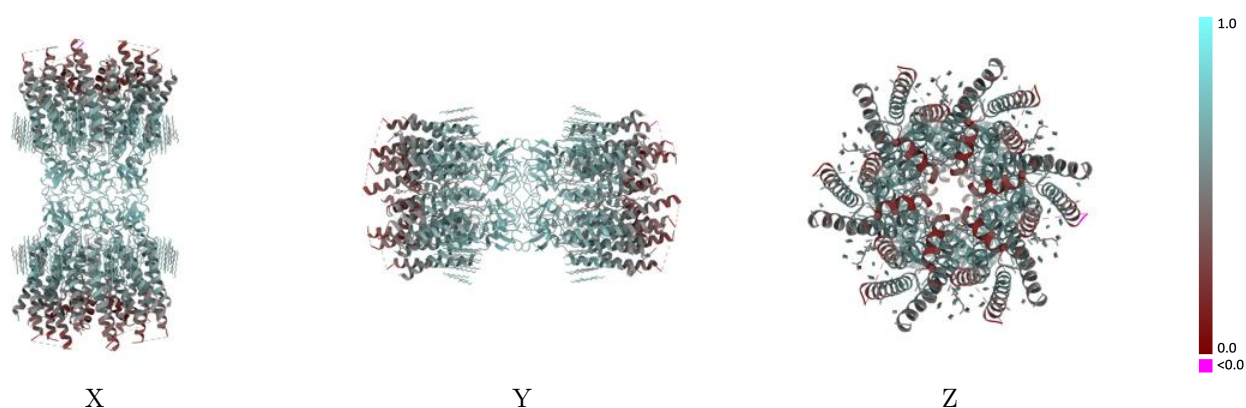
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73900 and PDB model 9Z8M. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)

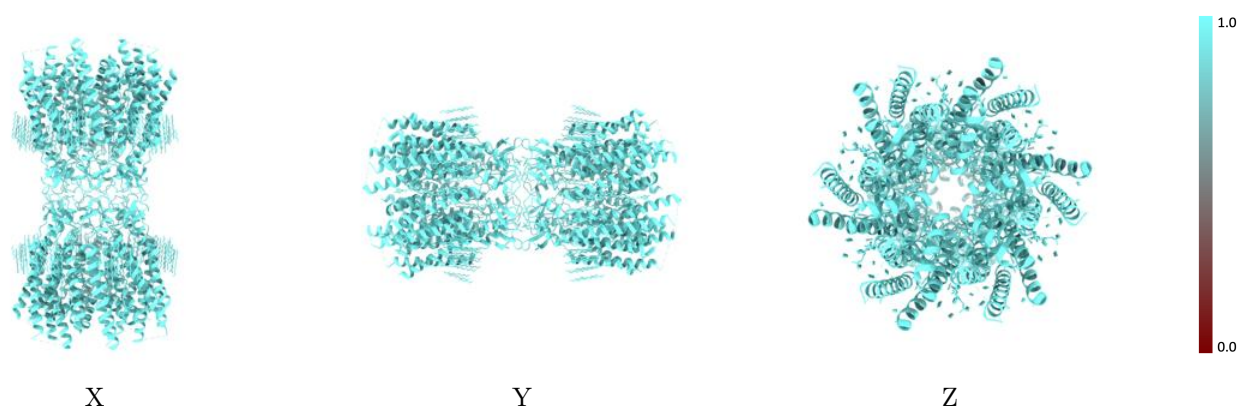
This section was not generated.

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



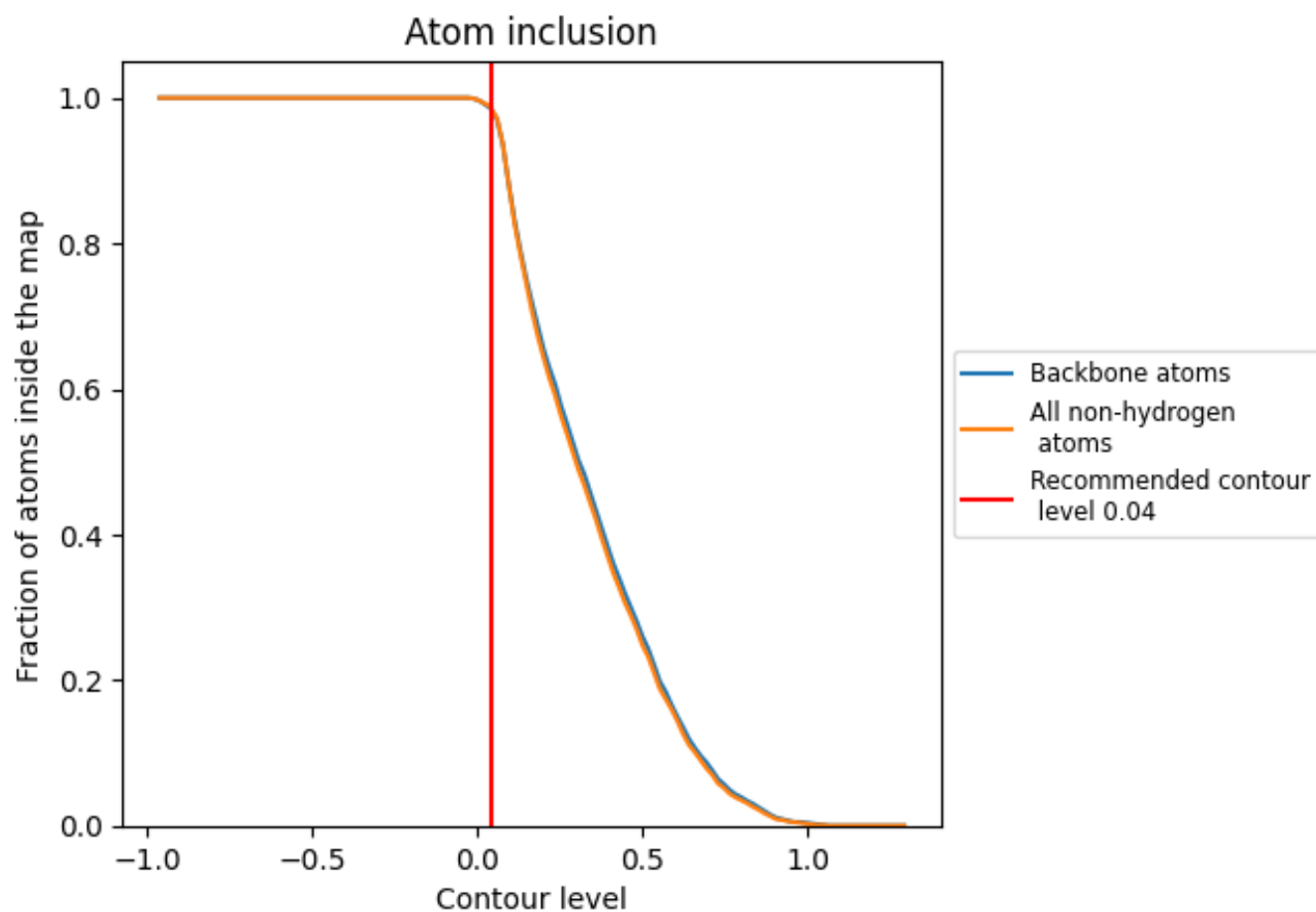
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9880	0.5560
A	0.9890	0.5580
B	0.9880	0.5550
C	0.9880	0.5560
D	0.9900	0.5570
E	0.9870	0.5540
F	0.9880	0.5550
G	0.9870	0.5570
H	0.9900	0.5580
I	0.9870	0.5570
J	0.9870	0.5560
K	0.9900	0.5530
L	0.9880	0.5540

1.0

0.0

<0.0