



## Full wwPDB EM Validation Report ⓘ

Jun 24, 2024 – 02:48 pm BST

PDB ID : 8QOJ  
EMDB ID : EMD-18540  
Title : human connexin-36 gap junction channel in complex with mefloquine  
Authors : Ding, X.Y.; Blum, T.B.; Korkhov, V.M.  
Deposited on : 2023-09-29  
Resolution : 2.13 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.dev92  
Mogul : 1.8.4, 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 : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

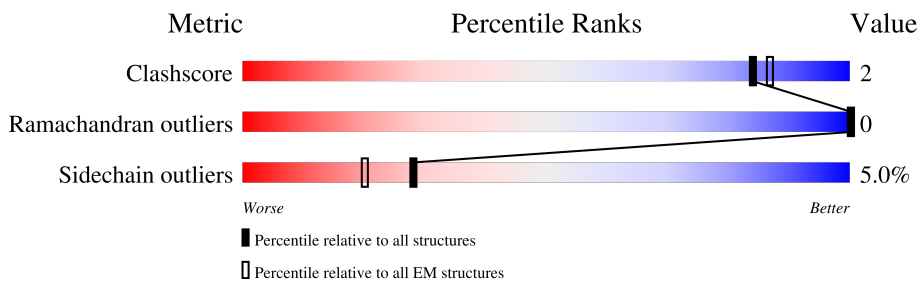
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.13 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.



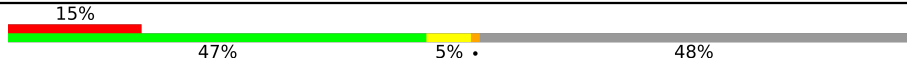
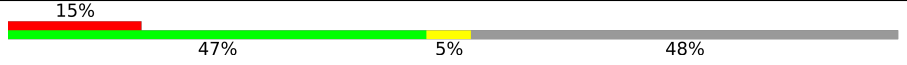
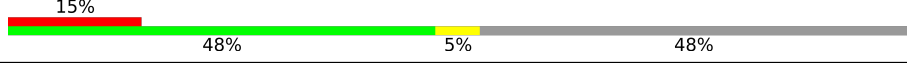

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	330	
1	B	330	
1	C	330	
1	D	330	
1	E	330	
1	F	330	
1	G	330	
1	H	330	

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Mol	Chain	Length	Quality of chain
1	I	330	
1	J	330	
1	K	330	
1	L	330	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 34302 atoms, of which 17100 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	H	N	O	S		
1	A	173	2803	920	1409	225	236	13	0	0
1	B	173	2803	920	1409	225	236	13	0	0
1	C	173	2803	920	1409	225	236	13	0	0
1	D	173	2803	920	1409	225	236	13	0	0
1	E	173	2803	920	1409	225	236	13	0	0
1	F	173	2803	920	1409	225	236	13	0	0
1	G	173	2803	920	1409	225	236	13	0	0
1	H	173	2803	920	1409	225	236	13	0	0
1	I	173	2803	920	1409	225	236	13	0	0
1	J	173	2803	920	1409	225	236	13	0	0
1	K	173	2803	920	1409	225	236	13	0	0
1	L	173	2803	920	1409	225	236	13	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	322	ALA	-	expression tag	UNP Q9UKL4
A	323	ALA	-	expression tag	UNP Q9UKL4
A	324	ALA	-	expression tag	UNP Q9UKL4
A	325	LEU	-	expression tag	UNP Q9UKL4
A	326	GLU	-	expression tag	UNP Q9UKL4
A	327	VAL	-	expression tag	UNP Q9UKL4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	328	LEU	-	expression tag	UNP Q9UKL4
A	329	PHE	-	expression tag	UNP Q9UKL4
A	330	GLN	-	expression tag	UNP Q9UKL4
B	322	ALA	-	expression tag	UNP Q9UKL4
B	323	ALA	-	expression tag	UNP Q9UKL4
B	324	ALA	-	expression tag	UNP Q9UKL4
B	325	LEU	-	expression tag	UNP Q9UKL4
B	326	GLU	-	expression tag	UNP Q9UKL4
B	327	VAL	-	expression tag	UNP Q9UKL4
B	328	LEU	-	expression tag	UNP Q9UKL4
B	329	PHE	-	expression tag	UNP Q9UKL4
B	330	GLN	-	expression tag	UNP Q9UKL4
C	322	ALA	-	expression tag	UNP Q9UKL4
C	323	ALA	-	expression tag	UNP Q9UKL4
C	324	ALA	-	expression tag	UNP Q9UKL4
C	325	LEU	-	expression tag	UNP Q9UKL4
C	326	GLU	-	expression tag	UNP Q9UKL4
C	327	VAL	-	expression tag	UNP Q9UKL4
C	328	LEU	-	expression tag	UNP Q9UKL4
C	329	PHE	-	expression tag	UNP Q9UKL4
C	330	GLN	-	expression tag	UNP Q9UKL4
D	322	ALA	-	expression tag	UNP Q9UKL4
D	323	ALA	-	expression tag	UNP Q9UKL4
D	324	ALA	-	expression tag	UNP Q9UKL4
D	325	LEU	-	expression tag	UNP Q9UKL4
D	326	GLU	-	expression tag	UNP Q9UKL4
D	327	VAL	-	expression tag	UNP Q9UKL4
D	328	LEU	-	expression tag	UNP Q9UKL4
D	329	PHE	-	expression tag	UNP Q9UKL4
D	330	GLN	-	expression tag	UNP Q9UKL4
E	322	ALA	-	expression tag	UNP Q9UKL4
E	323	ALA	-	expression tag	UNP Q9UKL4
E	324	ALA	-	expression tag	UNP Q9UKL4
E	325	LEU	-	expression tag	UNP Q9UKL4
E	326	GLU	-	expression tag	UNP Q9UKL4
E	327	VAL	-	expression tag	UNP Q9UKL4
E	328	LEU	-	expression tag	UNP Q9UKL4
E	329	PHE	-	expression tag	UNP Q9UKL4
E	330	GLN	-	expression tag	UNP Q9UKL4
F	322	ALA	-	expression tag	UNP Q9UKL4
F	323	ALA	-	expression tag	UNP Q9UKL4
F	324	ALA	-	expression tag	UNP Q9UKL4

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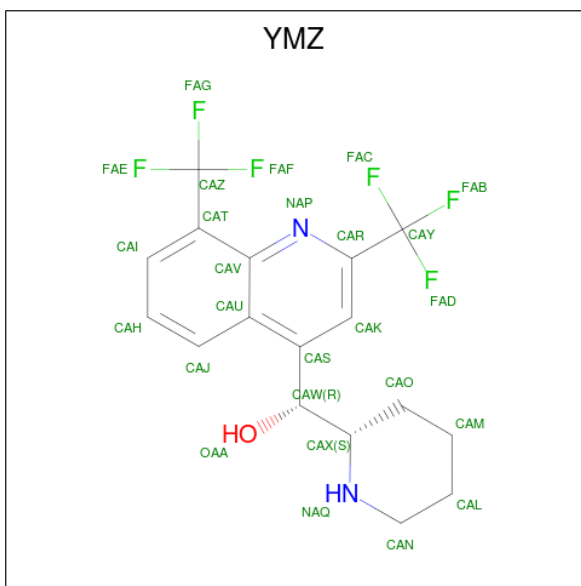
Chain	Residue	Modelled	Actual	Comment	Reference
F	325	LEU	-	expression tag	UNP Q9UKL4
F	326	GLU	-	expression tag	UNP Q9UKL4
F	327	VAL	-	expression tag	UNP Q9UKL4
F	328	LEU	-	expression tag	UNP Q9UKL4
F	329	PHE	-	expression tag	UNP Q9UKL4
F	330	GLN	-	expression tag	UNP Q9UKL4
G	322	ALA	-	expression tag	UNP Q9UKL4
G	323	ALA	-	expression tag	UNP Q9UKL4
G	324	ALA	-	expression tag	UNP Q9UKL4
G	325	LEU	-	expression tag	UNP Q9UKL4
G	326	GLU	-	expression tag	UNP Q9UKL4
G	327	VAL	-	expression tag	UNP Q9UKL4
G	328	LEU	-	expression tag	UNP Q9UKL4
G	329	PHE	-	expression tag	UNP Q9UKL4
G	330	GLN	-	expression tag	UNP Q9UKL4
H	322	ALA	-	expression tag	UNP Q9UKL4
H	323	ALA	-	expression tag	UNP Q9UKL4
H	324	ALA	-	expression tag	UNP Q9UKL4
H	325	LEU	-	expression tag	UNP Q9UKL4
H	326	GLU	-	expression tag	UNP Q9UKL4
H	327	VAL	-	expression tag	UNP Q9UKL4
H	328	LEU	-	expression tag	UNP Q9UKL4
H	329	PHE	-	expression tag	UNP Q9UKL4
H	330	GLN	-	expression tag	UNP Q9UKL4
I	322	ALA	-	expression tag	UNP Q9UKL4
I	323	ALA	-	expression tag	UNP Q9UKL4
I	324	ALA	-	expression tag	UNP Q9UKL4
I	325	LEU	-	expression tag	UNP Q9UKL4
I	326	GLU	-	expression tag	UNP Q9UKL4
I	327	VAL	-	expression tag	UNP Q9UKL4
I	328	LEU	-	expression tag	UNP Q9UKL4
I	329	PHE	-	expression tag	UNP Q9UKL4
I	330	GLN	-	expression tag	UNP Q9UKL4
J	322	ALA	-	expression tag	UNP Q9UKL4
J	323	ALA	-	expression tag	UNP Q9UKL4
J	324	ALA	-	expression tag	UNP Q9UKL4
J	325	LEU	-	expression tag	UNP Q9UKL4
J	326	GLU	-	expression tag	UNP Q9UKL4
J	327	VAL	-	expression tag	UNP Q9UKL4
J	328	LEU	-	expression tag	UNP Q9UKL4
J	329	PHE	-	expression tag	UNP Q9UKL4
J	330	GLN	-	expression tag	UNP Q9UKL4

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Chain	Residue	Modelled	Actual	Comment	Reference
K	322	ALA	-	expression tag	UNP Q9UKL4
K	323	ALA	-	expression tag	UNP Q9UKL4
K	324	ALA	-	expression tag	UNP Q9UKL4
K	325	LEU	-	expression tag	UNP Q9UKL4
K	326	GLU	-	expression tag	UNP Q9UKL4
K	327	VAL	-	expression tag	UNP Q9UKL4
K	328	LEU	-	expression tag	UNP Q9UKL4
K	329	PHE	-	expression tag	UNP Q9UKL4
K	330	GLN	-	expression tag	UNP Q9UKL4
L	322	ALA	-	expression tag	UNP Q9UKL4
L	323	ALA	-	expression tag	UNP Q9UKL4
L	324	ALA	-	expression tag	UNP Q9UKL4
L	325	LEU	-	expression tag	UNP Q9UKL4
L	326	GLU	-	expression tag	UNP Q9UKL4
L	327	VAL	-	expression tag	UNP Q9UKL4
L	328	LEU	-	expression tag	UNP Q9UKL4
L	329	PHE	-	expression tag	UNP Q9UKL4
L	330	GLN	-	expression tag	UNP Q9UKL4

- Molecule 2 is Mefloquine (three-letter code: YMZ) (formula:  $C_{17}H_{16}F_6N_2O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	F	H	N		O
2	A	1	Total	C	F	H	N	O	0
			42	17	6	16	2	1	
2	B	1	Total	C	F	H	N	O	0
			42	17	6	16	2	1	

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Mol	Chain	Residues	Atoms					AltConf	
2	C	1	Total	C	F	H	N	O	0
			42	17	6	16	2	1	
2	D	1	Total	C	F	H	N	O	0
			42	17	6	16	2	1	
2	E	1	Total	C	F	H	N	O	0
			42	17	6	16	2	1	
2	F	1	Total	C	F	H	N	O	0
			42	17	6	16	2	1	
2	G	1	Total	C	F	H	N	O	0
			42	17	6	16	2	1	
2	H	1	Total	C	F	H	N	O	0
			42	17	6	16	2	1	
2	I	1	Total	C	F	H	N	O	0
			42	17	6	16	2	1	
2	J	1	Total	C	F	H	N	O	0
			42	17	6	16	2	1	
2	K	1	Total	C	F	H	N	O	0
			42	17	6	16	2	1	
2	L	1	Total	C	F	H	N	O	0
			42	17	6	16	2	1	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		AltConf
3	A	12	Total	O	0
			12	12	
3	B	13	Total	O	0
			13	13	
3	C	15	Total	O	0
			15	15	
3	D	13	Total	O	0
			13	13	
3	E	14	Total	O	0
			14	14	
3	F	15	Total	O	0
			15	15	
3	G	14	Total	O	0
			14	14	
3	H	13	Total	O	0
			13	13	
3	I	13	Total	O	0
			13	13	

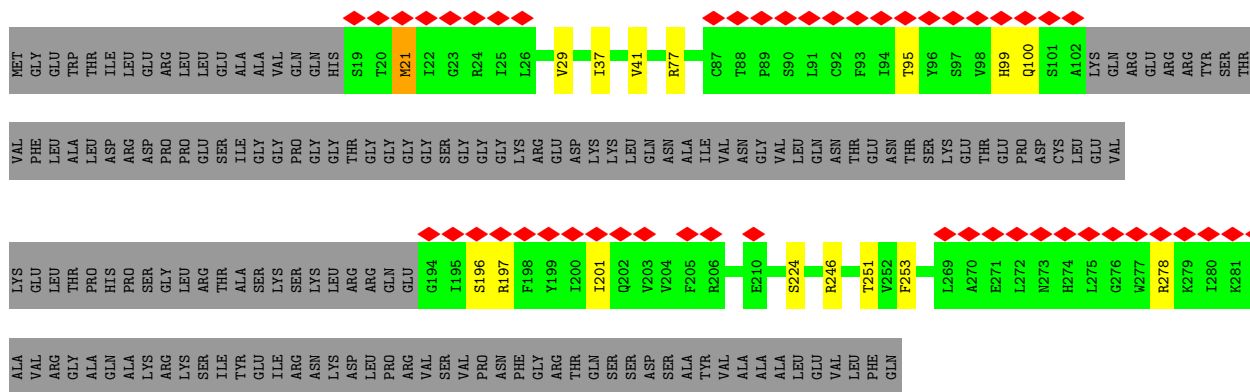
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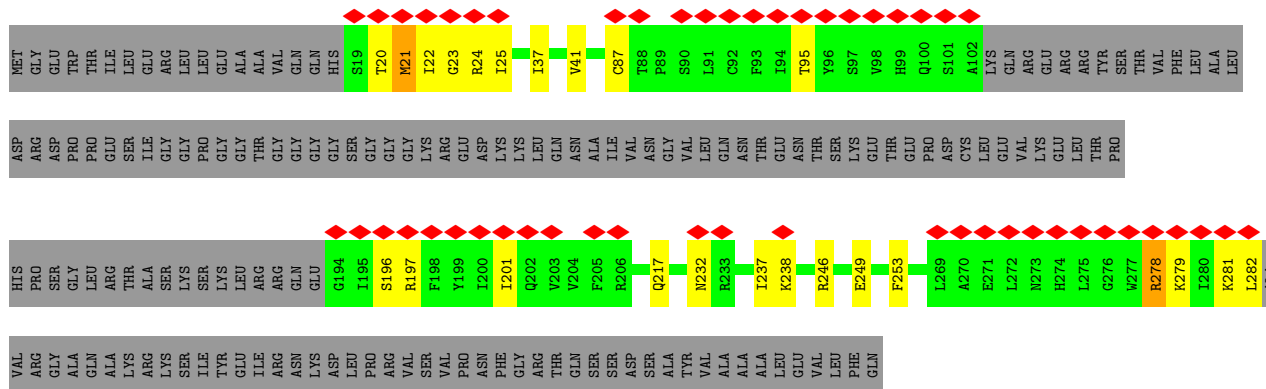
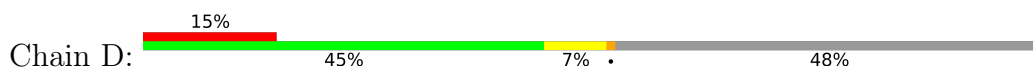
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Mol	Chain	Residues	Atoms		AltConf
3	J	13	Total 13	O 13	0
3	K	13	Total 13	O 13	0
3	L	14	Total 14	O 14	0

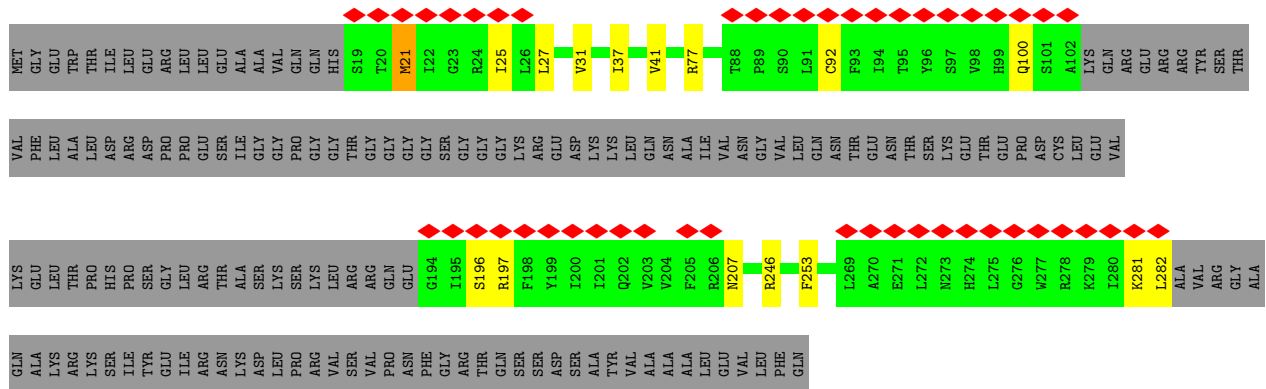




• Molecule 1: Gap junction delta-2 protein

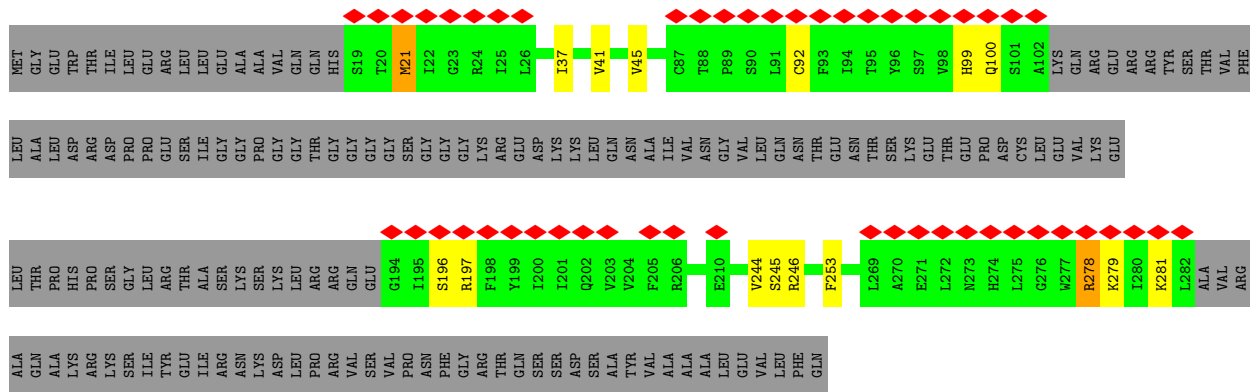


• Molecule 1: Gap junction delta-2 protein

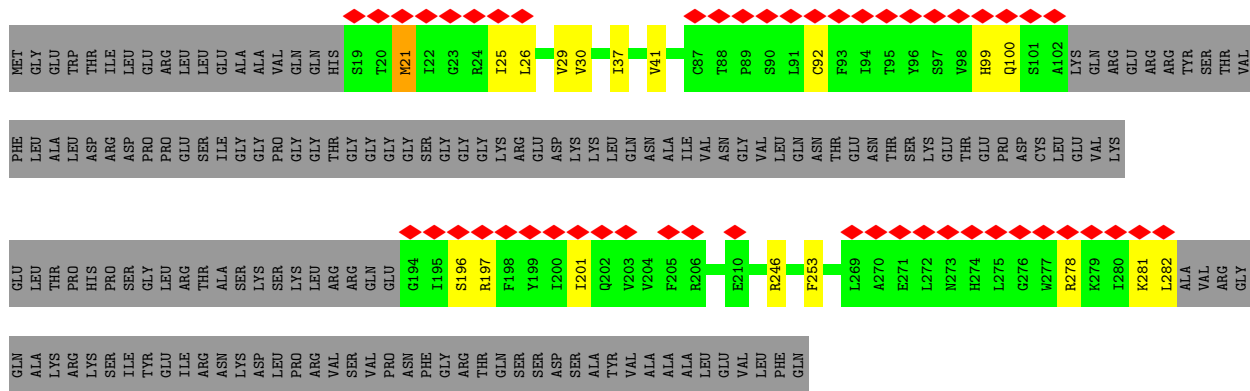


• Molecule 1: Gap junction delta-2 protein

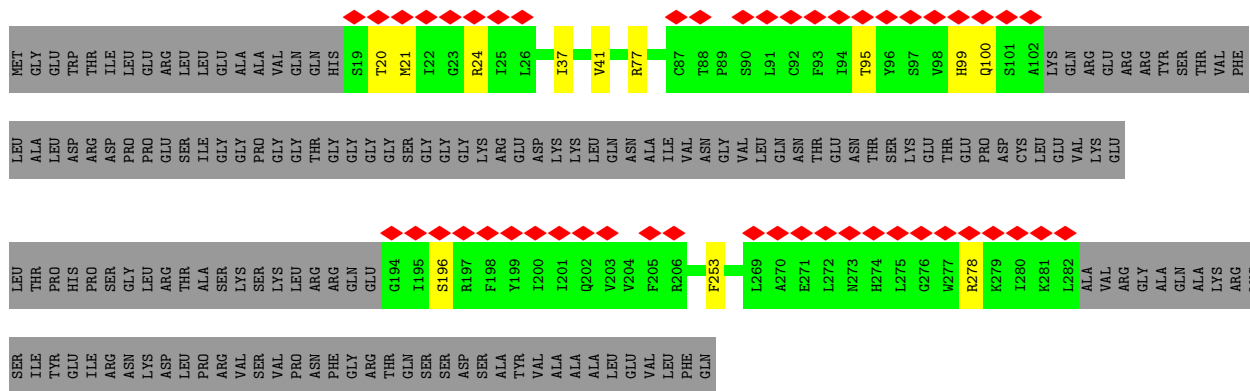




• Molecule 1: Gap junction delta-2 protein



• Molecule 1: Gap junction delta-2 protein



• Molecule 1: Gap junction delta-2 protein





MET	GLY	GLU	TRP	THR	ILE	LEU	GLU	ARG	LEU	LEU	ALA	ALA	VAL	GLN	GLN	HIS	S19	T20	M21	I22	G23	R24	I25	L26	V29	I37	V41	T88	P89	S90	L91	C92	F93	I94	T95	Y96	S97	V98	H99	Q100	S101	A102	LYS	GLN	ARG	GLU	ARG	ARG	TYR	SER	THR	VAL	PHE	LEU	
ALA	LEU	ASP	ARG	ASP	PRO	PRO	GLU	SER	GLY	ILE	LEU	GLY	PRO	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	SER	GLY	GLY	GLY	GLY	VAL	ASN	GLN	THR	GLU	ASN	THR	SER	LYS	GLU	THR	GLU	PRO	ASP	CYS	LEU	GLU	VAL	LYS	GLU	LEU	VAL	GLY	LEU		
THR	PRO	HIS	PRO	SER	GLY	LEU	ARG	THR	ALA	THR	LYS	SER	LYS	VAL	LYS	LYS	G194	I195	S196	R197	F198	Y199	I200	I201	Q202	V203	V204	F205	R206	R246	F253	L269	A270	E271	L272	R273	H274	L275	G276	W277	R278	R279	I280	R281	L282	ALA	VAL	ARG	GLY	ALA	GLN	ALA	LYS	ARG	
LYS	SER	ILE	TYR	LEU	ILE	ARG	ASN	LYS	ASP	LEU	PRO	ARG	VAL	SER	PRO	ASN	PHE	GLY	ARG	THR	GLN	SER	SER	ASP	SER	ALA	VAL	VAL	VAL	LEU	PHE	GLN	L269	A270	E271	L272	R273	H274	L275	G276	W277	R278	R279	I280	R281	L282	ALA	VAL	ARG	GLY	ALA	GLN	ALA	LYS	ARG

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102585	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	55	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.077	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.031	Depositor
Map size ( $\text{\AA}$ )	264.0, 264.0, 264.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.66, 0.66, 0.66	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: YMZ

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	0.26	0/1428	0.47	0/1940
1	B	0.27	0/1428	0.48	0/1940
1	C	0.27	0/1428	0.49	0/1940
1	D	0.26	0/1428	0.47	0/1940
1	E	0.26	0/1428	0.47	0/1940
1	F	0.26	0/1428	0.48	0/1940
1	G	0.26	0/1428	0.48	0/1940
1	H	0.26	0/1428	0.47	0/1940
1	I	0.26	0/1428	0.47	0/1940
1	J	0.27	0/1428	0.50	0/1940
1	K	0.26	0/1428	0.48	0/1940
1	L	0.27	0/1428	0.47	0/1940
All	All	0.26	0/17136	0.48	0/23280

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	1394	1409	1409	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1394	1409	1409	5	0
1	C	1394	1409	1409	9	0
1	D	1394	1409	1409	12	0
1	E	1394	1409	1409	7	0
1	F	1394	1409	1409	7	0
1	G	1394	1409	1409	8	0
1	H	1394	1409	1409	4	0
1	I	1394	1409	1409	10	0
1	J	1394	1409	1409	8	0
1	K	1394	1409	1409	8	0
1	L	1394	1409	1409	7	0
2	A	26	16	0	0	0
2	B	26	16	0	0	0
2	C	26	16	0	0	0
2	D	26	16	0	0	0
2	E	26	16	0	0	0
2	F	26	16	0	0	0
2	G	26	16	0	0	0
2	H	26	16	0	0	0
2	I	26	16	0	0	0
2	J	26	16	0	0	0
2	K	26	16	0	0	0
2	L	26	16	0	0	0
3	A	12	0	0	0	0
3	B	13	0	0	0	0
3	C	15	0	0	0	0
3	D	13	0	0	1	0
3	E	14	0	0	0	0
3	F	15	0	0	0	0
3	G	14	0	0	0	0
3	H	13	0	0	0	0
3	I	13	0	0	0	0
3	J	13	0	0	0	0
3	K	13	0	0	0	0
3	L	14	0	0	0	0
All	All	17202	17100	16908	78	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 (78) 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:237:ILE:HG22	1:D:238:LYS:HD2	1.68	0.75
1:K:37:ILE:O	1:K:41:VAL:HG22	1.97	0.65
1:C:37:ILE:O	1:C:41:VAL:HG22	1.98	0.64
1:H:37:ILE:O	1:H:41:VAL:HG22	1.98	0.63
1:A:37:ILE:O	1:A:41:VAL:HG22	1.98	0.63
1:L:37:ILE:O	1:L:41:VAL:HG22	1.99	0.63
1:B:37:ILE:O	1:B:41:VAL:HG22	1.99	0.62
1:G:37:ILE:O	1:G:41:VAL:HG22	1.99	0.62
1:I:37:ILE:O	1:I:41:VAL:HG22	1.99	0.62
1:F:37:ILE:O	1:F:41:VAL:HG22	1.99	0.62
1:E:37:ILE:O	1:E:41:VAL:HG22	1.99	0.62
1:J:37:ILE:O	1:J:41:VAL:HG22	2.01	0.60
1:D:37:ILE:O	1:D:41:VAL:HG22	2.01	0.60
1:D:87:CYS:SG	3:D:508:HOH:O	2.56	0.60
1:A:21:MET:SD	1:A:21:MET:N	2.78	0.57
1:C:95:THR:HG22	1:D:25:ILE:HD12	1.91	0.52
1:D:95:THR:HG22	1:E:25:ILE:HD12	1.91	0.52
1:J:206:ARG:NH1	1:J:268:ASN:OD1	2.43	0.52
1:J:232:ASN:CG	1:J:232:ASN:O	2.49	0.52
1:K:92:CYS:SG	1:L:29:VAL:HG21	2.50	0.51
1:L:100:GLN:HA	1:L:100:GLN:OE1	2.11	0.50
1:F:21:MET:H	1:F:21:MET:CE	2.25	0.50
1:G:25:ILE:HD12	1:L:95:THR:HG22	1.94	0.50
1:B:272:LEU:HD21	1:B:277:TRP:HZ3	1.77	0.50
1:D:197:ARG:O	1:D:201:ILE:HD12	2.12	0.49
1:E:21:MET:SD	1:E:21:MET:N	2.81	0.49
1:J:21:MET:H	1:J:21:MET:CE	2.26	0.49
1:I:21:MET:H	1:I:21:MET:CE	2.26	0.49
1:C:21:MET:H	1:C:21:MET:CE	2.26	0.49
1:G:26:LEU:O	1:G:30:VAL:HG23	2.12	0.48
1:B:92:CYS:SG	1:C:29:VAL:HG21	2.54	0.48
1:L:21:MET:CE	1:L:21:MET:H	2.27	0.48
1:K:21:MET:SD	1:K:21:MET:N	2.86	0.48
1:G:21:MET:H	1:G:21:MET:CE	2.27	0.47
1:B:100:GLN:HA	1:B:100:GLN:OE1	2.13	0.47
1:I:278:ARG:HD2	1:I:279:LYS:N	2.29	0.47
1:J:26:LEU:O	1:J:30:VAL:HG23	2.15	0.46
1:K:21:MET:H	1:K:21:MET:CE	2.28	0.46
1:E:197:ARG:NH2	1:E:282:LEU:O	2.49	0.46
1:H:77:ARG:HD3	1:I:45:VAL:HG22	1.98	0.45
1:C:21:MET:H	1:C:21:MET:HE3	1.80	0.45
1:G:29:VAL:HG21	1:L:92:CYS:SG	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:197:ARG:O	1:I:201:ILE:HD12	2.17	0.45
1:F:100:GLN:HA	1:F:100:GLN:OE1	2.16	0.44
1:J:77:ARG:NE	1:K:249:GLU:OE2	2.47	0.44
1:K:280:ILE:O	1:K:280:ILE:HG22	2.18	0.44
1:C:77:ARG:NE	1:D:249:GLU:OE2	2.47	0.44
1:C:224:SER:HA	1:C:251:THR:HG23	2.00	0.44
1:L:21:MET:SD	1:L:21:MET:N	2.89	0.44
1:H:95:THR:HG22	1:I:25:ILE:HD12	2.01	0.43
1:D:278:ARG:HD2	1:D:279:LYS:N	2.34	0.43
1:I:77:ARG:NE	1:J:249:GLU:OE2	2.48	0.43
1:D:197:ARG:NH2	1:D:282:LEU:O	2.51	0.43
1:G:197:ARG:NH2	1:G:282:LEU:O	2.52	0.43
1:A:21:MET:H	1:A:21:MET:CE	2.32	0.42
1:C:197:ARG:O	1:C:201:ILE:HD12	2.19	0.42
1:I:21:MET:H	1:I:21:MET:HE3	1.83	0.42
1:I:224:SER:HA	1:I:251:THR:HG23	2.00	0.42
1:A:197:ARG:O	1:A:201:ILE:HD12	2.20	0.42
1:E:27:LEU:O	1:E:31:VAL:HG23	2.19	0.42
1:J:21:MET:O	1:J:25:ILE:HG12	2.20	0.42
1:E:77:ARG:HD3	1:F:45:VAL:HG22	2.02	0.42
1:G:197:ARG:O	1:G:201:ILE:HD12	2.19	0.42
1:B:21:MET:N	1:B:21:MET:HE3	2.35	0.42
1:D:21:MET:H	1:D:21:MET:CE	2.32	0.41
1:E:21:MET:H	1:E:21:MET:CE	2.32	0.41
1:H:20:THR:OG1	1:H:24:ARG:NH1	2.53	0.41
1:G:100:GLN:OE1	1:G:100:GLN:HA	2.21	0.41
1:D:20:THR:OG1	1:D:24:ARG:NH1	2.53	0.41
1:K:99:HIS:CD2	1:K:99:HIS:C	2.93	0.41
1:K:100:GLN:OE1	1:K:100:GLN:HA	2.21	0.41
1:F:21:MET:H	1:F:21:MET:HE3	1.86	0.41
1:C:100:GLN:OE1	1:C:100:GLN:HA	2.21	0.40
1:F:278:ARG:H	1:F:278:ARG:HD3	1.86	0.40
1:A:244:VAL:HG12	1:A:245:SER:N	2.37	0.40
1:D:22:ILE:HD12	1:D:23:GLY:N	2.37	0.40
1:F:244:VAL:HG12	1:F:245:SER:N	2.37	0.40
1:I:100:GLN:HA	1:I:100:GLN:OE1	2.21	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	169/330 (51%)	168 (99%)	1 (1%)	0	100	100
1	B	169/330 (51%)	167 (99%)	2 (1%)	0	100	100
1	C	169/330 (51%)	168 (99%)	1 (1%)	0	100	100
1	D	169/330 (51%)	167 (99%)	2 (1%)	0	100	100
1	E	169/330 (51%)	168 (99%)	1 (1%)	0	100	100
1	F	169/330 (51%)	168 (99%)	1 (1%)	0	100	100
1	G	169/330 (51%)	168 (99%)	1 (1%)	0	100	100
1	H	169/330 (51%)	168 (99%)	1 (1%)	0	100	100
1	I	169/330 (51%)	167 (99%)	2 (1%)	0	100	100
1	J	169/330 (51%)	168 (99%)	1 (1%)	0	100	100
1	K	169/330 (51%)	168 (99%)	1 (1%)	0	100	100
1	L	169/330 (51%)	168 (99%)	1 (1%)	0	100	100
All	All	2028/3960 (51%)	2013 (99%)	15 (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	156/285 (55%)	148 (95%)	8 (5%)	24	19
1	B	156/285 (55%)	147 (94%)	9 (6%)	20	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	156/285 (55%)	150 (96%)	6 (4%)	33	30
1	D	156/285 (55%)	148 (95%)	8 (5%)	24	19
1	E	156/285 (55%)	148 (95%)	8 (5%)	24	19
1	F	156/285 (55%)	146 (94%)	10 (6%)	17	12
1	G	156/285 (55%)	148 (95%)	8 (5%)	24	19
1	H	156/285 (55%)	150 (96%)	6 (4%)	33	30
1	I	156/285 (55%)	148 (95%)	8 (5%)	24	19
1	J	156/285 (55%)	148 (95%)	8 (5%)	24	19
1	K	156/285 (55%)	147 (94%)	9 (6%)	20	15
1	L	156/285 (55%)	151 (97%)	5 (3%)	39	37
All	All	1872/3420 (55%)	1779 (95%)	93 (5%)	28	20

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	92	CYS
1	A	100	GLN
1	A	196	SER
1	A	197	ARG
1	A	207	ASN
1	A	253	PHE
1	A	278	ARG
1	B	21	MET
1	B	92	CYS
1	B	99	HIS
1	B	196	SER
1	B	246	ARG
1	B	253	PHE
1	B	278	ARG
1	B	279	LYS
1	B	281	LYS
1	C	21	MET
1	C	99	HIS
1	C	196	SER
1	C	246	ARG
1	C	253	PHE
1	C	278	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	21	MET
1	D	196	SER
1	D	217	GLN
1	D	232	ASN
1	D	246	ARG
1	D	253	PHE
1	D	278	ARG
1	D	281	LYS
1	E	21	MET
1	E	92	CYS
1	E	100	GLN
1	E	196	SER
1	E	207	ASN
1	E	246	ARG
1	E	253	PHE
1	E	281	LYS
1	F	21	MET
1	F	92	CYS
1	F	99	HIS
1	F	196	SER
1	F	197	ARG
1	F	246	ARG
1	F	253	PHE
1	F	278	ARG
1	F	279	LYS
1	F	281	LYS
1	G	21	MET
1	G	92	CYS
1	G	99	HIS
1	G	196	SER
1	G	246	ARG
1	G	253	PHE
1	G	278	ARG
1	G	281	LYS
1	H	21	MET
1	H	99	HIS
1	H	100	GLN
1	H	196	SER
1	H	253	PHE
1	H	278	ARG
1	I	21	MET
1	I	92	CYS

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Mol	Chain	Res	Type
1	I	99	HIS
1	I	196	SER
1	I	246	ARG
1	I	253	PHE
1	I	278	ARG
1	I	281	LYS
1	J	21	MET
1	J	69	ARG
1	J	99	HIS
1	J	196	SER
1	J	224	SER
1	J	253	PHE
1	J	278	ARG
1	J	281	LYS
1	K	21	MET
1	K	69	ARG
1	K	101	SER
1	K	196	SER
1	K	197	ARG
1	K	207	ASN
1	K	253	PHE
1	K	278	ARG
1	K	279	LYS
1	L	21	MET
1	L	99	HIS
1	L	196	SER
1	L	246	ARG
1	L	253	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	99	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 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	YMZ	D	401	-	28,28,28	0.70	0	41,43,43	0.81	1 (2%)
2	YMZ	E	401	-	28,28,28	0.70	0	41,43,43	0.80	1 (2%)
2	YMZ	H	401	-	28,28,28	0.70	0	41,43,43	0.80	1 (2%)
2	YMZ	B	401	-	28,28,28	0.69	0	41,43,43	0.80	1 (2%)
2	YMZ	F	401	-	28,28,28	0.71	0	41,43,43	0.81	1 (2%)
2	YMZ	C	401	-	28,28,28	0.70	0	41,43,43	0.81	1 (2%)
2	YMZ	K	401	-	28,28,28	0.71	0	41,43,43	0.81	1 (2%)
2	YMZ	J	401	-	28,28,28	0.71	0	41,43,43	0.83	1 (2%)
2	YMZ	L	401	-	28,28,28	0.70	0	41,43,43	0.81	1 (2%)
2	YMZ	I	401	-	28,28,28	0.71	0	41,43,43	0.85	1 (2%)
2	YMZ	A	401	-	28,28,28	0.71	0	41,43,43	0.80	1 (2%)
2	YMZ	G	401	-	28,28,28	0.69	0	41,43,43	0.80	1 (2%)

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. '2' means no outliers of that kind were identified.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YMZ	D	401	-	-	5/20/28/28	0/3/3/3
2	YMZ	E	401	-	-	4/20/28/28	0/3/3/3
2	YMZ	H	401	-	-	4/20/28/28	0/3/3/3
2	YMZ	B	401	-	-	4/20/28/28	0/3/3/3
2	YMZ	F	401	-	-	4/20/28/28	0/3/3/3
2	YMZ	C	401	-	-	4/20/28/28	0/3/3/3
2	YMZ	K	401	-	-	0/20/28/28	0/3/3/3
2	YMZ	J	401	-	-	2/20/28/28	0/3/3/3
2	YMZ	L	401	-	-	4/20/28/28	0/3/3/3
2	YMZ	I	401	-	-	2/20/28/28	0/3/3/3
2	YMZ	A	401	-	-	4/20/28/28	0/3/3/3
2	YMZ	G	401	-	-	0/20/28/28	0/3/3/3

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	401	YMZ	CAY-CAR-NAP	2.50	117.02	114.79
2	J	401	YMZ	CAY-CAR-NAP	2.42	116.95	114.79
2	K	401	YMZ	CAY-CAR-NAP	2.37	116.91	114.79
2	D	401	YMZ	CAY-CAR-NAP	2.36	116.90	114.79
2	L	401	YMZ	CAY-CAR-NAP	2.32	116.86	114.79
2	F	401	YMZ	CAY-CAR-NAP	2.30	116.84	114.79
2	G	401	YMZ	CAY-CAR-NAP	2.30	116.84	114.79
2	C	401	YMZ	CAY-CAR-NAP	2.29	116.84	114.79
2	A	401	YMZ	CAY-CAR-NAP	2.29	116.83	114.79
2	E	401	YMZ	CAY-CAR-NAP	2.29	116.83	114.79
2	B	401	YMZ	CAY-CAR-NAP	2.28	116.83	114.79
2	H	401	YMZ	CAY-CAR-NAP	2.27	116.81	114.79

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	YMZ	NAP-CAR-CAY-FAC
2	A	401	YMZ	NAP-CAR-CAY-FAC
2	H	401	YMZ	NAP-CAR-CAY-FAC
2	B	401	YMZ	NAP-CAR-CAY-FAD
2	B	401	YMZ	NAP-CAR-CAY-FAB
2	D	401	YMZ	NAP-CAR-CAY-FAC

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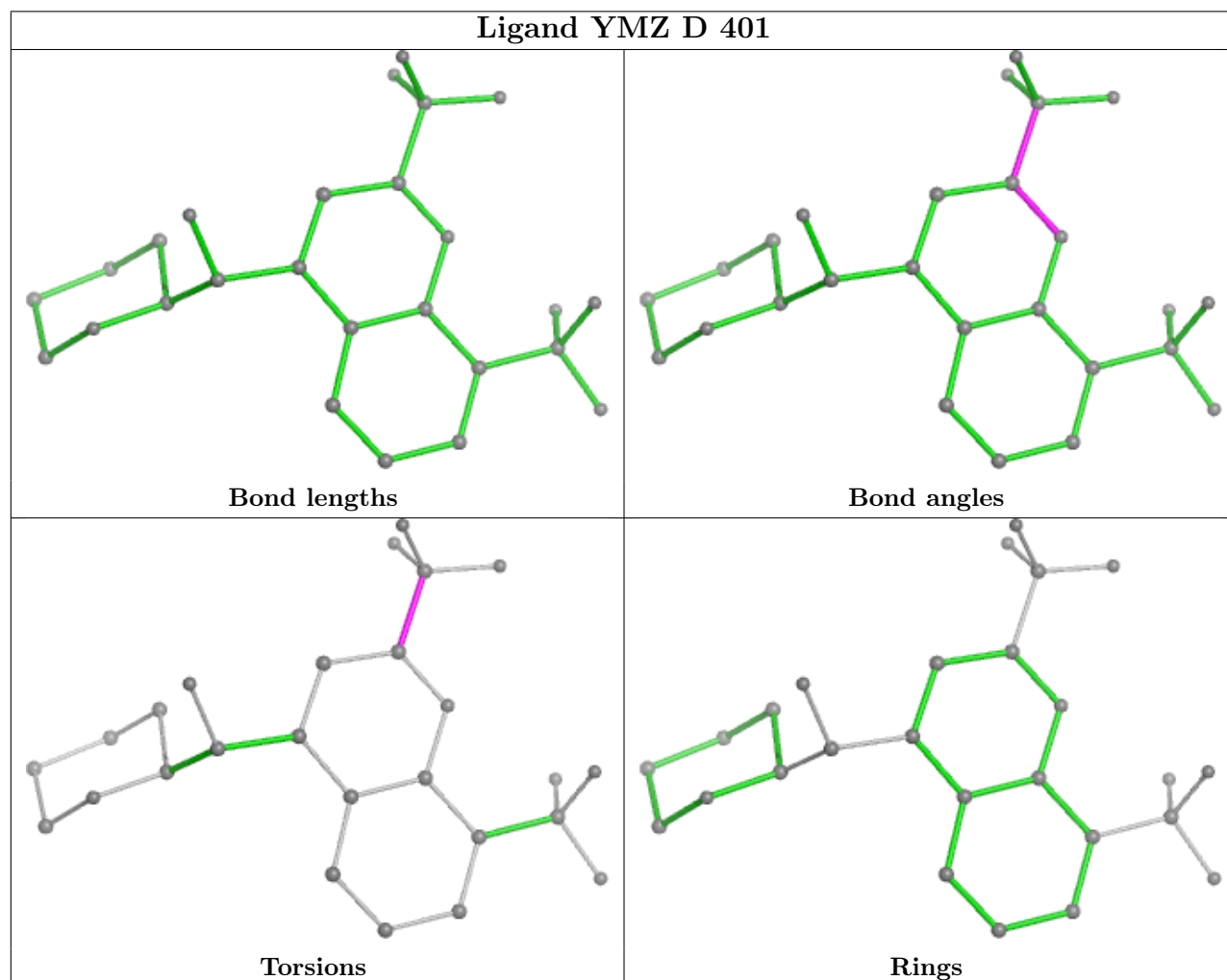
Mol	Chain	Res	Type	Atoms
2	A	401	YMZ	NAP-CAR-CAY-FAD
2	C	401	YMZ	NAP-CAR-CAY-FAC
2	F	401	YMZ	NAP-CAR-CAY-FAC
2	H	401	YMZ	NAP-CAR-CAY-FAD
2	A	401	YMZ	NAP-CAR-CAY-FAB
2	D	401	YMZ	NAP-CAR-CAY-FAB
2	E	401	YMZ	NAP-CAR-CAY-FAC
2	H	401	YMZ	NAP-CAR-CAY-FAB
2	L	401	YMZ	NAP-CAR-CAY-FAC
2	D	401	YMZ	NAP-CAR-CAY-FAD
2	D	401	YMZ	CAK-CAR-CAY-FAC
2	A	401	YMZ	CAK-CAR-CAY-FAC
2	C	401	YMZ	NAP-CAR-CAY-FAB
2	E	401	YMZ	NAP-CAR-CAY-FAB
2	F	401	YMZ	NAP-CAR-CAY-FAB
2	J	401	YMZ	NAP-CAR-CAY-FAC
2	L	401	YMZ	NAP-CAR-CAY-FAB
2	H	401	YMZ	CAK-CAR-CAY-FAC
2	F	401	YMZ	NAP-CAR-CAY-FAD
2	B	401	YMZ	CAK-CAR-CAY-FAC
2	C	401	YMZ	NAP-CAR-CAY-FAD
2	J	401	YMZ	NAP-CAR-CAY-FAB
2	L	401	YMZ	NAP-CAR-CAY-FAD
2	E	401	YMZ	NAP-CAR-CAY-FAD
2	I	401	YMZ	NAP-CAR-CAY-FAC
2	C	401	YMZ	CAK-CAR-CAY-FAB
2	D	401	YMZ	CAK-CAR-CAY-FAB
2	E	401	YMZ	CAK-CAR-CAY-FAB
2	F	401	YMZ	CAK-CAR-CAY-FAB
2	L	401	YMZ	CAK-CAR-CAY-FAB
2	I	401	YMZ	NAP-CAR-CAY-FAB

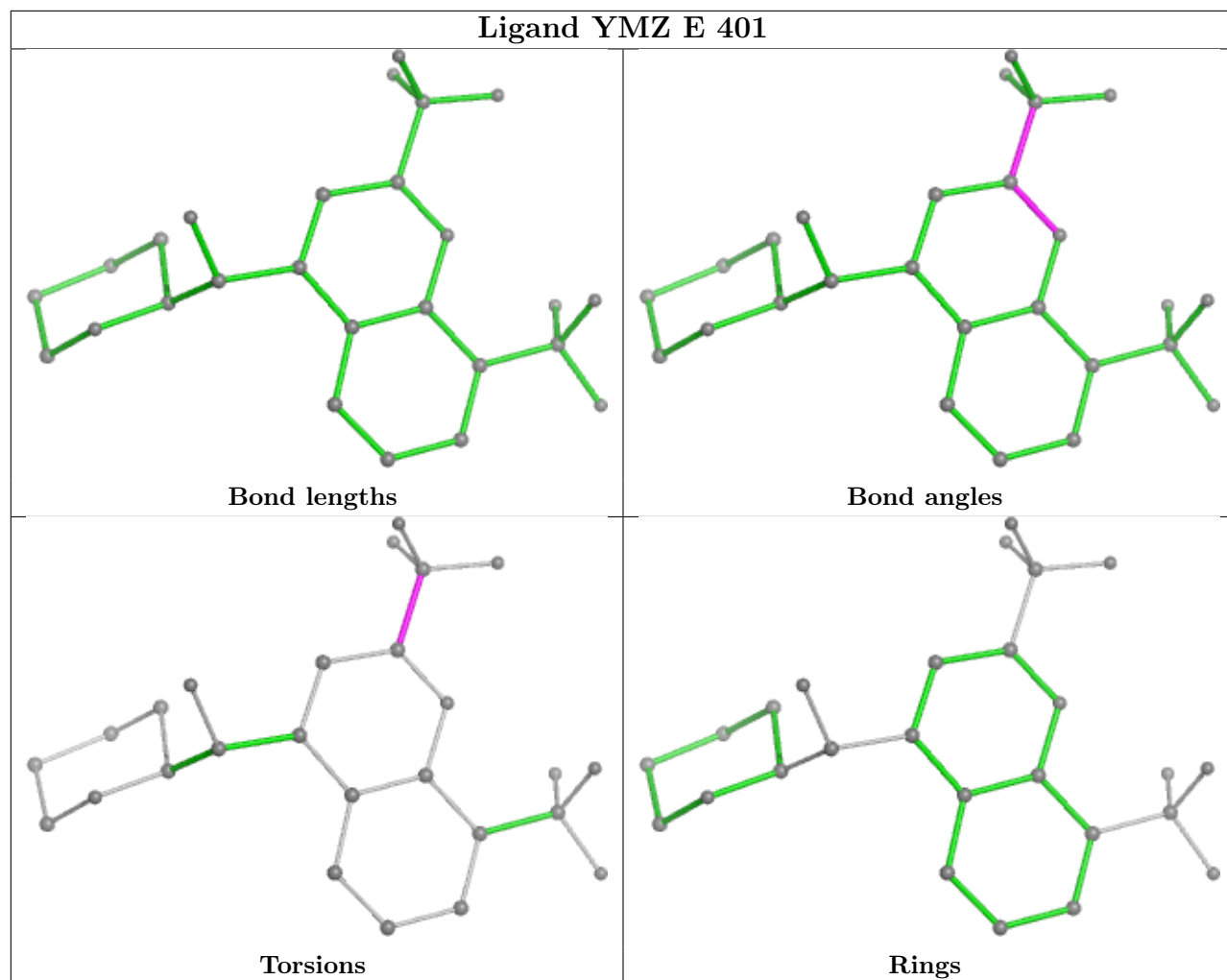
There are no ring outliers.

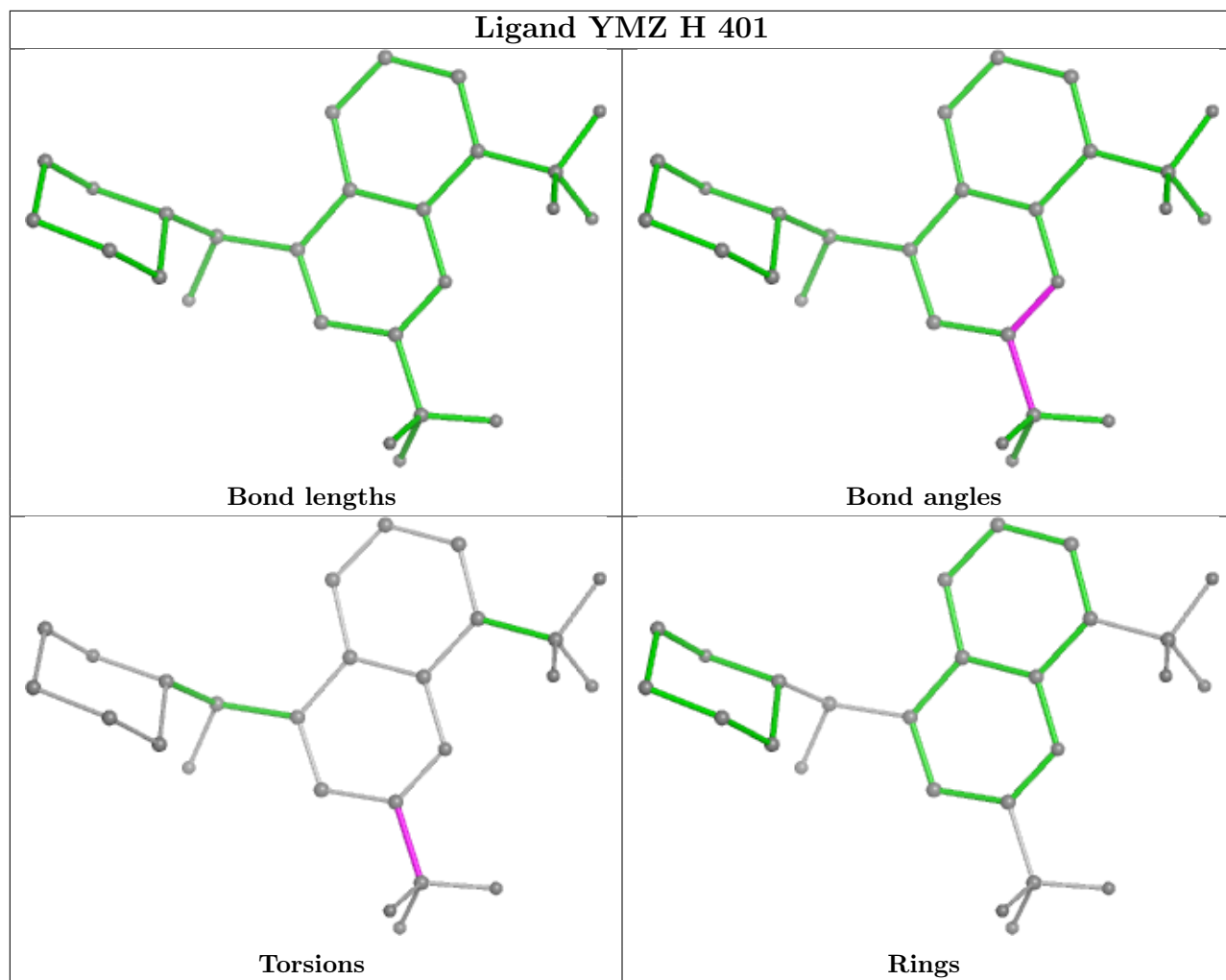
No monomer is involved in short contacts.

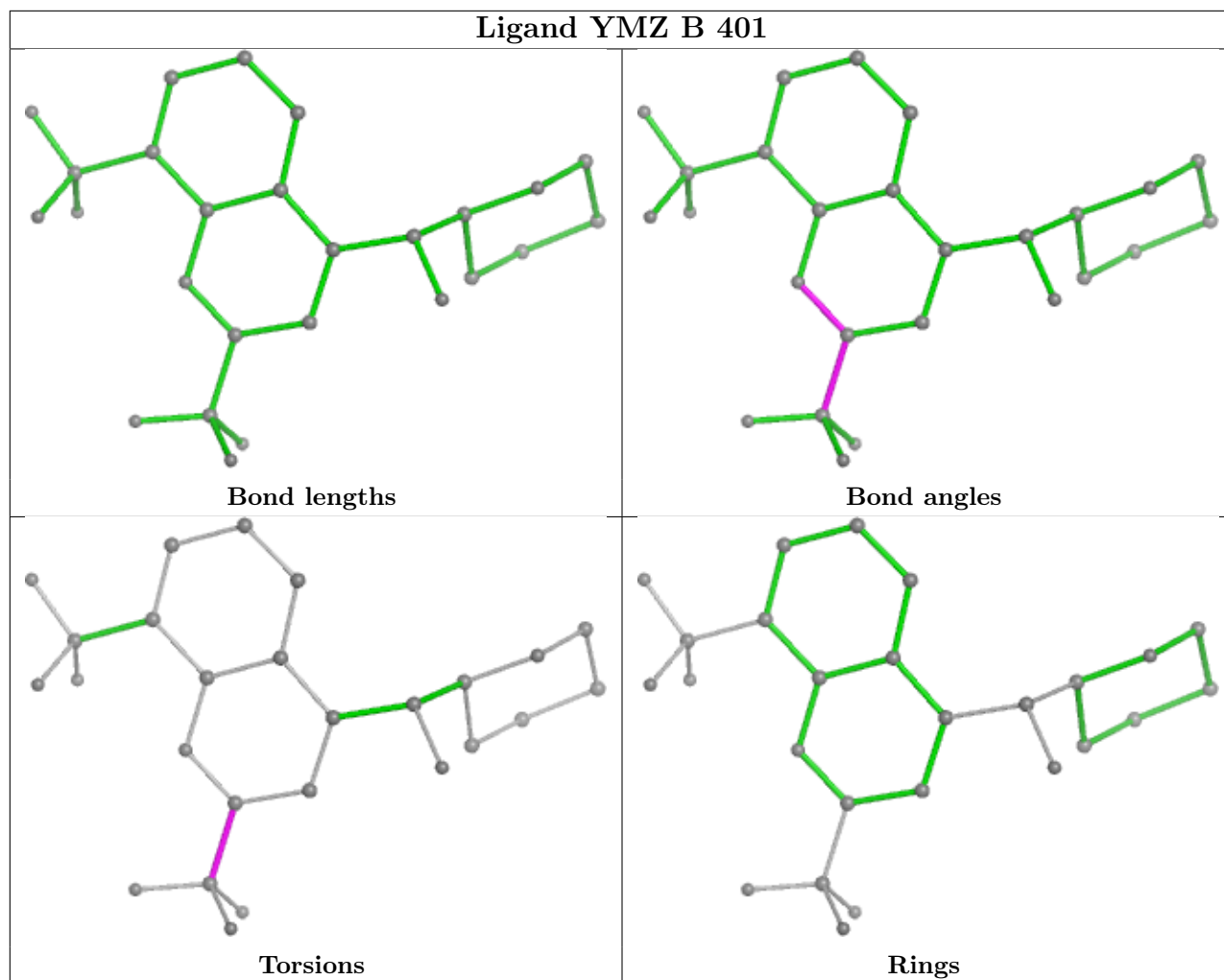
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

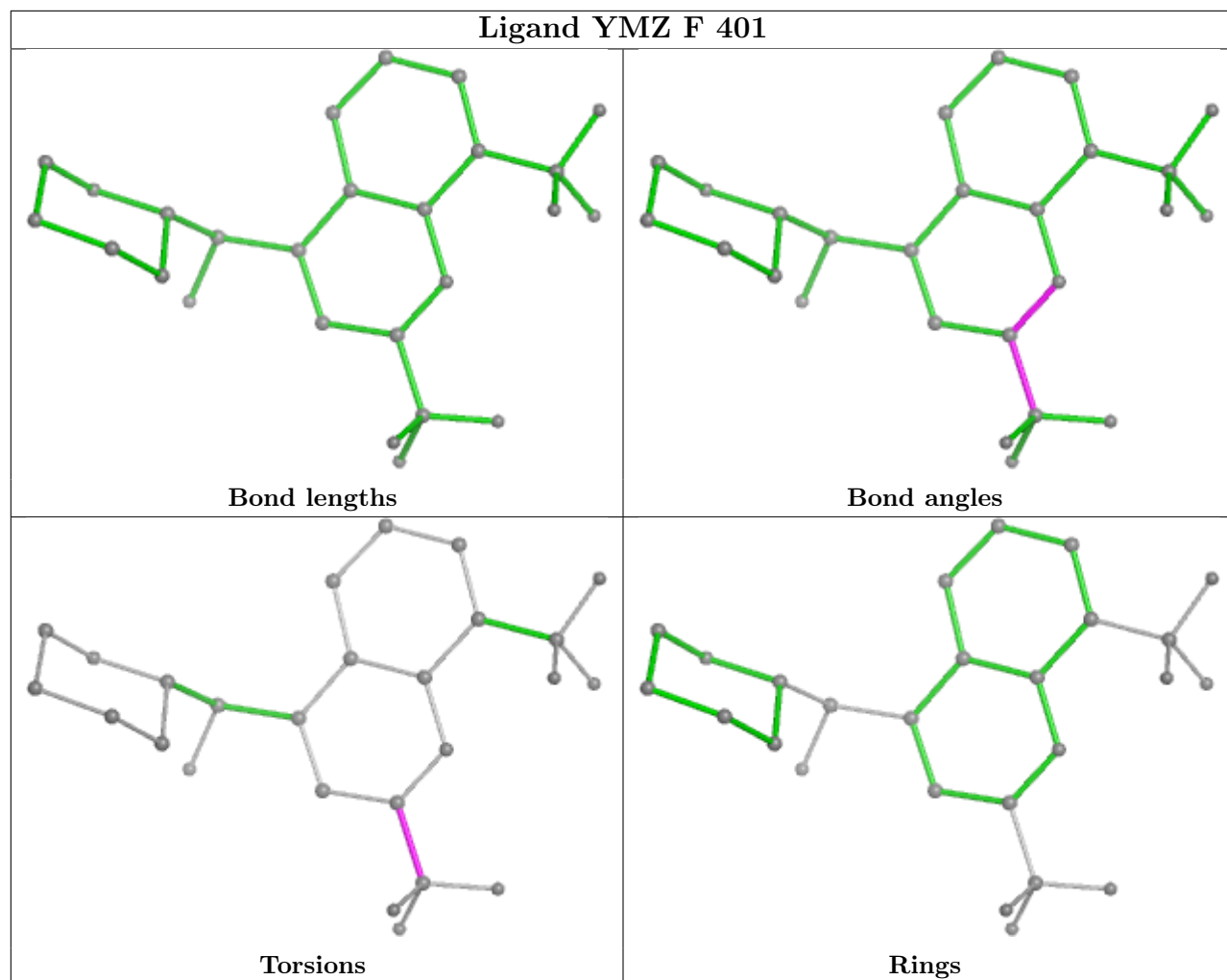
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents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

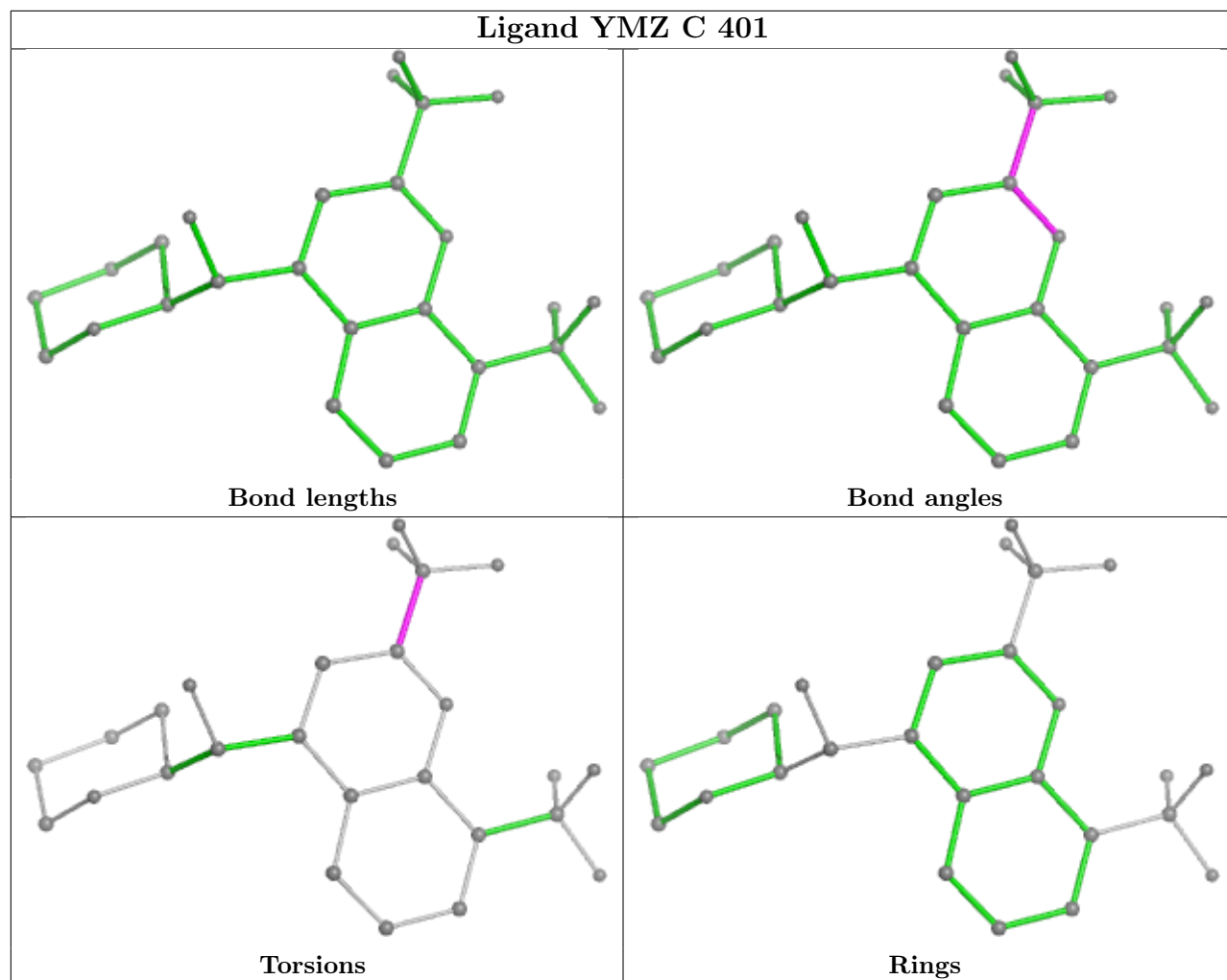




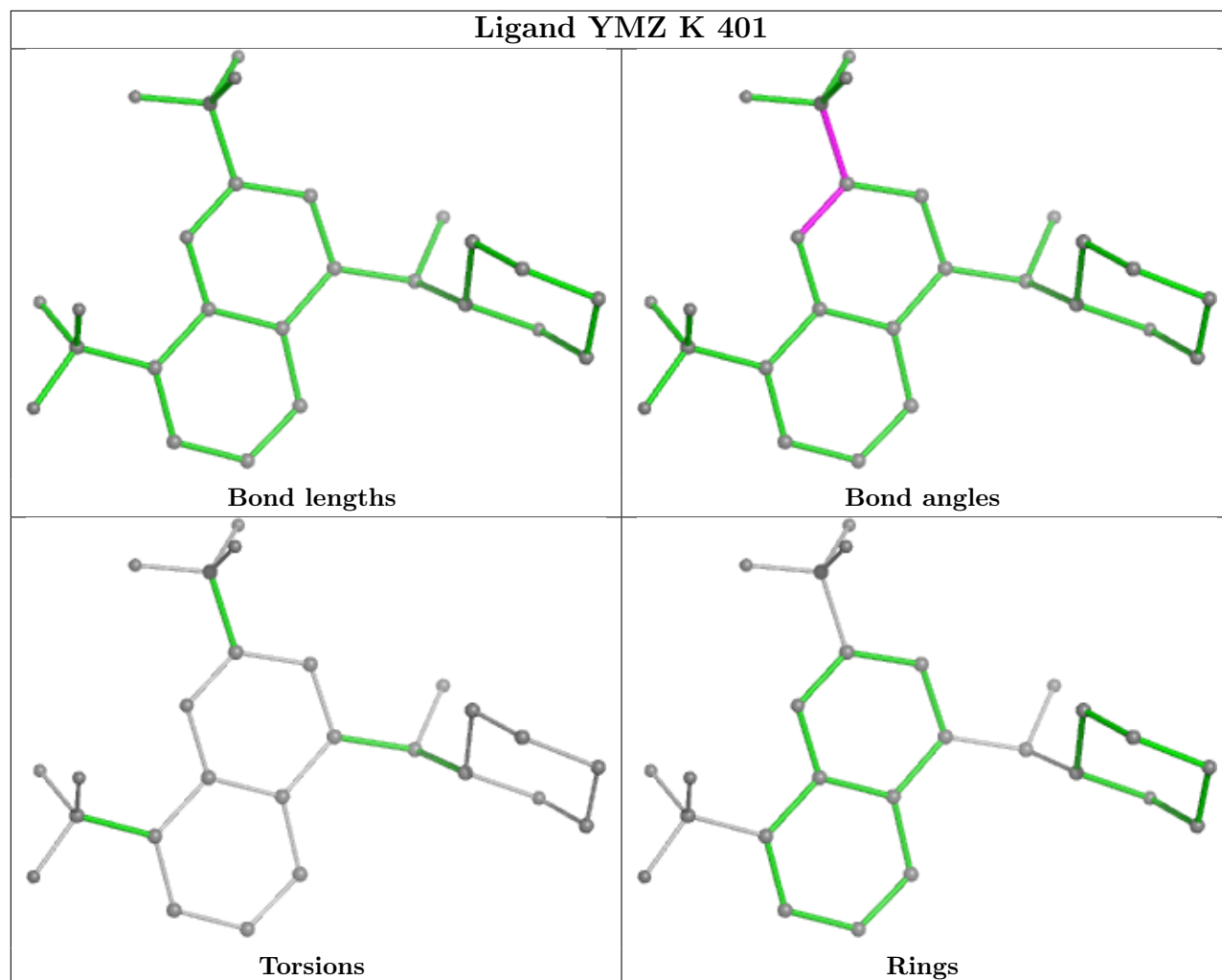


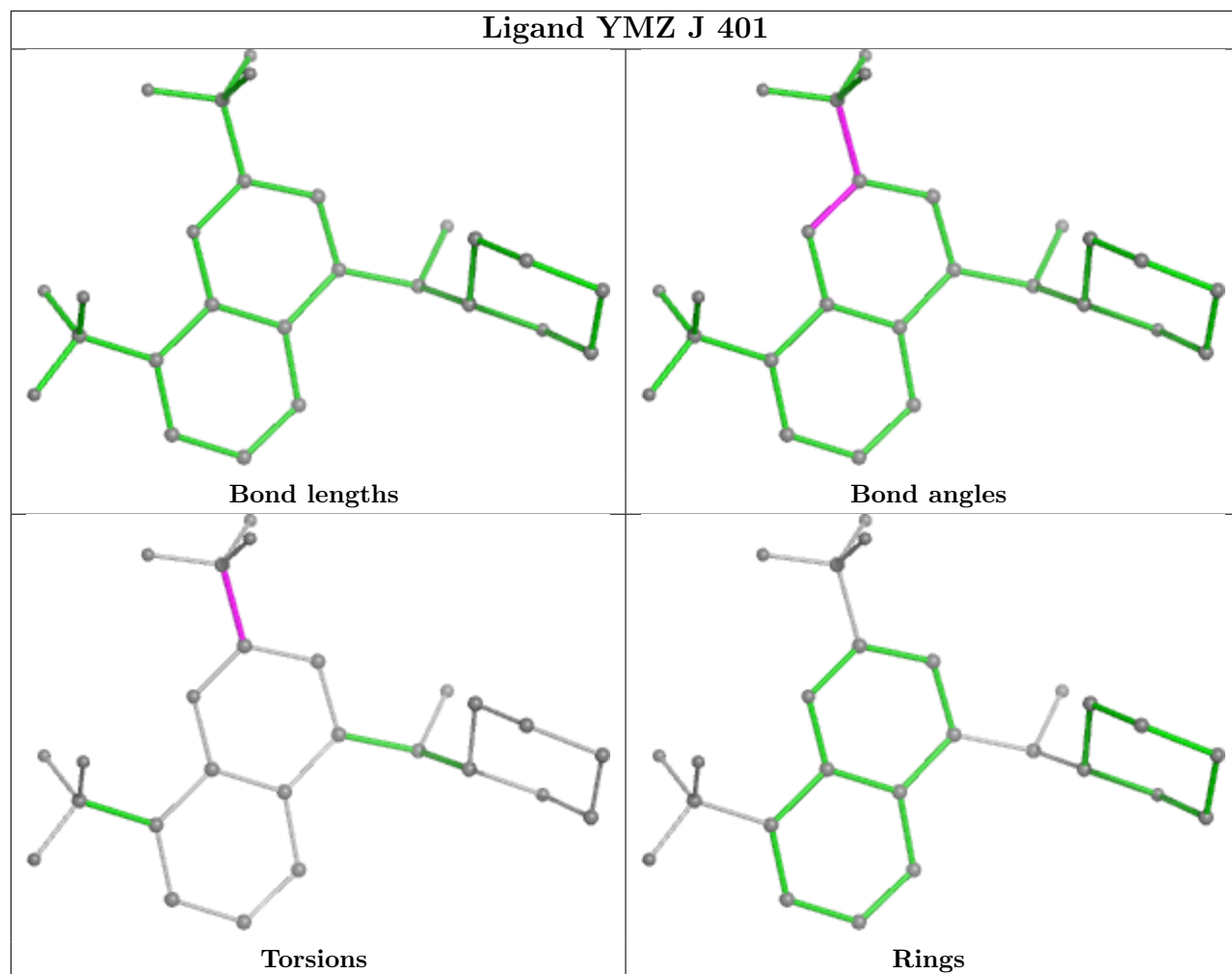


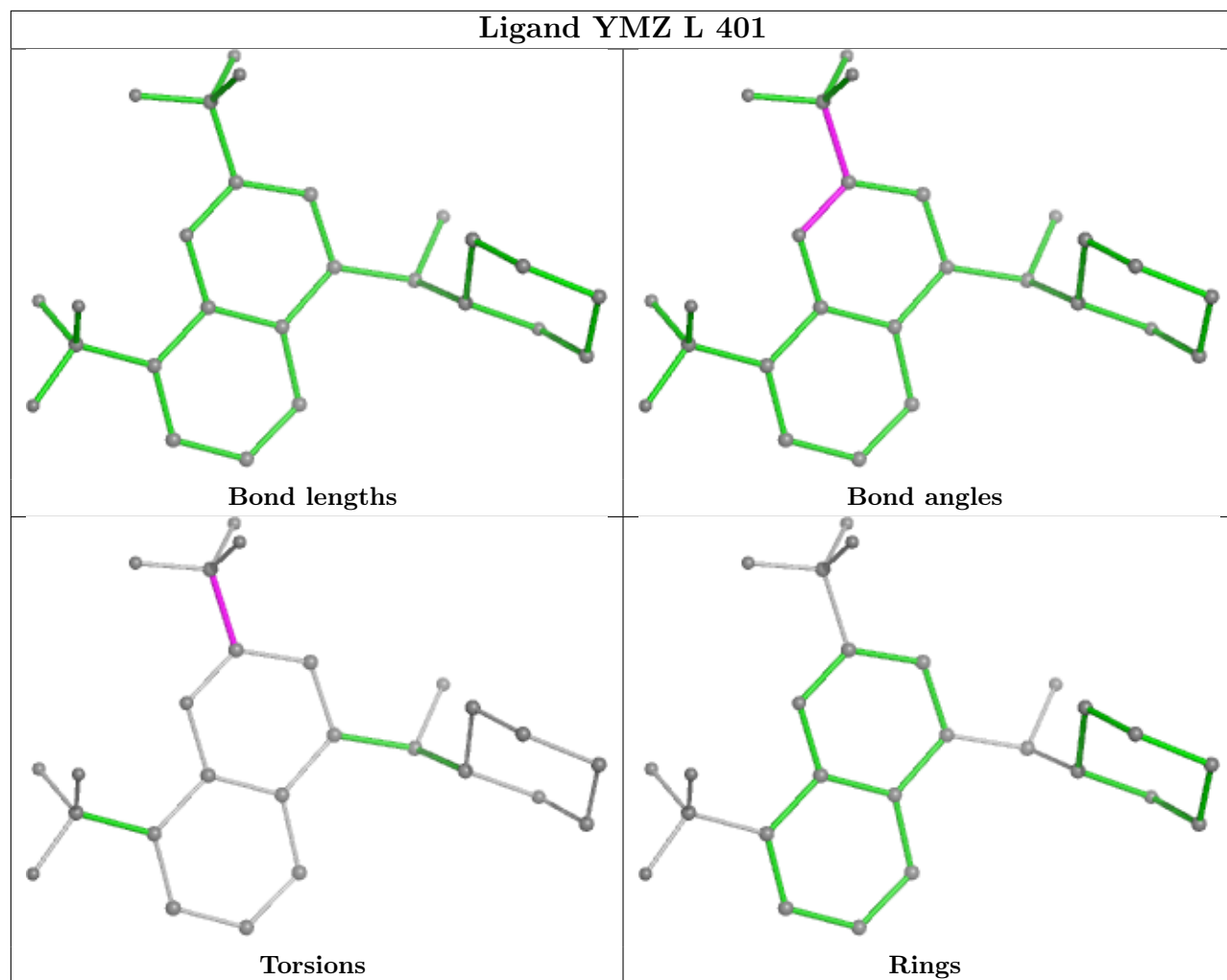


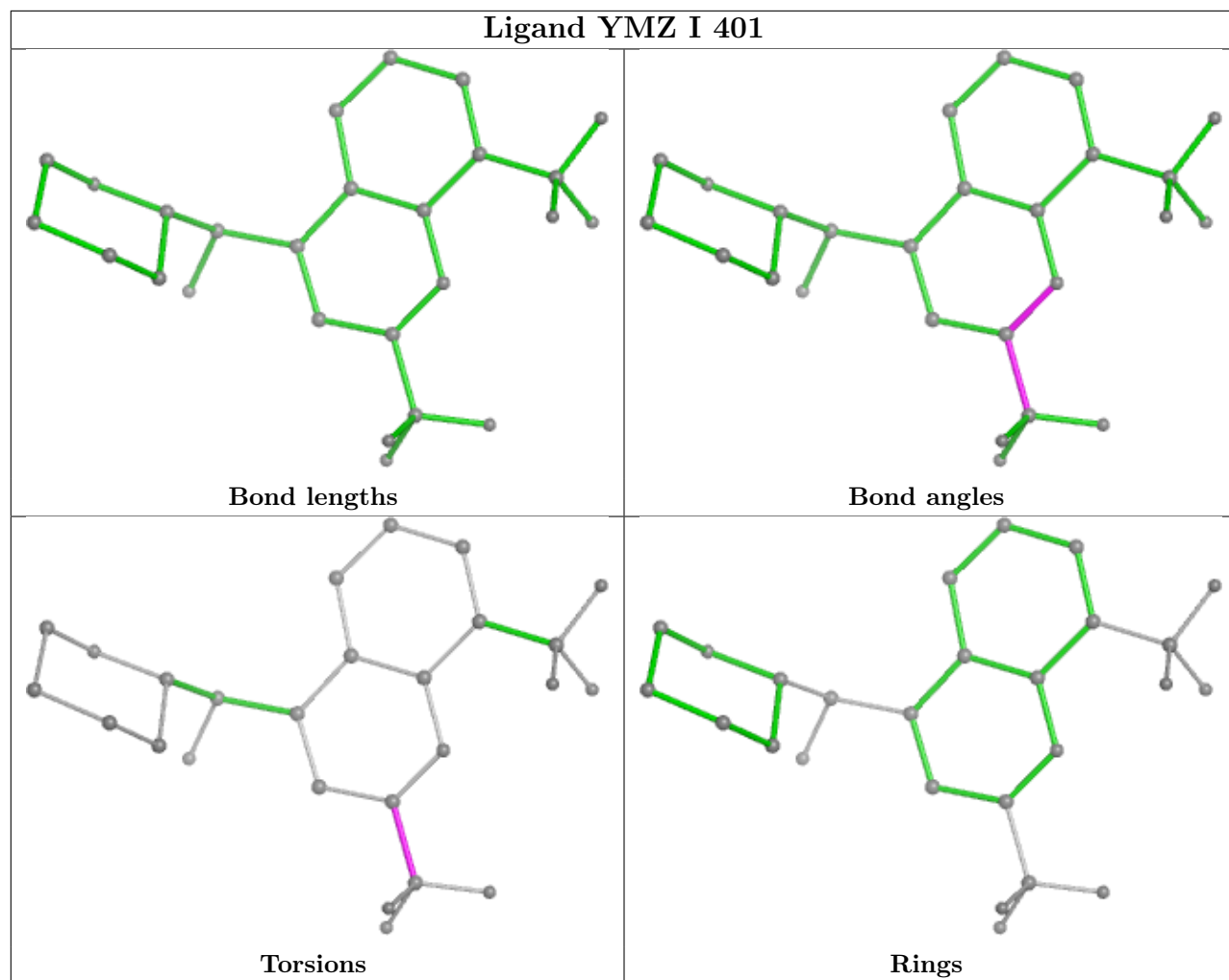


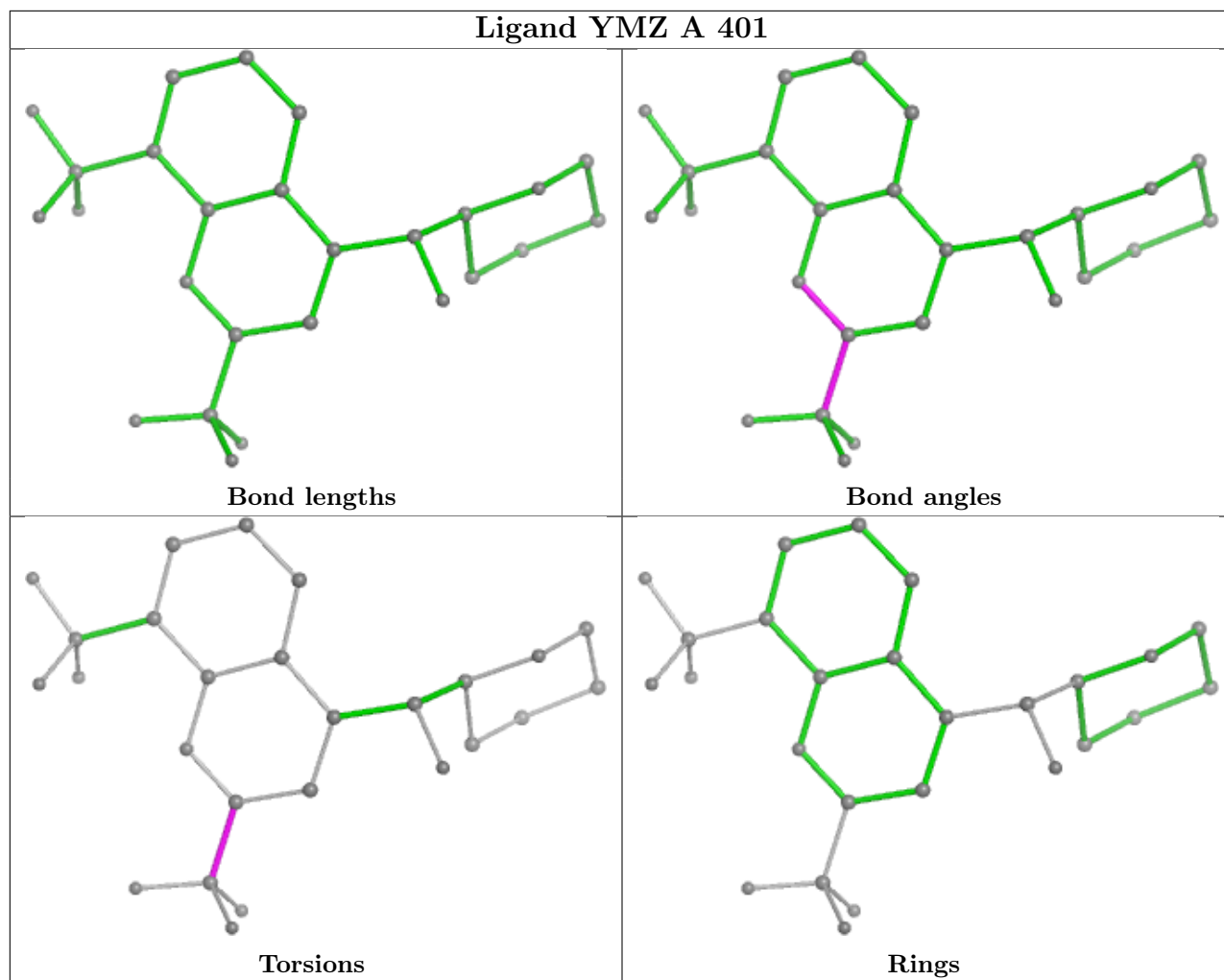


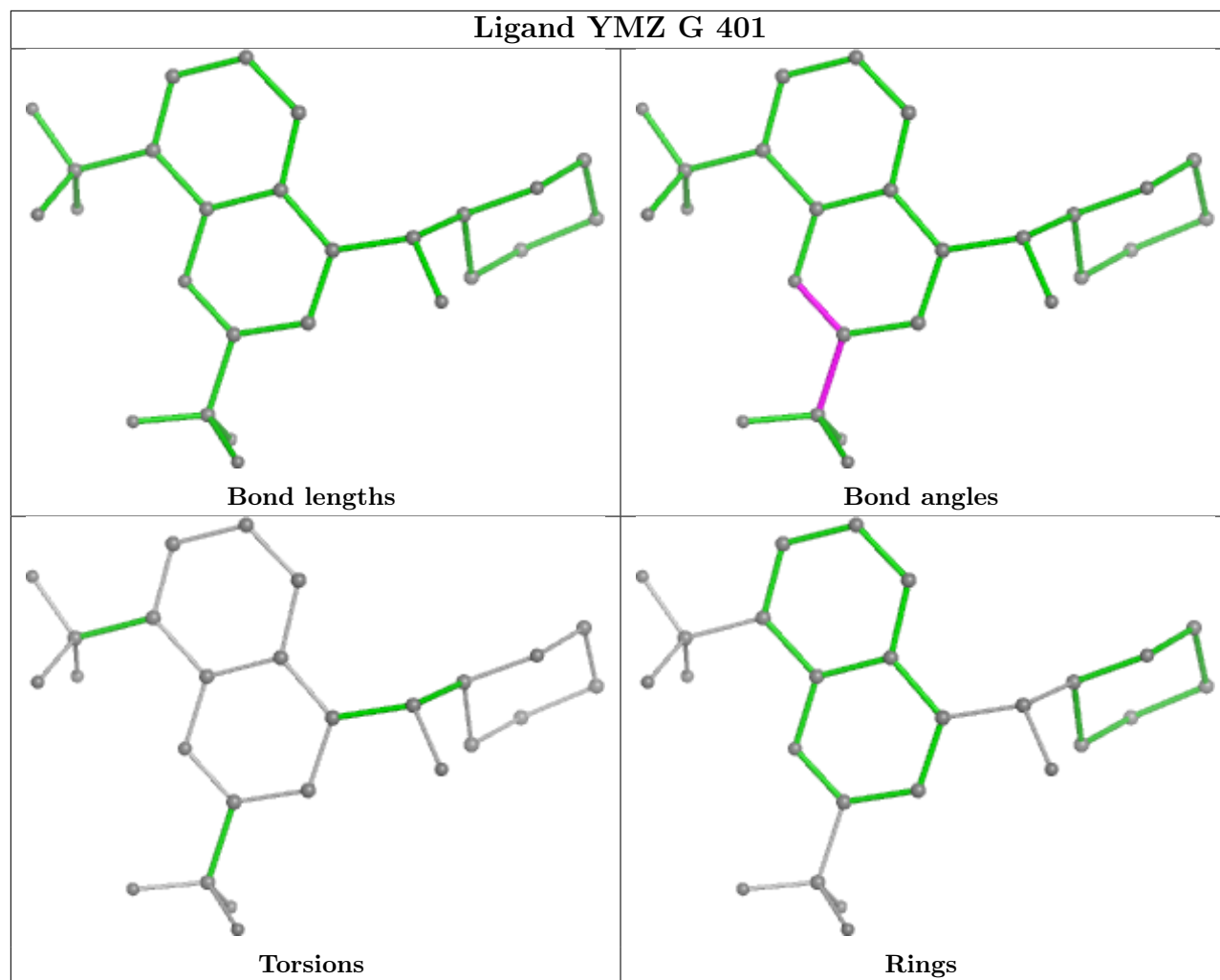












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

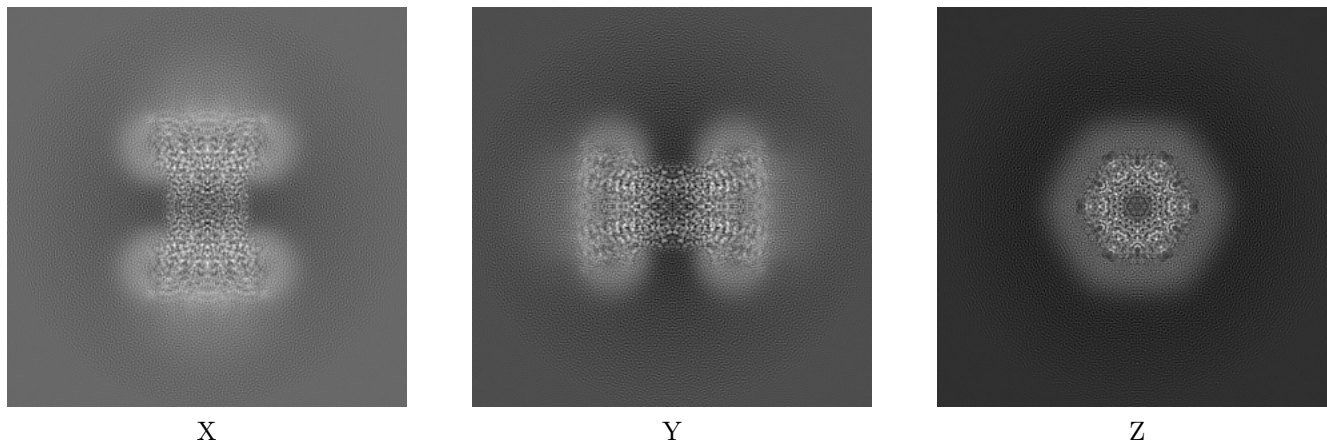
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18540. These allow visual inspection of the internal detail of the map and identification of artifacts.

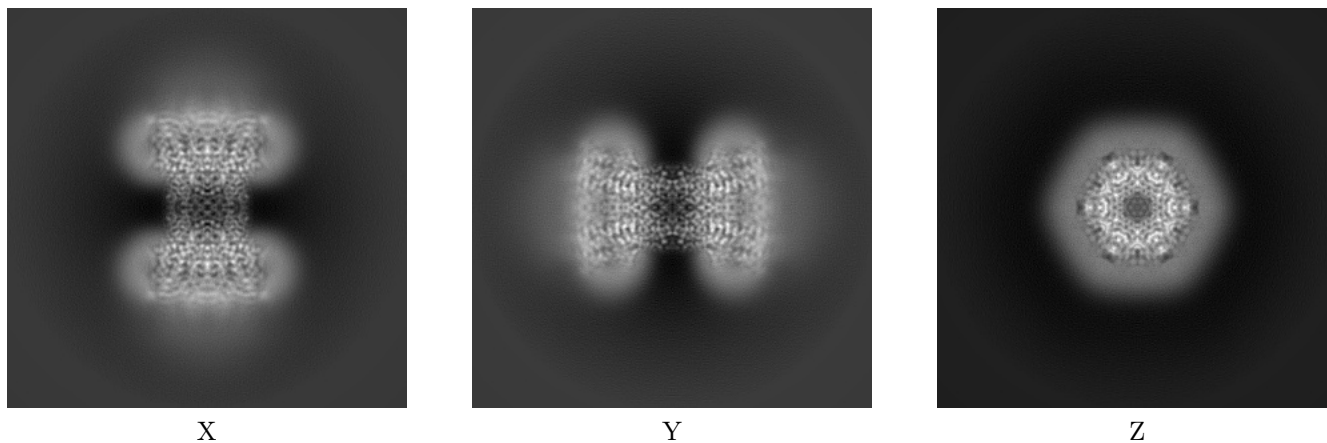
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



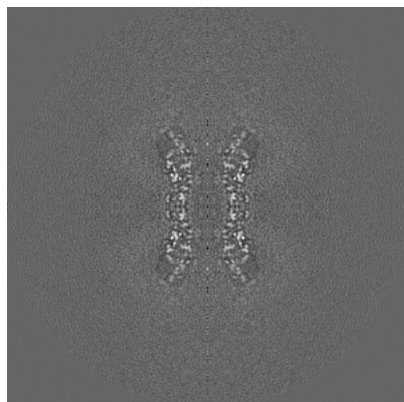
#### 6.1.2 Raw map



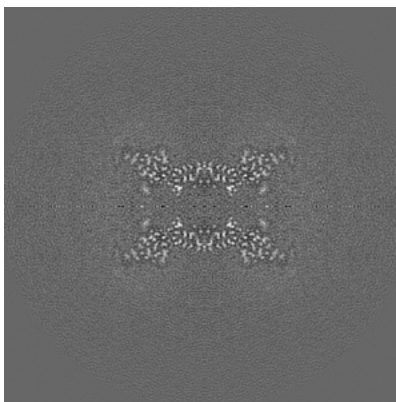
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

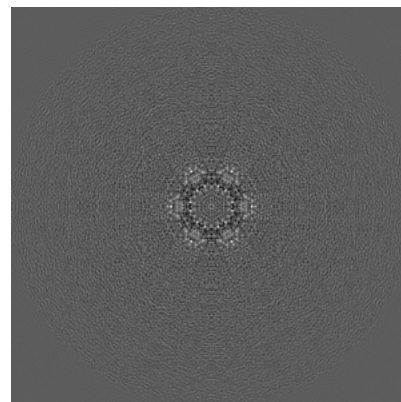
### 6.2.1 Primary map



X Index: 200

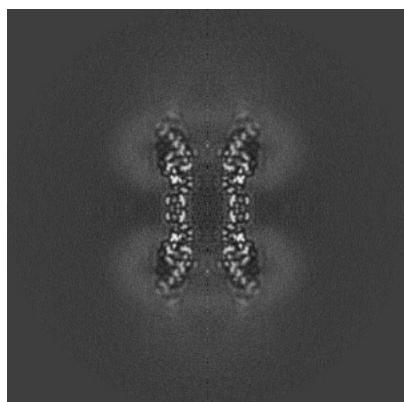


Y Index: 200

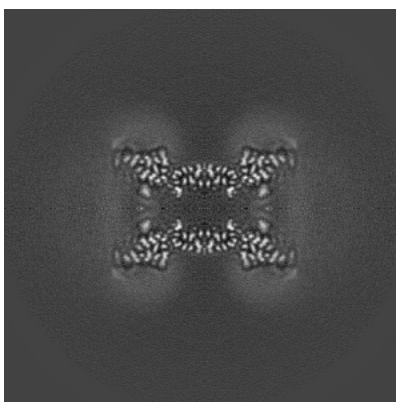


Z Index: 200

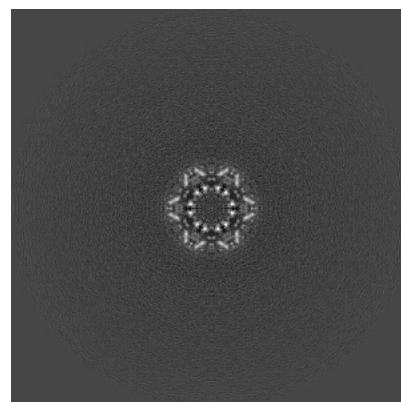
### 6.2.2 Raw map



X Index: 200



Y Index: 200



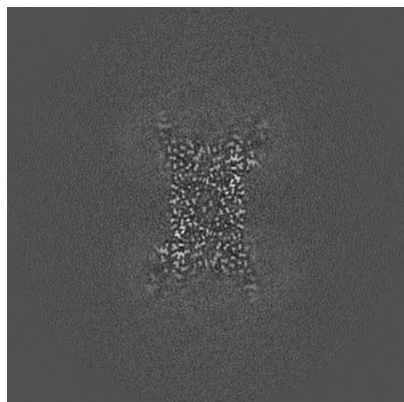
Z Index: 200

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

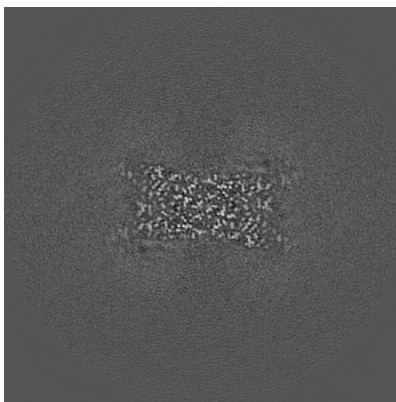


## 6.3 Largest variance slices [i](#)

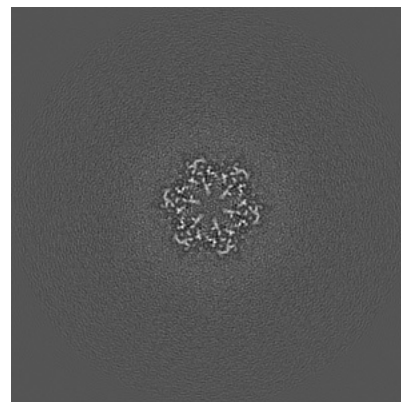
### 6.3.1 Primary map



X Index: 219

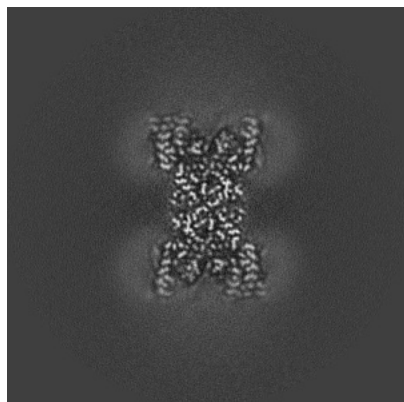


Y Index: 225

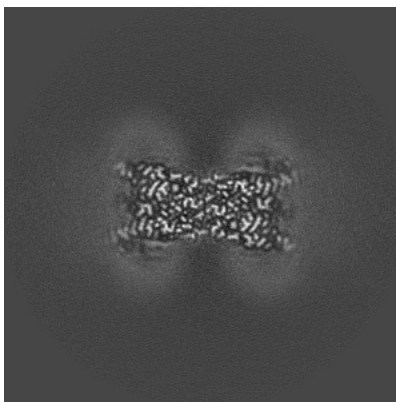


Z Index: 162

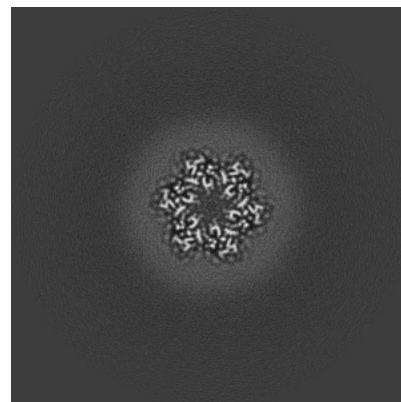
### 6.3.2 Raw map



X Index: 177



Y Index: 226

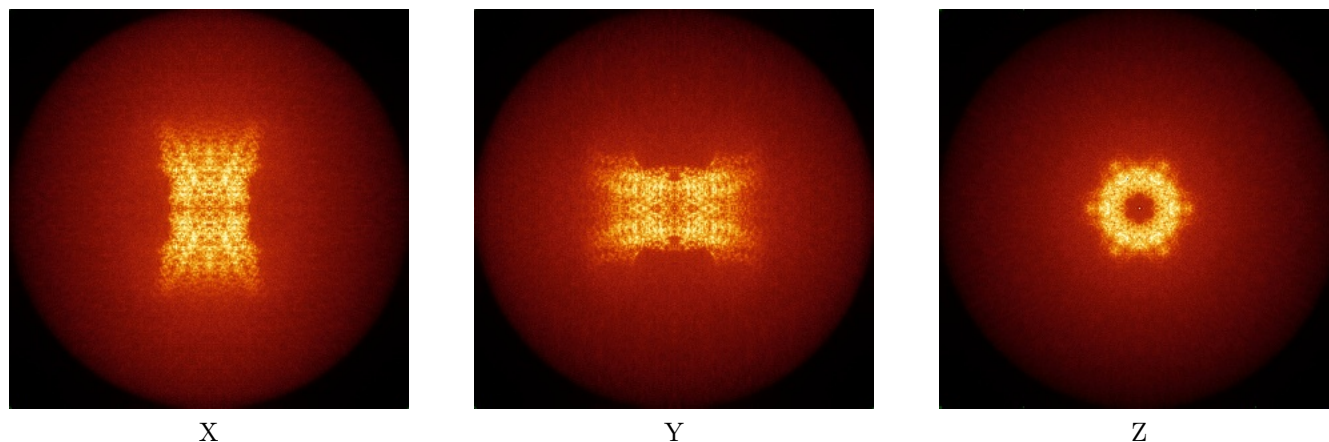


Z Index: 161

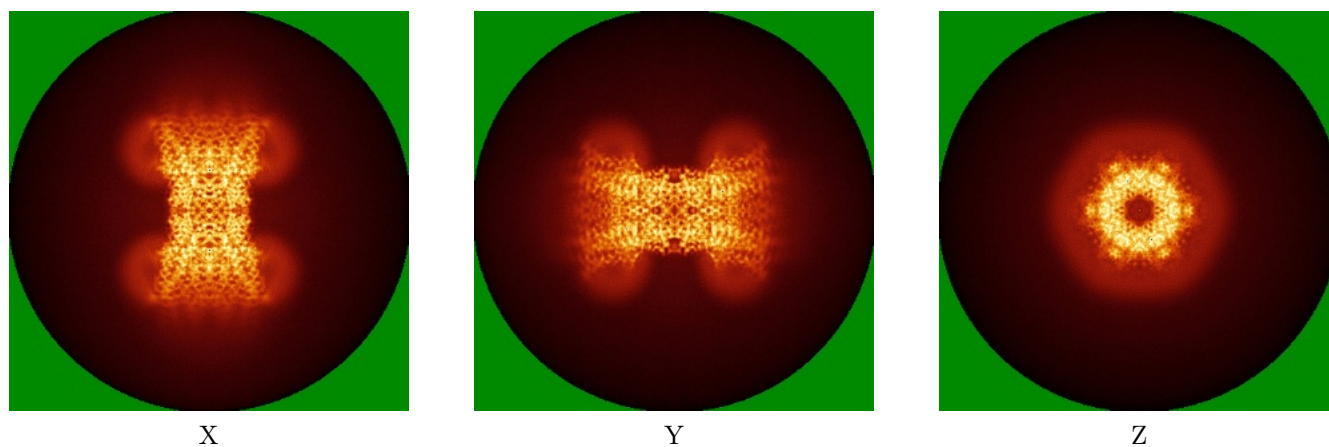
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



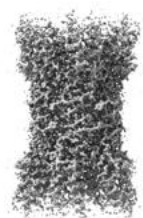
### 6.4.2 Raw map



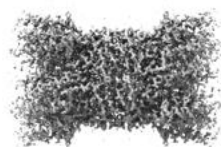
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

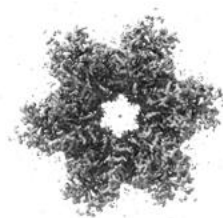
### 6.5.1 Primary map



X



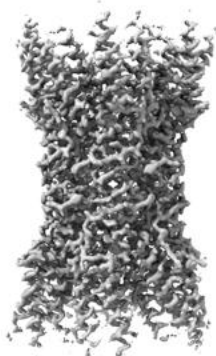
Y



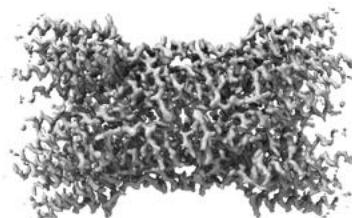
Z

The images above show the 3D surface view of the map at the recommended contour level 0.031. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

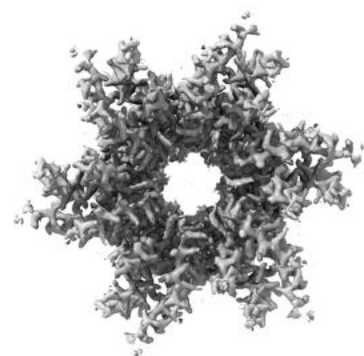
### 6.5.2 Raw map



X



Y



Z

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

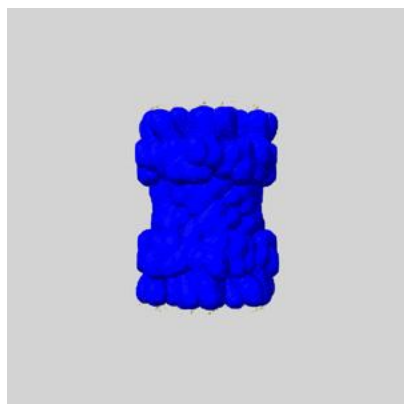
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

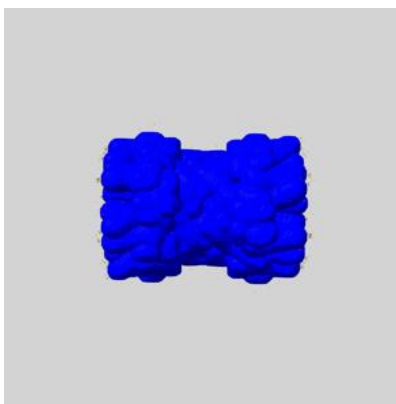
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

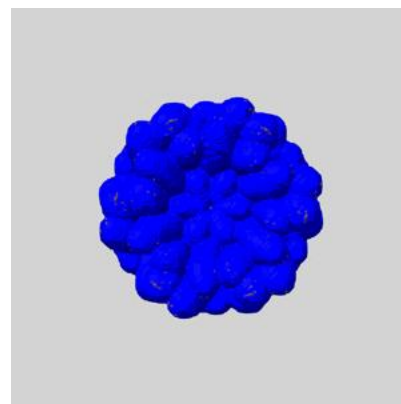
### 6.6.1 emd\_18540\_msk\_1.map [i](#)



X



Y

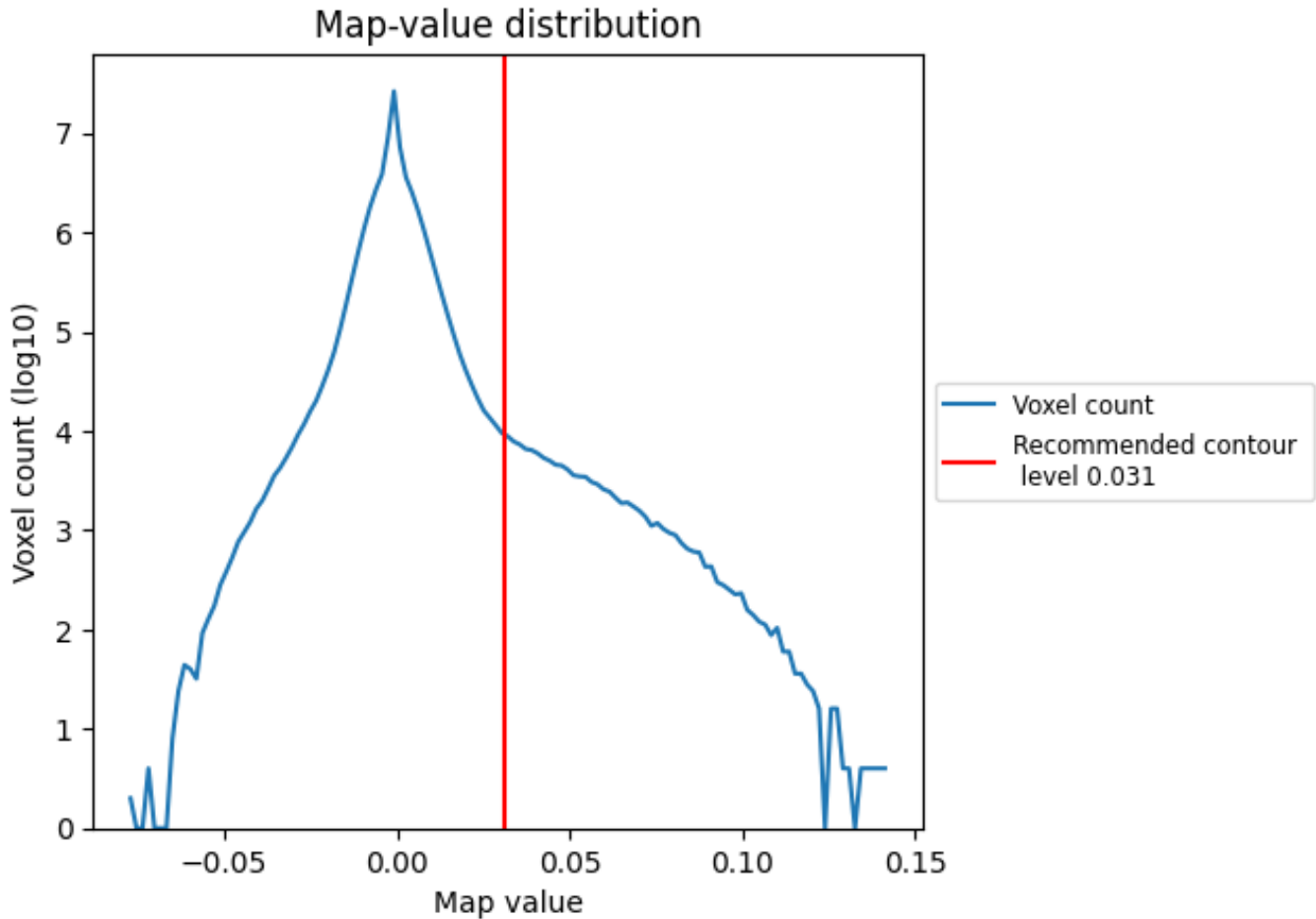


Z

## 7 Map analysis [i](#)

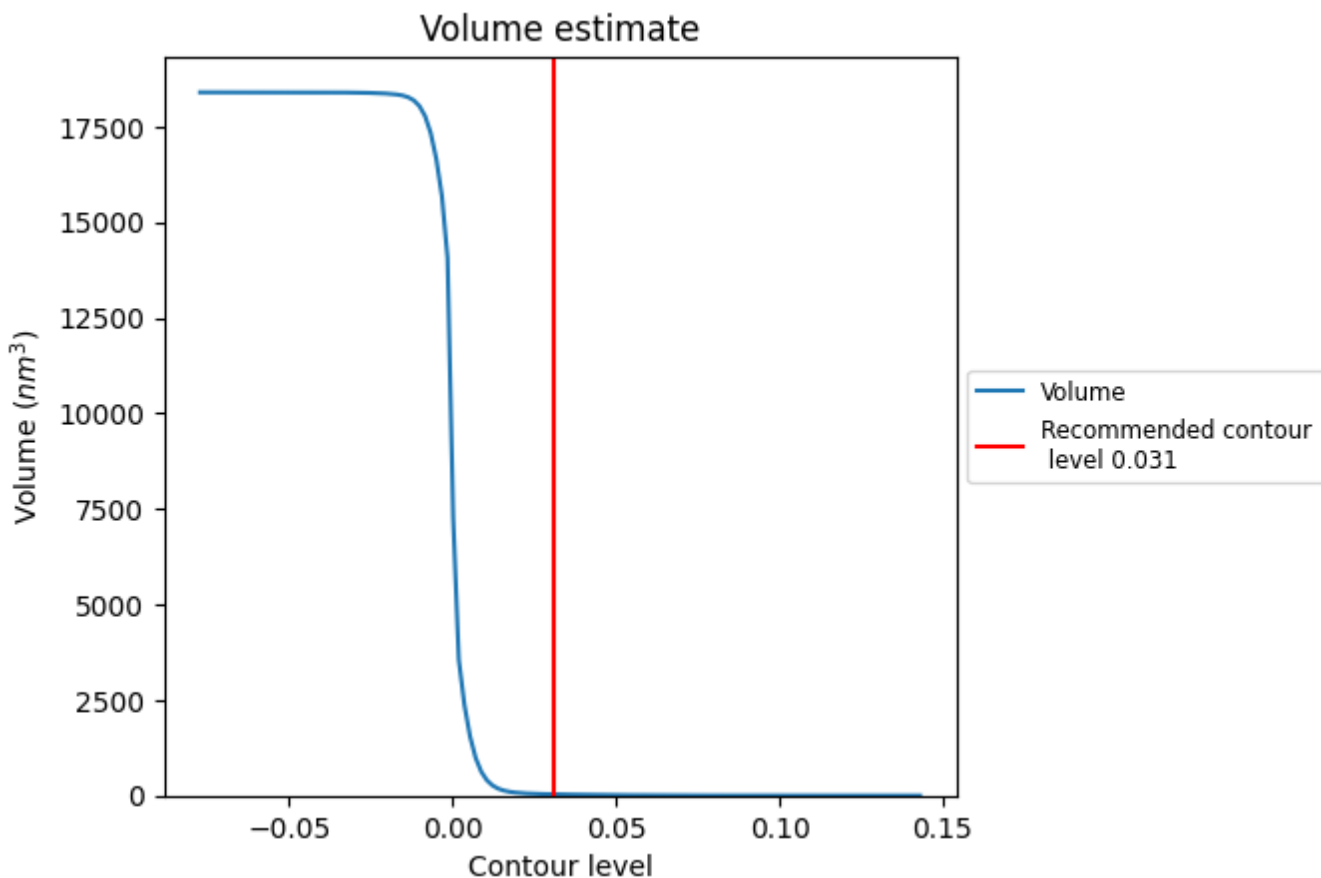
This section contains the results of statistical analysis of the map.

### 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.

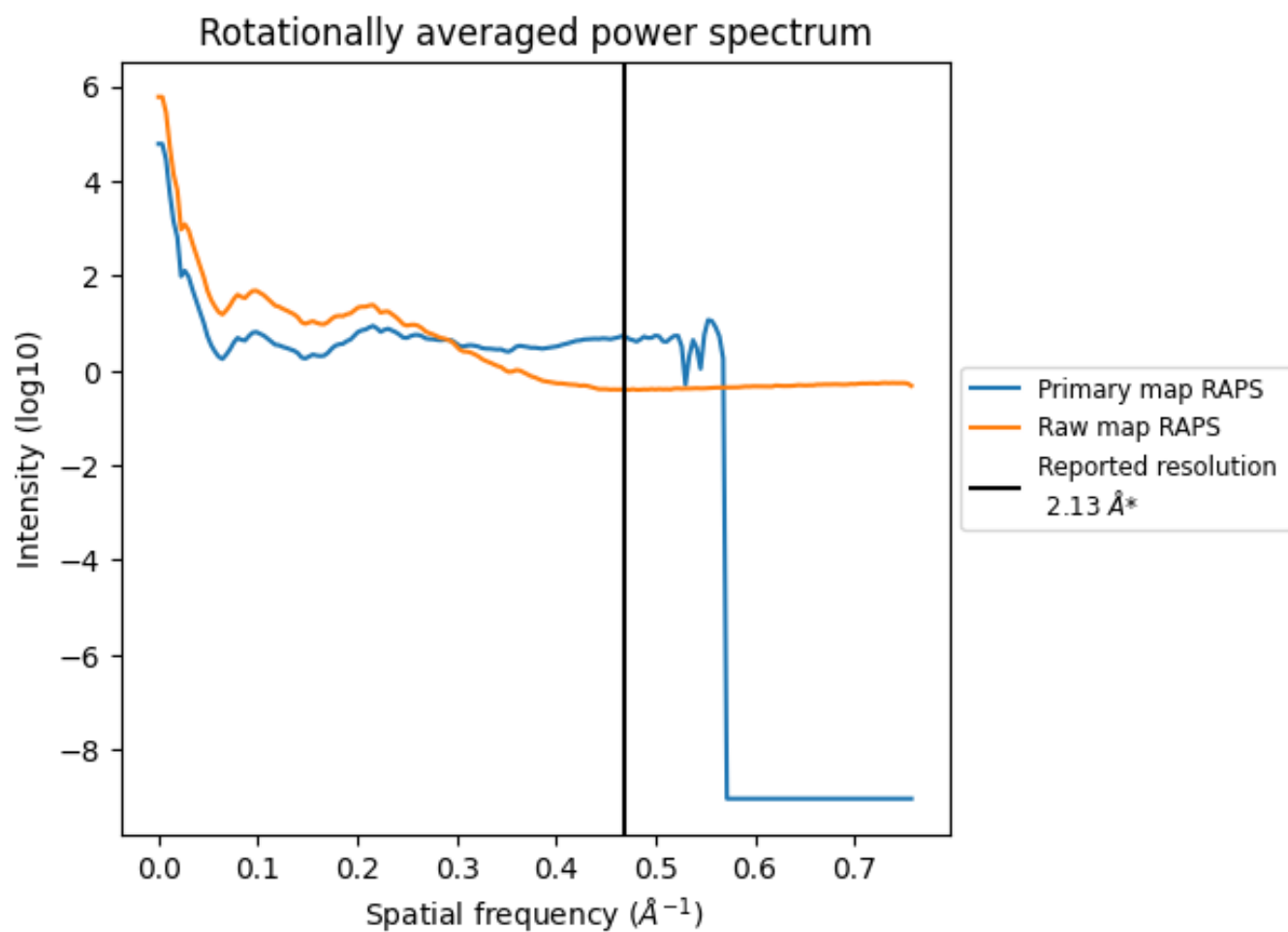
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 33 nm<sup>3</sup>; this corresponds to an approximate mass of 30 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](#)

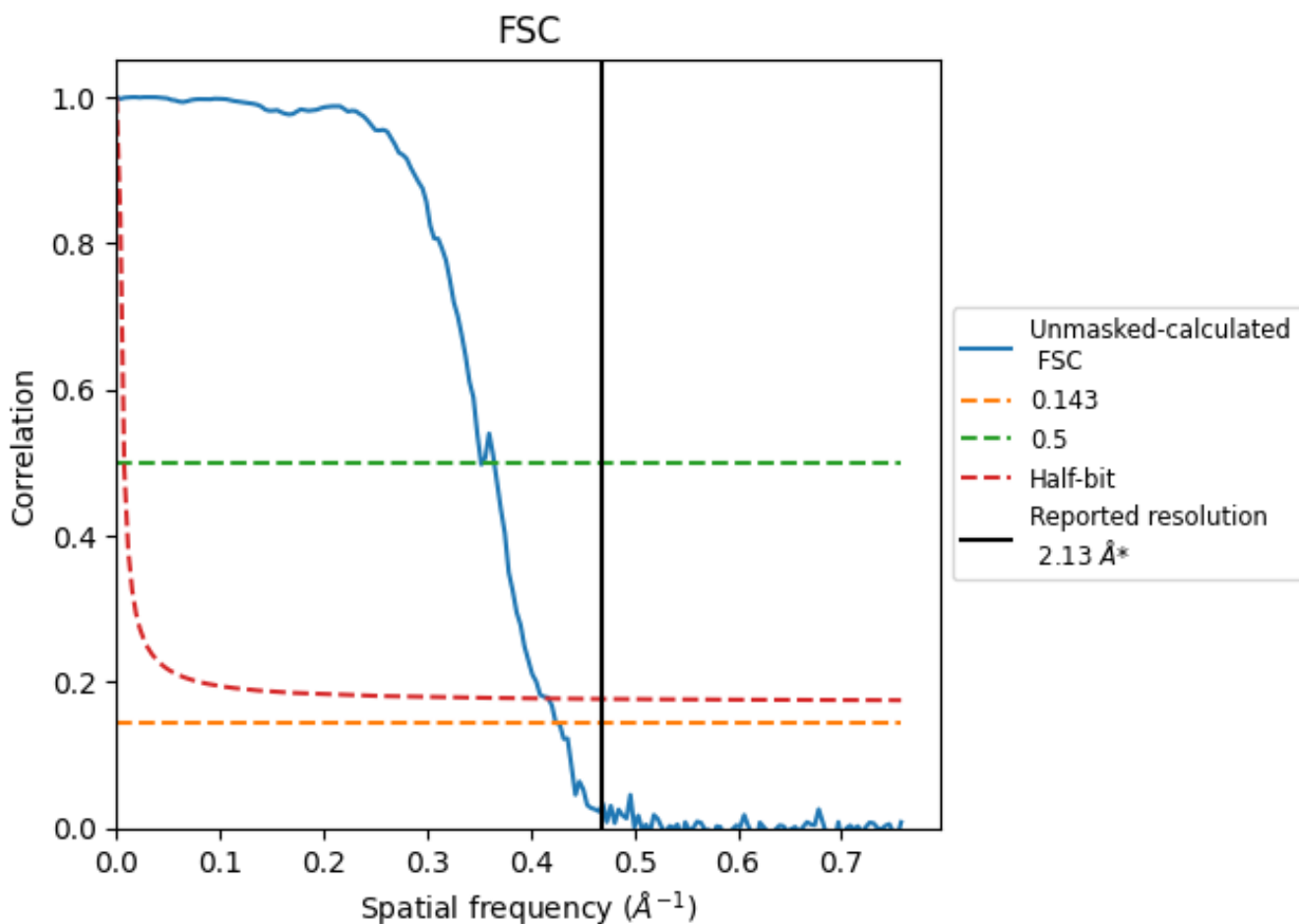


\*Reported resolution corresponds to spatial frequency of 0.469 Å<sup>-1</sup>

## 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 0.469 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

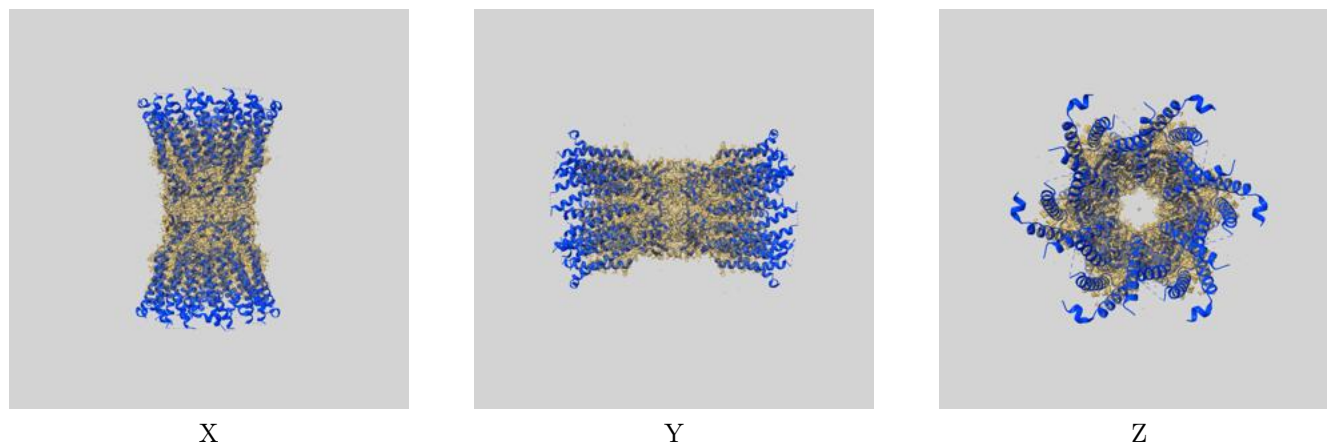
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.13	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.35	2.84	2.40

\*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 2.35 differs from the reported value 2.13 by more than 10 %

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

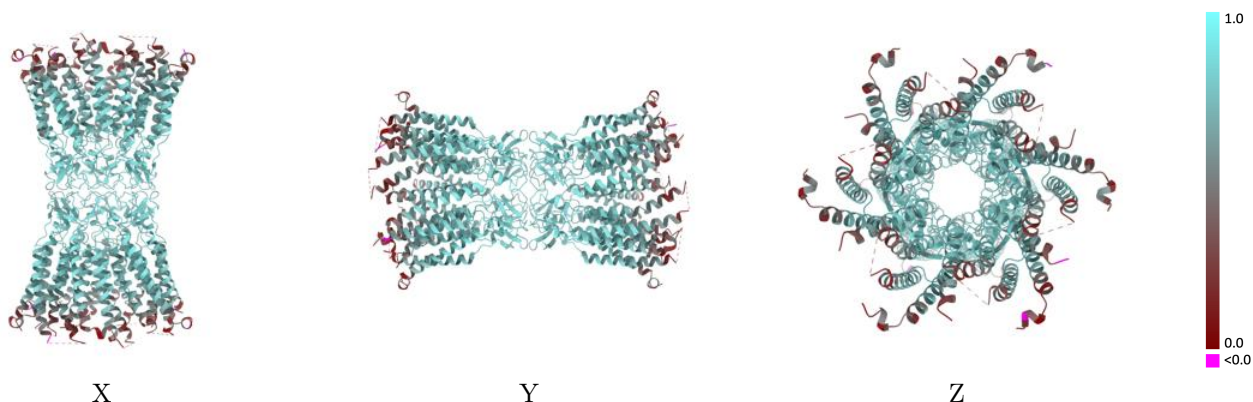
This section contains information regarding the fit between EMDB map EMD-18540 and PDB model 8QOJ. Per-residue inclusion information can be found in section 3 on page 10.

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



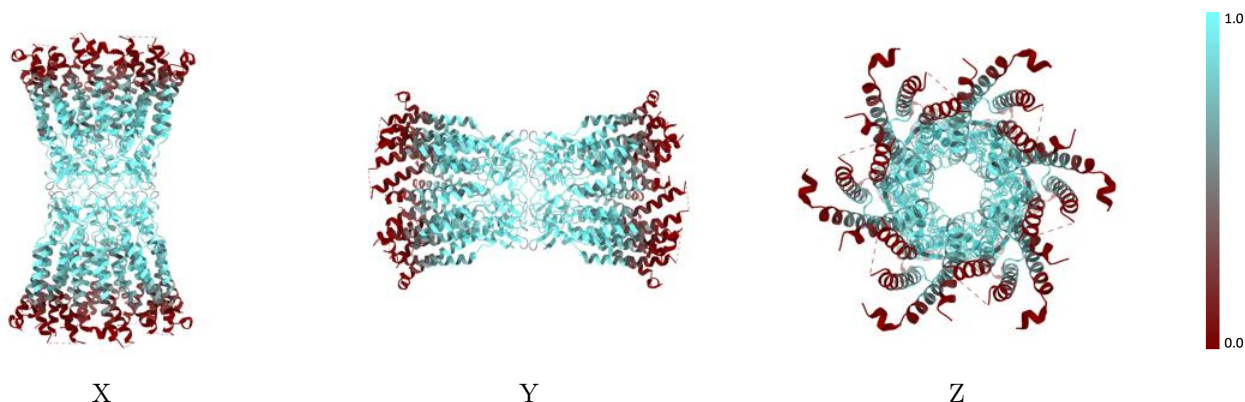
The images above show the 3D surface view of the map at the recommended contour level 0.031 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



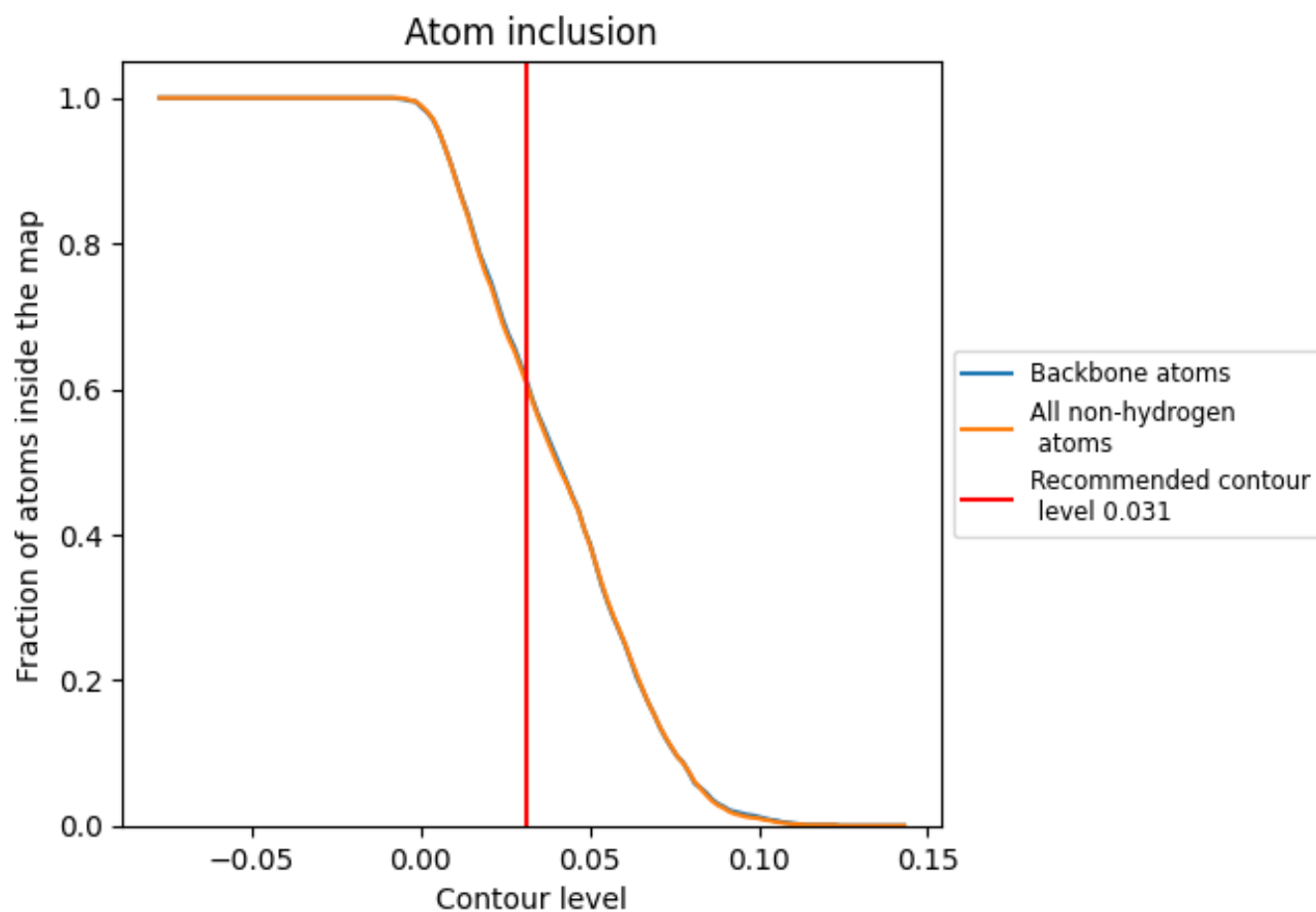
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.031).



























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 61% 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 (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6120	 0.6570
A	 0.6280	 0.6560
B	 0.6260	 0.6610
C	 0.6260	 0.6570
D	 0.6130	 0.6480
E	 0.6260	 0.6590
F	 0.6270	 0.6590
G	 0.6240	 0.6640
H	 0.6280	 0.6620
I	 0.6260	 0.6620
J	 0.6110	 0.6360
K	 0.6300	 0.6590
L	 0.6240	 0.6640

