



## Full wwPDB EM Validation Report ⓘ

Aug 22, 2023 – 12:20 AM JST

PDB ID : 7XL8  
EMDB ID : EMD-33274  
Title : Human Cx36/GJD2 (N-terminal deletion mutant) gap junction channel in soybean lipids (D6 symmetry)  
Authors : Lee, S.N.; Cho, H.J.; Jeong, H.; Ryu, B.; Lee, H.J.; Lee, H.H.; Woo, J.S.  
Deposited on : 2022-04-21  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

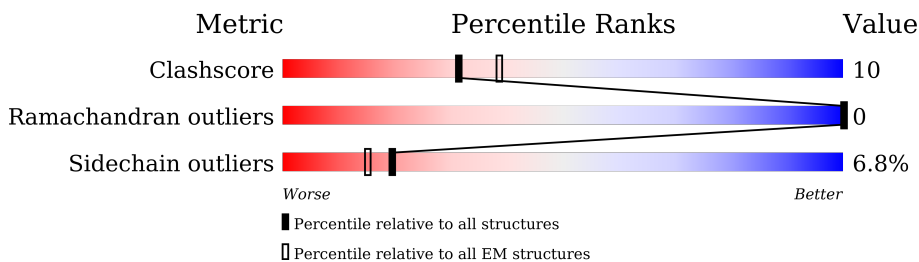
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*


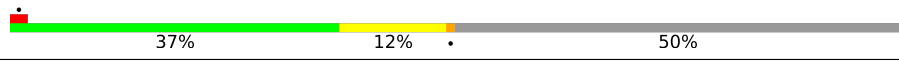
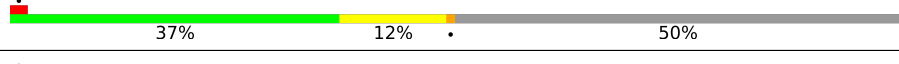




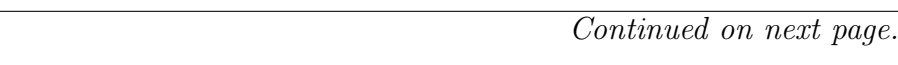
The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	325	
1	B	325	
1	C	325	
1	D	325	
1	E	325	
1	F	325	
1	G	325	
1	H	325	

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Mol	Chain	Length	Quality of chain
1	I	325	
1	J	325	
1	K	325	
1	L	325	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19188 atoms, of which 2268 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 delta-2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	163	1312	865	209	225	13	0	0
1	B	163	1312	865	209	225	13	0	0
1	C	163	1312	865	209	225	13	0	0
1	D	163	1312	865	209	225	13	0	0
1	E	163	1312	865	209	225	13	0	0
1	F	163	1312	865	209	225	13	0	0
1	G	163	1312	865	209	225	13	0	0
1	H	163	1312	865	209	225	13	0	0
1	I	163	1312	865	209	225	13	0	0
1	J	163	1312	865	209	225	13	0	0
1	K	163	1312	865	209	225	13	0	0
1	L	163	1312	865	209	225	13	0	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	initiating methionine	UNP Q9UKL4
A	322	SER	-	expression tag	UNP Q9UKL4
A	323	ARG	-	expression tag	UNP Q9UKL4
A	324	GLY	-	expression tag	UNP Q9UKL4
A	325	ASP	-	expression tag	UNP Q9UKL4
A	326	MET	-	expression tag	UNP Q9UKL4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	327	LEU	-	expression tag	UNP Q9UKL4
A	328	GLU	-	expression tag	UNP Q9UKL4
A	329	VAL	-	expression tag	UNP Q9UKL4
A	330	LEU	-	expression tag	UNP Q9UKL4
A	331	PHE	-	expression tag	UNP Q9UKL4
A	332	GLN	-	expression tag	UNP Q9UKL4
B	8	MET	-	initiating methionine	UNP Q9UKL4
B	322	SER	-	expression tag	UNP Q9UKL4
B	323	ARG	-	expression tag	UNP Q9UKL4
B	324	GLY	-	expression tag	UNP Q9UKL4
B	325	ASP	-	expression tag	UNP Q9UKL4
B	326	MET	-	expression tag	UNP Q9UKL4
B	327	LEU	-	expression tag	UNP Q9UKL4
B	328	GLU	-	expression tag	UNP Q9UKL4
B	329	VAL	-	expression tag	UNP Q9UKL4
B	330	LEU	-	expression tag	UNP Q9UKL4
B	331	PHE	-	expression tag	UNP Q9UKL4
B	332	GLN	-	expression tag	UNP Q9UKL4
C	8	MET	-	initiating methionine	UNP Q9UKL4
C	322	SER	-	expression tag	UNP Q9UKL4
C	323	ARG	-	expression tag	UNP Q9UKL4
C	324	GLY	-	expression tag	UNP Q9UKL4
C	325	ASP	-	expression tag	UNP Q9UKL4
C	326	MET	-	expression tag	UNP Q9UKL4
C	327	LEU	-	expression tag	UNP Q9UKL4
C	328	GLU	-	expression tag	UNP Q9UKL4
C	329	VAL	-	expression tag	UNP Q9UKL4
C	330	LEU	-	expression tag	UNP Q9UKL4
C	331	PHE	-	expression tag	UNP Q9UKL4
C	332	GLN	-	expression tag	UNP Q9UKL4
D	8	MET	-	initiating methionine	UNP Q9UKL4
D	322	SER	-	expression tag	UNP Q9UKL4
D	323	ARG	-	expression tag	UNP Q9UKL4
D	324	GLY	-	expression tag	UNP Q9UKL4
D	325	ASP	-	expression tag	UNP Q9UKL4
D	326	MET	-	expression tag	UNP Q9UKL4
D	327	LEU	-	expression tag	UNP Q9UKL4
D	328	GLU	-	expression tag	UNP Q9UKL4
D	329	VAL	-	expression tag	UNP Q9UKL4
D	330	LEU	-	expression tag	UNP Q9UKL4
D	331	PHE	-	expression tag	UNP Q9UKL4
D	332	GLN	-	expression tag	UNP Q9UKL4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	8	MET	-	initiating methionine	UNP Q9UKL4
E	322	SER	-	expression tag	UNP Q9UKL4
E	323	ARG	-	expression tag	UNP Q9UKL4
E	324	GLY	-	expression tag	UNP Q9UKL4
E	325	ASP	-	expression tag	UNP Q9UKL4
E	326	MET	-	expression tag	UNP Q9UKL4
E	327	LEU	-	expression tag	UNP Q9UKL4
E	328	GLU	-	expression tag	UNP Q9UKL4
E	329	VAL	-	expression tag	UNP Q9UKL4
E	330	LEU	-	expression tag	UNP Q9UKL4
E	331	PHE	-	expression tag	UNP Q9UKL4
E	332	GLN	-	expression tag	UNP Q9UKL4
F	8	MET	-	initiating methionine	UNP Q9UKL4
F	322	SER	-	expression tag	UNP Q9UKL4
F	323	ARG	-	expression tag	UNP Q9UKL4
F	324	GLY	-	expression tag	UNP Q9UKL4
F	325	ASP	-	expression tag	UNP Q9UKL4
F	326	MET	-	expression tag	UNP Q9UKL4
F	327	LEU	-	expression tag	UNP Q9UKL4
F	328	GLU	-	expression tag	UNP Q9UKL4
F	329	VAL	-	expression tag	UNP Q9UKL4
F	330	LEU	-	expression tag	UNP Q9UKL4
F	331	PHE	-	expression tag	UNP Q9UKL4
F	332	GLN	-	expression tag	UNP Q9UKL4
G	8	MET	-	initiating methionine	UNP Q9UKL4
G	322	SER	-	expression tag	UNP Q9UKL4
G	323	ARG	-	expression tag	UNP Q9UKL4
G	324	GLY	-	expression tag	UNP Q9UKL4
G	325	ASP	-	expression tag	UNP Q9UKL4
G	326	MET	-	expression tag	UNP Q9UKL4
G	327	LEU	-	expression tag	UNP Q9UKL4
G	328	GLU	-	expression tag	UNP Q9UKL4
G	329	VAL	-	expression tag	UNP Q9UKL4
G	330	LEU	-	expression tag	UNP Q9UKL4
G	331	PHE	-	expression tag	UNP Q9UKL4
G	332	GLN	-	expression tag	UNP Q9UKL4
H	8	MET	-	initiating methionine	UNP Q9UKL4
H	322	SER	-	expression tag	UNP Q9UKL4
H	323	ARG	-	expression tag	UNP Q9UKL4
H	324	GLY	-	expression tag	UNP Q9UKL4
H	325	ASP	-	expression tag	UNP Q9UKL4
H	326	MET	-	expression tag	UNP Q9UKL4

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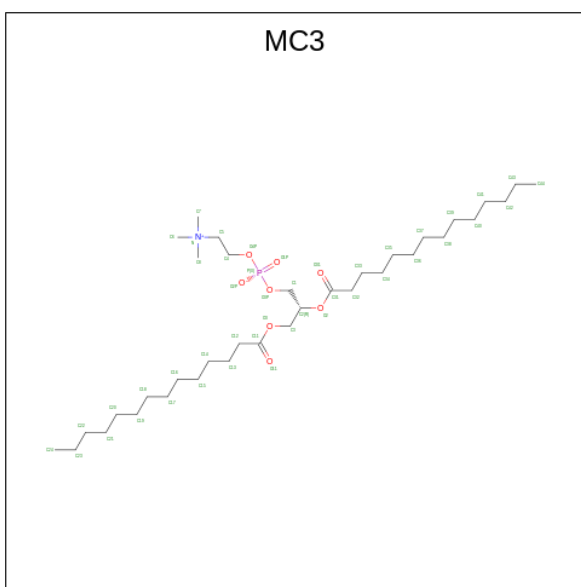
Chain	Residue	Modelled	Actual	Comment	Reference
H	327	LEU	-	expression tag	UNP Q9UKL4
H	328	GLU	-	expression tag	UNP Q9UKL4
H	329	VAL	-	expression tag	UNP Q9UKL4
H	330	LEU	-	expression tag	UNP Q9UKL4
H	331	PHE	-	expression tag	UNP Q9UKL4
H	332	GLN	-	expression tag	UNP Q9UKL4
I	8	MET	-	initiating methionine	UNP Q9UKL4
I	322	SER	-	expression tag	UNP Q9UKL4
I	323	ARG	-	expression tag	UNP Q9UKL4
I	324	GLY	-	expression tag	UNP Q9UKL4
I	325	ASP	-	expression tag	UNP Q9UKL4
I	326	MET	-	expression tag	UNP Q9UKL4
I	327	LEU	-	expression tag	UNP Q9UKL4
I	328	GLU	-	expression tag	UNP Q9UKL4
I	329	VAL	-	expression tag	UNP Q9UKL4
I	330	LEU	-	expression tag	UNP Q9UKL4
I	331	PHE	-	expression tag	UNP Q9UKL4
I	332	GLN	-	expression tag	UNP Q9UKL4
J	8	MET	-	initiating methionine	UNP Q9UKL4
J	322	SER	-	expression tag	UNP Q9UKL4
J	323	ARG	-	expression tag	UNP Q9UKL4
J	324	GLY	-	expression tag	UNP Q9UKL4
J	325	ASP	-	expression tag	UNP Q9UKL4
J	326	MET	-	expression tag	UNP Q9UKL4
J	327	LEU	-	expression tag	UNP Q9UKL4
J	328	GLU	-	expression tag	UNP Q9UKL4
J	329	VAL	-	expression tag	UNP Q9UKL4
J	330	LEU	-	expression tag	UNP Q9UKL4
J	331	PHE	-	expression tag	UNP Q9UKL4
J	332	GLN	-	expression tag	UNP Q9UKL4
K	8	MET	-	initiating methionine	UNP Q9UKL4
K	322	SER	-	expression tag	UNP Q9UKL4
K	323	ARG	-	expression tag	UNP Q9UKL4
K	324	GLY	-	expression tag	UNP Q9UKL4
K	325	ASP	-	expression tag	UNP Q9UKL4
K	326	MET	-	expression tag	UNP Q9UKL4
K	327	LEU	-	expression tag	UNP Q9UKL4
K	328	GLU	-	expression tag	UNP Q9UKL4
K	329	VAL	-	expression tag	UNP Q9UKL4
K	330	LEU	-	expression tag	UNP Q9UKL4
K	331	PHE	-	expression tag	UNP Q9UKL4
K	332	GLN	-	expression tag	UNP Q9UKL4

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Chain	Residue	Modelled	Actual	Comment	Reference
L	8	MET	-	initiating methionine	UNP Q9UKL4
L	322	SER	-	expression tag	UNP Q9UKL4
L	323	ARG	-	expression tag	UNP Q9UKL4
L	324	GLY	-	expression tag	UNP Q9UKL4
L	325	ASP	-	expression tag	UNP Q9UKL4
L	326	MET	-	expression tag	UNP Q9UKL4
L	327	LEU	-	expression tag	UNP Q9UKL4
L	328	GLU	-	expression tag	UNP Q9UKL4
L	329	VAL	-	expression tag	UNP Q9UKL4
L	330	LEU	-	expression tag	UNP Q9UKL4
L	331	PHE	-	expression tag	UNP Q9UKL4
L	332	GLN	-	expression tag	UNP Q9UKL4

- Molecule 2 is 1,2-DIMYRISTOYL-RAC-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: MC3) (formula:  $C_{36}H_{72}NO_8P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
2	A	1	41	14	27	0
2	A	1	41	14	27	0
2	A	1	41	14	27	0
2	A	1	41	14	27	0
2	A	1	41	14	27	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
2	A	1	41	14	27	0
2	A	1	41	14	27	0
2	B	1	41	14	27	0
2	B	1	41	14	27	0
2	B	1	41	14	27	0
2	B	1	41	14	27	0
2	B	1	41	14	27	0
2	B	1	41	14	27	0
2	B	1	41	14	27	0
2	C	1	41	14	27	0
2	C	1	41	14	27	0
2	C	1	41	14	27	0
2	C	1	41	14	27	0
2	C	1	41	14	27	0
2	C	1	41	14	27	0
2	C	1	41	14	27	0
2	D	1	41	14	27	0
2	D	1	41	14	27	0
2	D	1	41	14	27	0
2	D	1	41	14	27	0
2	D	1	41	14	27	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
2	D	1	41	14	27	0
2	D	1	41	14	27	0
2	E	1	41	14	27	0
2	E	1	41	14	27	0
2	E	1	41	14	27	0
2	E	1	41	14	27	0
2	E	1	41	14	27	0
2	E	1	41	14	27	0
2	E	1	41	14	27	0
2	F	1	41	14	27	0
2	F	1	41	14	27	0
2	F	1	41	14	27	0
2	F	1	41	14	27	0
2	F	1	41	14	27	0
2	F	1	41	14	27	0
2	F	1	41	14	27	0
2	F	1	41	14	27	0
2	G	1	41	14	27	0
2	G	1	41	14	27	0
2	G	1	41	14	27	0
2	G	1	41	14	27	0
2	G	1	41	14	27	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
2	G	1	41	14	27	0
2	G	1	41	14	27	0
2	H	1	41	14	27	0
2	H	1	41	14	27	0
2	H	1	41	14	27	0
2	H	1	41	14	27	0
2	H	1	41	14	27	0
2	H	1	41	14	27	0
2	H	1	41	14	27	0
2	I	1	41	14	27	0
2	I	1	41	14	27	0
2	I	1	41	14	27	0
2	I	1	41	14	27	0
2	I	1	41	14	27	0
2	I	1	41	14	27	0
2	I	1	41	14	27	0
2	I	1	41	14	27	0
2	J	1	41	14	27	0
2	J	1	41	14	27	0
2	J	1	41	14	27	0
2	J	1	41	14	27	0
2	J	1	41	14	27	0

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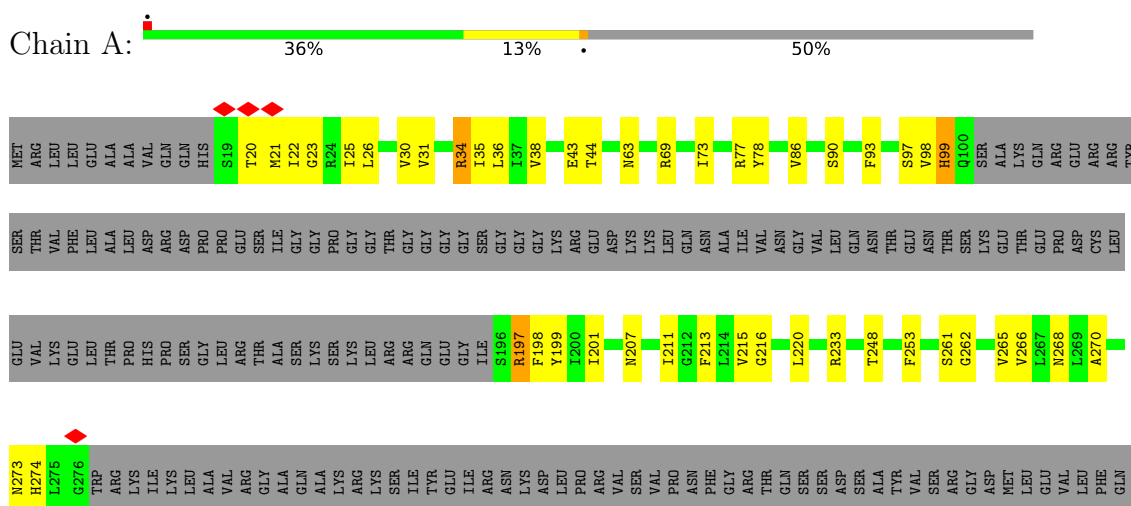
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
2	J	1	41	14	27	0
2	J	1	41	14	27	0
2	K	1	41	14	27	0
2	K	1	41	14	27	0
2	K	1	41	14	27	0
2	K	1	41	14	27	0
2	K	1	41	14	27	0
2	K	1	41	14	27	0
2	K	1	41	14	27	0
2	L	1	41	14	27	0
2	L	1	41	14	27	0
2	L	1	41	14	27	0
2	L	1	41	14	27	0
2	L	1	41	14	27	0
2	L	1	41	14	27	0
2	L	1	41	14	27	0

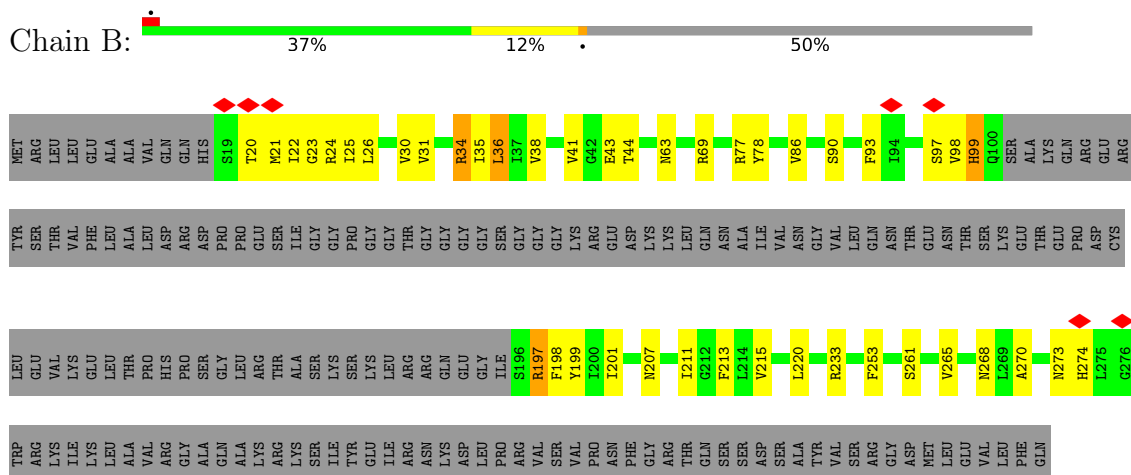
### 3 Residue-property plots i

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.

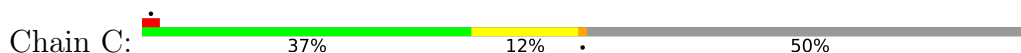
- Molecule 1: Gap junction delta-2 protein



- Molecule 1: Gap junction delta-2 protein

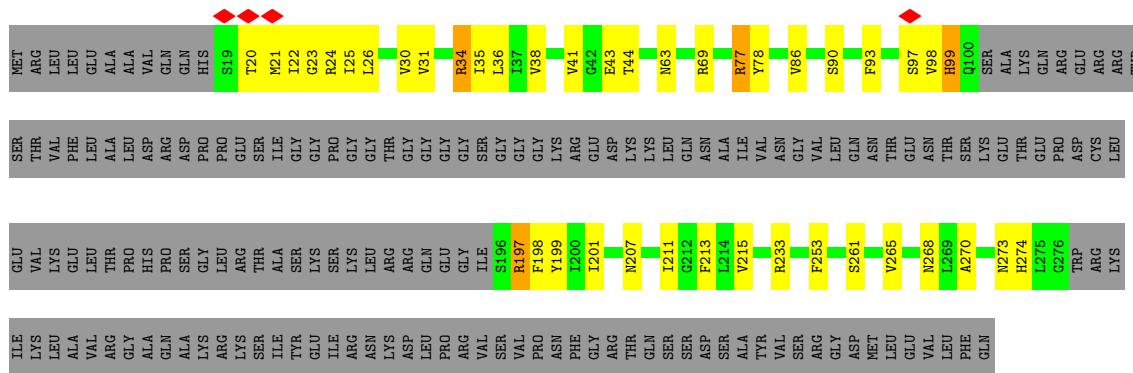


- Molecule 1: Gap junction delta-2 protein

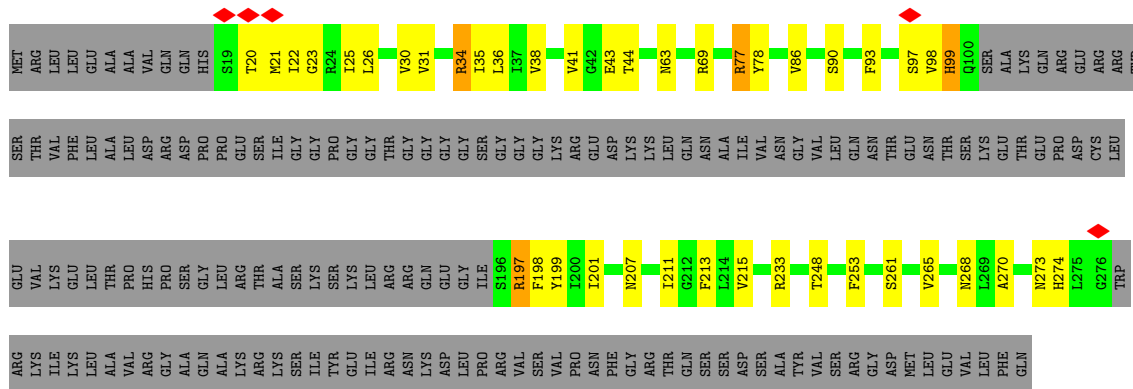
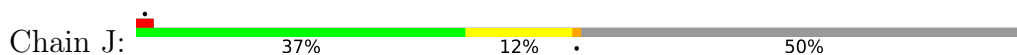




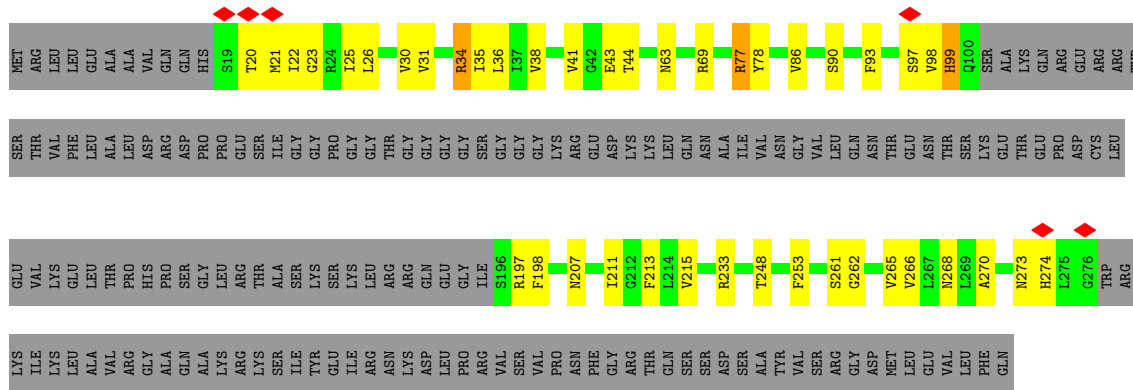
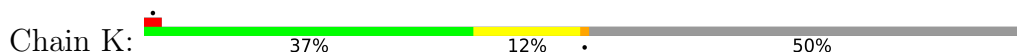




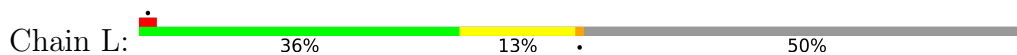
• Molecule 1: Gap junction delta-2 protein



• Molecule 1: Gap junction delta-2 protein



• Molecule 1: Gap junction delta-2 protein





MET	ARG	LEU	LEU	ALA	ALA	VAL	GLN	HIS	S19	T20	M21	I22	G23	R24	I25	L26	V30	V31	R34	I35	L36	I37	V38	V41	E43	T44	M63	R69	R77	Y78	V86	S90	F93	S97	V98	H99	Q100	SER	ALA	ALA	LYS	GLN	ARG	GLU	ARG	TYR										
SER	THR	VAL	PHE	LEU	LEU	ALA	LEU	ASP	ASP	PRO	PRO	GLU	SER	ILE	GLY	GLY	PRO	GLY	GLY	THR	THR	GLY	GLY	ARG	GLU	ASP	LYS	LEU	GLN	ASN	ALA	ILE	VAL	ASN	GLY	VAL	LEU	GLN	ASN	THR	THR	GLU	ASN	THR	SER	LYS	GLU	LYS	THR	THR	GLU	PRO	ARG	ASP	CYS	LEU
GLU	VAL	LYS	LEU	THR	PRO	HIS	PRO	SER	GLY	LEU	ARG	THR	ALA	ALA	SER	LYS	LYS	LEU	ARG	ARG	GLN	GLU	GLY	ILE	S196	R197	F198	Y199	T200	T201	N207	I211	G212	F213	L214	V215	L220	R233	T248	F253	S261	G262	V265	V266	L267	N268	L269	A270	N273							
H274	L275	G276	TRP	ARG	LYS	ILE	LYS	LEU	ALA	VAL	ARG	GLY	ALA	GLN	ALA	LYS	ARG	LYS	SER	ILE	TTR	GLU	ILE	ASN	LYS	ASP	LEU	PRO	ARG	VAL	SER	VAL	PRO	ASN	PHE	GLY	ARG	THR	GLN	SER	SER	ASP	ALA	TYR	VAL	SER	ARG	GLY	ASP	MET	LEU	GLU	VAL	LEU	PHE	GLN

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	460806	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	61	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.884	Depositor
Minimum map value	-1.348	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	302.94, 302.94, 302.94	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8415, 0.8415, 0.8415	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	0.50	0/1344	0.60	0/1828
1	B	0.50	0/1344	0.61	0/1828
1	C	0.50	0/1344	0.61	0/1828
1	D	0.50	0/1344	0.60	0/1828
1	E	0.50	0/1344	0.61	0/1828
1	F	0.50	0/1344	0.61	0/1828
1	G	0.50	0/1344	0.61	0/1828
1	H	0.50	0/1344	0.60	0/1828
1	I	0.50	0/1344	0.60	0/1828
1	J	0.50	0/1344	0.60	0/1828
1	K	0.50	0/1344	0.60	0/1828
1	L	0.50	0/1344	0.60	0/1828
All	All	0.50	0/16128	0.60	0/21936

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	1312	0	1314	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1312	0	1314	29	0
1	C	1312	0	1314	29	0
1	D	1312	0	1314	27	0
1	E	1312	0	1314	29	0
1	F	1312	0	1314	26	0
1	G	1312	0	1314	26	0
1	H	1312	0	1314	30	0
1	I	1312	0	1314	27	0
1	J	1312	0	1314	29	0
1	K	1312	0	1314	28	0
1	L	1312	0	1314	30	0
2	A	98	189	189	5	0
2	B	98	189	189	1	0
2	C	98	189	189	1	0
2	D	98	189	189	2	0
2	E	98	189	189	2	0
2	F	98	189	189	4	0
2	G	98	189	189	1	0
2	H	98	189	189	4	0
2	I	98	189	189	0	0
2	J	98	189	189	1	0
2	K	98	189	189	2	0
2	L	98	189	189	2	0
All	All	16920	2268	18036	335	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 10.

All (335) 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:22:ILE:O	1:D:25:ILE:HG13	1.44	1.17
1:K:22:ILE:O	1:K:25:ILE:HG13	1.44	1.17
1:E:22:ILE:O	1:E:25:ILE:HG13	1.44	1.17
1:A:22:ILE:O	1:A:25:ILE:HG13	1.44	1.17
1:H:22:ILE:O	1:H:25:ILE:HG13	1.44	1.17
1:L:22:ILE:O	1:L:25:ILE:HG13	1.44	1.17
1:G:22:ILE:O	1:G:25:ILE:HG13	1.44	1.16
1:F:22:ILE:O	1:F:25:ILE:HG13	1.44	1.16
1:B:22:ILE:O	1:B:25:ILE:HG13	1.44	1.13
1:J:22:ILE:O	1:J:25:ILE:HG13	1.44	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:22:ILE:O	1:I:25:ILE:HG13	1.44	1.13
1:C:22:ILE:O	1:C:25:ILE:HG13	1.44	1.13
1:A:22:ILE:O	1:A:25:ILE:CG1	2.25	0.85
1:D:22:ILE:O	1:D:25:ILE:CG1	2.25	0.85
1:J:22:ILE:O	1:J:25:ILE:CG1	2.25	0.85
1:K:22:ILE:O	1:K:25:ILE:CG1	2.25	0.85
1:C:22:ILE:O	1:C:25:ILE:CG1	2.25	0.85
1:H:22:ILE:O	1:H:25:ILE:CG1	2.25	0.85
1:I:22:ILE:O	1:I:25:ILE:CG1	2.25	0.83
1:B:22:ILE:O	1:B:25:ILE:CG1	2.25	0.83
1:L:22:ILE:O	1:L:25:ILE:CG1	2.25	0.83
1:E:22:ILE:O	1:E:25:ILE:CG1	2.25	0.83
1:G:22:ILE:O	1:G:25:ILE:CG1	2.25	0.82
1:F:22:ILE:O	1:F:25:ILE:CG1	2.25	0.81
1:L:34:ARG:HH12	1:L:86:VAL:HG21	1.54	0.73
1:E:34:ARG:HH12	1:E:86:VAL:HG21	1.54	0.73
1:B:34:ARG:HH12	1:B:86:VAL:HG21	1.54	0.73
1:I:34:ARG:HH12	1:I:86:VAL:HG21	1.54	0.73
1:C:34:ARG:HH12	1:C:86:VAL:HG21	1.54	0.72
1:J:34:ARG:HH12	1:J:86:VAL:HG21	1.54	0.72
1:K:34:ARG:HH12	1:K:86:VAL:HG21	1.54	0.72
1:D:34:ARG:HH12	1:D:86:VAL:HG21	1.54	0.72
1:F:34:ARG:HH12	1:F:86:VAL:HG21	1.54	0.72
1:G:34:ARG:HH12	1:G:86:VAL:HG21	1.54	0.72
1:A:34:ARG:HH12	1:A:86:VAL:HG21	1.54	0.72
1:H:34:ARG:HH12	1:H:86:VAL:HG21	1.54	0.72
1:F:43:GLU:HG3	1:F:44:THR:HG23	1.79	0.65
1:G:43:GLU:HG3	1:G:44:THR:HG23	1.79	0.65
1:A:43:GLU:HG3	1:A:44:THR:HG23	1.79	0.65
1:H:43:GLU:HG3	1:H:44:THR:HG23	1.79	0.65
1:E:43:GLU:HG3	1:E:44:THR:HG23	1.79	0.64
1:L:43:GLU:HG3	1:L:44:THR:HG23	1.79	0.64
1:C:43:GLU:HG3	1:C:44:THR:HG23	1.79	0.64
1:J:43:GLU:HG3	1:J:44:THR:HG23	1.79	0.64
1:I:43:GLU:HG3	1:I:44:THR:HG23	1.79	0.64
1:B:43:GLU:HG3	1:B:44:THR:HG23	1.79	0.63
1:D:43:GLU:HG3	1:D:44:THR:HG23	1.79	0.63
1:K:43:GLU:HG3	1:K:44:THR:HG23	1.79	0.63
1:A:34:ARG:NH1	1:A:86:VAL:HG21	2.15	0.62
1:H:34:ARG:NH1	1:H:86:VAL:HG21	2.15	0.62
1:B:34:ARG:NH1	1:B:86:VAL:HG21	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:ARG:NH1	1:F:86:VAL:HG21	2.15	0.62
1:G:34:ARG:NH1	1:G:86:VAL:HG21	2.15	0.62
1:I:34:ARG:NH1	1:I:86:VAL:HG21	2.15	0.62
1:L:34:ARG:NH1	1:L:86:VAL:HG21	2.15	0.62
1:E:34:ARG:NH1	1:E:86:VAL:HG21	2.15	0.61
1:C:34:ARG:NH1	1:C:86:VAL:HG21	2.15	0.61
1:K:34:ARG:NH1	1:K:86:VAL:HG21	2.15	0.61
1:D:34:ARG:NH1	1:D:86:VAL:HG21	2.15	0.61
1:J:34:ARG:NH1	1:J:86:VAL:HG21	2.15	0.61
1:D:207:ASN:OD1	1:D:268:ASN:HB3	2.01	0.60
1:K:207:ASN:OD1	1:K:268:ASN:HB3	2.01	0.60
1:J:207:ASN:OD1	1:J:268:ASN:HB3	2.01	0.60
1:B:207:ASN:OD1	1:B:268:ASN:HB3	2.01	0.60
1:C:207:ASN:OD1	1:C:268:ASN:HB3	2.02	0.60
1:A:207:ASN:OD1	1:A:268:ASN:HB3	2.01	0.59
1:G:207:ASN:OD1	1:G:268:ASN:HB3	2.01	0.59
1:I:207:ASN:OD1	1:I:268:ASN:HB3	2.01	0.59
1:F:207:ASN:OD1	1:F:268:ASN:HB3	2.01	0.59
1:B:41:VAL:HG13	1:C:77:ARG:HG3	1.84	0.59
1:H:207:ASN:OD1	1:H:268:ASN:HB3	2.01	0.59
1:B:20:THR:HG21	1:B:274:HIS:CD2	2.38	0.59
1:I:20:THR:HG21	1:I:274:HIS:CD2	2.38	0.59
1:A:220:LEU:HG	2:A:406:MC3:H172	1.85	0.58
1:C:20:THR:HG21	1:C:274:HIS:CD2	2.38	0.58
1:G:20:THR:HG21	1:G:274:HIS:CD2	2.38	0.58
1:F:20:THR:HG21	1:F:274:HIS:CD2	2.38	0.58
1:L:207:ASN:OD1	1:L:268:ASN:HB3	2.01	0.58
1:H:20:THR:HG21	1:H:274:HIS:CD2	2.38	0.58
1:J:20:THR:HG21	1:J:274:HIS:CD2	2.38	0.58
1:D:20:THR:HG21	1:D:274:HIS:CD2	2.38	0.58
1:A:20:THR:HG21	1:A:274:HIS:CD2	2.38	0.58
1:K:20:THR:HG21	1:K:274:HIS:CD2	2.38	0.58
1:E:207:ASN:OD1	1:E:268:ASN:HB3	2.02	0.58
1:L:20:THR:HG21	1:L:274:HIS:CD2	2.38	0.58
1:E:20:THR:HG21	1:E:274:HIS:CD2	2.38	0.57
1:C:93:PHE:HA	1:C:198:PHE:CE2	2.40	0.57
1:J:93:PHE:HA	1:J:198:PHE:CE2	2.40	0.57
1:B:93:PHE:HA	1:B:198:PHE:CE2	2.40	0.57
1:I:93:PHE:HA	1:I:198:PHE:CE2	2.40	0.57
1:K:93:PHE:HA	1:K:198:PHE:CE2	2.40	0.57
1:D:93:PHE:HA	1:D:198:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ARG:HD3	1:B:233:ARG:HD2	1.88	0.56
1:I:69:ARG:HD3	1:I:233:ARG:HD2	1.88	0.56
1:G:69:ARG:HD3	1:G:233:ARG:HD2	1.88	0.56
1:H:93:PHE:HA	1:H:198:PHE:CE2	2.40	0.56
1:F:69:ARG:HD3	1:F:233:ARG:HD2	1.88	0.56
1:E:69:ARG:HD3	1:E:233:ARG:HD2	1.88	0.56
1:A:69:ARG:HD3	1:A:233:ARG:HD2	1.88	0.56
1:A:93:PHE:HA	1:A:198:PHE:CE2	2.40	0.56
1:E:93:PHE:HA	1:E:198:PHE:CE2	2.40	0.56
1:J:69:ARG:HD3	1:J:233:ARG:HD2	1.88	0.56
1:L:69:ARG:HD3	1:L:233:ARG:HD2	1.88	0.56
1:C:69:ARG:HD3	1:C:233:ARG:HD2	1.88	0.56
1:H:69:ARG:HD3	1:H:233:ARG:HD2	1.88	0.56
1:L:93:PHE:HA	1:L:198:PHE:CE2	2.40	0.56
1:D:69:ARG:HD3	1:D:233:ARG:HD2	1.88	0.55
1:K:69:ARG:HD3	1:K:233:ARG:HD2	1.88	0.55
1:G:93:PHE:HA	1:G:198:PHE:CE2	2.40	0.55
1:F:93:PHE:HA	1:F:198:PHE:CE2	2.40	0.55
1:D:31:VAL:O	1:D:35:ILE:HG13	2.08	0.54
1:K:31:VAL:O	1:K:35:ILE:HG13	2.08	0.53
1:J:31:VAL:O	1:J:35:ILE:HG13	2.08	0.53
1:C:31:VAL:O	1:C:35:ILE:HG13	2.08	0.53
1:A:31:VAL:O	1:A:35:ILE:HG13	2.08	0.53
1:G:31:VAL:O	1:G:35:ILE:HG13	2.08	0.53
1:H:31:VAL:O	1:H:35:ILE:HG13	2.08	0.53
1:F:31:VAL:O	1:F:35:ILE:HG13	2.08	0.52
1:H:220:LEU:HG	2:H:603:MC3:H172	1.91	0.52
1:I:31:VAL:O	1:I:35:ILE:HG13	2.08	0.52
1:L:31:VAL:O	1:L:35:ILE:HG13	2.08	0.52
1:B:31:VAL:O	1:B:35:ILE:HG13	2.08	0.52
1:E:31:VAL:O	1:E:35:ILE:HG13	2.08	0.52
1:A:216:GLY:HA2	2:A:407:MC3:H192	1.91	0.52
1:B:98:VAL:HG23	1:B:99:HIS:ND1	2.27	0.50
1:I:98:VAL:HG23	1:I:99:HIS:ND1	2.27	0.50
1:C:98:VAL:HG23	1:C:99:HIS:ND1	2.27	0.50
1:J:98:VAL:HG23	1:J:99:HIS:ND1	2.27	0.50
1:D:98:VAL:HG23	1:D:99:HIS:ND1	2.27	0.50
1:K:98:VAL:HG23	1:K:99:HIS:ND1	2.27	0.50
1:H:98:VAL:HG23	1:H:99:HIS:ND1	2.27	0.50
1:A:98:VAL:HG23	1:A:99:HIS:ND1	2.27	0.49
1:E:98:VAL:HG23	1:E:99:HIS:ND1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:98:VAL:HG23	1:L:99:HIS:ND1	2.27	0.49
1:C:22:ILE:HD12	1:C:23:GLY:N	2.28	0.49
1:J:22:ILE:HD12	1:J:23:GLY:N	2.28	0.49
1:F:220:LEU:HG	2:F:603:MC3:H172	1.95	0.49
1:G:22:ILE:HD12	1:G:23:GLY:N	2.28	0.49
1:L:22:ILE:HD12	1:L:23:GLY:N	2.28	0.49
1:D:22:ILE:HD12	1:D:23:GLY:N	2.28	0.49
1:E:22:ILE:HD12	1:E:23:GLY:N	2.28	0.49
1:F:22:ILE:HD12	1:F:23:GLY:N	2.28	0.49
1:G:98:VAL:HG23	1:G:99:HIS:ND1	2.27	0.49
1:K:22:ILE:HD12	1:K:23:GLY:N	2.28	0.49
1:B:22:ILE:HD12	1:B:23:GLY:N	2.28	0.49
1:I:22:ILE:HD12	1:I:23:GLY:N	2.28	0.49
1:F:98:VAL:HG23	1:F:99:HIS:ND1	2.27	0.48
1:H:22:ILE:HD12	1:H:23:GLY:N	2.28	0.48
1:A:22:ILE:HD12	1:A:23:GLY:N	2.28	0.48
1:E:26:LEU:O	1:E:30:VAL:HG13	2.14	0.48
1:J:261:SER:O	1:J:265:VAL:HG23	2.14	0.48
1:C:261:SER:O	1:C:265:VAL:HG23	2.14	0.48
1:D:26:LEU:O	1:D:30:VAL:HG13	2.14	0.48
1:K:26:LEU:O	1:K:30:VAL:HG13	2.14	0.48
1:L:26:LEU:O	1:L:30:VAL:HG13	2.14	0.48
1:E:261:SER:O	1:E:265:VAL:HG23	2.14	0.47
1:L:261:SER:O	1:L:265:VAL:HG23	2.14	0.47
1:F:261:SER:O	1:F:265:VAL:HG23	2.14	0.47
1:G:261:SER:O	1:G:265:VAL:HG23	2.14	0.47
1:F:26:LEU:O	1:F:30:VAL:HG13	2.14	0.47
1:I:26:LEU:O	1:I:30:VAL:HG13	2.14	0.47
1:I:261:SER:O	1:I:265:VAL:HG23	2.14	0.47
1:B:26:LEU:O	1:B:30:VAL:HG13	2.14	0.47
1:B:261:SER:O	1:B:265:VAL:HG23	2.14	0.47
1:C:26:LEU:O	1:C:30:VAL:HG13	2.14	0.47
1:G:26:LEU:O	1:G:30:VAL:HG13	2.14	0.47
1:J:26:LEU:O	1:J:30:VAL:HG13	2.14	0.47
1:G:77:ARG:HG3	1:L:41:VAL:HG13	1.96	0.47
1:H:216:GLY:HA2	2:H:604:MC3:H192	1.96	0.47
1:A:261:SER:O	1:A:265:VAL:HG23	2.14	0.46
1:H:261:SER:O	1:H:265:VAL:HG23	2.14	0.46
1:H:26:LEU:O	1:H:30:VAL:HG13	2.14	0.46
1:K:261:SER:O	1:K:265:VAL:HG23	2.14	0.46
1:A:26:LEU:O	1:A:30:VAL:HG13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:SER:O	1:D:265:VAL:HG23	2.14	0.46
1:I:41:VAL:HG13	1:J:77:ARG:HG3	1.98	0.46
2:F:602:MC3:H243	2:F:602:MC3:H211	1.83	0.46
1:K:41:VAL:HG13	1:L:77:ARG:HG3	1.97	0.46
1:B:78:TYR:OH	1:B:213:PHE:O	2.34	0.46
1:I:78:TYR:OH	1:I:213:PHE:O	2.34	0.46
1:J:78:TYR:OH	1:J:213:PHE:O	2.34	0.46
1:A:78:TYR:OH	1:A:213:PHE:O	2.34	0.45
1:C:78:TYR:OH	1:C:213:PHE:O	2.34	0.45
1:C:34:ARG:NH1	1:C:86:VAL:CG2	2.80	0.45
1:D:34:ARG:NH1	1:D:86:VAL:CG2	2.80	0.45
1:F:78:TYR:OH	1:F:213:PHE:O	2.34	0.45
1:H:78:TYR:OH	1:H:213:PHE:O	2.34	0.45
1:K:34:ARG:NH1	1:K:86:VAL:CG2	2.80	0.45
1:B:34:ARG:NH1	1:B:86:VAL:CG2	2.80	0.45
1:G:78:TYR:OH	1:G:213:PHE:O	2.34	0.45
1:L:34:ARG:NH1	1:L:86:VAL:CG2	2.80	0.45
1:E:34:ARG:NH1	1:E:86:VAL:CG2	2.80	0.45
1:E:211:ILE:O	1:E:215:VAL:HG23	2.17	0.45
1:K:211:ILE:O	1:K:215:VAL:HG23	2.17	0.45
1:D:35:ILE:O	1:D:35:ILE:HG22	2.17	0.44
1:D:211:ILE:O	1:D:215:VAL:HG23	2.17	0.44
1:E:35:ILE:O	1:E:35:ILE:HG22	2.17	0.44
1:E:78:TYR:OH	1:E:213:PHE:O	2.34	0.44
1:K:35:ILE:O	1:K:35:ILE:HG22	2.17	0.44
1:L:211:ILE:O	1:L:215:VAL:HG23	2.17	0.44
1:A:34:ARG:NH1	1:A:86:VAL:CG2	2.80	0.44
1:B:211:ILE:O	1:B:215:VAL:HG23	2.17	0.44
1:D:270:ALA:O	1:D:273:ASN:ND2	2.51	0.44
1:H:34:ARG:NH1	1:H:86:VAL:CG2	2.80	0.44
1:I:211:ILE:O	1:I:215:VAL:HG23	2.18	0.44
1:K:270:ALA:O	1:K:273:ASN:ND2	2.51	0.44
1:L:35:ILE:O	1:L:35:ILE:HG22	2.18	0.44
1:G:34:ARG:NH1	1:G:86:VAL:CG2	2.80	0.44
1:J:211:ILE:O	1:J:215:VAL:HG23	2.17	0.44
1:L:78:TYR:OH	1:L:213:PHE:O	2.34	0.44
1:A:73:ILE:HD11	2:A:405:MC3:H161	1.99	0.44
1:F:34:ARG:NH1	1:F:86:VAL:CG2	2.80	0.44
1:F:270:ALA:O	1:F:273:ASN:ND2	2.50	0.44
1:G:270:ALA:O	1:G:273:ASN:ND2	2.51	0.44
1:H:211:ILE:O	1:H:215:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ILE:O	1:A:215:VAL:HG23	2.17	0.44
1:C:211:ILE:O	1:C:215:VAL:HG23	2.17	0.44
1:D:78:TYR:OH	1:D:213:PHE:O	2.34	0.44
1:L:270:ALA:O	1:L:273:ASN:ND2	2.51	0.44
1:C:35:ILE:HG22	1:C:35:ILE:O	2.18	0.44
1:E:270:ALA:O	1:E:273:ASN:ND2	2.51	0.44
1:F:35:ILE:O	1:F:35:ILE:HG22	2.17	0.44
1:F:211:ILE:O	1:F:215:VAL:HG23	2.17	0.44
1:J:35:ILE:HG22	1:J:35:ILE:O	2.17	0.44
1:K:78:TYR:OH	1:K:213:PHE:O	2.34	0.44
1:C:270:ALA:O	1:C:273:ASN:ND2	2.50	0.43
1:G:211:ILE:O	1:G:215:VAL:HG23	2.17	0.43
1:J:270:ALA:O	1:J:273:ASN:ND2	2.50	0.43
1:B:270:ALA:O	1:B:273:ASN:ND2	2.50	0.43
1:G:35:ILE:O	1:G:35:ILE:HG22	2.18	0.43
1:A:270:ALA:O	1:A:273:ASN:ND2	2.51	0.43
2:D:602:MC3:H211	2:D:602:MC3:H243	1.83	0.43
1:H:270:ALA:O	1:H:273:ASN:ND2	2.50	0.43
1:I:270:ALA:O	1:I:273:ASN:ND2	2.50	0.43
2:H:602:MC3:H243	2:H:602:MC3:H211	1.82	0.43
2:K:602:MC3:H211	2:K:602:MC3:H243	1.82	0.43
1:B:35:ILE:O	1:B:35:ILE:HG22	2.18	0.43
1:F:73:ILE:HD11	2:F:602:MC3:H161	2.01	0.43
1:A:35:ILE:O	1:A:35:ILE:HG22	2.18	0.43
1:G:35:ILE:HD13	1:G:35:ILE:HG21	1.75	0.43
1:H:35:ILE:O	1:H:35:ILE:HG22	2.18	0.43
1:H:41:VAL:HG13	1:I:77:ARG:HG3	2.00	0.43
1:I:35:ILE:O	1:I:35:ILE:HG22	2.18	0.43
1:D:35:ILE:HD13	1:D:35:ILE:HG21	1.75	0.42
2:A:405:MC3:H211	2:A:405:MC3:H243	1.82	0.42
1:I:34:ARG:NH1	1:I:86:VAL:CG2	2.80	0.42
1:J:41:VAL:HG13	1:K:77:ARG:HG3	2.01	0.42
1:J:34:ARG:NH1	1:J:86:VAL:CG2	2.80	0.42
1:L:220:LEU:HG	2:L:603:MC3:H172	2.02	0.42
1:B:36:LEU:CD1	1:C:84:ILE:HD13	2.50	0.42
1:D:38:VAL:O	1:D:38:VAL:HG12	2.20	0.42
1:K:38:VAL:O	1:K:38:VAL:HG12	2.20	0.42
1:D:30:VAL:O	1:D:34:ARG:HB3	2.20	0.42
1:K:35:ILE:HD13	1:K:35:ILE:HG21	1.75	0.42
1:K:30:VAL:O	1:K:34:ARG:HB3	2.20	0.42
1:D:248:THR:HG23	2:D:607:MC3:H142	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:30:VAL:O	1:I:34:ARG:HB3	2.20	0.42
1:L:38:VAL:O	1:L:38:VAL:HG12	2.20	0.42
1:B:30:VAL:O	1:B:34:ARG:HB3	2.20	0.41
1:C:38:VAL:O	1:C:38:VAL:HG12	2.20	0.41
1:C:41:VAL:HG13	1:D:77:ARG:HG3	2.01	0.41
1:G:30:VAL:O	1:G:34:ARG:HB3	2.20	0.41
1:H:30:VAL:O	1:H:34:ARG:HB3	2.20	0.41
1:J:38:VAL:O	1:J:38:VAL:HG12	2.20	0.41
1:K:248:THR:HG23	2:K:607:MC3:H142	2.02	0.41
1:C:30:VAL:O	1:C:34:ARG:HB3	2.20	0.41
1:F:30:VAL:O	1:F:34:ARG:HB3	2.20	0.41
1:J:30:VAL:O	1:J:34:ARG:HB3	2.20	0.41
1:A:30:VAL:O	1:A:34:ARG:HB3	2.20	0.41
1:E:38:VAL:O	1:E:38:VAL:HG12	2.20	0.41
1:E:35:ILE:HG21	1:E:35:ILE:HD13	1.75	0.41
1:G:38:VAL:O	1:G:38:VAL:HG12	2.20	0.41
1:F:38:VAL:O	1:F:38:VAL:HG12	2.20	0.41
1:H:38:VAL:O	1:H:38:VAL:HG12	2.20	0.41
1:B:38:VAL:O	1:B:38:VAL:HG12	2.20	0.41
1:E:248:THR:HG23	2:E:607:MC3:H142	2.02	0.41
1:E:267:LEU:HD23	1:E:267:LEU:HA	1.97	0.41
1:G:248:THR:HG23	2:G:403:MC3:H142	2.02	0.41
1:J:248:THR:HG23	2:J:607:MC3:H142	2.02	0.41
1:A:38:VAL:O	1:A:38:VAL:HG12	2.20	0.41
1:A:248:THR:HG23	2:A:403:MC3:H142	2.02	0.41
1:C:248:THR:HG23	2:C:607:MC3:H142	2.02	0.41
1:H:248:THR:HG23	2:H:607:MC3:H142	2.02	0.41
1:I:38:VAL:O	1:I:38:VAL:HG12	2.20	0.41
1:L:30:VAL:O	1:L:34:ARG:HB3	2.20	0.41
1:A:38:VAL:O	1:A:38:VAL:CG1	2.69	0.41
1:D:38:VAL:O	1:D:38:VAL:CG1	2.69	0.41
1:E:24:ARG:H	1:E:24:ARG:HG3	1.71	0.41
1:E:30:VAL:O	1:E:34:ARG:HB3	2.20	0.41
1:F:197:ARG:O	1:F:201:ILE:HG12	2.21	0.41
1:F:248:THR:HG23	2:F:607:MC3:H142	2.02	0.41
1:G:197:ARG:O	1:G:201:ILE:HG12	2.21	0.41
1:H:38:VAL:O	1:H:38:VAL:CG1	2.69	0.41
1:B:35:ILE:O	1:B:35:ILE:CG2	2.69	0.41
1:I:35:ILE:O	1:I:35:ILE:CG2	2.69	0.41
1:K:38:VAL:O	1:K:38:VAL:CG1	2.69	0.41
1:L:248:THR:HG23	2:L:607:MC3:H142	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:PHE:CE1	1:B:199:TYR:HD1	2.40	0.40
1:B:197:ARG:O	1:B:201:ILE:HG12	2.21	0.40
1:B:220:LEU:HG	2:B:603:MC3:H172	2.02	0.40
1:E:220:LEU:HG	2:E:603:MC3:H172	2.03	0.40
1:F:38:VAL:O	1:F:38:VAL:CG1	2.69	0.40
1:I:93:PHE:CE1	1:I:199:TYR:HD1	2.40	0.40
1:I:197:ARG:O	1:I:201:ILE:HG12	2.21	0.40
1:L:38:VAL:O	1:L:38:VAL:CG1	2.69	0.40
1:A:93:PHE:CE1	1:A:199:TYR:HD1	2.40	0.40
1:E:197:ARG:O	1:E:201:ILE:HG12	2.21	0.40
1:J:38:VAL:O	1:J:38:VAL:CG1	2.69	0.40
1:K:262:GLY:O	1:K:266:VAL:HG23	2.22	0.40
1:B:24:ARG:H	1:B:24:ARG:HG3	1.71	0.40
1:C:34:ARG:HH12	1:C:86:VAL:CG2	2.29	0.40
1:C:197:ARG:O	1:C:201:ILE:HG12	2.21	0.40
1:D:41:VAL:HG13	1:E:77:ARG:HG3	2.03	0.40
1:D:262:GLY:O	1:D:266:VAL:HG23	2.22	0.40
1:G:38:VAL:O	1:G:38:VAL:CG1	2.69	0.40
1:J:34:ARG:HH12	1:J:86:VAL:CG2	2.29	0.40
1:J:93:PHE:CE1	1:J:199:TYR:HD1	2.40	0.40
1:K:34:ARG:HH12	1:K:86:VAL:CG2	2.29	0.40
1:L:197:ARG:O	1:L:201:ILE:HG12	2.21	0.40
1:L:267:LEU:HD23	1:L:267:LEU:HA	1.97	0.40
1:C:38:VAL:O	1:C:38:VAL:CG1	2.69	0.40
1:E:38:VAL:O	1:E:38:VAL:CG1	2.69	0.40
1:H:93:PHE:CE1	1:H:199:TYR:HD1	2.40	0.40
1:J:197:ARG:O	1:J:201:ILE:HG12	2.21	0.40
1:L:93:PHE:CE1	1:L:199:TYR:HD1	2.40	0.40
1:L:262:GLY:O	1:L:266:VAL:HG23	2.22	0.40
1:A:197:ARG:O	1:A:201:ILE:HG12	2.21	0.40
1:A:262:GLY:O	1:A:266:VAL:HG23	2.22	0.40
1:B:38:VAL:O	1:B:38:VAL:CG1	2.69	0.40
1:C:93:PHE:CE1	1:C:199:TYR:HD1	2.40	0.40
1:H:35:ILE:O	1:H:35:ILE:CG2	2.69	0.40
1:H:197:ARG:O	1:H:201:ILE:HG12	2.21	0.40
1:H:262:GLY:O	1:H:266:VAL:HG23	2.22	0.40
1:I:24:ARG:H	1:I:24:ARG:HG3	1.71	0.40
1:J:35:ILE:O	1:J:35:ILE:CG2	2.69	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	159/325 (49%)	157 (99%)	2 (1%)	0	100	100
1	B	159/325 (49%)	157 (99%)	2 (1%)	0	100	100
1	C	159/325 (49%)	157 (99%)	2 (1%)	0	100	100
1	D	159/325 (49%)	157 (99%)	2 (1%)	0	100	100
1	E	159/325 (49%)	157 (99%)	2 (1%)	0	100	100
1	F	159/325 (49%)	157 (99%)	2 (1%)	0	100	100
1	G	159/325 (49%)	157 (99%)	2 (1%)	0	100	100
1	H	159/325 (49%)	157 (99%)	2 (1%)	0	100	100
1	I	159/325 (49%)	157 (99%)	2 (1%)	0	100	100
1	J	159/325 (49%)	157 (99%)	2 (1%)	0	100	100
1	K	159/325 (49%)	157 (99%)	2 (1%)	0	100	100
1	L	159/325 (49%)	157 (99%)	2 (1%)	0	100	100
All	All	1908/3900 (49%)	1884 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	148/283 (52%)	138 (93%)	10 (7%)	16	48
1	B	148/283 (52%)	138 (93%)	10 (7%)	16	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	148/283 (52%)	138 (93%)	10 (7%)	16	48
1	D	148/283 (52%)	138 (93%)	10 (7%)	16	48
1	E	148/283 (52%)	138 (93%)	10 (7%)	16	48
1	F	148/283 (52%)	138 (93%)	10 (7%)	16	48
1	G	148/283 (52%)	138 (93%)	10 (7%)	16	48
1	H	148/283 (52%)	138 (93%)	10 (7%)	16	48
1	I	148/283 (52%)	138 (93%)	10 (7%)	16	48
1	J	148/283 (52%)	138 (93%)	10 (7%)	16	48
1	K	148/283 (52%)	138 (93%)	10 (7%)	16	48
1	L	148/283 (52%)	138 (93%)	10 (7%)	16	48
All	All	1776/3396 (52%)	1656 (93%)	120 (7%)	19	48

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	34	ARG
1	A	36	LEU
1	A	63	ASN
1	A	77	ARG
1	A	90	SER
1	A	97	SER
1	A	99	HIS
1	A	197	ARG
1	A	253	PHE
1	B	21	MET
1	B	34	ARG
1	B	36	LEU
1	B	63	ASN
1	B	77	ARG
1	B	90	SER
1	B	97	SER
1	B	99	HIS
1	B	197	ARG
1	B	253	PHE
1	C	21	MET
1	C	34	ARG
1	C	36	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	63	ASN
1	C	77	ARG
1	C	90	SER
1	C	97	SER
1	C	99	HIS
1	C	197	ARG
1	C	253	PHE
1	D	21	MET
1	D	34	ARG
1	D	36	LEU
1	D	63	ASN
1	D	77	ARG
1	D	90	SER
1	D	97	SER
1	D	99	HIS
1	D	197	ARG
1	D	253	PHE
1	E	21	MET
1	E	34	ARG
1	E	36	LEU
1	E	63	ASN
1	E	77	ARG
1	E	90	SER
1	E	97	SER
1	E	99	HIS
1	E	197	ARG
1	E	253	PHE
1	F	21	MET
1	F	34	ARG
1	F	36	LEU
1	F	63	ASN
1	F	77	ARG
1	F	90	SER
1	F	97	SER
1	F	99	HIS
1	F	197	ARG
1	F	253	PHE
1	G	21	MET
1	G	34	ARG
1	G	36	LEU
1	G	63	ASN
1	G	77	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	90	SER
1	G	97	SER
1	G	99	HIS
1	G	197	ARG
1	G	253	PHE
1	H	21	MET
1	H	34	ARG
1	H	36	LEU
1	H	63	ASN
1	H	77	ARG
1	H	90	SER
1	H	97	SER
1	H	99	HIS
1	H	197	ARG
1	H	253	PHE
1	I	21	MET
1	I	34	ARG
1	I	36	LEU
1	I	63	ASN
1	I	77	ARG
1	I	90	SER
1	I	97	SER
1	I	99	HIS
1	I	197	ARG
1	I	253	PHE
1	J	21	MET
1	J	34	ARG
1	J	36	LEU
1	J	63	ASN
1	J	77	ARG
1	J	90	SER
1	J	97	SER
1	J	99	HIS
1	J	197	ARG
1	J	253	PHE
1	K	21	MET
1	K	34	ARG
1	K	36	LEU
1	K	63	ASN
1	K	77	ARG
1	K	90	SER
1	K	97	SER

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Mol	Chain	Res	Type
1	K	99	HIS
1	K	197	ARG
1	K	253	PHE
1	L	21	MET
1	L	34	ARG
1	L	36	LEU
1	L	63	ASN
1	L	77	ARG
1	L	90	SER
1	L	97	SER
1	L	99	HIS
1	L	197	ARG
1	L	253	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	ASN
1	B	273	ASN
1	C	59	GLN
1	C	273	ASN
1	D	59	GLN
1	D	273	ASN
1	E	273	ASN
1	F	273	ASN
1	G	59	GLN
1	G	273	ASN
1	H	59	GLN
1	H	273	ASN
1	I	59	GLN
1	I	273	ASN
1	J	59	GLN
1	J	273	ASN
1	K	273	ASN
1	L	273	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

84 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	L	604	-	13,13,45	0.29	0	12,12,53	0.38	0
2	MC3	H	604	-	13,13,45	0.29	0	12,12,53	0.38	0
2	MC3	I	606	-	13,13,45	0.13	0	12,12,53	0.79	0
2	MC3	A	407	-	13,13,45	0.29	0	12,12,53	0.38	0
2	MC3	L	607	-	13,13,45	0.20	0	12,12,53	0.82	0
2	MC3	G	406	-	13,13,45	0.16	0	12,12,53	0.88	0
2	MC3	A	402	-	13,13,45	0.13	0	12,12,53	0.79	0
2	MC3	J	601	-	13,13,45	0.20	0	12,12,53	0.43	0
2	MC3	J	603	-	13,13,45	0.16	0	12,12,53	0.88	0
2	MC3	L	601	-	13,13,45	0.20	0	12,12,53	0.43	0
2	MC3	H	601	-	13,13,45	0.20	0	12,12,53	0.43	0
2	MC3	L	606	-	13,13,45	0.13	0	12,12,53	0.79	0
2	MC3	E	603	-	13,13,45	0.16	0	12,12,53	0.88	0
2	MC3	H	606	-	13,13,45	0.13	0	12,12,53	0.79	0
2	MC3	I	605	-	13,13,45	0.19	0	12,12,53	0.53	0
2	MC3	B	604	-	13,13,45	0.29	0	12,12,53	0.38	0
2	MC3	G	407	-	13,13,45	0.29	0	12,12,53	0.38	0
2	MC3	C	603	-	13,13,45	0.16	0	12,12,53	0.88	0
2	MC3	D	605	-	13,13,45	0.19	0	12,12,53	0.53	0
2	MC3	B	607	-	13,13,45	0.20	0	12,12,53	0.82	0
2	MC3	L	603	-	13,13,45	0.16	0	12,12,53	0.88	0
2	MC3	I	603	-	13,13,45	0.16	0	12,12,53	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MC3	I	604	-	13,13,45	0.29	0	12,12,53	0.37	0
2	MC3	J	604	-	13,13,45	0.29	0	12,12,53	0.38	0
2	MC3	J	606	-	13,13,45	0.13	0	12,12,53	0.80	0
2	MC3	D	602	-	13,13,45	0.15	0	12,12,53	1.27	2 (16%)
2	MC3	E	602	-	13,13,45	0.15	0	12,12,53	1.27	3 (25%)
2	MC3	A	401	-	13,13,45	0.19	0	12,12,53	0.53	0
2	MC3	A	405	-	13,13,45	0.15	0	12,12,53	1.27	3 (25%)
2	MC3	K	602	-	13,13,45	0.15	0	12,12,53	1.27	2 (16%)
2	MC3	G	402	-	13,13,45	0.13	0	12,12,53	0.79	0
2	MC3	G	404	-	13,13,45	0.20	0	12,12,53	0.42	0
2	MC3	F	607	-	13,13,45	0.20	0	12,12,53	0.82	0
2	MC3	C	607	-	13,13,45	0.20	0	12,12,53	0.81	0
2	MC3	D	601	-	13,13,45	0.21	0	12,12,53	0.43	0
2	MC3	C	602	-	13,13,45	0.15	0	12,12,53	1.27	2 (16%)
2	MC3	F	605	-	13,13,45	0.19	0	12,12,53	0.53	0
2	MC3	H	607	-	13,13,45	0.20	0	12,12,53	0.82	0
2	MC3	C	601	-	13,13,45	0.21	0	12,12,53	0.43	0
2	MC3	A	403	-	13,13,45	0.20	0	12,12,53	0.82	0
2	MC3	C	605	-	13,13,45	0.19	0	12,12,53	0.53	0
2	MC3	B	603	-	13,13,45	0.16	0	12,12,53	0.88	0
2	MC3	F	606	-	13,13,45	0.13	0	12,12,53	0.79	0
2	MC3	I	607	-	13,13,45	0.20	0	12,12,53	0.82	0
2	MC3	I	602	-	13,13,45	0.15	0	12,12,53	1.27	2 (16%)
2	MC3	J	602	-	13,13,45	0.15	0	12,12,53	1.27	2 (16%)
2	MC3	G	401	-	13,13,45	0.19	0	12,12,53	0.54	0
2	MC3	K	605	-	13,13,45	0.19	0	12,12,53	0.53	0
2	MC3	F	601	-	13,13,45	0.20	0	12,12,53	0.43	0
2	MC3	H	605	-	13,13,45	0.19	0	12,12,53	0.53	0
2	MC3	J	605	-	13,13,45	0.19	0	12,12,53	0.53	0
2	MC3	D	604	-	13,13,45	0.28	0	12,12,53	0.37	0
2	MC3	E	604	-	13,13,45	0.29	0	12,12,53	0.38	0
2	MC3	B	602	-	13,13,45	0.15	0	12,12,53	1.27	2 (16%)
2	MC3	H	602	-	13,13,45	0.15	0	12,12,53	1.27	3 (25%)
2	MC3	E	606	-	13,13,45	0.13	0	12,12,53	0.79	0
2	MC3	B	601	-	13,13,45	0.20	0	12,12,53	0.43	0
2	MC3	K	604	-	13,13,45	0.28	0	12,12,53	0.37	0
2	MC3	H	603	-	13,13,45	0.16	0	12,12,53	0.88	0
2	MC3	D	607	-	13,13,45	0.20	0	12,12,53	0.82	0
2	MC3	A	406	-	13,13,45	0.16	0	12,12,53	0.88	0
2	MC3	A	404	-	13,13,45	0.21	0	12,12,53	0.43	0
2	MC3	F	603	-	13,13,45	0.16	0	12,12,53	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MC3	B	606	-	13,13,45	0.13	0	12,12,53	0.79	0
2	MC3	E	601	-	13,13,45	0.20	0	12,12,53	0.43	0
2	MC3	F	602	-	13,13,45	0.15	0	12,12,53	1.27	2 (16%)
2	MC3	D	606	-	13,13,45	0.13	0	12,12,53	0.79	0
2	MC3	K	607	-	13,13,45	0.20	0	12,12,53	0.82	0
2	MC3	J	607	-	13,13,45	0.20	0	12,12,53	0.81	0
2	MC3	K	601	-	13,13,45	0.20	0	12,12,53	0.43	0
2	MC3	L	605	-	13,13,45	0.19	0	12,12,53	0.53	0
2	MC3	B	605	-	13,13,45	0.19	0	12,12,53	0.53	0
2	MC3	E	607	-	13,13,45	0.20	0	12,12,53	0.82	0
2	MC3	E	605	-	13,13,45	0.19	0	12,12,53	0.53	0
2	MC3	L	602	-	13,13,45	0.15	0	12,12,53	1.27	3 (25%)
2	MC3	K	606	-	13,13,45	0.13	0	12,12,53	0.79	0
2	MC3	C	604	-	13,13,45	0.29	0	12,12,53	0.38	0
2	MC3	G	405	-	13,13,45	0.15	0	12,12,53	1.27	2 (16%)
2	MC3	C	606	-	13,13,45	0.13	0	12,12,53	0.79	0
2	MC3	G	403	-	13,13,45	0.20	0	12,12,53	0.82	0
2	MC3	D	603	-	13,13,45	0.16	0	12,12,53	0.88	0
2	MC3	I	601	-	13,13,45	0.20	0	12,12,53	0.43	0
2	MC3	K	603	-	13,13,45	0.16	0	12,12,53	0.88	0
2	MC3	F	604	-	13,13,45	0.29	0	12,12,53	0.37	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	L	604	-	-	5/11/11/49	-
2	MC3	H	604	-	-	5/11/11/49	-
2	MC3	I	606	-	-	7/11/11/49	-
2	MC3	A	407	-	-	5/11/11/49	-
2	MC3	L	607	-	-	6/11/11/49	-
2	MC3	G	406	-	-	6/11/11/49	-
2	MC3	A	402	-	-	7/11/11/49	-
2	MC3	J	601	-	-	6/11/11/49	-
2	MC3	J	603	-	-	6/11/11/49	-
2	MC3	L	601	-	-	6/11/11/49	-
2	MC3	H	601	-	-	6/11/11/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	L	606	-	-	7/11/11/49	-
2	MC3	E	603	-	-	6/11/11/49	-
2	MC3	H	606	-	-	7/11/11/49	-
2	MC3	I	605	-	-	8/11/11/49	-
2	MC3	B	604	-	-	5/11/11/49	-
2	MC3	G	407	-	-	5/11/11/49	-
2	MC3	C	603	-	-	6/11/11/49	-
2	MC3	D	605	-	-	8/11/11/49	-
2	MC3	B	607	-	-	6/11/11/49	-
2	MC3	L	603	-	-	6/11/11/49	-
2	MC3	I	603	-	-	6/11/11/49	-
2	MC3	I	604	-	-	5/11/11/49	-
2	MC3	J	604	-	-	5/11/11/49	-
2	MC3	J	606	-	-	7/11/11/49	-
2	MC3	D	602	-	-	4/11/11/49	-
2	MC3	E	602	-	-	4/11/11/49	-
2	MC3	A	401	-	-	8/11/11/49	-
2	MC3	A	405	-	-	4/11/11/49	-
2	MC3	K	602	-	-	4/11/11/49	-
2	MC3	G	402	-	-	7/11/11/49	-
2	MC3	G	404	-	-	6/11/11/49	-
2	MC3	F	607	-	-	6/11/11/49	-
2	MC3	C	607	-	-	6/11/11/49	-
2	MC3	D	601	-	-	6/11/11/49	-
2	MC3	C	602	-	-	4/11/11/49	-
2	MC3	F	605	-	-	8/11/11/49	-
2	MC3	H	607	-	-	6/11/11/49	-
2	MC3	C	601	-	-	6/11/11/49	-
2	MC3	A	403	-	-	6/11/11/49	-
2	MC3	C	605	-	-	8/11/11/49	-
2	MC3	B	603	-	-	6/11/11/49	-
2	MC3	F	606	-	-	7/11/11/49	-
2	MC3	I	607	-	-	6/11/11/49	-
2	MC3	I	602	-	-	4/11/11/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	J	602	-	-	4/11/11/49	-
2	MC3	G	401	-	-	8/11/11/49	-
2	MC3	K	605	-	-	8/11/11/49	-
2	MC3	F	601	-	-	6/11/11/49	-
2	MC3	H	605	-	-	8/11/11/49	-
2	MC3	J	605	-	-	8/11/11/49	-
2	MC3	D	604	-	-	5/11/11/49	-
2	MC3	E	604	-	-	5/11/11/49	-
2	MC3	B	602	-	-	4/11/11/49	-
2	MC3	H	602	-	-	4/11/11/49	-
2	MC3	E	606	-	-	7/11/11/49	-
2	MC3	B	601	-	-	6/11/11/49	-
2	MC3	K	604	-	-	5/11/11/49	-
2	MC3	H	603	-	-	6/11/11/49	-
2	MC3	D	607	-	-	6/11/11/49	-
2	MC3	A	406	-	-	6/11/11/49	-
2	MC3	A	404	-	-	6/11/11/49	-
2	MC3	F	603	-	-	6/11/11/49	-
2	MC3	B	606	-	-	7/11/11/49	-
2	MC3	E	601	-	-	6/11/11/49	-
2	MC3	F	602	-	-	4/11/11/49	-
2	MC3	D	606	-	-	7/11/11/49	-
2	MC3	K	607	-	-	6/11/11/49	-
2	MC3	J	607	-	-	6/11/11/49	-
2	MC3	K	601	-	-	6/11/11/49	-
2	MC3	L	605	-	-	8/11/11/49	-
2	MC3	B	605	-	-	8/11/11/49	-
2	MC3	E	607	-	-	6/11/11/49	-
2	MC3	E	605	-	-	8/11/11/49	-
2	MC3	L	602	-	-	4/11/11/49	-
2	MC3	K	606	-	-	7/11/11/49	-
2	MC3	C	604	-	-	5/11/11/49	-
2	MC3	G	405	-	-	4/11/11/49	-
2	MC3	C	606	-	-	7/11/11/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MC3	G	403	-	-	6/11/11/49	-
2	MC3	D	603	-	-	6/11/11/49	-
2	MC3	I	601	-	-	6/11/11/49	-
2	MC3	K	603	-	-	6/11/11/49	-
2	MC3	F	604	-	-	5/11/11/49	-

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	602	MC3	C20-C19-C18	-2.27	102.92	114.42
2	C	602	MC3	C20-C19-C18	-2.25	102.98	114.42
2	K	602	MC3	C20-C19-C18	-2.25	102.98	114.42
2	F	602	MC3	C20-C19-C18	-2.25	102.98	114.42
2	I	602	MC3	C20-C19-C18	-2.25	102.98	114.42
2	B	602	MC3	C20-C19-C18	-2.25	102.99	114.42
2	D	602	MC3	C20-C19-C18	-2.25	102.99	114.42
2	A	405	MC3	C20-C19-C18	-2.25	102.99	114.42
2	J	602	MC3	C20-C19-C18	-2.25	102.99	114.42
2	E	602	MC3	C20-C19-C18	-2.25	103.01	114.42
2	G	405	MC3	C20-C19-C18	-2.25	103.01	114.42
2	H	602	MC3	C20-C19-C18	-2.25	103.01	114.42
2	J	602	MC3	C19-C18-C17	2.05	124.83	114.42
2	K	602	MC3	C19-C18-C17	2.05	124.83	114.42
2	G	405	MC3	C19-C18-C17	2.05	124.81	114.42
2	H	602	MC3	C19-C18-C17	2.05	124.81	114.42
2	I	602	MC3	C19-C18-C17	2.04	124.80	114.42
2	D	602	MC3	C19-C18-C17	2.04	124.79	114.42
2	B	602	MC3	C19-C18-C17	2.04	124.79	114.42
2	E	602	MC3	C19-C18-C17	2.04	124.79	114.42
2	F	602	MC3	C19-C18-C17	2.04	124.78	114.42
2	L	602	MC3	C19-C18-C17	2.04	124.78	114.42
2	C	602	MC3	C19-C18-C17	2.04	124.76	114.42
2	A	405	MC3	C19-C18-C17	2.03	124.75	114.42
2	E	602	MC3	C15-C14-C13	-2.00	104.26	114.42
2	H	602	MC3	C15-C14-C13	-2.00	104.26	114.42
2	L	602	MC3	C15-C14-C13	-2.00	104.27	114.42
2	A	405	MC3	C15-C14-C13	-2.00	104.27	114.42

There are no chirality outliers.

All (504) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	607	MC3	C19-C20-C21-C22
2	A	403	MC3	C16-C17-C18-C19
2	A	403	MC3	C19-C20-C21-C22
2	A	404	MC3	C18-C19-C20-C21
2	B	601	MC3	C18-C19-C20-C21
2	B	607	MC3	C16-C17-C18-C19
2	B	607	MC3	C19-C20-C21-C22
2	C	601	MC3	C18-C19-C20-C21
2	C	607	MC3	C16-C17-C18-C19
2	C	607	MC3	C19-C20-C21-C22
2	D	601	MC3	C18-C19-C20-C21
2	D	607	MC3	C16-C17-C18-C19
2	D	607	MC3	C19-C20-C21-C22
2	E	601	MC3	C18-C19-C20-C21
2	E	607	MC3	C16-C17-C18-C19
2	E	607	MC3	C19-C20-C21-C22
2	F	601	MC3	C18-C19-C20-C21
2	F	607	MC3	C16-C17-C18-C19
2	F	607	MC3	C19-C20-C21-C22
2	G	403	MC3	C16-C17-C18-C19
2	G	403	MC3	C19-C20-C21-C22
2	G	404	MC3	C18-C19-C20-C21
2	H	601	MC3	C18-C19-C20-C21
2	H	607	MC3	C16-C17-C18-C19
2	H	607	MC3	C19-C20-C21-C22
2	I	601	MC3	C18-C19-C20-C21
2	I	607	MC3	C16-C17-C18-C19
2	I	607	MC3	C19-C20-C21-C22
2	J	601	MC3	C18-C19-C20-C21
2	J	607	MC3	C16-C17-C18-C19
2	K	601	MC3	C18-C19-C20-C21
2	K	607	MC3	C16-C17-C18-C19
2	K	607	MC3	C19-C20-C21-C22
2	L	601	MC3	C18-C19-C20-C21
2	L	607	MC3	C16-C17-C18-C19
2	L	607	MC3	C19-C20-C21-C22
2	G	407	MC3	C15-C16-C17-C18
2	H	604	MC3	C15-C16-C17-C18
2	A	407	MC3	C15-C16-C17-C18
2	B	604	MC3	C15-C16-C17-C18
2	C	604	MC3	C15-C16-C17-C18
2	D	604	MC3	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
2	E	604	MC3	C15-C16-C17-C18
2	F	604	MC3	C15-C16-C17-C18
2	I	604	MC3	C15-C16-C17-C18
2	J	604	MC3	C15-C16-C17-C18
2	K	604	MC3	C15-C16-C17-C18
2	L	604	MC3	C15-C16-C17-C18
2	A	407	MC3	C20-C21-C22-C23
2	B	604	MC3	C20-C21-C22-C23
2	C	604	MC3	C20-C21-C22-C23
2	D	604	MC3	C20-C21-C22-C23
2	E	604	MC3	C20-C21-C22-C23
2	F	604	MC3	C20-C21-C22-C23
2	G	407	MC3	C20-C21-C22-C23
2	H	604	MC3	C20-C21-C22-C23
2	I	604	MC3	C20-C21-C22-C23
2	J	604	MC3	C20-C21-C22-C23
2	K	604	MC3	C20-C21-C22-C23
2	L	604	MC3	C20-C21-C22-C23
2	A	401	MC3	C15-C16-C17-C18
2	B	605	MC3	C15-C16-C17-C18
2	C	605	MC3	C15-C16-C17-C18
2	D	605	MC3	C15-C16-C17-C18
2	E	605	MC3	C15-C16-C17-C18
2	F	605	MC3	C15-C16-C17-C18
2	G	401	MC3	C15-C16-C17-C18
2	H	605	MC3	C15-C16-C17-C18
2	I	605	MC3	C15-C16-C17-C18
2	J	605	MC3	C15-C16-C17-C18
2	K	605	MC3	C15-C16-C17-C18
2	L	605	MC3	C15-C16-C17-C18
2	A	404	MC3	C20-C21-C22-C23
2	C	601	MC3	C20-C21-C22-C23
2	E	601	MC3	C20-C21-C22-C23
2	F	601	MC3	C20-C21-C22-C23
2	G	404	MC3	C20-C21-C22-C23
2	J	601	MC3	C20-C21-C22-C23
2	K	601	MC3	C20-C21-C22-C23
2	B	601	MC3	C20-C21-C22-C23
2	D	601	MC3	C20-C21-C22-C23
2	H	601	MC3	C20-C21-C22-C23
2	I	601	MC3	C20-C21-C22-C23
2	L	601	MC3	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
2	A	401	MC3	C20-C21-C22-C23
2	B	605	MC3	C20-C21-C22-C23
2	C	605	MC3	C20-C21-C22-C23
2	D	605	MC3	C20-C21-C22-C23
2	E	605	MC3	C20-C21-C22-C23
2	F	605	MC3	C20-C21-C22-C23
2	G	401	MC3	C20-C21-C22-C23
2	H	605	MC3	C20-C21-C22-C23
2	I	605	MC3	C20-C21-C22-C23
2	J	605	MC3	C20-C21-C22-C23
2	K	605	MC3	C20-C21-C22-C23
2	L	605	MC3	C20-C21-C22-C23
2	A	404	MC3	C16-C17-C18-C19
2	B	601	MC3	C16-C17-C18-C19
2	C	601	MC3	C16-C17-C18-C19
2	D	601	MC3	C16-C17-C18-C19
2	F	601	MC3	C16-C17-C18-C19
2	H	601	MC3	C16-C17-C18-C19
2	I	601	MC3	C16-C17-C18-C19
2	K	601	MC3	C16-C17-C18-C19
2	L	601	MC3	C16-C17-C18-C19
2	A	402	MC3	C18-C19-C20-C21
2	B	606	MC3	C18-C19-C20-C21
2	C	606	MC3	C18-C19-C20-C21
2	D	606	MC3	C18-C19-C20-C21
2	E	601	MC3	C16-C17-C18-C19
2	E	606	MC3	C18-C19-C20-C21
2	F	606	MC3	C18-C19-C20-C21
2	G	402	MC3	C18-C19-C20-C21
2	G	404	MC3	C16-C17-C18-C19
2	H	606	MC3	C18-C19-C20-C21
2	I	606	MC3	C18-C19-C20-C21
2	J	601	MC3	C16-C17-C18-C19
2	J	606	MC3	C18-C19-C20-C21
2	K	606	MC3	C18-C19-C20-C21
2	L	606	MC3	C18-C19-C20-C21
2	A	404	MC3	C12-C13-C14-C15
2	B	601	MC3	C12-C13-C14-C15
2	C	601	MC3	C12-C13-C14-C15
2	D	601	MC3	C12-C13-C14-C15
2	G	404	MC3	C12-C13-C14-C15
2	H	601	MC3	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
2	J	601	MC3	C12-C13-C14-C15
2	K	601	MC3	C12-C13-C14-C15
2	A	406	MC3	C13-C14-C15-C16
2	B	603	MC3	C13-C14-C15-C16
2	C	603	MC3	C13-C14-C15-C16
2	D	603	MC3	C13-C14-C15-C16
2	E	601	MC3	C12-C13-C14-C15
2	E	603	MC3	C13-C14-C15-C16
2	F	601	MC3	C12-C13-C14-C15
2	F	603	MC3	C13-C14-C15-C16
2	G	406	MC3	C13-C14-C15-C16
2	H	603	MC3	C13-C14-C15-C16
2	I	601	MC3	C12-C13-C14-C15
2	I	603	MC3	C13-C14-C15-C16
2	J	603	MC3	C13-C14-C15-C16
2	K	603	MC3	C13-C14-C15-C16
2	L	601	MC3	C12-C13-C14-C15
2	L	603	MC3	C13-C14-C15-C16
2	A	401	MC3	C17-C18-C19-C20
2	A	402	MC3	C19-C20-C21-C22
2	B	605	MC3	C17-C18-C19-C20
2	B	606	MC3	C19-C20-C21-C22
2	C	605	MC3	C17-C18-C19-C20
2	C	606	MC3	C19-C20-C21-C22
2	D	605	MC3	C17-C18-C19-C20
2	D	606	MC3	C19-C20-C21-C22
2	E	605	MC3	C17-C18-C19-C20
2	E	606	MC3	C19-C20-C21-C22
2	F	605	MC3	C17-C18-C19-C20
2	F	606	MC3	C19-C20-C21-C22
2	G	401	MC3	C17-C18-C19-C20
2	G	402	MC3	C19-C20-C21-C22
2	H	605	MC3	C17-C18-C19-C20
2	H	606	MC3	C19-C20-C21-C22
2	I	605	MC3	C17-C18-C19-C20
2	I	606	MC3	C19-C20-C21-C22
2	J	605	MC3	C17-C18-C19-C20
2	J	606	MC3	C19-C20-C21-C22
2	K	605	MC3	C17-C18-C19-C20
2	K	606	MC3	C19-C20-C21-C22
2	L	605	MC3	C17-C18-C19-C20
2	L	606	MC3	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
2	A	401	MC3	C13-C14-C15-C16
2	B	605	MC3	C13-C14-C15-C16
2	C	605	MC3	C13-C14-C15-C16
2	D	605	MC3	C13-C14-C15-C16
2	E	605	MC3	C13-C14-C15-C16
2	F	605	MC3	C13-C14-C15-C16
2	G	401	MC3	C13-C14-C15-C16
2	H	605	MC3	C13-C14-C15-C16
2	I	605	MC3	C13-C14-C15-C16
2	J	605	MC3	C13-C14-C15-C16
2	K	605	MC3	C13-C14-C15-C16
2	L	605	MC3	C13-C14-C15-C16
2	F	603	MC3	C12-C13-C14-C15
2	I	603	MC3	C12-C13-C14-C15
2	K	603	MC3	C12-C13-C14-C15
2	A	406	MC3	C12-C13-C14-C15
2	B	603	MC3	C12-C13-C14-C15
2	C	603	MC3	C12-C13-C14-C15
2	D	603	MC3	C12-C13-C14-C15
2	E	603	MC3	C12-C13-C14-C15
2	G	406	MC3	C12-C13-C14-C15
2	H	603	MC3	C12-C13-C14-C15
2	J	603	MC3	C12-C13-C14-C15
2	L	603	MC3	C12-C13-C14-C15
2	A	401	MC3	C11-C12-C13-C14
2	B	605	MC3	C11-C12-C13-C14
2	C	605	MC3	C11-C12-C13-C14
2	D	605	MC3	C11-C12-C13-C14
2	E	605	MC3	C11-C12-C13-C14
2	F	605	MC3	C11-C12-C13-C14
2	G	401	MC3	C11-C12-C13-C14
2	H	605	MC3	C11-C12-C13-C14
2	I	605	MC3	C11-C12-C13-C14
2	J	605	MC3	C11-C12-C13-C14
2	L	605	MC3	C11-C12-C13-C14
2	K	605	MC3	C11-C12-C13-C14
2	G	402	MC3	C12-C13-C14-C15
2	J	606	MC3	C12-C13-C14-C15
2	A	402	MC3	C12-C13-C14-C15
2	B	606	MC3	C12-C13-C14-C15
2	C	606	MC3	C12-C13-C14-C15
2	D	606	MC3	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
2	E	606	MC3	C12-C13-C14-C15
2	F	606	MC3	C12-C13-C14-C15
2	H	606	MC3	C12-C13-C14-C15
2	I	606	MC3	C12-C13-C14-C15
2	K	606	MC3	C12-C13-C14-C15
2	L	606	MC3	C12-C13-C14-C15
2	A	402	MC3	C11-C12-C13-C14
2	B	606	MC3	C11-C12-C13-C14
2	C	606	MC3	C11-C12-C13-C14
2	D	606	MC3	C11-C12-C13-C14
2	E	606	MC3	C11-C12-C13-C14
2	F	606	MC3	C11-C12-C13-C14
2	G	402	MC3	C11-C12-C13-C14
2	H	606	MC3	C11-C12-C13-C14
2	J	606	MC3	C11-C12-C13-C14
2	K	606	MC3	C11-C12-C13-C14
2	L	606	MC3	C11-C12-C13-C14
2	I	606	MC3	C11-C12-C13-C14
2	A	403	MC3	C15-C16-C17-C18
2	B	607	MC3	C15-C16-C17-C18
2	C	607	MC3	C15-C16-C17-C18
2	D	607	MC3	C15-C16-C17-C18
2	E	607	MC3	C15-C16-C17-C18
2	F	607	MC3	C15-C16-C17-C18
2	G	403	MC3	C15-C16-C17-C18
2	H	607	MC3	C15-C16-C17-C18
2	J	607	MC3	C15-C16-C17-C18
2	K	607	MC3	C15-C16-C17-C18
2	L	607	MC3	C15-C16-C17-C18
2	I	607	MC3	C15-C16-C17-C18
2	B	604	MC3	C16-C17-C18-C19
2	C	604	MC3	C16-C17-C18-C19
2	D	604	MC3	C16-C17-C18-C19
2	E	604	MC3	C16-C17-C18-C19
2	F	604	MC3	C16-C17-C18-C19
2	G	407	MC3	C16-C17-C18-C19
2	H	604	MC3	C16-C17-C18-C19
2	I	604	MC3	C16-C17-C18-C19
2	J	604	MC3	C16-C17-C18-C19
2	K	604	MC3	C16-C17-C18-C19
2	L	604	MC3	C16-C17-C18-C19
2	A	407	MC3	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
2	F	602	MC3	C13-C14-C15-C16
2	I	602	MC3	C13-C14-C15-C16
2	J	602	MC3	C13-C14-C15-C16
2	A	405	MC3	C13-C14-C15-C16
2	B	602	MC3	C13-C14-C15-C16
2	C	602	MC3	C13-C14-C15-C16
2	D	602	MC3	C13-C14-C15-C16
2	E	602	MC3	C13-C14-C15-C16
2	G	405	MC3	C13-C14-C15-C16
2	H	602	MC3	C13-C14-C15-C16
2	K	602	MC3	C13-C14-C15-C16
2	L	602	MC3	C13-C14-C15-C16
2	A	404	MC3	C21-C22-C23-C24
2	B	601	MC3	C21-C22-C23-C24
2	C	601	MC3	C21-C22-C23-C24
2	E	601	MC3	C21-C22-C23-C24
2	G	404	MC3	C21-C22-C23-C24
2	H	601	MC3	C21-C22-C23-C24
2	I	601	MC3	C21-C22-C23-C24
2	J	601	MC3	C21-C22-C23-C24
2	K	601	MC3	C21-C22-C23-C24
2	L	601	MC3	C21-C22-C23-C24
2	D	601	MC3	C21-C22-C23-C24
2	F	601	MC3	C21-C22-C23-C24
2	A	401	MC3	C21-C22-C23-C24
2	C	605	MC3	C21-C22-C23-C24
2	D	605	MC3	C21-C22-C23-C24
2	E	605	MC3	C21-C22-C23-C24
2	J	605	MC3	C21-C22-C23-C24
2	L	605	MC3	C21-C22-C23-C24
2	B	605	MC3	C21-C22-C23-C24
2	F	605	MC3	C21-C22-C23-C24
2	G	401	MC3	C21-C22-C23-C24
2	H	605	MC3	C21-C22-C23-C24
2	I	605	MC3	C21-C22-C23-C24
2	K	605	MC3	C21-C22-C23-C24
2	H	605	MC3	C14-C15-C16-C17
2	I	605	MC3	C14-C15-C16-C17
2	A	401	MC3	C14-C15-C16-C17
2	B	605	MC3	C14-C15-C16-C17
2	C	605	MC3	C14-C15-C16-C17
2	D	605	MC3	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
2	E	605	MC3	C14-C15-C16-C17
2	F	605	MC3	C14-C15-C16-C17
2	G	401	MC3	C14-C15-C16-C17
2	J	605	MC3	C14-C15-C16-C17
2	K	605	MC3	C14-C15-C16-C17
2	L	605	MC3	C14-C15-C16-C17
2	C	603	MC3	C21-C22-C23-C24
2	A	406	MC3	C21-C22-C23-C24
2	E	603	MC3	C21-C22-C23-C24
2	G	406	MC3	C21-C22-C23-C24
2	K	603	MC3	C21-C22-C23-C24
2	B	603	MC3	C21-C22-C23-C24
2	D	603	MC3	C21-C22-C23-C24
2	H	603	MC3	C21-C22-C23-C24
2	I	603	MC3	C21-C22-C23-C24
2	J	603	MC3	C21-C22-C23-C24
2	L	603	MC3	C21-C22-C23-C24
2	F	603	MC3	C21-C22-C23-C24
2	A	402	MC3	C14-C15-C16-C17
2	C	606	MC3	C14-C15-C16-C17
2	D	606	MC3	C14-C15-C16-C17
2	G	402	MC3	C14-C15-C16-C17
2	J	606	MC3	C14-C15-C16-C17
2	K	606	MC3	C14-C15-C16-C17
2	L	606	MC3	C14-C15-C16-C17
2	B	606	MC3	C14-C15-C16-C17
2	E	606	MC3	C14-C15-C16-C17
2	F	606	MC3	C14-C15-C16-C17
2	H	606	MC3	C14-C15-C16-C17
2	I	606	MC3	C14-C15-C16-C17
2	A	403	MC3	C12-C13-C14-C15
2	C	607	MC3	C12-C13-C14-C15
2	D	607	MC3	C12-C13-C14-C15
2	E	607	MC3	C12-C13-C14-C15
2	F	603	MC3	C11-C12-C13-C14
2	F	607	MC3	C12-C13-C14-C15
2	G	403	MC3	C12-C13-C14-C15
2	H	607	MC3	C12-C13-C14-C15
2	I	607	MC3	C12-C13-C14-C15
2	K	607	MC3	C12-C13-C14-C15
2	L	607	MC3	C12-C13-C14-C15
2	A	406	MC3	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	B	603	MC3	C11-C12-C13-C14
2	B	607	MC3	C12-C13-C14-C15
2	C	603	MC3	C11-C12-C13-C14
2	D	603	MC3	C11-C12-C13-C14
2	E	603	MC3	C11-C12-C13-C14
2	G	406	MC3	C11-C12-C13-C14
2	H	603	MC3	C11-C12-C13-C14
2	I	603	MC3	C11-C12-C13-C14
2	J	603	MC3	C11-C12-C13-C14
2	J	607	MC3	C12-C13-C14-C15
2	K	603	MC3	C11-C12-C13-C14
2	L	603	MC3	C11-C12-C13-C14
2	F	601	MC3	C13-C14-C15-C16
2	G	404	MC3	C13-C14-C15-C16
2	J	601	MC3	C13-C14-C15-C16
2	B	601	MC3	C13-C14-C15-C16
2	C	601	MC3	C13-C14-C15-C16
2	D	601	MC3	C13-C14-C15-C16
2	E	601	MC3	C13-C14-C15-C16
2	K	601	MC3	C13-C14-C15-C16
2	L	601	MC3	C13-C14-C15-C16
2	A	404	MC3	C13-C14-C15-C16
2	H	601	MC3	C13-C14-C15-C16
2	I	601	MC3	C13-C14-C15-C16
2	B	607	MC3	C11-C12-C13-C14
2	C	606	MC3	C16-C17-C18-C19
2	D	606	MC3	C16-C17-C18-C19
2	E	606	MC3	C16-C17-C18-C19
2	I	606	MC3	C16-C17-C18-C19
2	J	606	MC3	C16-C17-C18-C19
2	L	607	MC3	C11-C12-C13-C14
2	A	402	MC3	C16-C17-C18-C19
2	A	403	MC3	C11-C12-C13-C14
2	C	607	MC3	C11-C12-C13-C14
2	D	607	MC3	C11-C12-C13-C14
2	E	607	MC3	C11-C12-C13-C14
2	F	607	MC3	C11-C12-C13-C14
2	G	402	MC3	C16-C17-C18-C19
2	G	403	MC3	C11-C12-C13-C14
2	H	606	MC3	C16-C17-C18-C19
2	H	607	MC3	C11-C12-C13-C14
2	I	607	MC3	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	J	607	MC3	C11-C12-C13-C14
2	K	606	MC3	C16-C17-C18-C19
2	K	607	MC3	C11-C12-C13-C14
2	B	606	MC3	C16-C17-C18-C19
2	F	606	MC3	C16-C17-C18-C19
2	L	606	MC3	C16-C17-C18-C19
2	A	406	MC3	C14-C15-C16-C17
2	G	406	MC3	C14-C15-C16-C17
2	I	603	MC3	C14-C15-C16-C17
2	L	603	MC3	C14-C15-C16-C17
2	B	603	MC3	C14-C15-C16-C17
2	D	603	MC3	C14-C15-C16-C17
2	E	603	MC3	C14-C15-C16-C17
2	F	603	MC3	C14-C15-C16-C17
2	H	603	MC3	C14-C15-C16-C17
2	J	603	MC3	C14-C15-C16-C17
2	K	603	MC3	C14-C15-C16-C17
2	C	603	MC3	C14-C15-C16-C17
2	L	604	MC3	C17-C18-C19-C20
2	F	604	MC3	C17-C18-C19-C20
2	I	604	MC3	C17-C18-C19-C20
2	A	407	MC3	C17-C18-C19-C20
2	B	604	MC3	C17-C18-C19-C20
2	E	604	MC3	C17-C18-C19-C20
2	G	407	MC3	C17-C18-C19-C20
2	C	604	MC3	C17-C18-C19-C20
2	D	604	MC3	C17-C18-C19-C20
2	H	604	MC3	C17-C18-C19-C20
2	J	604	MC3	C17-C18-C19-C20
2	K	604	MC3	C17-C18-C19-C20
2	F	607	MC3	C18-C19-C20-C21
2	A	403	MC3	C18-C19-C20-C21
2	B	607	MC3	C18-C19-C20-C21
2	C	607	MC3	C18-C19-C20-C21
2	E	607	MC3	C18-C19-C20-C21
2	G	403	MC3	C18-C19-C20-C21
2	H	607	MC3	C18-C19-C20-C21
2	J	607	MC3	C18-C19-C20-C21
2	K	607	MC3	C18-C19-C20-C21
2	L	607	MC3	C18-C19-C20-C21
2	D	607	MC3	C18-C19-C20-C21
2	I	607	MC3	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
2	J	606	MC3	C20-C21-C22-C23
2	G	402	MC3	C20-C21-C22-C23
2	G	405	MC3	C20-C21-C22-C23
2	H	602	MC3	C20-C21-C22-C23
2	I	606	MC3	C20-C21-C22-C23
2	K	602	MC3	C20-C21-C22-C23
2	K	606	MC3	C20-C21-C22-C23
2	B	602	MC3	C20-C21-C22-C23
2	C	602	MC3	C20-C21-C22-C23
2	D	602	MC3	C20-C21-C22-C23
2	E	606	MC3	C20-C21-C22-C23
2	F	606	MC3	C20-C21-C22-C23
2	I	602	MC3	C20-C21-C22-C23
2	A	402	MC3	C20-C21-C22-C23
2	A	405	MC3	C20-C21-C22-C23
2	B	606	MC3	C20-C21-C22-C23
2	C	606	MC3	C20-C21-C22-C23
2	E	602	MC3	C20-C21-C22-C23
2	F	602	MC3	C20-C21-C22-C23
2	J	602	MC3	C20-C21-C22-C23
2	L	602	MC3	C20-C21-C22-C23
2	H	606	MC3	C20-C21-C22-C23
2	L	606	MC3	C20-C21-C22-C23
2	D	606	MC3	C20-C21-C22-C23
2	E	604	MC3	C12-C13-C14-C15
2	C	604	MC3	C12-C13-C14-C15
2	B	604	MC3	C12-C13-C14-C15
2	D	604	MC3	C12-C13-C14-C15
2	G	407	MC3	C12-C13-C14-C15
2	H	604	MC3	C12-C13-C14-C15
2	L	604	MC3	C12-C13-C14-C15
2	A	407	MC3	C12-C13-C14-C15
2	F	604	MC3	C12-C13-C14-C15
2	I	604	MC3	C12-C13-C14-C15
2	J	604	MC3	C12-C13-C14-C15
2	K	604	MC3	C12-C13-C14-C15
2	F	603	MC3	C20-C21-C22-C23
2	J	603	MC3	C20-C21-C22-C23
2	E	603	MC3	C20-C21-C22-C23
2	G	406	MC3	C20-C21-C22-C23
2	L	603	MC3	C20-C21-C22-C23
2	B	603	MC3	C20-C21-C22-C23

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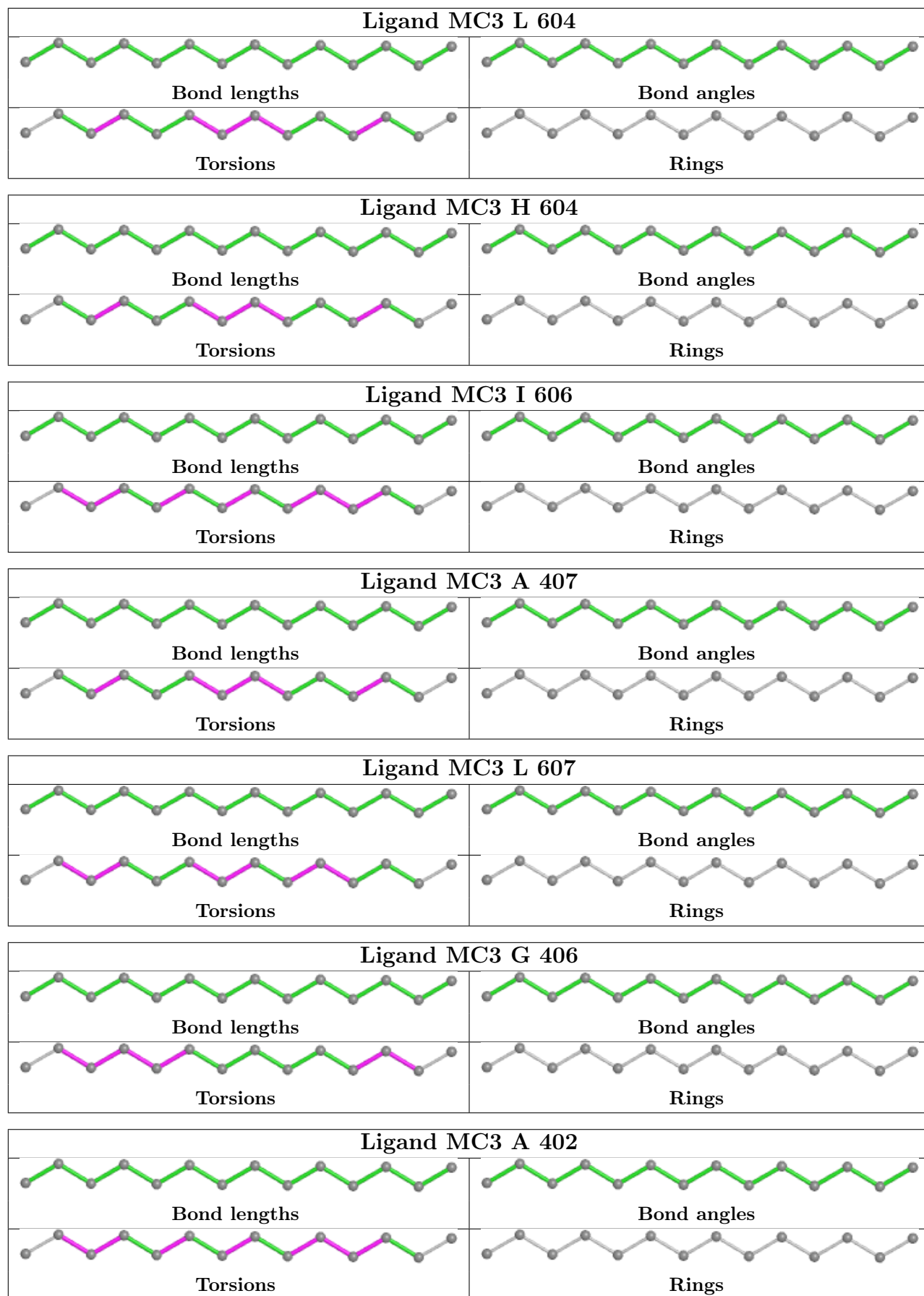
Mol	Chain	Res	Type	Atoms
2	D	603	MC3	C20-C21-C22-C23
2	C	603	MC3	C20-C21-C22-C23
2	I	603	MC3	C20-C21-C22-C23
2	K	603	MC3	C20-C21-C22-C23
2	A	406	MC3	C20-C21-C22-C23
2	H	603	MC3	C20-C21-C22-C23
2	G	405	MC3	C18-C19-C20-C21
2	L	602	MC3	C18-C19-C20-C21
2	E	602	MC3	C18-C19-C20-C21
2	F	602	MC3	C18-C19-C20-C21
2	I	602	MC3	C18-C19-C20-C21
2	J	602	MC3	C18-C19-C20-C21
2	K	602	MC3	C18-C19-C20-C21
2	A	405	MC3	C18-C19-C20-C21
2	B	602	MC3	C18-C19-C20-C21
2	D	602	MC3	C18-C19-C20-C21
2	H	602	MC3	C18-C19-C20-C21
2	C	602	MC3	C18-C19-C20-C21
2	D	605	MC3	C12-C13-C14-C15
2	H	605	MC3	C12-C13-C14-C15
2	B	605	MC3	C12-C13-C14-C15
2	E	605	MC3	C12-C13-C14-C15
2	G	401	MC3	C12-C13-C14-C15
2	I	605	MC3	C12-C13-C14-C15
2	J	605	MC3	C12-C13-C14-C15
2	K	605	MC3	C12-C13-C14-C15
2	A	401	MC3	C12-C13-C14-C15
2	F	605	MC3	C12-C13-C14-C15
2	C	605	MC3	C12-C13-C14-C15
2	L	605	MC3	C12-C13-C14-C15
2	F	602	MC3	C17-C18-C19-C20
2	G	405	MC3	C17-C18-C19-C20
2	E	602	MC3	C17-C18-C19-C20
2	B	602	MC3	C17-C18-C19-C20
2	A	405	MC3	C17-C18-C19-C20
2	D	602	MC3	C17-C18-C19-C20
2	H	602	MC3	C17-C18-C19-C20
2	K	602	MC3	C17-C18-C19-C20
2	C	602	MC3	C17-C18-C19-C20
2	I	602	MC3	C17-C18-C19-C20
2	J	602	MC3	C17-C18-C19-C20
2	L	602	MC3	C17-C18-C19-C20

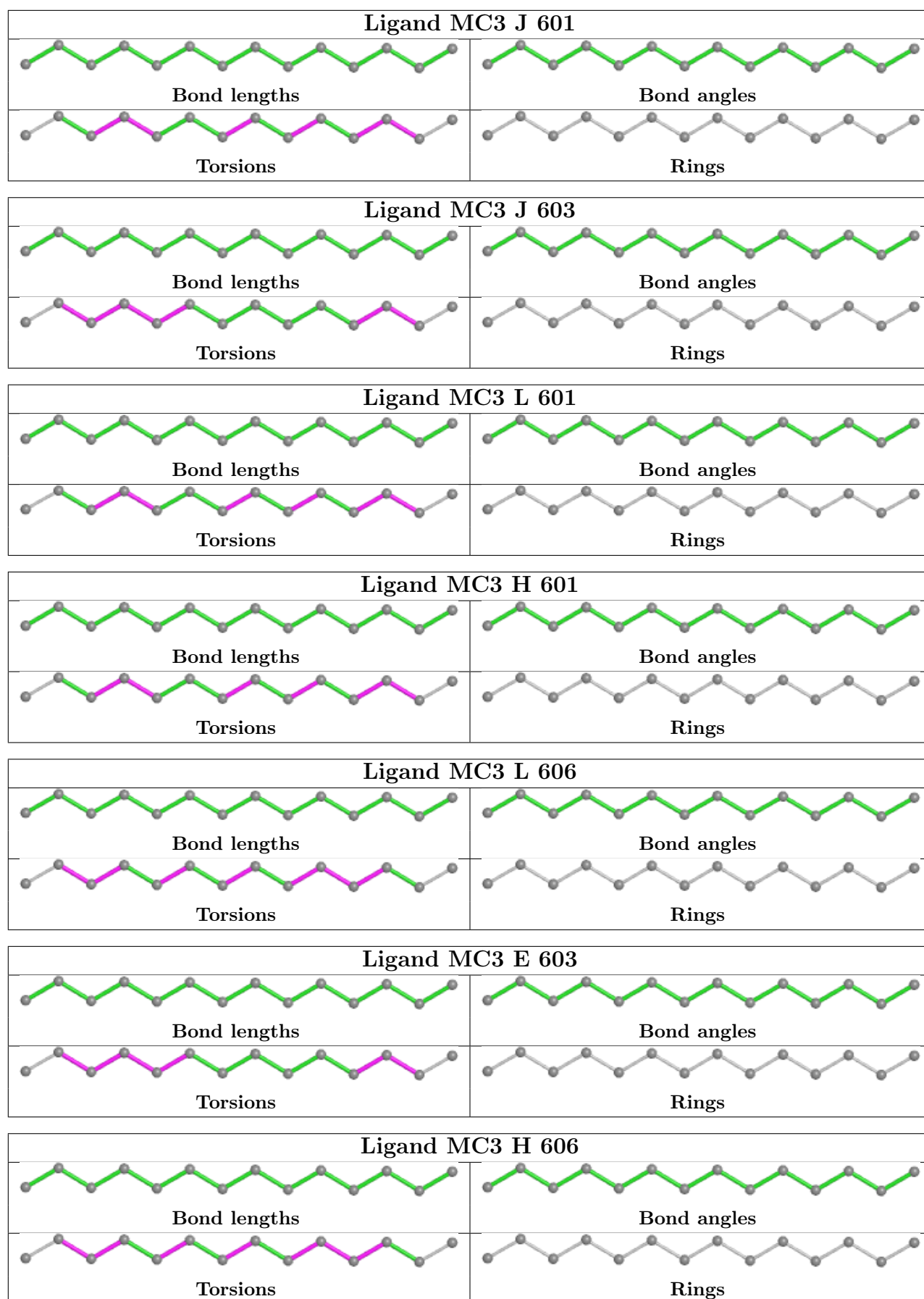
There are no ring outliers.

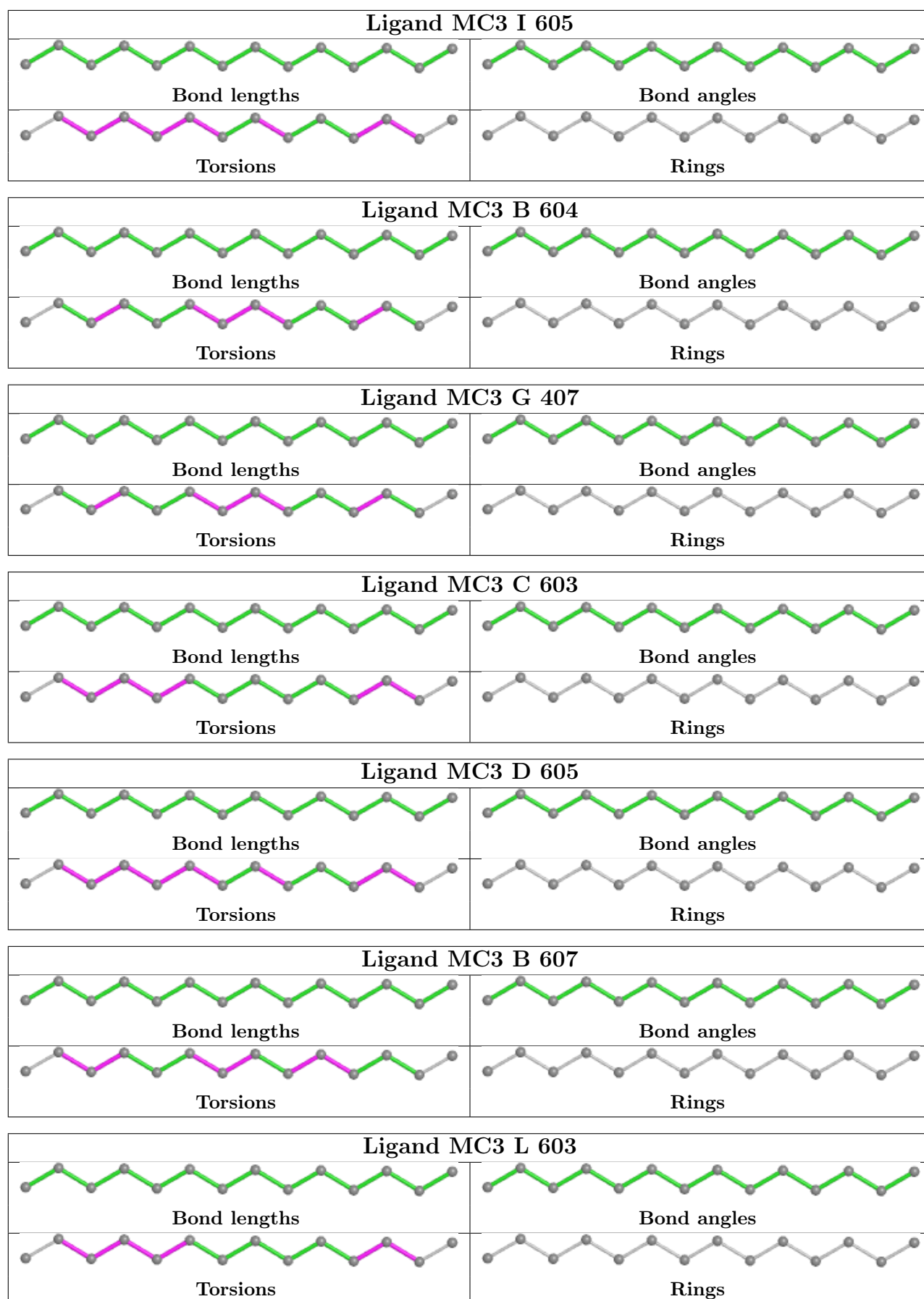
23 monomers are involved in 25 short contacts:

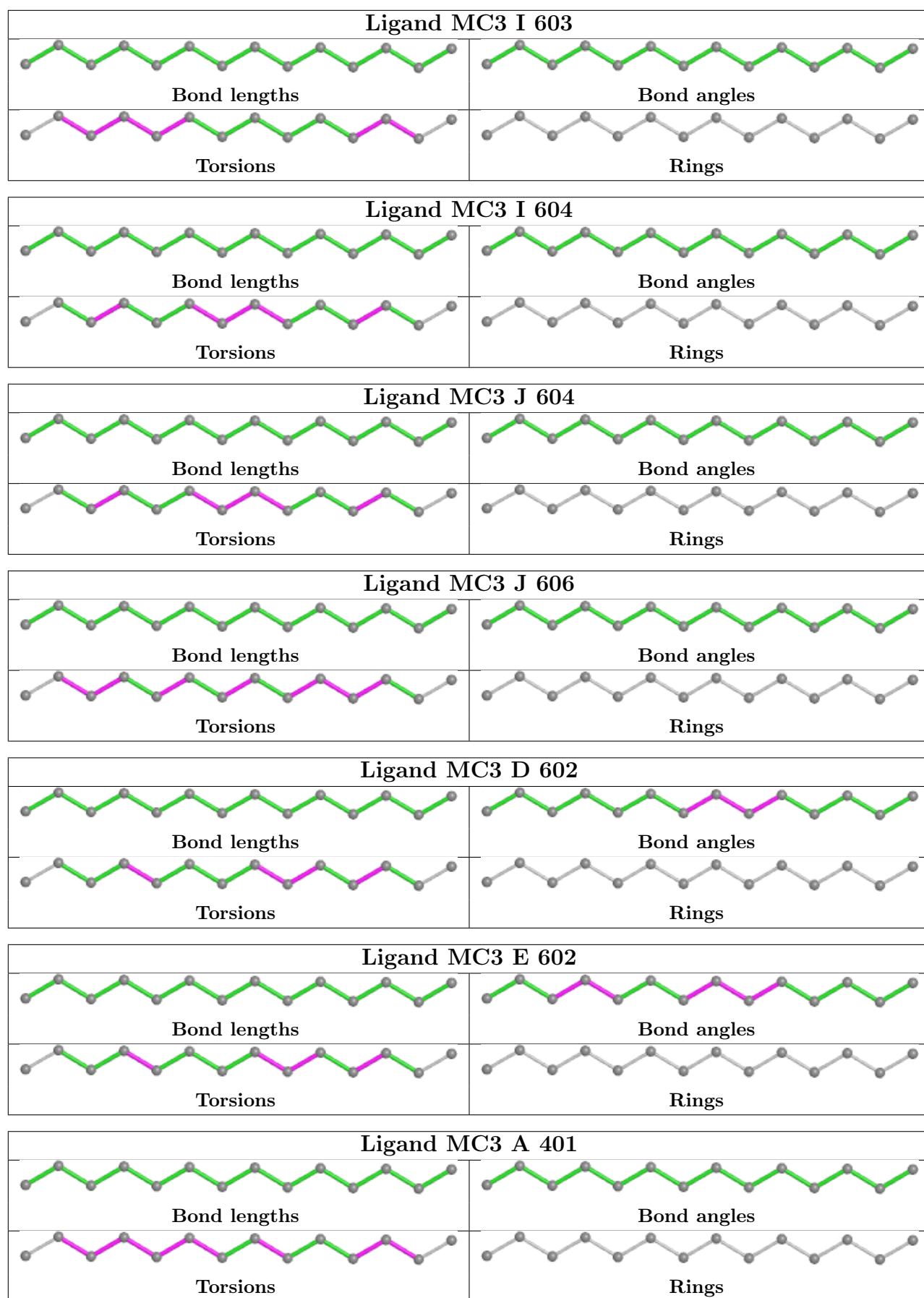
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	604	MC3	1	0
2	A	407	MC3	1	0
2	L	607	MC3	1	0
2	E	603	MC3	1	0
2	L	603	MC3	1	0
2	D	602	MC3	1	0
2	A	405	MC3	2	0
2	K	602	MC3	1	0
2	F	607	MC3	1	0
2	C	607	MC3	1	0
2	H	607	MC3	1	0
2	A	403	MC3	1	0
2	B	603	MC3	1	0
2	H	602	MC3	1	0
2	H	603	MC3	1	0
2	D	607	MC3	1	0
2	A	406	MC3	1	0
2	F	603	MC3	1	0
2	F	602	MC3	2	0
2	K	607	MC3	1	0
2	J	607	MC3	1	0
2	E	607	MC3	1	0
2	G	403	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.

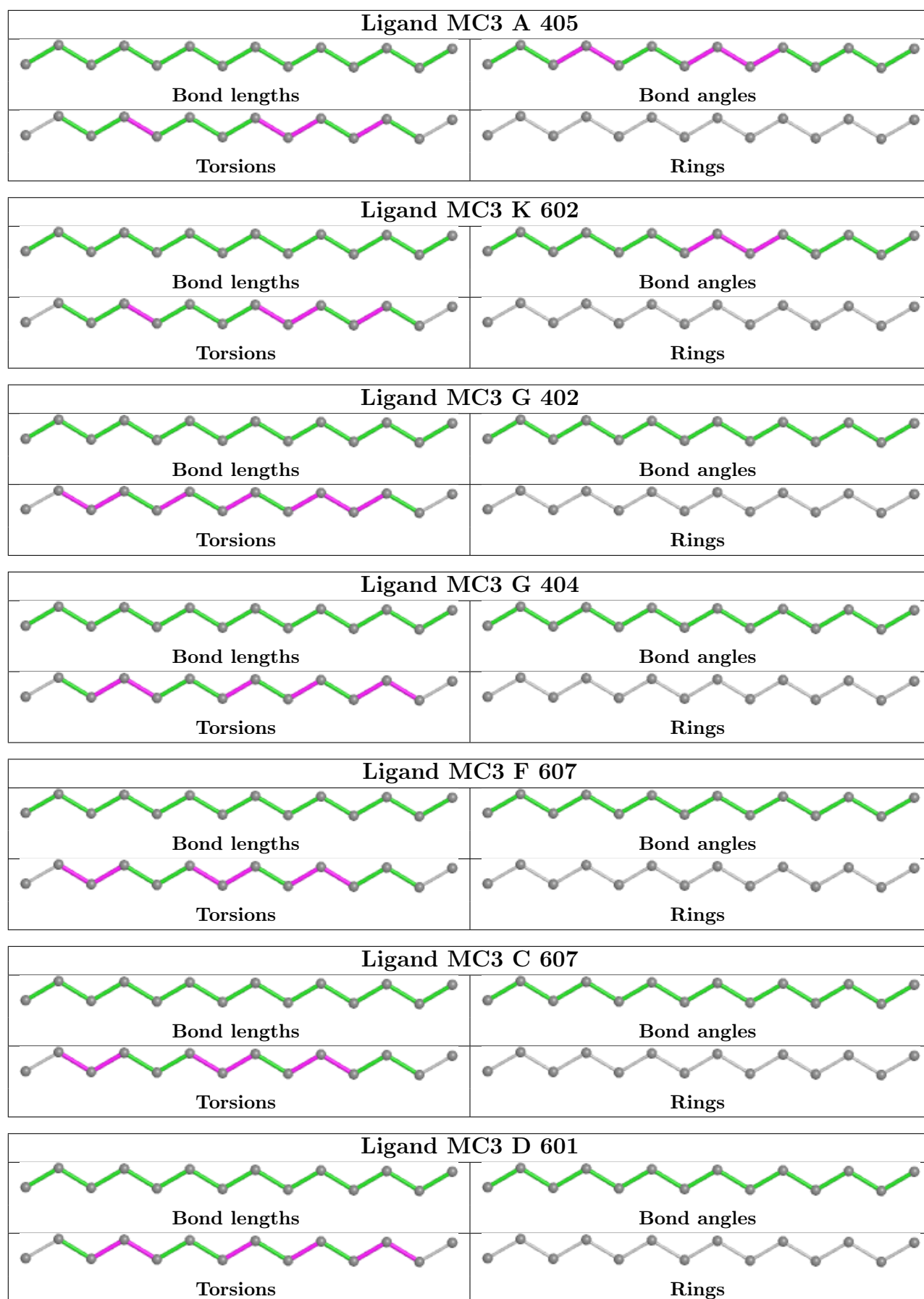


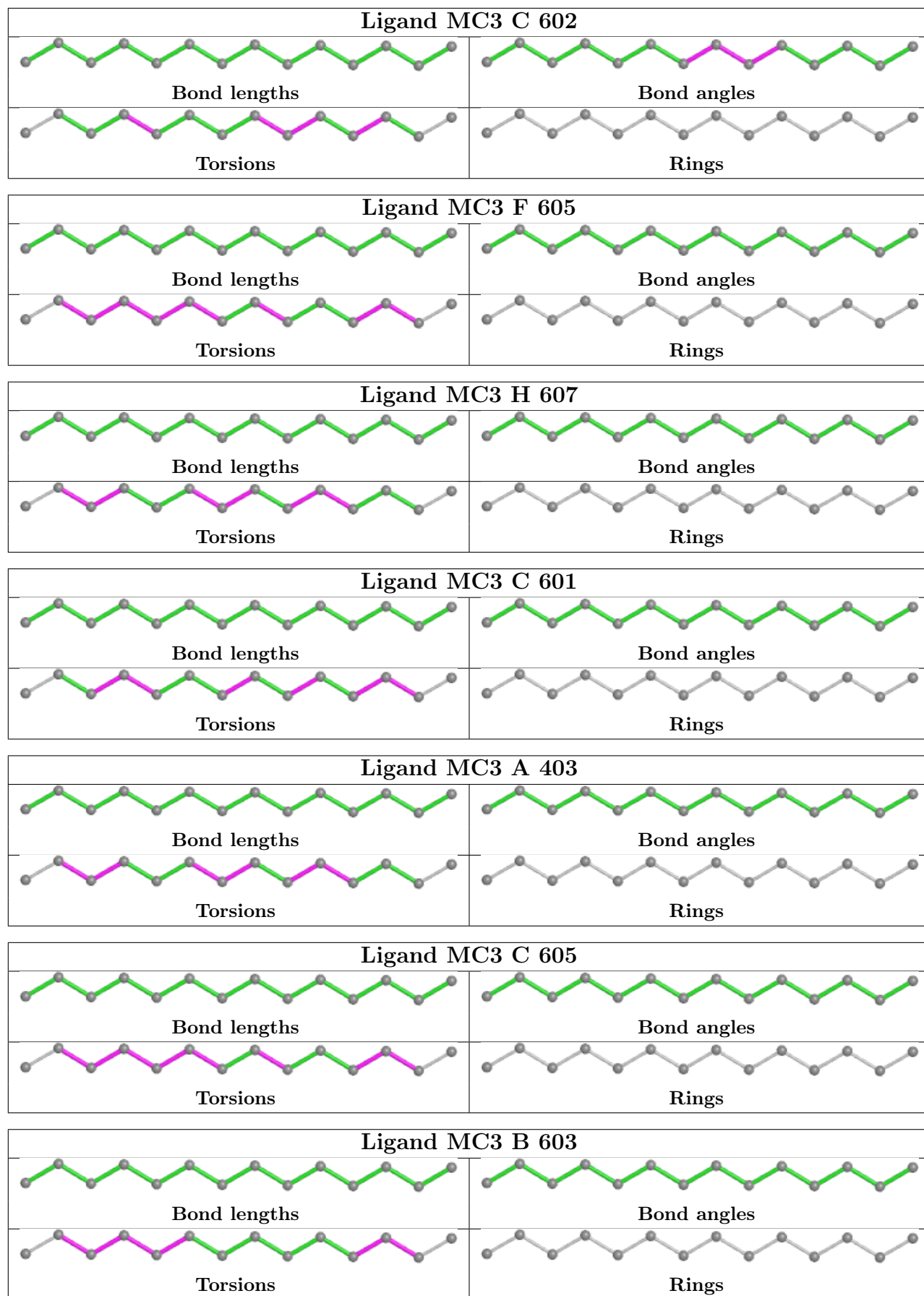


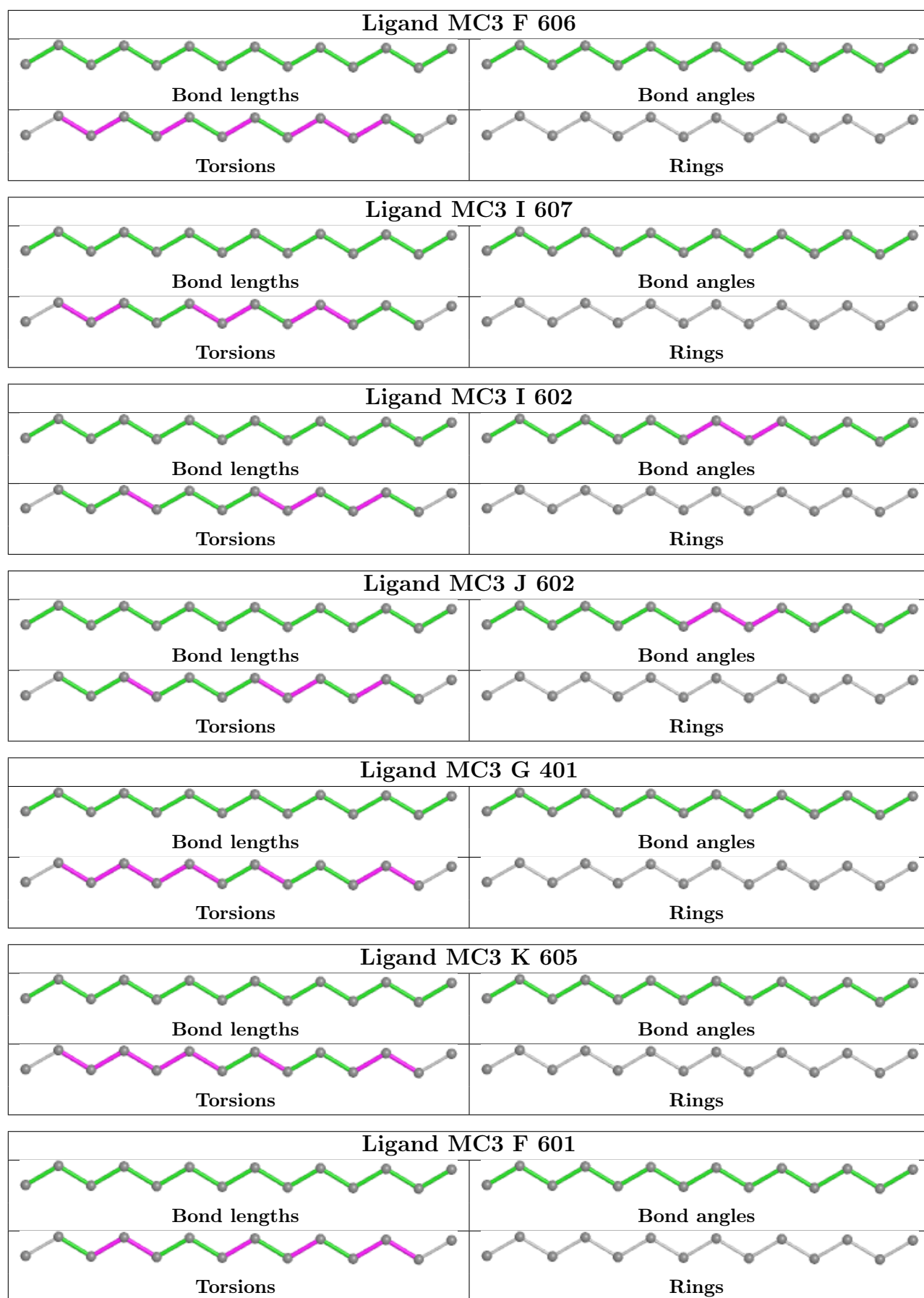


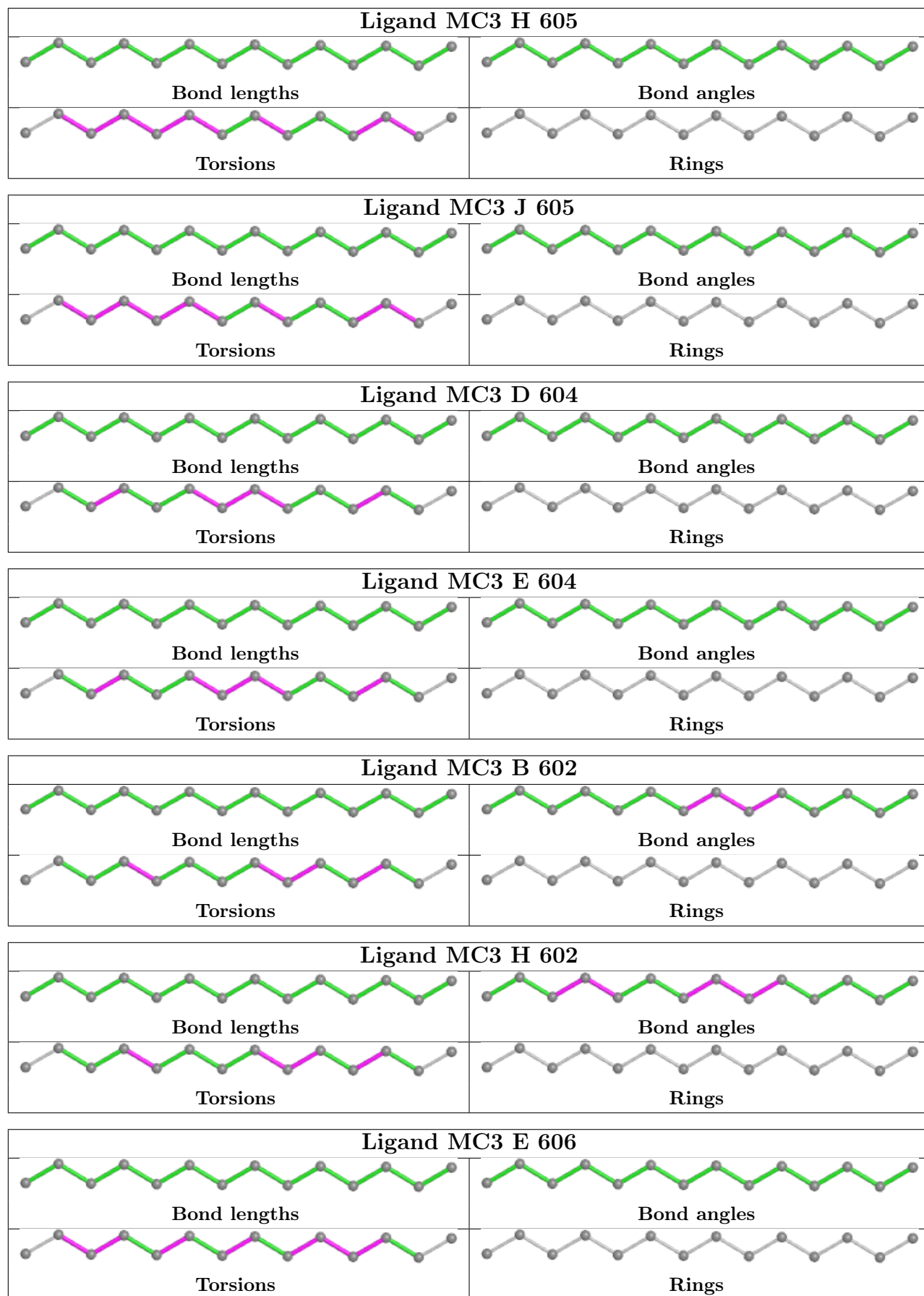


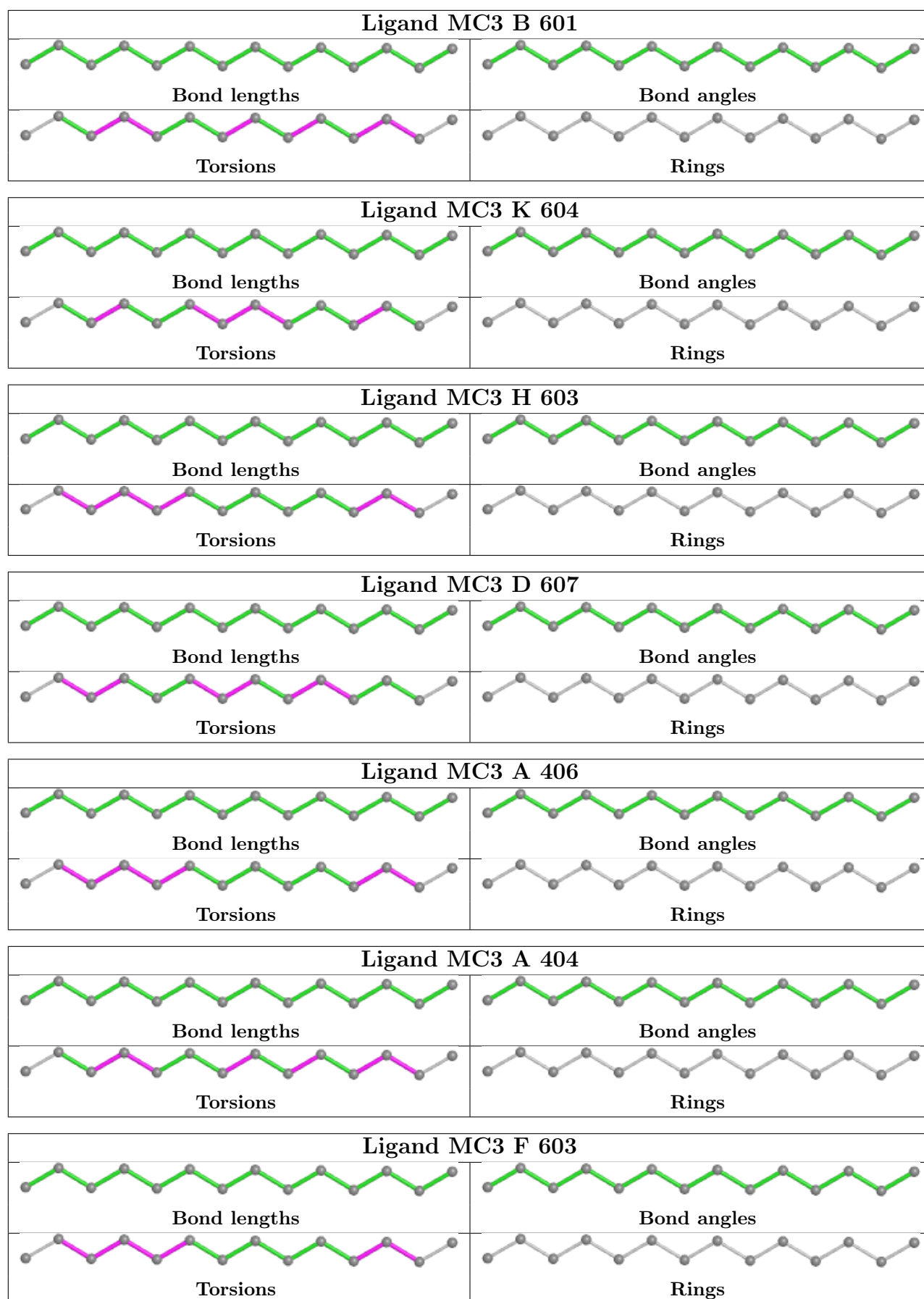


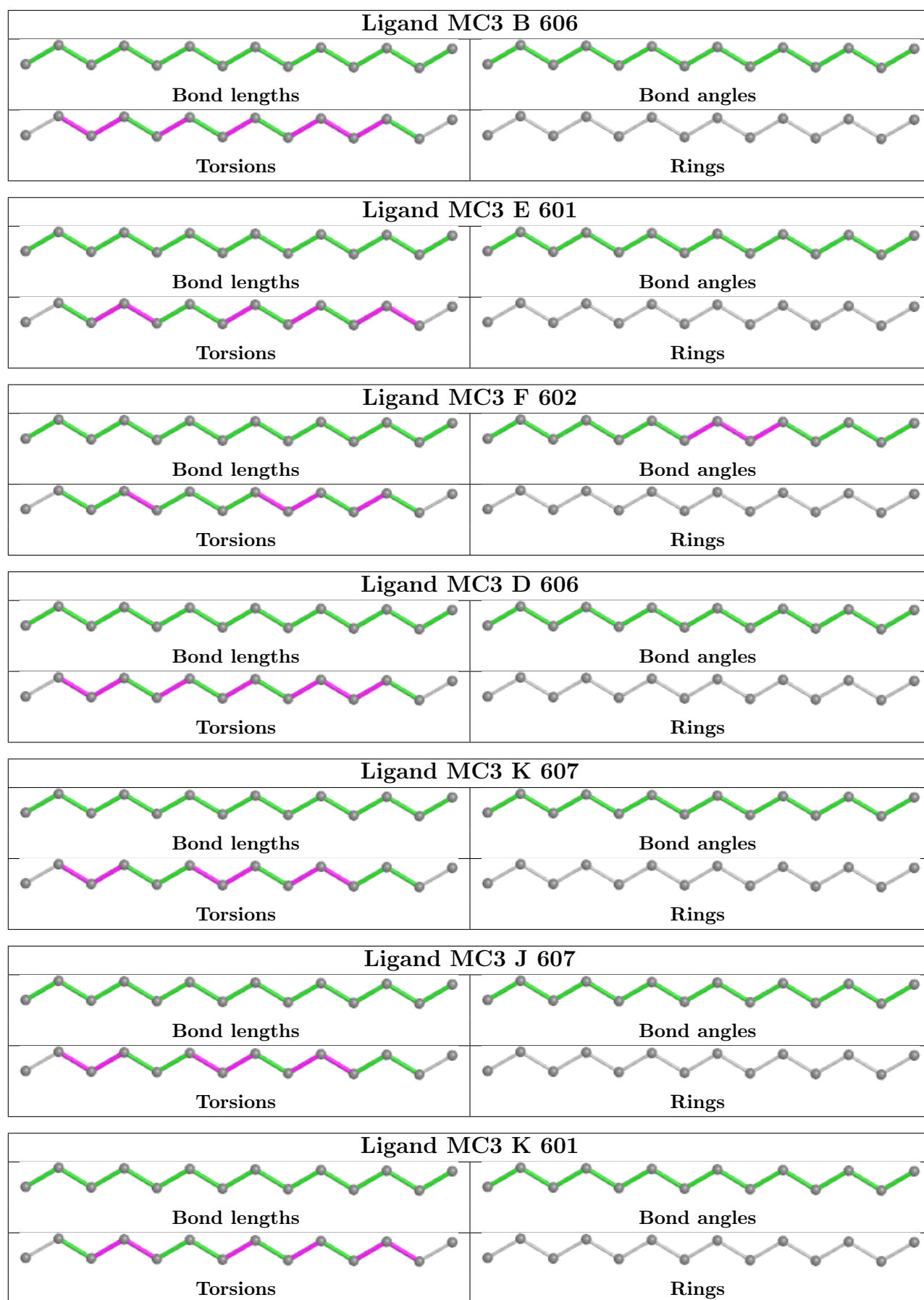


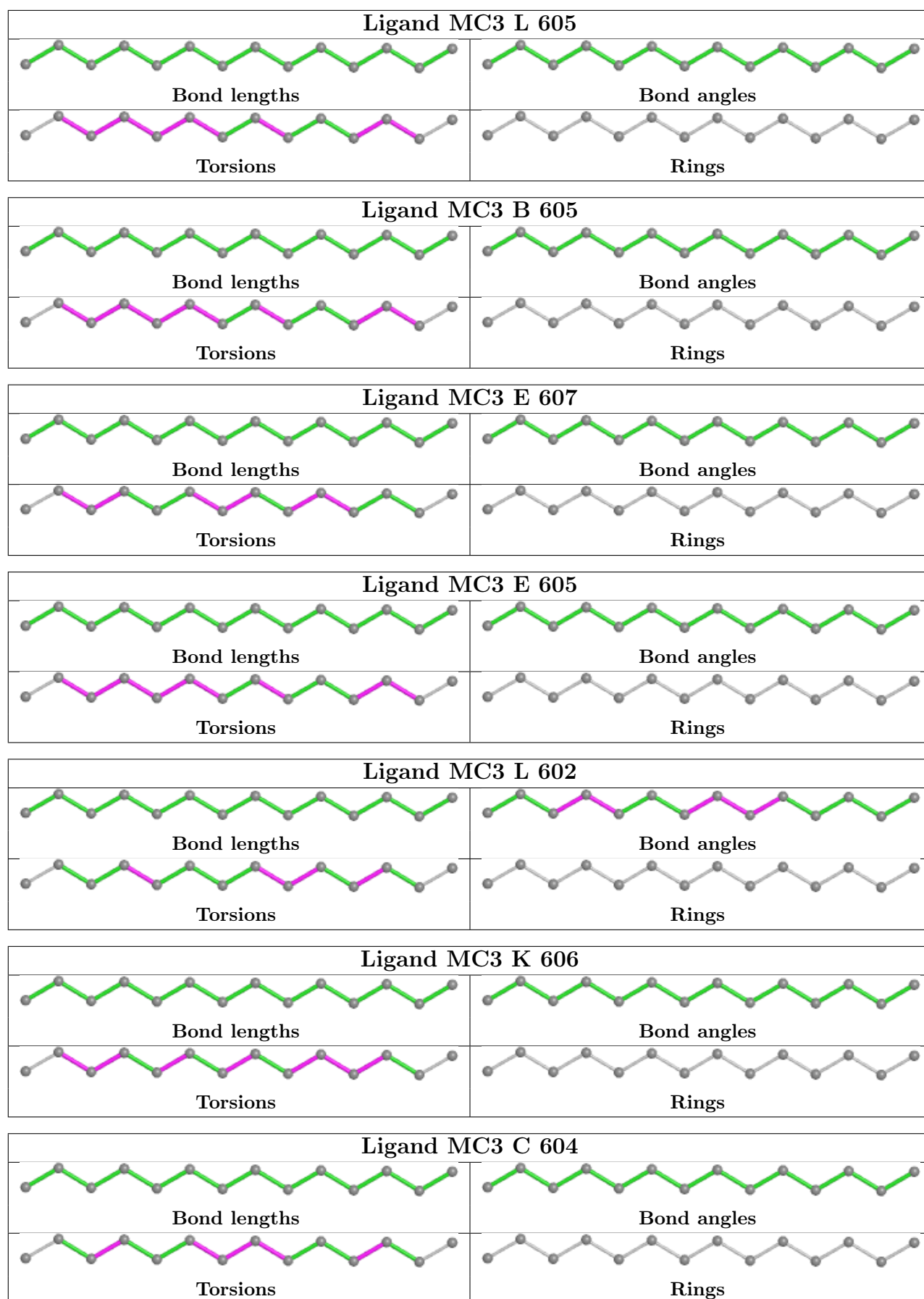




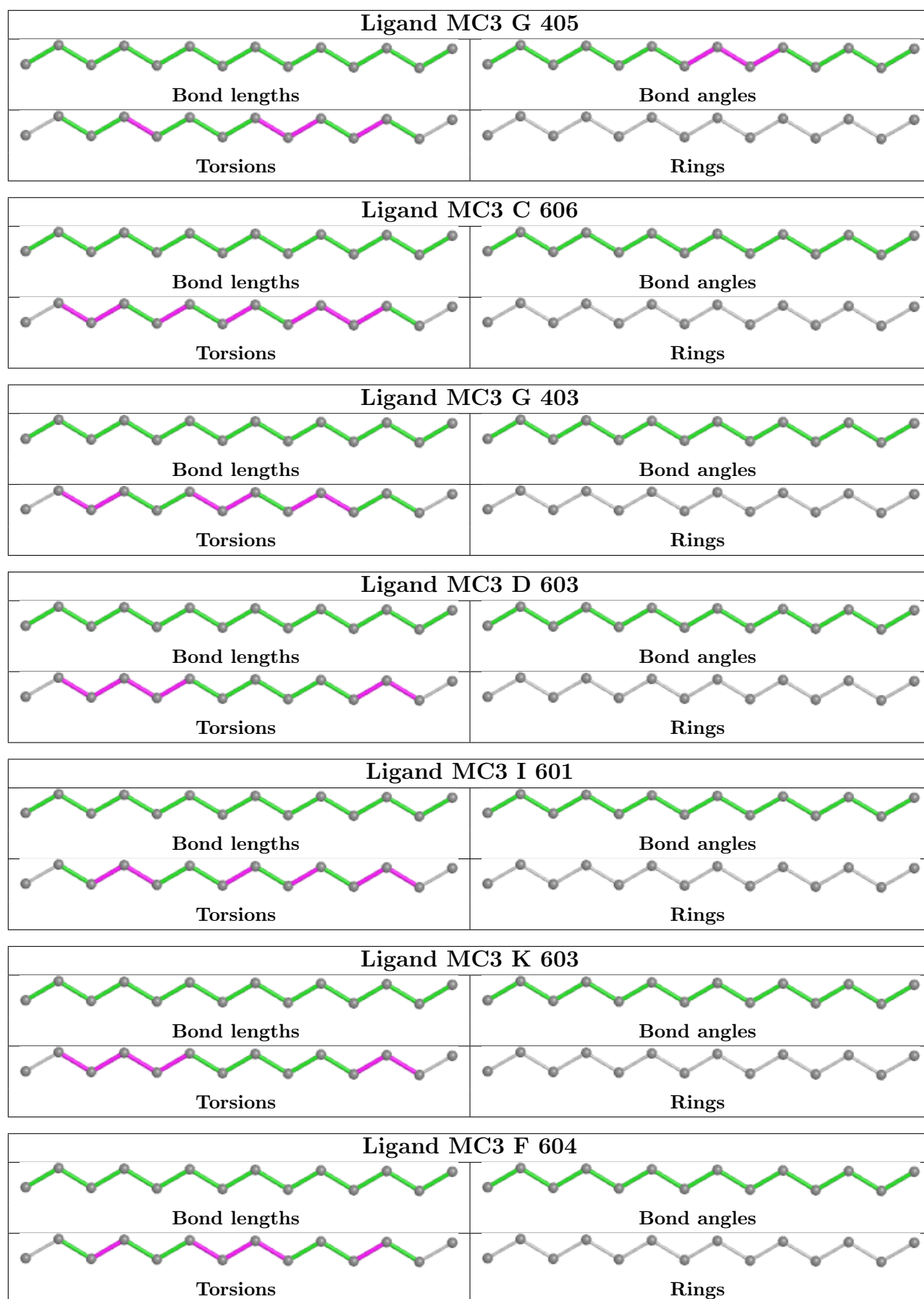














## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

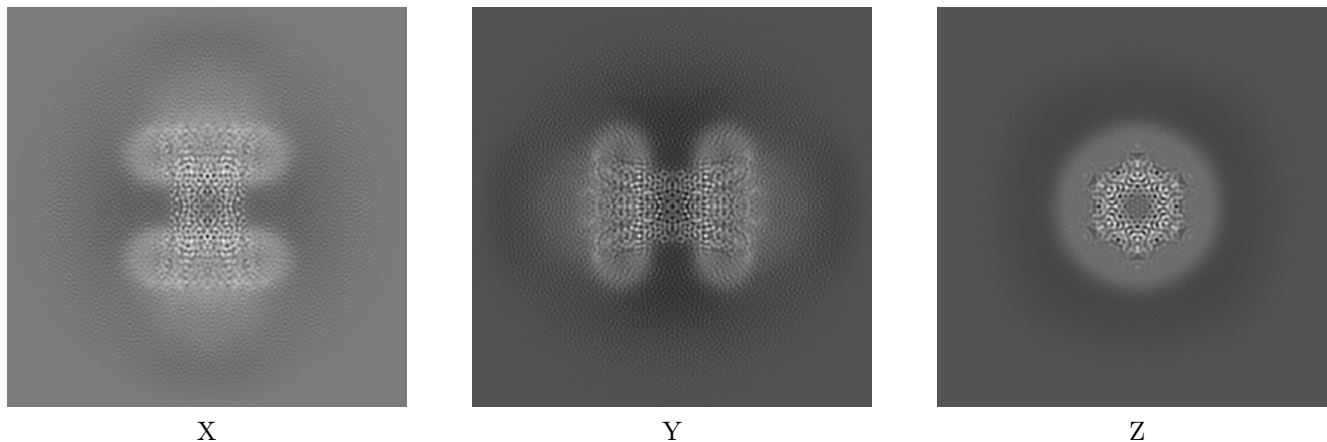
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33274. These allow visual inspection of the internal detail of the map and identification of artifacts.

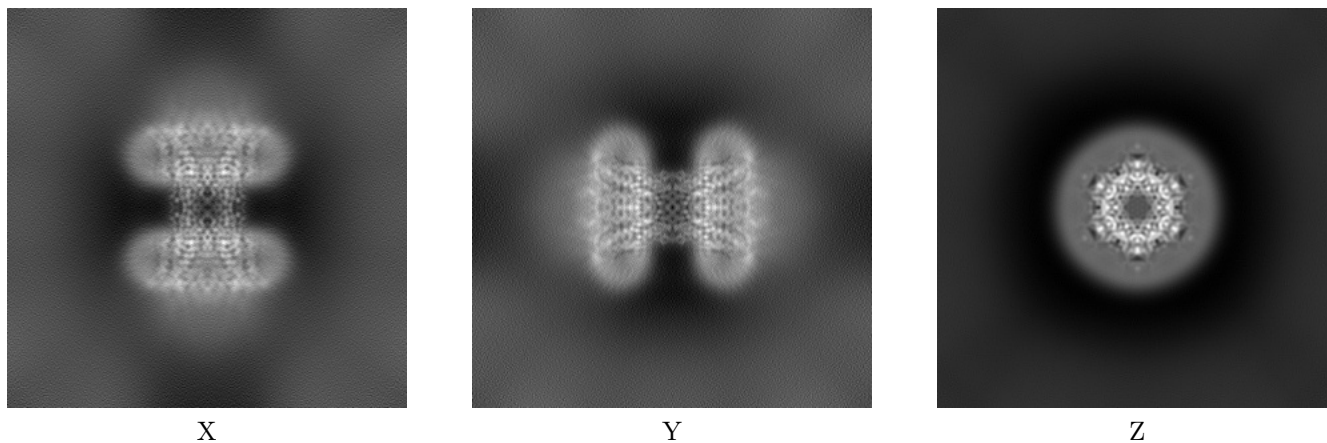
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



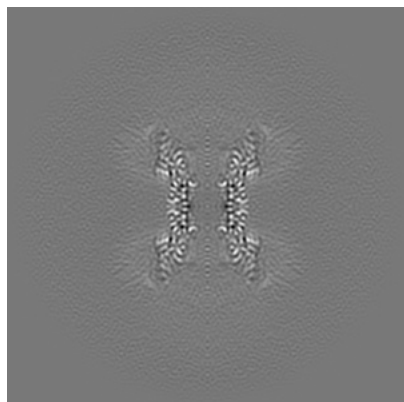
#### 6.1.2 Raw map



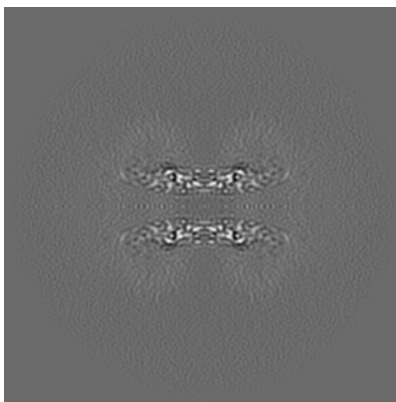
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

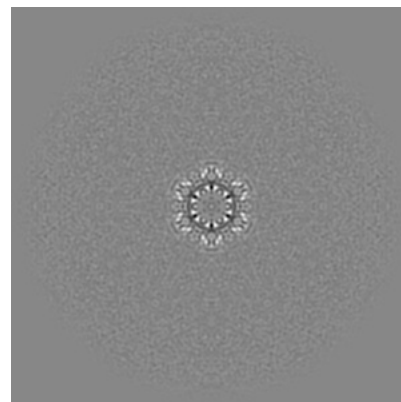
### 6.2.1 Primary map



X Index: 180

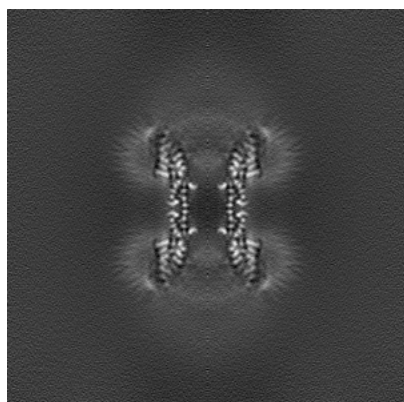


Y Index: 180

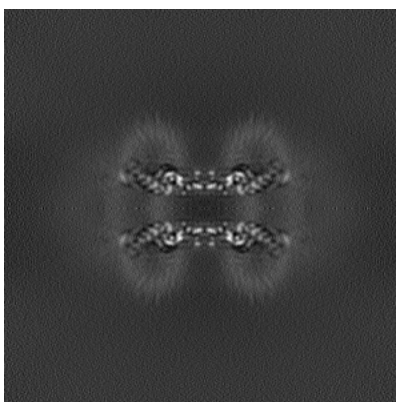


Z Index: 180

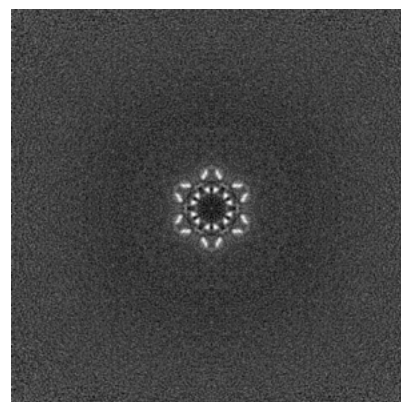
### 6.2.2 Raw map



X Index: 180



Y Index: 180

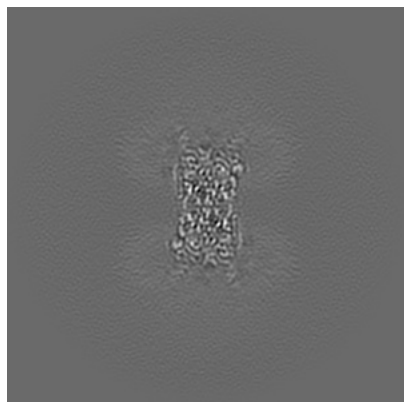


Z Index: 180

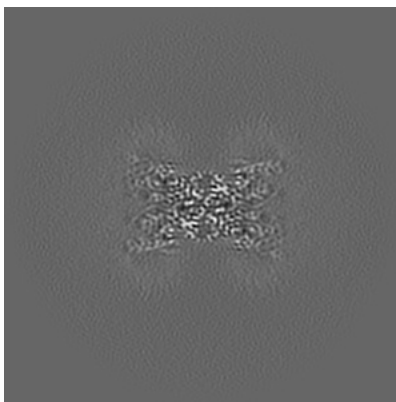
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

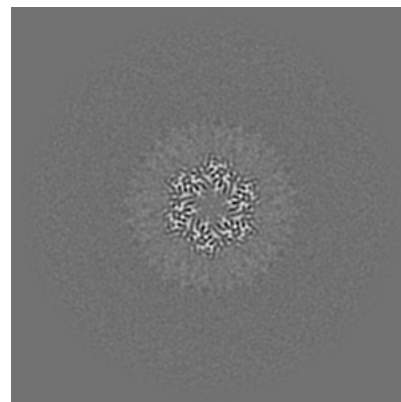
### 6.3.1 Primary map



X Index: 200

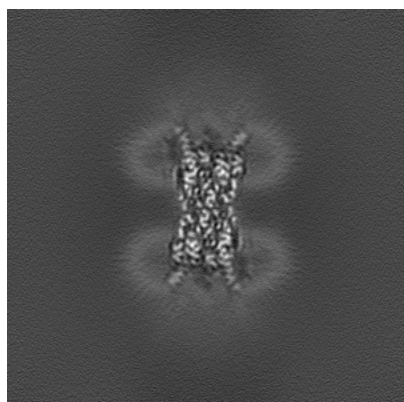


Y Index: 198

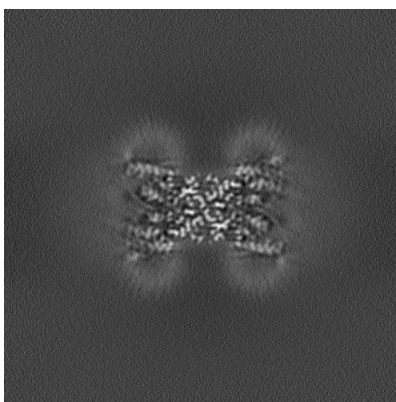


Z Index: 150

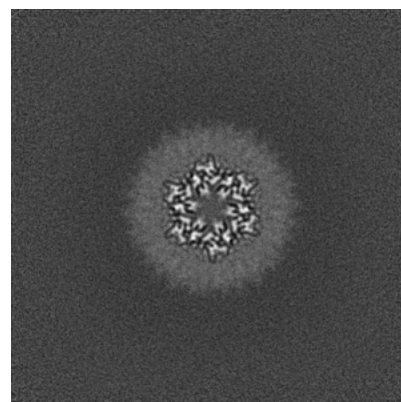
### 6.3.2 Raw map



X Index: 201



Y Index: 162

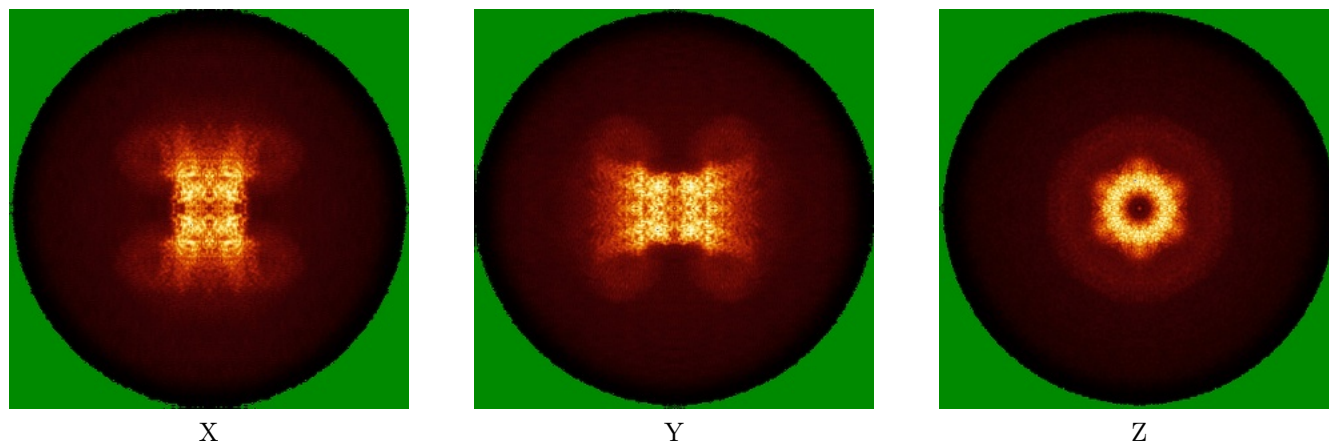


Z Index: 210

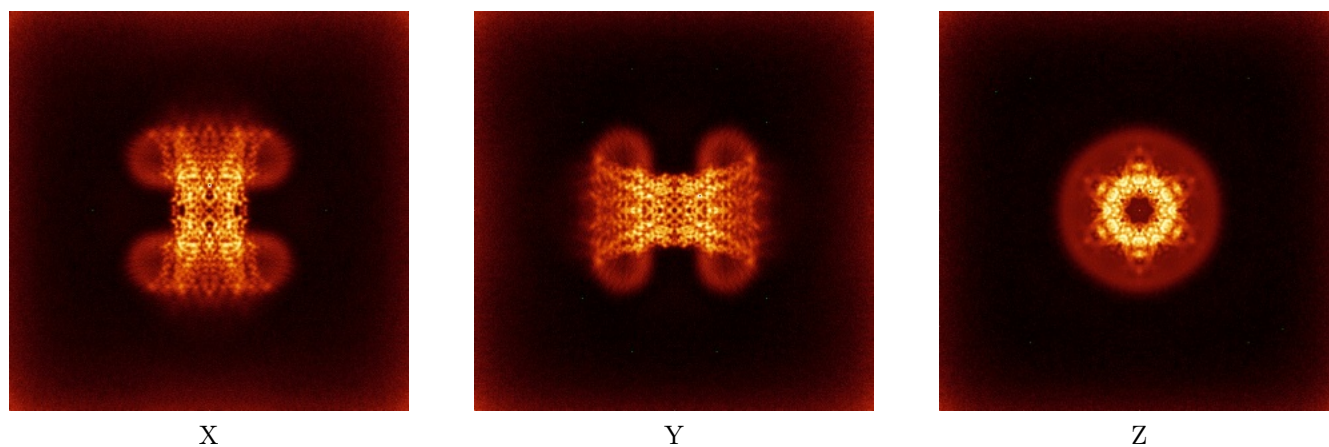
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map

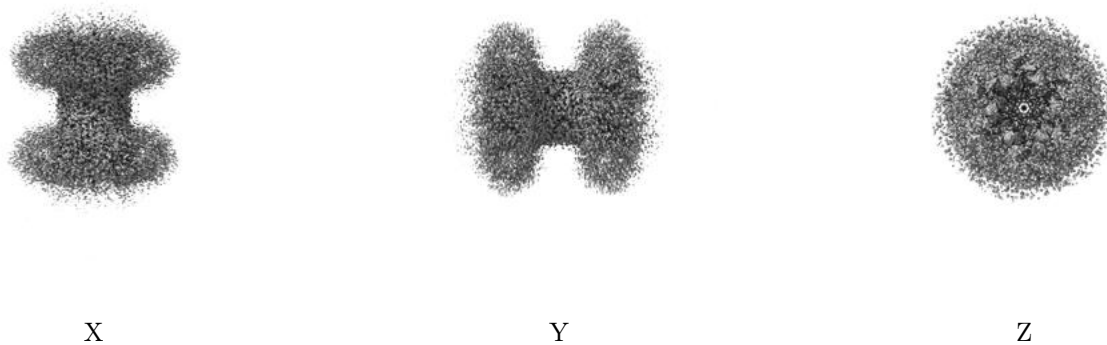


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



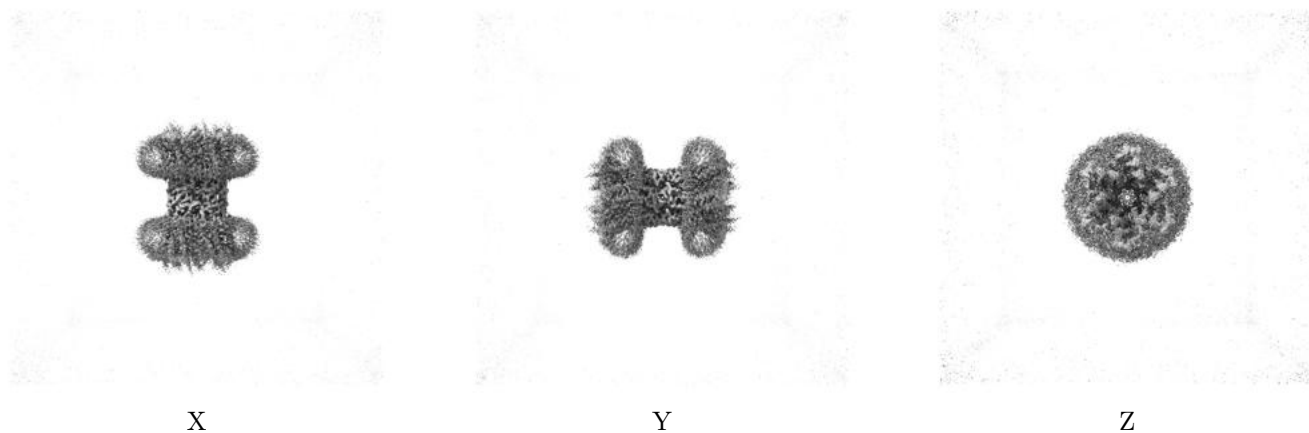
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

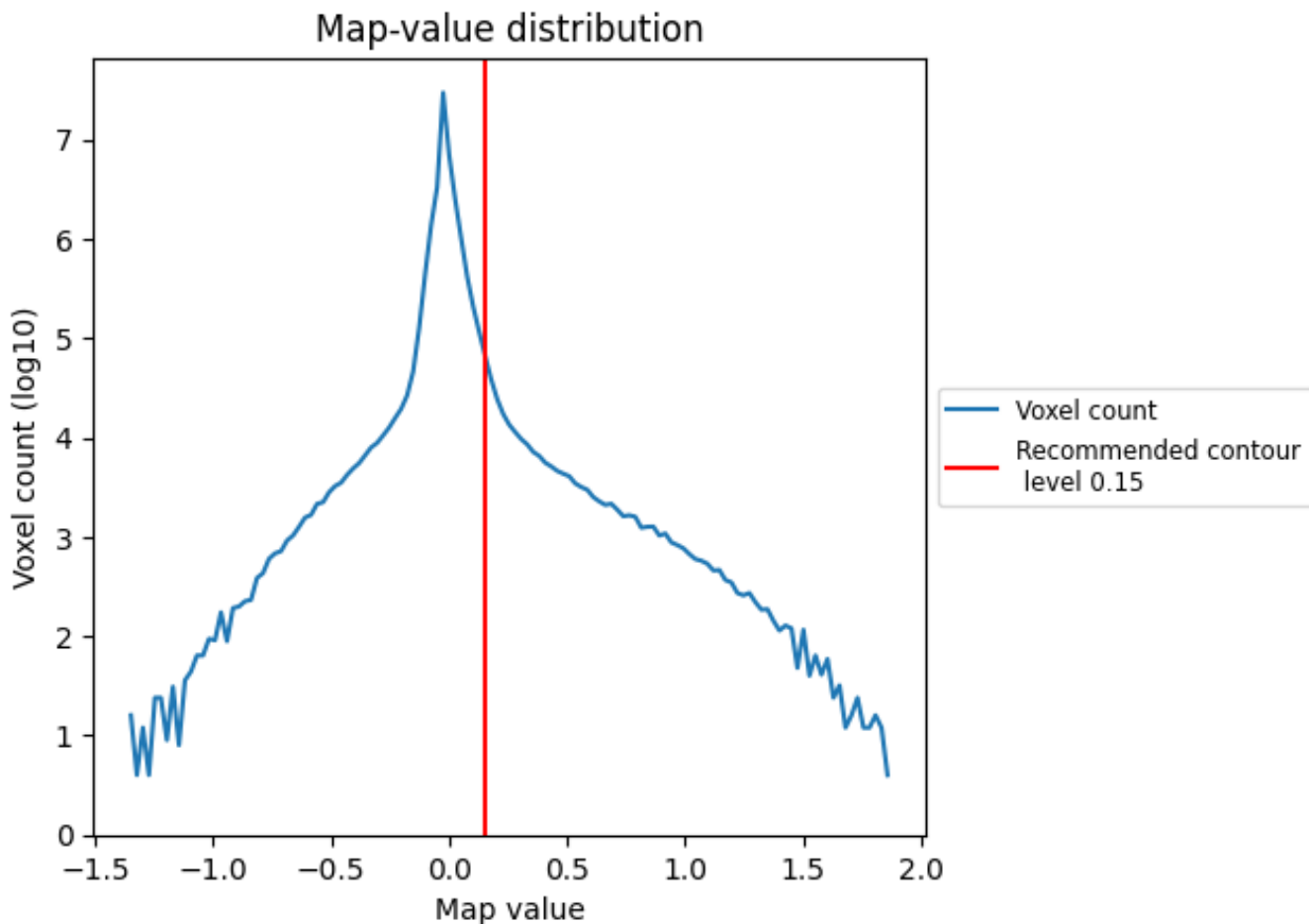
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

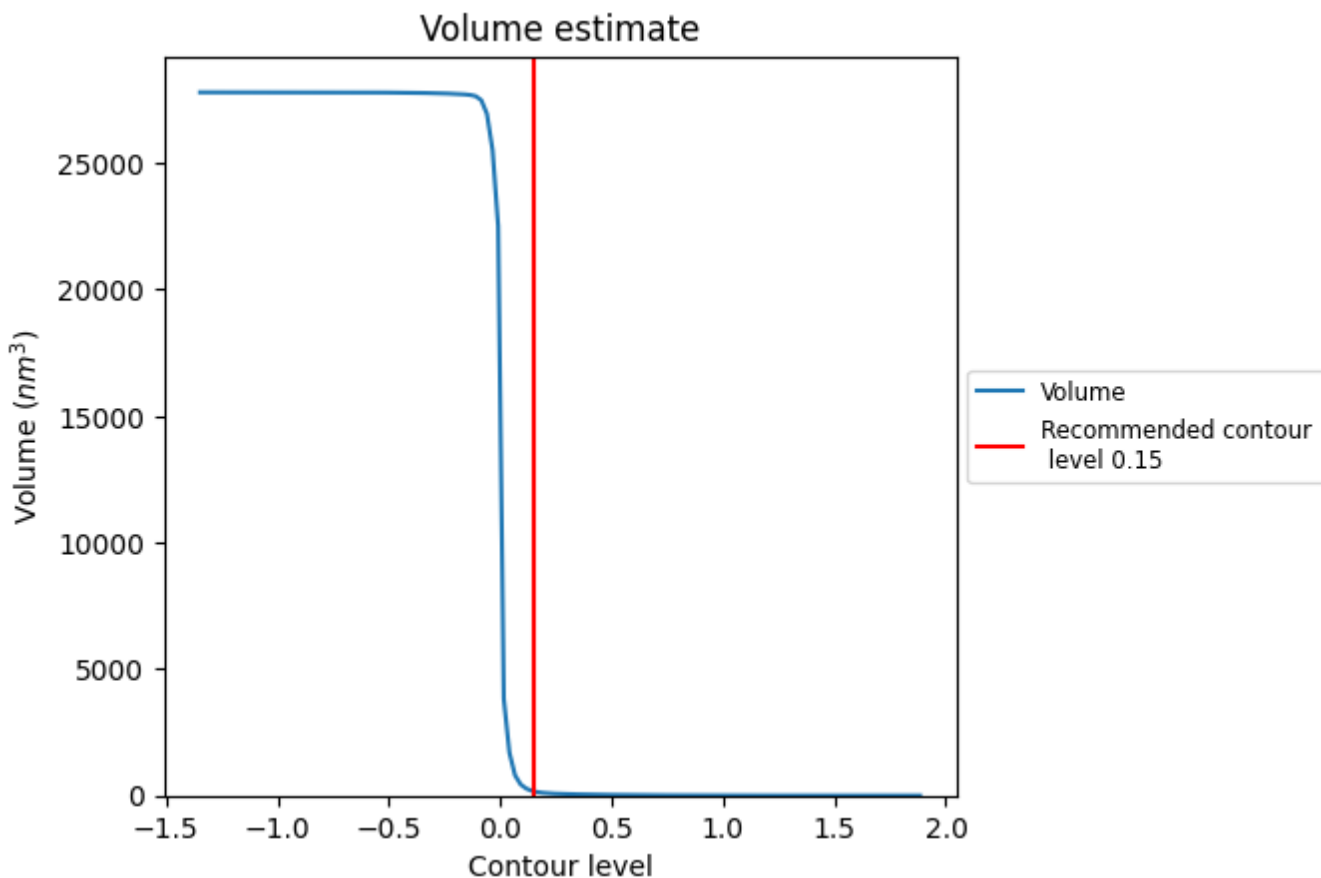
This section contains the results of statistical analysis of the map.

### 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](#)

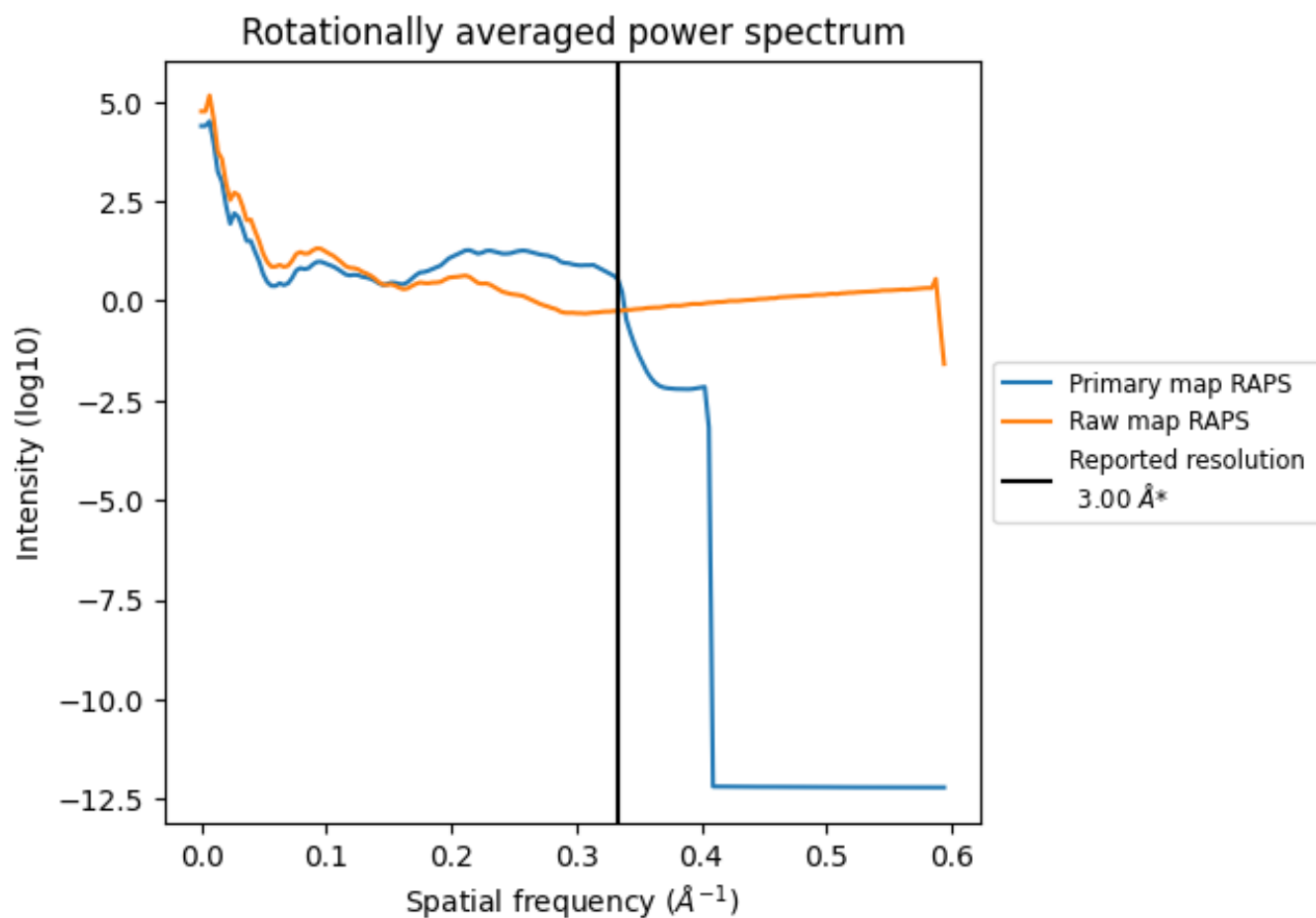


The volume at the recommended contour level is 170 nm<sup>3</sup>; this corresponds to an approximate mass of 153 kDa.

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 [i](#)

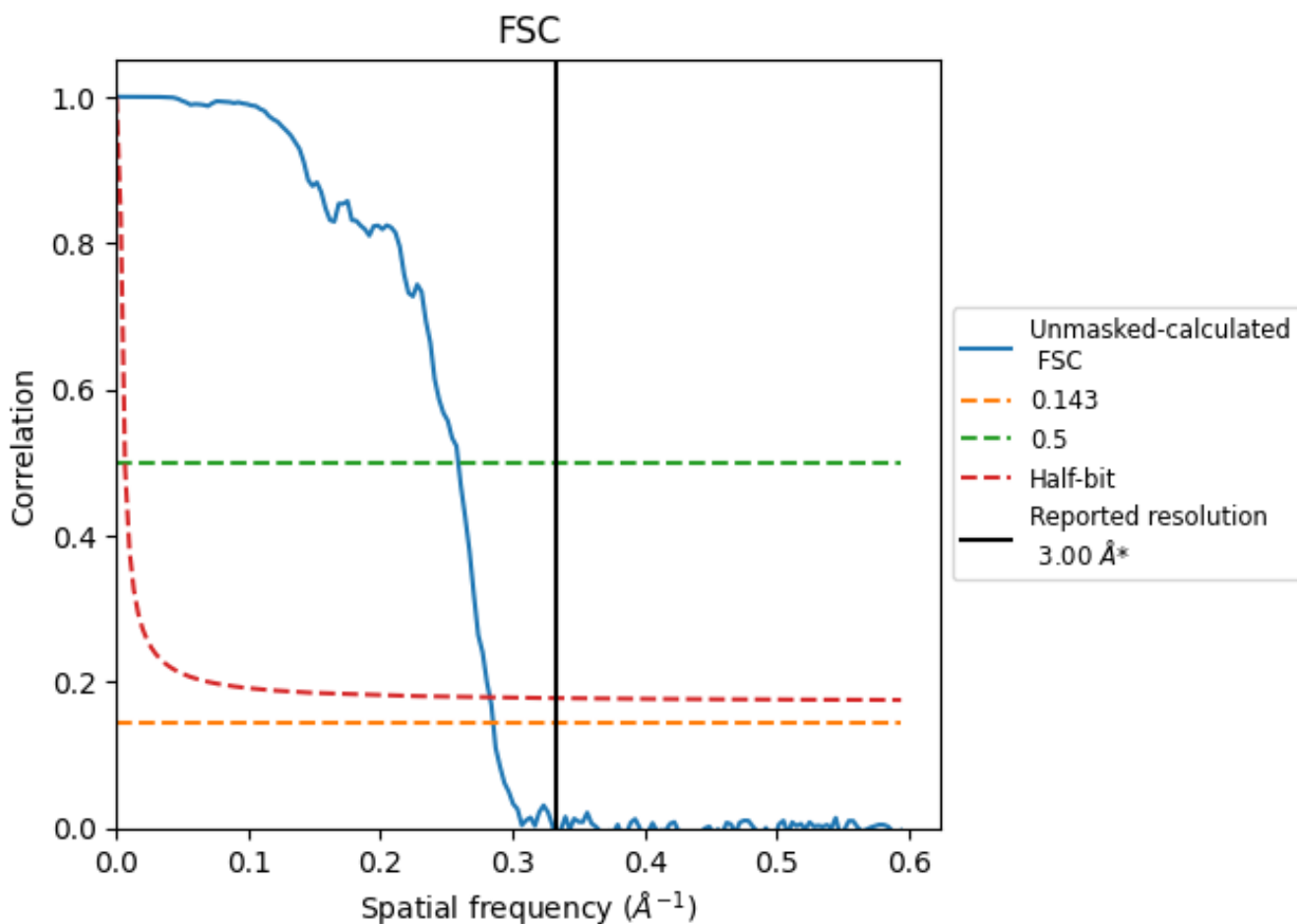


\*Reported resolution corresponds to spatial frequency of 0.333 Å<sup>-1</sup>

## 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 0.333 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

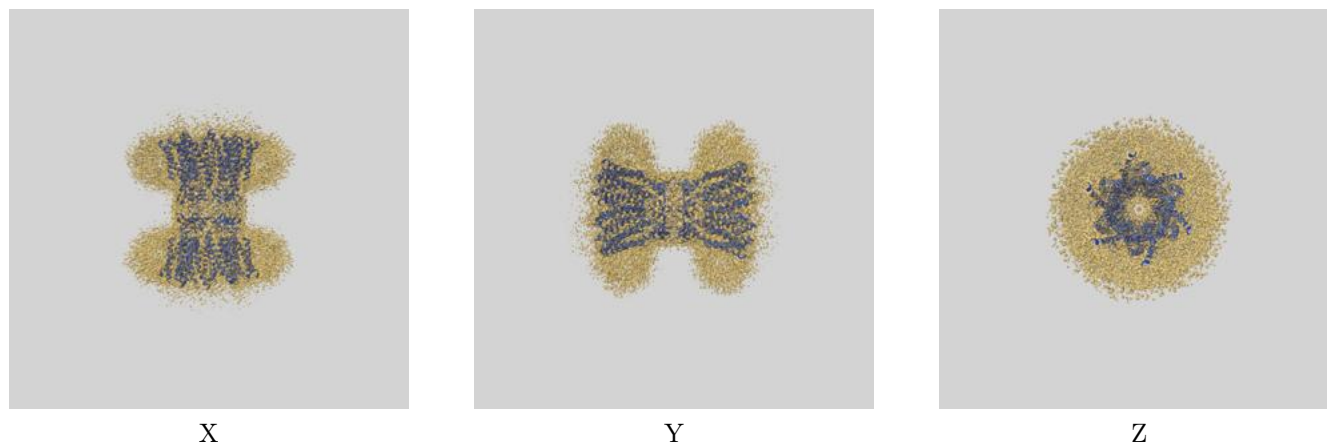
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.51	3.86	3.54

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.51 differs from the reported value 3.0 by more than 10 %

## 9 Map-model fit [i](#)

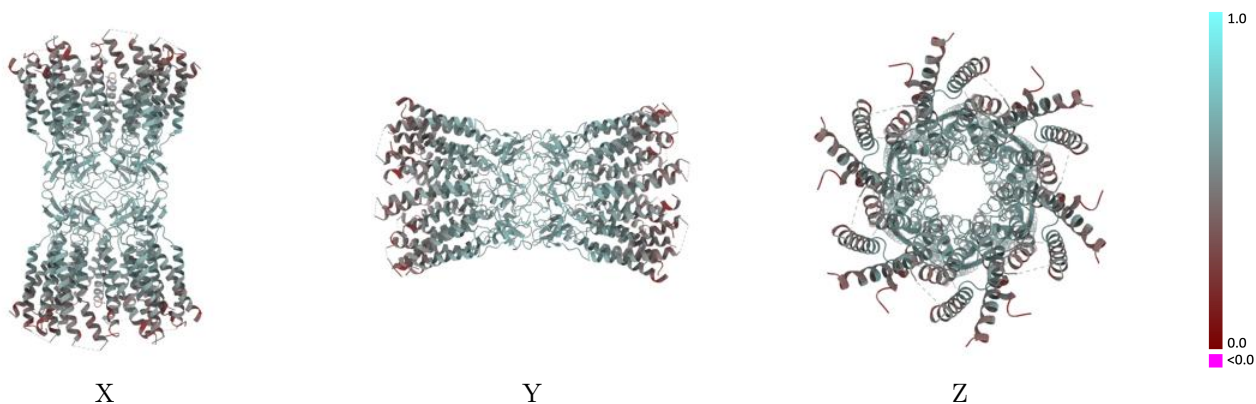
This section contains information regarding the fit between EMDB map EMD-33274 and PDB model 7XL8. Per-residue inclusion information can be found in section 3 on page 13.

### 9.1 Map-model overlay [i](#)



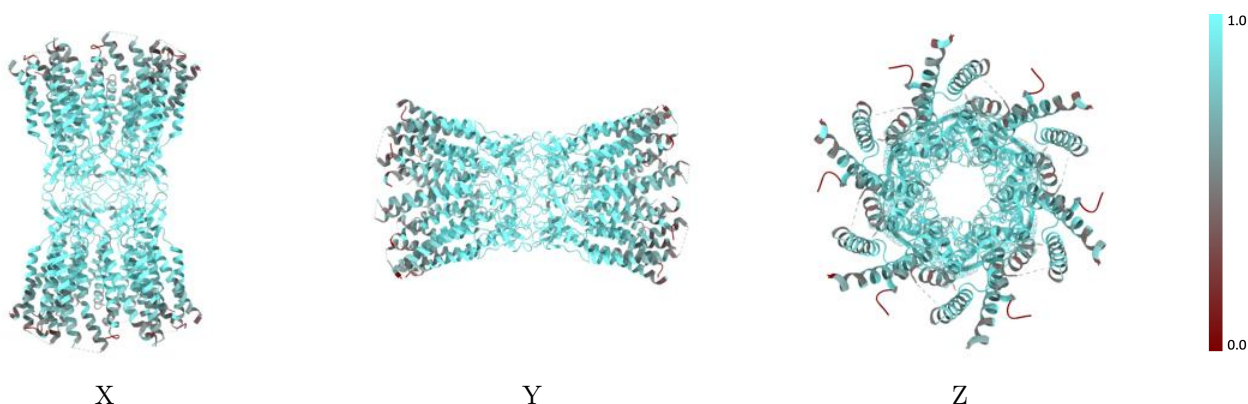
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



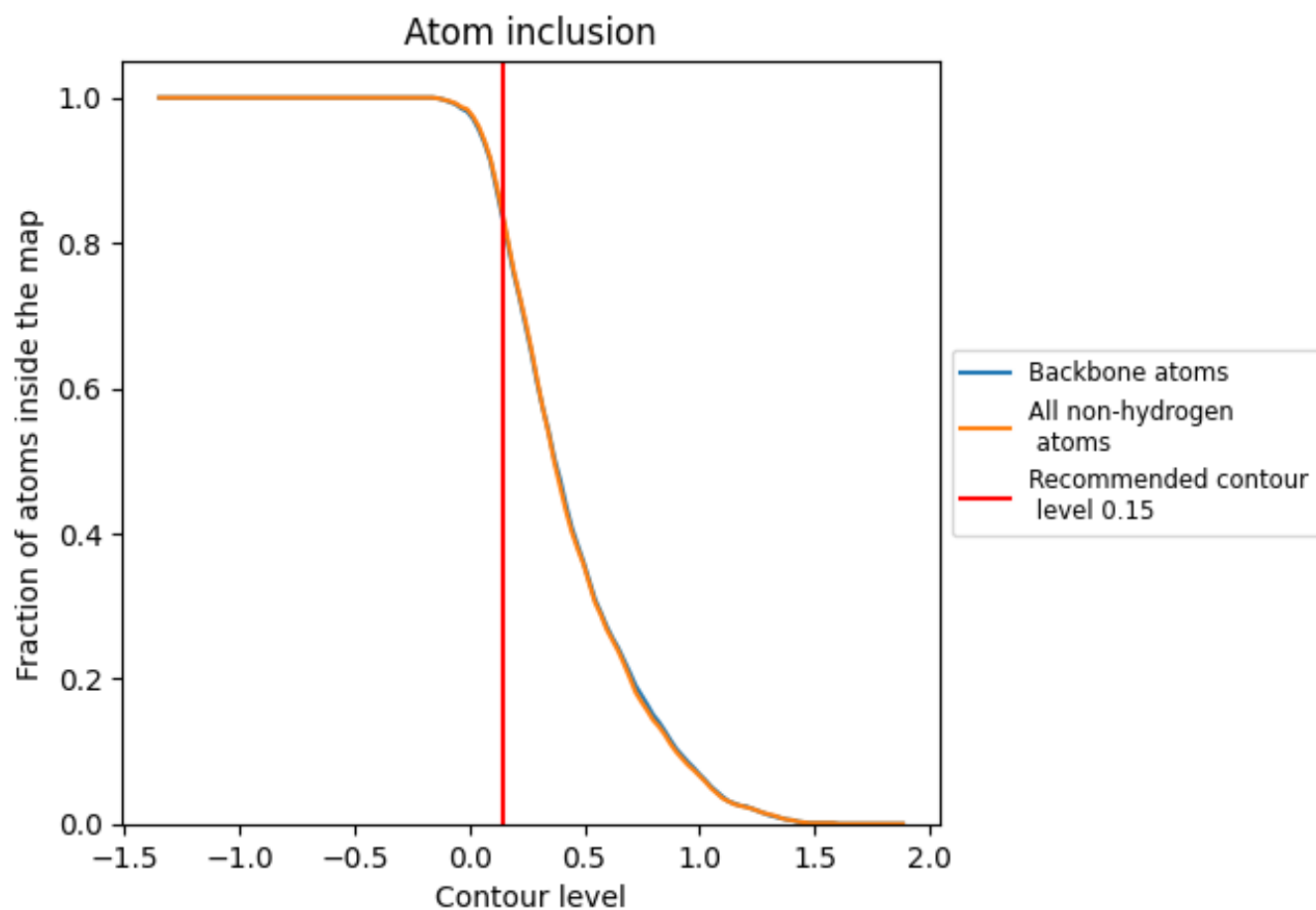
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8310	 0.5320
A	 0.8320	 0.5320
B	 0.8320	 0.5290
C	 0.8370	 0.5330
D	 0.8330	 0.5340
E	 0.8290	 0.5320
F	 0.8270	 0.5310
G	 0.8330	 0.5320
H	 0.8370	 0.5340
I	 0.8370	 0.5330
J	 0.8370	 0.5330
K	 0.8340	 0.5330
L	 0.8330	 0.5320

