



wwPDB EM Validation Summary Report ⓘ

Nov 13, 2022 – 09:08 AM EST

PDB ID : 6UD4
EMDB ID : EMD-20733
Title : GluA2 in complex with its auxiliary subunit CNIH3 in AS map II - (LBD-TMD-C3(AS) II)- with antagonist ZK200775, without NTD
Authors : Nakagawa, T.
Deposited on : 2019-09-18
Resolution : 3.30 Å(reported)

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

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

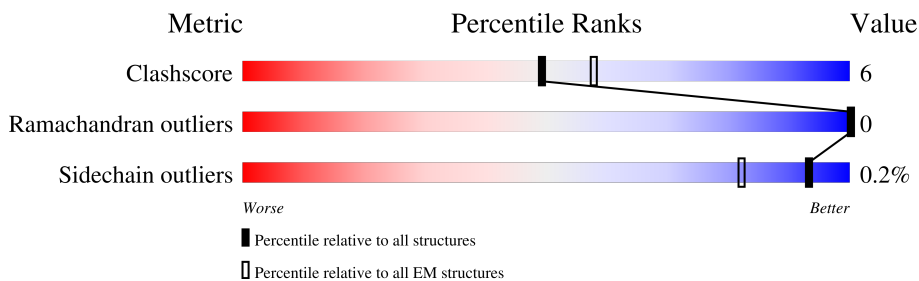
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.30 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 ≥ 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	889	
1	B	889	
1	C	889	
1	D	889	
2	E	174	
2	F	174	
2	G	174	
2	H	174	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 32038 atoms, of which 15866 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	378	5658	1847	2809	458	526	18	0	0
1	B	378	5731	1865	2855	466	527	18	0	0
1	C	378	5675	1850	2820	461	526	18	0	0
1	D	378	5731	1865	2855	466	527	18	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	586	ARG	GLN	conflict	UNP P19491
A	848	ASP	-	expression tag	UNP P19491
A	849	TYR	-	expression tag	UNP P19491
A	850	LYS	-	expression tag	UNP P19491
A	851	ASP	-	expression tag	UNP P19491
A	852	ASP	-	expression tag	UNP P19491
A	853	ASP	-	expression tag	UNP P19491
A	854	ASP	-	expression tag	UNP P19491
A	855	LYS	-	expression tag	UNP P19491
A	856	GLU	-	expression tag	UNP P19491
A	857	GLY	-	expression tag	UNP P19491
A	858	TYR	-	expression tag	UNP P19491
A	859	ASN	-	expression tag	UNP P19491
A	860	VAL	-	expression tag	UNP P19491
A	861	TYR	-	expression tag	UNP P19491
A	862	GLY	-	expression tag	UNP P19491
A	863	ILE	-	expression tag	UNP P19491
A	864	GLU	-	expression tag	UNP P19491
A	865	SER	-	expression tag	UNP P19491
A	866	VAL	-	expression tag	UNP P19491
A	867	LYS	-	expression tag	UNP P19491
A	868	ILE	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	586	ARG	GLN	conflict	UNP P19491
B	848	ASP	-	expression tag	UNP P19491
B	849	TYR	-	expression tag	UNP P19491
B	850	LYS	-	expression tag	UNP P19491
B	851	ASP	-	expression tag	UNP P19491
B	852	ASP	-	expression tag	UNP P19491
B	853	ASP	-	expression tag	UNP P19491
B	854	ASP	-	expression tag	UNP P19491
B	855	LYS	-	expression tag	UNP P19491
B	856	GLU	-	expression tag	UNP P19491
B	857	GLY	-	expression tag	UNP P19491
B	858	TYR	-	expression tag	UNP P19491
B	859	ASN	-	expression tag	UNP P19491
B	860	VAL	-	expression tag	UNP P19491
B	861	TYR	-	expression tag	UNP P19491
B	862	GLY	-	expression tag	UNP P19491
B	863	ILE	-	expression tag	UNP P19491
B	864	GLU	-	expression tag	UNP P19491
B	865	SER	-	expression tag	UNP P19491
B	866	VAL	-	expression tag	UNP P19491
B	867	LYS	-	expression tag	UNP P19491
B	868	ILE	-	expression tag	UNP P19491
C	586	ARG	GLN	conflict	UNP P19491
C	848	ASP	-	expression tag	UNP P19491
C	849	TYR	-	expression tag	UNP P19491
C	850	LYS	-	expression tag	UNP P19491
C	851	ASP	-	expression tag	UNP P19491
C	852	ASP	-	expression tag	UNP P19491
C	853	ASP	-	expression tag	UNP P19491
C	854	ASP	-	expression tag	UNP P19491
C	855	LYS	-	expression tag	UNP P19491
C	856	GLU	-	expression tag	UNP P19491
C	857	GLY	-	expression tag	UNP P19491
C	858	TYR	-	expression tag	UNP P19491
C	859	ASN	-	expression tag	UNP P19491
C	860	VAL	-	expression tag	UNP P19491
C	861	TYR	-	expression tag	UNP P19491
C	862	GLY	-	expression tag	UNP P19491
C	863	ILE	-	expression tag	UNP P19491
C	864	GLU	-	expression tag	UNP P19491
C	865	SER	-	expression tag	UNP P19491
C	866	VAL	-	expression tag	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
C	867	LYS	-	expression tag	UNP P19491
C	868	ILE	-	expression tag	UNP P19491
D	586	ARG	GLN	conflict	UNP P19491
D	848	ASP	-	expression tag	UNP P19491
D	849	TYR	-	expression tag	UNP P19491
D	850	LYS	-	expression tag	UNP P19491
D	851	ASP	-	expression tag	UNP P19491
D	852	ASP	-	expression tag	UNP P19491
D	853	ASP	-	expression tag	UNP P19491
D	854	ASP	-	expression tag	UNP P19491
D	855	LYS	-	expression tag	UNP P19491
D	856	GLU	-	expression tag	UNP P19491
D	857	GLY	-	expression tag	UNP P19491
D	858	TYR	-	expression tag	UNP P19491
D	859	ASN	-	expression tag	UNP P19491
D	860	VAL	-	expression tag	UNP P19491
D	861	TYR	-	expression tag	UNP P19491
D	862	GLY	-	expression tag	UNP P19491
D	863	ILE	-	expression tag	UNP P19491
D	864	GLU	-	expression tag	UNP P19491
D	865	SER	-	expression tag	UNP P19491
D	866	VAL	-	expression tag	UNP P19491
D	867	LYS	-	expression tag	UNP P19491
D	868	ILE	-	expression tag	UNP P19491

- Molecule 2 is a protein called Protein cornichon homolog 3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	E	132	Total	C	H	N	O	S	0	0
			2112	741	1026	162	171	12		
2	F	134	Total	C	H	N	O	S	0	0
			2147	758	1035	166	176	12		
2	G	132	Total	C	H	N	O	S	0	0
			2121	741	1035	162	171	12		
2	H	134	Total	C	H	N	O	S	0	0
			2147	758	1035	166	176	12		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	161	GLY	-	linker	UNP Q6ZWS4
E	162	GLY	-	linker	UNP Q6ZWS4

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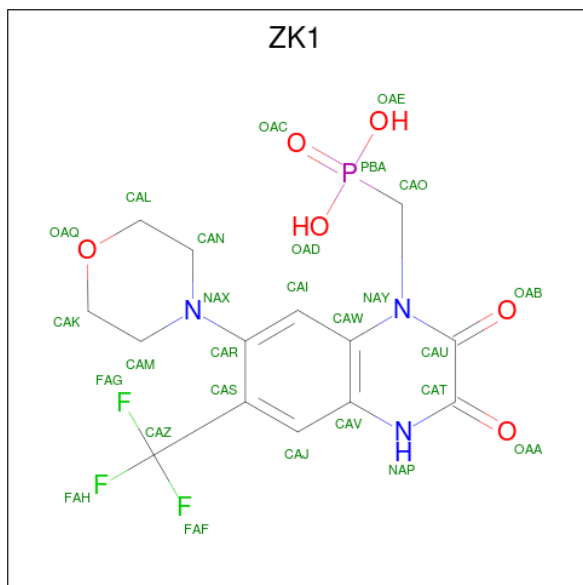
Chain	Residue	Modelled	Actual	Comment	Reference
E	163	ARG	-	linker	UNP Q6ZWS4
E	164	GLY	-	linker	UNP Q6ZWS4
E	165	GLY	-	linker	UNP Q6ZWS4
E	166	THR	-	expression tag	UNP Q6ZWS4
E	167	GLU	-	expression tag	UNP Q6ZWS4
E	168	THR	-	expression tag	UNP Q6ZWS4
E	169	SER	-	expression tag	UNP Q6ZWS4
E	170	GLN	-	expression tag	UNP Q6ZWS4
E	171	VAL	-	expression tag	UNP Q6ZWS4
E	172	ALA	-	expression tag	UNP Q6ZWS4
E	173	PRO	-	expression tag	UNP Q6ZWS4
E	174	ALA	-	expression tag	UNP Q6ZWS4
F	161	GLY	-	linker	UNP Q6ZWS4
F	162	GLY	-	linker	UNP Q6ZWS4
F	163	ARG	-	linker	UNP Q6ZWS4
F	164	GLY	-	linker	UNP Q6ZWS4
F	165	GLY	-	linker	UNP Q6ZWS4
F	166	THR	-	expression tag	UNP Q6ZWS4
F	167	GLU	-	expression tag	UNP Q6ZWS4
F	168	THR	-	expression tag	UNP Q6ZWS4
F	169	SER	-	expression tag	UNP Q6ZWS4
F	170	GLN	-	expression tag	UNP Q6ZWS4
F	171	VAL	-	expression tag	UNP Q6ZWS4
F	172	ALA	-	expression tag	UNP Q6ZWS4
F	173	PRO	-	expression tag	UNP Q6ZWS4
F	174	ALA	-	expression tag	UNP Q6ZWS4
G	161	GLY	-	linker	UNP Q6ZWS4
G	162	GLY	-	linker	UNP Q6ZWS4
G	163	ARG	-	linker	UNP Q6ZWS4
G	164	GLY	-	linker	UNP Q6ZWS4
G	165	GLY	-	linker	UNP Q6ZWS4
G	166	THR	-	expression tag	UNP Q6ZWS4
G	167	GLU	-	expression tag	UNP Q6ZWS4
G	168	THR	-	expression tag	UNP Q6ZWS4
G	169	SER	-	expression tag	UNP Q6ZWS4
G	170	GLN	-	expression tag	UNP Q6ZWS4
G	171	VAL	-	expression tag	UNP Q6ZWS4
G	172	ALA	-	expression tag	UNP Q6ZWS4
G	173	PRO	-	expression tag	UNP Q6ZWS4
G	174	ALA	-	expression tag	UNP Q6ZWS4
H	161	GLY	-	linker	UNP Q6ZWS4
H	162	GLY	-	linker	UNP Q6ZWS4

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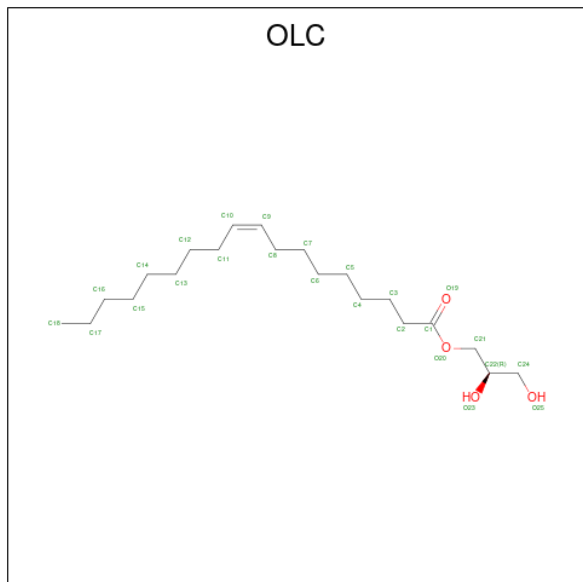
Chain	Residue	Modelled	Actual	Comment	Reference
H	163	ARG	-	linker	UNP Q6ZWS4
H	164	GLY	-	linker	UNP Q6ZWS4
H	165	GLY	-	linker	UNP Q6ZWS4
H	166	THR	-	expression tag	UNP Q6ZWS4
H	167	GLU	-	expression tag	UNP Q6ZWS4
H	168	THR	-	expression tag	UNP Q6ZWS4
H	169	SER	-	expression tag	UNP Q6ZWS4
H	170	GLN	-	expression tag	UNP Q6ZWS4
H	171	VAL	-	expression tag	UNP Q6ZWS4
H	172	ALA	-	expression tag	UNP Q6ZWS4
H	173	PRO	-	expression tag	UNP Q6ZWS4
H	174	ALA	-	expression tag	UNP Q6ZWS4

- Molecule 3 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-yl]methyl}phosphonic acid (three-letter code: ZK1) (formula: C₁₄H₁₅F₃N₃O₆P) (labeled as "Ligand of Interest" by depositor).



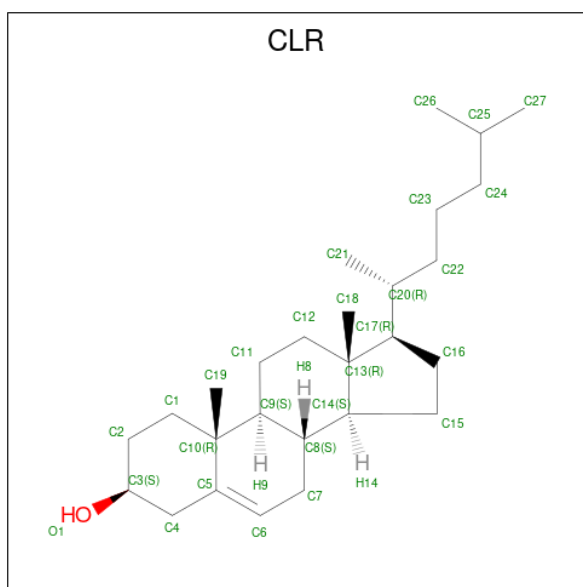
Mol	Chain	Residues	Atoms						AltConf	
			Total	C	F	H	N	O		P
3	A	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	
3	B	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	
3	C	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	
3	D	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	

- Molecule 4 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄) (labeled as "Ligand of Interest" by depositor).

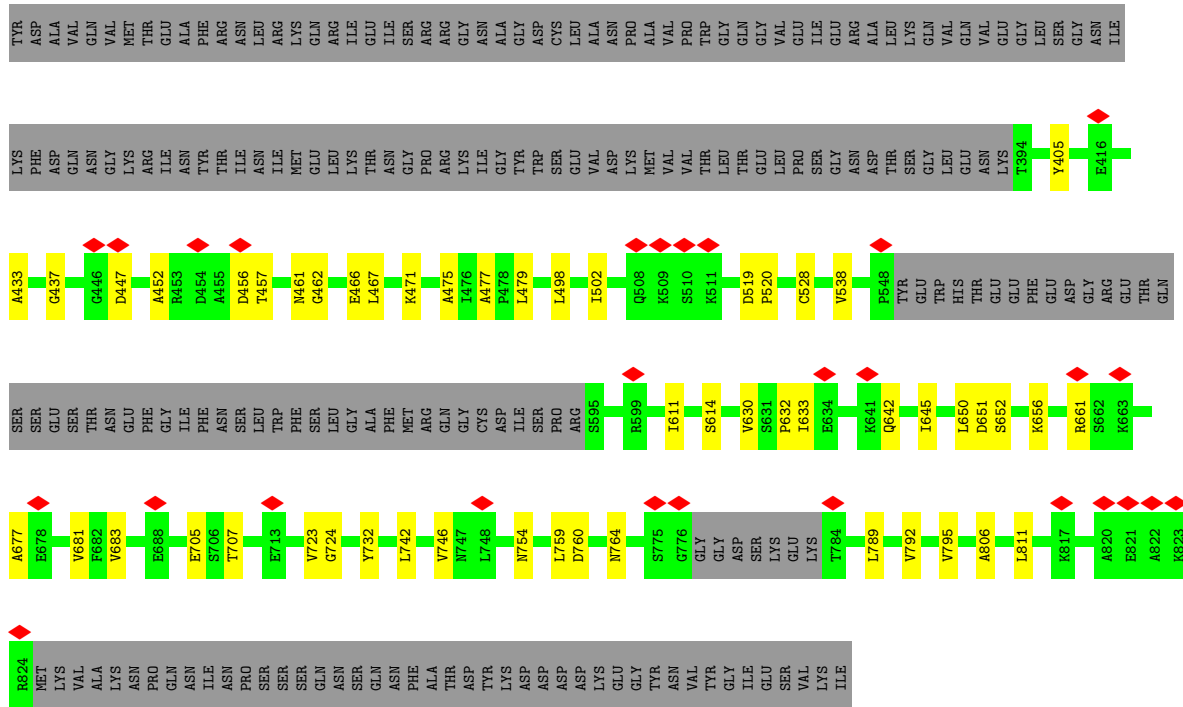


Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
4	A	1	65	21	40	4	0
4	B	1	65	21	40	4	0
4	C	1	65	21	40	4	0
4	D	1	65	21	40	4	0

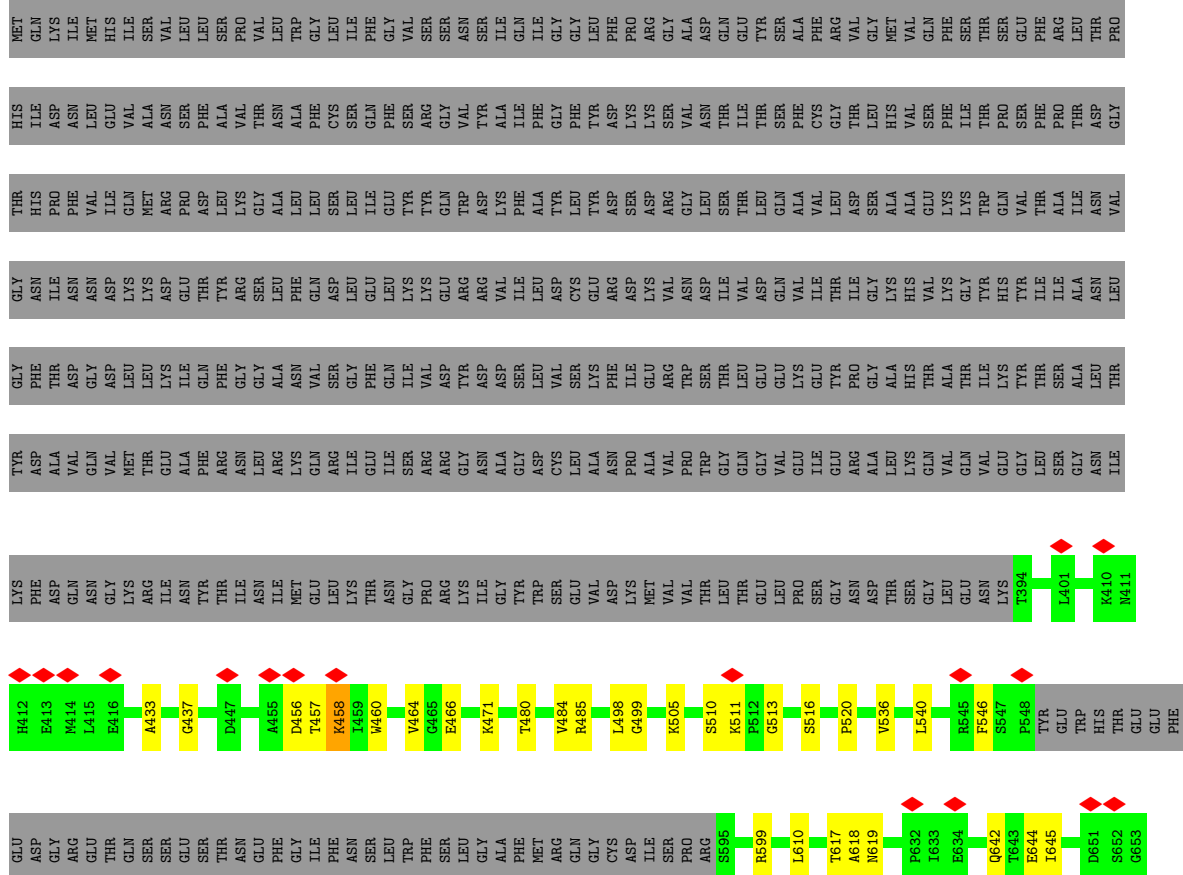
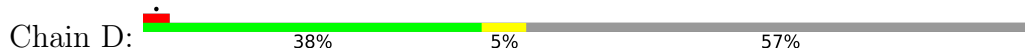
- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: C₂₇H₄₆O) (labeled as "Ligand of Interest" by depositor).

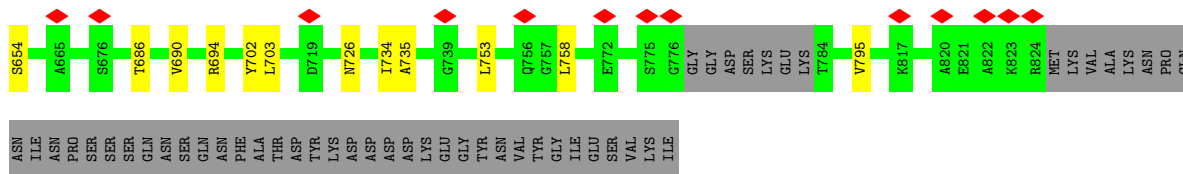


Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
5	A	1	74	27	46	1	0
5	F	1	74	27	46	1	0
5	G	1	74	27	46	1	0
5	H	1	74	27	46	1	0

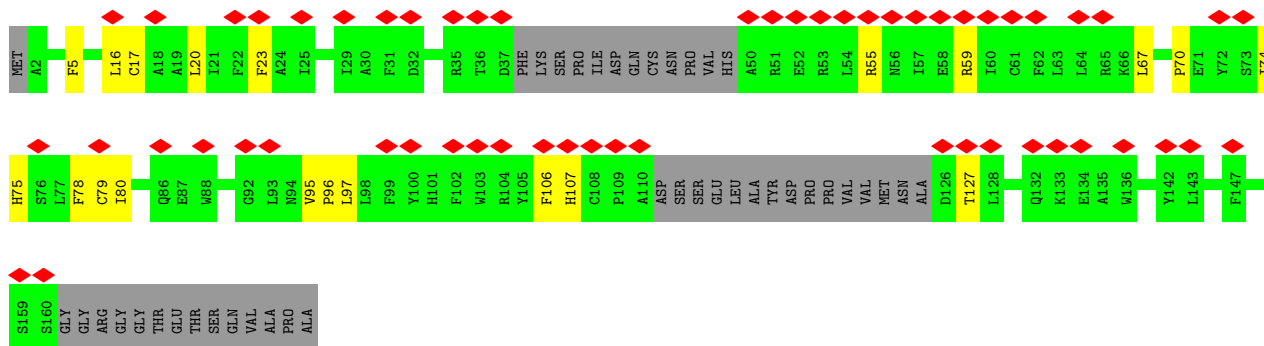


● Molecule 1: Glutamate receptor 2

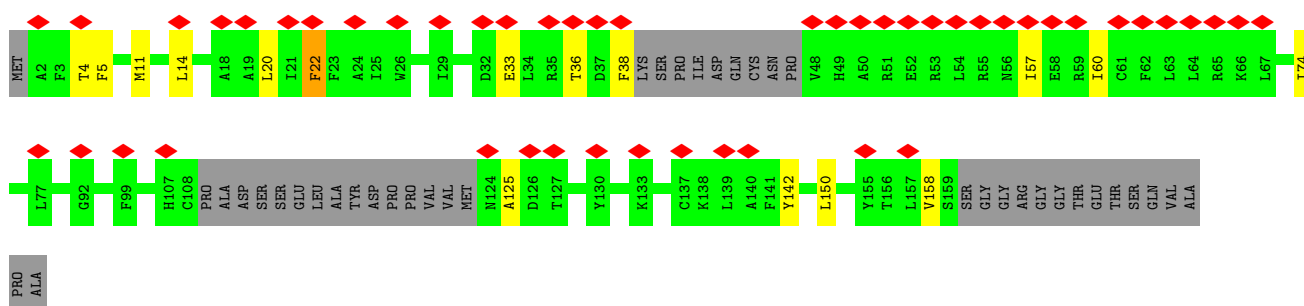




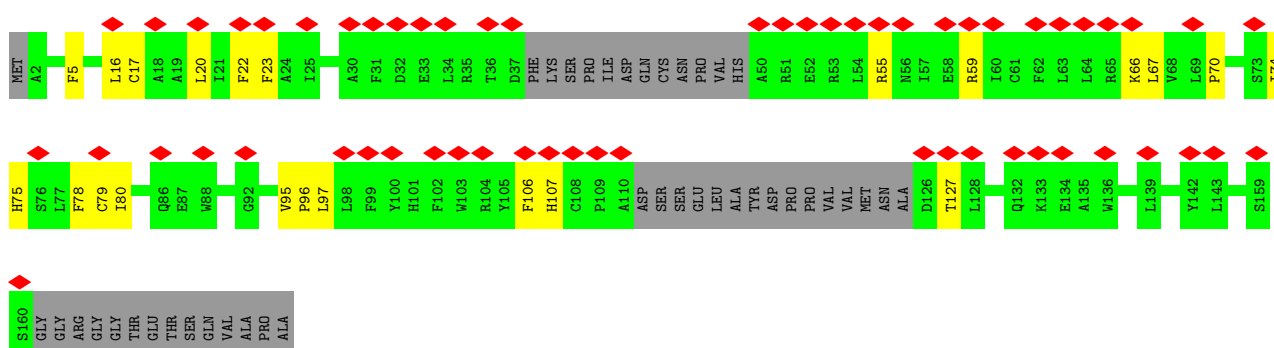
• Molecule 2: Protein cornichon homolog 3



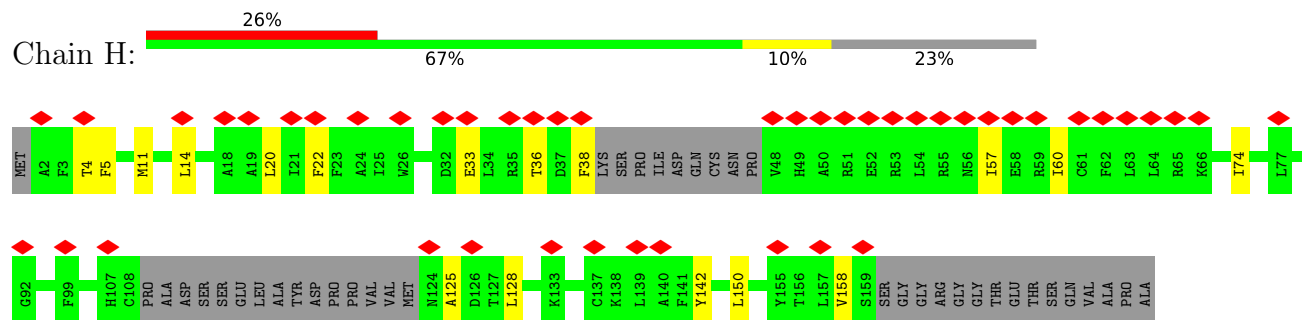
• Molecule 2: Protein cornichon homolog 3



• Molecule 2: Protein cornichon homolog 3



• Molecule 2: Protein cornichon homolog 3



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	84584	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 ($e^-/\text{\AA}^2$)	58.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0248	Depositor
Map size (Å)	383.76, 383.76, 383.76	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.066, 1.066, 1.066	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: CLR, OLC, ZK1

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	0.28	0/2908	0.42	0/3941
1	B	0.28	0/2935	0.41	0/3973
1	C	0.28	0/2914	0.42	0/3948
1	D	0.28	0/2935	0.41	0/3973
2	E	0.26	0/1123	0.35	0/1527
2	F	0.27	0/1149	0.36	0/1561
2	G	0.26	0/1123	0.35	0/1527
2	H	0.27	0/1149	0.36	0/1561
All	All	0.28	0/16236	0.40	0/22011

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	2849	2809	2808	38	0
1	B	2876	2855	2867	37	0
1	C	2855	2820	2819	40	0
1	D	2876	2855	2867	31	0
2	E	1086	1026	1047	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1112	1035	1071	14	0
2	G	1086	1035	1047	17	0
2	H	1112	1035	1071	15	0
3	A	27	13	13	0	0
3	B	27	13	13	2	0
3	C	27	13	13	0	0
3	D	27	13	13	3	0
4	A	25	40	40	2	0
4	B	25	40	40	1	0
4	C	25	40	40	2	0
4	D	25	40	40	0	0
5	A	28	46	46	1	0
5	F	28	46	46	2	0
5	G	28	46	46	1	0
5	H	28	46	46	3	0
All	All	16172	15866	15993	195	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 6.

The worst 5 of 195 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:B:545:ARG:NH1	2:G:66:LYS:O	2.02	0.92
2:E:20:LEU:HD21	2:E:74:ILE:HD11	1.66	0.77
2:G:20:LEU:HD21	2:G:74:ILE:HD11	1.66	0.77
5:H:201:CLR:H212	5:H:201:CLR:H183	1.75	0.69
1:C:452:ALA:N	1:C:461:ASN:OD1	2.25	0.69

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	372/889 (42%)	349 (94%)	23 (6%)	0	100	100
1	B	372/889 (42%)	350 (94%)	22 (6%)	0	100	100
1	C	372/889 (42%)	350 (94%)	22 (6%)	0	100	100
1	D	372/889 (42%)	350 (94%)	22 (6%)	0	100	100
2	E	126/174 (72%)	120 (95%)	6 (5%)	0	100	100
2	F	128/174 (74%)	127 (99%)	1 (1%)	0	100	100
2	G	126/174 (72%)	120 (95%)	6 (5%)	0	100	100
2	H	128/174 (74%)	127 (99%)	1 (1%)	0	100	100
All	All	1996/4252 (47%)	1893 (95%)	103 (5%)	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	292/761 (38%)	292 (100%)	0	100	100
1	B	299/761 (39%)	298 (100%)	1 (0%)	92	96
1	C	293/761 (38%)	293 (100%)	0	100	100
1	D	299/761 (39%)	298 (100%)	1 (0%)	92	96
2	E	111/153 (72%)	111 (100%)	0	100	100
2	F	114/153 (74%)	113 (99%)	1 (1%)	78	87
2	G	111/153 (72%)	111 (100%)	0	100	100
2	H	114/153 (74%)	113 (99%)	1 (1%)	78	87
All	All	1633/3656 (45%)	1629 (100%)	4 (0%)	93	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	458	LYS
2	F	22	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	22	PHE
1	D	458	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	791	ASN
1	C	791	ASN

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
4	OLC	C	902	-	24,24,24	1.36	4 (16%)	25,25,25	1.00	2 (8%)
4	OLC	B	902	-	24,24,24	1.40	4 (16%)	25,25,25	1.04	2 (8%)
3	ZK1	B	901	-	28,29,29	3.57	8 (28%)	42,45,45	1.54	7 (16%)
3	ZK1	D	901	-	28,29,29	3.60	8 (28%)	42,45,45	1.52	8 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OLC	A	902	-	24,24,24	1.36	4 (16%)	25,25,25	0.99	2 (8%)
4	OLC	D	902	-	24,24,24	1.38	4 (16%)	25,25,25	0.97	2 (8%)
5	CLR	A	903	-	31,31,31	1.04	3 (9%)	48,48,48	1.73	10 (20%)
3	ZK1	C	901	-	28,29,29	3.59	8 (28%)	42,45,45	1.51	8 (19%)
5	CLR	F	201	-	31,31,31	1.03	2 (6%)	48,48,48	1.62	10 (20%)
3	ZK1	A	901	-	28,29,29	3.59	8 (28%)	42,45,45	1.52	8 (19%)
5	CLR	H	201	-	31,31,31	1.15	3 (9%)	48,48,48	1.68	11 (22%)
5	CLR	G	201	-	31,31,31	1.00	3 (9%)	48,48,48	1.54	7 (14%)

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
4	OLC	C	902	-	-	13/24/24/24	-
4	OLC	B	902	-	-	12/24/24/24	-
3	ZK1	B	901	-	-	7/13/23/23	0/3/3/3
3	ZK1	D	901	-	-	7/13/23/23	0/3/3/3
4	OLC	A	902	-	-	12/24/24/24	-
4	OLC	D	902	-	-	12/24/24/24	-
5	CLR	A	903	-	-	7/10/68/68	0/4/4/4
3	ZK1	C	901	-	-	7/13/23/23	0/3/3/3
5	CLR	F	201	-	-	2/10/68/68	0/4/4/4
3	ZK1	A	901	-	-	6/13/23/23	0/3/3/3
5	CLR	H	201	-	-	4/10/68/68	0/4/4/4
5	CLR	G	201	-	-	0/10/68/68	0/4/4/4

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	ZK1	OAA-CAT	8.73	1.40	1.23
3	C	901	ZK1	OAA-CAT	8.73	1.40	1.23
3	D	901	ZK1	OAA-CAT	8.60	1.40	1.23
3	B	901	ZK1	OAA-CAT	8.53	1.39	1.23
3	B	901	ZK1	OAB-CAU	8.08	1.40	1.23

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	201	CLR	C17-C13-C14	5.20	106.23	100.07
5	A	903	CLR	C19-C10-C9	-5.04	105.67	111.68
5	H	201	CLR	C19-C10-C9	-4.80	105.95	111.68
5	F	201	CLR	C19-C10-C9	-4.74	106.03	111.68
5	G	201	CLR	C19-C10-C9	-4.51	106.31	111.68

There are no chirality outliers.

5 of 89 torsion outliers are listed below:

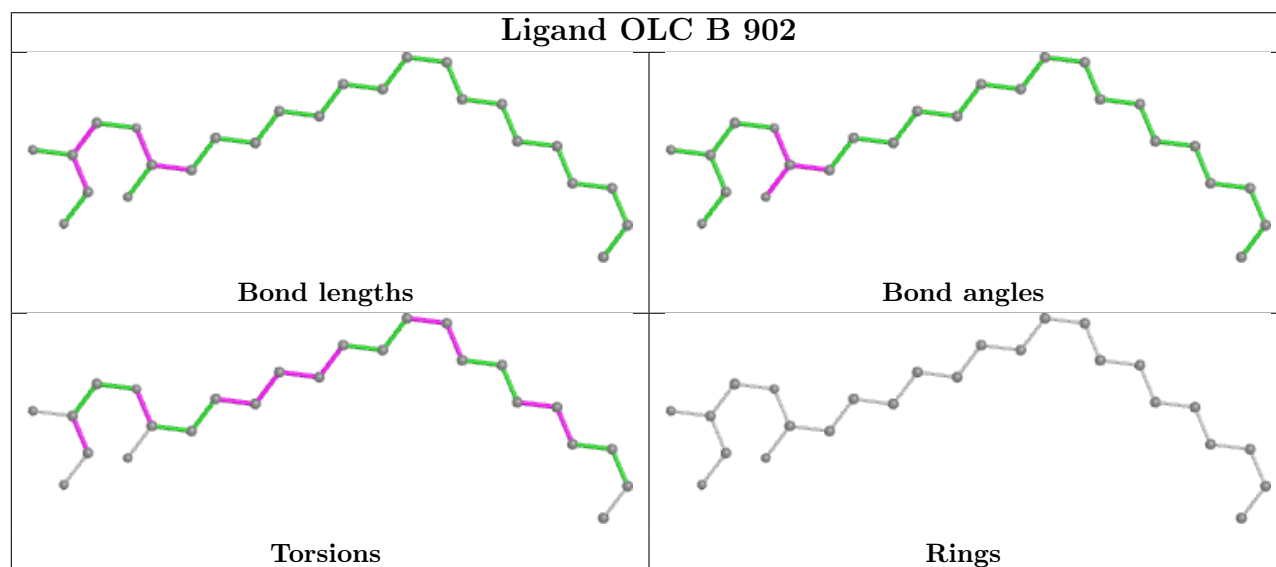
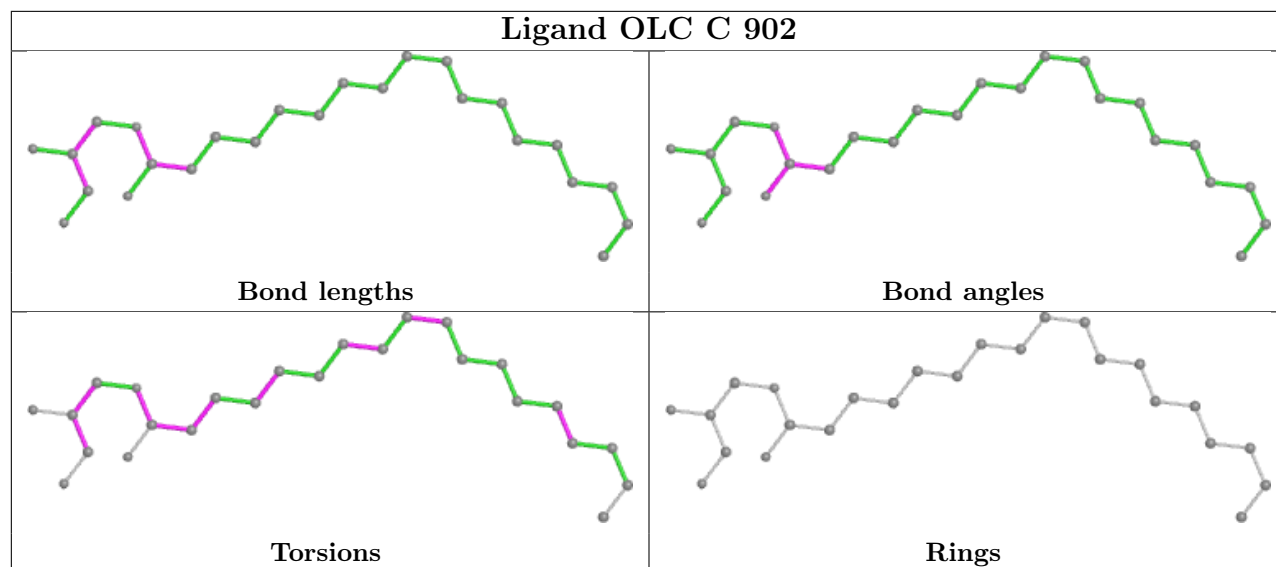
Mol	Chain	Res	Type	Atoms
3	B	901	ZK1	NAY-CAO-PBA-OAD
3	C	901	ZK1	NAY-CAO-PBA-OAD
4	B	902	OLC	C21-C22-C24-O25
4	B	902	OLC	C2-C1-O20-C21
4	B	902	OLC	O19-C1-O20-C21

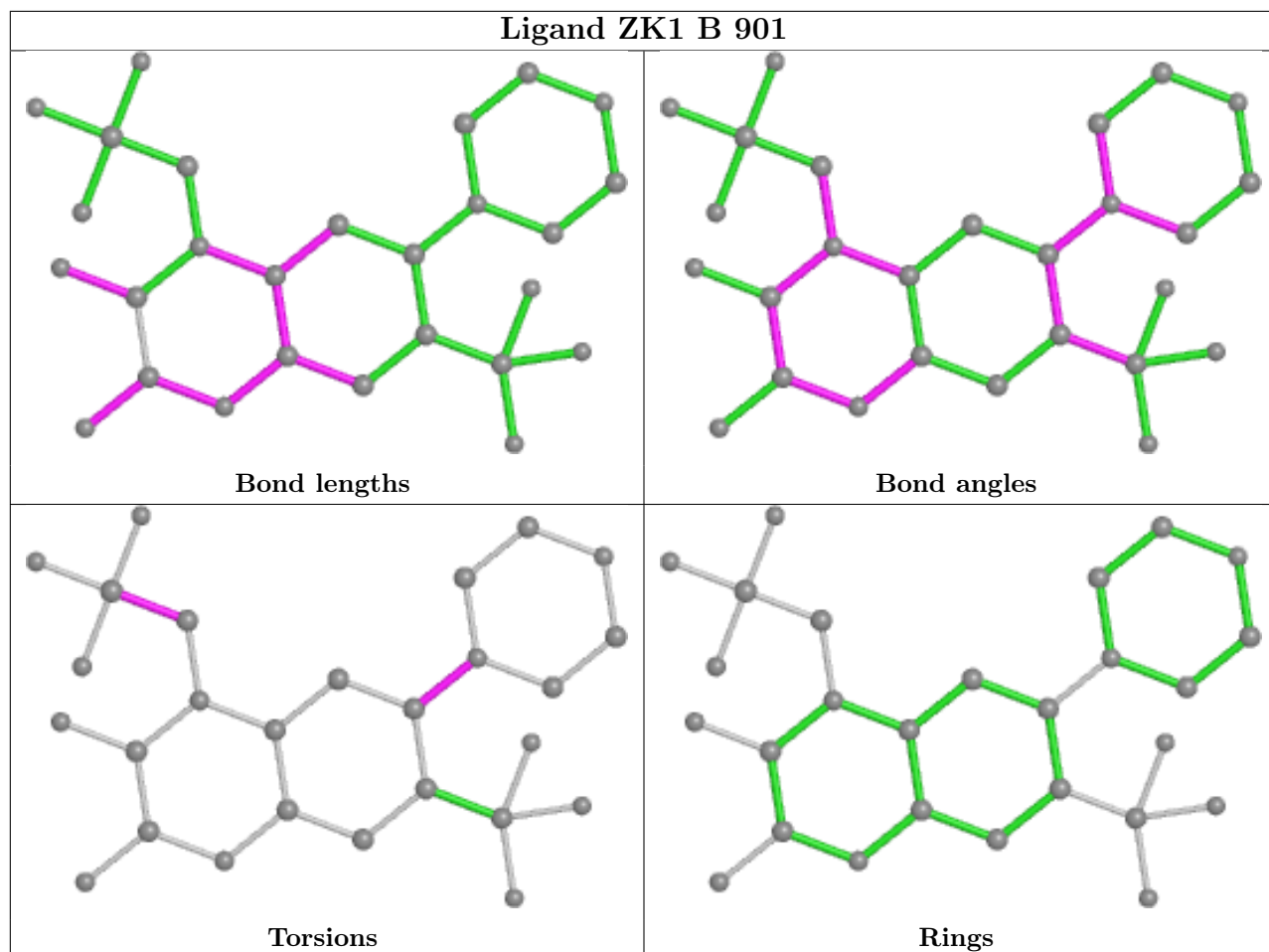
There are no ring outliers.

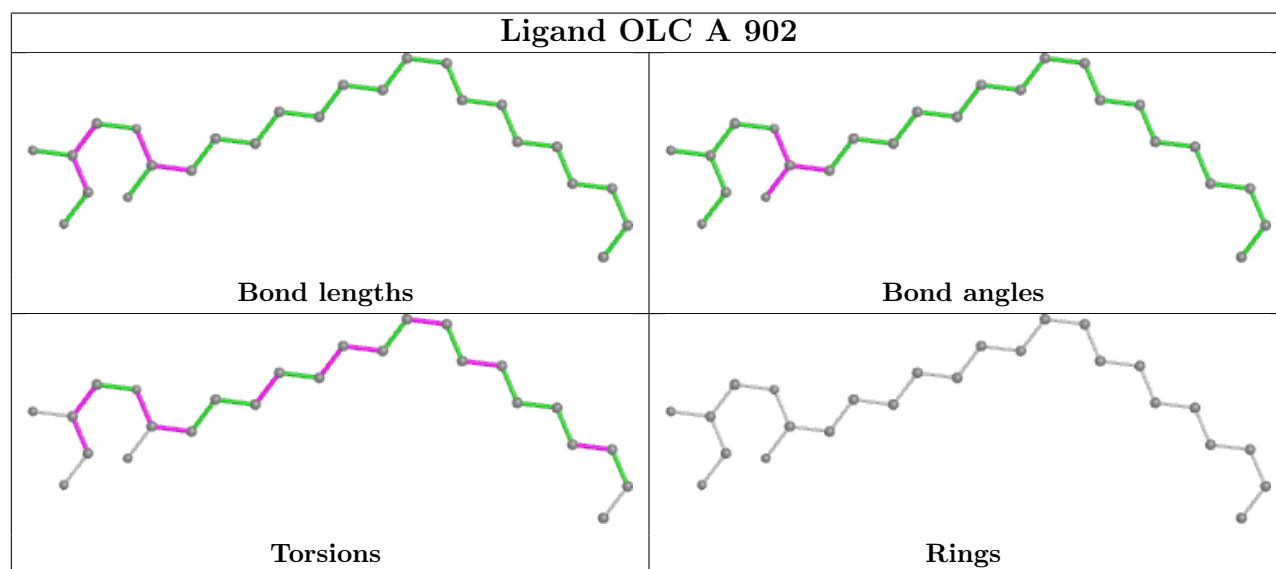
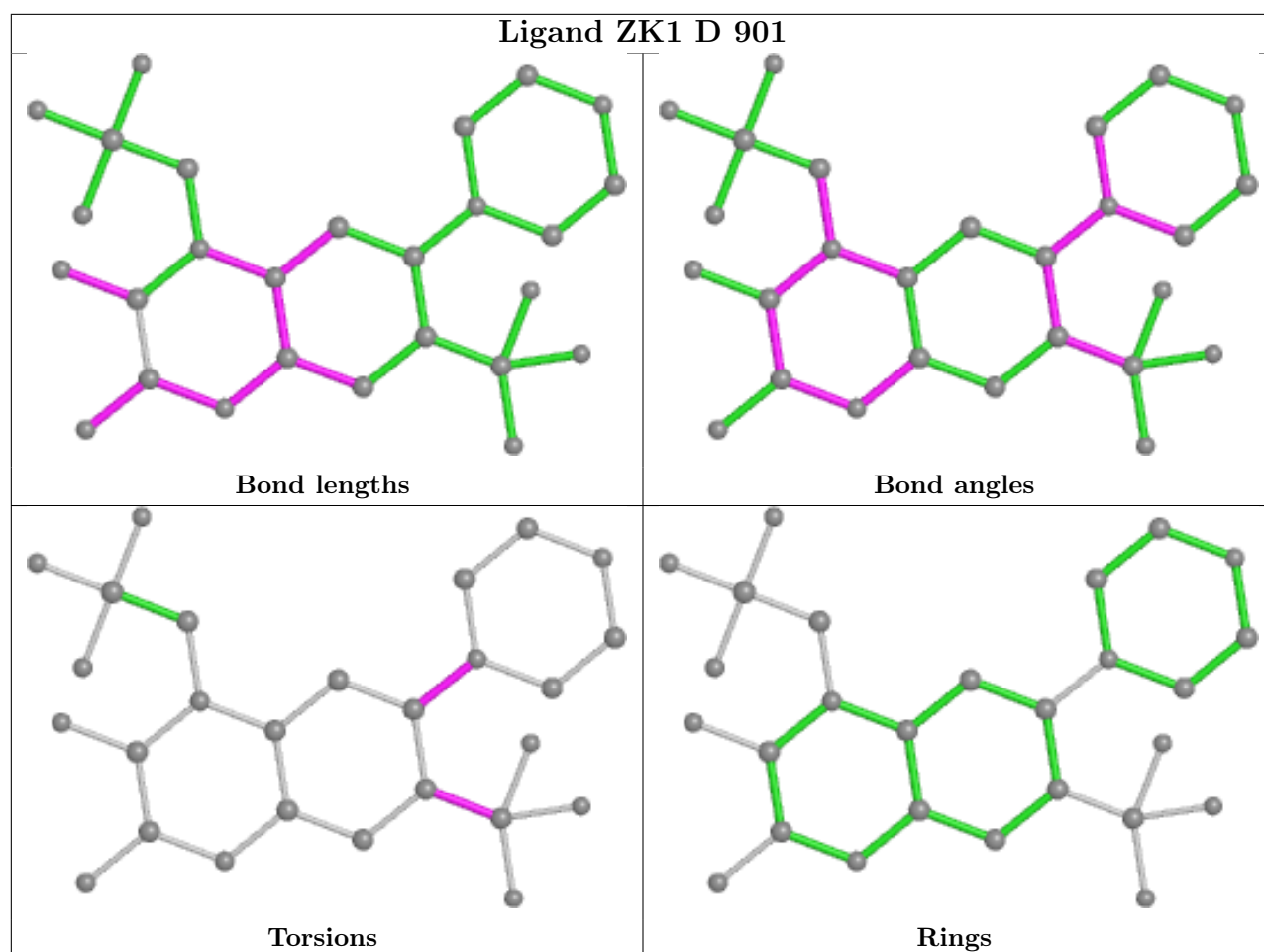
9 monomers are involved in 17 short contacts:

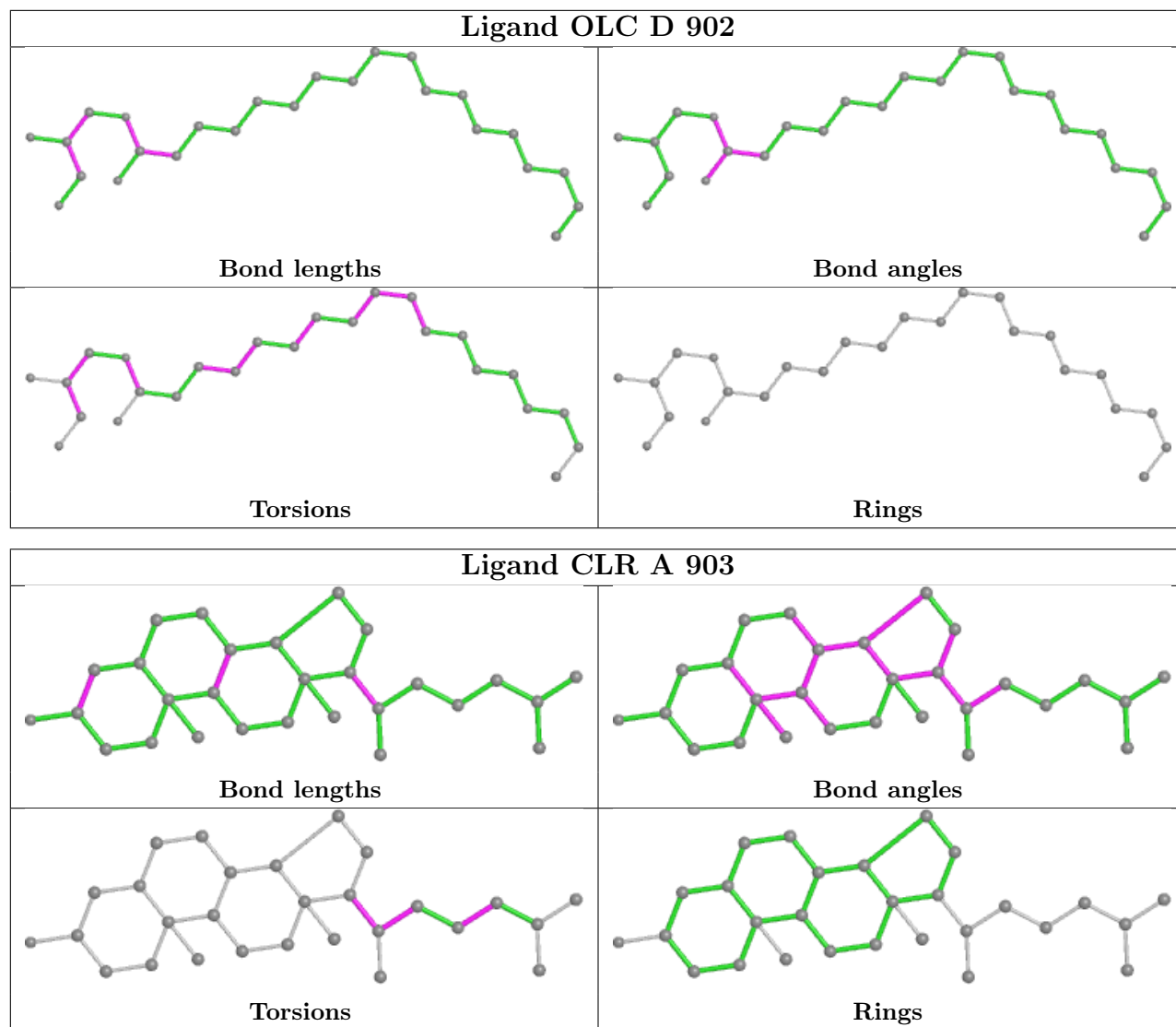
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	902	OLC	2	0
4	B	902	OLC	1	0
3	B	901	ZK1	2	0
3	D	901	ZK1	3	0
4	A	902	OLC	2	0
5	A	903	CLR	1	0
5	F	201	CLR	2	0
5	H	201	CLR	3	0
5	G	201	CLR	1	0

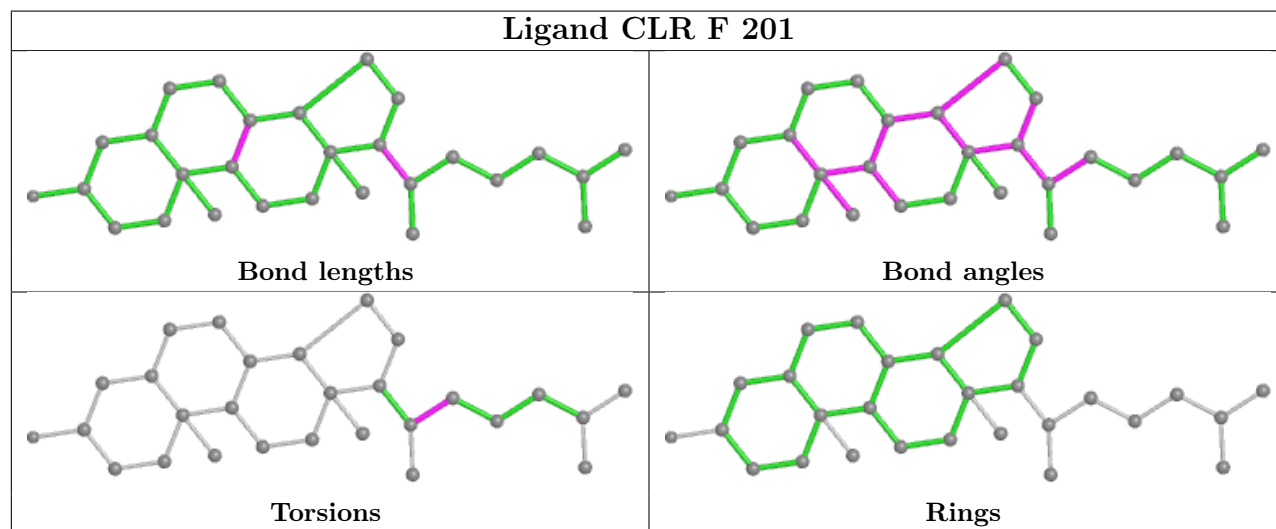
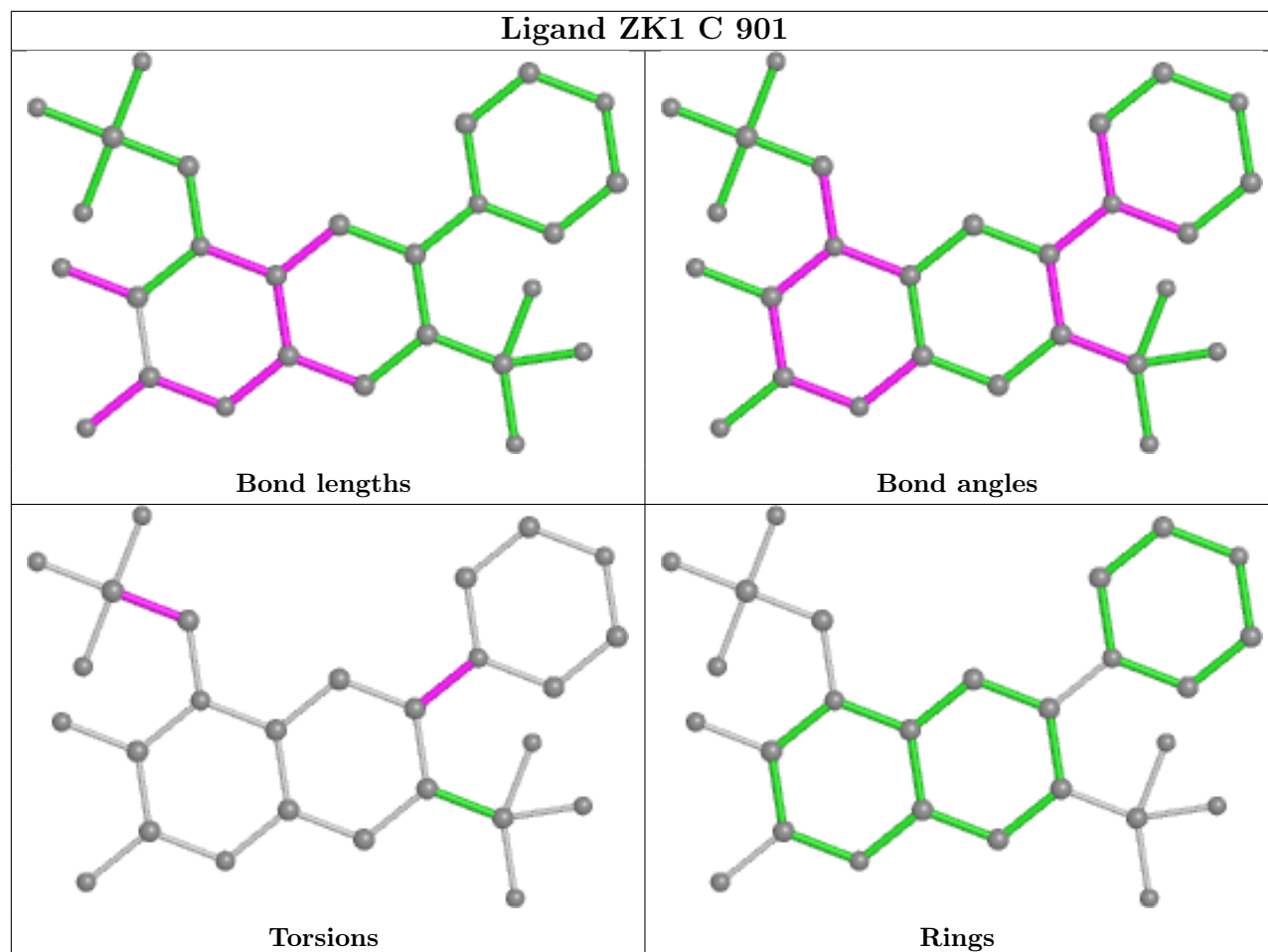
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

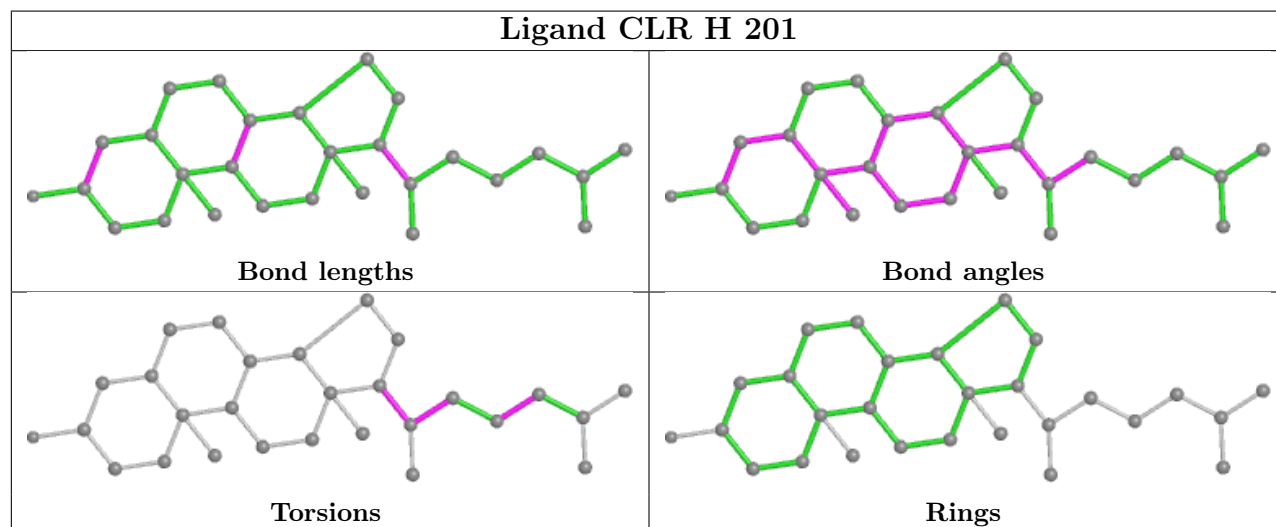
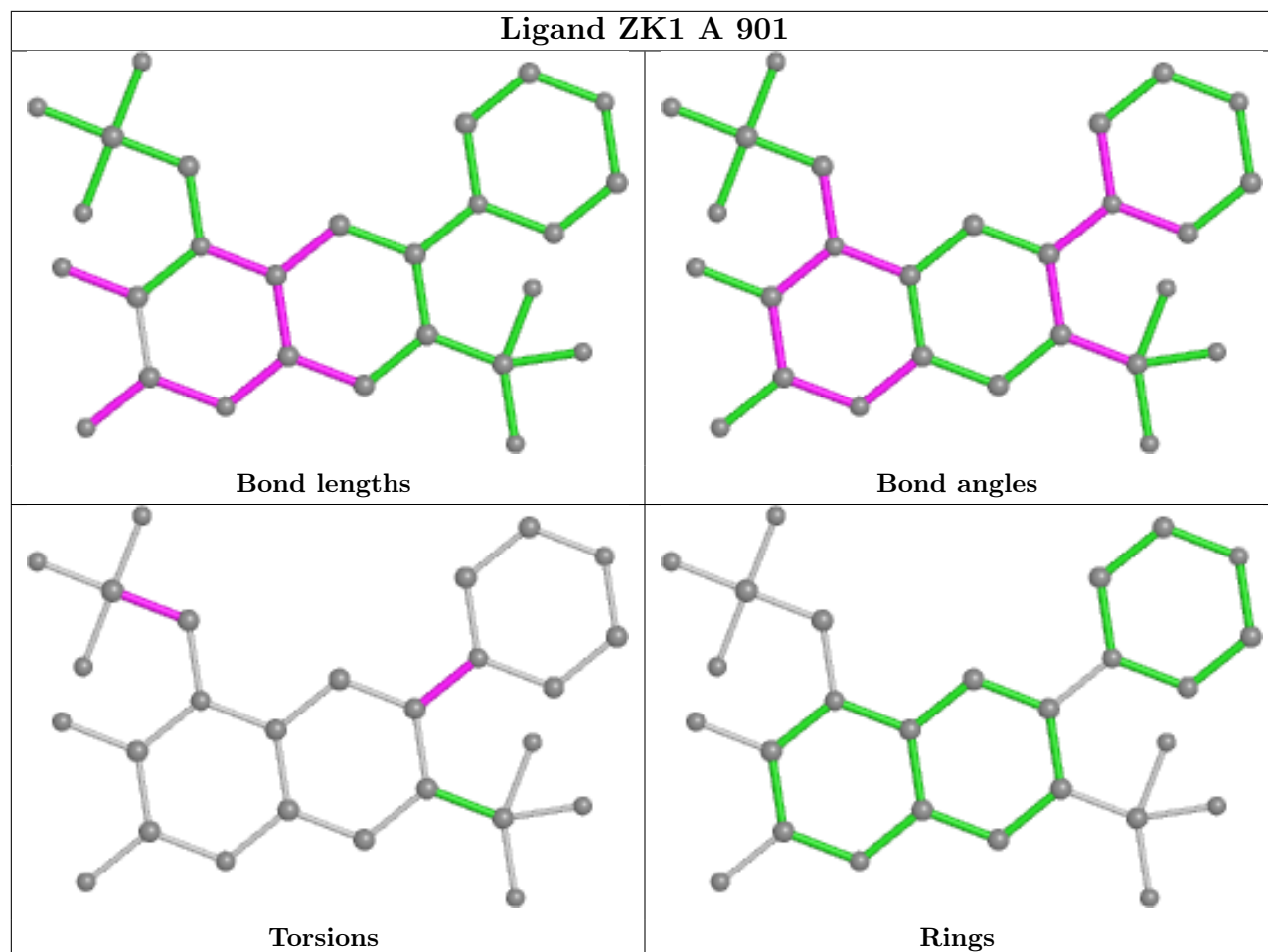


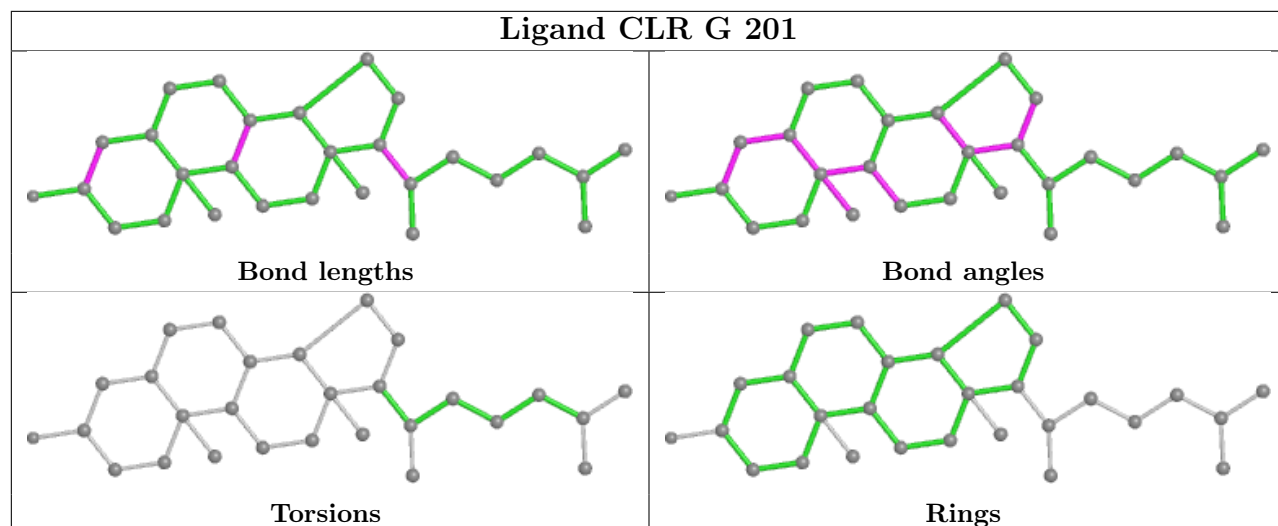












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

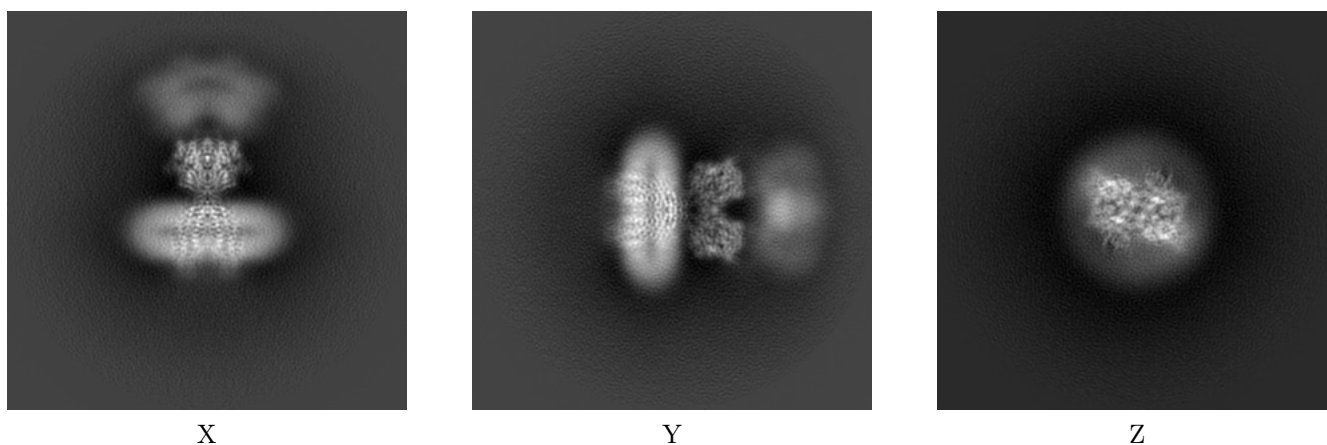
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20733. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

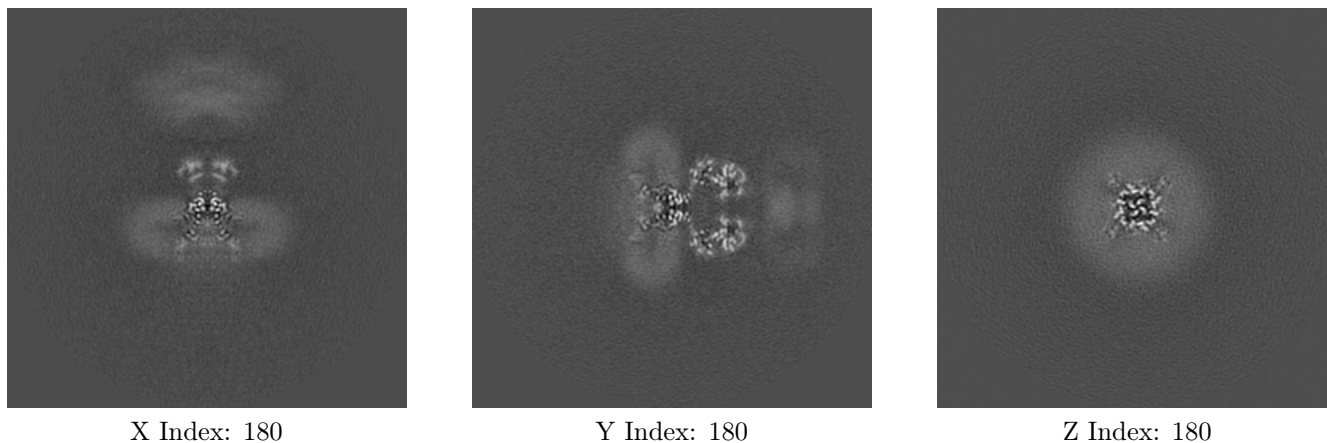
6.1.1 Primary map



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

6.2 Central slices [i](#)

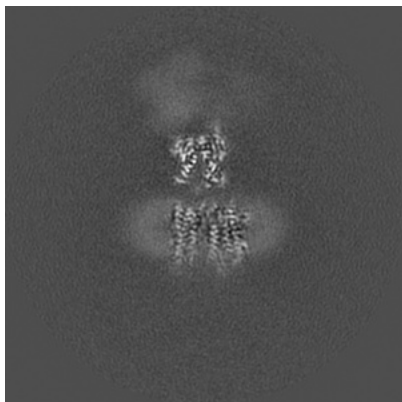
6.2.1 Primary map



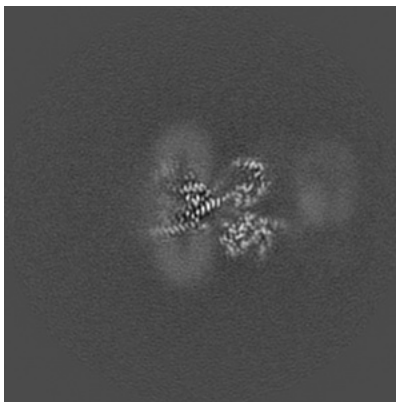
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

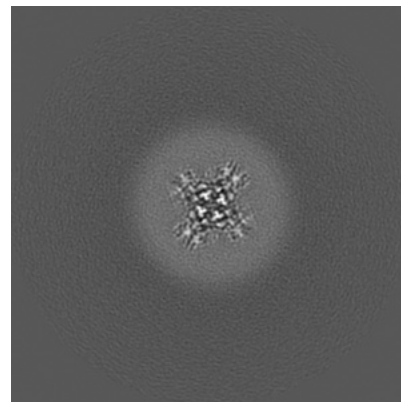
6.3.1 Primary map



X Index: 201



Y Index: 173

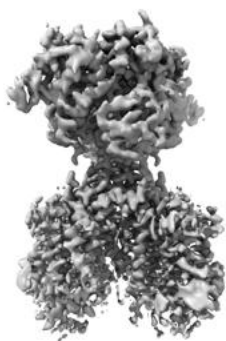


Z Index: 170

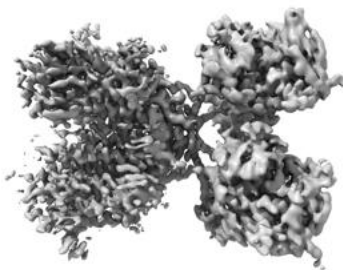
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

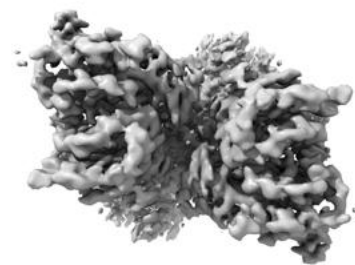
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0248. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

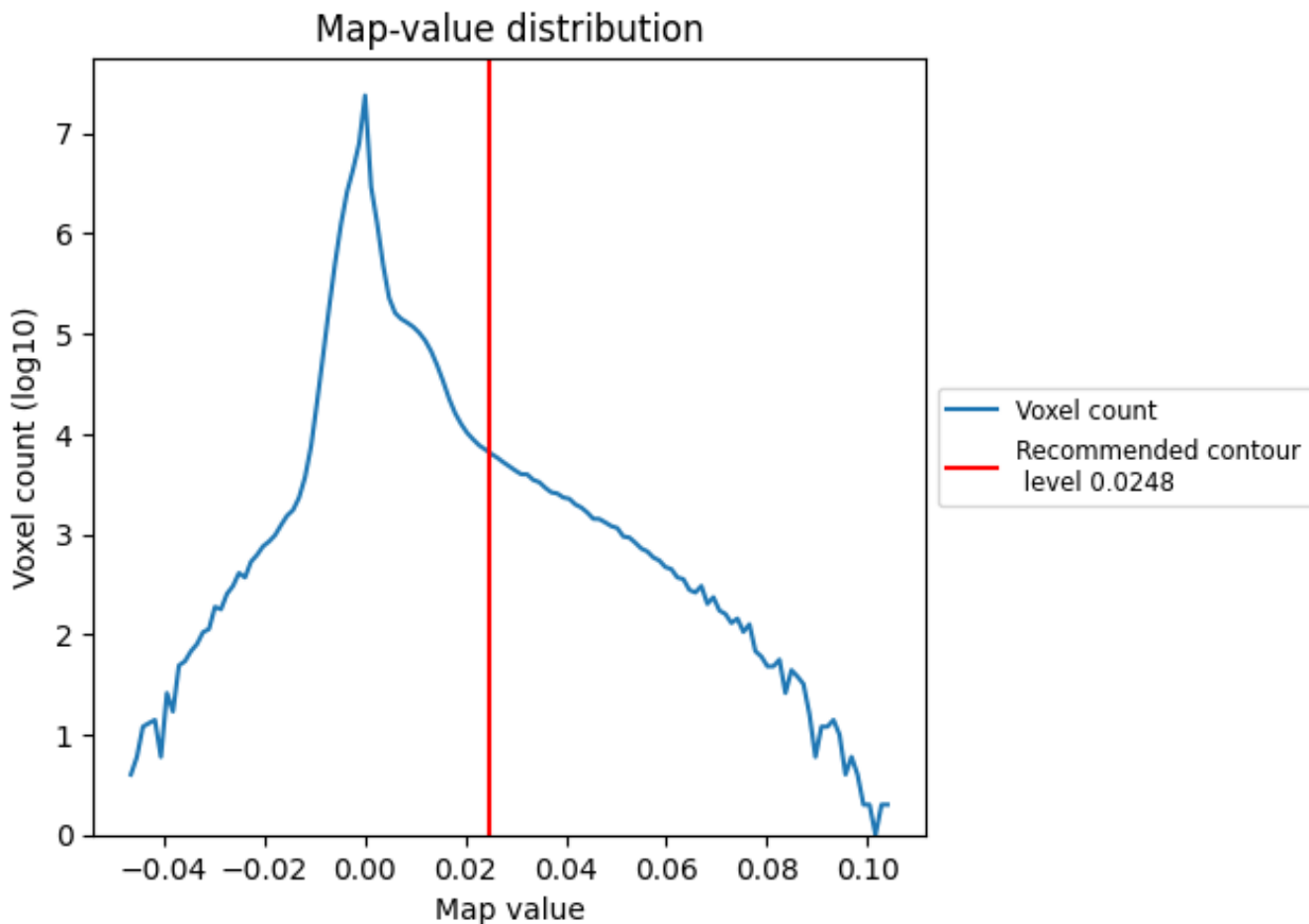
6.5 Mask visualisation

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

7 Map analysis [i](#)

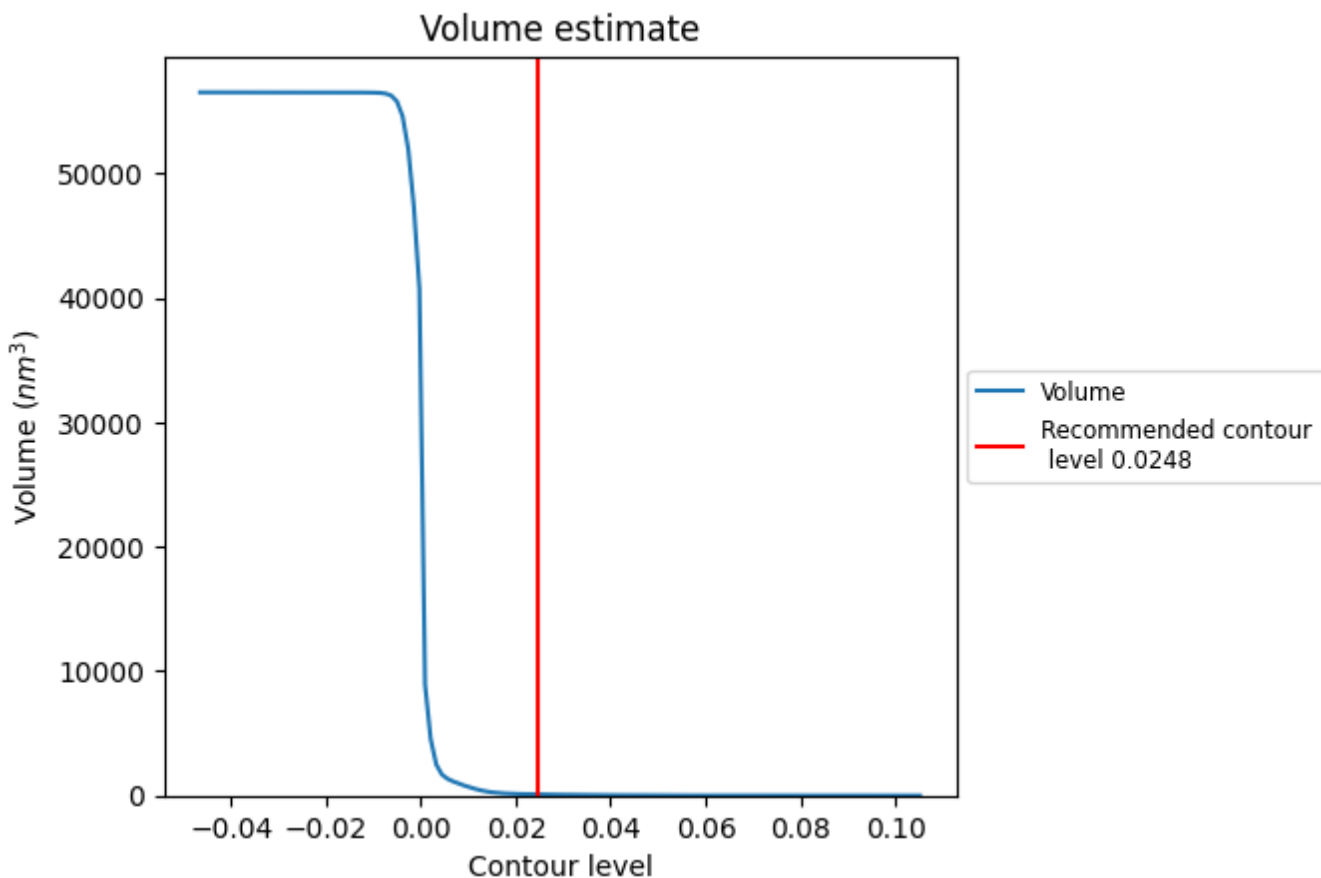
This section contains the results of statistical analysis of the map.

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.

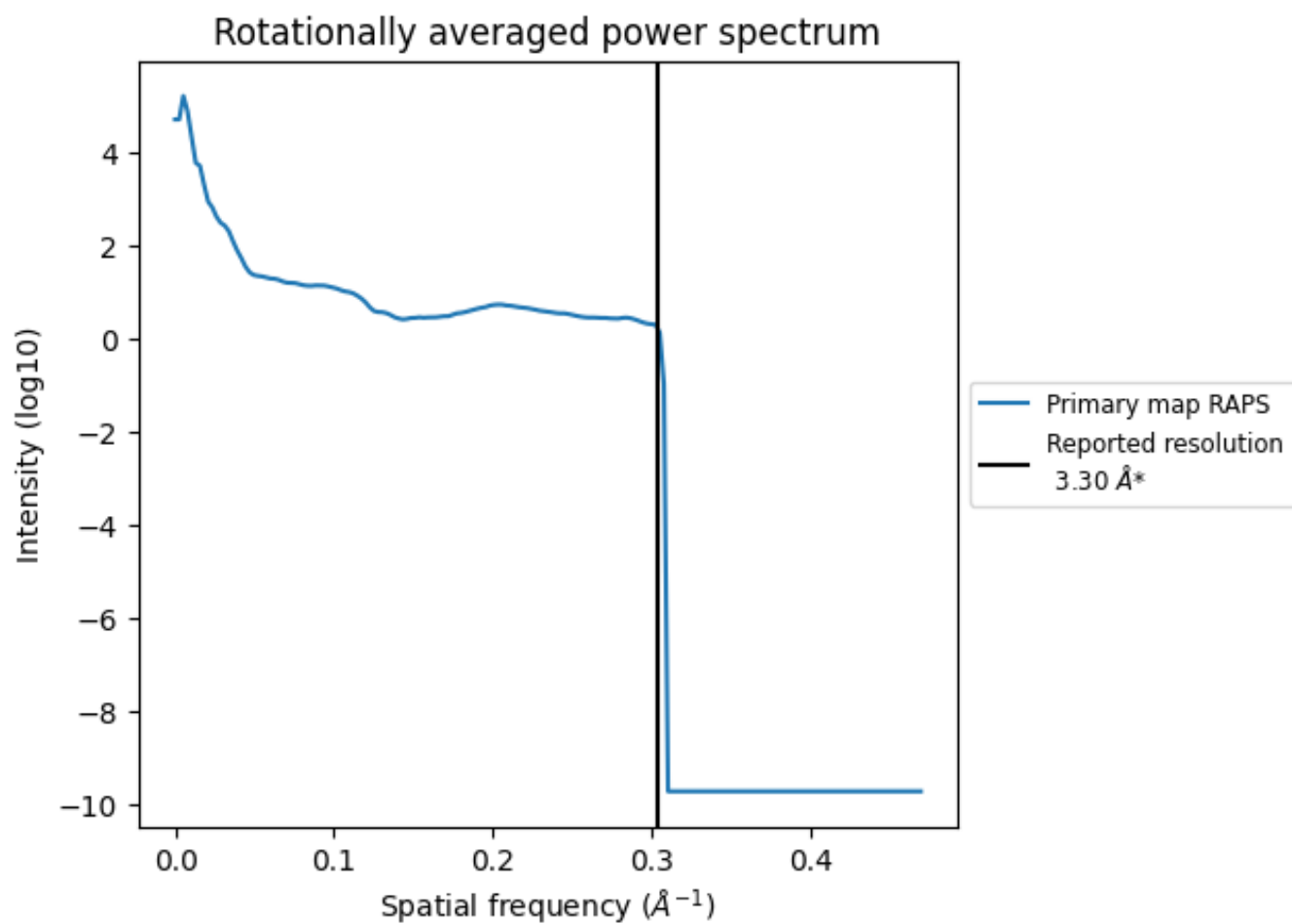
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 94 nm^3 ; this corresponds to an approximate mass of 85 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 [\(i\)](#)

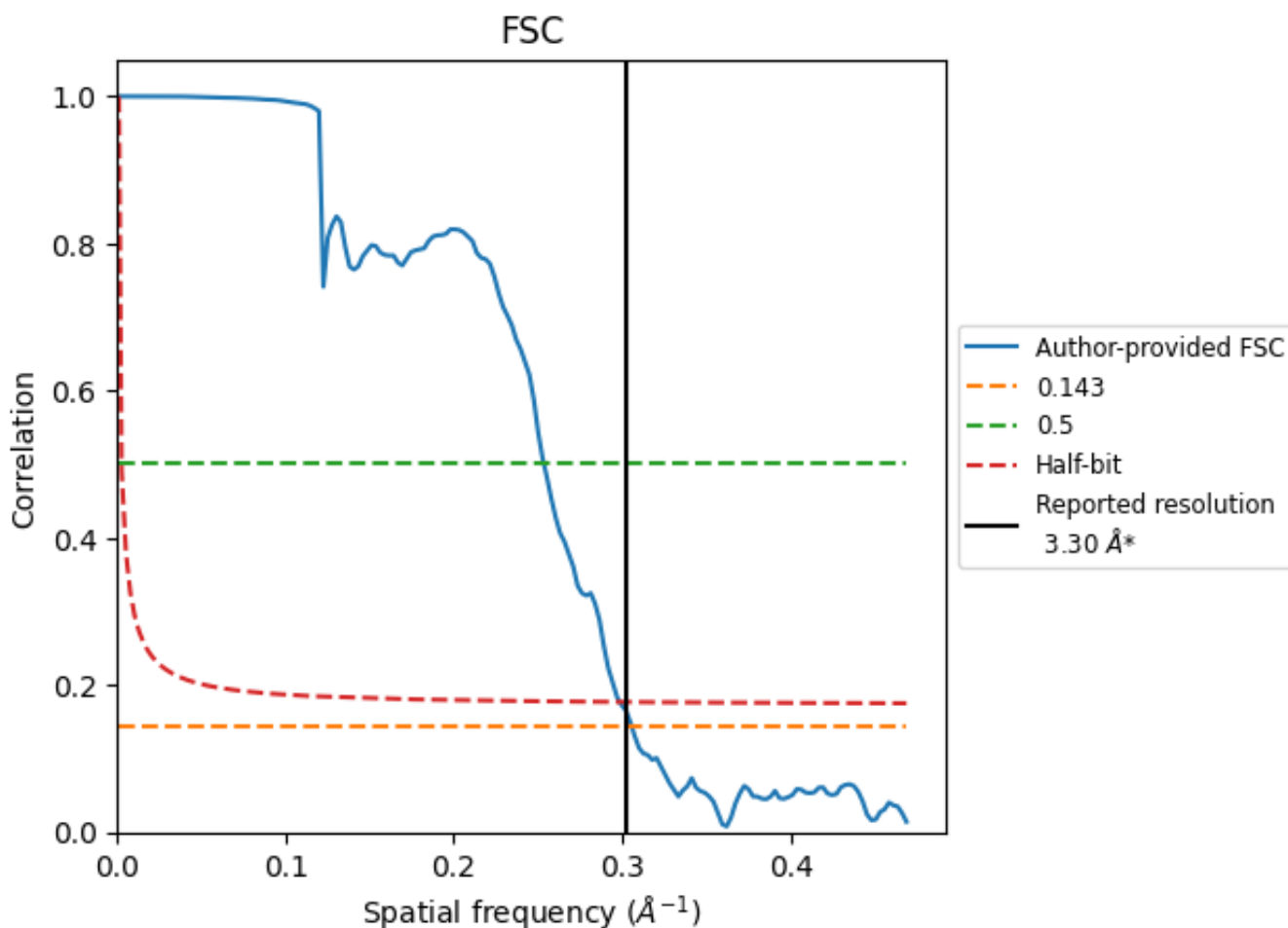


*Reported resolution corresponds to spatial frequency of 0.303\AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

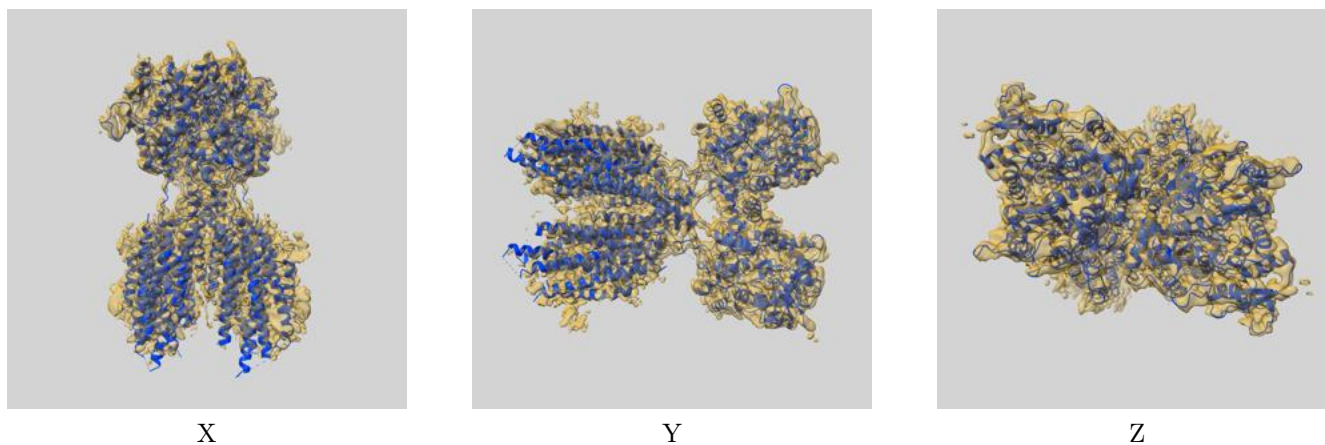
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.94	3.35
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

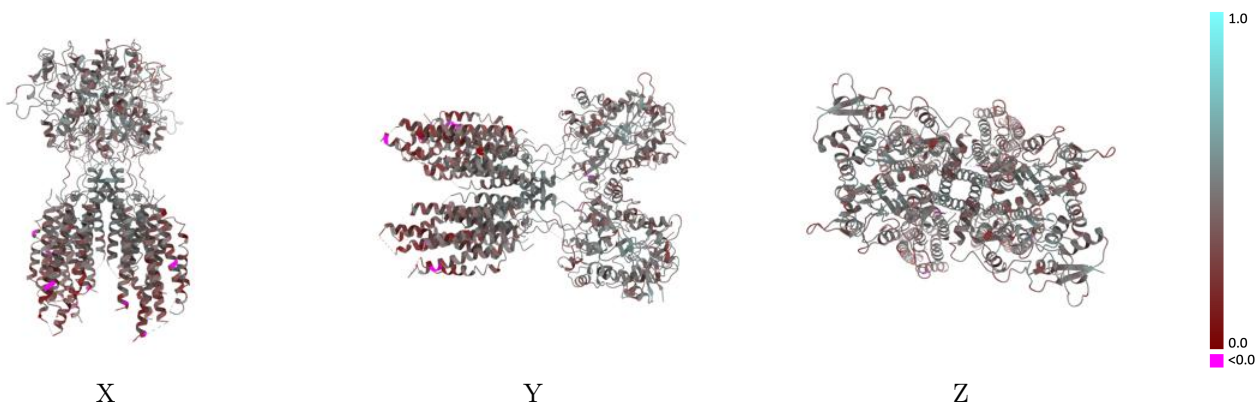
This section contains information regarding the fit between EMDB map EMD-20733 and PDB model 6UD4. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



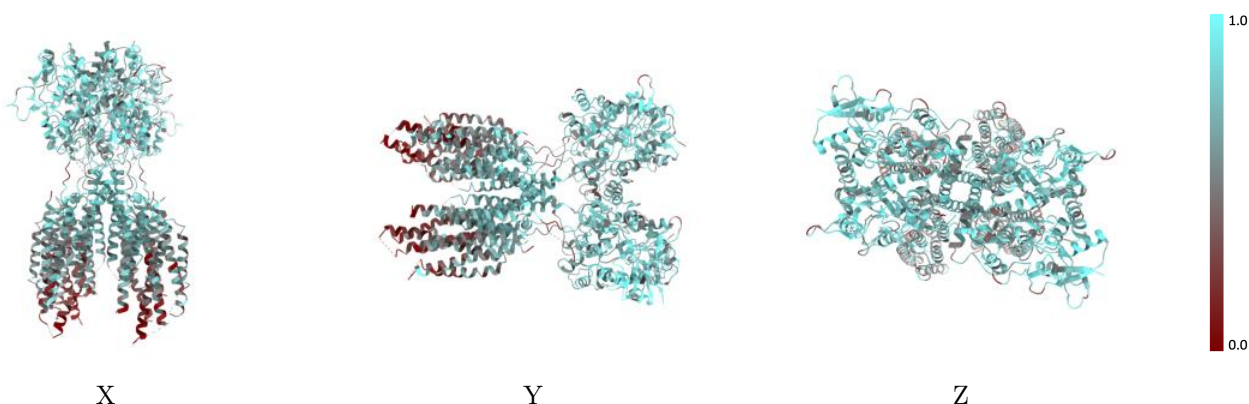
The images above show the 3D surface view of the map at the recommended contour level 0.0248 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



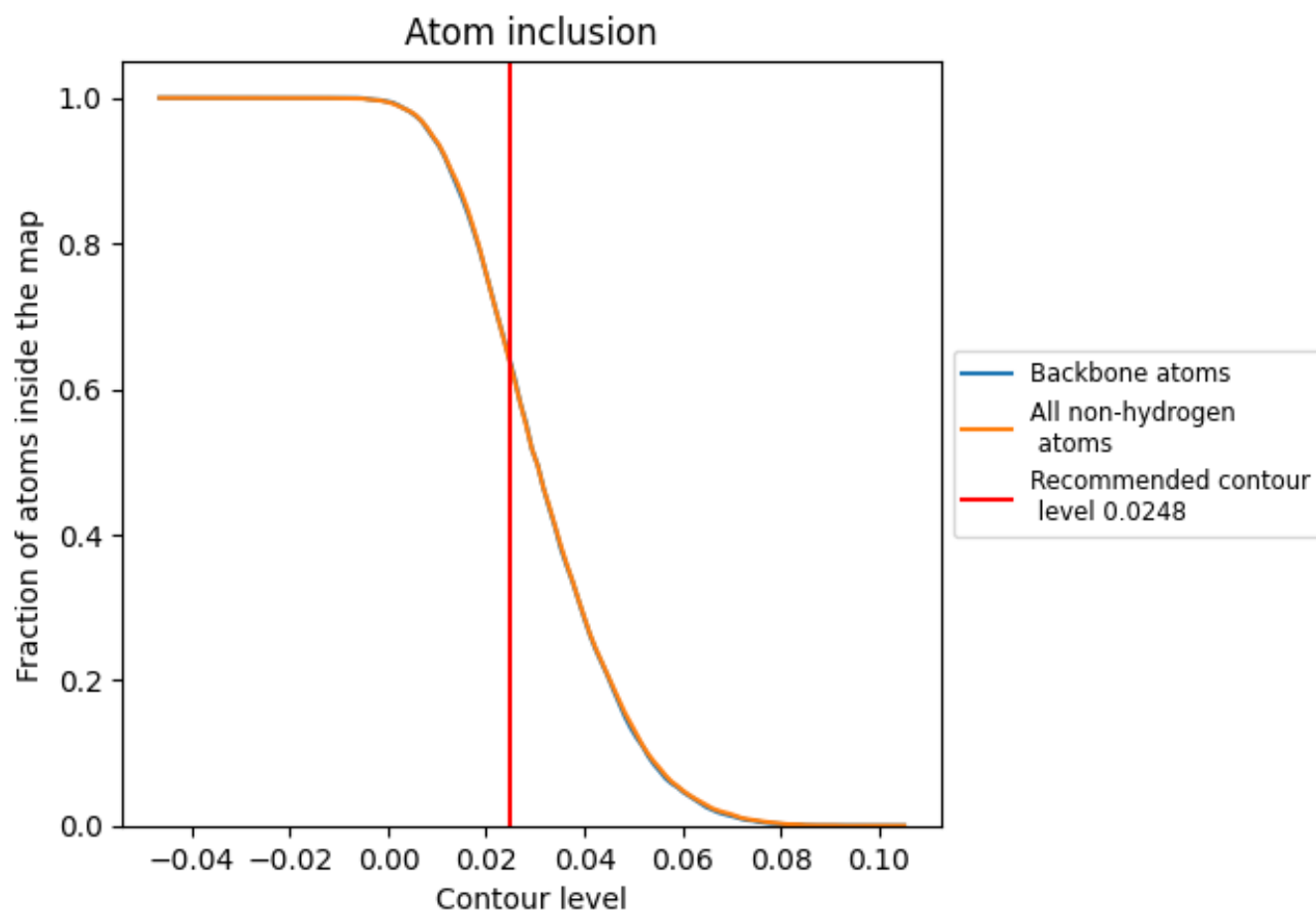
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0248).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 64% 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 (0.0248) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6375	 0.4120
A	 0.7121	 0.4450
B	 0.7090	 0.4380
C	 0.7121	 0.4460
D	 0.7027	 0.4320
E	 0.4586	 0.3280
F	 0.4794	 0.3450
G	 0.4487	 0.3380
H	 0.4812	 0.3430

