



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 03:59 PM UTC

PDB ID : 9ZA3 / pdb_00009za3
EMDB ID : EMD-73965
Title : Asymmetrically gated state sheep connexin-46 in DMPC nanodiscs at low pH
Authors : Jarodsky, J.M.; Myers, J.B.; Reichow, S.L.
Deposited on : 2025-11-19
Resolution : 2.40 Å(reported)
Based on initial model : 7jkc

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

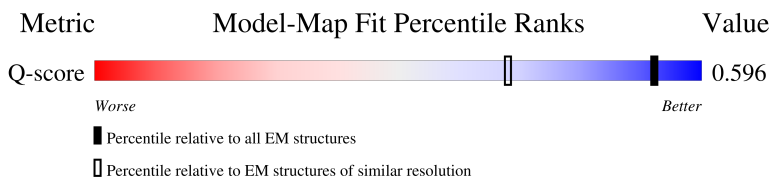
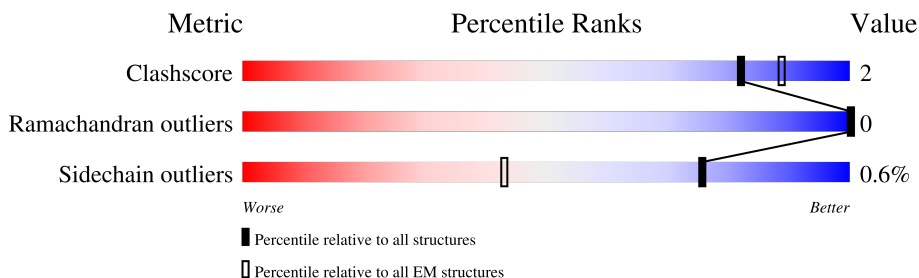
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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	413	
1	B	413	
1	C	413	
1	D	413	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	413	 41% . 56%
1	F	413	 41% . 56%
1	G	413	 42% . 55%
1	H	413	 42% . 55%
1	I	413	 42% . 55%
1	J	413	 42% . 55%
1	K	413	 42% . 55%
1	L	413	 42% . 55%

2 Entry composition

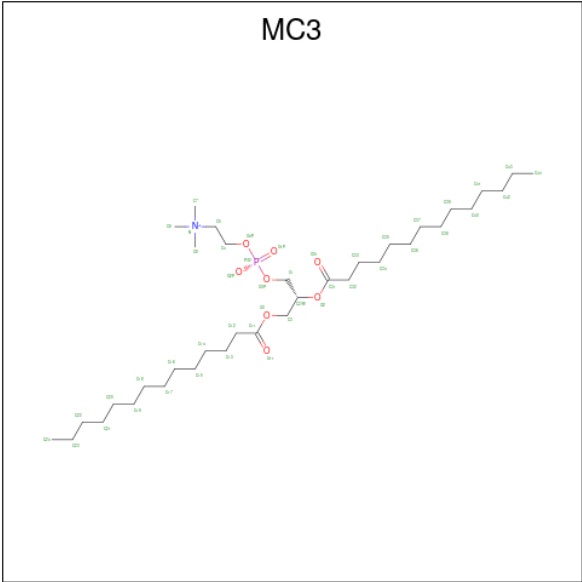
There are 3 unique types of molecules in this entry. The entry contains 44016 atoms, of which 22830 are hydrogens and 0 are deuteriums.

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	183	Total	C	H	N	O	S	0	0
			2971	988	1485	239	251	8		
1	B	183	Total	C	H	N	O	S	0	0
			2971	988	1485	239	251	8		
1	C	183	Total	C	H	N	O	S	0	0
			2971	988	1485	239	251	8		
1	D	183	Total	C	H	N	O	S	0	0
			2971	988	1485	239	251	8		
1	E	183	Total	C	H	N	O	S	0	0
			2971	988	1485	239	251	8		
1	F	183	Total	C	H	N	O	S	0	0
			2971	988	1485	239	251	8		
1	G	185	Total	C	H	N	O	S	0	0
			2869	964	1417	235	244	9		
1	H	185	Total	C	H	N	O	S	0	0
			2869	964	1417	235	244	9		
1	I	185	Total	C	H	N	O	S	0	0
			2869	964	1417	235	244	9		
1	J	185	Total	C	H	N	O	S	0	0
			2869	964	1417	235	244	9		
1	K	185	Total	C	H	N	O	S	0	0
			2869	964	1417	235	244	9		
1	L	185	Total	C	H	N	O	S	0	0
			2869	964	1417	235	244	9		

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



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	H	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 30	C 10	H 20	0	
2	F	1	Total 33	C 11	H 22	0	
2	F	1	Total 27	C 9	H 18	0	
2	F	1	Total 30	C 10	H 20	0	
2	F	1	Total 24	C 8	H 16	0	
2	F	1	Total 33	C 11	H 22	0	
2	F	1	Total 39	C 13	H 26	0	
2	F	1	Total 36	C 12	H 24	0	
2	F	1	Total 30	C 10	H 20	0	
2	F	1	Total 39	C 13	H 26	0	
2	F	1	Total 27	C 9	H 18	0	
2	F	1	Total 33	C 11	H 22	0	
2	F	1	Total 30	C 10	H 20	0	
2	F	1	Total 18	C 6	H 12	0	
2	F	1	Total 30	C 10	H 20	0	
2	F	1	Total 24	C 8	H 16	0	
2	G	1	Total 27	C 9	H 18	0	
2	G	1	Total 52	C 16	H 27 O 8 P 1	0	
2	G	1	Total 33	C 11	H 22	0	
2	G	1	Total 39	C 13	H 26	0	
2	G	1	Total 36	C 12	H 24	0	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	G	1	Total	C	H			0
			33	11	22			
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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
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
			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
			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
			36	12	24			
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
			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
			36	12	24			
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			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
2	J	1	Total	C	H			0
			36	12	24			
2	J	1	Total	C	H			0
			27	9	18			
2	J	1	Total	C	H			0
			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
			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
			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
			36	12	24			
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	

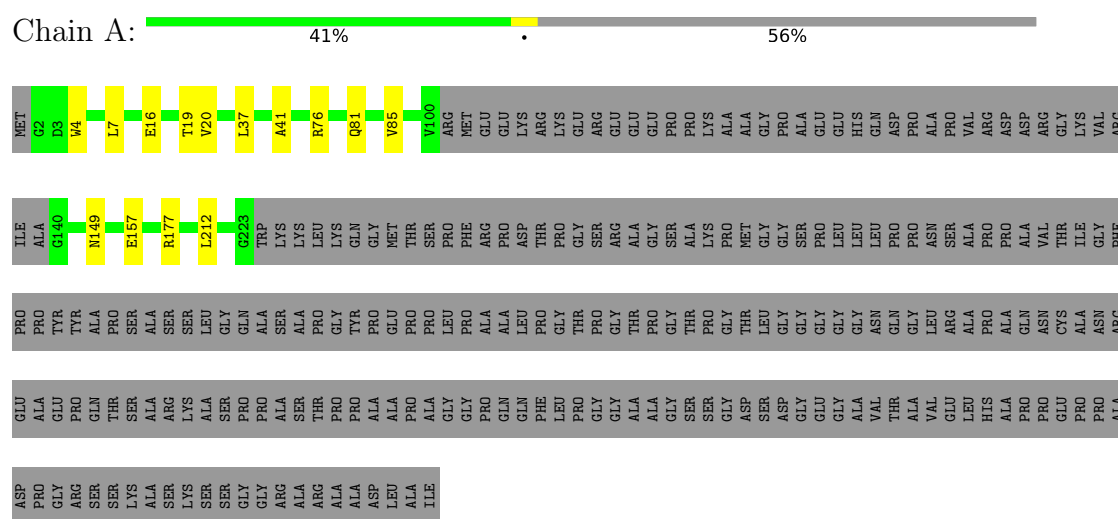
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	63	Total	O	0
			63	63	
3	B	63	Total	O	0
			63	63	
3	C	63	Total	O	0
			63	63	
3	D	63	Total	O	0
			63	63	
3	E	63	Total	O	0
			63	63	
3	F	63	Total	O	0
			63	63	
3	G	55	Total	O	0
			55	55	
3	H	55	Total	O	0
			55	55	
3	I	55	Total	O	0
			55	55	
3	J	55	Total	O	0
			55	55	
3	K	55	Total	O	0
			55	55	
3	L	55	Total	O	0
			55	55	

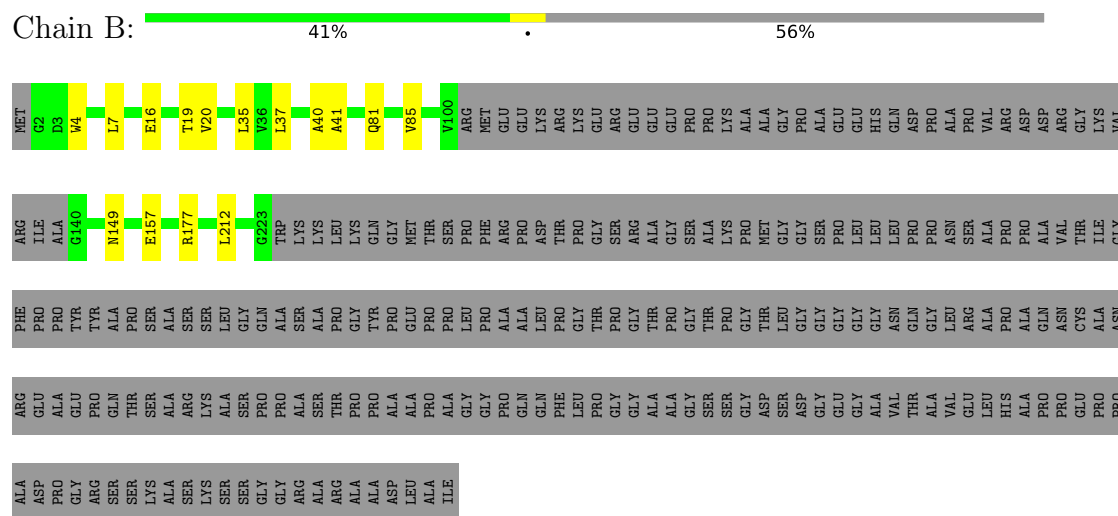
3 Residue-property plots [i](#)

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

- Molecule 1: Gap junction alpha-3 protein



- Molecule 1: Gap junction alpha-3 protein



- Molecule 1: Gap junction alpha-3 protein

[illegible]

Chain D: 41% . 56%

[illegible]

Chain E: 41% 0% 56%

GLY	GLU	TYR	G140	MET
ARG	PRO	TYR		G2
SER	GLN	ALA	N149	D3
SER	THR	PRO		N4
LYS	SER	SER	E157	
ALA	ALA	ALA		L7
SER	ARG	SER	R177	E16
SER	LYS	SER		
SER	ALA	LEU	L212	T19
SER	SER	GLY		V20
GLY	PRO	GLN	G223	
GLY	PRO	ALA	TRP	L37
ARG	ALA	SER	LYS	
ALA	SER	ALA	LYS	A41
ALA	THR	PRO	LEU	
ALA	PRO	TYR	LYS	Q61
ALA	PRO	PRO	GLN	
ASP	ALA	PRO	GLY	V85
LEU	ALA	GLU	MET	
ALA	PRO	PRO	THR	V100
ILE	ALA	PRO	SER	ARG
	GLY	LEU	PRO	
	GLY	PRO	PHE	GLU
	PRO	ALA	ARG	
	GLN	ALA	PRO	GLU
	GLN	LEU	ASP	LYS
	PHE	PRO	THR	ARG
	LEU	THR	PRO	LYS
	PRO	THR	GLY	GLU
	GLY	PRO	SER	ARG
	GLY	GLY	ARG	
	ALA	THR	ALA	GLU
	ALA	PRO	ALA	GLY
	GLY	GLY	SER	PRO
	SER	THR	ALA	PRO
	SER	PRO	LYS	LYS
	GLY	PRO	PRO	ALA
	GLY	THR	MET	ALA
	ASP	THR	GLY	ALA
	SER	LEU	GLY	GLY
	SER	GLY	SER	PRO
	GLY	GLY	ALA	ALA
	GLU	GLY	PRO	GLU
	GLY	GLY	LEU	GLU
	ALA	GLY	LEU	HIS
	VAL	ASN	LEU	GLN
	THR	GLN	PRO	ASP
	ALA	GLY	PRO	PRO
	VAL	LEU	ASN	ALA
	GLU	ARG	SER	PRO
	GLY	ALA	ALA	VAL
	HIS	PRO	PRO	ARG
	ALA	ALA	PRO	ASP
	PRO	GLN	ALA	ASP
	PRO	ASN	VAL	ARG
	GLU	CYS	THR	GLY
	PRO	ALA	ILE	LYS
	PRO	ASN	PHE	VAL
	ALA	ARG	GLY	ARG
	PRO	ALA	PRO	ILE
	THR	ALA	PRO	ALA

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

SER
SER
GLY
GLY
ARG
ALA
ARG
ALA
ALA
ALA
ASP
LEU
ALA
ILE

● Molecule 1: Gap junction alpha-3 protein



MET
GLY
ASP
W4
L37
A40
A41
E42
E43
V44
D51
F52
T53
E104
LYS
ARG
LYS
GLU
ARG
GLY
SER
GLU
GLU
PRO
PRO
LYS
LYS
ALA
SER
ALA
GLY
PRO
LEU
LEU
ALA
GLN
HIS
GLN
ASN
SER
ASP
PRO
ALA
PRO
VAL
VAL
ARG
ASP
THR
ILE
A139
N149
K173
P174
L222

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

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

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

GLY
GLY
ARG
ALA
ARG
ALA
ALA
ASP
LEU
ALA
ILE

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	0.13	0/1529	0.33	0/2084
1	B	0.14	0/1529	0.33	0/2084
1	C	0.14	0/1529	0.33	0/2084
1	D	0.14	0/1529	0.33	0/2084
1	E	0.14	0/1529	0.33	0/2084
1	F	0.14	0/1529	0.33	0/2084
1	G	0.09	0/1492	0.21	0/2037
1	H	0.09	0/1492	0.21	0/2037
1	I	0.09	0/1492	0.21	0/2037
1	J	0.09	0/1492	0.21	0/2037
1	K	0.09	0/1492	0.21	0/2037
1	L	0.09	0/1492	0.21	0/2037
All	All	0.11	0/18126	0.28	0/24726

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	1486	1485	1478	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1486	1485	1478	13	0
1	C	1486	1485	1478	10	0
1	D	1486	1485	1478	12	0
1	E	1486	1485	1478	12	0
1	F	1486	1485	1478	11	0
1	G	1452	1417	1414	6	0
1	H	1452	1417	1414	6	0
1	I	1452	1417	1414	6	0
1	J	1452	1417	1414	6	0
1	K	1452	1417	1414	6	0
1	L	1452	1417	1414	5	0
2	A	199	398	343	0	0
2	B	199	398	343	0	0
2	C	199	398	343	0	0
2	D	199	398	343	0	0
2	E	199	398	343	0	0
2	F	199	398	343	0	0
2	G	276	505	441	0	0
2	H	276	505	441	0	0
2	I	276	505	441	0	0
2	J	276	505	441	0	0
2	K	276	505	441	0	0
2	L	276	505	441	0	0
3	A	63	0	0	1	0
3	B	63	0	0	1	0
3	C	63	0	0	1	0
3	D	63	0	0	2	0
3	E	63	0	0	1	0
3	F	63	0	0	1	0
3	G	55	0	0	1	0
3	H	55	0	0	1	0
3	I	55	0	0	1	0
3	J	55	0	0	1	0
3	K	55	0	0	1	0
3	L	55	0	0	1	0
All	All	21186	22830	22056	105	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (105) 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:D:4:TRP:CE3	1:D:7:LEU:HD23	2.24	0.72
1:E:4:TRP:CE3	1:E:7:LEU:HD23	2.24	0.72
1:B:4:TRP:CE3	1:B:7:LEU:HD23	2.24	0.72
1:A:4:TRP:CE3	1:A:7:LEU:HD23	2.24	0.72
1:C:4:TRP:CE3	1:C:7:LEU:HD23	2.25	0.72
1:F:4:TRP:CE3	1:F:7:LEU:HD23	2.25	0.71
1:A:4:TRP:CZ3	1:A:7:LEU:HD23	2.39	0.57
1:F:4:TRP:CZ3	1:F:7:LEU:HD23	2.40	0.57
1:B:4:TRP:CZ3	1:B:7:LEU:HD23	2.39	0.57
1:C:4:TRP:CZ3	1:C:7:LEU:HD23	2.40	0.57
1:E:4:TRP:CZ3	1:E:7:LEU:HD23	2.40	0.56
1:D:4:TRP:CZ3	1:D:7:LEU:HD23	2.39	0.56
1:D:177:ARG:HD2	3:D:651:HOH:O	2.08	0.54
1:A:177:ARG:HD2	3:A:651:HOH:O	2.08	0.53
1:C:177:ARG:HD2	3:C:652:HOH:O	2.09	0.53
1:K:173:LYS:HE3	1:K:174:PRO:HD2	1.91	0.53
1:G:173:LYS:HE3	1:G:174:PRO:HD2	1.91	0.52
1:L:173:LYS:HE3	1:L:174:PRO:HD2	1.91	0.52
1:H:173:LYS:HE3	1:H:174:PRO:HD2	1.92	0.52
1:J:173:LYS:HE3	1:J:174:PRO:HD2	1.91	0.52
1:I:173:LYS:HE3	1:I:174:PRO:HD2	1.91	0.52
1:A:4:TRP:CZ3	1:A:7:LEU:CD2	2.93	0.52
1:B:4:TRP:CZ3	1:B:7:LEU:CD2	2.93	0.52
1:F:4:TRP:CZ3	1:F:7:LEU:CD2	2.93	0.51
1:E:4:TRP:CZ3	1:E:7:LEU:CD2	2.93	0.51
1:C:4:TRP:CZ3	1:C:7:LEU:CD2	2.93	0.50
1:D:4:TRP:CZ3	1:D:7:LEU:CD2	2.93	0.50
1:J:40:ALA:O	1:J:44:VAL:HG23	2.12	0.50
1:K:40:ALA:O	1:K:44:VAL:HG23	2.11	0.50
1:I:40:ALA:O	1:I:44:VAL:HG23	2.12	0.50
1:G:40:ALA:O	1:G:44:VAL:HG23	2.12	0.49
1:H:40:ALA:O	1:H:44:VAL:HG23	2.12	0.49
1:L:40:ALA:O	1:L:44:VAL:HG23	2.12	0.49
1:F:177:ARG:HD2	3:F:653:HOH:O	2.12	0.49
1:B:177:ARG:HD2	3:B:654:HOH:O	2.12	0.48
1:D:4:TRP:HE3	1:D:7:LEU:HD23	1.78	0.48
1:C:4:TRP:HE3	1:C:7:LEU:HD23	1.78	0.48
1:L:43:GLU:HG3	3:L:610:HOH:O	2.13	0.47
1:F:19:THR:HG22	1:F:20:VAL:N	2.30	0.47
1:A:19:THR:HG22	1:A:20:VAL:N	2.30	0.47
1:E:177:ARG:HD2	3:E:654:HOH:O	2.14	0.47
1:G:37:LEU:HD12	1:G:41:ALA:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:37:LEU:HD12	1:H:41:ALA:HB3	1.97	0.46
1:K:37:LEU:HD12	1:K:41:ALA:HB3	1.97	0.46
1:I:43:GLU:HG3	3:I:609:HOH:O	2.14	0.46
1:J:37:LEU:HD12	1:J:41:ALA:HB3	1.97	0.46
1:E:16:GLU:HA	1:E:16:GLU:OE1	2.16	0.46
1:E:19:THR:HG22	1:E:20:VAL:N	2.30	0.46
1:B:4:TRP:HE3	1:B:7:LEU:HD23	1.78	0.46
1:E:4:TRP:HE3	1:E:7:LEU:HD23	1.78	0.46
1:B:16:GLU:HA	1:B:16:GLU:OE1	2.16	0.46
1:C:16:GLU:HA	1:C:16:GLU:OE1	2.16	0.46
1:A:16:GLU:HA	1:A:16:GLU:OE1	2.16	0.46
1:D:16:GLU:HA	1:D:16:GLU:OE1	2.16	0.46
1:L:37:LEU:HD12	1:L:41:ALA:HB3	1.97	0.46
1:F:4:TRP:HE3	1:F:7:LEU:HD23	1.78	0.46
1:A:4:TRP:CE3	1:A:7:LEU:CD2	2.98	0.45
1:B:19:THR:HG22	1:B:20:VAL:N	2.30	0.45
1:D:19:THR:HG22	1:D:20:VAL:N	2.30	0.45
1:L:51:ASP:O	1:L:53:THR:HG23	2.17	0.45
1:C:37:LEU:HD12	1:C:41:ALA:HB3	1.99	0.45
1:A:4:TRP:HE3	1:A:7:LEU:HD23	1.78	0.45
1:B:37:LEU:HD12	1:B:41:ALA:HB3	1.99	0.45
1:D:37:LEU:HD12	1:D:41:ALA:HB3	1.99	0.45
1:I:37:LEU:HD12	1:I:41:ALA:HB3	1.97	0.45
1:D:4:TRP:CE3	1:D:7:LEU:CD2	2.98	0.45
1:F:4:TRP:CE3	1:F:7:LEU:CD2	2.98	0.45
1:G:51:ASP:O	1:G:53:THR:HG23	2.17	0.45
1:C:19:THR:HG22	1:C:20:VAL:N	2.30	0.45
1:F:16:GLU:HA	1:F:16:GLU:OE1	2.16	0.45
1:K:51:ASP:O	1:K:53:THR:HG23	2.17	0.45
1:E:4:TRP:CE3	1:E:7:LEU:CD2	2.98	0.45
1:A:37:LEU:HD12	1:A:41:ALA:HB3	1.99	0.45
1:B:4:TRP:CE3	1:B:7:LEU:CD2	2.98	0.45
1:H:51:ASP:O	1:H:53:THR:HG23	2.17	0.45
1:J:51:ASP:O	1:J:53:THR:HG23	2.17	0.45
1:F:37:LEU:HD12	1:F:41:ALA:HB3	1.99	0.44
1:I:51:ASP:O	1:I:53:THR:HG23	2.17	0.44
1:E:37:LEU:HD12	1:E:41:ALA:HB3	1.98	0.44
1:H:43:GLU:HG3	3:H:618:HOH:O	2.16	0.44
1:K:43:GLU:HG3	3:K:613:HOH:O	2.17	0.42
1:J:43:GLU:HG3	3:J:614:HOH:O	2.18	0.42
1:G:43:GLU:HG3	3:G:614:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:GLN:O	1:E:85:VAL:HG22	2.20	0.41
1:F:81:GLN:O	1:F:85:VAL:HG22	2.20	0.41
1:J:191:ILE:HD12	1:J:191:ILE:N	2.36	0.41
1:C:81:GLN:O	1:C:85:VAL:HG22	2.20	0.41
1:B:81:GLN:O	1:B:85:VAL:HG22	2.20	0.41
1:K:191:ILE:N	1:K:191:ILE:HD12	2.36	0.41
1:A:4:TRP:HZ3	1:A:7:LEU:CD2	2.33	0.41
1:A:81:GLN:O	1:A:85:VAL:HG22	2.20	0.41
1:D:81:GLN:O	1:D:85:VAL:HG22	2.20	0.41
1:A:76:ARG:HG3	1:B:40:ALA:HB1	2.03	0.41
1:A:157:GLU:HB2	1:A:212:LEU:HD21	2.03	0.41
1:B:157:GLU:HB2	1:B:212:LEU:HD21	2.03	0.41
1:D:177:ARG:CD	3:D:651:HOH:O	2.69	0.41
1:I:191:ILE:HD12	1:I:191:ILE:N	2.36	0.41
1:C:4:TRP:CE3	1:C:7:LEU:CD2	2.98	0.41
1:E:4:TRP:HZ3	1:E:7:LEU:CD2	2.34	0.41
1:A:4:TRP:CE3	1:B:35:LEU:HD21	2.56	0.40
1:G:191:ILE:HD12	1:G:191:ILE:N	2.36	0.40
1:D:157:GLU:HB2	1:D:212:LEU:HD21	2.03	0.40
1:F:157:GLU:HB2	1:F:212:LEU:HD21	2.03	0.40
1:E:157:GLU:HB2	1:E:212:LEU:HD21	2.03	0.40
1:H:191:ILE:HD12	1:H:191:ILE:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	179/413 (43%)	176 (98%)	3 (2%)	0	100	100
1	B	179/413 (43%)	176 (98%)	3 (2%)	0	100	100
1	C	179/413 (43%)	176 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	179/413 (43%)	176 (98%)	3 (2%)	0	100	100
1	E	179/413 (43%)	176 (98%)	3 (2%)	0	100	100
1	F	179/413 (43%)	176 (98%)	3 (2%)	0	100	100
1	G	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
1	H	181/413 (44%)	179 (99%)	2 (1%)	0	100	100
1	I	181/413 (44%)	179 (99%)	2 (1%)	0	100	100
1	J	181/413 (44%)	180 (99%)	1 (1%)	0	100	100
1	K	181/413 (44%)	179 (99%)	2 (1%)	0	100	100
1	L	181/413 (44%)	179 (99%)	2 (1%)	0	100	100
All	All	2160/4956 (44%)	2132 (99%)	28 (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	162/325 (50%)	161 (99%)	1 (1%)	78	89
1	B	162/325 (50%)	161 (99%)	1 (1%)	78	89
1	C	162/325 (50%)	161 (99%)	1 (1%)	78	89
1	D	162/325 (50%)	161 (99%)	1 (1%)	78	89
1	E	162/325 (50%)	161 (99%)	1 (1%)	78	89
1	F	162/325 (50%)	161 (99%)	1 (1%)	78	89
1	G	151/325 (46%)	150 (99%)	1 (1%)	76	88
1	H	151/325 (46%)	150 (99%)	1 (1%)	76	88
1	I	151/325 (46%)	150 (99%)	1 (1%)	76	88
1	J	151/325 (46%)	150 (99%)	1 (1%)	76	88
1	K	151/325 (46%)	150 (99%)	1 (1%)	76	88
1	L	151/325 (46%)	150 (99%)	1 (1%)	76	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1878/3900 (48%)	1866 (99%)	12 (1%)	76 89

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

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [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	H	523	-	7,7,45	0.35	0	6,6,53	0.74	0
2	MC3	L	515	-	10,10,45	0.33	0	9,9,53	0.80	0
2	MC3	G	505	-	11,11,45	0.33	0	10,10,53	0.82	0
2	MC3	D	517	-	5,5,45	0.36	0	4,4,53	0.62	0
2	MC3	E	505	-	10,10,45	0.36	0	9,9,53	0.84	0
2	MC3	H	507	-	12,12,45	0.34	0	11,11,53	0.84	0
2	MC3	B	515	-	10,10,45	0.36	0	9,9,53	0.82	0
2	MC3	J	521	-	11,11,45	0.34	0	10,10,53	0.84	0
2	MC3	L	514	-	11,11,45	0.32	0	10,10,53	0.81	0
2	MC3	L	519	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	A	511	-	7,7,45	0.36	0	6,6,53	0.76	0
2	MC3	J	519	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	C	509	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	J	520	-	9,9,45	0.34	0	8,8,53	0.79	0
2	MC3	I	513	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	L	506	-	9,9,45	0.34	0	8,8,53	0.80	0
2	MC3	J	515	-	24,24,45	0.53	0	27,29,53	0.73	1 (3%)
2	MC3	I	503	-	10,10,45	0.32	0	9,9,53	0.80	0
2	MC3	J	504	-	12,12,45	0.33	0	11,11,53	0.83	0
2	MC3	E	516	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	L	511	-	24,24,45	0.83	1 (4%)	27,29,53	1.26	2 (7%)
2	MC3	L	513	-	12,12,45	0.33	0	11,11,53	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	C	515	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	D	502	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	F	516	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	E	519	-	7,7,45	0.37	0	6,6,53	0.76	0
2	MC3	D	515	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	J	522	-	8,8,45	0.35	0	7,7,53	0.78	0
2	MC3	A	503	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	G	515	-	24,24,45	0.53	0	27,29,53	0.73	1 (3%)
2	MC3	G	517	-	11,11,45	0.32	0	10,10,53	0.84	0
2	MC3	G	523	-	7,7,45	0.36	0	6,6,53	0.74	0
2	MC3	E	503	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	K	515	-	24,24,45	0.52	0	27,29,53	0.73	1 (3%)
2	MC3	B	508	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	E	502	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	H	503	-	10,10,45	0.32	0	9,9,53	0.80	0
2	MC3	H	514	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	F	515	-	10,10,45	0.36	0	9,9,53	0.82	0
2	MC3	F	517	-	5,5,45	0.36	0	4,4,53	0.62	0
2	MC3	C	505	-	10,10,45	0.36	0	9,9,53	0.83	0
2	MC3	I	504	-	12,12,45	0.32	0	11,11,53	0.82	0
2	MC3	J	506	-	10,10,45	0.34	0	9,9,53	0.81	0
2	MC3	C	516	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	J	516	-	12,12,45	0.31	0	11,11,53	0.83	0
2	MC3	L	518	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	B	510	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	B	513	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	I	507	-	12,12,45	0.34	0	11,11,53	0.83	0
2	MC3	C	511	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	D	506	-	8,8,45	0.37	0	7,7,53	0.79	0
2	MC3	J	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	J	518	-	12,12,45	0.33	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	J	502	-	24,24,45	0.83	1 (4%)	27,29,53	1.26	2 (7%)
2	MC3	B	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	K	511	-	10,10,45	0.34	0	9,9,53	0.82	0
2	MC3	G	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	D	511	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	G	518	-	12,12,45	0.33	0	11,11,53	0.85	0
2	MC3	F	511	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	J	510	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	J	511	-	10,10,45	0.34	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	L	505	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	B	502	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	E	518	-	9,9,45	0.36	0	8,8,53	0.83	0
2	MC3	K	514	-	8,8,45	0.35	0	7,7,53	0.79	0
2	MC3	L	509	-	7,7,45	0.35	0	6,6,53	0.74	0
2	MC3	K	501	-	8,8,45	0.24	0	7,7,53	0.20	0
2	MC3	E	506	-	8,8,45	0.37	0	7,7,53	0.79	0
2	MC3	I	520	-	9,9,45	0.34	0	8,8,53	0.79	0
2	MC3	C	506	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	J	513	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	K	506	-	10,10,45	0.33	0	9,9,53	0.81	0
2	MC3	D	501	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	H	512	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	L	523	-	8,8,45	0.35	0	7,7,53	0.79	0
2	MC3	F	503	-	11,11,45	0.36	0	10,10,53	0.85	0
2	MC3	I	519	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	I	521	-	11,11,45	0.34	0	10,10,53	0.84	0
2	MC3	G	511	-	10,10,45	0.34	0	9,9,53	0.82	0
2	MC3	D	507	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	I	508	-	4,4,45	0.37	0	3,3,53	0.57	0
2	MC3	C	510	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	F	501	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	G	512	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	C	519	-	7,7,45	0.36	0	6,6,53	0.76	0
2	MC3	E	517	-	5,5,45	0.37	0	4,4,53	0.62	0
2	MC3	A	515	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	K	520	-	9,9,45	0.34	0	8,8,53	0.79	0
2	MC3	L	516	-	12,12,45	0.34	0	11,11,53	0.84	0
2	MC3	F	502	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	G	521	-	11,11,45	0.34	0	10,10,53	0.84	0
2	MC3	K	504	-	12,12,45	0.33	0	11,11,53	0.83	0
2	MC3	A	517	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	C	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	B	512	-	9,9,45	0.36	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	I	523	-	7,7,45	0.35	0	6,6,53	0.74	0
2	MC3	J	509	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	H	504	-	12,12,45	0.33	0	11,11,53	0.83	0
2	MC3	K	521	-	11,11,45	0.34	0	10,10,53	0.84	0
2	MC3	H	517	-	11,11,45	0.33	0	10,10,53	0.84	0
2	MC3	K	522	-	8,8,45	0.35	0	7,7,53	0.78	0
2	MC3	D	505	-	10,10,45	0.36	0	9,9,53	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	G	509	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	H	522	-	8,8,45	0.35	0	7,7,53	0.78	0
2	MC3	I	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	H	505	-	11,11,45	0.33	0	10,10,53	0.82	0
2	MC3	H	508	-	4,4,45	0.37	0	3,3,53	0.58	0
2	MC3	K	505	-	11,11,45	0.32	0	10,10,53	0.82	0
2	MC3	J	508	-	4,4,45	0.37	0	3,3,53	0.57	0
2	MC3	L	520	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	F	505	-	10,10,45	0.36	0	9,9,53	0.83	0
2	MC3	K	509	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	A	514	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	I	502	-	24,24,45	0.83	1 (4%)	27,29,53	1.26	2 (7%)
2	MC3	G	516	-	12,12,45	0.31	0	11,11,53	0.83	0
2	MC3	J	517	-	11,11,45	0.33	0	10,10,53	0.84	0
2	MC3	A	501	-	10,10,45	0.35	0	9,9,53	0.83	0
2	MC3	L	510	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	C	517	-	5,5,45	0.36	0	4,4,53	0.62	0
2	MC3	B	517	-	5,5,45	0.37	0	4,4,53	0.62	0
2	MC3	G	519	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	K	516	-	12,12,45	0.31	0	11,11,53	0.83	0
2	MC3	B	506	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	A	518	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	A	502	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	E	508	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	H	515	-	24,24,45	0.51	0	27,29,53	0.75	1 (3%)
2	MC3	A	507	-	10,10,45	0.36	0	9,9,53	0.82	0
2	MC3	C	503	-	11,11,45	0.36	0	10,10,53	0.85	0
2	MC3	I	518	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	H	518	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	L	504	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	G	502	-	24,24,45	0.83	1 (4%)	27,29,53	1.26	2 (7%)
2	MC3	A	508	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	L	507	-	11,11,45	0.34	0	10,10,53	0.84	0
2	MC3	D	504	-	9,9,45	0.36	0	8,8,53	0.82	0
2	MC3	H	519	-	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	K	502	-	24,24,45	0.83	1 (4%)	27,29,53	1.26	2 (7%)
2	MC3	F	506	-	8,8,45	0.36	0	7,7,53	0.79	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	K	513	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	H	511	-	10,10,45	0.34	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	L	508	-	8,8,45	0.35	0	7,7,53	0.78	0
2	MC3	I	522	-	8,8,45	0.35	0	7,7,53	0.78	0
2	MC3	L	512	-	10,10,45	0.32	0	9,9,53	0.80	0
2	MC3	B	511	-	11,11,45	0.35	0	10,10,53	0.84	0
2	MC3	G	506	-	10,10,45	0.33	0	9,9,53	0.81	0
2	MC3	G	520	-	9,9,45	0.34	0	8,8,53	0.79	0
2	MC3	J	507	-	12,12,45	0.34	0	11,11,53	0.84	0
2	MC3	C	507	-	9,9,45	0.36	0	8,8,53	0.82	0
2	MC3	G	514	-	8,8,45	0.35	0	7,7,53	0.79	0
2	MC3	E	504	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	F	510	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	E	509	-	10,10,45	0.35	0	9,9,53	0.82	0
2	MC3	K	503	-	10,10,45	0.32	0	9,9,53	0.80	0
2	MC3	I	515	-	24,24,45	0.52	0	27,29,53	0.72	1 (3%)
2	MC3	F	514	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	K	519	-	12,12,45	0.34	0	11,11,53	0.85	0
2	MC3	G	522	-	8,8,45	0.35	0	7,7,53	0.78	0
2	MC3	E	507	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	A	505	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	G	503	-	10,10,45	0.32	0	9,9,53	0.80	0
2	MC3	F	504	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	A	509	-	5,5,45	0.37	0	4,4,53	0.62	0
2	MC3	L	517	-	4,4,45	0.37	0	3,3,53	0.57	0
2	MC3	F	518	-	9,9,45	0.35	0	8,8,53	0.82	0
2	MC3	K	507	-	12,12,45	0.34	0	11,11,53	0.84	0
2	MC3	J	512	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	F	507	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	A	516	-	10,10,45	0.36	0	9,9,53	0.84	0
2	MC3	L	503	-	11,11,45	0.33	0	10,10,53	0.84	0
2	MC3	G	510	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	I	506	-	10,10,45	0.33	0	9,9,53	0.80	0
2	MC3	I	511	-	10,10,45	0.34	0	9,9,53	0.82	0
2	MC3	H	516	-	12,12,45	0.32	0	11,11,53	0.83	0
2	MC3	K	510	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	B	503	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	E	512	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	C	518	-	9,9,45	0.36	0	8,8,53	0.82	0
2	MC3	K	518	-	12,12,45	0.33	0	11,11,53	0.85	0
2	MC3	G	507	-	12,12,45	0.34	0	11,11,53	0.83	0
2	MC3	B	505	-	10,10,45	0.36	0	9,9,53	0.84	0
2	MC3	A	506	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	D	519	-	7,7,45	0.37	0	6,6,53	0.76	0
2	MC3	G	508	-	4,4,45	0.37	0	3,3,53	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	H	520	-	9,9,45	0.34	0	8,8,53	0.79	0
2	MC3	K	512	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	A	513	-	12,12,45	0.36	0	11,11,53	0.86	0
2	MC3	B	509	-	10,10,45	0.35	0	9,9,53	0.83	0
2	MC3	F	512	-	9,9,45	0.36	0	8,8,53	0.80	0
2	MC3	H	506	-	10,10,45	0.34	0	9,9,53	0.81	0
2	MC3	D	503	-	11,11,45	0.36	0	10,10,53	0.85	0
2	MC3	D	509	-	10,10,45	0.35	0	9,9,53	0.83	0
2	MC3	J	523	-	7,7,45	0.35	0	6,6,53	0.74	0
2	MC3	H	521	-	11,11,45	0.34	0	10,10,53	0.84	0
2	MC3	L	501	-	24,24,45	0.52	0	27,29,53	0.72	1 (3%)
2	MC3	E	513	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	F	519	-	7,7,45	0.37	0	6,6,53	0.76	0
2	MC3	J	503	-	10,10,45	0.32	0	9,9,53	0.80	0
2	MC3	D	508	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	J	514	-	8,8,45	0.35	0	7,7,53	0.79	0
2	MC3	L	502	-	12,12,45	0.31	0	11,11,53	0.83	0
2	MC3	I	510	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	B	516	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	A	519	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	C	514	-	8,8,45	0.36	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	F	509	-	10,10,45	0.36	0	9,9,53	0.83	0
2	MC3	D	510	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	H	510	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	B	519	-	7,7,45	0.37	0	6,6,53	0.76	0
2	MC3	C	501	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	H	513	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	A	504	-	9,9,45	0.35	0	8,8,53	0.80	0
2	MC3	H	502	-	24,24,45	0.83	1 (4%)	27,29,53	1.26	2 (7%)
2	MC3	D	518	-	9,9,45	0.35	0	8,8,53	0.82	0
2	MC3	D	516	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	J	505	-	11,11,45	0.33	0	10,10,53	0.82	0
2	MC3	D	513	-	12,12,45	0.35	0	11,11,53	0.84	0
2	MC3	K	517	-	11,11,45	0.33	0	10,10,53	0.84	0
2	MC3	K	523	-	7,7,45	0.35	0	6,6,53	0.74	0
2	MC3	C	502	-	12,12,45	0.36	0	11,11,53	0.86	0
2	MC3	E	514	-	8,8,45	0.36	0	7,7,53	0.79	0
2	MC3	I	512	-	7,7,45	0.36	0	6,6,53	0.76	0
2	MC3	H	501	-	8,8,45	0.24	0	7,7,53	0.19	0
2	MC3	D	512	-	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MC3	I	514	-	8,8,45	0.35	0	7,7,53	0.79	0
2	MC3	C	508	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	K	508	-	4,4,45	0.37	0	3,3,53	0.58	0
2	MC3	G	513	-	9,9,45	0.35	0	8,8,53	0.81	0
2	MC3	F	508	-	7,7,45	0.36	0	6,6,53	0.75	0
2	MC3	E	511	-	11,11,45	0.35	0	10,10,53	0.85	0
2	MC3	I	505	-	11,11,45	0.33	0	10,10,53	0.82	0
2	MC3	A	510	-	9,9,45	0.36	0	8,8,53	0.82	0
2	MC3	L	521	-	7,7,45	0.35	0	6,6,53	0.75	0
2	MC3	C	513	-	12,12,45	0.35	0	11,11,53	0.84	0
2	MC3	L	522	-	9,9,45	0.34	0	8,8,53	0.81	0
2	MC3	E	501	-	12,12,45	0.35	0	11,11,53	0.86	0
2	MC3	I	509	-	11,11,45	0.34	0	10,10,53	0.83	0
2	MC3	F	513	-	12,12,45	0.35	0	11,11,53	0.85	0
2	MC3	B	518	-	9,9,45	0.35	0	8,8,53	0.82	0
2	MC3	B	504	-	9,9,45	0.36	0	8,8,53	0.81	0
2	MC3	I	516	-	12,12,45	0.31	0	11,11,53	0.83	0
2	MC3	A	512	-	12,12,45	0.35	0	11,11,53	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	H	523	-	-	0/5/5/49	-
2	MC3	L	515	-	-	0/8/8/49	-
2	MC3	G	505	-	-	0/9/9/49	-
2	MC3	D	517	-	-	0/3/3/49	-
2	MC3	E	505	-	-	0/8/8/49	-
2	MC3	H	507	-	-	0/10/10/49	-
2	MC3	B	515	-	-	0/8/8/49	-
2	MC3	J	521	-	-	0/9/9/49	-
2	MC3	L	514	-	-	0/9/9/49	-
2	MC3	L	519	-	-	0/9/9/49	-
2	MC3	A	511	-	-	0/5/5/49	-
2	MC3	J	519	-	-	0/10/10/49	-
2	MC3	C	509	-	-	0/8/8/49	-
2	MC3	J	520	-	-	0/7/7/49	-
2	MC3	I	513	-	-	0/7/7/49	-
2	MC3	L	506	-	-	0/7/7/49	-
2	MC3	J	515	-	-	11/26/26/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	I	503	-	-	0/8/8/49	-
2	MC3	J	504	-	-	0/10/10/49	-
2	MC3	E	516	-	-	0/7/7/49	-
2	MC3	L	511	-	-	9/26/26/49	-
2	MC3	L	513	-	-	0/10/10/49	-
2	MC3	C	515	-	-	0/8/8/49	-
2	MC3	D	502	-	-	0/10/10/49	-
2	MC3	F	516	-	-	0/7/7/49	-
2	MC3	E	519	-	-	0/5/5/49	-
2	MC3	D	515	-	-	0/8/8/49	-
2	MC3	J	522	-	-	0/6/6/49	-
2	MC3	A	503	-	-	0/9/9/49	-
2	MC3	G	515	-	-	11/26/26/49	-
2	MC3	G	517	-	-	0/9/9/49	-
2	MC3	G	523	-	-	0/5/5/49	-
2	MC3	E	503	-	-	0/9/9/49	-
2	MC3	K	515	-	-	10/26/26/49	-
2	MC3	B	508	-	-	0/5/5/49	-
2	MC3	E	502	-	-	0/10/10/49	-
2	MC3	H	503	-	-	0/8/8/49	-
2	MC3	H	514	-	-	0/6/6/49	-
2	MC3	F	515	-	-	0/8/8/49	-
2	MC3	F	517	-	-	0/3/3/49	-
2	MC3	C	505	-	-	0/8/8/49	-
2	MC3	I	504	-	-	0/10/10/49	-
2	MC3	J	506	-	-	0/8/8/49	-
2	MC3	C	516	-	-	0/7/7/49	-
2	MC3	J	516	-	-	0/10/10/49	-
2	MC3	L	518	-	-	0/9/9/49	-
2	MC3	B	510	-	-	0/10/10/49	-
2	MC3	B	513	-	-	0/10/10/49	-
2	MC3	I	507	-	-	0/10/10/49	-
2	MC3	C	511	-	-	0/9/9/49	-
2	MC3	D	506	-	-	0/6/6/49	-
2	MC3	J	501	-	-	1/6/6/49	-
2	MC3	J	518	-	-	0/10/10/49	-
2	MC3	H	509	-	-	0/9/9/49	-
2	MC3	J	502	-	-	9/26/26/49	-
2	MC3	B	501	-	-	0/10/10/49	-
2	MC3	G	504	-	-	0/10/10/49	-
2	MC3	K	511	-	-	0/8/8/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	G	501	-	-	1/6/6/49	-
2	MC3	D	511	-	-	0/9/9/49	-
2	MC3	G	518	-	-	0/10/10/49	-
2	MC3	F	511	-	-	0/9/9/49	-
2	MC3	J	510	-	-	0/9/9/49	-
2	MC3	J	511	-	-	0/8/8/49	-
2	MC3	L	505	-	-	0/10/10/49	-
2	MC3	B	502	-	-	0/10/10/49	-
2	MC3	E	518	-	-	0/7/7/49	-
2	MC3	K	514	-	-	0/6/6/49	-
2	MC3	L	509	-	-	0/5/5/49	-
2	MC3	K	501	-	-	1/6/6/49	-
2	MC3	E	506	-	-	0/6/6/49	-
2	MC3	I	520	-	-	0/7/7/49	-
2	MC3	C	506	-	-	0/6/6/49	-
2	MC3	J	513	-	-	0/7/7/49	-
2	MC3	K	506	-	-	0/8/8/49	-
2	MC3	D	501	-	-	0/10/10/49	-
2	MC3	H	512	-	-	0/5/5/49	-
2	MC3	L	523	-	-	0/6/6/49	-
2	MC3	F	503	-	-	0/9/9/49	-
2	MC3	I	519	-	-	0/10/10/49	-
2	MC3	I	521	-	-	0/9/9/49	-
2	MC3	G	511	-	-	0/8/8/49	-
2	MC3	D	507	-	-	0/7/7/49	-
2	MC3	I	508	-	-	0/2/2/49	-
2	MC3	C	510	-	-	0/10/10/49	-
2	MC3	F	501	-	-	0/10/10/49	-
2	MC3	G	512	-	-	0/5/5/49	-
2	MC3	C	519	-	-	0/5/5/49	-
2	MC3	E	517	-	-	0/3/3/49	-
2	MC3	A	515	-	-	0/7/7/49	-
2	MC3	K	520	-	-	0/7/7/49	-
2	MC3	L	516	-	-	0/10/10/49	-
2	MC3	F	502	-	-	0/10/10/49	-
2	MC3	G	521	-	-	0/9/9/49	-
2	MC3	K	504	-	-	0/10/10/49	-
2	MC3	A	517	-	-	0/6/6/49	-
2	MC3	C	512	-	-	0/7/7/49	-
2	MC3	C	504	-	-	0/7/7/49	-
2	MC3	B	512	-	-	0/7/7/49	-
2	MC3	D	514	-	-	0/6/6/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	I	523	-	-	0/5/5/49	-
2	MC3	J	509	-	-	0/9/9/49	-
2	MC3	H	504	-	-	0/10/10/49	-
2	MC3	K	521	-	-	0/9/9/49	-
2	MC3	H	517	-	-	0/9/9/49	-
2	MC3	K	522	-	-	0/6/6/49	-
2	MC3	D	505	-	-	0/8/8/49	-
2	MC3	G	509	-	-	0/9/9/49	-
2	MC3	H	522	-	-	0/6/6/49	-
2	MC3	I	501	-	-	1/6/6/49	-
2	MC3	H	505	-	-	0/9/9/49	-
2	MC3	H	508	-	-	0/2/2/49	-
2	MC3	K	505	-	-	0/9/9/49	-
2	MC3	J	508	-	-	0/2/2/49	-
2	MC3	L	520	-	-	0/8/8/49	-
2	MC3	F	505	-	-	0/8/8/49	-
2	MC3	K	509	-	-	0/9/9/49	-
2	MC3	A	514	-	-	0/9/9/49	-
2	MC3	I	502	-	-	9/26/26/49	-
2	MC3	G	516	-	-	0/10/10/49	-
2	MC3	J	517	-	-	0/9/9/49	-
2	MC3	A	501	-	-	0/8/8/49	-
2	MC3	L	510	-	-	1/6/6/49	-
2	MC3	C	517	-	-	0/3/3/49	-
2	MC3	B	517	-	-	0/3/3/49	-
2	MC3	G	519	-	-	0/10/10/49	-
2	MC3	K	516	-	-	0/10/10/49	-
2	MC3	B	506	-	-	0/6/6/49	-
2	MC3	A	518	-	-	0/7/7/49	-
2	MC3	A	502	-	-	0/10/10/49	-
2	MC3	E	508	-	-	0/5/5/49	-
2	MC3	H	515	-	-	10/26/26/49	-
2	MC3	A	507	-	-	0/8/8/49	-
2	MC3	C	503	-	-	0/9/9/49	-
2	MC3	I	518	-	-	0/10/10/49	-
2	MC3	H	518	-	-	0/10/10/49	-
2	MC3	L	504	-	-	0/10/10/49	-
2	MC3	G	502	-	-	9/26/26/49	-
2	MC3	A	508	-	-	0/7/7/49	-
2	MC3	L	507	-	-	0/9/9/49	-
2	MC3	D	504	-	-	0/7/7/49	-
2	MC3	H	519	-	-	0/10/10/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	I	517	-	-	0/9/9/49	-
2	MC3	K	502	-	-	9/26/26/49	-
2	MC3	F	506	-	-	0/6/6/49	-
2	MC3	B	507	-	-	0/7/7/49	-
2	MC3	E	515	-	-	0/8/8/49	-
2	MC3	K	513	-	-	0/7/7/49	-
2	MC3	H	511	-	-	0/8/8/49	-
2	MC3	L	508	-	-	0/6/6/49	-
2	MC3	I	522	-	-	0/6/6/49	-
2	MC3	L	512	-	-	0/8/8/49	-
2	MC3	B	511	-	-	0/9/9/49	-
2	MC3	G	506	-	-	0/8/8/49	-
2	MC3	G	520	-	-	0/7/7/49	-
2	MC3	J	507	-	-	0/10/10/49	-
2	MC3	C	507	-	-	0/7/7/49	-
2	MC3	G	514	-	-	0/6/6/49	-
2	MC3	E	504	-	-	0/7/7/49	-
2	MC3	F	510	-	-	0/10/10/49	-
2	MC3	E	509	-	-	0/8/8/49	-
2	MC3	K	503	-	-	0/8/8/49	-
2	MC3	I	515	-	-	18/26/26/49	-
2	MC3	F	514	-	-	0/6/6/49	-
2	MC3	K	519	-	-	0/10/10/49	-
2	MC3	G	522	-	-	0/6/6/49	-
2	MC3	E	507	-	-	0/7/7/49	-
2	MC3	A	505	-	-	0/10/10/49	-
2	MC3	G	503	-	-	0/8/8/49	-
2	MC3	F	504	-	-	0/7/7/49	-
2	MC3	A	509	-	-	0/3/3/49	-
2	MC3	L	517	-	-	0/2/2/49	-
2	MC3	F	518	-	-	0/7/7/49	-
2	MC3	K	507	-	-	0/10/10/49	-
2	MC3	J	512	-	-	0/5/5/49	-
2	MC3	F	507	-	-	0/7/7/49	-
2	MC3	A	516	-	-	0/8/8/49	-
2	MC3	L	503	-	-	0/9/9/49	-
2	MC3	G	510	-	-	0/9/9/49	-
2	MC3	I	506	-	-	0/8/8/49	-
2	MC3	I	511	-	-	0/8/8/49	-
2	MC3	H	516	-	-	0/10/10/49	-
2	MC3	K	510	-	-	0/9/9/49	-
2	MC3	B	503	-	-	0/9/9/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	E	512	-	-	0/7/7/49	-
2	MC3	C	518	-	-	0/7/7/49	-
2	MC3	K	518	-	-	0/10/10/49	-
2	MC3	G	507	-	-	0/10/10/49	-
2	MC3	B	505	-	-	0/8/8/49	-
2	MC3	A	506	-	-	0/6/6/49	-
2	MC3	D	519	-	-	0/5/5/49	-
2	MC3	G	508	-	-	0/2/2/49	-
2	MC3	H	520	-	-	0/7/7/49	-
2	MC3	K	512	-	-	0/5/5/49	-
2	MC3	A	513	-	-	0/10/10/49	-
2	MC3	B	509	-	-	0/8/8/49	-
2	MC3	F	512	-	-	0/7/7/49	-
2	MC3	H	506	-	-	0/8/8/49	-
2	MC3	D	503	-	-	0/9/9/49	-
2	MC3	D	509	-	-	0/8/8/49	-
2	MC3	J	523	-	-	0/5/5/49	-
2	MC3	H	521	-	-	0/9/9/49	-
2	MC3	L	501	-	-	16/26/26/49	-
2	MC3	E	513	-	-	0/10/10/49	-
2	MC3	F	519	-	-	0/5/5/49	-
2	MC3	J	503	-	-	0/8/8/49	-
2	MC3	D	508	-	-	0/5/5/49	-
2	MC3	J	514	-	-	0/6/6/49	-
2	MC3	L	502	-	-	0/10/10/49	-
2	MC3	I	510	-	-	0/9/9/49	-
2	MC3	B	516	-	-	0/7/7/49	-
2	MC3	A	519	-	-	0/5/5/49	-
2	MC3	C	514	-	-	0/6/6/49	-
2	MC3	B	514	-	-	0/6/6/49	-
2	MC3	F	509	-	-	0/8/8/49	-
2	MC3	D	510	-	-	0/10/10/49	-
2	MC3	H	510	-	-	0/9/9/49	-
2	MC3	B	519	-	-	0/5/5/49	-
2	MC3	C	501	-	-	0/10/10/49	-
2	MC3	H	513	-	-	0/7/7/49	-
2	MC3	A	504	-	-	0/7/7/49	-
2	MC3	H	502	-	-	9/26/26/49	-
2	MC3	D	518	-	-	0/7/7/49	-
2	MC3	D	516	-	-	0/7/7/49	-
2	MC3	J	505	-	-	0/9/9/49	-
2	MC3	D	513	-	-	0/10/10/49	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	K	517	-	-	0/9/9/49	-
2	MC3	K	523	-	-	0/5/5/49	-
2	MC3	C	502	-	-	0/10/10/49	-
2	MC3	E	514	-	-	0/6/6/49	-
2	MC3	I	512	-	-	0/5/5/49	-
2	MC3	H	501	-	-	1/6/6/49	-
2	MC3	D	512	-	-	0/7/7/49	-
2	MC3	E	510	-	-	0/10/10/49	-
2	MC3	I	514	-	-	0/6/6/49	-
2	MC3	C	508	-	-	0/5/5/49	-
2	MC3	K	508	-	-	0/2/2/49	-
2	MC3	G	513	-	-	0/7/7/49	-
2	MC3	F	508	-	-	0/5/5/49	-
2	MC3	E	511	-	-	0/9/9/49	-
2	MC3	I	505	-	-	0/9/9/49	-
2	MC3	A	510	-	-	0/7/7/49	-
2	MC3	L	521	-	-	0/5/5/49	-
2	MC3	C	513	-	-	0/10/10/49	-
2	MC3	L	522	-	-	0/7/7/49	-
2	MC3	E	501	-	-	0/10/10/49	-
2	MC3	I	509	-	-	0/9/9/49	-
2	MC3	F	513	-	-	0/10/10/49	-
2	MC3	B	518	-	-	0/7/7/49	-
2	MC3	B	504	-	-	0/7/7/49	-
2	MC3	I	516	-	-	0/10/10/49	-
2	MC3	A	512	-	-	0/10/10/49	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	511	MC3	P-O4P	2.85	1.65	1.54
2	G	502	MC3	P-O4P	2.84	1.65	1.54
2	H	502	MC3	P-O4P	2.84	1.65	1.54
2	K	502	MC3	P-O4P	2.84	1.65	1.54
2	I	502	MC3	P-O4P	2.83	1.65	1.54
2	J	502	MC3	P-O4P	2.83	1.65	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	502	MC3	O4P-P-O3P	-5.18	93.17	106.67
2	L	511	MC3	O4P-P-O3P	-5.17	93.19	106.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	502	MC3	O4P-P-O3P	-5.16	93.21	106.67
2	J	502	MC3	O4P-P-O3P	-5.16	93.22	106.67
2	I	502	MC3	O4P-P-O3P	-5.16	93.22	106.67
2	G	502	MC3	O4P-P-O3P	-5.15	93.24	106.67
2	H	502	MC3	O2P-P-O1P	2.29	119.75	110.83
2	L	511	MC3	O2P-P-O1P	2.29	119.75	110.83
2	K	502	MC3	O2P-P-O1P	2.28	119.73	110.83
2	I	502	MC3	O2P-P-O1P	2.28	119.71	110.83
2	G	502	MC3	O2P-P-O1P	2.28	119.71	110.83
2	J	502	MC3	O2P-P-O1P	2.28	119.71	110.83
2	I	515	MC3	O2P-P-O1P	2.23	119.53	110.83
2	L	501	MC3	O2P-P-O1P	2.23	119.52	110.83
2	K	515	MC3	O2P-P-O1P	2.21	119.44	110.83
2	H	515	MC3	O2P-P-O1P	2.18	119.33	110.83
2	J	515	MC3	O2P-P-O1P	2.18	119.33	110.83
2	G	515	MC3	O2P-P-O1P	2.18	119.33	110.83

There are no chirality outliers.

All (136) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	515	MC3	O3P-C1-C2-O2
2	G	515	MC3	C1-O3P-P-O4P
2	H	515	MC3	C1-O3P-P-O4P
2	I	515	MC3	C1-O3P-P-O1P
2	J	515	MC3	O3P-C1-C2-O2
2	J	515	MC3	C1-O3P-P-O4P
2	K	515	MC3	C1-O3P-P-O1P
2	L	501	MC3	C1-O3P-P-O1P
2	G	502	MC3	O11-C11-O3-C3
2	H	502	MC3	O11-C11-O3-C3
2	I	502	MC3	O11-C11-O3-C3
2	J	502	MC3	O11-C11-O3-C3
2	K	502	MC3	O11-C11-O3-C3
2	L	511	MC3	O11-C11-O3-C3
2	G	502	MC3	C12-C11-O3-C3
2	H	502	MC3	C12-C11-O3-C3
2	I	502	MC3	C12-C11-O3-C3
2	J	502	MC3	C12-C11-O3-C3
2	K	502	MC3	C12-C11-O3-C3
2	L	511	MC3	C12-C11-O3-C3
2	I	515	MC3	C12-C11-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	L	501	MC3	C12-C11-O3-C3
2	G	515	MC3	C11-C12-C13-C14
2	J	515	MC3	C11-C12-C13-C14
2	H	515	MC3	O3P-C1-C2-O2
2	I	515	MC3	O3P-C1-C2-O2
2	K	515	MC3	O3P-C1-C2-O2
2	L	501	MC3	O3P-C1-C2-O2
2	H	515	MC3	C11-C12-C13-C14
2	K	515	MC3	C11-C12-C13-C14
2	I	515	MC3	C11-C12-C13-C14
2	L	501	MC3	C11-C12-C13-C14
2	L	501	MC3	O11-C11-O3-C3
2	I	515	MC3	O11-C11-O3-C3
2	G	502	MC3	C32-C31-O2-C2
2	H	502	MC3	C32-C31-O2-C2
2	I	502	MC3	C32-C31-O2-C2
2	J	502	MC3	C32-C31-O2-C2
2	K	502	MC3	C32-C31-O2-C2
2	L	511	MC3	C32-C31-O2-C2
2	G	502	MC3	O31-C31-O2-C2
2	H	502	MC3	O31-C31-O2-C2
2	I	502	MC3	O31-C31-O2-C2
2	J	502	MC3	O31-C31-O2-C2
2	K	502	MC3	O31-C31-O2-C2
2	L	511	MC3	O31-C31-O2-C2
2	L	501	MC3	C12-C13-C14-C15
2	G	515	MC3	C12-C13-C14-C15
2	I	515	MC3	C12-C13-C14-C15
2	I	515	MC3	C1-C2-C3-O3
2	L	501	MC3	C1-C2-C3-O3
2	H	515	MC3	C12-C13-C14-C15
2	J	515	MC3	C12-C13-C14-C15
2	H	515	MC3	C33-C34-C35-C36
2	K	515	MC3	C12-C13-C14-C15
2	K	515	MC3	C33-C34-C35-C36
2	I	515	MC3	C33-C34-C35-C36
2	H	515	MC3	C31-C32-C33-C34
2	L	501	MC3	C33-C34-C35-C36
2	G	501	MC3	C17-C18-C19-C20
2	H	501	MC3	C17-C18-C19-C20
2	I	501	MC3	C17-C18-C19-C20
2	J	501	MC3	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	K	501	MC3	C17-C18-C19-C20
2	L	510	MC3	C17-C18-C19-C20
2	H	515	MC3	O3P-C1-C2-C3
2	I	515	MC3	O3P-C1-C2-C3
2	J	515	MC3	O3P-C1-C2-C3
2	L	501	MC3	O3P-C1-C2-C3
2	G	515	MC3	C1-O3P-P-O1P
2	H	515	MC3	C1-O3P-P-O1P
2	J	515	MC3	C1-O3P-P-O1P
2	G	502	MC3	C34-C35-C36-C37
2	H	502	MC3	C34-C35-C36-C37
2	I	502	MC3	C34-C35-C36-C37
2	J	502	MC3	C34-C35-C36-C37
2	K	502	MC3	C34-C35-C36-C37
2	L	511	MC3	C34-C35-C36-C37
2	I	515	MC3	C31-C32-C33-C34
2	L	501	MC3	C31-C32-C33-C34
2	H	515	MC3	C34-C35-C36-C37
2	G	515	MC3	O3P-C1-C2-C3
2	K	515	MC3	O3P-C1-C2-C3
2	G	502	MC3	C32-C33-C34-C35
2	H	502	MC3	C32-C33-C34-C35
2	I	502	MC3	C32-C33-C34-C35
2	J	502	MC3	C32-C33-C34-C35
2	K	502	MC3	C32-C33-C34-C35
2	L	511	MC3	C32-C33-C34-C35
2	G	515	MC3	C33-C34-C35-C36
2	K	515	MC3	C31-C32-C33-C34
2	J	515	MC3	C32-C33-C34-C35
2	K	515	MC3	C34-C35-C36-C37
2	I	515	MC3	C34-C35-C36-C37
2	L	501	MC3	C34-C35-C36-C37
2	I	515	MC3	C1-O3P-P-O4P
2	K	515	MC3	C1-O3P-P-O4P
2	L	501	MC3	C1-O3P-P-O4P
2	J	515	MC3	C33-C34-C35-C36
2	L	501	MC3	O2-C2-C3-O3
2	G	515	MC3	C32-C33-C34-C35
2	G	502	MC3	C31-C32-C33-C34
2	H	502	MC3	C31-C32-C33-C34
2	I	502	MC3	C31-C32-C33-C34
2	J	502	MC3	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

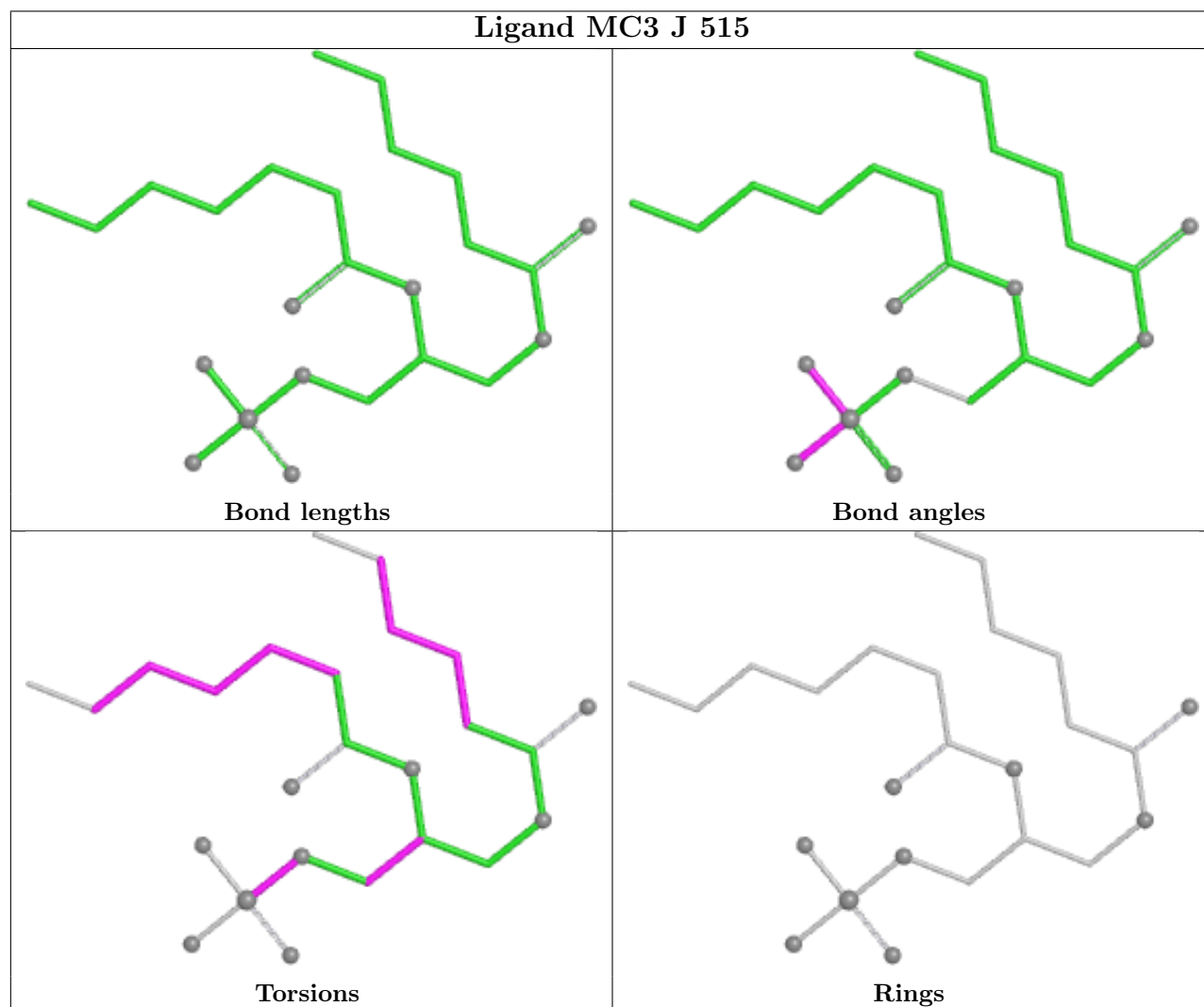
Mol	Chain	Res	Type	Atoms
2	K	502	MC3	C31-C32-C33-C34
2	G	502	MC3	O3P-C1-C2-O2
2	H	502	MC3	O3P-C1-C2-O2
2	I	502	MC3	O3P-C1-C2-O2
2	J	502	MC3	O3P-C1-C2-O2
2	K	502	MC3	O3P-C1-C2-O2
2	L	511	MC3	O3P-C1-C2-O2
2	L	511	MC3	C31-C32-C33-C34
2	L	501	MC3	C32-C33-C34-C35
2	I	515	MC3	O2-C2-C3-O3
2	K	515	MC3	C32-C33-C34-C35
2	I	515	MC3	C32-C33-C34-C35
2	I	515	MC3	C3-C2-O2-C31
2	L	501	MC3	C3-C2-O2-C31
2	G	515	MC3	C31-C32-C33-C34
2	G	515	MC3	C34-C35-C36-C37
2	H	515	MC3	C32-C33-C34-C35
2	G	502	MC3	O3P-C1-C2-C3
2	H	502	MC3	O3P-C1-C2-C3
2	I	502	MC3	O3P-C1-C2-C3
2	J	502	MC3	O3P-C1-C2-C3
2	K	502	MC3	O3P-C1-C2-C3
2	L	511	MC3	O3P-C1-C2-C3
2	G	515	MC3	C1-O3P-P-O2P
2	I	515	MC3	C1-C2-O2-C31
2	L	501	MC3	C1-C2-O2-C31
2	J	515	MC3	C34-C35-C36-C37
2	J	515	MC3	C13-C14-C15-C16
2	J	515	MC3	C31-C32-C33-C34
2	I	515	MC3	O31-C31-O2-C2
2	I	515	MC3	C32-C31-O2-C2

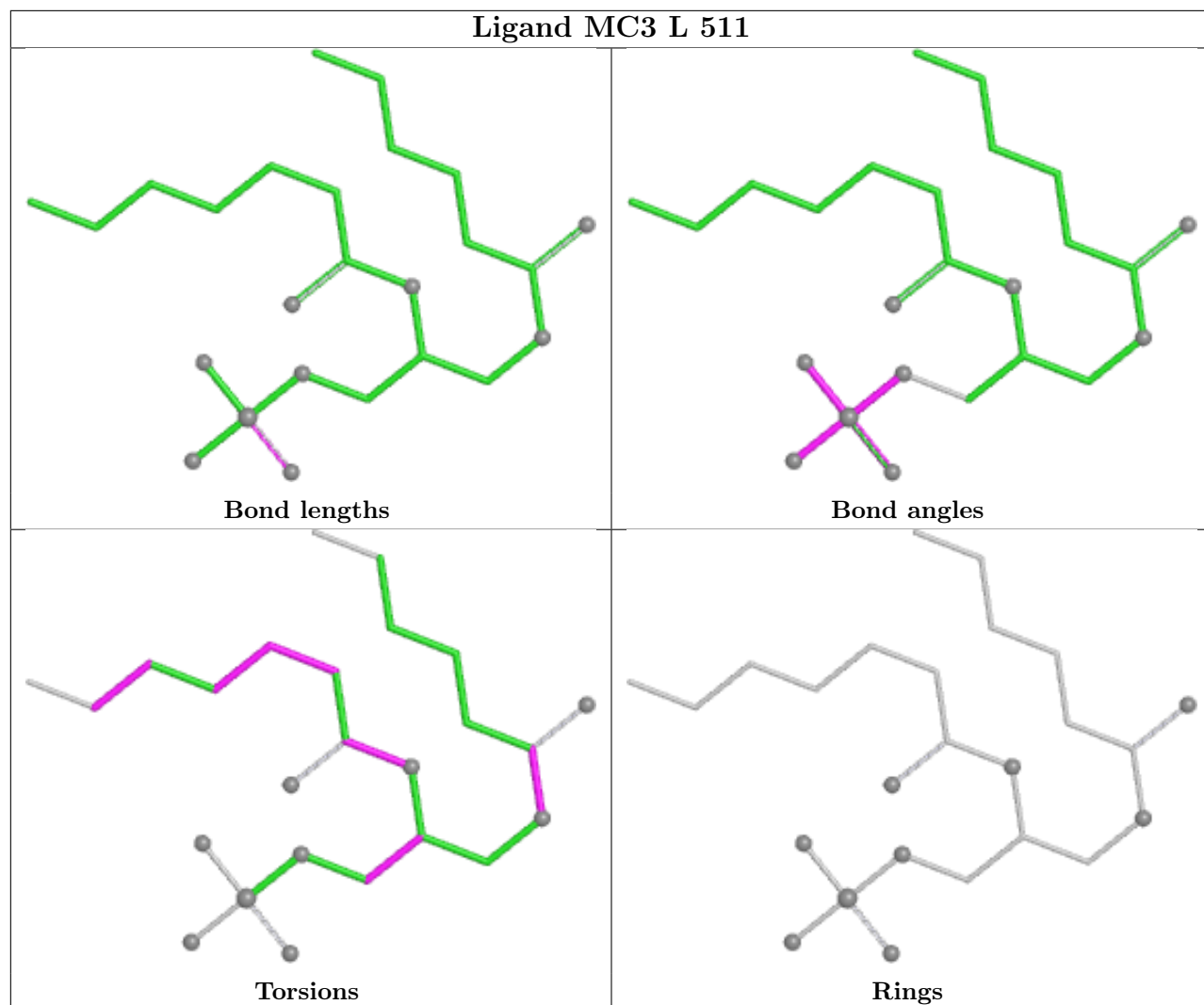
There are no ring outliers.

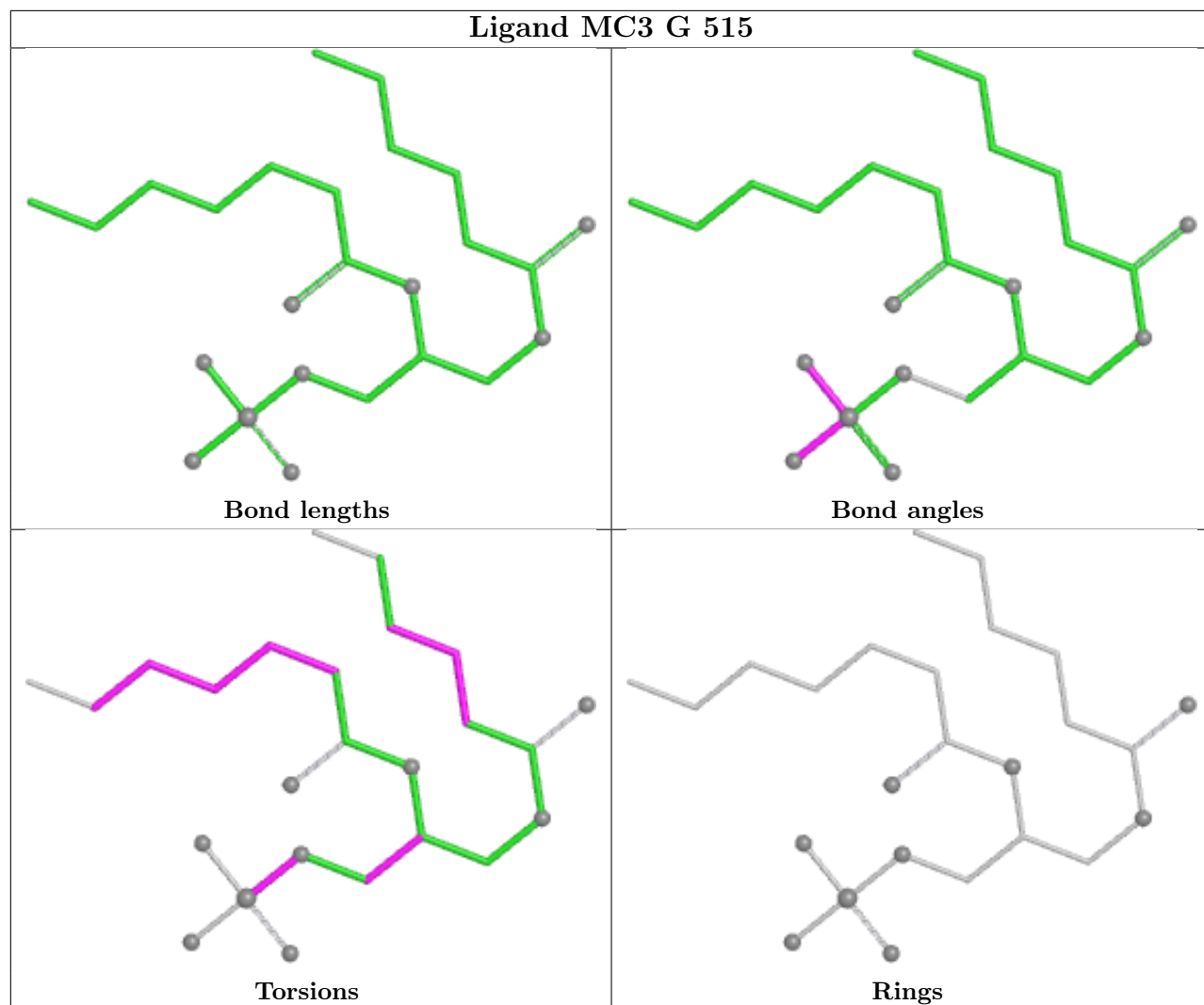
No monomer is involved in short contacts.

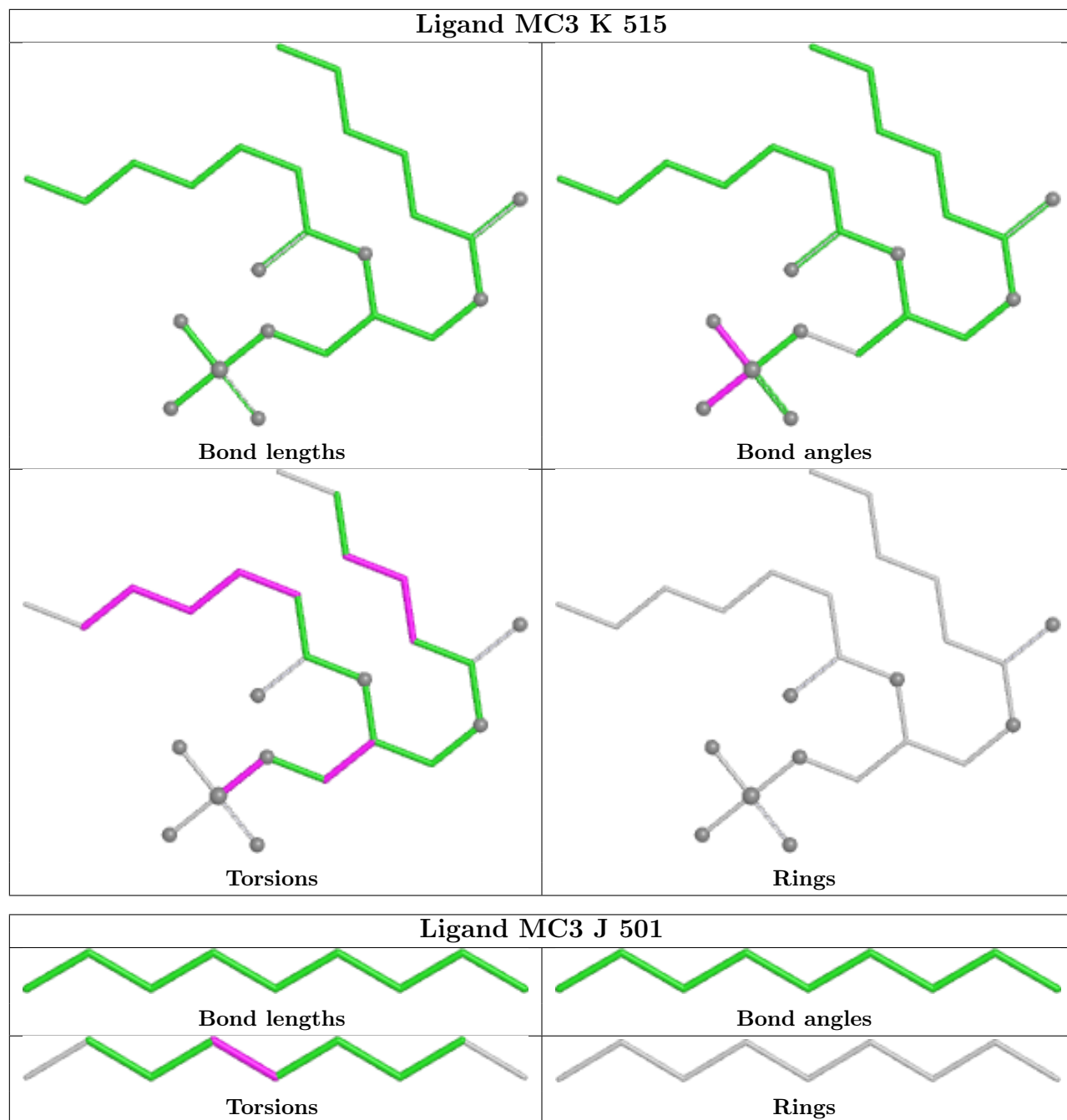
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

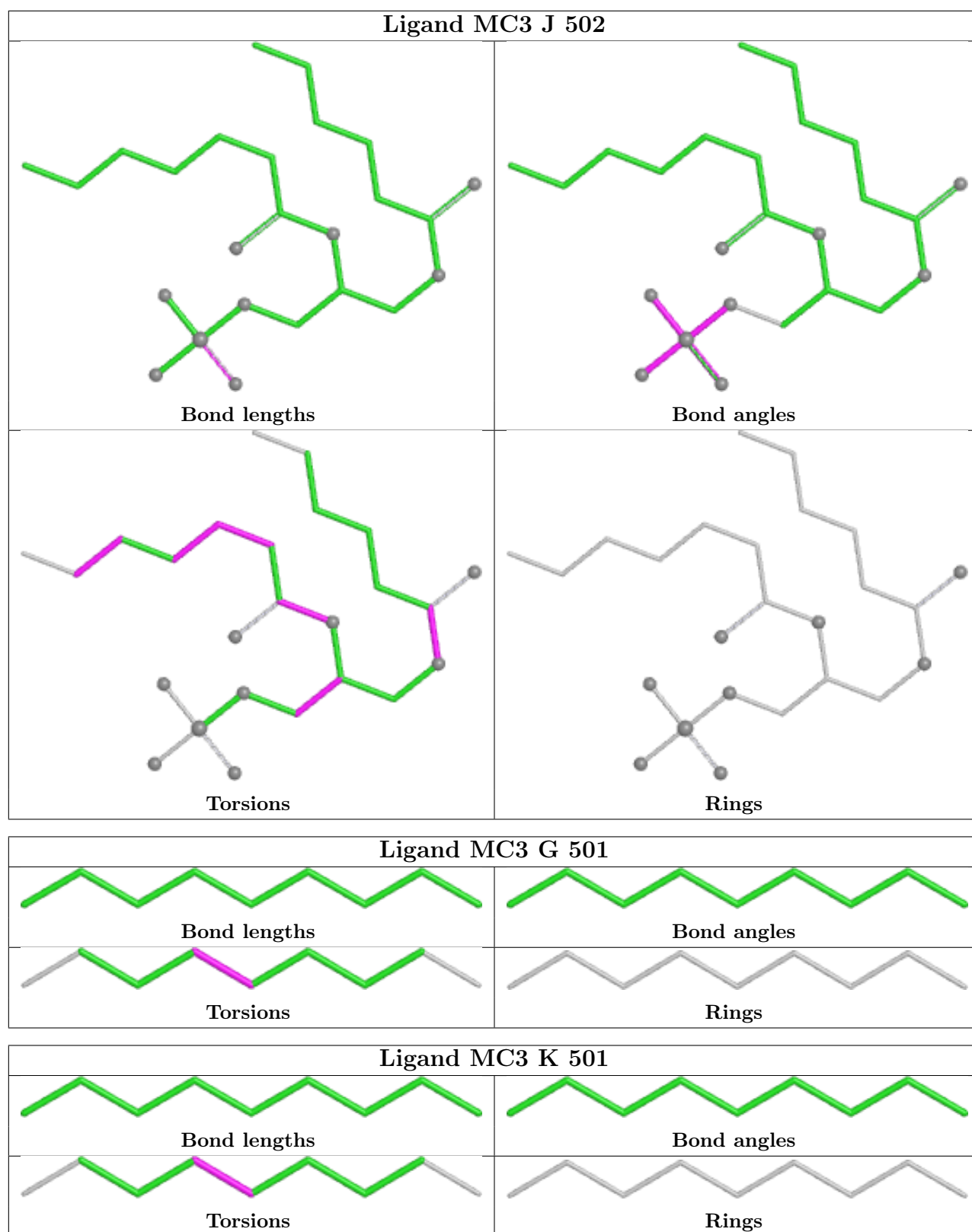
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

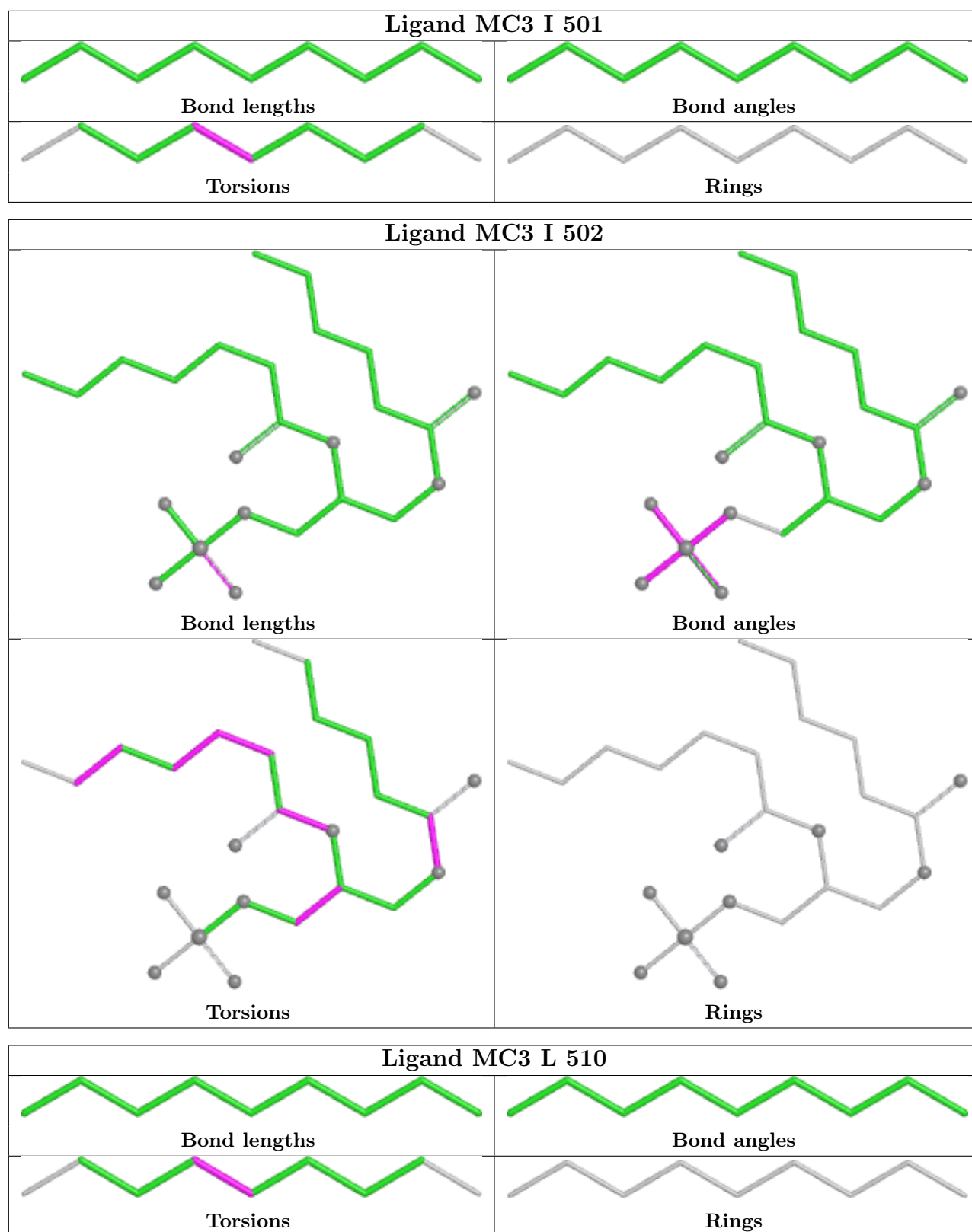


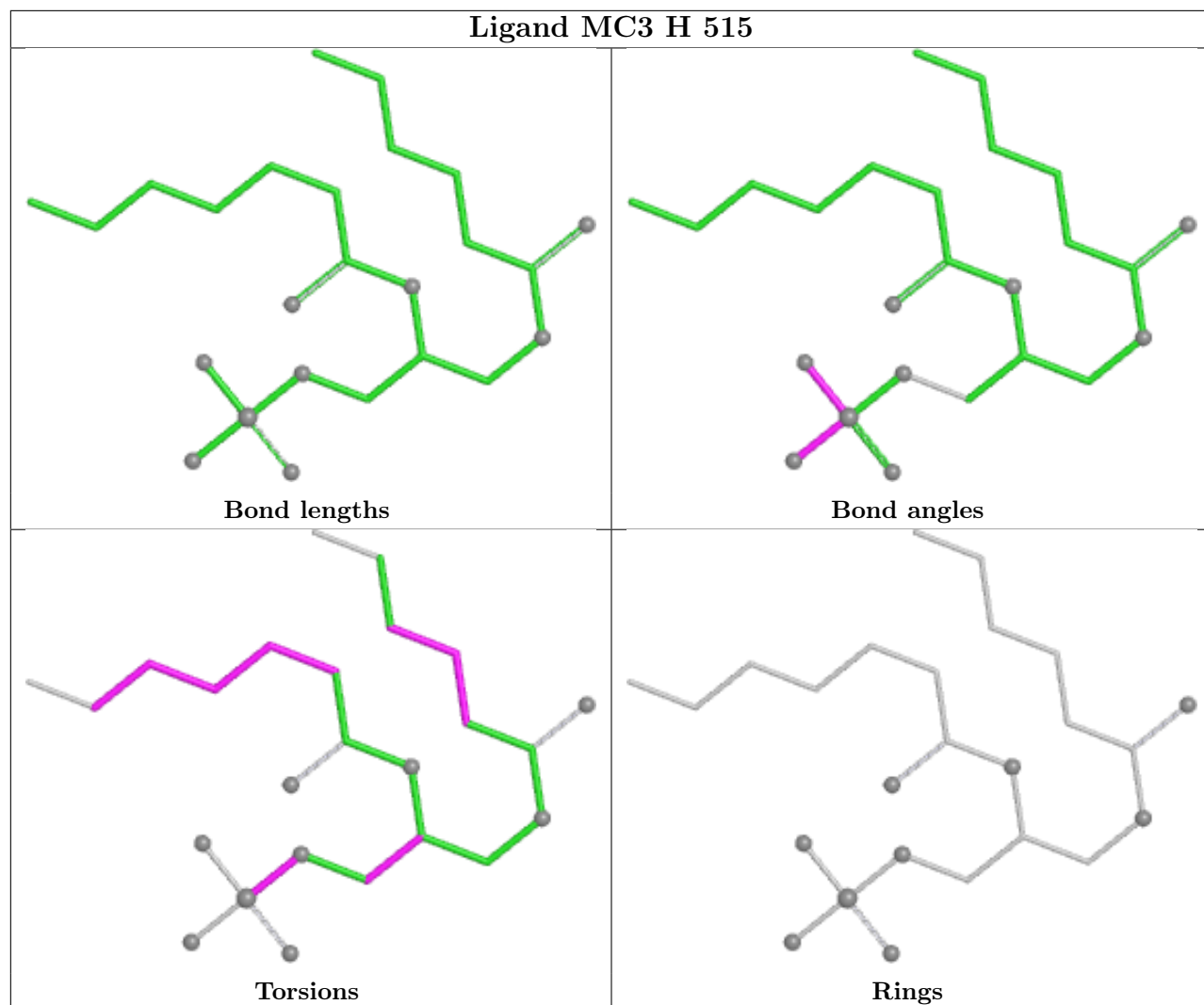


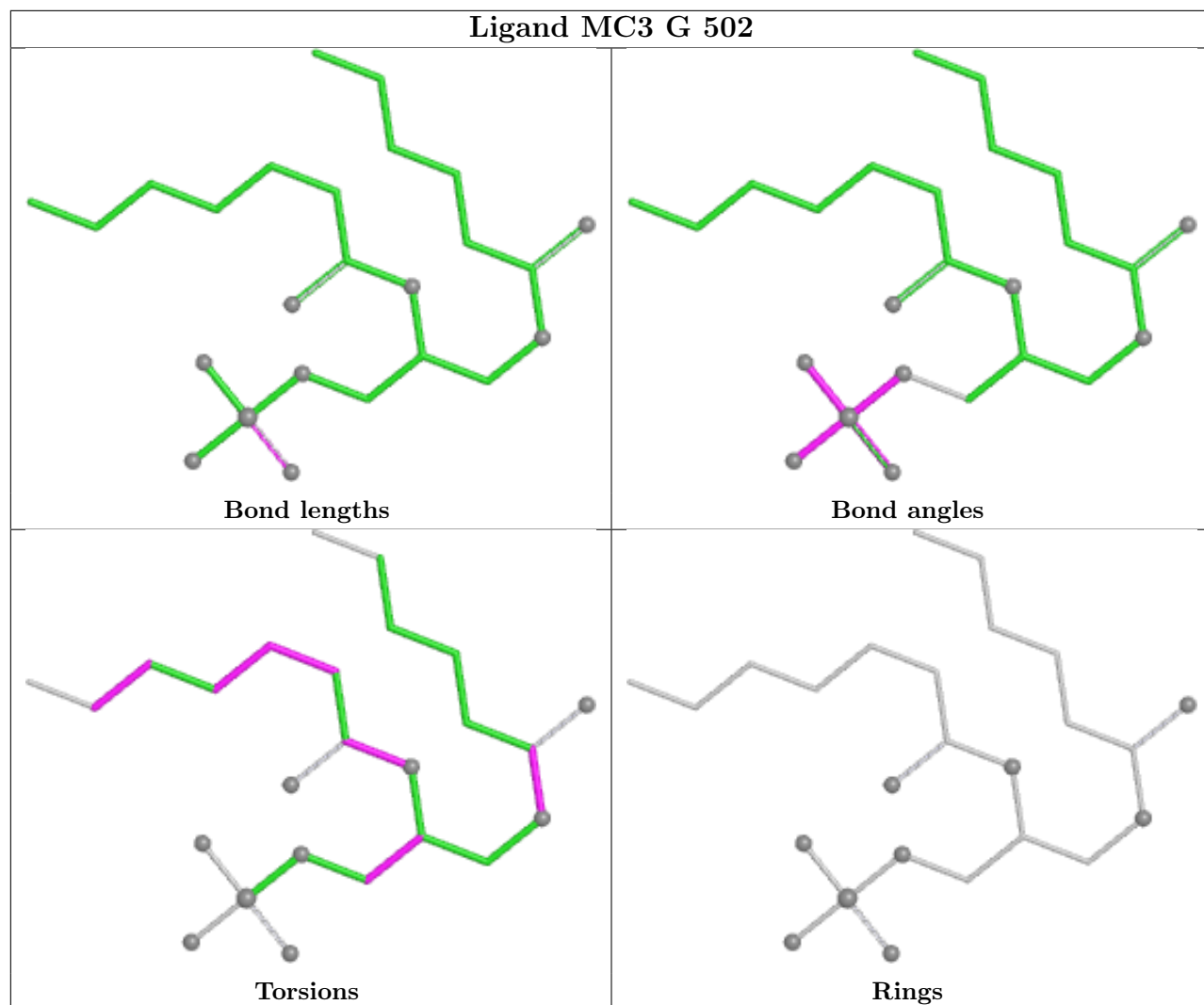


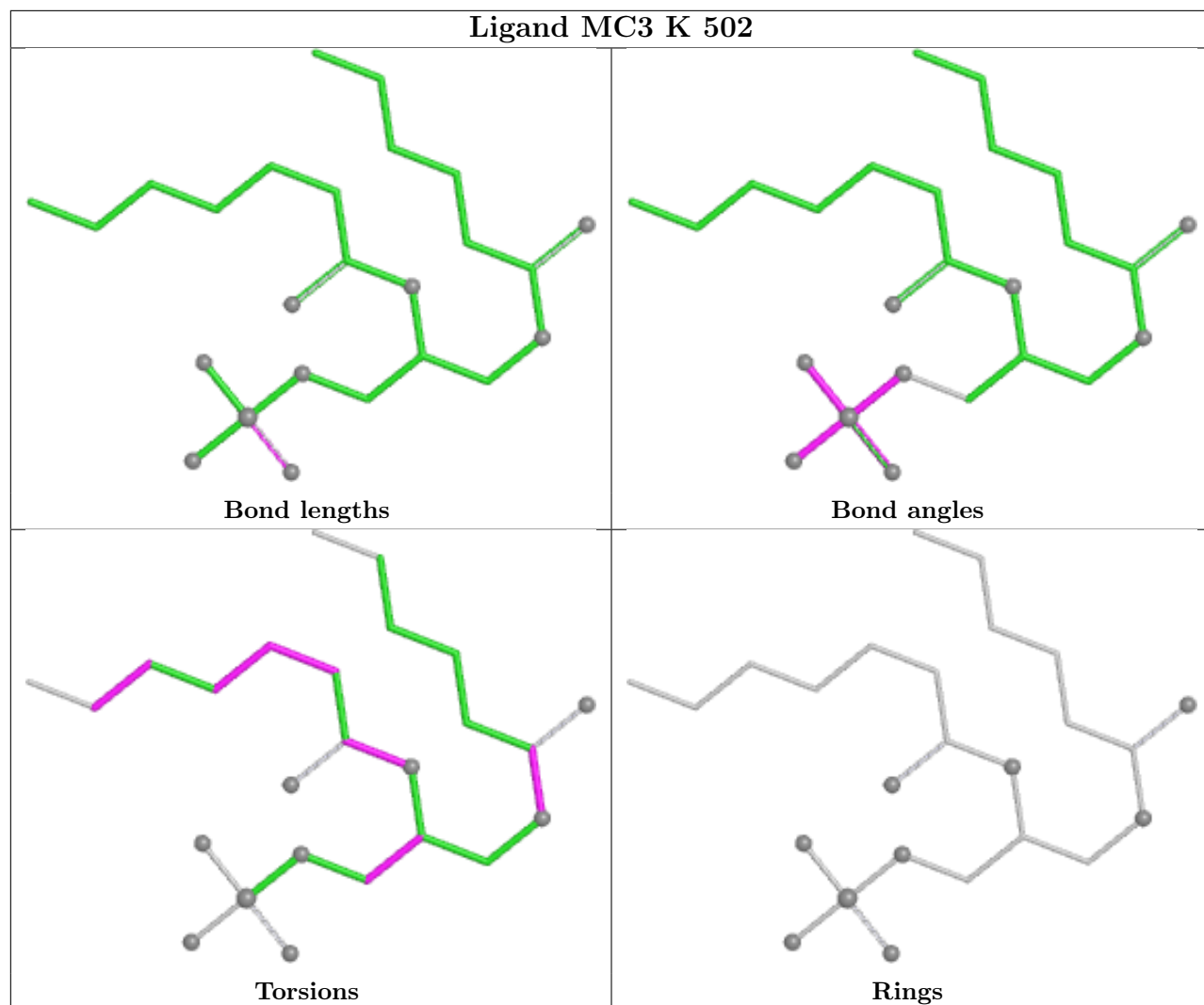




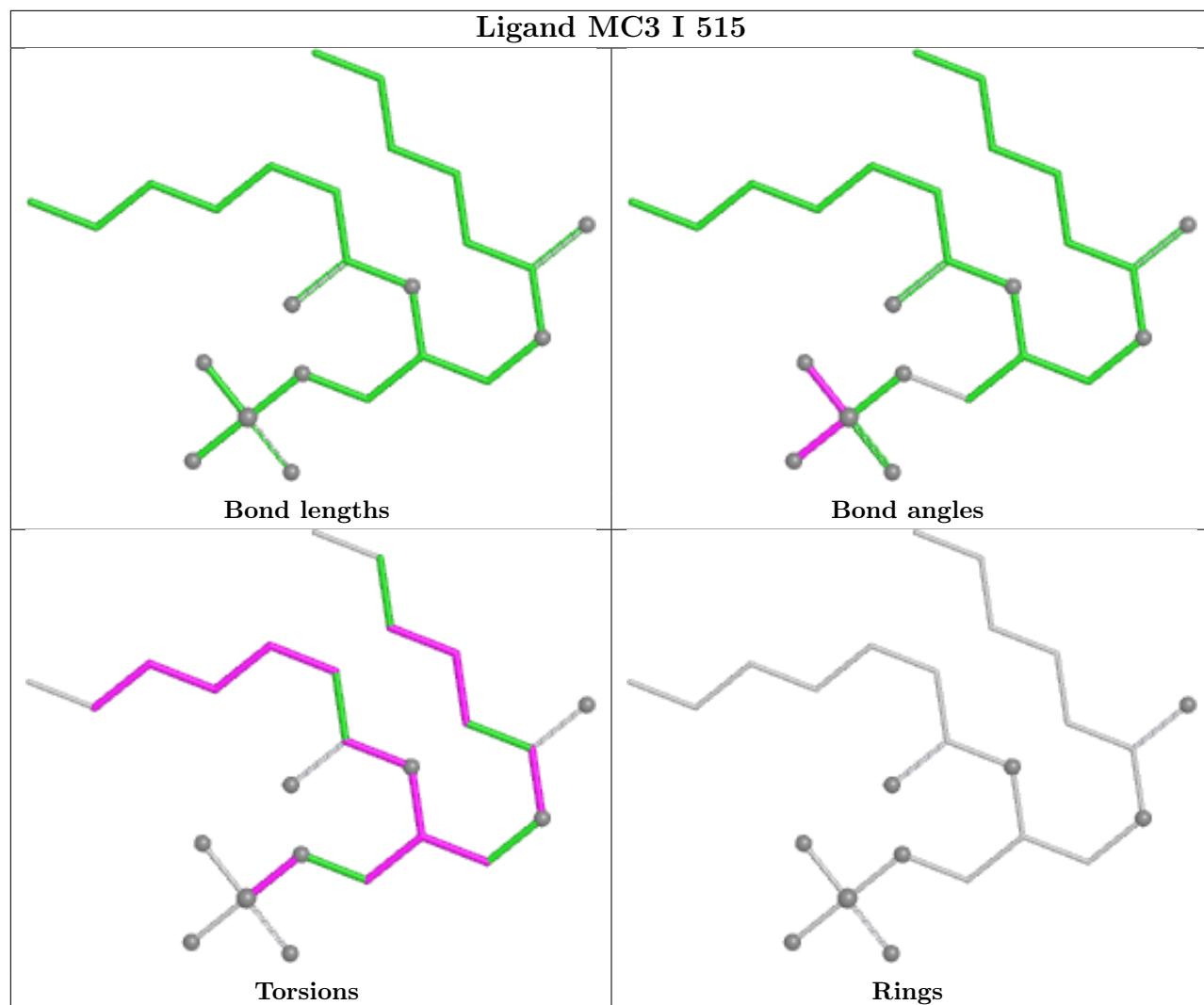


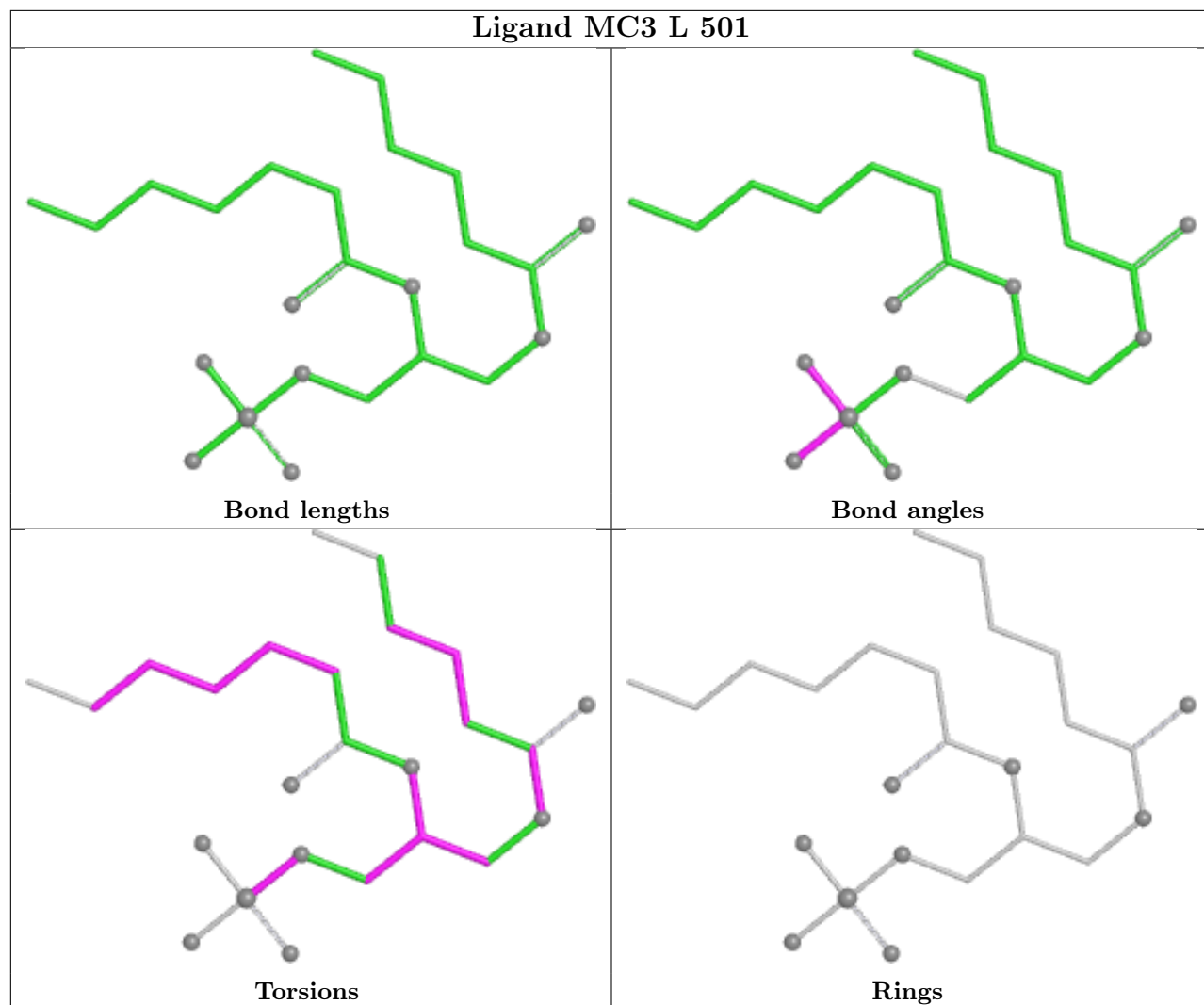


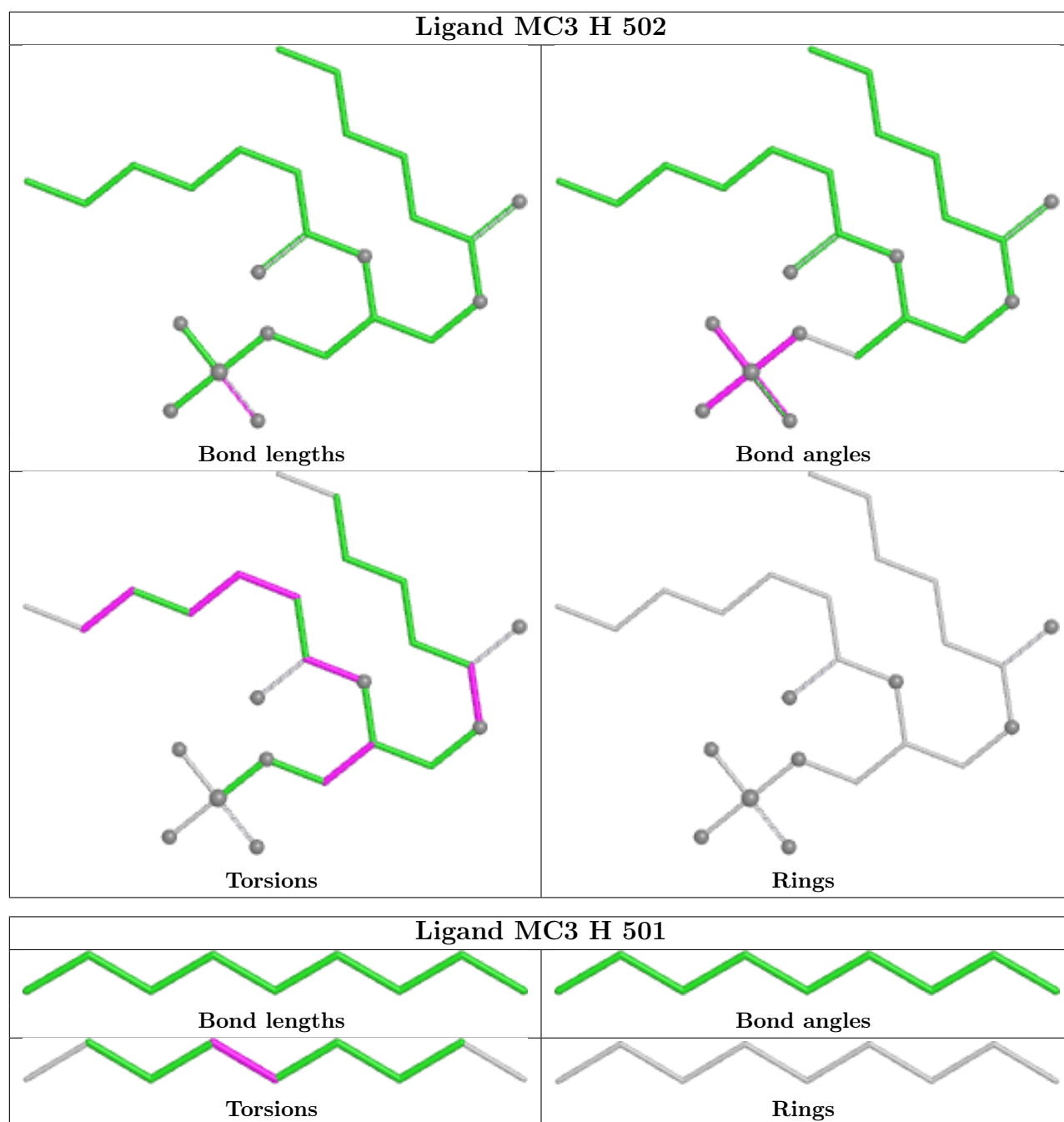




Ligand MC3 I 515







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.

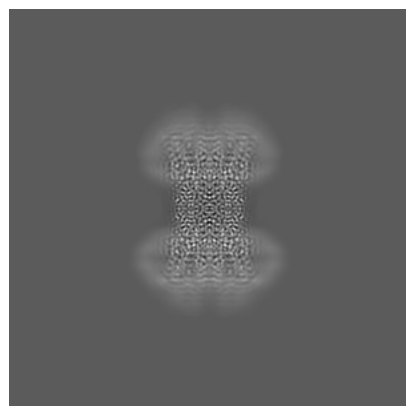
6 Map visualisation [i](#)

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.

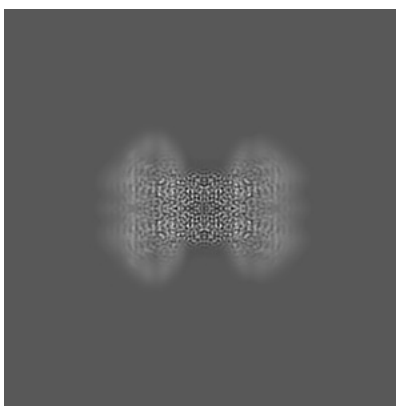
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

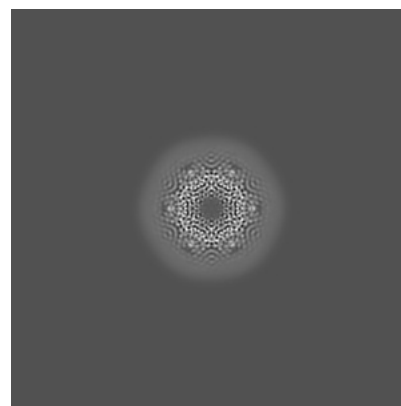
6.1.1 Primary map



X

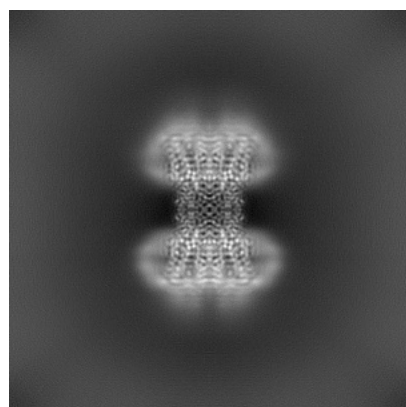


Y

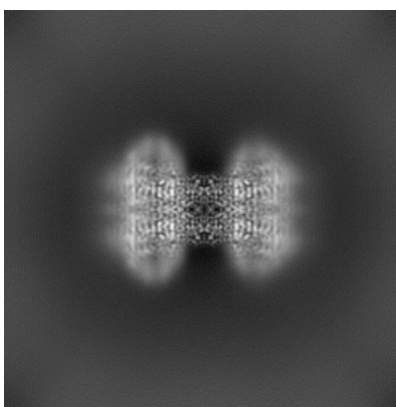


Z

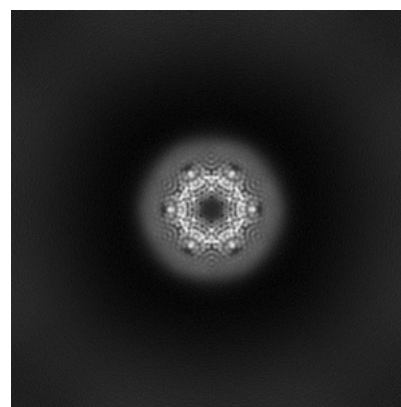
6.1.2 Raw map



X



Y

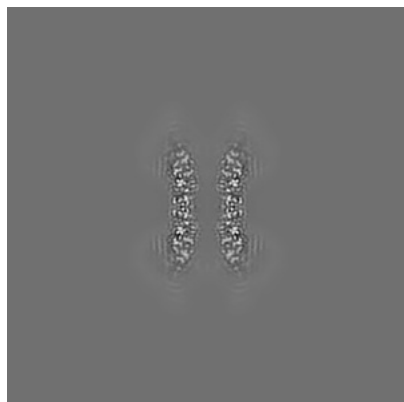


Z

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

6.2 Central slices [i](#)

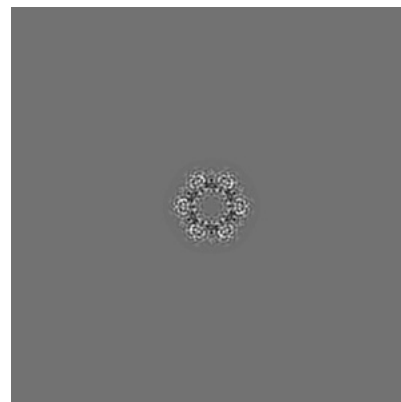
6.2.1 Primary map



X Index: 192

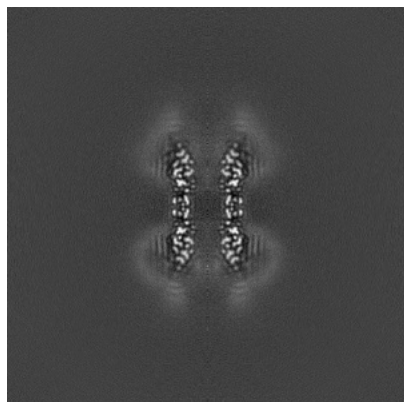


Y Index: 192

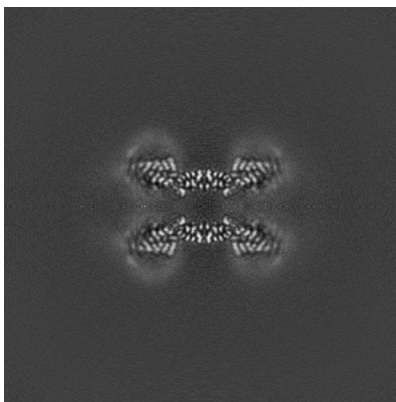


Z Index: 192

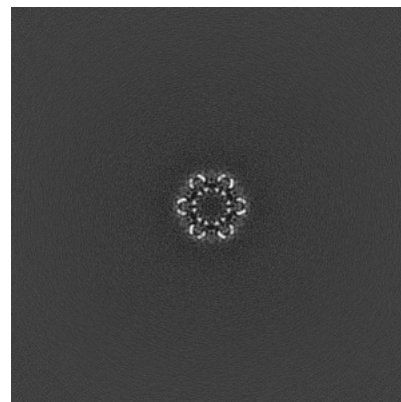
6.2.2 Raw map



X Index: 192



Y Index: 192

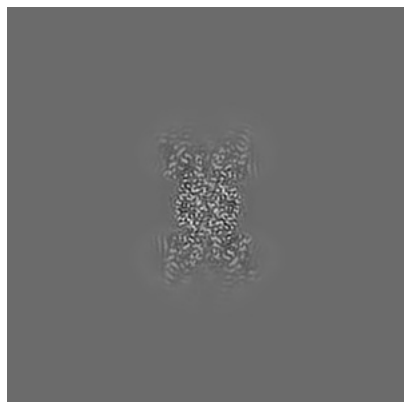


Z Index: 192

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

6.3 Largest variance slices [i](#)

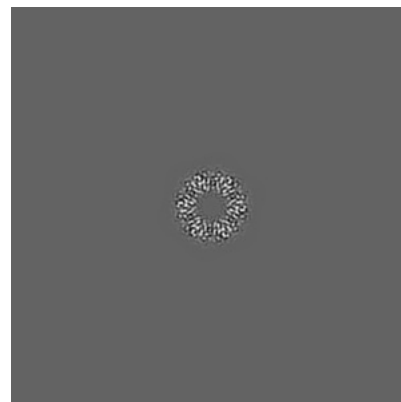
6.3.1 Primary map



X Index: 175

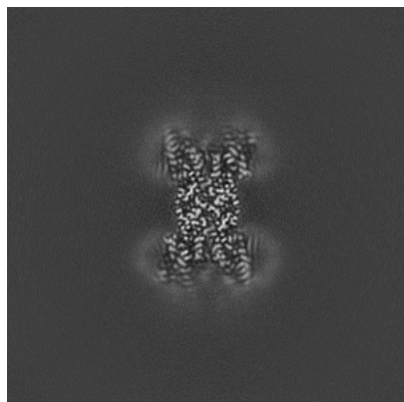


Y Index: 212

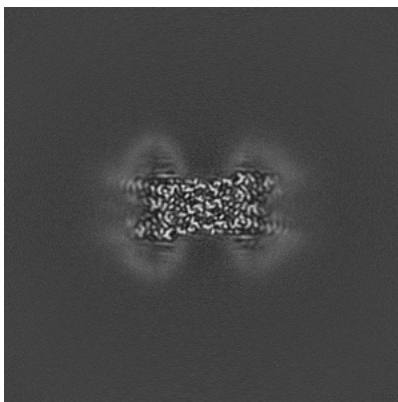


Z Index: 180

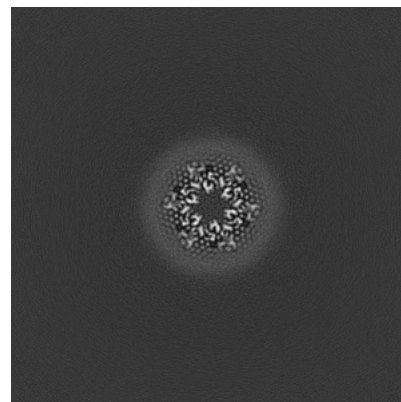
6.3.2 Raw map



X Index: 209



Y Index: 172

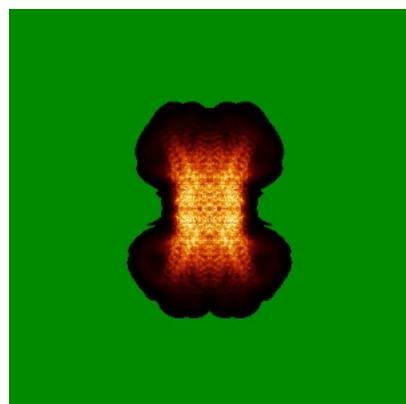


Z Index: 161

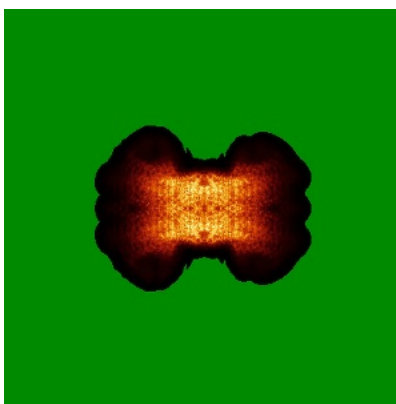
The images above show the largest variance slices of the map in three orthogonal directions.

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

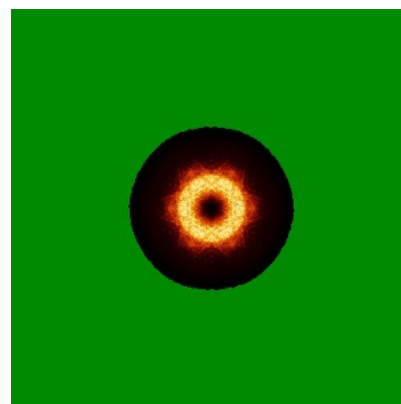
6.4.1 Primary map



X

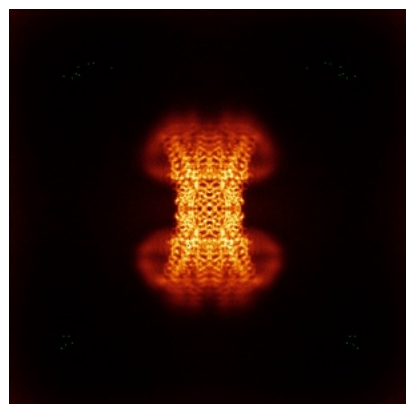


Y

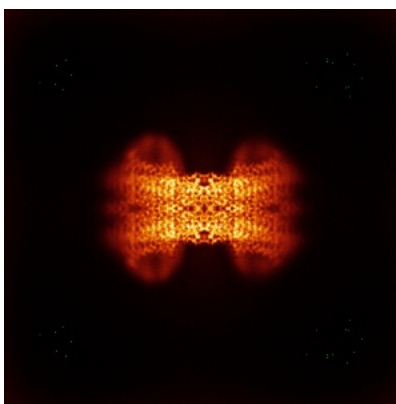


Z

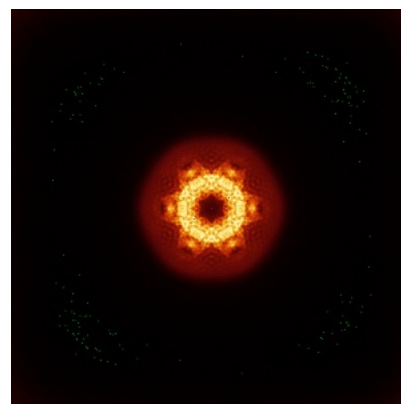
6.4.2 Raw map



X



Y

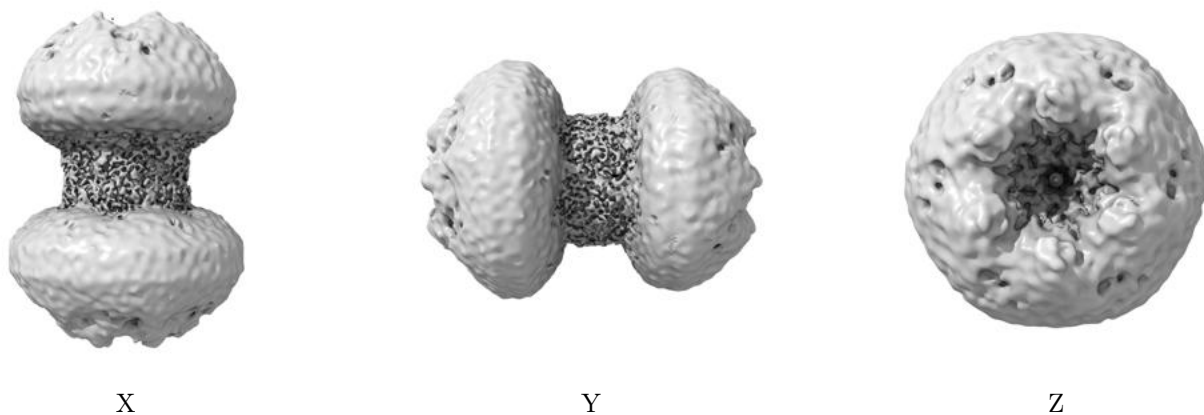


Z

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

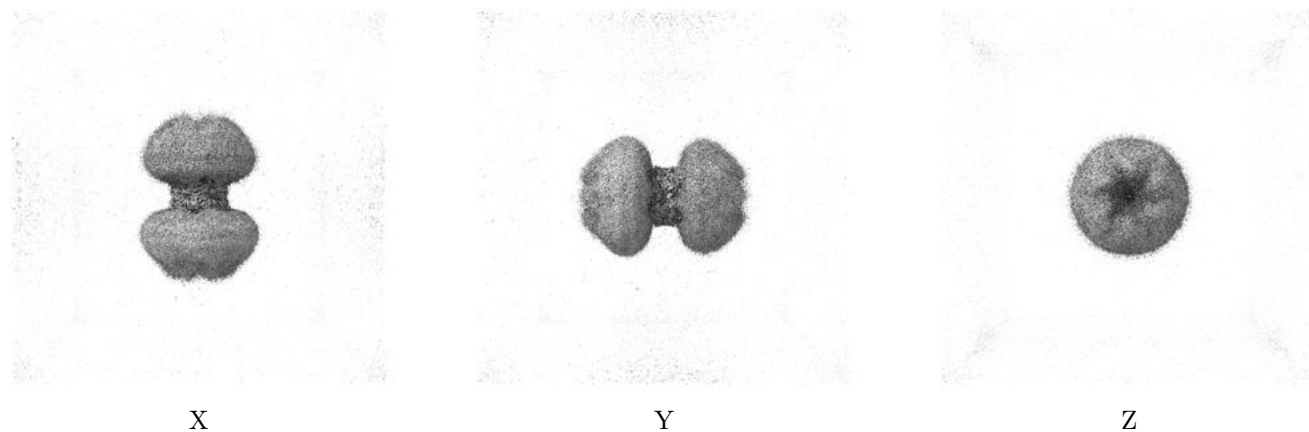
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

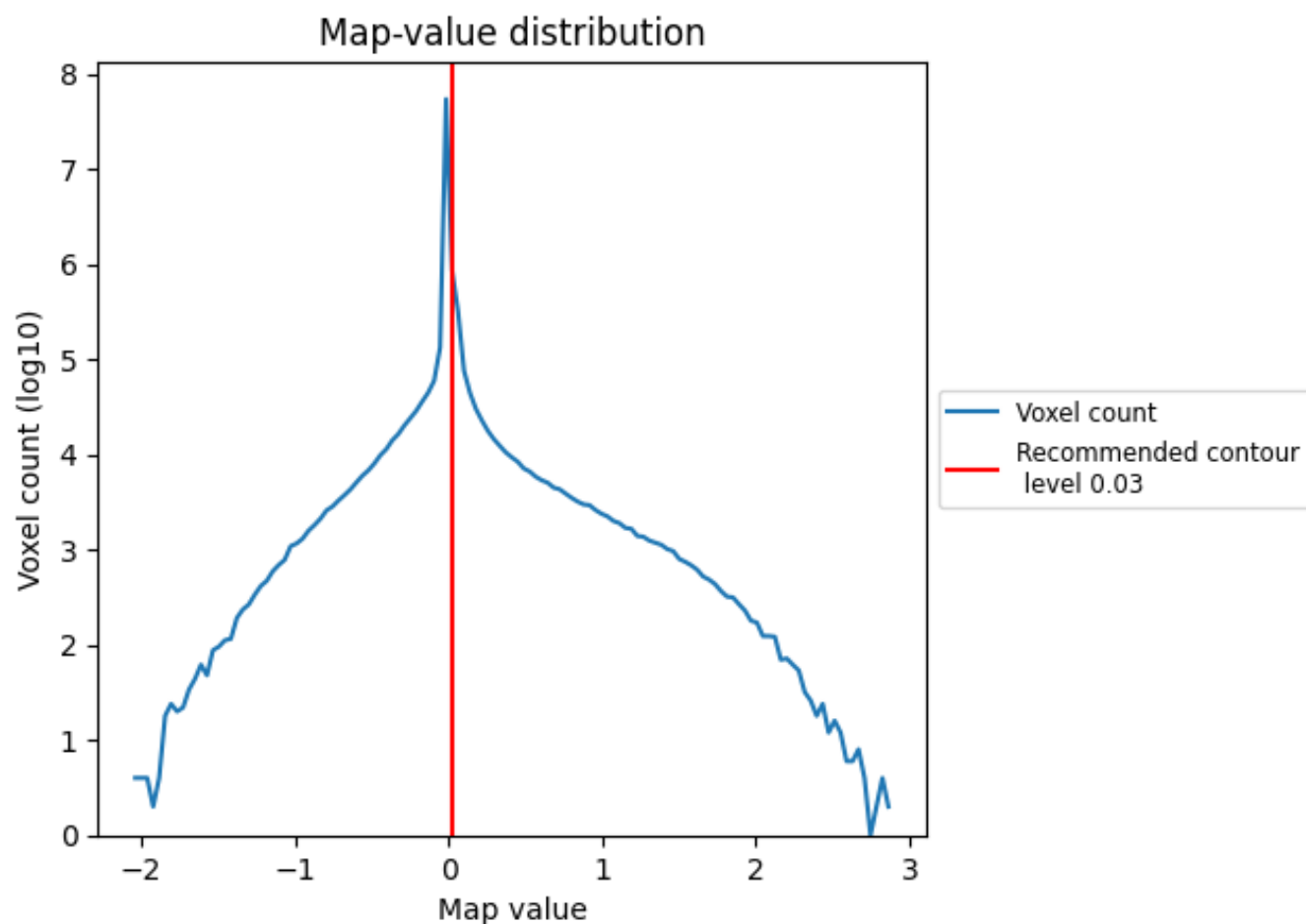
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

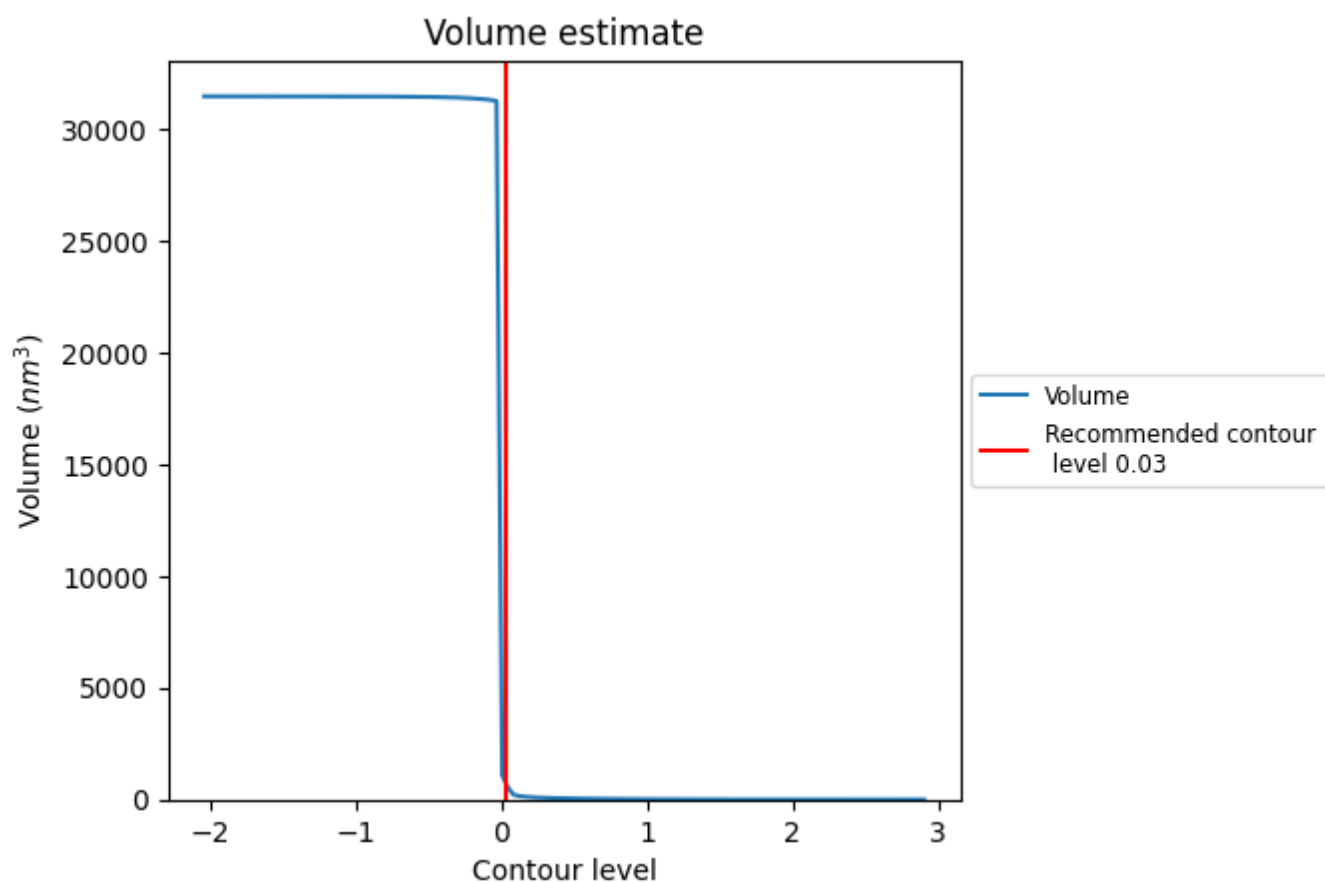
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

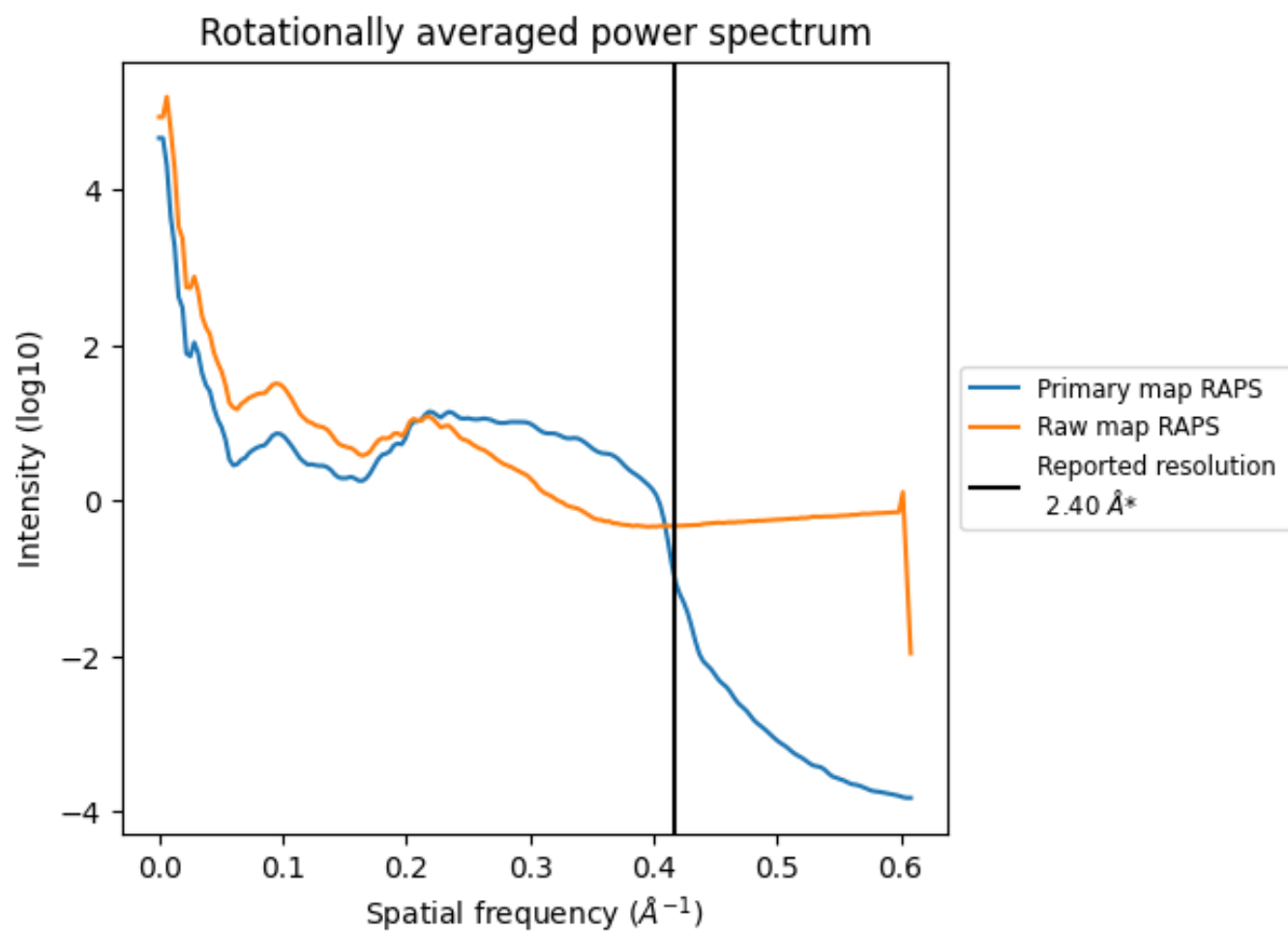
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 764 nm^3 ; 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 ⓘ

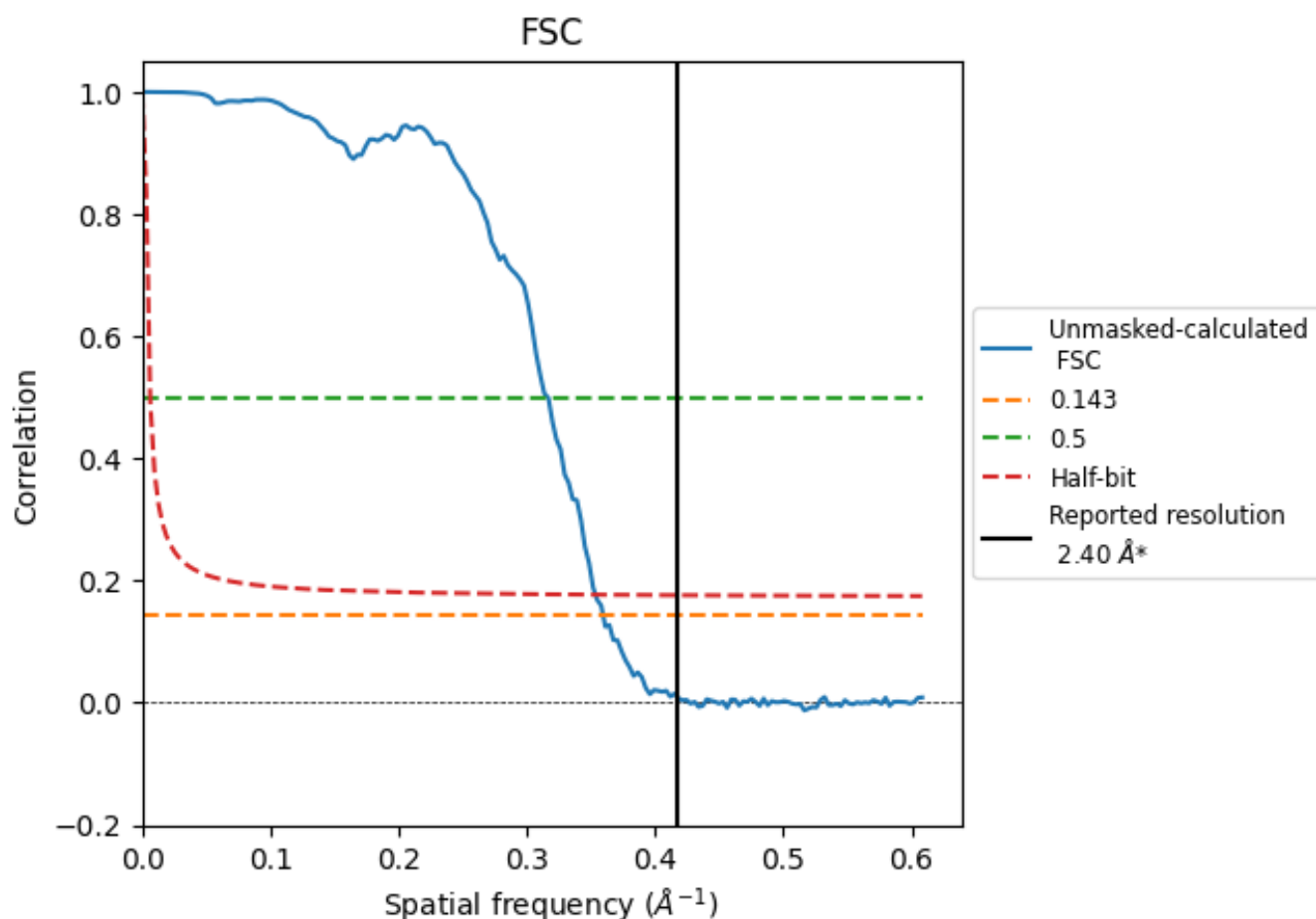


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

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 $0.417 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

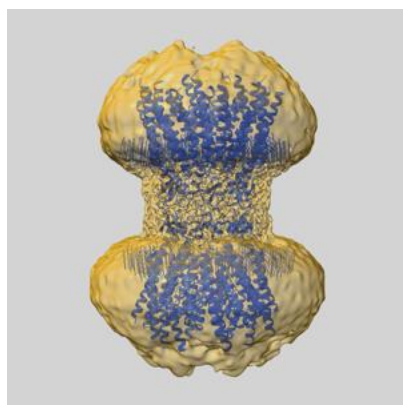
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.78	3.16	2.83

*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 %

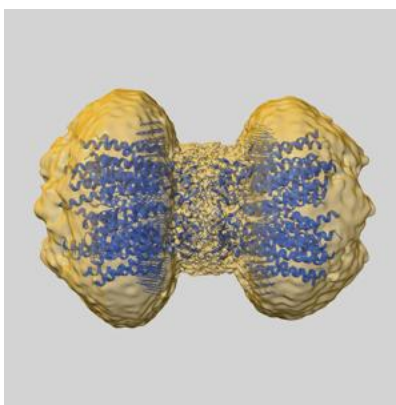
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-73965 and PDB model 9ZA3. Per-residue inclusion information can be found in section [3](#) on page [18](#).

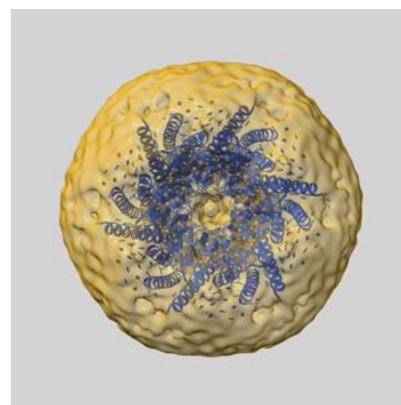
9.1 Map-model overlay [i](#)



X



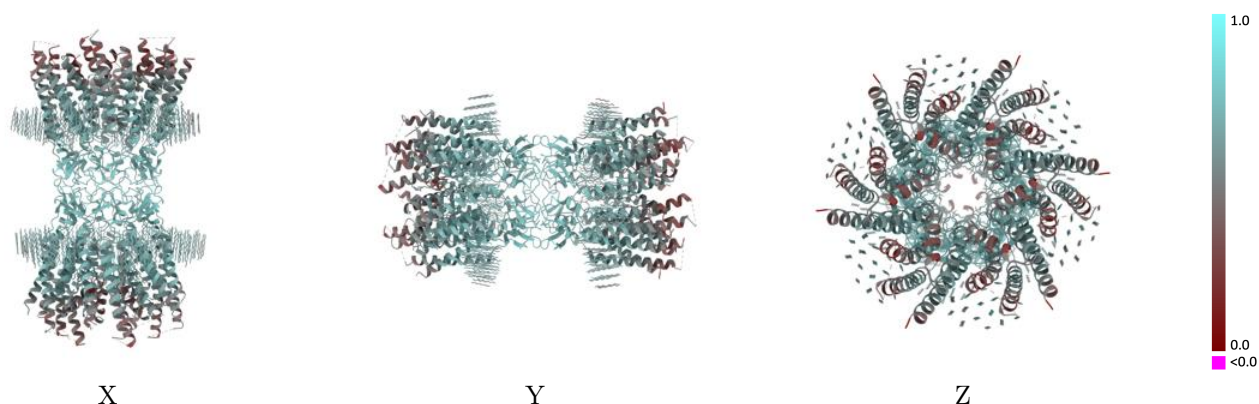
Y



Z

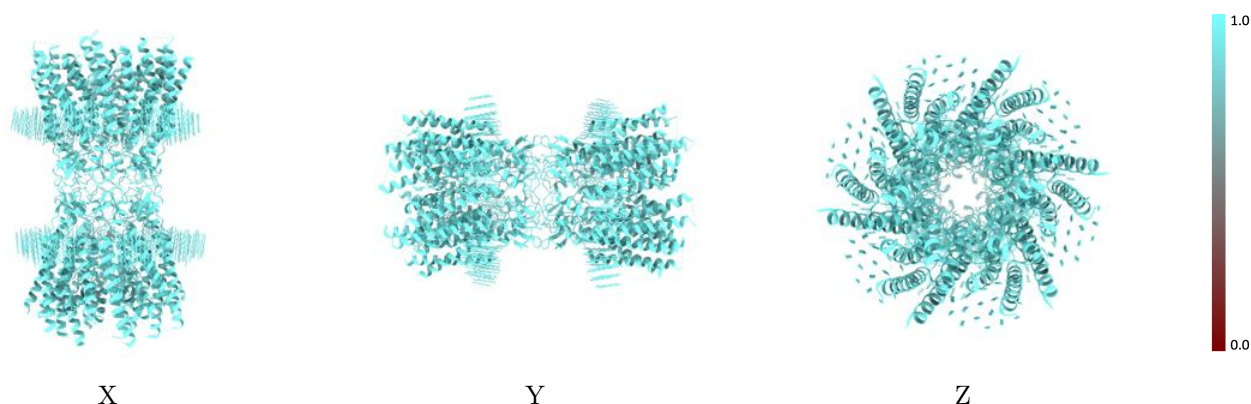
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



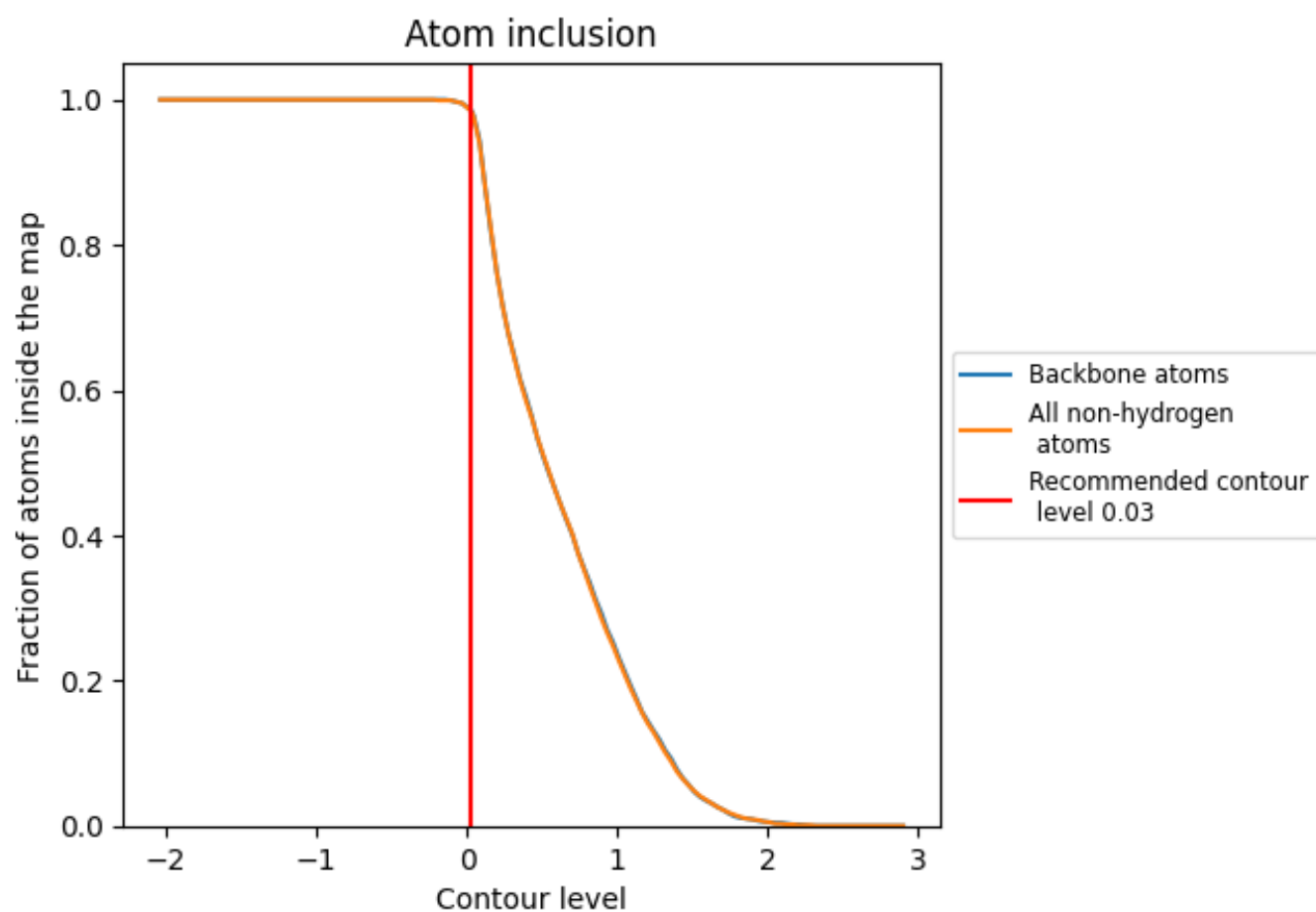
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.9840	0.5960
A	0.9800	0.5790
B	0.9800	0.5770
C	0.9800	0.5760
D	0.9800	0.5750
E	0.9800	0.5750
F	0.9810	0.5750
G	0.9920	0.6160
H	0.9910	0.6160
I	0.9910	0.6170
J	0.9910	0.6140
K	0.9920	0.6130
L	0.9910	0.6150

1.0

0.0

<0.0