



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 02:41 PM UTC

PDB ID : 9ZA4 / pdb_00009za4
EMDB ID : EMD-73965
Title : Asymmetrically gated state sheep connexin-50 in DMPC nanodiscs at low pH
Authors : Jarodsky, J.M.; Myers, J.B.; Reichow, S.L.
Deposited on : 2025-11-19
Resolution : 2.40 Å (reported)
Based on initial model : 7jjp

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

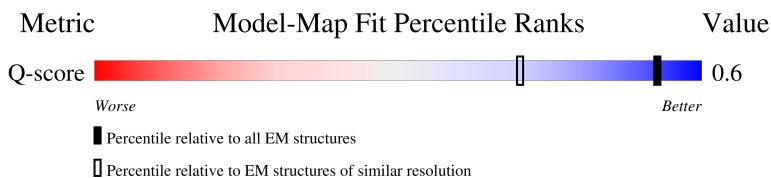
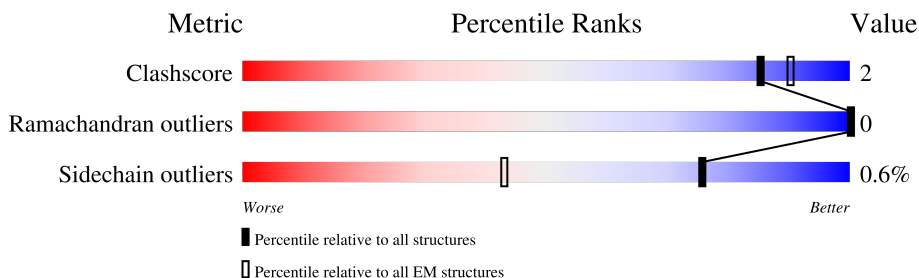
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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	5628 (1.90 - 2.90)

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	440	
1	B	440	
1	C	440	
1	D	440	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	440	 39% 58%
1	F	440	 39% 58%
1	G	440	 40% 58%
1	H	440	 40% 58%
1	I	440	 40% 58%
1	J	440	 40% 58%
1	K	440	 40% 58%
1	L	440	 40% 58%

2 Entry composition

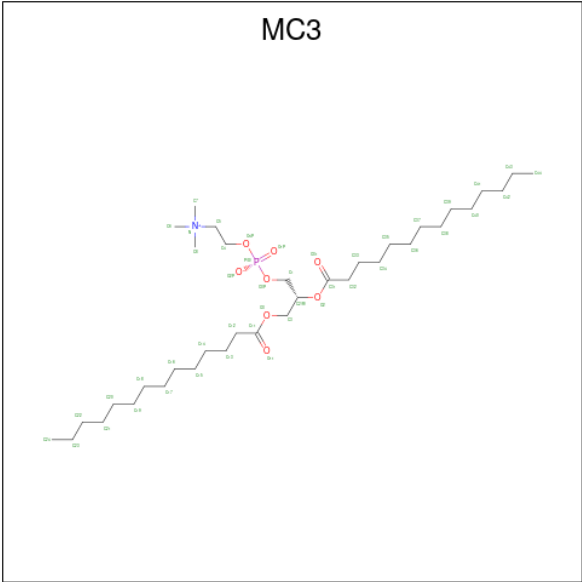
There are 3 unique types of molecules in this entry. The entry contains 43524 atoms, of which 22482 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Gap junction alpha-8 protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	183	Total	C	H	N	O	S	0	0
			2956	983	1473	240	251	9		
1	B	183	Total	C	H	N	O	S	0	0
			2956	983	1473	240	251	9		
1	C	183	Total	C	H	N	O	S	0	0
			2956	983	1473	240	251	9		
1	D	183	Total	C	H	N	O	S	0	0
			2956	983	1473	240	251	9		
1	E	183	Total	C	H	N	O	S	0	0
			2956	983	1473	240	251	9		
1	F	183	Total	C	H	N	O	S	0	0
			2956	983	1473	240	251	9		
1	G	184	Total	C	H	N	O	S	0	0
			2802	946	1371	235	240	10		
1	H	184	Total	C	H	N	O	S	0	0
			2802	946	1371	235	240	10		
1	I	184	Total	C	H	N	O	S	0	0
			2802	946	1371	235	240	10		
1	J	184	Total	C	H	N	O	S	0	0
			2802	946	1371	235	240	10		
1	K	184	Total	C	H	N	O	S	0	0
			2802	946	1371	235	240	10		
1	L	184	Total	C	H	N	O	S	0	0
			2802	946	1371	235	240	10		

- 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
			33	11	22	
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
			30	10	20	
2	A	1	Total	C	H	0
			39	13	26	
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
			30	10	20	
2	A	1	Total	C	H	0
			18	6	12	
2	A	1	Total	C	H	0
			30	10	20	
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
			39	13	26	
2	A	1	Total	C	H	0
			36	12	24	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
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
			27	9	18		
2	F	1	Total	C	H		0
			30	10	20		
2	F	1	Total	C	H		0
			24	8	16		
2	F	1	Total	C	H		0
			33	11	22		
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
			30	10	20		
2	F	1	Total	C	H		0
			39	13	26		
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
			30	10	20		
2	F	1	Total	C	H		0
			18	6	12		
2	F	1	Total	C	H		0
			30	10	20		
2	F	1	Total	C	H		0
			24	8	16		
2	G	1	Total	C	H		0
			27	9	18		
2	G	1	Total	C	H	O	P
			52	16	27	8	1
2	G	1	Total	C	H		0
			33	11	22		
2	G	1	Total	C	H		0
			39	13	26		
2	G	1	Total	C	H		0
			33	11	22		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	G	1	Total	C	H			0
			38	13	25			
2	G	1	Total	C	H			0
			15	5	10			
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
			33	11	22			
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			0
			27	9	18			
2	G	1	Total	C	H	O	P	0
			52	16	27	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
			39	13	26			
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
			36	12	24			
2	G	1	Total	C	H			0
			27	9	18			
2	G	1	Total	C	H			0
			24	8	16			
2	H	1	Total	C	H			0
			27	9	18			
2	H	1	Total	C	H	O	P	0
			52	16	27	8	1	
2	H	1	Total	C	H			0
			33	11	22			
2	H	1	Total	C	H			0
			39	13	26			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	H	1	Total	C	H			0
			36	12	24			
2	H	1	Total	C	H			0
			33	11	22			
2	H	1	Total	C	H			0
			38	13	25			
2	H	1	Total	C	H			0
			15	5	10			
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
			33	11	22			
2	H	1	Total	C	H			0
			24	8	16			
2	H	1	Total	C	H			0
			30	10	20			
2	H	1	Total	C	H			0
			27	9	18			
2	H	1	Total	C	H	O	P	0
			52	16	27	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
			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
			36	12	24			
2	H	1	Total	C	H			0
			27	9	18			
2	H	1	Total	C	H			0
			24	8	16			
2	I	1	Total	C	H			0
			27	9	18			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	I	1	Total	C	H	O	P	0
			52	16	27	8	1	
2	I	1	Total	C	H			0
			33	11	22			
2	I	1	Total	C	H			0
			39	13	26			
2	I	1	Total	C	H			0
			33	11	22			
2	I	1	Total	C	H			0
			38	13	25			
2	I	1	Total	C	H			0
			15	5	10			
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
			33	11	22			
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			0
			27	9	18			
2	I	1	Total	C	H	O	P	0
			52	16	27	8	1	
2	I	1	Total	C	H			0
			39	13	26			
2	I	1	Total	C	H			0
			36	12	24			
2	I	1	Total	C	H			0
			36	12	24			
2	I	1	Total	C	H			0
			39	13	26			
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
			36	12	24			
2	I	1	Total	C	H			0
			27	9	18			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	I	1	Total	C	H			0
			24	8	16			
2	J	1	Total	C	H			0
			27	9	18			
2	J	1	Total	C	H	O	P	0
			52	16	27	8	1	
2	J	1	Total	C	H			0
			33	11	22			
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
			38	13	25			
2	J	1	Total	C	H			0
			15	5	10			
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
			33	11	22			
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			0
			27	9	18			
2	J	1	Total	C	H	O	P	0
			52	16	27	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
			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
			36	12	24			

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
			24	8	16			
2	K	1	Total	C	H			0
			27	9	18			
2	K	1	Total	C	H	O	P	0
			52	16	27	8	1	
2	K	1	Total	C	H			0
			33	11	22			
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
			33	11	22			
2	K	1	Total	C	H			0
			38	13	25			
2	K	1	Total	C	H			0
			15	5	10			
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
			33	11	22			
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			0
			27	9	18			
2	K	1	Total	C	H	O	P	0
			52	16	27	8	1	
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
			39	13	26			

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
			30	10	20			
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
			24	8	16			
2	L	1	Total	C	H	O	P	0
			52	16	27	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
			39	13	26			
2	L	1	Total	C	H			0
			39	13	26			
2	L	1	Total	C	H			0
			30	10	20			
2	L	1	Total	C	H			0
			36	12	24			
2	L	1	Total	C	H			0
			27	9	18			
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	O	P	0
			52	16	27	8	1	
2	L	1	Total	C	H			0
			33	11	22			
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
			38	13	25			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf
2	L	1	Total	C	H	0
			15	5	10	
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
			33	11	22	
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	0
			27	9	18	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	61	Total	O	0
			61	61	
3	B	62	Total	O	0
			62	62	
3	C	62	Total	O	0
			62	62	
3	D	62	Total	O	0
			62	62	
3	E	62	Total	O	0
			62	62	
3	F	62	Total	O	0
			62	62	
3	G	57	Total	O	0
			57	57	
3	H	56	Total	O	0
			56	56	
3	I	56	Total	O	0
			56	56	
3	J	56	Total	O	0
			56	56	
3	K	56	Total	O	0
			56	56	
3	L	56	Total	O	0
			56	56	

GLU	GLN	LEU	LYS	MET
LYS	GLY	GLU	PHE	C2
VAL	VAL	GLY	ARG	E13
SER	GLY	GLY	LEU	V14
LYS	GLY	ILE	GLU	N15
GLN	GLU	VAL	G152	E16
LEU	GLN	SER	HIS	H17
THR	PRO	TYR	T157	S18
PRO	ILE	PHE	C160	T19
GLY	GLU	PRO	H161	V20
ALA	ALA	LEU	E169	T39
PRO	GLY	GLU	V174	V100
SER	PRO	VAL	G189	ARG
CYS	GLY	GLY	G235	GLU
ALA	VAL	MET	LEU	LYS
GLU	GLY	VAL	ILE	GLY
LEU	GLY	GLU	ALA	ARG
GLY	ASP	ALA	SER	GLY
PRO	LYS	PRO	LEU	ALA
GLY	SER	PRO	LEU	GLU
GLU	SER	ALA	SER	GLU
THR	GLN	GLY	LYS	GLY
ARG	GLU	ALA	ALA	SER
PRO	ARG	LYS	PHE	GLY
PRO	VAL	PHE	PRO	ASN
GLY	SER	SER	LEU	GLY
SER	THR	SER	GLY	GLY
ARG	LEU	VAL	GLY	GLY
ARG	ALA	GLY	ILE	GLU
ALA	VAL	PRO	PRO	ARG
SER	GLY	LEU	GLU	ALA
ASP	GLU	GLY	LYS	PRO
ASP	GLU	ASP	SER	LEU
LEU	LYS	VAL	LEU	ALA
THR	VAL	GLY	LEU	ALA
VAL	GLY	SER	HIS	ASP
	PRO	ARG	TLE	GLN
	PRO	ALA	ALA	GLY
	GLY	TYR	VAL	SER
	VAL	GLN	SER	LYS
	GLY	THR	ILE	LYS
	GLY	LEU	TLE	LYS
	ALA	PRO	GLN	SER
	GLY	SER	LYS	SER
	GLY	TYR	ALA	SER
	LYS	ALA	LYS	SER
	GLY	VAL	GLY	SER
	THR	GLN	TYR	LYS
	PRO	GLY	GLN	GLY
	PRO	ALA	LEU	THR

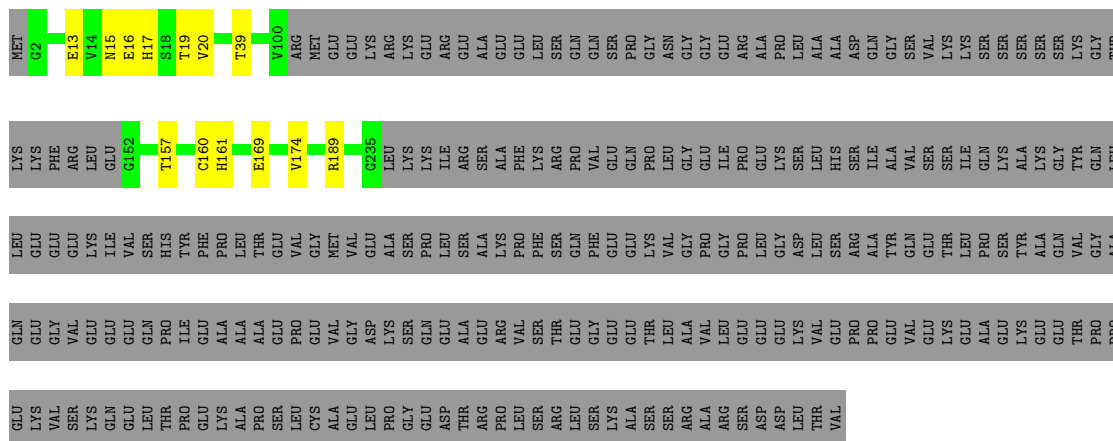
Chain D: 39% . 58%

VAL	GLY	GLU	PHE	MET
SER	VAL	GLU	ARG	G2
LYS	GLU	LYS	LEU	E13
GLN	GLU	ILE	GLU	V14
GLU	GLN	SER	G152	V14
LEU	PRO	HIS	T157	H15
THR	ILE	TYR	TYR	E16
PRO	GLU	PHE	C160	H17
GLU	ALA	PRO	H161	S18
LYS	ALA	LEU	E169	T19
ALA	ALA	THR	V174	V20
PRO	GLU	GLU	R189	V100
SER	PRO	VAL	G235	ARG
LEU	ASP	VAL	LEU	MET
PRO	LYS	ALA	LYS	GLU
GLY	GLN	PRO	LYS	GLU
LEU	GLU	LEU	ILE	ARG
SER	ALA	SER	ARG	GLU
ARG	GLU	ALA	SER	ALA
THR	VAL	ARG	ALA	GLU
PRO	VAL	PRO	PHE	GLU
GLY	THR	PHE	LYS	LEU
LYS	GLU	GLN	ARG	SER
ALA	THR	PHE	PRO	GLN
GLU	LEU	GLU	VAL	GLN
THR	VAL	LYS	GLY	SER
SER	ALA	VAL	GLU	GLY
ARG	VAL	PRO	ILE	GLY
ALA	LEU	PRO	PRO	GLU
ALA	GLU	LEU	GLU	ARG
ASP	GLU	GLY	ASP	ALA
SER	GLY	ASP	LYS	PRO
LEU	VAL	LEU	SER	LEU
THR	GLU	SER	LEU	ALA
VAL	GLU	PRO	HIS	ALA
	PRO	ARG	SER	ASP
	PRO	ALA	ILE	GLN
	GLU	TYR	VAL	GLY
	VAL	GLN	VAL	SER
	GLU	GLU	SER	VAL
	LYS	THR	LEU	LYS
	GLU	PRO	ILE	LYS
	ALA	PRO	GLN	SER
	GLU	SER	LYS	SER
	GLY	TYR	ALA	SER
	GLU	ALA	LYS	SER
	GLU	GLN	GLY	SER
	PRO	GLY	GLN	LYS
	PRO	ALA	LEU	THR
	GLY	GLN	LEU	LYS

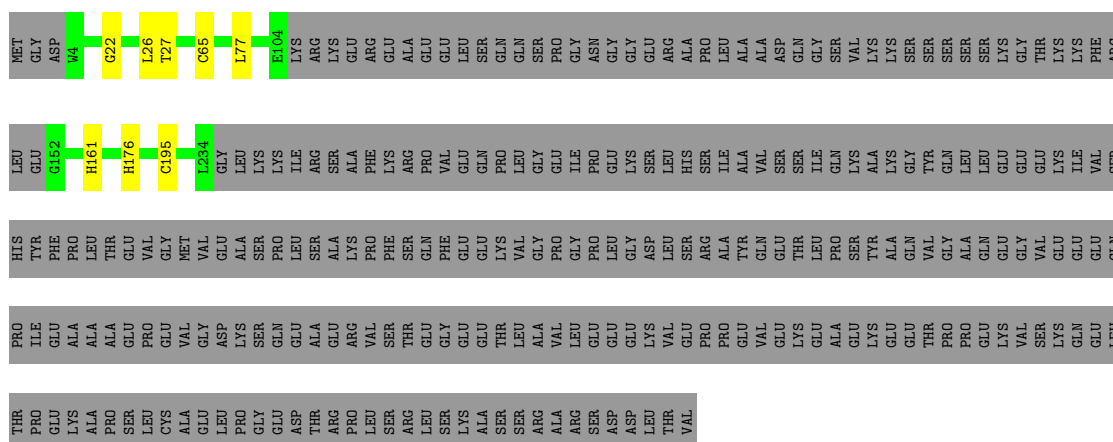
Chain E: 39% 0% 58%

VAL	GLY	GLU	PHE	MET
SER	VAL	GLU	ARG	C2
LYS	GLU	LYS	LEU	E13
GLN	GLU	ILE	GLU	V44
GLU	GLN	VAL	G152	N15
LEU	SER	SER		E16
THR	PRO	HIS	T157	H17
PRO	ILE	TYR		S18
GLU	GLU	PHE	C160	T19
LYS	ALA	PRO	H161	V20
ALA	ALA	LEU		
PRO	ALA	THR	E169	V100
SER	GLU	GLU		ARG
LEU	PRO	VAL	V174	MET
CYS	GLU	GLY		GLU
ALA	VAL	MET	R189	GLU
GLY	GLY	VAL		LYS
LEU	ASP	GLU	G235	ARG
PRO	LYS	ALA	LEU	ARG
GLY	SER	SER	LYS	LYS
GLU	GLN	PRO	LYS	GLU
THR	ALA	LEU	ILE	ARG
THR	ALA	SER	ARG	GLU
ARG	GLU	ALA	SER	ALA
PRO	ARG	LYS	ALA	GLU
LEU	VAL	PRO	PHE	GLU
SER	SER	PHE	LYS	LEU
ARG	THR	THR	ARG	SER
LEU	GLY	GLN	PRO	GLN
SER	GLY	PHE	VAL	GLN
LYS	GLU	GLU	GLU	SER
ALA	GLU	GLU	GLN	PRO
SER	THR	LYS	PRO	GLY
SER	LEU	VAL	LEU	ASN
ARG	ALA	GLY	GLY	GLY
ALA	VAL	PRO	GLU	GLY
ARG	LEU	GLY	ILE	GLY
SER	GLU	PRO	PRO	ARG
ASP	GLU	LEU	GLU	ALA
ASP	GLU	LYS	LYS	PRO
LEU	LYS	ASP	SER	LEU
THR	VAL	LEU	LEU	ALA
VAL	GLU	SER	HIS	ALA
	PRO	ARG	SER	ASP
	PRO	GLU	ALA	GLN
	GLU	TYR	ILE	GLY
	VAL	GLN	VAL	SER
	GLY	GLU	SER	VAL
	LEU	THR	SER	LYS
	GLU	LEU	ILE	LYS
	ALA	PRO	GLN	SER
	GLY	THR	LYS	SER
	LYS	TYR	ALA	SER
	GLU	ALA	LYS	SER
	GLU	GLN	GLY	LYS
	THR	VAL	TYR	GLY
	PRO	GLY	GLN	THR
	PRO	ALA	LEU	LYS
	GLY	GLN	LEU	LYS

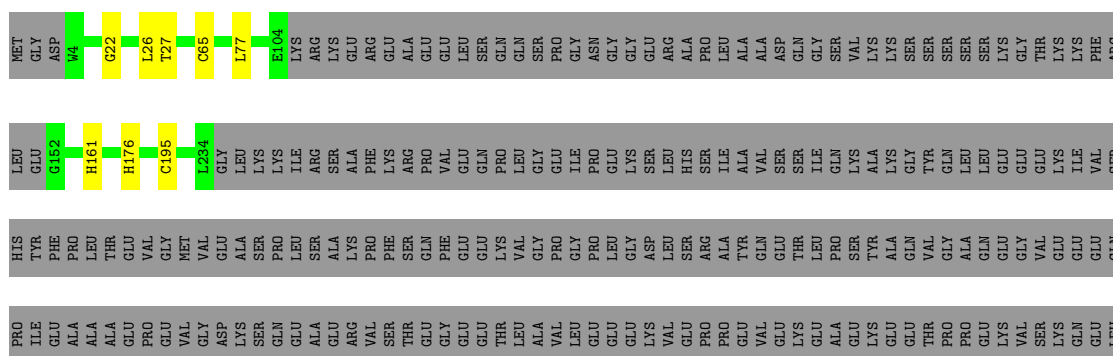
Chain F: 39% 1% 58%



Chain G: 40% 1% 58%



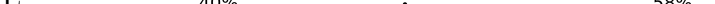
Chain H: 40% . 58%



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

[illegible]

- Molecule 1: Gap junction alpha-8 protein

Chain L:  40% . 58%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	162334	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)	500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.902	Depositor
Minimum map value	-2.039	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.050	Depositor
Recommended contour level	0.03	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	0.18	0/1528	0.32	0/2084
1	B	0.19	0/1528	0.32	0/2084
1	C	0.19	0/1528	0.32	0/2084
1	D	0.19	0/1528	0.32	0/2084
1	E	0.19	0/1528	0.32	0/2084
1	F	0.19	0/1528	0.32	0/2084
1	G	0.16	0/1473	0.27	0/2012
1	H	0.17	0/1473	0.27	0/2012
1	I	0.17	0/1473	0.28	0/2012
1	J	0.17	0/1473	0.28	0/2012
1	K	0.17	0/1473	0.28	0/2012
1	L	0.17	0/1473	0.28	0/2012
All	All	0.18	0/18006	0.30	0/24576

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	1483	1473	1463	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1483	1473	1463	12	0
1	C	1483	1473	1463	12	0
1	D	1483	1473	1463	11	0
1	E	1483	1473	1463	12	0
1	F	1483	1473	1463	12	0
1	G	1431	1371	1362	4	0
1	H	1431	1371	1362	4	0
1	I	1431	1371	1362	5	0
1	J	1431	1371	1362	4	0
1	K	1431	1371	1362	4	0
1	L	1431	1371	1362	4	0
2	A	199	398	343	0	0
2	B	199	398	343	1	0
2	C	199	398	343	1	0
2	D	199	398	343	1	0
2	E	199	398	343	1	0
2	F	199	398	343	1	0
2	G	264	481	418	0	0
2	H	288	529	464	0	0
2	I	276	505	441	1	0
2	J	264	481	418	0	0
2	K	288	529	464	0	0
2	L	276	505	441	0	0
3	A	61	0	0	1	0
3	B	62	0	0	1	0
3	C	62	0	0	1	0
3	D	62	0	0	1	0
3	E	62	0	0	1	0
3	F	62	0	0	1	0
3	G	57	0	0	0	0
3	H	56	0	0	0	0
3	I	56	0	0	0	0
3	J	56	0	0	0	0
3	K	56	0	0	0	0
3	L	56	0	0	0	0
All	All	21042	22482	21654	92	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.

The worst 5 of 92 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:C:157:THR:HA	1:C:160:CYS:SG	2.16	0.86
1:A:157:THR:HA	1:A:160:CYS:SG	2.15	0.86
1:B:157:THR:HA	1:B:160:CYS:SG	2.15	0.85
1:D:157:THR:HA	1:D:160:CYS:SG	2.16	0.85
1:E:157:THR:HA	1:E:160:CYS:SG	2.15	0.85

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	179/440 (41%)	176 (98%)	3 (2%)	0	100	100
1	B	179/440 (41%)	176 (98%)	3 (2%)	0	100	100
1	C	179/440 (41%)	176 (98%)	3 (2%)	0	100	100
1	D	179/440 (41%)	176 (98%)	3 (2%)	0	100	100
1	E	179/440 (41%)	176 (98%)	3 (2%)	0	100	100
1	F	179/440 (41%)	176 (98%)	3 (2%)	0	100	100
1	G	180/440 (41%)	179 (99%)	1 (1%)	0	100	100
1	H	180/440 (41%)	179 (99%)	1 (1%)	0	100	100
1	I	180/440 (41%)	179 (99%)	1 (1%)	0	100	100
1	J	180/440 (41%)	179 (99%)	1 (1%)	0	100	100
1	K	180/440 (41%)	179 (99%)	1 (1%)	0	100	100
1	L	180/440 (41%)	179 (99%)	1 (1%)	0	100	100
All	All	2154/5280 (41%)	2130 (99%)	24 (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	166/385 (43%)	165 (99%)	1 (1%)	78	89
1	B	166/385 (43%)	165 (99%)	1 (1%)	78	89
1	C	166/385 (43%)	165 (99%)	1 (1%)	78	89
1	D	166/385 (43%)	165 (99%)	1 (1%)	78	89
1	E	166/385 (43%)	165 (99%)	1 (1%)	78	89
1	F	166/385 (43%)	165 (99%)	1 (1%)	78	89
1	G	150/385 (39%)	149 (99%)	1 (1%)	76	88
1	H	150/385 (39%)	149 (99%)	1 (1%)	76	88
1	I	150/385 (39%)	149 (99%)	1 (1%)	76	88
1	J	150/385 (39%)	149 (99%)	1 (1%)	76	88
1	K	150/385 (39%)	149 (99%)	1 (1%)	76	88
1	L	150/385 (39%)	149 (99%)	1 (1%)	76	88
All	All	1896/4620 (41%)	1884 (99%)	12 (1%)	76	89

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

Mol	Chain	Res	Type
1	H	27	THR
1	I	27	THR
1	L	27	THR
1	J	27	THR
1	D	161	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	57	GLN
1	J	49	GLN
1	I	49	GLN
1	J	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	58	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

252 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	G	505	-	10,10,45	0.33	0	9,9,53	0.81	0
2	MC3	E	512	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	F	510	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	H	509	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	H	514	-	8,8,45	0.35	0	7,7,53	0.79	0
2	MC3	L	519	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	K	522	-	11,11,45	0.34	0	10,10,53	0.84	0
2	MC3	A	519	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	G	513	-	8,8,45	0.35	0	7,7,53	0.79	0
2	MC3	B	503	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	L	518	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	B	505	-	10,10,45	0.36	0	9,9,53	0.84	0
2	MC3	H	522	-	11,11,45	0.34	0	10,10,53	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	C	502	-	12,12,45	0.36	0	11,11,53	0.86	0
2	MC3	F	501	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	K	507	-	12,12,45	0.34	0	11,11,53	0.84	0
2	MC3	K	512	-	7,7,45	0.35	0	6,6,53	0.76	0
2	MC3	G	516	-	11,11,45	0.33	0	10,10,53	0.84	0
2	MC3	E	501	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	G	504	-	12,12,45	0.33	0	11,11,53	0.83	0
2	MC3	C	517	-	5,5,45	0.36	0	4,4,53	0.62	0
2	MC3	K	508	-	4,4,45	0.37	0	3,3,53	0.57	0
2	MC3	I	505	-	10,10,45	0.33	0	9,9,53	0.81	0
2	MC3	K	514	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	F	514	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	L	510	-	7,7,45	0.35	0	6,6,53	0.74	0
2	MC3	J	519	-	9,9,45	0.34	0	8,8,53	0.80	0
2	MC3	G	514	-	24,24,45	0.54	0	27,29,53	0.73	1 (3%)
2	MC3	J	508	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	B	517	-	5,5,45	0.37	0	4,4,53	0.62	0
2	MC3	K	524	-	7,7,45	0.35	0	6,6,53	0.74	0
2	MC3	A	513	-	12,12,45	0.36	0	11,11,53	0.86	0
2	MC3	A	516	-	10,10,45	0.36	0	9,9,53	0.84	0
2	MC3	B	510	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	L	522	-	9,9,45	0.34	0	8,8,53	0.81	0
2	MC3	K	523	-	8,8,45	0.34	0	7,7,53	0.78	0
2	MC3	B	506	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	E	511	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	G	506	-	12,12,45	0.34	0	11,11,53	0.83	0
2	MC3	G	511	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	L	520	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	I	502	-	24,24,45	0.82	1 (4%)	27,29,53	1.13	2 (7%)
2	MC3	D	502	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	B	504	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	A	512	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	D	519	-	7,7,45	0.37	0	6,6,53	0.76	0
2	MC3	F	504	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	F	503	-	11,11,45	0.36	0	10,10,53	0.85	0
2	MC3	J	502	-	24,24,45	0.82	1 (4%)	27,29,53	1.13	2 (7%)
2	MC3	D	517	-	5,5,45	0.36	0	4,4,53	0.62	0
2	MC3	K	518	-	11,11,45	0.33	0	10,10,53	0.84	0
2	MC3	F	519	-	7,7,45	0.37	0	6,6,53	0.76	0
2	MC3	H	523	-	8,8,45	0.35	0	7,7,53	0.79	0
2	MC3	D	506	-	8,8,45	0.37	0	7,7,53	0.79	0
2	MC3	D	515	-	10,10,45	0.35	0	9,9,53	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	J	517	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	D	513	-	12,12,45	0.35	0	11,11,53	0.84	0
2	MC3	B	508	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	F	518	-	9,9,45	0.35	0	8,8,53	0.82	0
2	MC3	E	518	-	9,9,45	0.36	0	8,8,53	0.83	0
2	MC3	G	512	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	C	515	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	C	513	-	12,12,45	0.35	0	11,11,53	0.84	0
2	MC3	A	504	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	I	510	-	10,10,45	0.34	0	9,9,53	0.82	0
2	MC3	J	503	-	10,10,45	0.32	0	9,9,53	0.80	0
2	MC3	J	505	-	10,10,45	0.33	0	9,9,53	0.80	0
2	MC3	K	513	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	C	510	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	K	515	-	24,24,45	0.52	0	27,29,53	0.77	1 (3%)
2	MC3	I	522	-	8,8,45	0.34	0	7,7,53	0.78	0
2	MC3	F	509	-	10,10,45	0.36	0	9,9,53	0.83	0
2	MC3	G	501	-	8,8,45	0.23	0	7,7,53	0.22	0
2	MC3	K	502	-	24,24,45	0.82	1 (4%)	27,29,53	1.13	2 (7%)
2	MC3	L	507	-	9,9,45	0.34	0	8,8,53	0.80	0
2	MC3	F	506	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	L	514	-	12,12,45	0.33	0	11,11,53	0.82	0
2	MC3	L	521	-	7,7,45	0.36	0	6,6,53	0.76	0
2	MC3	H	517	-	11,11,45	0.33	0	10,10,53	0.82	0
2	MC3	C	507	-	9,9,45	0.36	0	8,8,53	0.82	0
2	MC3	J	513	-	8,8,45	0.35	0	7,7,53	0.79	0
2	MC3	E	502	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	K	517	-	11,11,45	0.33	0	10,10,53	0.82	0
2	MC3	K	520	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	I	503	-	10,10,45	0.32	0	9,9,53	0.80	0
2	MC3	J	518	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	E	504	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	H	520	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	L	511	-	8,8,45	0.23	0	7,7,53	0.22	0
2	MC3	L	513	-	10,10,45	0.32	0	9,9,53	0.80	0
2	MC3	E	519	-	7,7,45	0.37	0	6,6,53	0.76	0
2	MC3	J	509	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	J	511	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	B	511	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	G	509	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	L	516	-	12,12,45	0.34	0	11,11,53	0.83	0
2	MC3	C	516	-	9,9,45	0.36	0	8,8,53	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	A	518	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	J	515	-	12,12,45	0.32	0	11,11,53	0.83	0
2	MC3	J	516	-	11,11,45	0.33	0	10,10,53	0.84	0
2	MC3	A	515	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	K	519	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	L	509	-	8,8,45	0.35	0	7,7,53	0.78	0
2	MC3	I	519	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	J	522	-	7,7,45	0.36	0	6,6,53	0.74	0
2	MC3	G	503	-	10,10,45	0.32	0	9,9,53	0.80	0
2	MC3	D	512	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	C	504	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	C	505	-	10,10,45	0.36	0	9,9,53	0.83	0
2	MC3	J	506	-	12,12,45	0.34	0	11,11,53	0.84	0
2	MC3	B	509	-	10,10,45	0.35	0	9,9,53	0.83	0
2	MC3	C	512	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	G	520	-	11,11,45	0.34	0	10,10,53	0.85	0
2	MC3	A	509	-	5,5,45	0.37	0	4,4,53	0.62	0
2	MC3	A	511	-	7,7,45	0.36	0	6,6,53	0.76	0
2	MC3	G	518	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	I	517	-	11,11,45	0.33	0	10,10,53	0.84	0
2	MC3	C	519	-	7,7,45	0.36	0	6,6,53	0.76	0
2	MC3	F	515	-	10,10,45	0.36	0	9,9,53	0.82	0
2	MC3	H	515	-	24,24,45	0.52	0	27,29,53	0.78	1 (3%)
2	MC3	L	506	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	H	516	-	12,12,45	0.32	0	11,11,53	0.83	0
2	MC3	I	515	-	12,12,45	0.31	0	11,11,53	0.83	0
2	MC3	I	513	-	8,8,45	0.35	0	7,7,53	0.79	0
2	MC3	K	516	-	12,12,45	0.32	0	11,11,53	0.83	0
2	MC3	D	504	-	9,9,45	0.36	0	8,8,53	0.82	0
2	MC3	A	501	-	10,10,45	0.35	0	9,9,53	0.83	0
2	MC3	I	521	-	11,11,45	0.34	0	10,10,53	0.84	0
2	MC3	L	503	-	11,11,45	0.33	0	10,10,53	0.82	0
2	MC3	C	506	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	F	517	-	5,5,45	0.36	0	4,4,53	0.62	0
2	MC3	H	508	-	4,4,45	0.37	0	3,3,53	0.57	0
2	MC3	I	506	-	12,12,45	0.34	0	11,11,53	0.84	0
2	MC3	J	510	-	10,10,45	0.34	0	9,9,53	0.82	0
2	MC3	L	512	-	24,24,45	0.82	1 (4%)	27,29,53	1.13	2 (7%)
2	MC3	A	507	-	10,10,45	0.36	0	9,9,53	0.82	0
2	MC3	D	511	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	G	519	-	9,9,45	0.34	0	8,8,53	0.80	0
2	MC3	C	509	-	10,10,45	0.35	0	9,9,53	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	K	509	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	A	505	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	B	507	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	E	515	-	10,10,45	0.36	0	9,9,53	0.81	0
2	MC3	F	511	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	H	511	-	10,10,45	0.34	0	9,9,53	0.82	0
2	MC3	H	519	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	J	514	-	24,24,45	0.53	0	27,29,53	0.72	1 (3%)
2	MC3	B	519	-	7,7,45	0.37	0	6,6,53	0.76	0
2	MC3	K	510	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	G	517	-	12,12,45	0.33	0	11,11,53	0.85	0
2	MC3	D	503	-	11,11,45	0.36	0	10,10,53	0.85	0
2	MC3	E	507	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	L	523	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	J	512	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	D	507	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	H	524	-	7,7,45	0.36	0	6,6,53	0.74	0
2	MC3	D	518	-	9,9,45	0.35	0	8,8,53	0.82	0
2	MC3	J	507	-	4,4,45	0.37	0	3,3,53	0.57	0
2	MC3	K	506	-	10,10,45	0.33	0	9,9,53	0.80	0
2	MC3	C	518	-	9,9,45	0.36	0	8,8,53	0.82	0
2	MC3	B	513	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	F	505	-	10,10,45	0.36	0	9,9,53	0.83	0
2	MC3	H	503	-	10,10,45	0.32	0	9,9,53	0.80	0
2	MC3	H	505	-	11,11,45	0.33	0	10,10,53	0.82	0
2	MC3	E	508	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	I	523	-	7,7,45	0.36	0	6,6,53	0.74	0
2	MC3	J	521	-	8,8,45	0.35	0	7,7,53	0.79	0
2	MC3	H	506	-	10,10,45	0.33	0	9,9,53	0.81	0
2	MC3	D	508	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	B	518	-	9,9,45	0.35	0	8,8,53	0.82	0
2	MC3	C	508	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	B	516	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	E	517	-	5,5,45	0.37	0	4,4,53	0.62	0
2	MC3	F	513	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	I	512	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	K	521	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	E	510	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	A	506	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	H	510	-	11,11,45	0.33	0	10,10,53	0.83	0
2	MC3	D	509	-	10,10,45	0.35	0	9,9,53	0.83	0
2	MC3	F	516	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	D	516	-	9,9,45	0.36	0	8,8,53	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	H	513	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	J	520	-	11,11,45	0.34	0	10,10,53	0.84	0
2	MC3	K	503	-	10,10,45	0.32	0	9,9,53	0.80	0
2	MC3	D	501	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	L	505	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	I	504	-	12,12,45	0.33	0	11,11,53	0.83	0
2	MC3	C	501	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	F	512	-	9,9,45	0.36	0	8,8,53	0.80	0
2	MC3	H	512	-	7,7,45	0.36	0	6,6,53	0.76	0
2	MC3	F	507	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	H	507	-	12,12,45	0.34	0	11,11,53	0.83	0
2	MC3	K	501	-	8,8,45	0.23	0	7,7,53	0.22	0
2	MC3	L	515	-	10,10,45	0.34	0	9,9,53	0.81	0
2	MC3	E	514	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	H	501	-	8,8,45	0.23	0	7,7,53	0.22	0
2	MC3	I	514	-	24,24,45	0.51	0	27,29,53	0.79	1 (3%)
2	MC3	I	520	-	9,9,45	0.34	0	8,8,53	0.80	0
2	MC3	D	514	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	E	505	-	10,10,45	0.36	0	9,9,53	0.84	0
2	MC3	C	514	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	L	508	-	11,11,45	0.34	0	10,10,53	0.84	0
2	MC3	L	517	-	4,4,45	0.37	0	3,3,53	0.58	0
2	MC3	E	513	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	G	515	-	12,12,45	0.32	0	11,11,53	0.83	0
2	MC3	I	511	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	B	502	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	K	505	-	11,11,45	0.33	0	10,10,53	0.82	0
2	MC3	A	508	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	C	511	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	D	505	-	10,10,45	0.36	0	9,9,53	0.84	0
2	MC3	E	516	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	G	507	-	4,4,45	0.37	0	3,3,53	0.57	0
2	MC3	B	512	-	9,9,45	0.36	0	8,8,53	0.80	0
2	MC3	B	515	-	10,10,45	0.36	0	9,9,53	0.82	0
2	MC3	L	501	-	24,24,45	0.51	0	27,29,53	0.78	1 (3%)
2	MC3	L	502	-	12,12,45	0.31	0	11,11,53	0.83	0
2	MC3	G	521	-	8,8,45	0.35	0	7,7,53	0.78	0
2	MC3	K	511	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	E	509	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	A	510	-	9,9,45	0.36	0	8,8,53	0.82	0
2	MC3	G	502	-	24,24,45	0.82	1 (4%)	27,29,53	1.13	2 (7%)
2	MC3	G	508	-	11,11,45	0.34	0	10,10,53	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	L	504	-	11,11,45	0.33	0	10,10,53	0.84	0
2	MC3	I	507	-	4,4,45	0.37	0	3,3,53	0.58	0
2	MC3	H	521	-	9,9,45	0.34	0	8,8,53	0.80	0
2	MC3	I	518	-	12,12,45	0.33	0	11,11,53	0.85	0
2	MC3	C	503	-	11,11,45	0.36	0	10,10,53	0.85	0
2	MC3	J	501	-	8,8,45	0.23	0	7,7,53	0.22	0
2	MC3	J	504	-	12,12,45	0.33	0	11,11,53	0.83	0
2	MC3	B	501	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	G	510	-	10,10,45	0.34	0	9,9,53	0.82	0
2	MC3	A	514	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	I	508	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	A	502	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	E	506	-	8,8,45	0.37	0	7,7,53	0.79	0
2	MC3	B	514	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	G	522	-	7,7,45	0.35	0	6,6,53	0.74	0
2	MC3	H	502	-	24,24,45	0.82	1 (4%)	27,29,53	1.13	2 (7%)
2	MC3	E	503	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	H	518	-	11,11,45	0.33	0	10,10,53	0.84	0
2	MC3	I	509	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	A	517	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	A	503	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	H	504	-	12,12,45	0.33	0	11,11,53	0.83	0
2	MC3	F	502	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	I	516	-	11,11,45	0.33	0	10,10,53	0.82	0
2	MC3	D	510	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	F	508	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	K	504	-	12,12,45	0.33	0	11,11,53	0.83	0
2	MC3	I	501	-	8,8,45	0.23	0	7,7,53	0.22	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	G	505	-	-	0/8/8/49	-
2	MC3	E	512	-	-	0/7/7/49	-
2	MC3	F	510	-	-	0/10/10/49	-
2	MC3	H	509	-	-	0/9/9/49	-
2	MC3	H	514	-	-	0/6/6/49	-
2	MC3	L	519	-	-	0/9/9/49	-
2	MC3	K	522	-	-	0/9/9/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	A	519	-	-	0/5/5/49	-
2	MC3	G	513	-	-	0/6/6/49	-
2	MC3	B	503	-	-	0/9/9/49	-
2	MC3	L	518	-	-	0/9/9/49	-
2	MC3	B	505	-	-	0/8/8/49	-
2	MC3	H	522	-	-	0/9/9/49	-
2	MC3	C	502	-	-	0/10/10/49	-
2	MC3	F	501	-	-	0/10/10/49	-
2	MC3	K	507	-	-	0/10/10/49	-
2	MC3	K	512	-	-	0/5/5/49	-
2	MC3	G	516	-	-	0/9/9/49	-
2	MC3	E	501	-	-	0/10/10/49	-
2	MC3	G	504	-	-	0/10/10/49	-
2	MC3	C	517	-	-	0/3/3/49	-
2	MC3	K	508	-	-	0/2/2/49	-
2	MC3	I	505	-	-	0/8/8/49	-
2	MC3	K	514	-	-	0/6/6/49	-
2	MC3	F	514	-	-	0/6/6/49	-
2	MC3	L	510	-	-	0/5/5/49	-
2	MC3	J	519	-	-	0/7/7/49	-
2	MC3	G	514	-	-	13/26/26/49	-
2	MC3	J	508	-	-	0/9/9/49	-
2	MC3	B	517	-	-	0/3/3/49	-
2	MC3	K	524	-	-	0/5/5/49	-
2	MC3	A	513	-	-	0/10/10/49	-
2	MC3	A	516	-	-	0/8/8/49	-
2	MC3	B	510	-	-	0/10/10/49	-
2	MC3	L	522	-	-	0/7/7/49	-
2	MC3	K	523	-	-	0/6/6/49	-
2	MC3	B	506	-	-	0/6/6/49	-
2	MC3	E	511	-	-	0/9/9/49	-
2	MC3	G	506	-	-	0/10/10/49	-
2	MC3	G	511	-	-	0/5/5/49	-
2	MC3	L	520	-	-	0/8/8/49	-
2	MC3	I	502	-	-	12/26/26/49	-
2	MC3	D	502	-	-	0/10/10/49	-
2	MC3	B	504	-	-	0/7/7/49	-
2	MC3	A	512	-	-	0/10/10/49	-
2	MC3	D	519	-	-	0/5/5/49	-
2	MC3	F	504	-	-	0/7/7/49	-
2	MC3	F	503	-	-	0/9/9/49	-
2	MC3	J	502	-	-	12/26/26/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	D	517	-	-	0/3/3/49	-
2	MC3	K	518	-	-	0/9/9/49	-
2	MC3	F	519	-	-	0/5/5/49	-
2	MC3	H	523	-	-	0/6/6/49	-
2	MC3	D	506	-	-	0/6/6/49	-
2	MC3	D	515	-	-	0/8/8/49	-
2	MC3	J	517	-	-	0/10/10/49	-
2	MC3	D	513	-	-	0/10/10/49	-
2	MC3	B	508	-	-	0/5/5/49	-
2	MC3	F	518	-	-	0/7/7/49	-
2	MC3	E	518	-	-	0/7/7/49	-
2	MC3	G	512	-	-	0/7/7/49	-
2	MC3	C	515	-	-	0/8/8/49	-
2	MC3	C	513	-	-	0/10/10/49	-
2	MC3	A	504	-	-	0/7/7/49	-
2	MC3	I	510	-	-	0/8/8/49	-
2	MC3	J	503	-	-	0/8/8/49	-
2	MC3	J	505	-	-	0/8/8/49	-
2	MC3	K	513	-	-	0/7/7/49	-
2	MC3	C	510	-	-	0/10/10/49	-
2	MC3	K	515	-	-	11/26/26/49	-
2	MC3	I	522	-	-	0/6/6/49	-
2	MC3	F	509	-	-	0/8/8/49	-
2	MC3	G	501	-	-	1/6/6/49	-
2	MC3	K	502	-	-	12/26/26/49	-
2	MC3	L	507	-	-	0/7/7/49	-
2	MC3	F	506	-	-	0/6/6/49	-
2	MC3	L	514	-	-	0/10/10/49	-
2	MC3	L	521	-	-	0/5/5/49	-
2	MC3	H	517	-	-	0/9/9/49	-
2	MC3	C	507	-	-	0/7/7/49	-
2	MC3	J	513	-	-	0/6/6/49	-
2	MC3	E	502	-	-	0/10/10/49	-
2	MC3	K	517	-	-	0/9/9/49	-
2	MC3	K	520	-	-	0/10/10/49	-
2	MC3	I	503	-	-	0/8/8/49	-
2	MC3	J	518	-	-	0/10/10/49	-
2	MC3	E	504	-	-	0/7/7/49	-
2	MC3	H	520	-	-	0/10/10/49	-
2	MC3	L	511	-	-	1/6/6/49	-
2	MC3	L	513	-	-	0/8/8/49	-
2	MC3	E	519	-	-	0/5/5/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	J	509	-	-	0/9/9/49	-
2	MC3	J	511	-	-	0/5/5/49	-
2	MC3	B	511	-	-	0/9/9/49	-
2	MC3	G	509	-	-	0/9/9/49	-
2	MC3	L	516	-	-	0/10/10/49	-
2	MC3	C	516	-	-	0/7/7/49	-
2	MC3	A	518	-	-	0/7/7/49	-
2	MC3	J	515	-	-	0/10/10/49	-
2	MC3	J	516	-	-	0/9/9/49	-
2	MC3	A	515	-	-	0/7/7/49	-
2	MC3	K	519	-	-	0/10/10/49	-
2	MC3	L	509	-	-	0/6/6/49	-
2	MC3	I	519	-	-	0/10/10/49	-
2	MC3	J	522	-	-	0/5/5/49	-
2	MC3	G	503	-	-	0/8/8/49	-
2	MC3	D	512	-	-	0/7/7/49	-
2	MC3	C	504	-	-	0/7/7/49	-
2	MC3	C	505	-	-	0/8/8/49	-
2	MC3	J	506	-	-	0/10/10/49	-
2	MC3	B	509	-	-	0/8/8/49	-
2	MC3	C	512	-	-	0/7/7/49	-
2	MC3	G	520	-	-	0/9/9/49	-
2	MC3	A	509	-	-	0/3/3/49	-
2	MC3	A	511	-	-	0/5/5/49	-
2	MC3	G	518	-	-	0/10/10/49	-
2	MC3	I	517	-	-	0/9/9/49	-
2	MC3	C	519	-	-	0/5/5/49	-
2	MC3	F	515	-	-	0/8/8/49	-
2	MC3	H	515	-	-	11/26/26/49	-
2	MC3	L	506	-	-	0/10/10/49	-
2	MC3	H	516	-	-	0/10/10/49	-
2	MC3	I	515	-	-	0/10/10/49	-
2	MC3	I	513	-	-	0/6/6/49	-
2	MC3	K	516	-	-	0/10/10/49	-
2	MC3	D	504	-	-	0/7/7/49	-
2	MC3	A	501	-	-	0/8/8/49	-
2	MC3	I	521	-	-	0/9/9/49	-
2	MC3	L	503	-	-	0/9/9/49	-
2	MC3	C	506	-	-	0/6/6/49	-
2	MC3	F	517	-	-	0/3/3/49	-
2	MC3	H	508	-	-	0/2/2/49	-
2	MC3	I	506	-	-	0/10/10/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	J	510	-	-	0/8/8/49	-
2	MC3	L	512	-	-	12/26/26/49	-
2	MC3	A	507	-	-	0/8/8/49	-
2	MC3	D	511	-	-	0/9/9/49	-
2	MC3	G	519	-	-	0/7/7/49	-
2	MC3	C	509	-	-	0/8/8/49	-
2	MC3	K	509	-	-	0/9/9/49	-
2	MC3	A	505	-	-	0/10/10/49	-
2	MC3	B	507	-	-	0/7/7/49	-
2	MC3	E	515	-	-	0/8/8/49	-
2	MC3	F	511	-	-	0/9/9/49	-
2	MC3	H	511	-	-	0/8/8/49	-
2	MC3	H	519	-	-	0/10/10/49	-
2	MC3	J	514	-	-	12/26/26/49	-
2	MC3	B	519	-	-	0/5/5/49	-
2	MC3	K	510	-	-	0/9/9/49	-
2	MC3	G	517	-	-	0/10/10/49	-
2	MC3	D	503	-	-	0/9/9/49	-
2	MC3	E	507	-	-	0/7/7/49	-
2	MC3	L	523	-	-	0/6/6/49	-
2	MC3	J	512	-	-	0/7/7/49	-
2	MC3	D	507	-	-	0/7/7/49	-
2	MC3	H	524	-	-	0/5/5/49	-
2	MC3	D	518	-	-	0/7/7/49	-
2	MC3	J	507	-	-	0/2/2/49	-
2	MC3	K	506	-	-	0/8/8/49	-
2	MC3	C	518	-	-	0/7/7/49	-
2	MC3	B	513	-	-	0/10/10/49	-
2	MC3	F	505	-	-	0/8/8/49	-
2	MC3	H	503	-	-	0/8/8/49	-
2	MC3	H	505	-	-	0/9/9/49	-
2	MC3	E	508	-	-	0/5/5/49	-
2	MC3	I	523	-	-	0/5/5/49	-
2	MC3	J	521	-	-	0/6/6/49	-
2	MC3	H	506	-	-	0/8/8/49	-
2	MC3	D	508	-	-	0/5/5/49	-
2	MC3	B	518	-	-	0/7/7/49	-
2	MC3	C	508	-	-	0/5/5/49	-
2	MC3	B	516	-	-	0/7/7/49	-
2	MC3	E	517	-	-	0/3/3/49	-
2	MC3	F	513	-	-	0/10/10/49	-
2	MC3	I	512	-	-	0/7/7/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	K	521	-	-	0/7/7/49	-
2	MC3	E	510	-	-	0/10/10/49	-
2	MC3	A	506	-	-	0/6/6/49	-
2	MC3	H	510	-	-	0/9/9/49	-
2	MC3	D	509	-	-	0/8/8/49	-
2	MC3	F	516	-	-	0/7/7/49	-
2	MC3	D	516	-	-	0/7/7/49	-
2	MC3	H	513	-	-	0/7/7/49	-
2	MC3	J	520	-	-	0/9/9/49	-
2	MC3	K	503	-	-	0/8/8/49	-
2	MC3	D	501	-	-	0/10/10/49	-
2	MC3	L	505	-	-	0/10/10/49	-
2	MC3	I	504	-	-	0/10/10/49	-
2	MC3	C	501	-	-	0/10/10/49	-
2	MC3	F	512	-	-	0/7/7/49	-
2	MC3	H	512	-	-	0/5/5/49	-
2	MC3	F	507	-	-	0/7/7/49	-
2	MC3	H	507	-	-	0/10/10/49	-
2	MC3	K	501	-	-	1/6/6/49	-
2	MC3	L	515	-	-	0/8/8/49	-
2	MC3	E	514	-	-	0/6/6/49	-
2	MC3	H	501	-	-	1/6/6/49	-
2	MC3	I	514	-	-	14/26/26/49	-
2	MC3	I	520	-	-	0/7/7/49	-
2	MC3	D	514	-	-	0/6/6/49	-
2	MC3	E	505	-	-	0/8/8/49	-
2	MC3	C	514	-	-	0/6/6/49	-
2	MC3	L	508	-	-	0/9/9/49	-
2	MC3	L	517	-	-	0/2/2/49	-
2	MC3	E	513	-	-	0/10/10/49	-
2	MC3	G	515	-	-	0/10/10/49	-
2	MC3	I	511	-	-	0/5/5/49	-
2	MC3	B	502	-	-	0/10/10/49	-
2	MC3	K	505	-	-	0/9/9/49	-
2	MC3	A	508	-	-	0/7/7/49	-
2	MC3	C	511	-	-	0/9/9/49	-
2	MC3	D	505	-	-	0/8/8/49	-
2	MC3	E	516	-	-	0/7/7/49	-
2	MC3	G	507	-	-	0/2/2/49	-
2	MC3	B	512	-	-	0/7/7/49	-
2	MC3	B	515	-	-	0/8/8/49	-
2	MC3	L	501	-	-	14/26/26/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	L	502	-	-	0/10/10/49	-
2	MC3	G	521	-	-	0/6/6/49	-
2	MC3	K	511	-	-	0/8/8/49	-
2	MC3	E	509	-	-	0/8/8/49	-
2	MC3	A	510	-	-	0/7/7/49	-
2	MC3	G	502	-	-	12/26/26/49	-
2	MC3	G	508	-	-	0/9/9/49	-
2	MC3	L	504	-	-	0/9/9/49	-
2	MC3	I	507	-	-	0/2/2/49	-
2	MC3	H	521	-	-	0/7/7/49	-
2	MC3	I	518	-	-	0/10/10/49	-
2	MC3	C	503	-	-	0/9/9/49	-
2	MC3	J	501	-	-	1/6/6/49	-
2	MC3	J	504	-	-	0/10/10/49	-
2	MC3	B	501	-	-	0/10/10/49	-
2	MC3	G	510	-	-	0/8/8/49	-
2	MC3	A	514	-	-	0/9/9/49	-
2	MC3	I	508	-	-	0/9/9/49	-
2	MC3	A	502	-	-	0/10/10/49	-
2	MC3	E	506	-	-	0/6/6/49	-
2	MC3	B	514	-	-	0/6/6/49	-
2	MC3	G	522	-	-	0/5/5/49	-
2	MC3	H	502	-	-	12/26/26/49	-
2	MC3	E	503	-	-	0/9/9/49	-
2	MC3	H	518	-	-	0/9/9/49	-
2	MC3	I	509	-	-	0/9/9/49	-
2	MC3	A	517	-	-	0/6/6/49	-
2	MC3	A	503	-	-	0/9/9/49	-
2	MC3	H	504	-	-	0/10/10/49	-
2	MC3	F	502	-	-	0/10/10/49	-
2	MC3	I	516	-	-	0/9/9/49	-
2	MC3	D	510	-	-	0/10/10/49	-
2	MC3	F	508	-	-	0/5/5/49	-
2	MC3	K	504	-	-	0/10/10/49	-
2	MC3	I	501	-	-	1/6/6/49	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	502	MC3	P-O4P	2.81	1.65	1.54
2	G	502	MC3	P-O4P	2.80	1.65	1.54
2	J	502	MC3	P-O4P	2.80	1.65	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	502	MC3	P-O4P	2.80	1.65	1.54
2	I	502	MC3	P-O4P	2.79	1.65	1.54

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	502	MC3	O4P-P-O3P	-4.03	96.17	106.67
2	I	502	MC3	O4P-P-O3P	-4.02	96.18	106.67
2	G	502	MC3	O4P-P-O3P	-4.02	96.20	106.67
2	J	502	MC3	O4P-P-O3P	-4.01	96.20	106.67
2	L	512	MC3	O4P-P-O3P	-4.01	96.21	106.67

There are no chirality outliers.

5 of 153 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	502	MC3	C32-C31-O2-C2
2	G	502	MC3	O31-C31-O2-C2
2	G	502	MC3	C1-O3P-P-O2P
2	G	514	MC3	C1-O3P-P-O4P
2	H	502	MC3	C32-C31-O2-C2

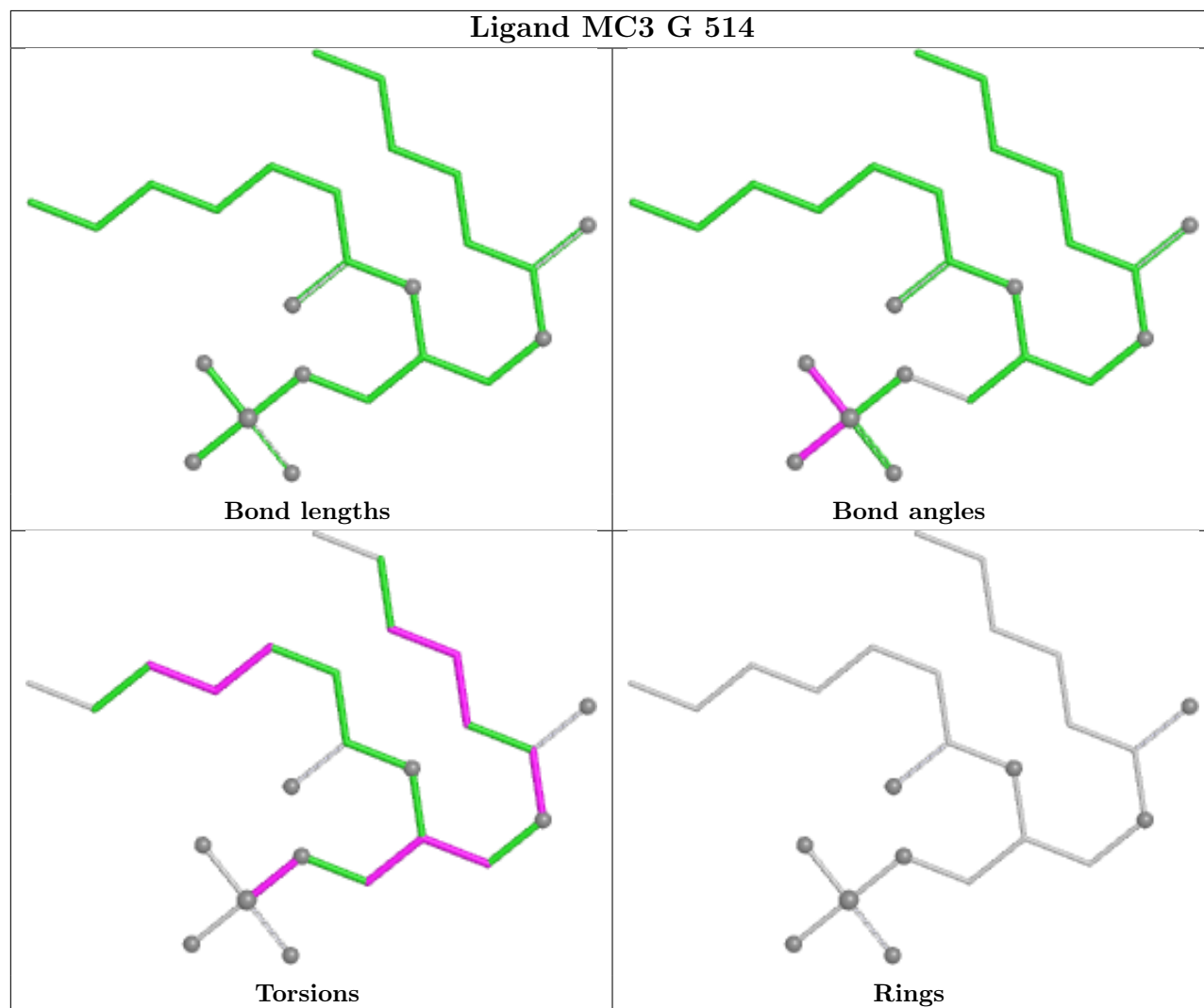
There are no ring outliers.

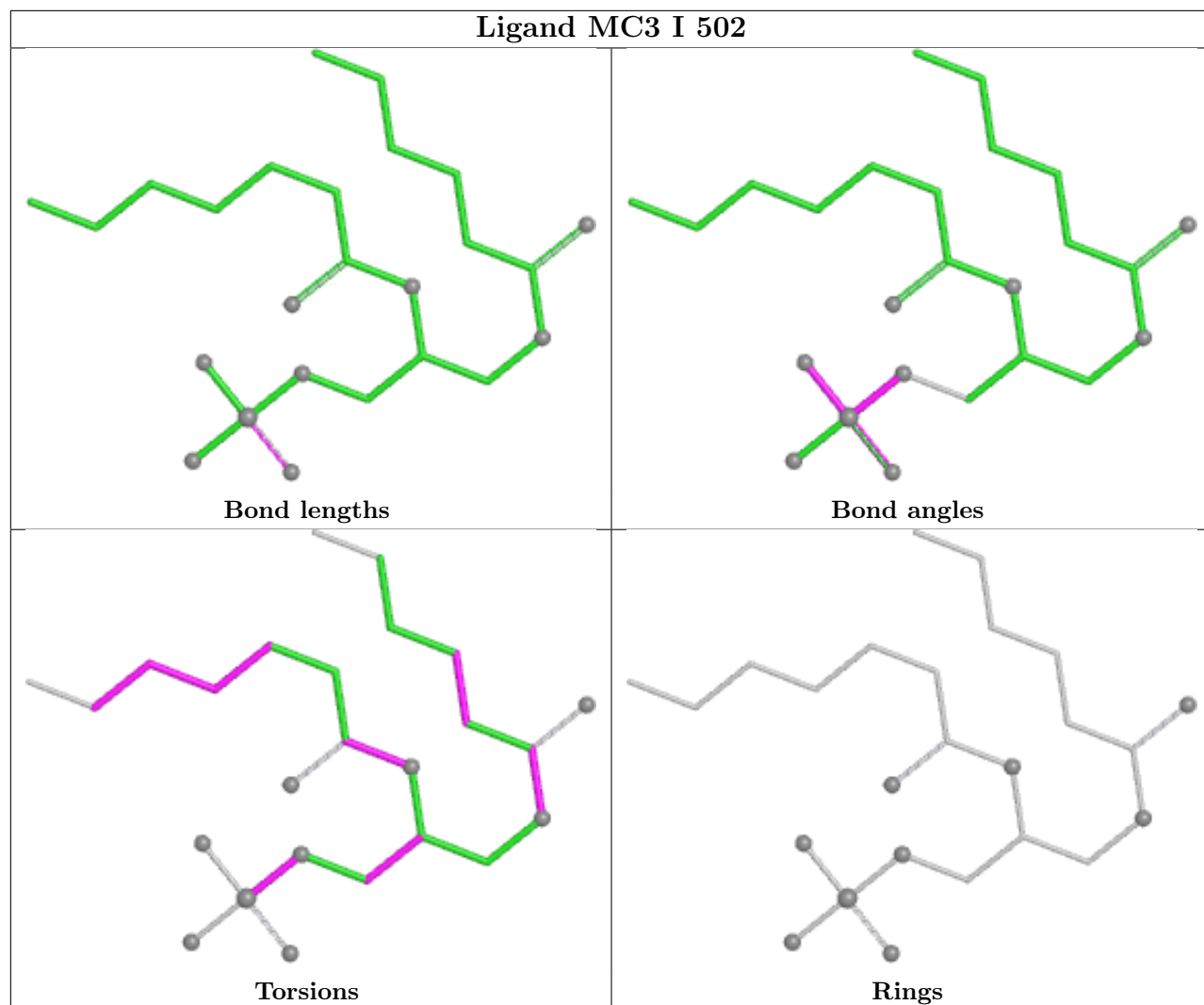
6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	512	MC3	1	0
2	D	512	MC3	1	0
2	C	512	MC3	1	0
2	F	512	MC3	1	0
2	I	514	MC3	1	0
2	B	512	MC3	1	0

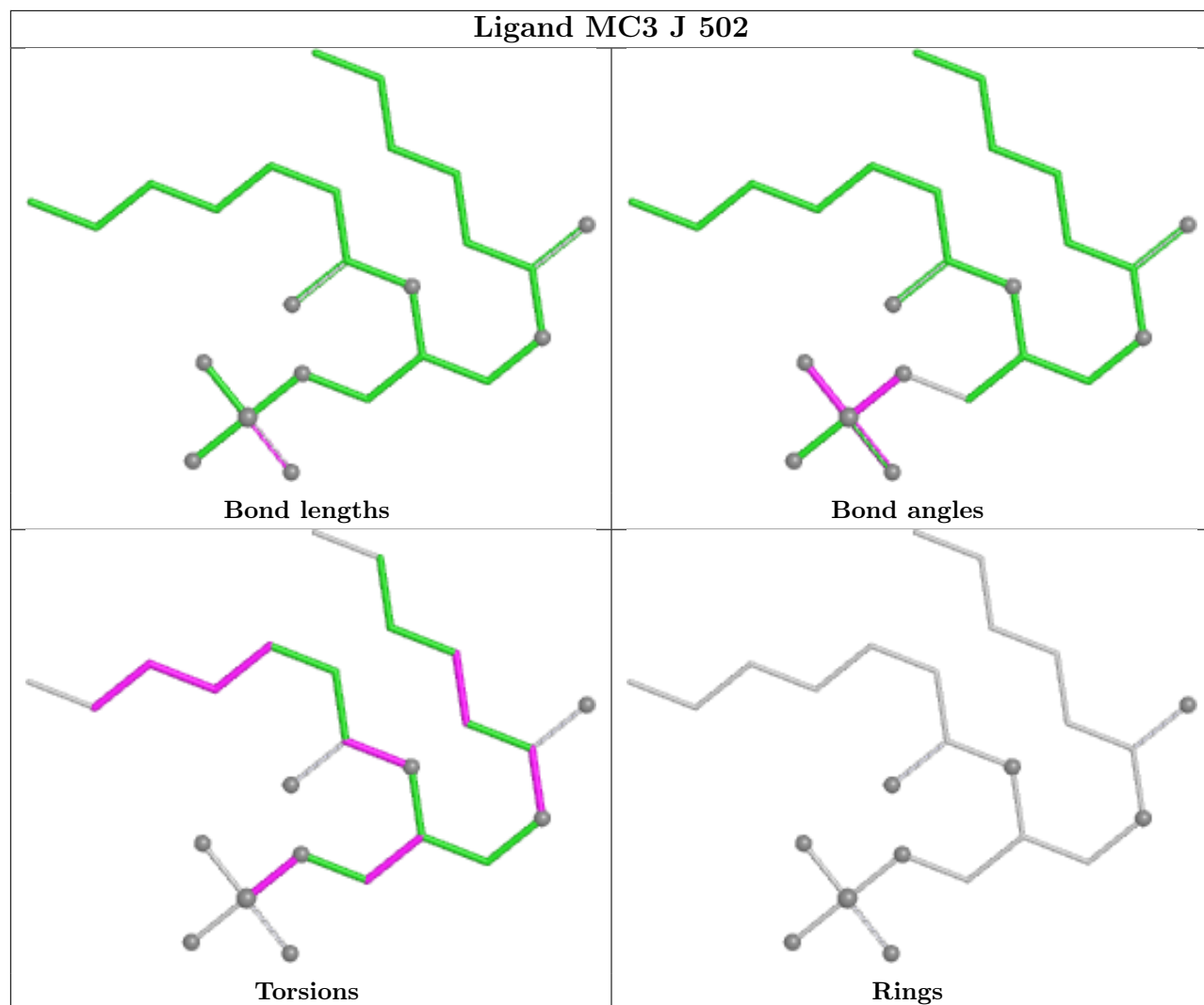
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

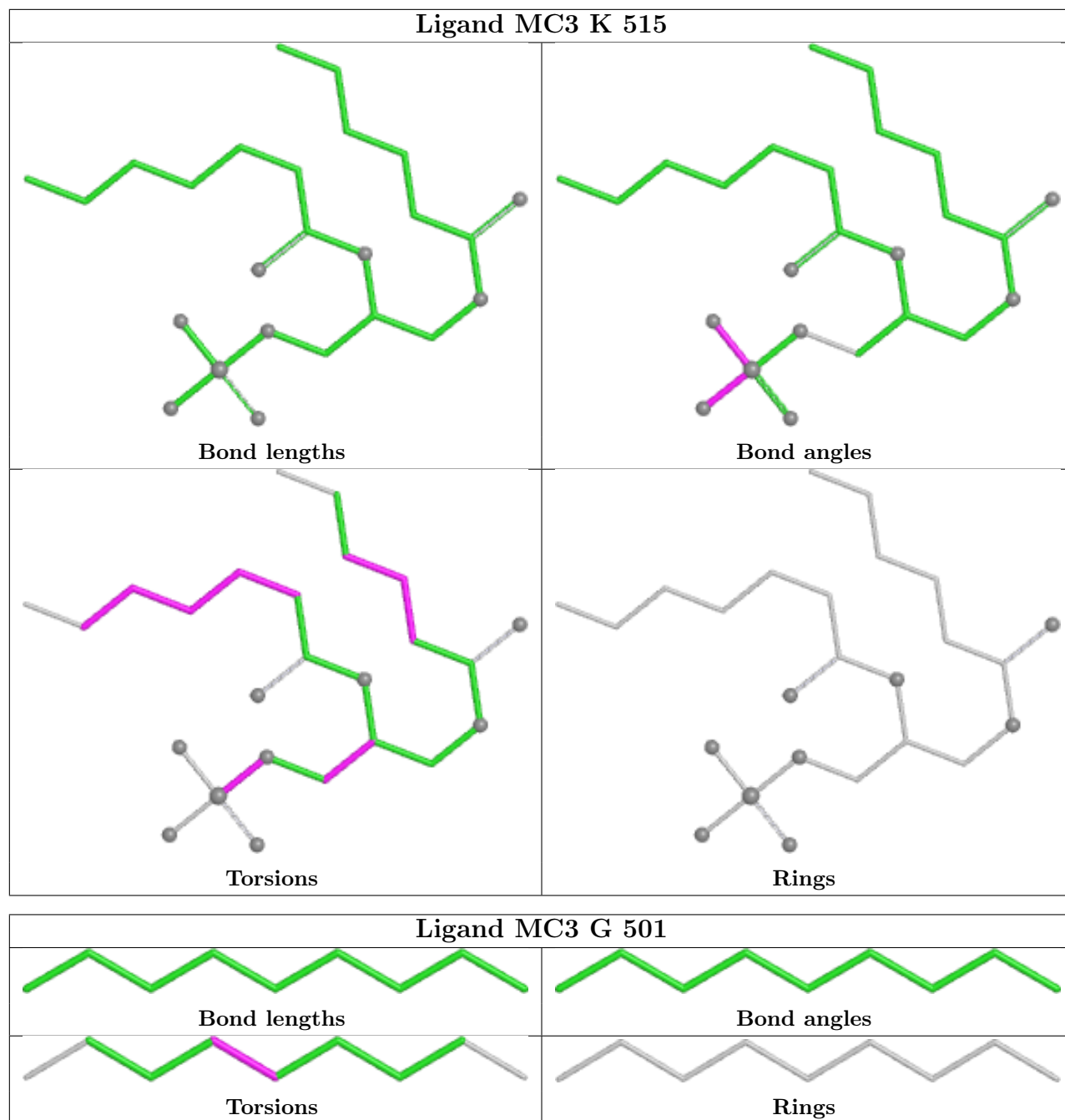
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

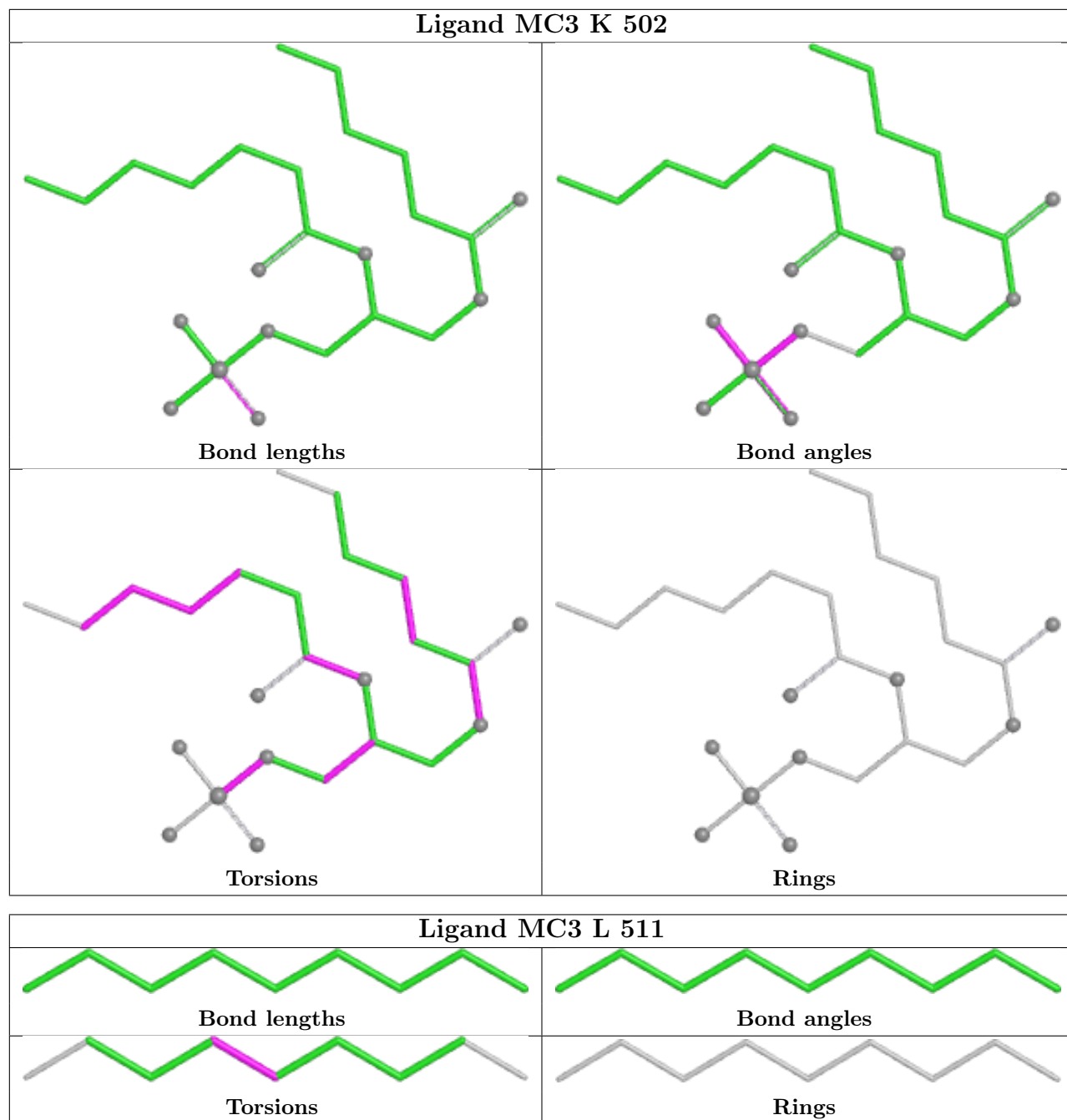


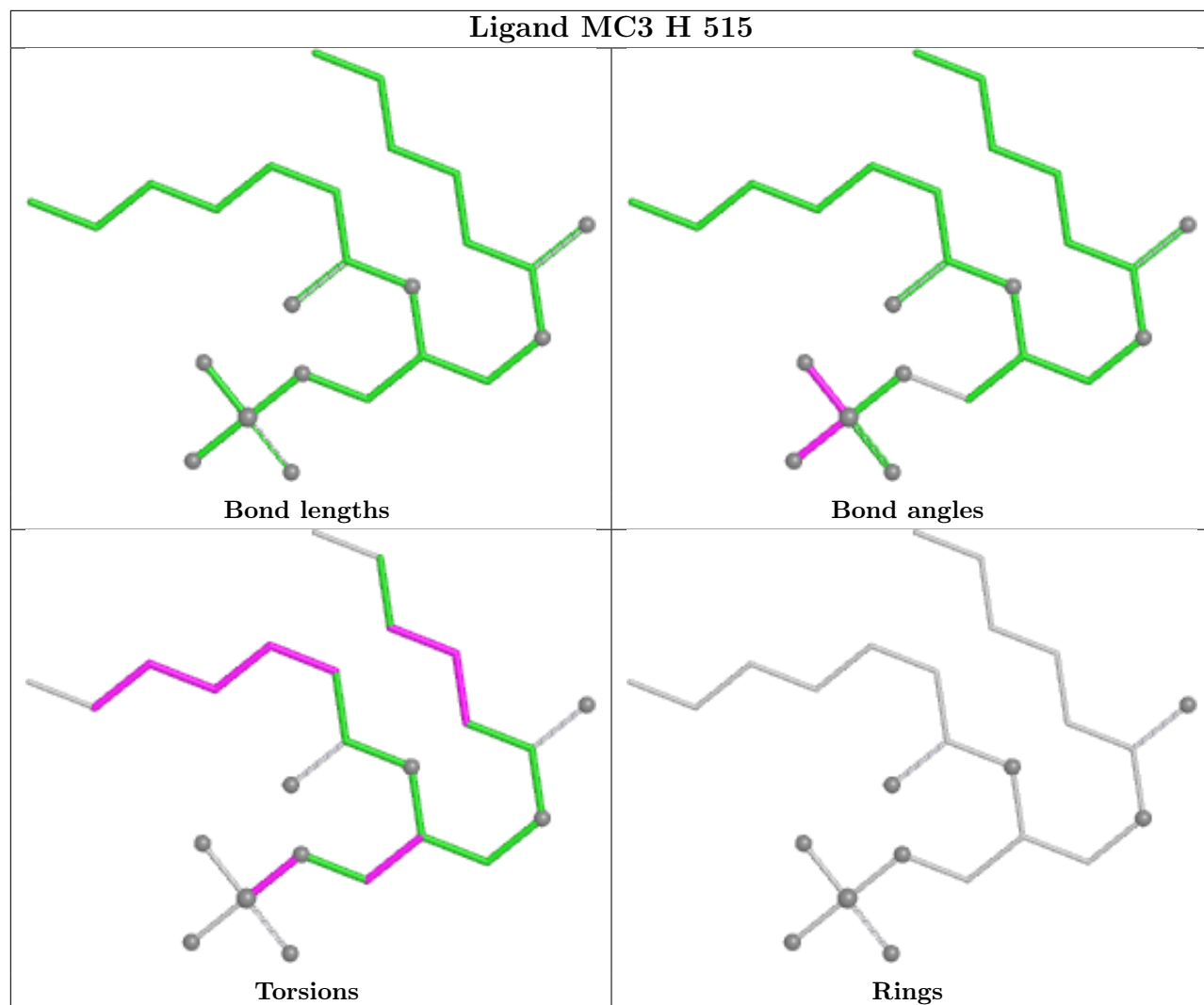


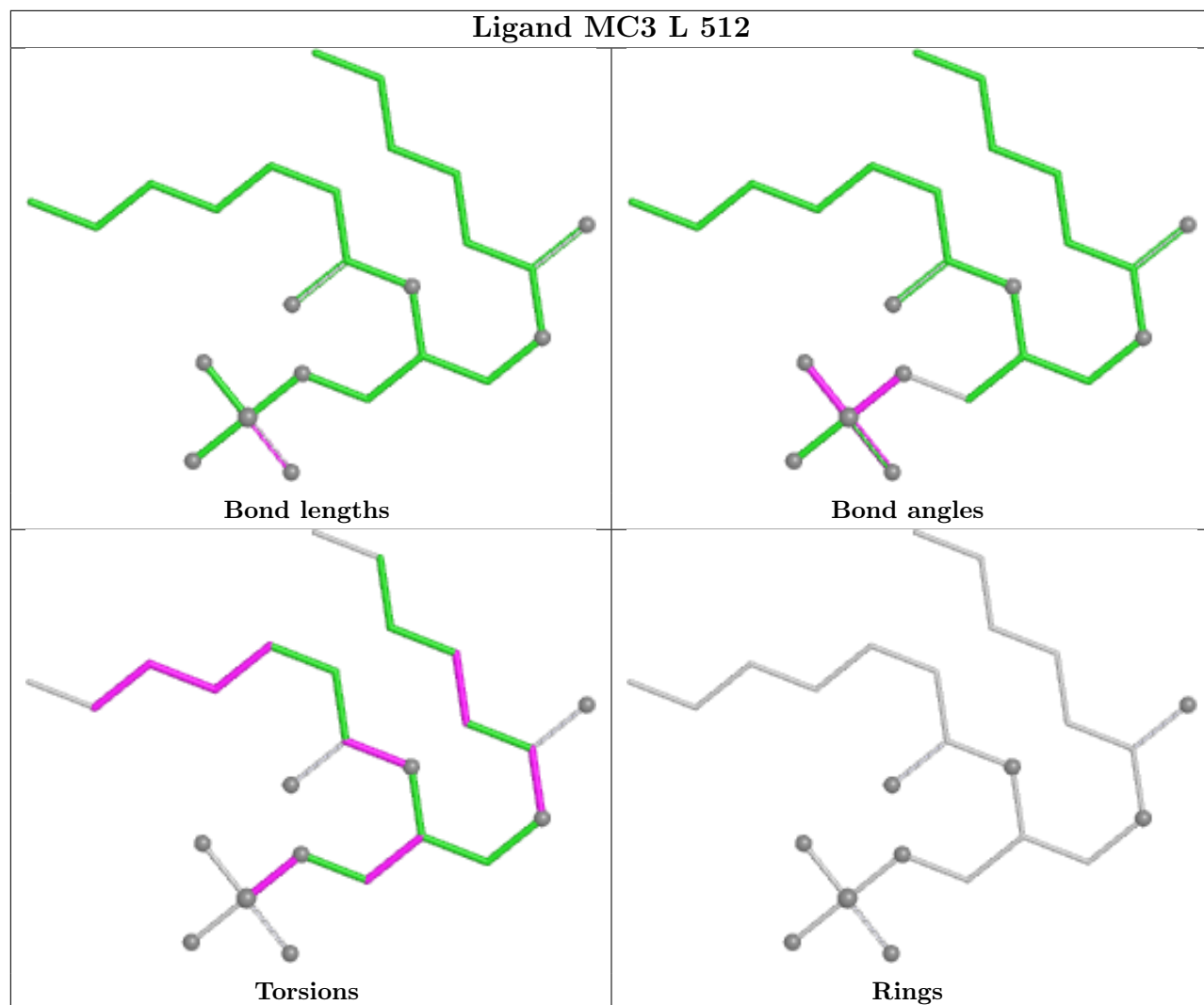
Ligand MC3 J 502

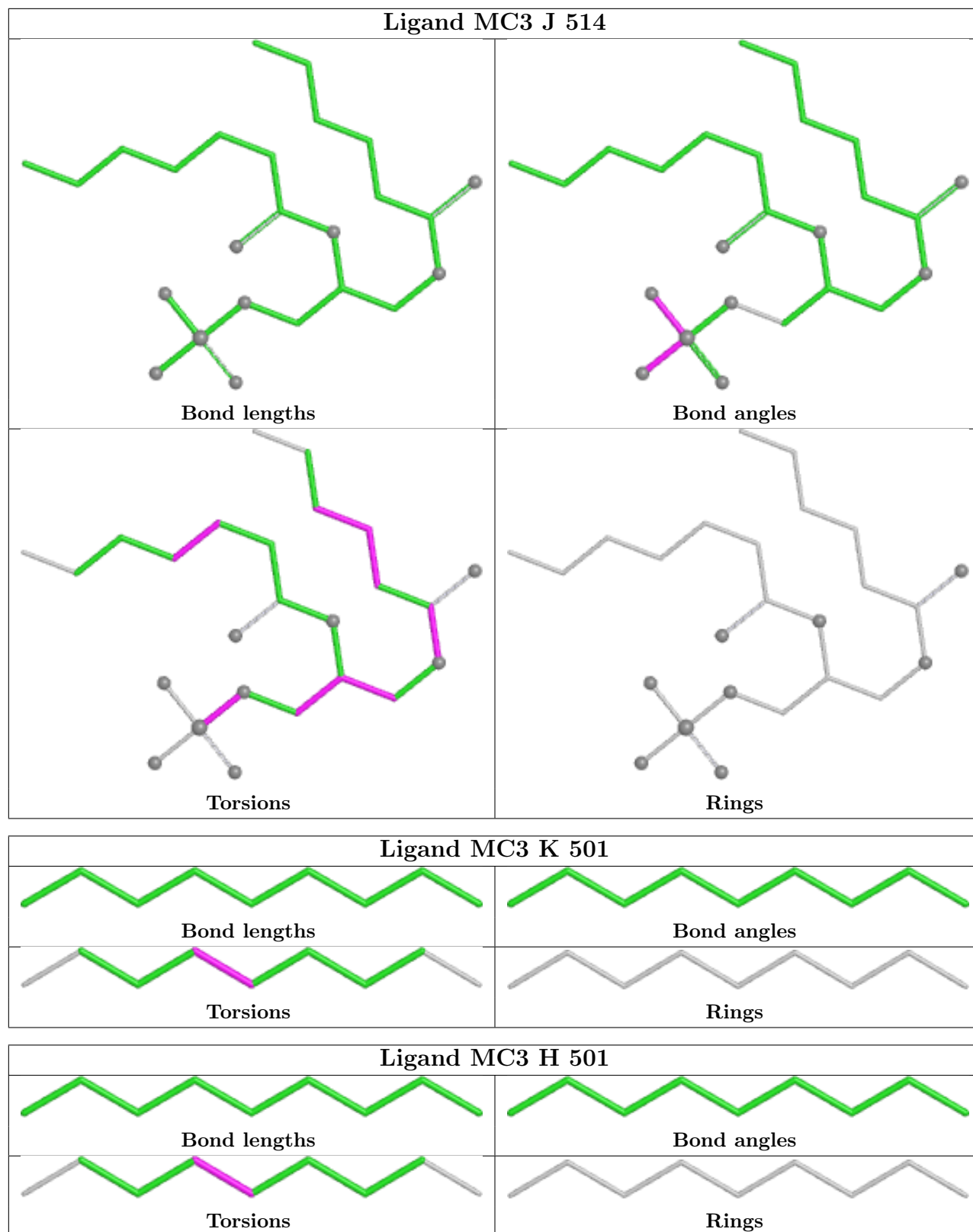




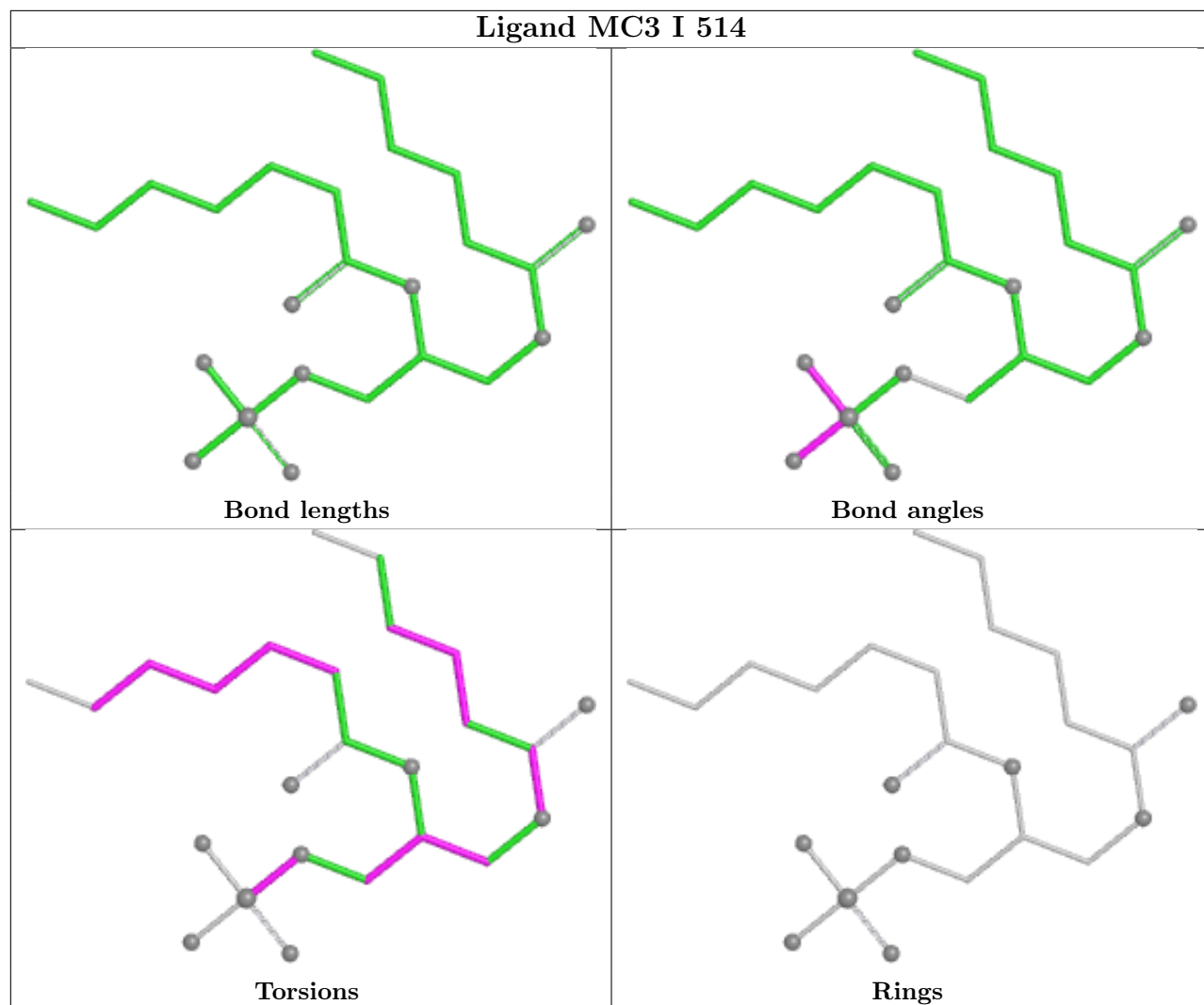


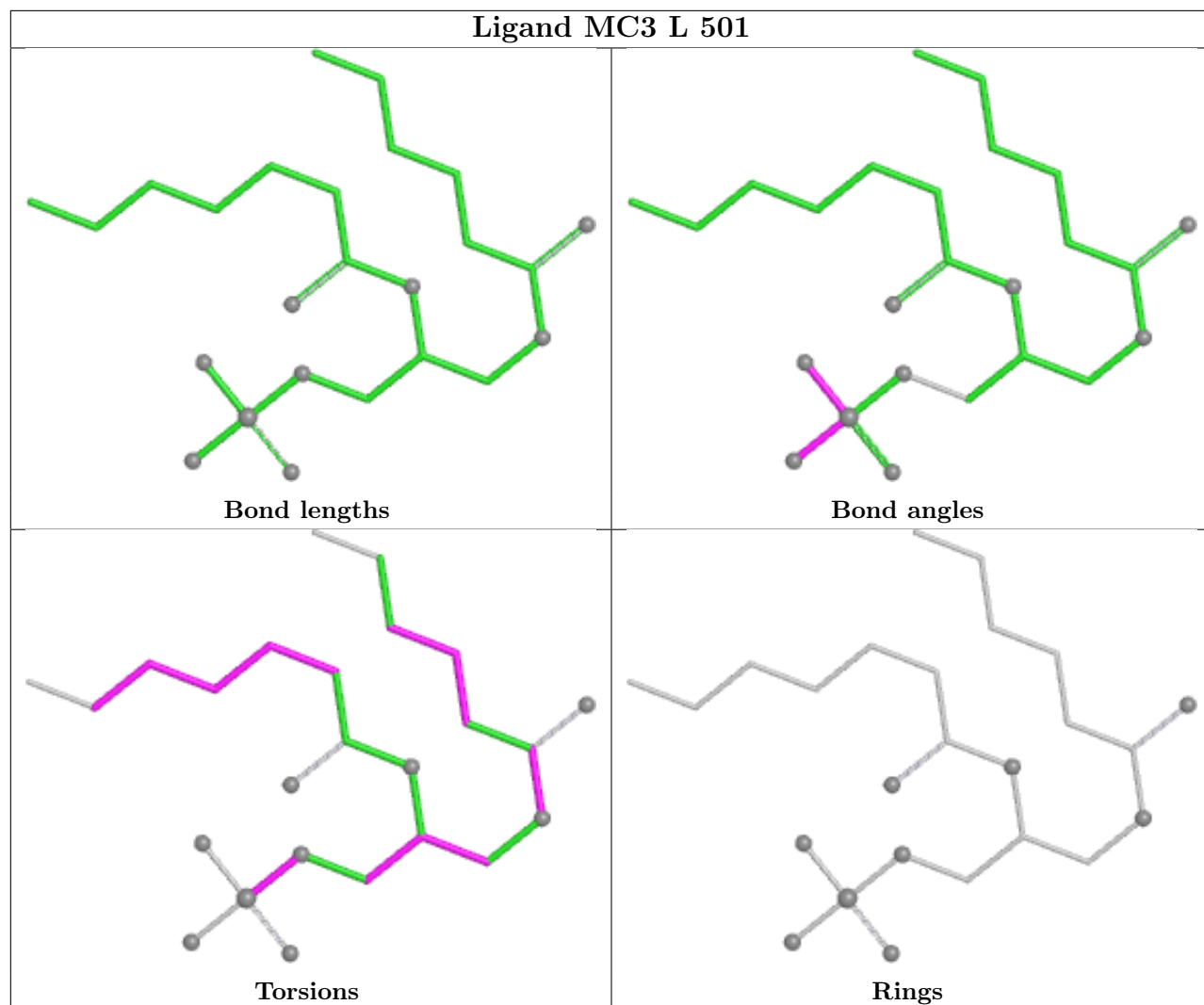


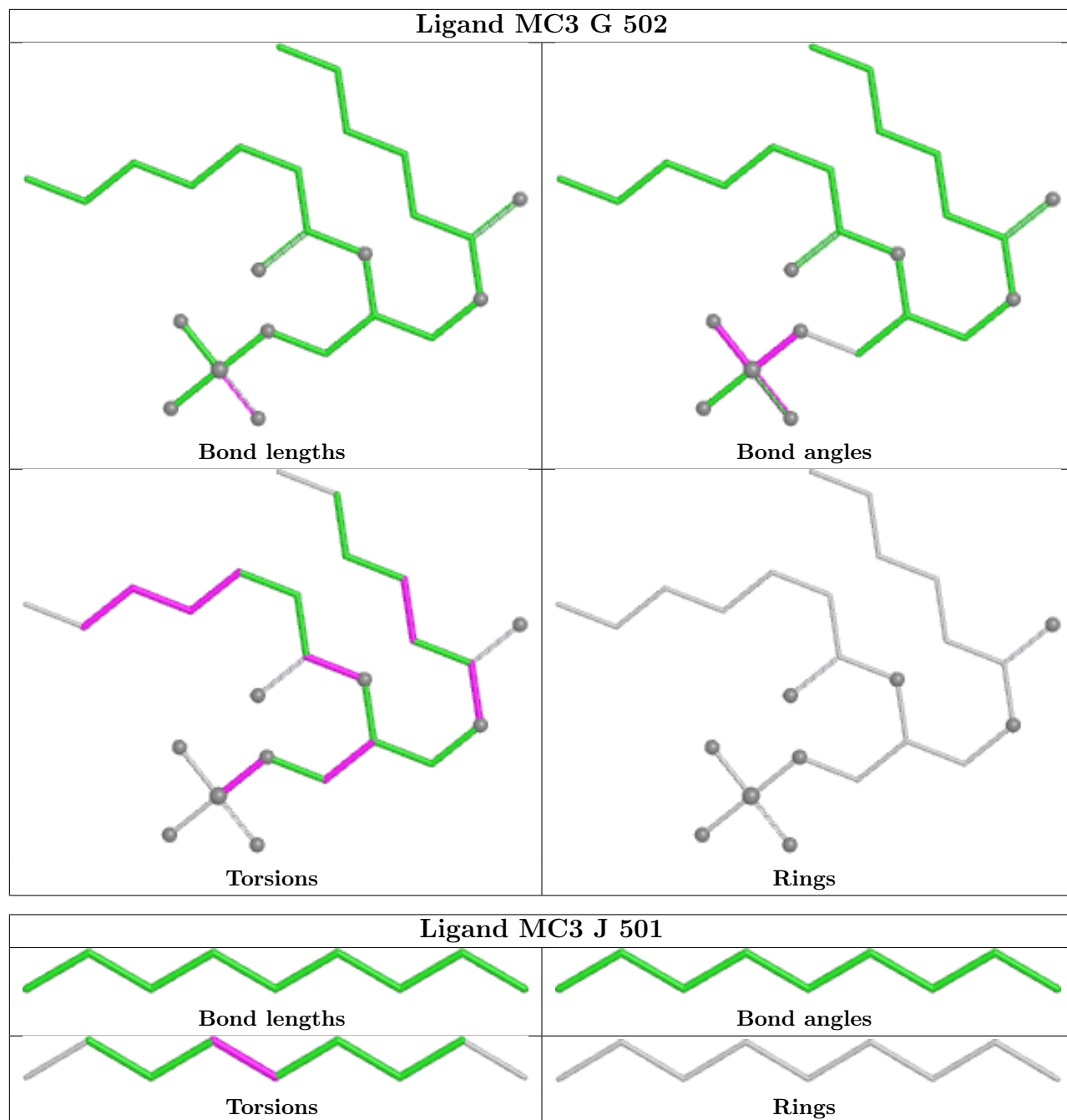


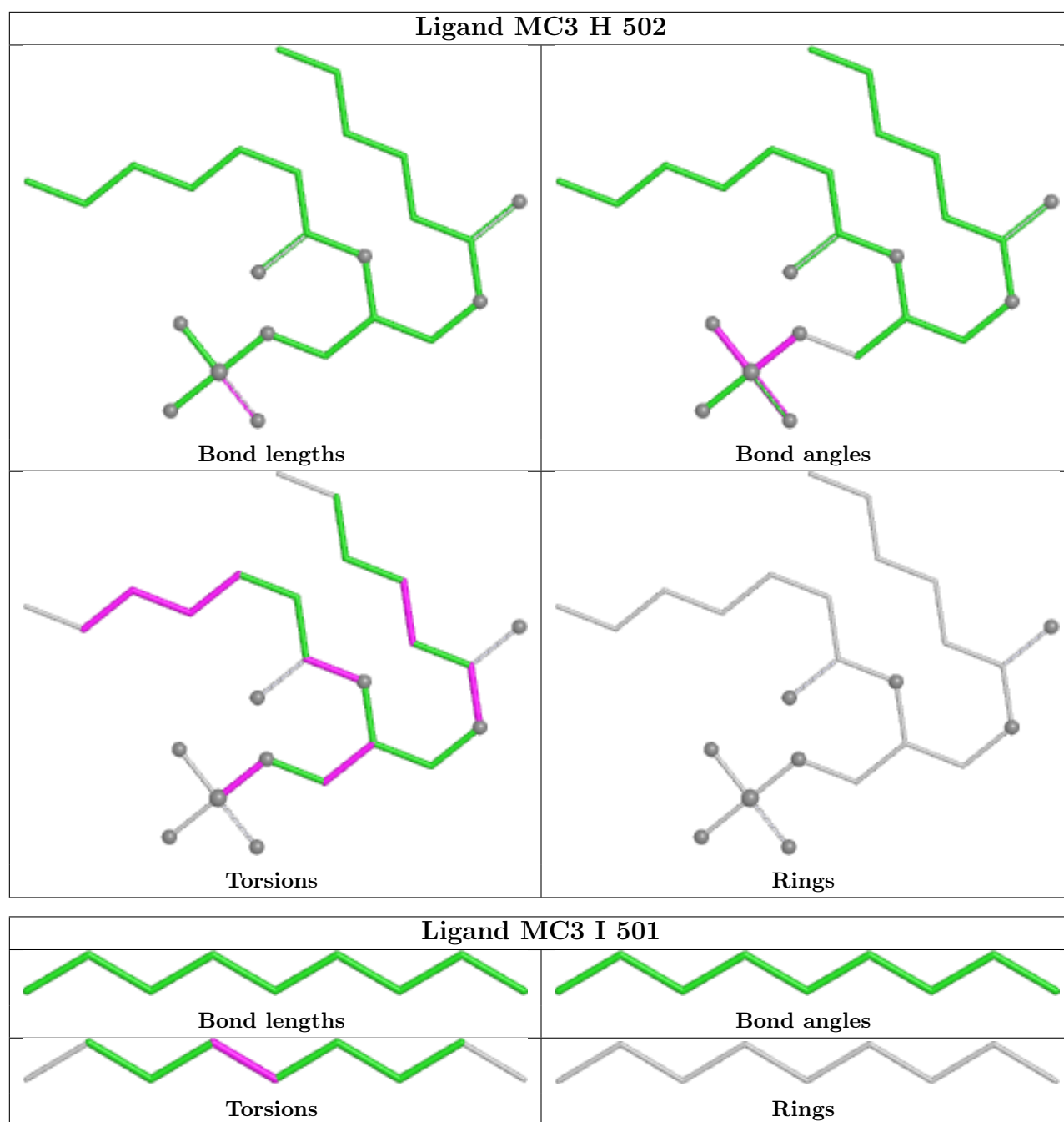


Ligand MC3 I 514









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.

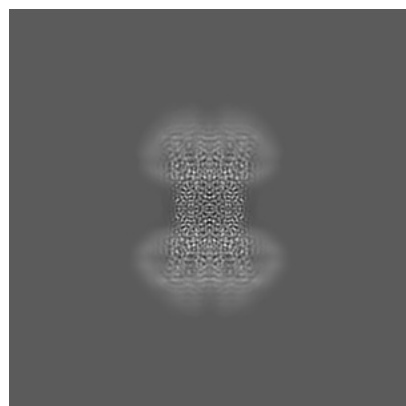
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-73965. These allow visual inspection of the internal detail of the map and identification of artifacts.

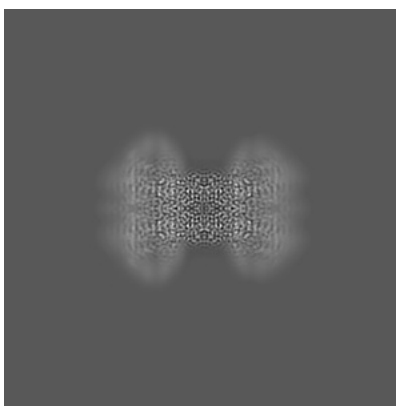
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

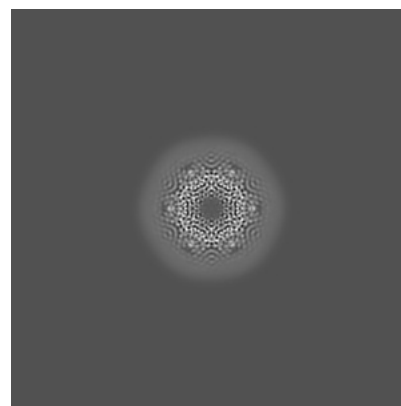
6.1.1 Primary map



X

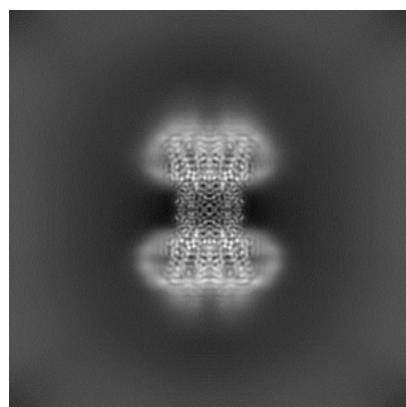


Y

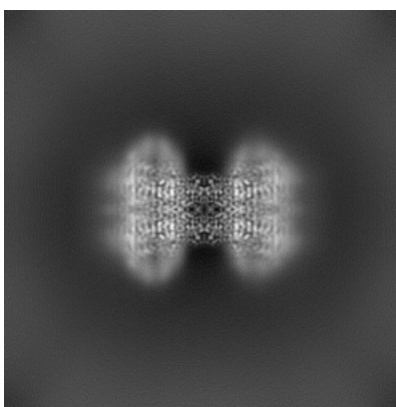


Z

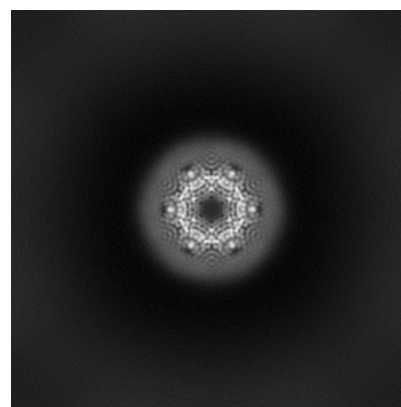
6.1.2 Raw map



X



Y

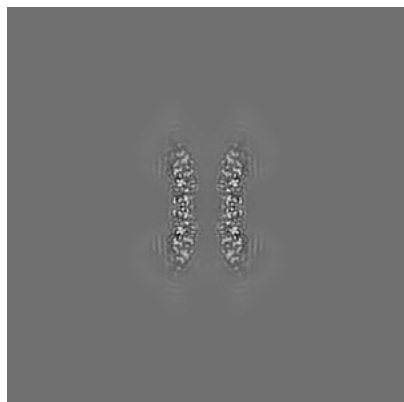


Z

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

6.2 Central slices [i](#)

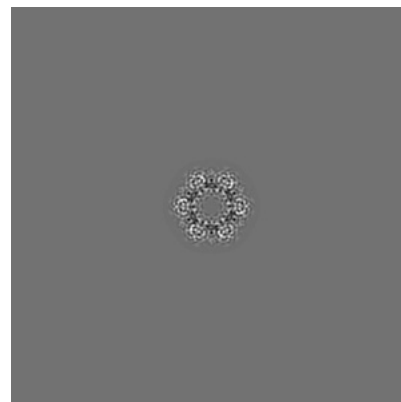
6.2.1 Primary map



X Index: 192

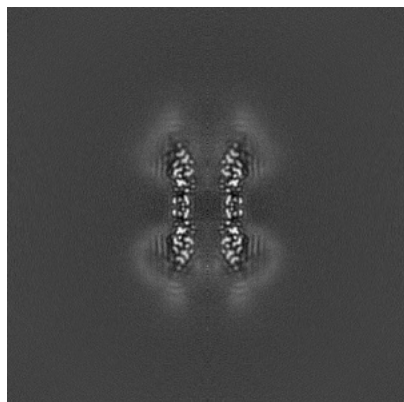


Y Index: 192

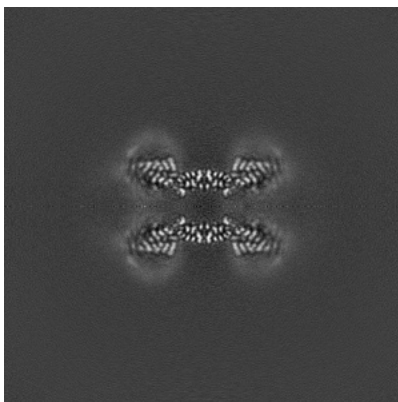


Z Index: 192

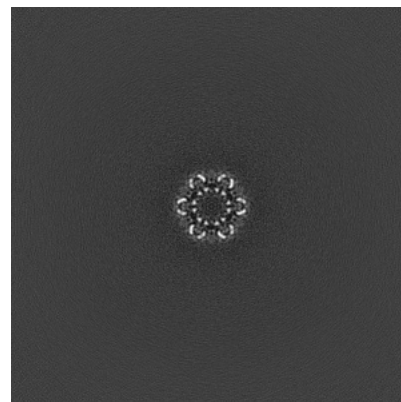
6.2.2 Raw map



X Index: 192



Y Index: 192

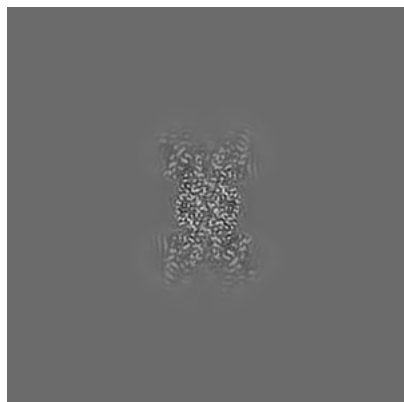


Z Index: 192

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

6.3 Largest variance slices [i](#)

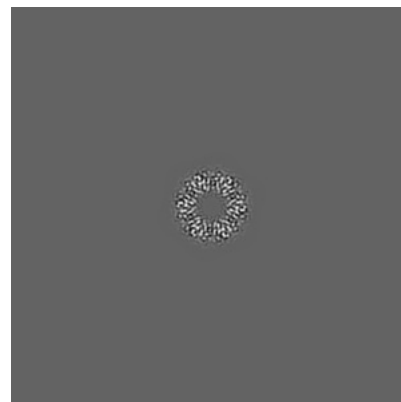
6.3.1 Primary map



X Index: 175

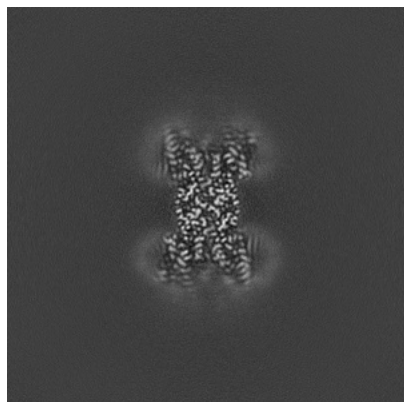


Y Index: 212

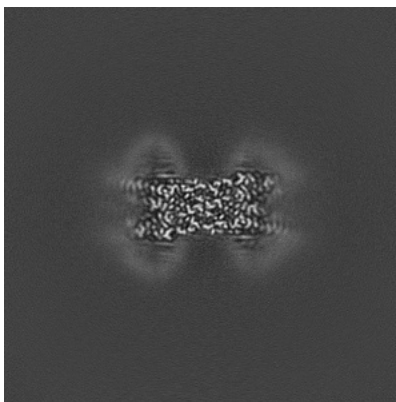


Z Index: 180

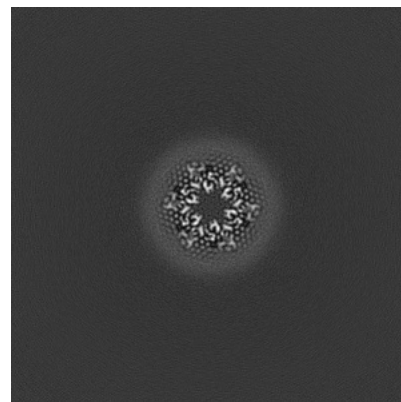
6.3.2 Raw map



X Index: 209



Y Index: 172

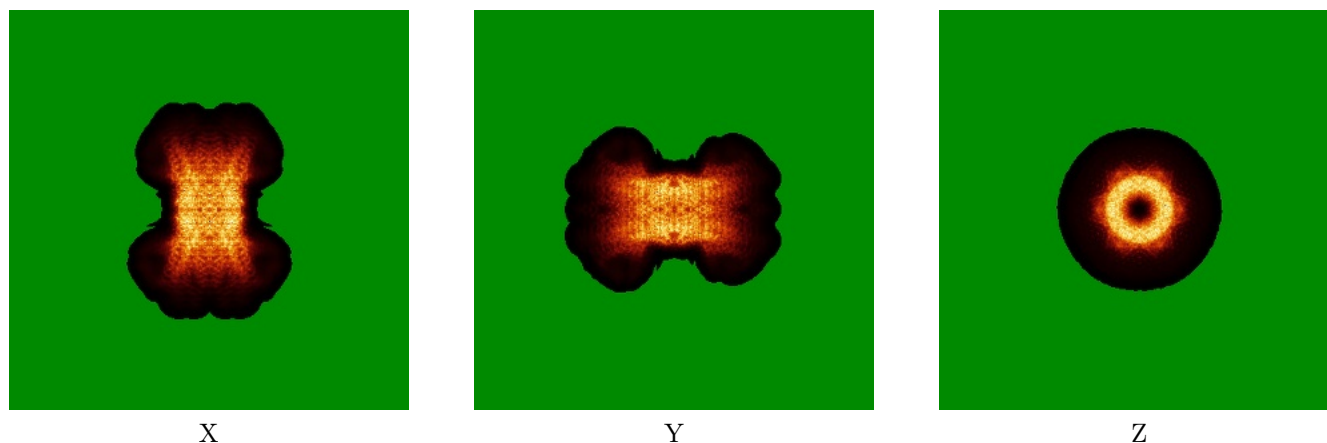


Z Index: 161

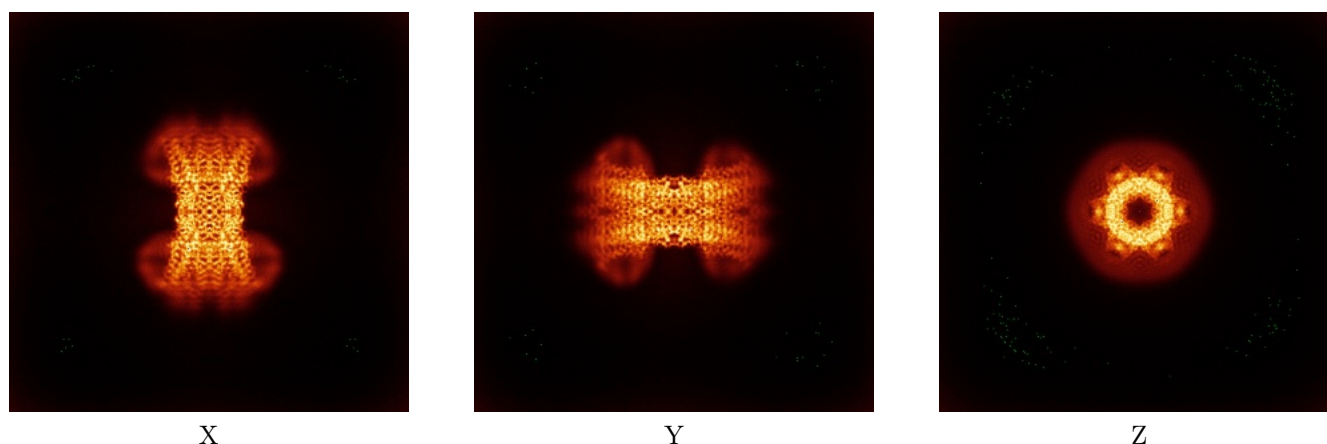
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

This section was not generated.

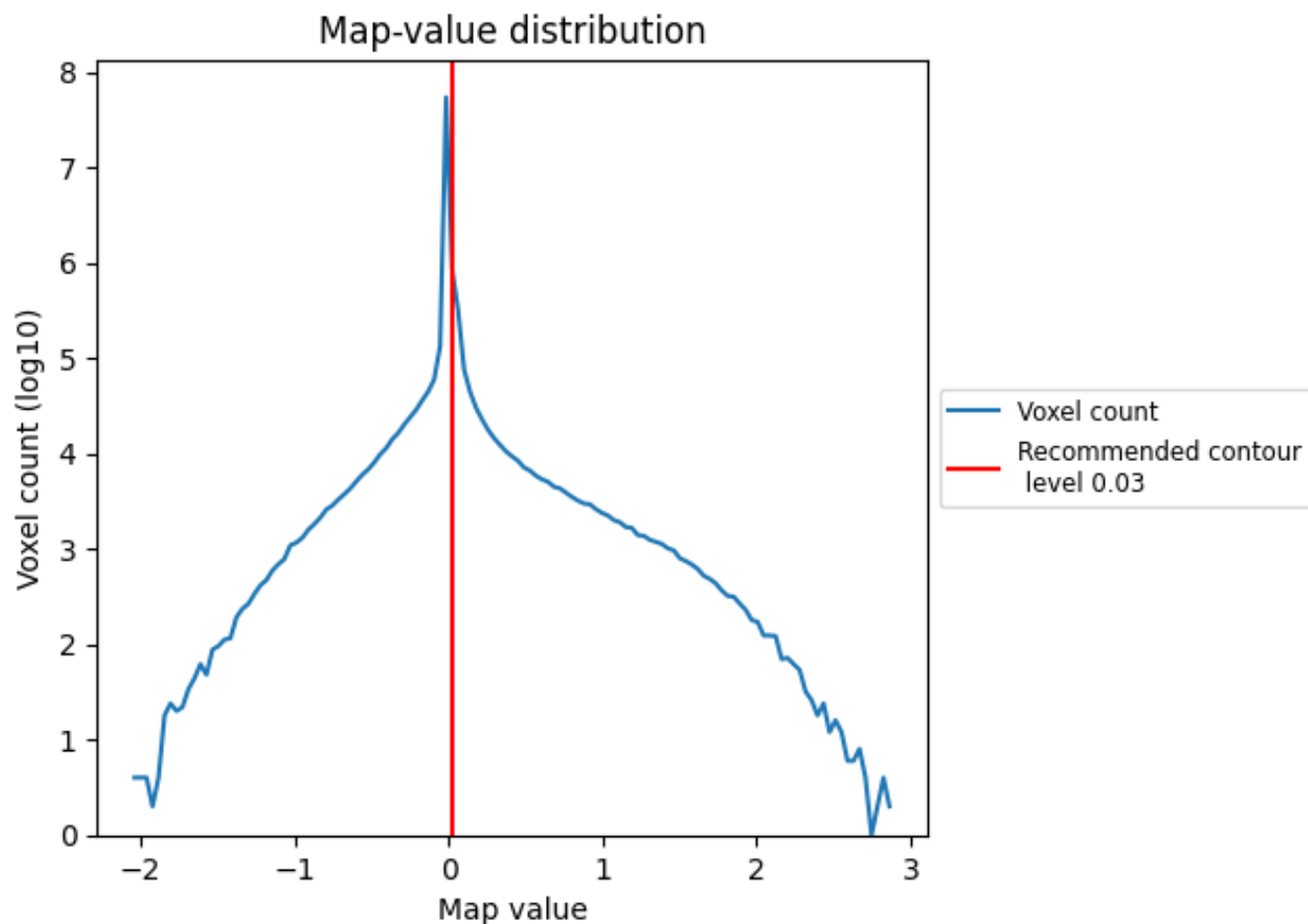
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

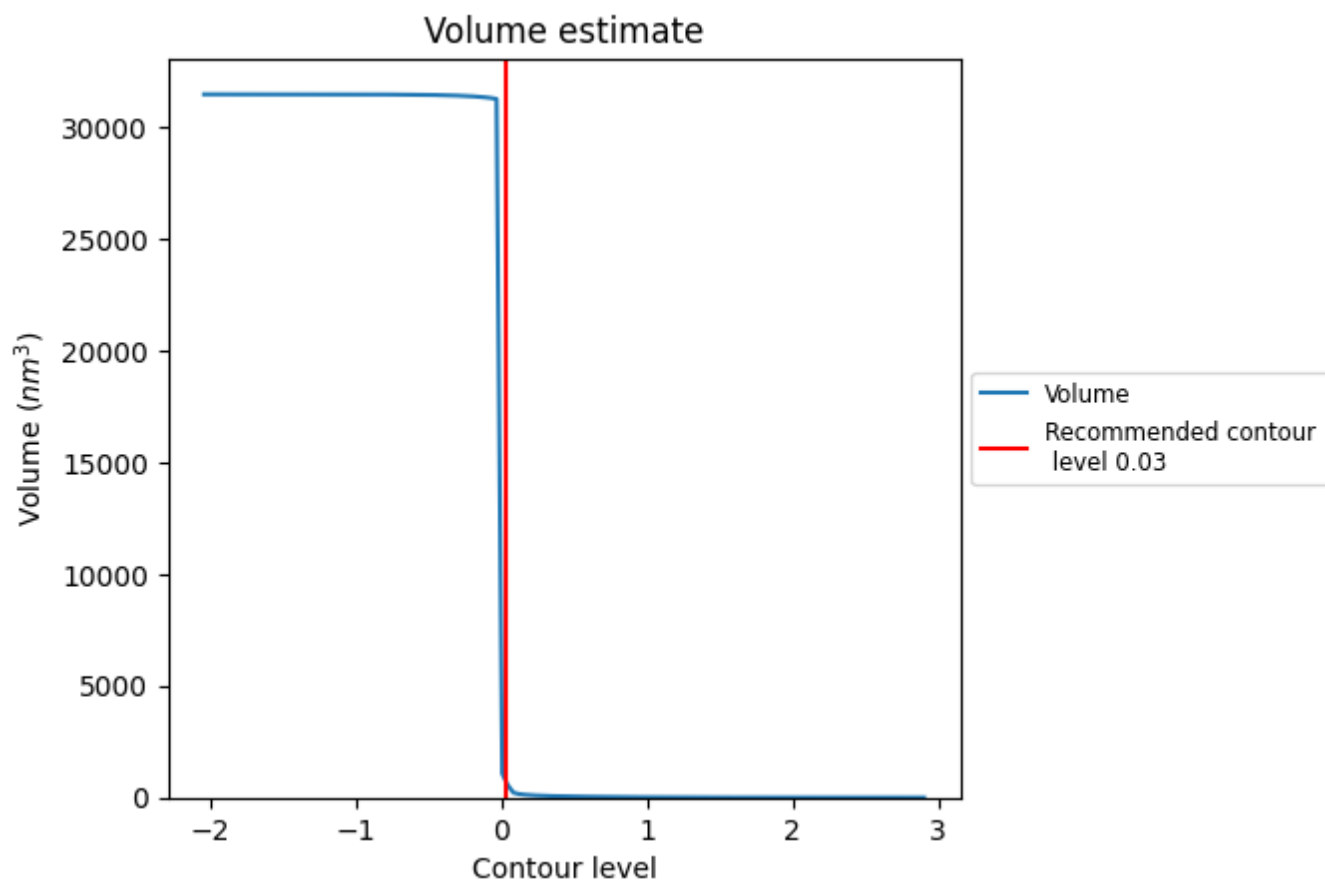
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

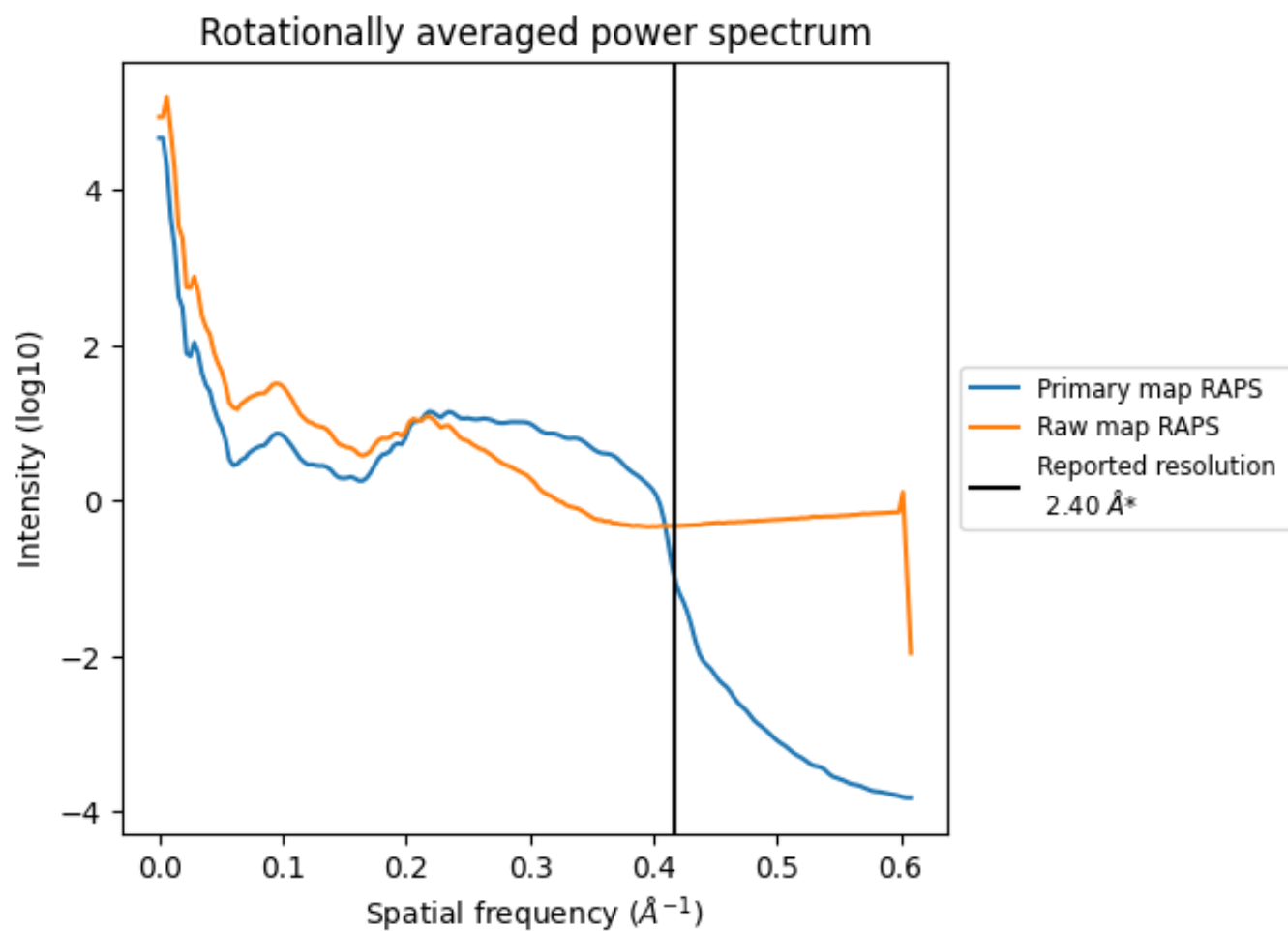
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 764 nm³; this corresponds to an approximate mass of 690 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 ⓘ

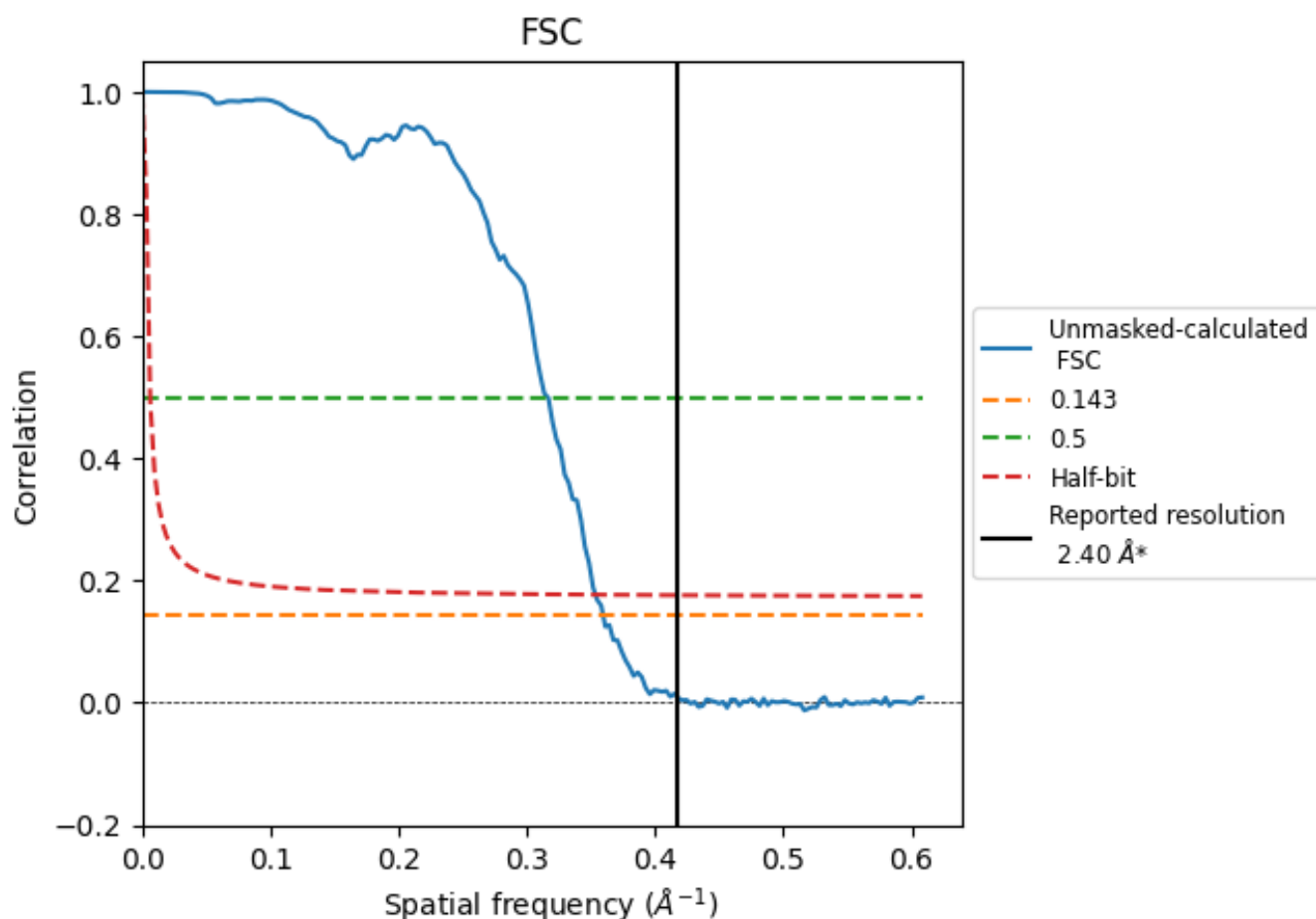


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

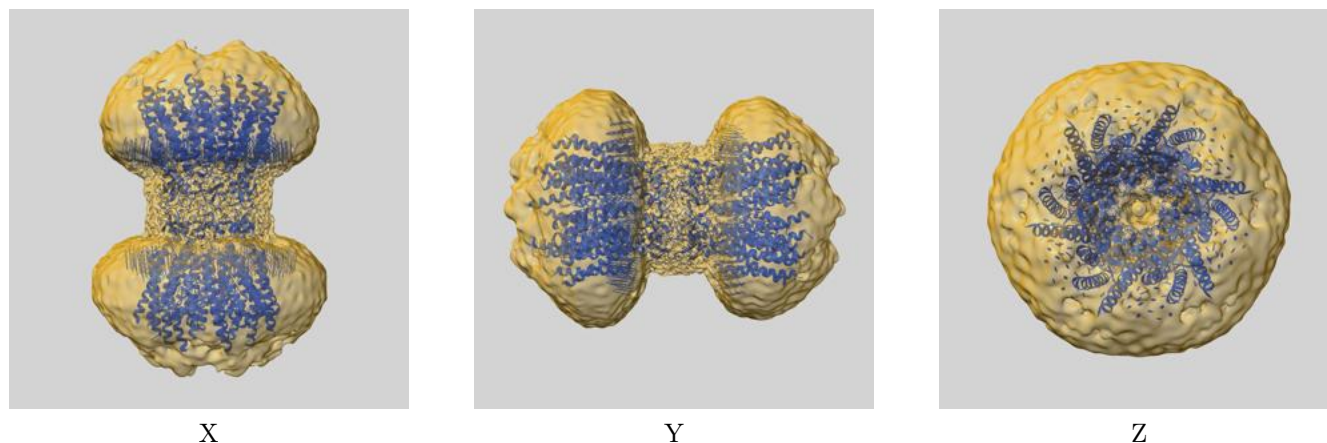
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.78	3.16	2.83

*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 2.78 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

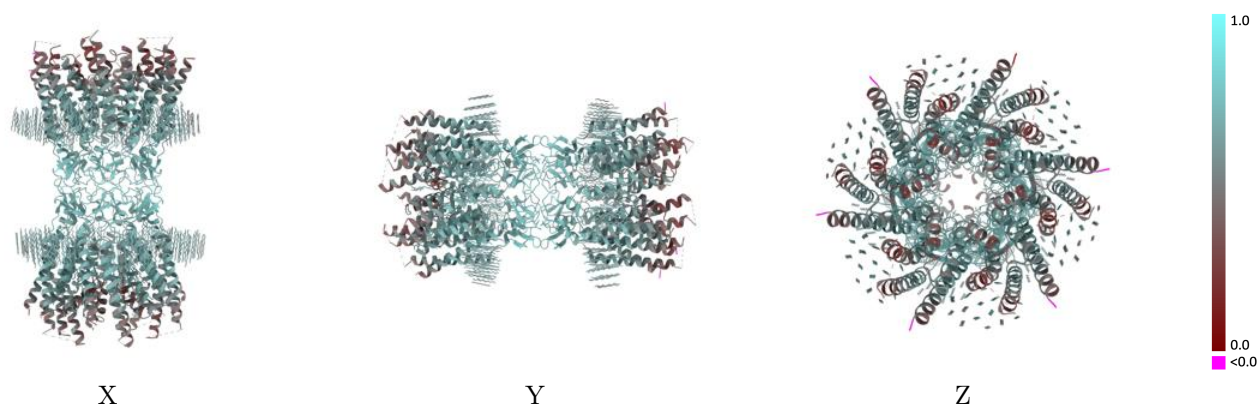
This section contains information regarding the fit between EMDB map EMD-73965 and PDB model 9ZA4. Per-residue inclusion information can be found in section [3](#) on page [18](#).

9.1 Map-model overlay [i](#)



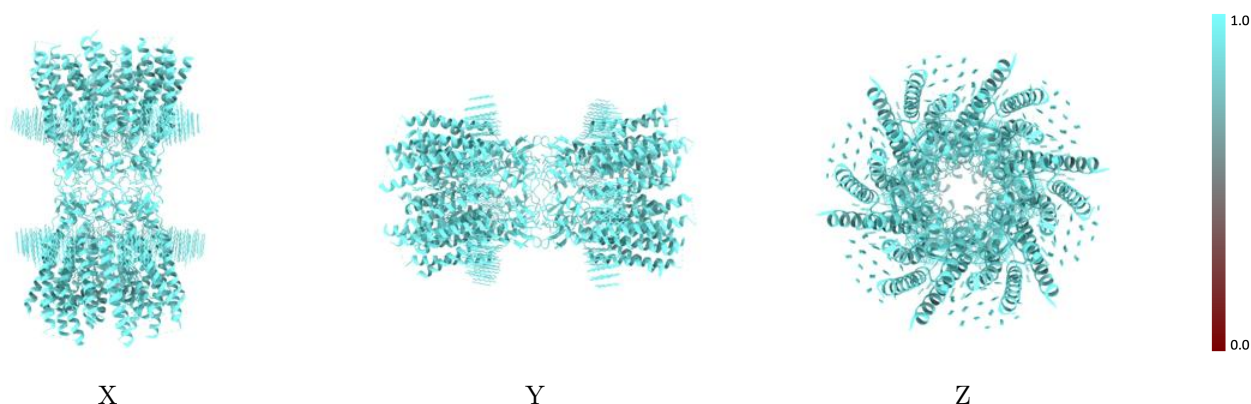
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



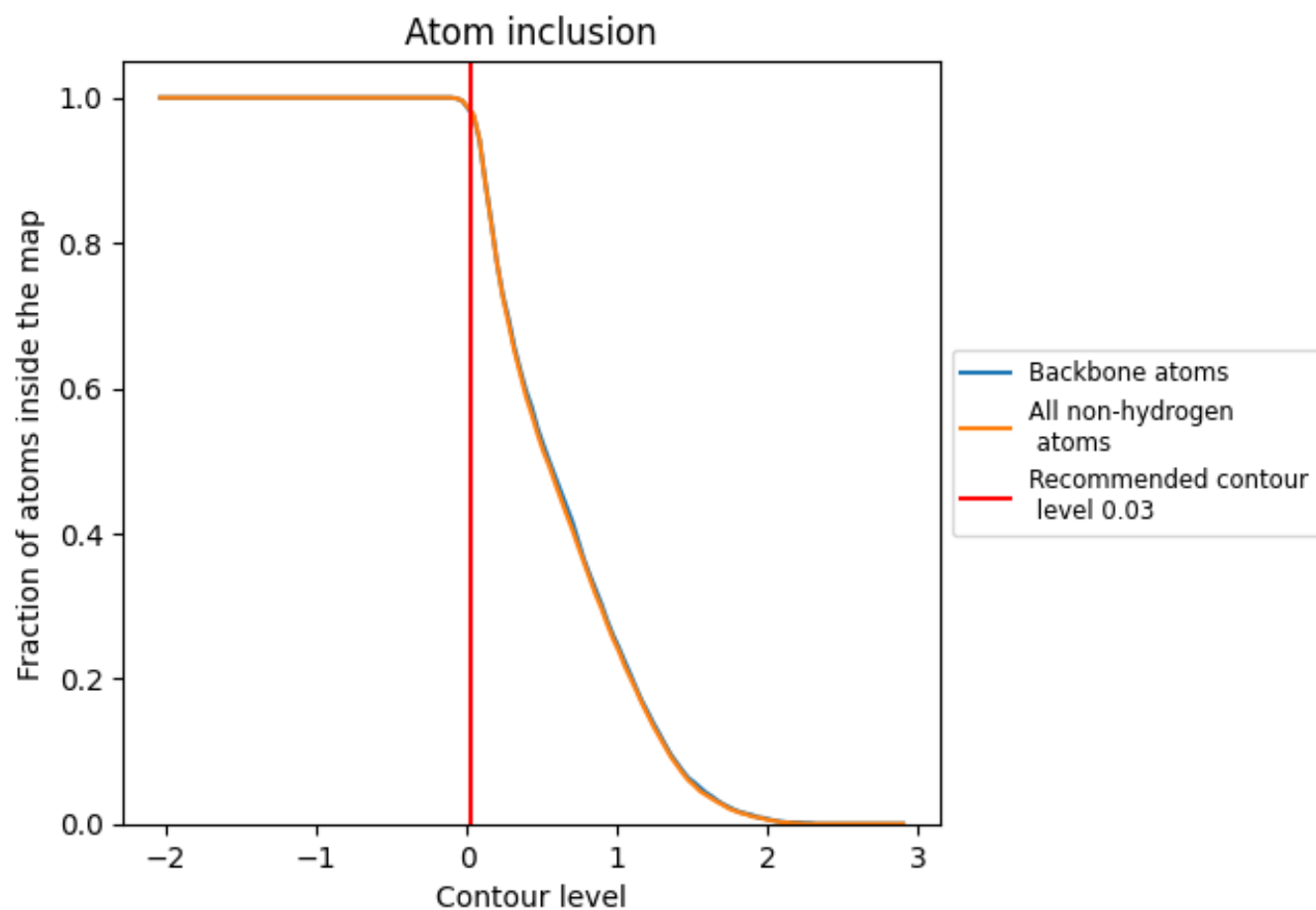
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9810	0.6000
A	0.9770	0.5830
B	0.9770	0.5820
C	0.9780	0.5810
D	0.9770	0.5800
E	0.9770	0.5810
F	0.9780	0.5820
G	0.9930	0.6210
H	0.9900	0.6190
I	0.9910	0.6190
J	0.9890	0.6170
K	0.9900	0.6160
L	0.9910	0.6180

1.0

0.0

<0.0