



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 12:48 PM UTC

PDB ID : 6UD8 / pdb_00006ud8
EMDB ID : EMD-20734
Title : GluA2 in complex with its auxiliary subunit CNIH3 - with antagonist ZK200775
Authors : Nakagawa, T.
Deposited on : 2019-09-18
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

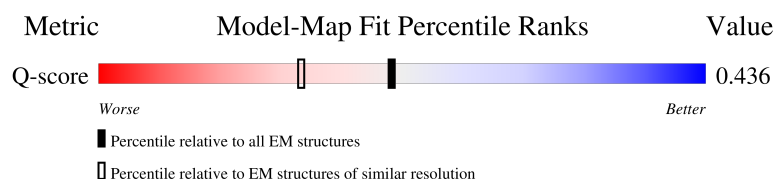
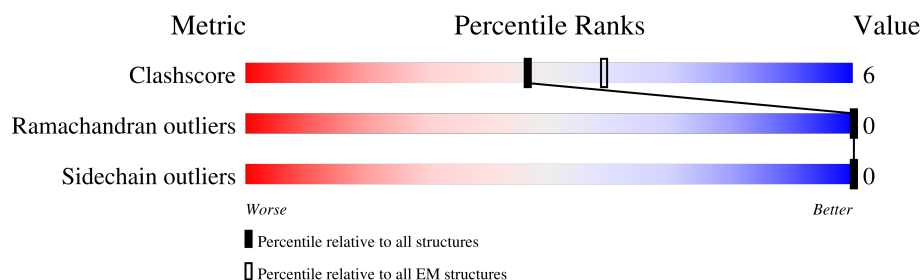
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	 37% 5% 57%
1	B	889	 36% 7% 57%
1	C	889	 37% 6% 57%
1	D	889	 35% 7% 57%

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Mol	Chain	Length	Quality of chain
2	E	174	
2	F	174	
2	G	174	
2	H	174	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32058 atoms, of which 15878 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
1	A	378	Total	C	H	N	O	S	0	0
			5675	1851	2819	461	526	18		
1	B	378	Total	C	H	N	O	S	0	0
			5742	1868	2863	467	526	18		
1	C	378	Total	C	H	N	O	S	0	0
			5675	1851	2819	461	526	18		
1	D	378	Total	C	H	N	O	S	0	0
			5742	1868	2863	467	526	18		

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
2	E	132	Total	C	H	N	O	S	0	0
			2107	740	1024	162	169	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
			2107	740	1024	162	169	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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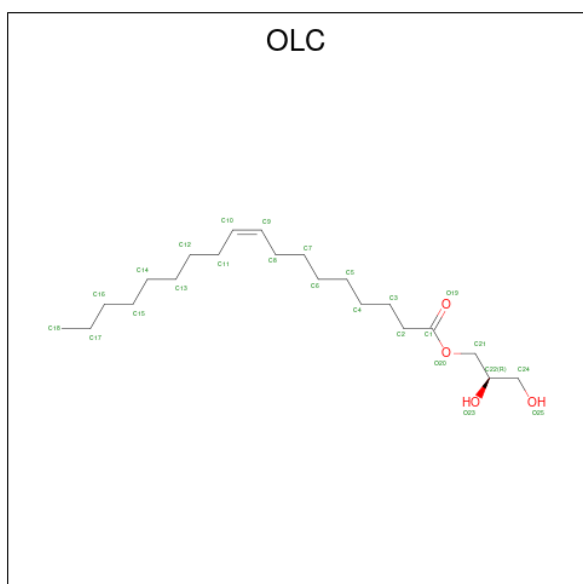
Chain	Residue	Modelled	Actual	Comment	Reference
E	163	ARG	-	linker	UNP Q6ZWS4
E	164	GLY	-	linker	UNP Q6ZWS4
E	165	GLY	-	linker	UNP Q6ZWS4
E	166	THR	-	expression tag	UNP Q6ZWS4
E	167	GLU	-	expression tag	UNP Q6ZWS4
E	168	THR	-	expression tag	UNP Q6ZWS4
E	169	SER	-	expression tag	UNP Q6ZWS4
E	170	GLN	-	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

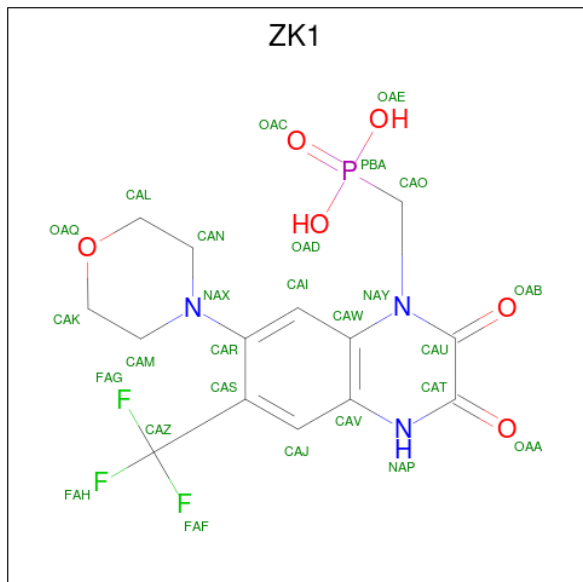
- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$) (labeled as "Ligand of Interest" by depositor).



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

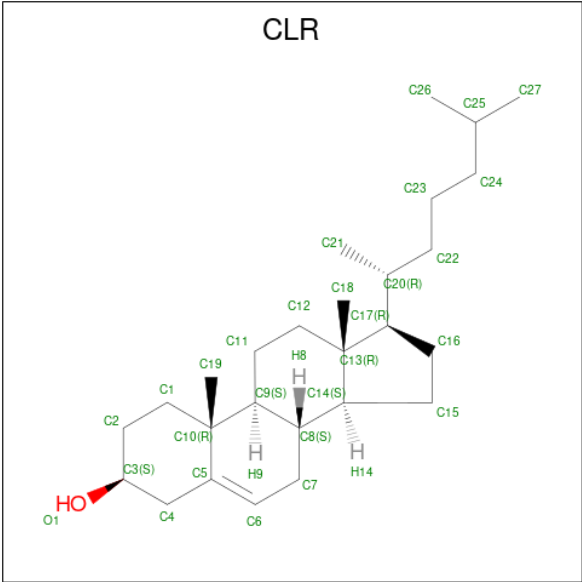
- Molecule 4 is {[7-morpholin-4-yl-2,3-dioxo-6-(trifluoromethyl)-3,4-dihydroquinoxalin-1(2H)-

yl)methyl}phosphonic acid (CCD ID: ZK1) (formula: $C_{14}H_{15}F_3N_3O_6P$) (labeled as "Ligand of Interest" by depositor).



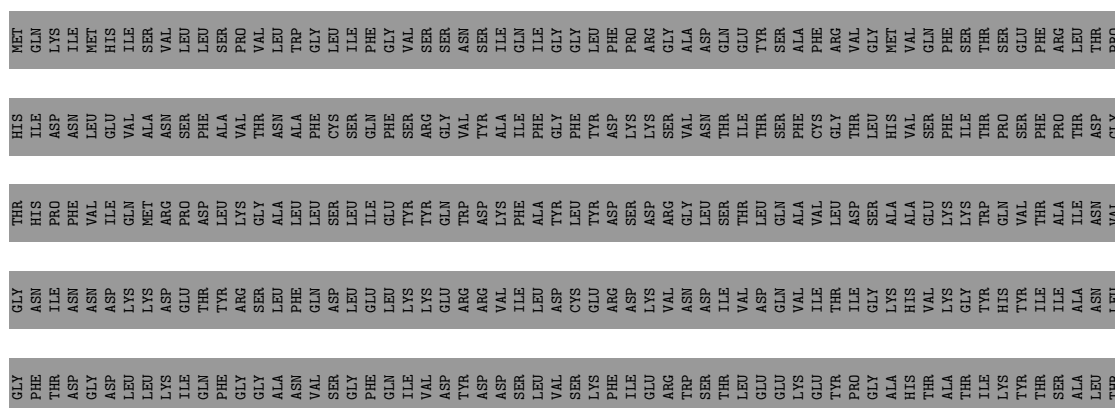
Mol	Chain	Residues	Atoms							AltConf
4	A	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	
4	B	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	
4	C	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	
4	D	1	Total	C	F	H	N	O	P	0
			40	14	3	13	3	6	1	

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by depositor).

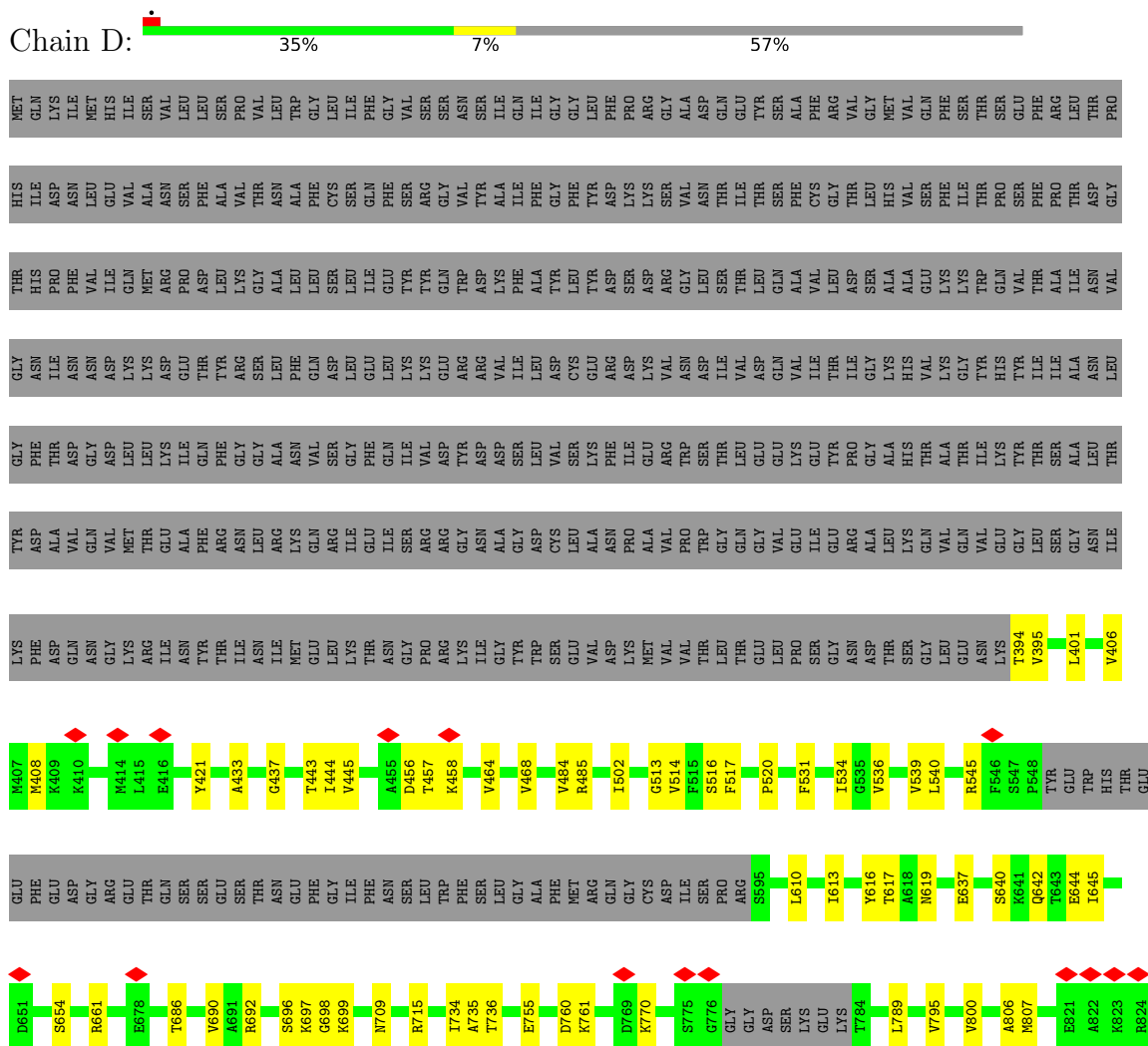


Mol	Chain	Residues	Atoms				AltConf
5	E	1	Total	C	H	O	0
			74	27	46	1	
5	F	1	Total	C	H	O	0
			74	27	46	1	
5	G	1	Total	C	H	O	0
			74	27	46	1	
5	H	1	Total	C	H	O	0
			74	27	46	1	

LYS	E644	GLU	W407	LYS	TYR	GLY	GLY	GLY	ASN	THR	THR	HIS	MET
VAL	1645	GLU	W408	PHE	ASP	ALA	PHE	THR	ASN	THR	PRO	GLN	GLN
ALA		PHE	W409	GLN	VAL	GLN	GLN	GLY	ASN	PHE	ASP	ASN	ILE
LYS	D651	ASP	W410	ASN	VAL	VAL	GLY	ASP	ASN	ILE	GLU	HIS	ILE
PRO		GLY		GLY	MET	MET	LEU	LEU	LYS	GLN	VAL	ILE	ILE
GLN	S654	ARG	W414	LYS	THR	THR	LEU	LEU	LYS	MET	GLN	VAL	ILE
ASN		THR	L415	ILE	GLU	GLU	GLU	GLU	ASN	ASN	VAL	ALA	SER
ASN	E678	THR	E416	ASN	ALA	ALA	ILE	ILE	GLU	PRO	ASN	LEU	VAL
PRO	T686	SER	W421	TYR	PHE	PHE	GLN	THR	THR	ASP	LEU	LEU	SER
SER		SER		THR	ARG	ARG	VAL	PHE	GLN	ASN	ALA	SER	LEU
SER	V690	GLU	A433	ILE	ASN	ASN	GLY	GLY	ARG	LYS	VAL	PRO	VAL
GLN	A691	SER		ASN	LEU	LEU	ALA	GLY	SER	GLY	THR	VAL	VAL
SER	B692	THR	Q437	ILE	ARG	ARG	ALA	ALA	LEU	ALA	ALA	THR	TRP
ASN		ASN		MET	LYS	GLN	VAL	ASN	PHE	GLN	PHE	GLY	GLY
SER	S696	GLU	T443	LEU	ARG	ILE	SER	GLY	ASN	LEU	LEU	ILE	ILE
GLN	K697	PHE	I444	LEU	THR	THR	PHE	PHE	GLN	GLU	GLN	GLN	PHE
ASN	G698	GLY	W446	LYS	ILE	ILE	GLY	GLY	LEU	LEU	SER	CYS	ILE
PHE	K699	ILE		LYS	THR	THR	GLY	GLY	ASN	ASP	ASN	ASN	ILE
ALA		PHE	A455	ASN	GLY	GLY	ASN	PHE	GLN	ILE	ILE	GLN	GLY
THR	W709	ASN	D456	THR	ARG	ARG	ASN	VAL	LYS	TYR	TYR	ARG	SER
ASP		SER	T457	PRO	ARG	ARG	ARG	ASP	GLY	GLN	GLN	SER	SER
TYR	R715	LEU	K458	LYS	LYS	LYS	TRP	TTR	ASP	TRP	TRP	VAL	ASN
LYS	I734	TRP		THR	GLY	GLY	ASP	ASP	GLY	ASP	ASP	VAL	ASN
ASP	A735	PHE	W464	ILE	ASN	ILE	ALA	ASP	ASN	ASP	ASP	ILE	ILE
ASP		SER	V468	TYR	GLY	GLY	GLY	SER	ASN	THR	PHE	GLN	GLN
ASP	E755	GLY		TRP	TRP	TRP	ASP	VAL	ASP	LEU	PHE	ILE	ILE
LYS		ALA	W484	SER	SER	SER	CYS	VAL	LEU	ASP	ILE	PHE	ILE
GLU	D760	PHE	R485	GLU	GLU	GLU	LEU	SER	LEU	CYS	LEU	GLY	GLY
GLY	K761	MET		VAL	VAL	VAL	ALA	SER	GLU	TYR	TYR	PHE	GLY
TYR		ARG		ASP	ASP	ASP	ALA	THR	ASN	ARG	ASP	ASN	ASN
ASN	D769	GLN	W502	LYS	LYS	LYS	GLN	ILE	PRO	ILE	SER	LYS	PRO
VAL	K770	GLY	G513	MET	MET	MET	ALA	GLU	ALA	GLU	ASP	LYS	ARG
TYR		CYS	W514	VAL	VAL	VAL	VAL	ARG	VAL	VAL	ARG	SER	GLY
GLY	S775	ASP	F515	VAL	VAL	VAL	PRO	TRP	PRO	TRP	GLY	VAL	ALA
ILE	G776	ILE	S516	THR	THR	THR	TRP	SER	GLY	SER	THR	THR	ASN
GLU		SER		LEU	LEU	LEU	GLY	THR	GLY	ILE	GLY	VAL	GLY
SER	GLY	PRO	P620	THR	THR	THR	GLN	GLU	GLN	VAL	SER	GLY	GLY
VAL		ARG		GLU	GLU	GLU	GLY	GLU	GLY	GLY	THR	THR	TYR
LYS	ASP	ASP	C528	LEU	LEU	LEU	VAL	GLU	VAL	GLN	SER	SER	SER
ILE	SER	SER		PRO	PRO	PRO	GLU	GLU	LYS	VAL	PHE	ALA	ALA
	LYS	GLU	F531	SER	SER	SER	ILE	GLU	ILE	VAL	PHE	ALA	ALA
	LYS	LYS	1611	GLY	GLY	GLY	GLU	TYR	THR	LEU	GLY	THR	ASN
			1612	ASN	ASN	ASN	ARG	PRO	ILE	ASP	THR	GLY	GLY
	I784		1613	ASP	ALA	ALA	ALA	PRO	GLY				

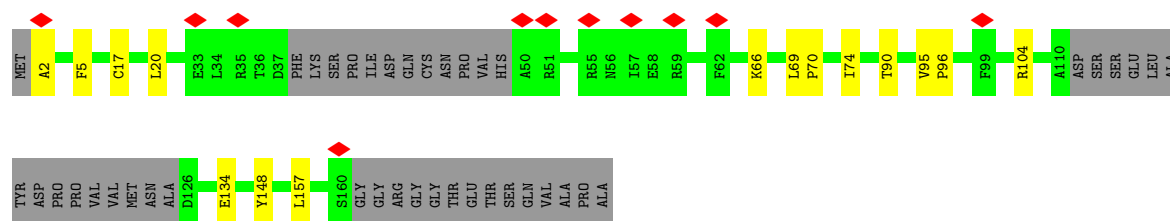


- Molecule 1: Glutamate receptor 2

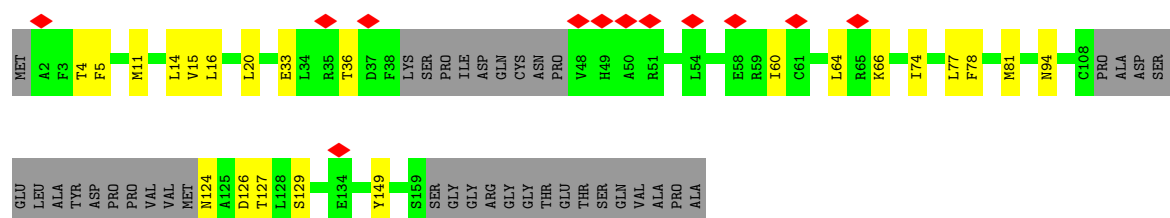


LYS VAL ALA LYS ASN PRO GLN ASN ILE PRO PRO SER SER SER GLN ASN LYS SER GLN ASN PHE ALA THR ASP TYR LYS ASP ASP ASP ASP LYS GLU GLY TYR ASN VAL TYR GLY ILE GLU SER VAL LYS ILE

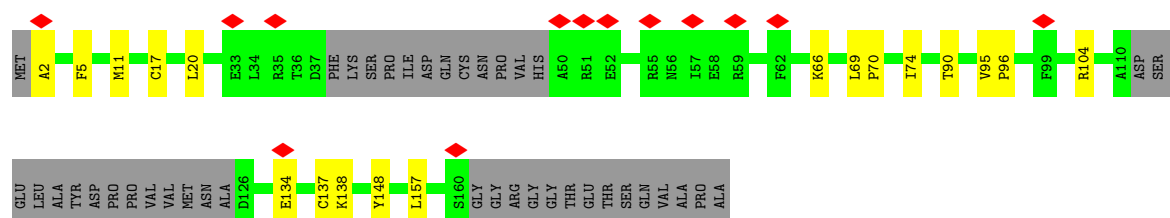
• Molecule 2: Protein cornichon homolog 3



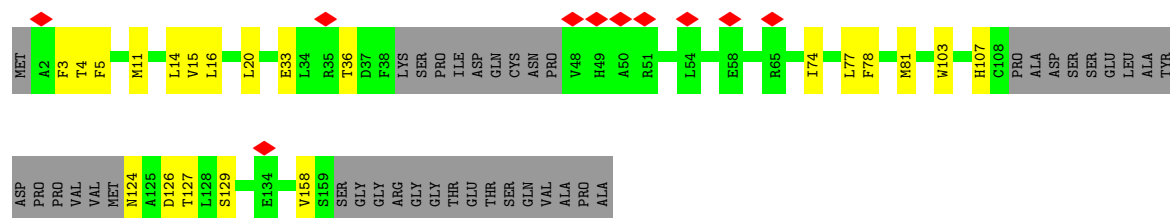
• Molecule 2: Protein cornichon homolog 3



• 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	76689	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	0.113	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0218	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZK1, CLR, OLC

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	0.16	0/2915	0.30	2/3951 (0.1%)
1	B	0.16	0/2938	0.25	0/3976
1	C	0.16	0/2915	0.30	2/3951 (0.1%)
1	D	0.16	0/2938	0.25	0/3976
2	E	0.13	0/1120	0.29	0/1523
2	F	0.14	0/1149	0.28	0/1561
2	G	0.13	0/1120	0.29	0/1523
2	H	0.14	0/1149	0.28	0/1561
All	All	0.15	0/16244	0.28	4/22022 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	VAL	CA-C-N	6.81	127.36	119.94
1	A	445	VAL	C-N-CA	6.81	127.36	119.94
1	C	445	VAL	CA-C-N	6.80	127.35	119.94
1	C	445	VAL	C-N-CA	6.80	127.35	119.94

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2856	2819	2818	35	0
1	B	2879	2863	2875	45	0
1	C	2856	2819	2818	40	0
1	D	2879	2863	2875	48	0
2	E	1083	1024	1045	10	0
2	F	1112	1035	1071	16	0
2	G	1083	1024	1045	13	0
2	H	1112	1035	1071	17	0
3	A	25	40	40	0	0
3	B	25	40	40	0	0
3	C	25	40	40	0	0
3	D	25	40	40	0	0
4	A	27	13	13	2	0
4	B	27	13	13	2	0
4	C	27	13	13	2	0
4	D	27	13	13	2	0
5	E	28	46	46	0	0
5	F	28	46	46	1	0
5	G	28	46	46	1	0
5	H	28	46	46	1	0
All	All	16180	15878	16014	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)
2:F:20:LEU:HD13	2:F:74:ILE:HD11	1.34	1.09
2:H:20:LEU:HD13	2:H:74:ILE:HD11	1.33	1.09
2:G:104:ARG:NH2	2:G:134:GLU:OE2	2.17	0.77
1:A:502:ILE:O	1:A:709:ASN:ND2	2.18	0.77
2:E:104:ARG:NH2	2:E:134:GLU:OE2	2.17	0.77

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/889 (42%)	347 (93%)	25 (7%)	0	100	100
1	B	372/889 (42%)	347 (93%)	25 (7%)	0	100	100
1	C	372/889 (42%)	347 (93%)	25 (7%)	0	100	100
1	D	372/889 (42%)	347 (93%)	25 (7%)	0	100	100
2	E	126/174 (72%)	124 (98%)	2 (2%)	0	100	100
2	F	128/174 (74%)	124 (97%)	4 (3%)	0	100	100
2	G	126/174 (72%)	124 (98%)	2 (2%)	0	100	100
2	H	128/174 (74%)	124 (97%)	4 (3%)	0	100	100
All	All	1996/4252 (47%)	1884 (94%)	112 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	293/761 (38%)	293 (100%)	0	100	100
1	B	299/761 (39%)	299 (100%)	0	100	100
1	C	293/761 (38%)	293 (100%)	0	100	100
1	D	299/761 (39%)	299 (100%)	0	100	100
2	E	110/153 (72%)	110 (100%)	0	100	100
2	F	114/153 (74%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	110/153 (72%)	110 (100%)	0	100	100
2	H	114/153 (74%)	114 (100%)	0	100	100
All	All	1632/3656 (45%)	1632 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	756	GLN
1	C	764	ASN
2	H	94	ASN
1	D	508	GLN
2	G	94	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 oligosaccharides 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	ZK1	C	902	-	29,29,29	3.72	11 (37%)	45,45,45	1.50	7 (15%)
5	CLR	F	201	-	31,31,31	1.12	4 (12%)	48,48,48	1.70	9 (18%)
3	OLC	D	901	-	24,24,24	1.41	4 (16%)	25,25,25	0.99	2 (8%)
3	OLC	B	901	-	24,24,24	1.41	4 (16%)	25,25,25	0.99	2 (8%)
5	CLR	G	201	-	31,31,31	1.01	4 (12%)	48,48,48	1.65	7 (14%)
3	OLC	C	901	-	24,24,24	1.59	4 (16%)	25,25,25	1.32	5 (20%)
3	OLC	A	901	-	24,24,24	1.58	4 (16%)	25,25,25	1.32	5 (20%)
4	ZK1	D	902	-	29,29,29	3.70	11 (37%)	45,45,45	1.54	8 (17%)
5	CLR	H	201	-	31,31,31	1.11	4 (12%)	48,48,48	1.70	9 (18%)
4	ZK1	A	902	-	29,29,29	3.71	11 (37%)	45,45,45	1.49	7 (15%)
4	ZK1	B	902	-	29,29,29	3.70	11 (37%)	45,45,45	1.53	7 (15%)
5	CLR	E	201	-	31,31,31	1.02	4 (12%)	48,48,48	1.66	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	ZK1	C	902	-	-	7/13/23/23	0/3/3/3
5	CLR	F	201	-	-	4/10/68/68	0/4/4/4
3	OLC	D	901	-	-	16/24/24/24	-
3	OLC	B	901	-	-	16/24/24/24	-
5	CLR	G	201	-	-	0/10/68/68	0/4/4/4
3	OLC	C	901	-	-	10/24/24/24	-
3	OLC	A	901	-	-	10/24/24/24	-
4	ZK1	D	902	-	-	4/13/23/23	0/3/3/3
5	CLR	H	201	-	-	4/10/68/68	0/4/4/4
4	ZK1	A	902	-	-	7/13/23/23	0/3/3/3
4	ZK1	B	902	-	-	7/13/23/23	0/3/3/3
5	CLR	E	201	-	-	0/10/68/68	0/4/4/4

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	ZK1	OAA-CAT	8.75	1.40	1.23
4	C	902	ZK1	OAA-CAT	8.71	1.40	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	902	ZK1	OAA-CAT	8.69	1.40	1.23
4	D	902	ZK1	OAA-CAT	8.65	1.40	1.23
4	C	902	ZK1	OAB-CAU	8.40	1.40	1.23

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	201	CLR	C19-C10-C9	-5.54	105.44	111.66
5	F	201	CLR	C19-C10-C9	-5.54	105.44	111.66
5	E	201	CLR	C19-C10-C9	-5.09	105.95	111.66
5	G	201	CLR	C19-C10-C9	-5.09	105.95	111.66
5	E	201	CLR	C17-C13-C14	4.60	105.38	100.10

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

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

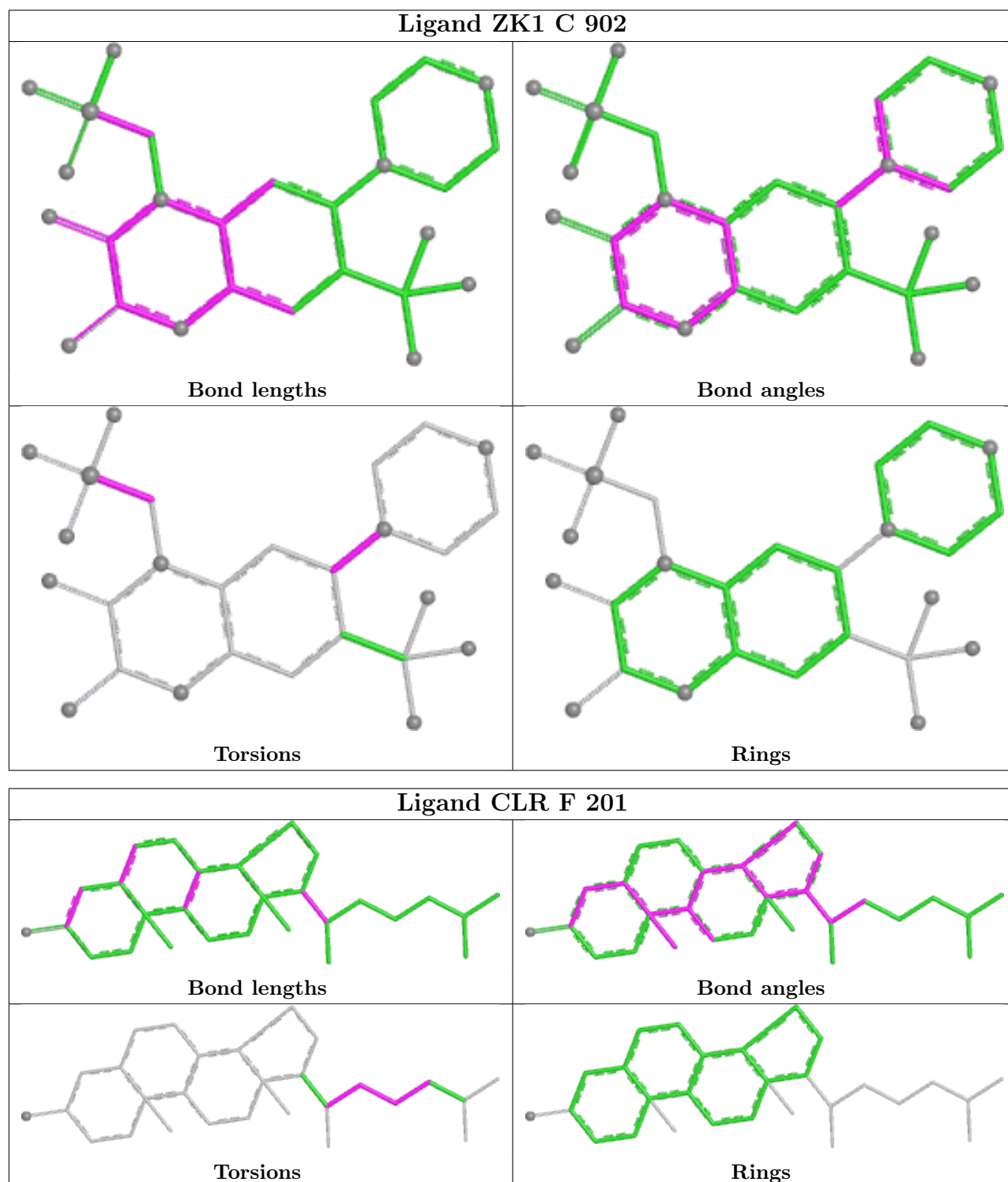
There are no ring outliers.

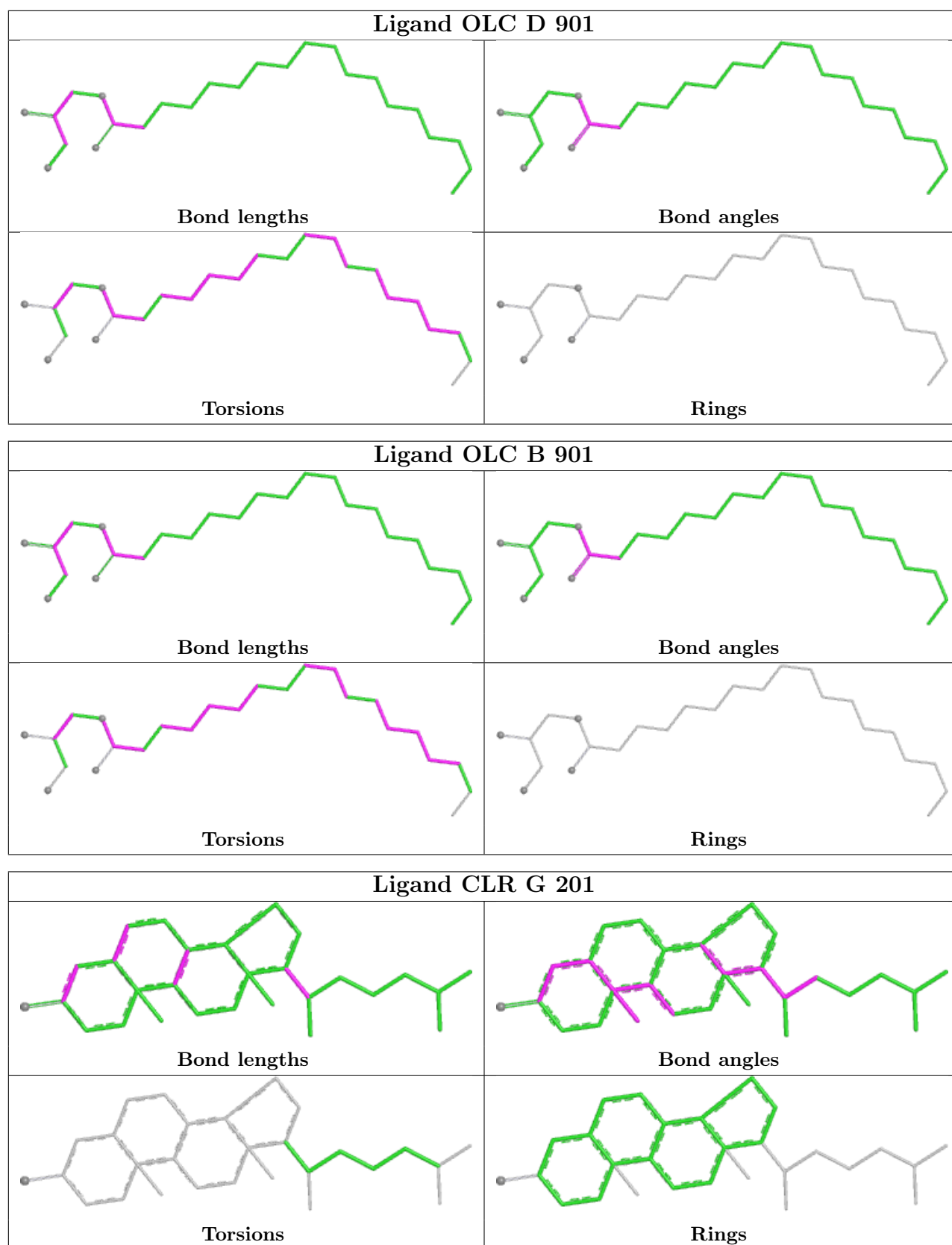
7 monomers are involved in 11 short contacts:

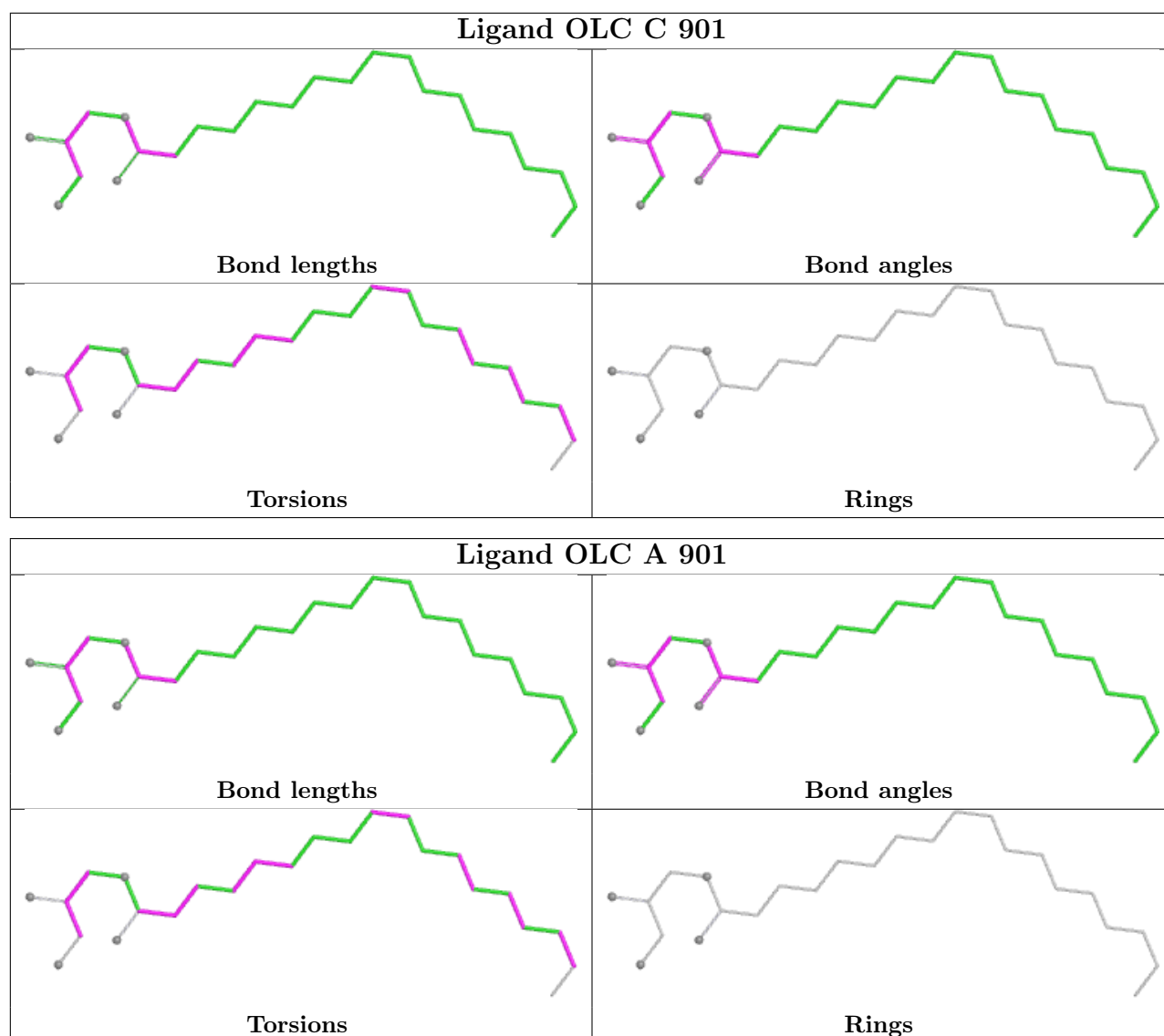
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	902	ZK1	2	0
5	F	201	CLR	1	0
5	G	201	CLR	1	0
4	D	902	ZK1	2	0
5	H	201	CLR	1	0
4	A	902	ZK1	2	0
4	B	902	ZK1	2	0

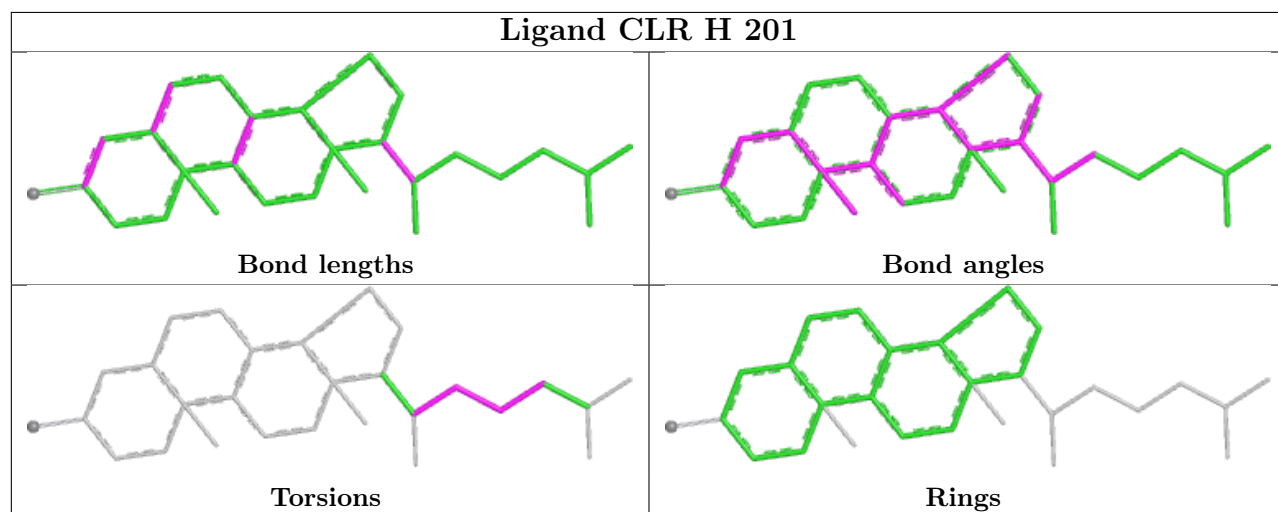
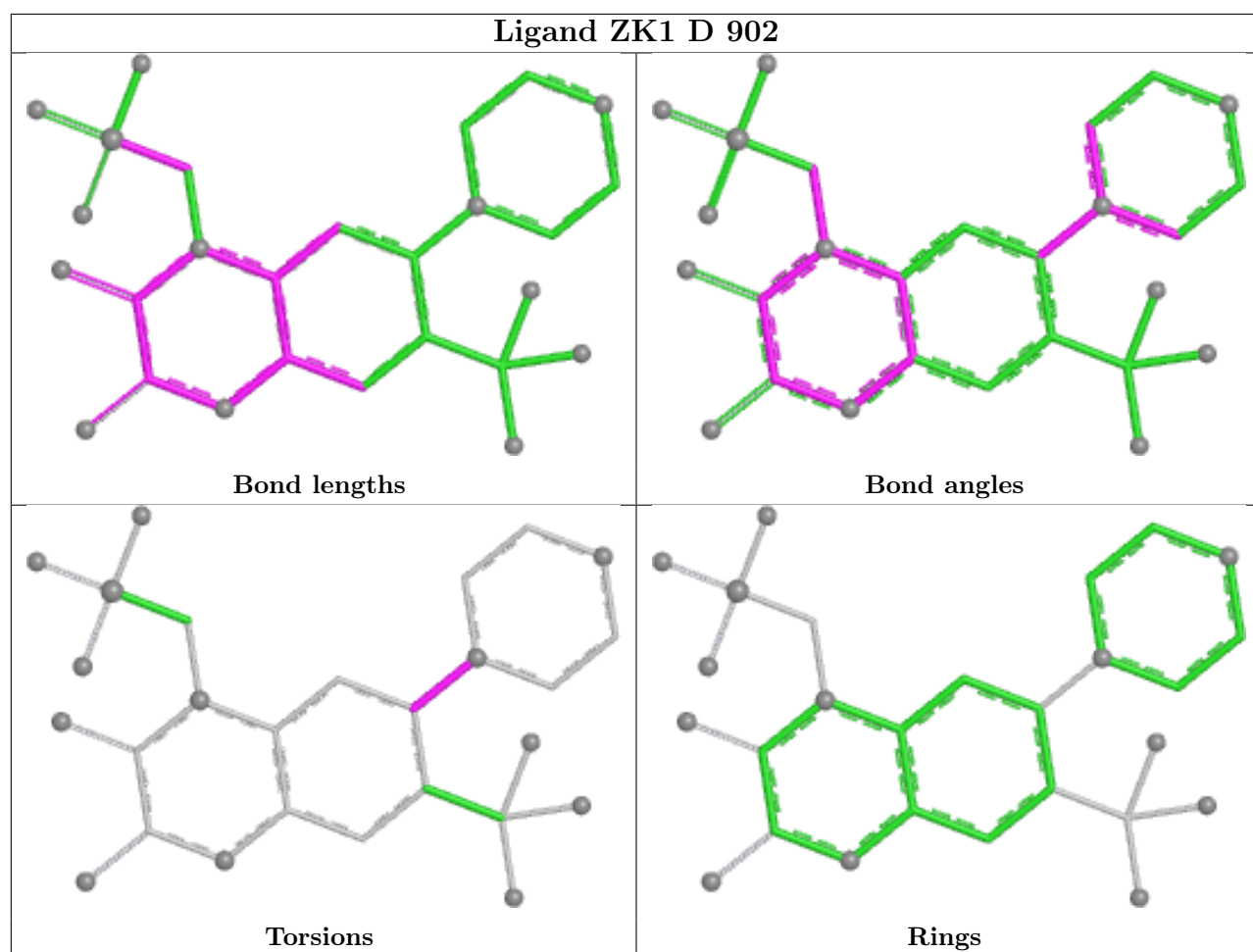
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

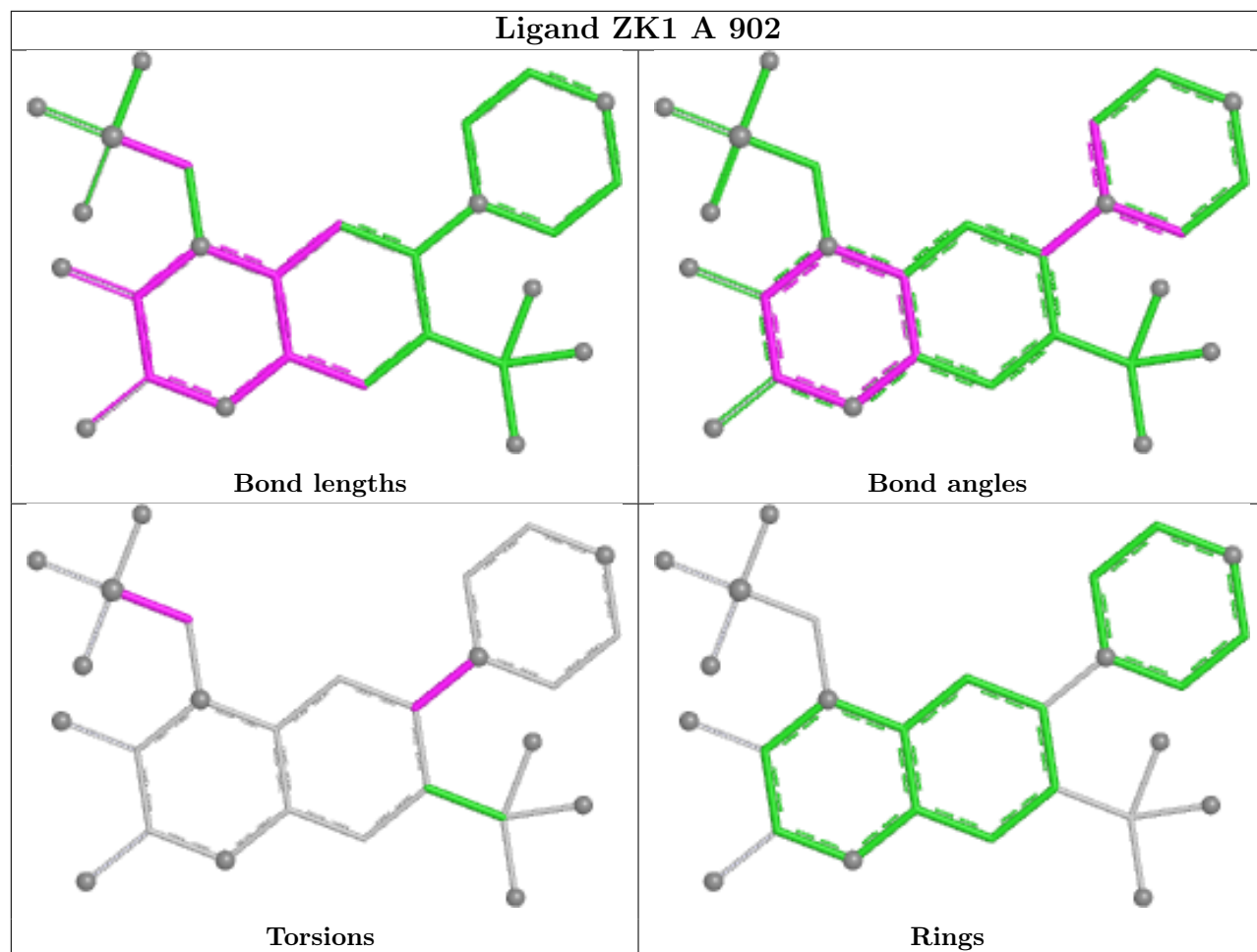
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

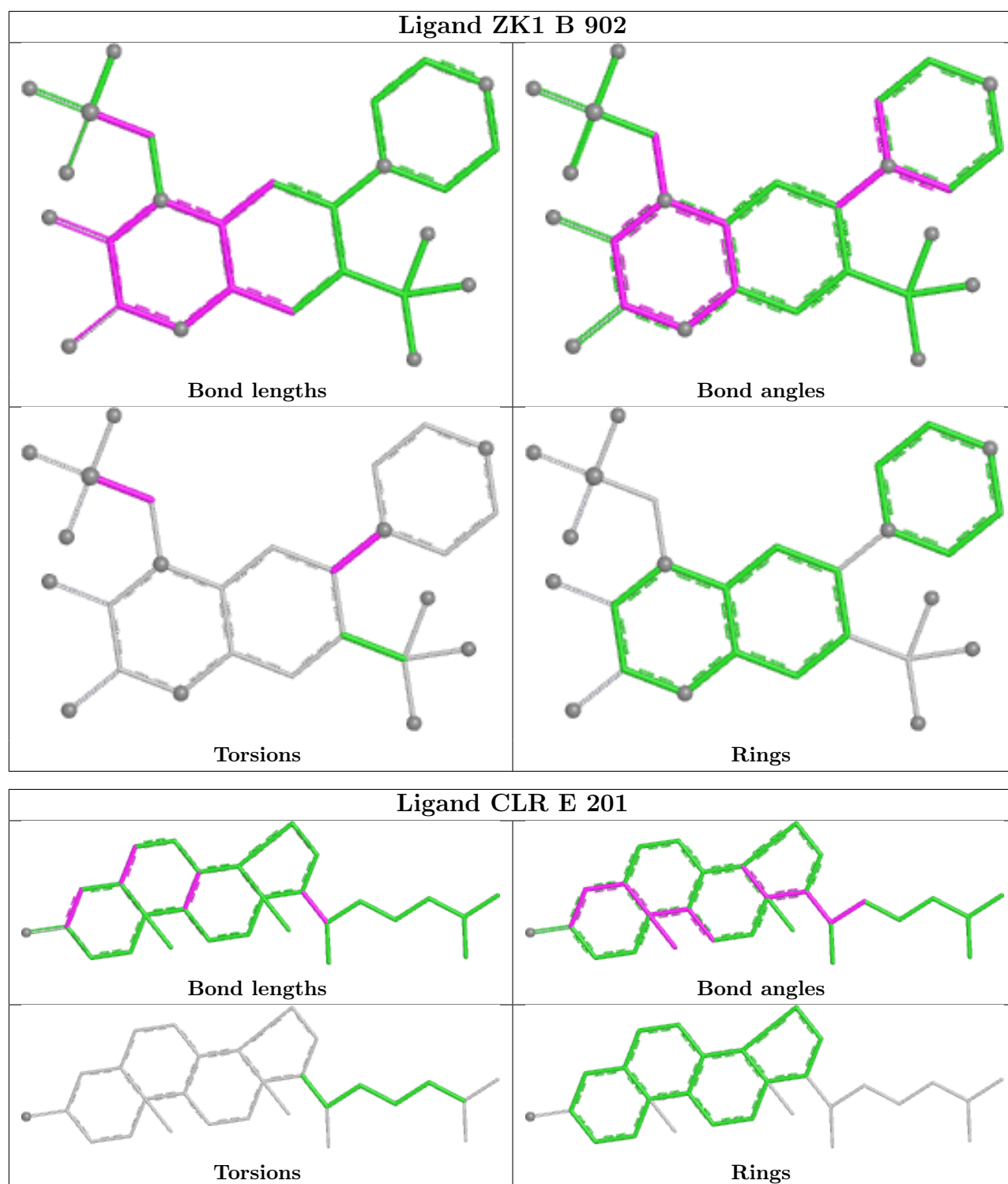












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

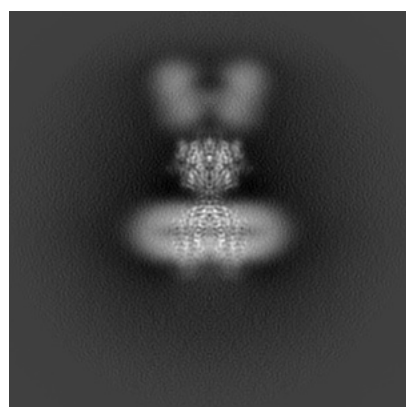
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20734. These allow visual inspection of the internal detail of the map and identification of artifacts.

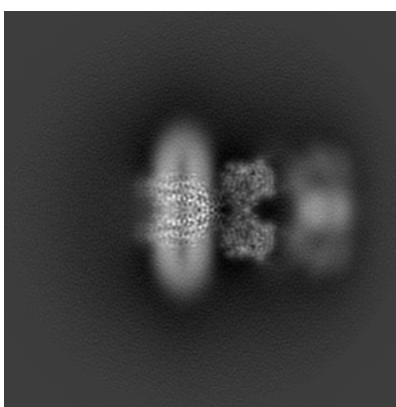
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

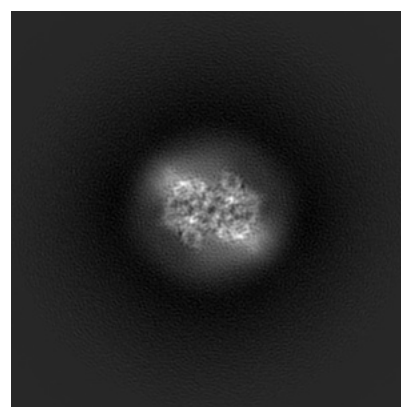
6.1.1 Primary map



X



Y

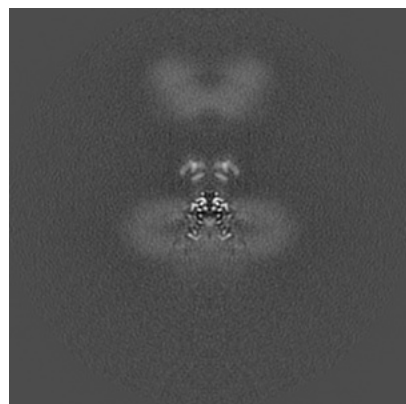


Z

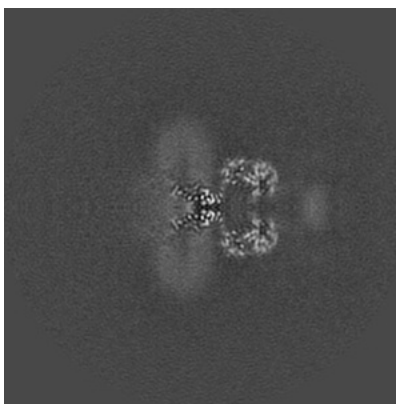
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

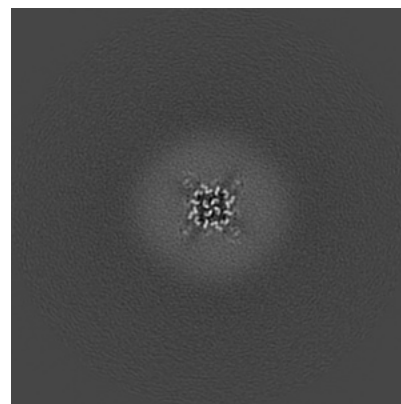
6.2.1 Primary map



X Index: 180



Y Index: 180

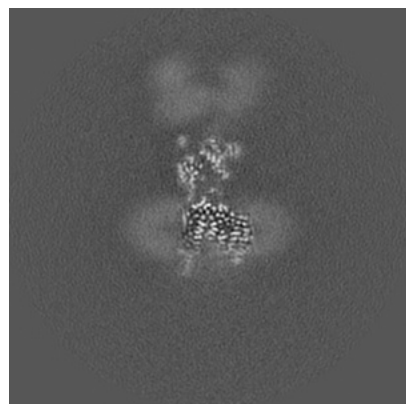


Z Index: 180

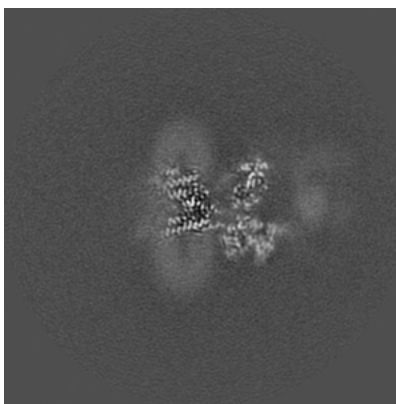
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

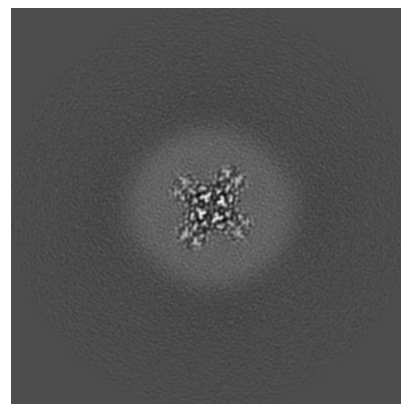
6.3.1 Primary map



X Index: 193



Y Index: 170

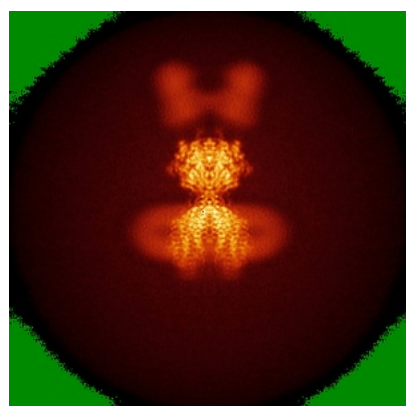


Z Index: 170

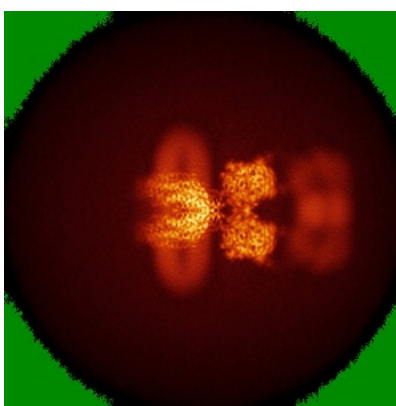
The images above show the largest variance slices of the map in three orthogonal directions.

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

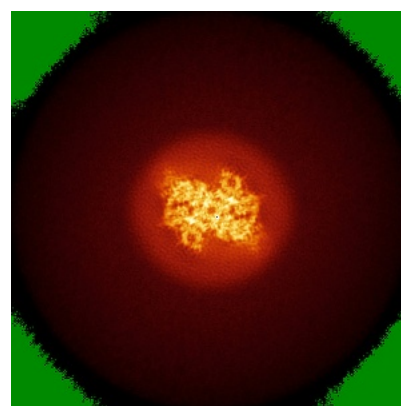
6.4.1 Primary map



X



Y



Z

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 0.0218. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

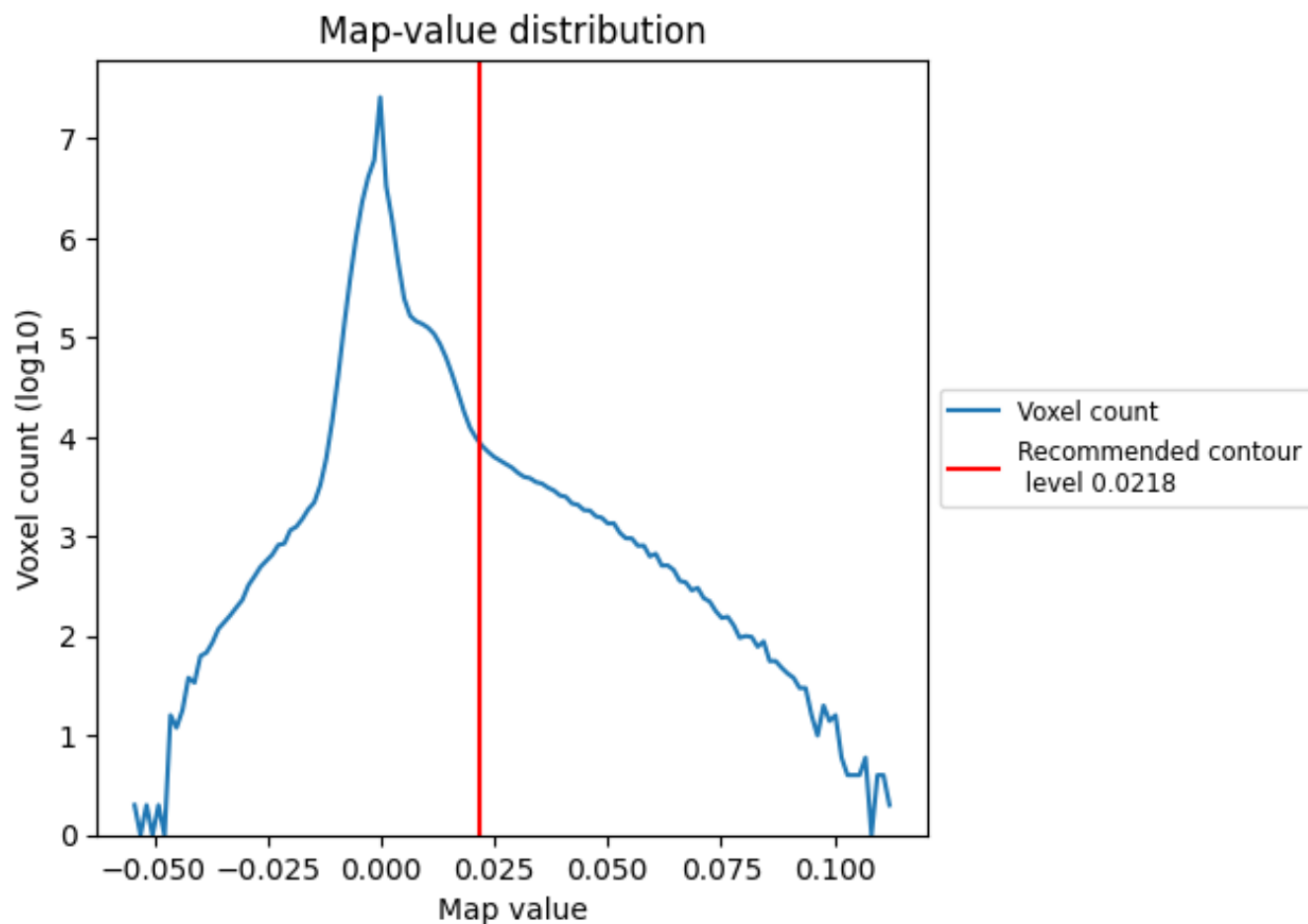
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

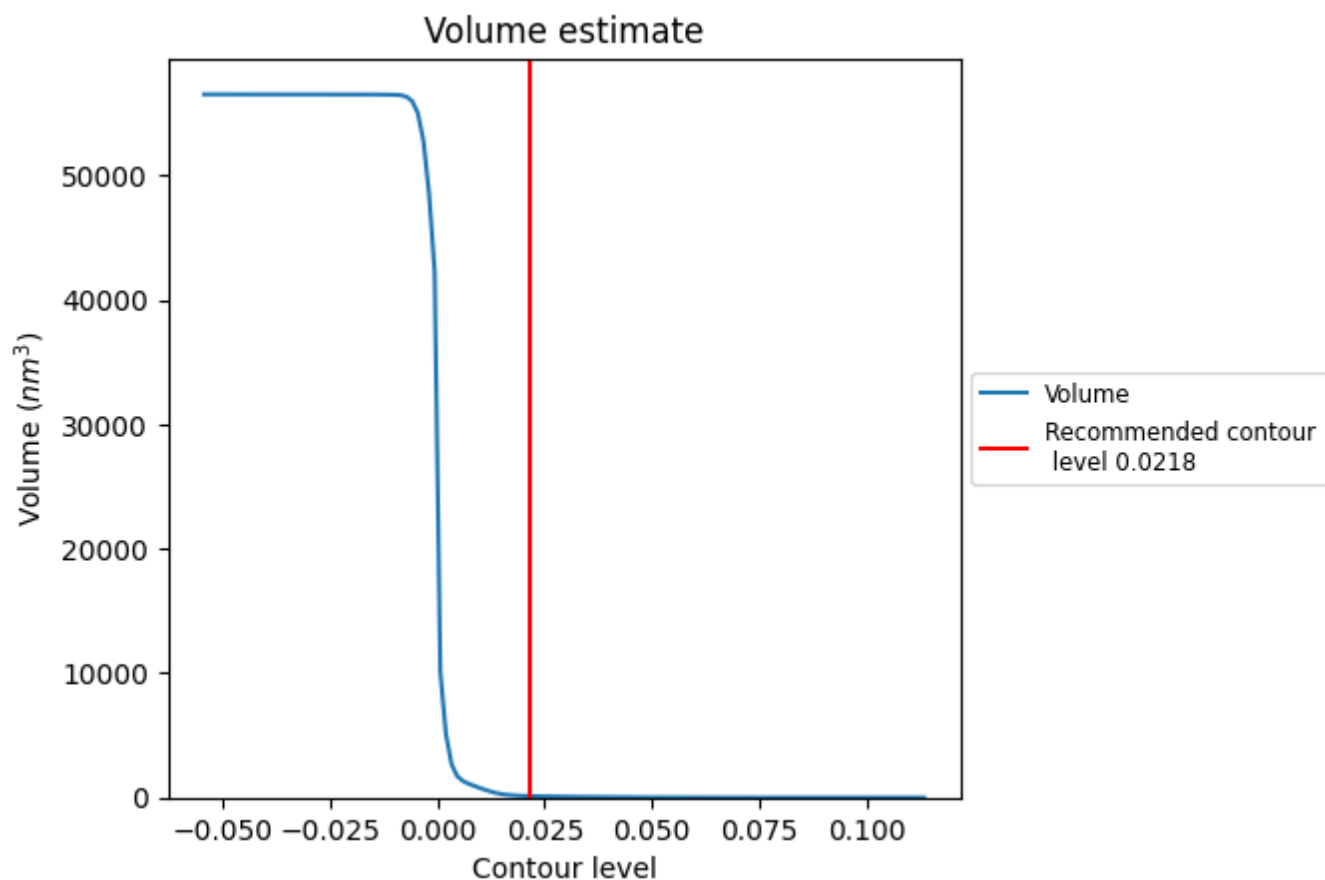
This section contains the results of statistical analysis of the map.

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.

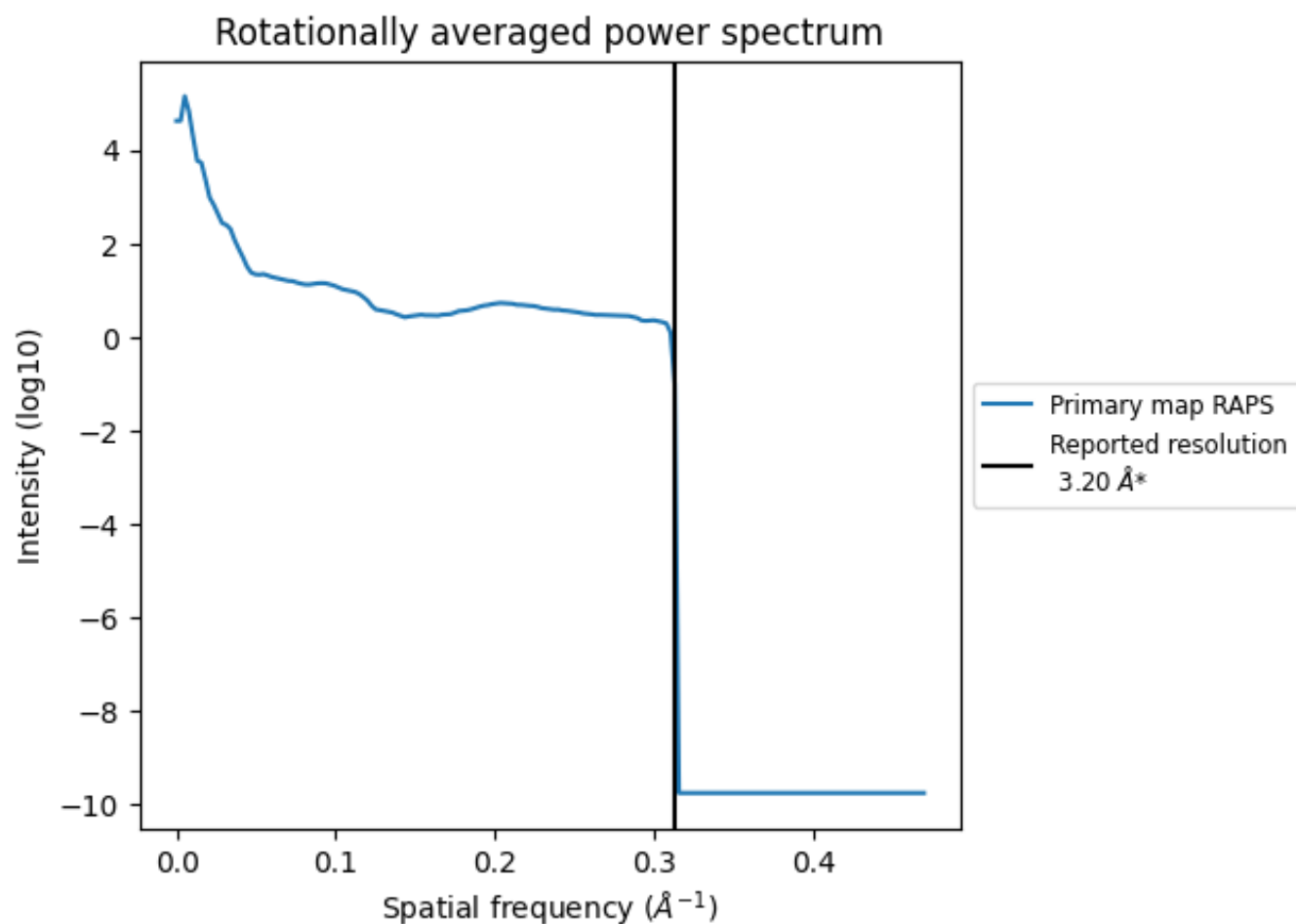
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 116 nm³; this corresponds to an approximate mass of 105 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

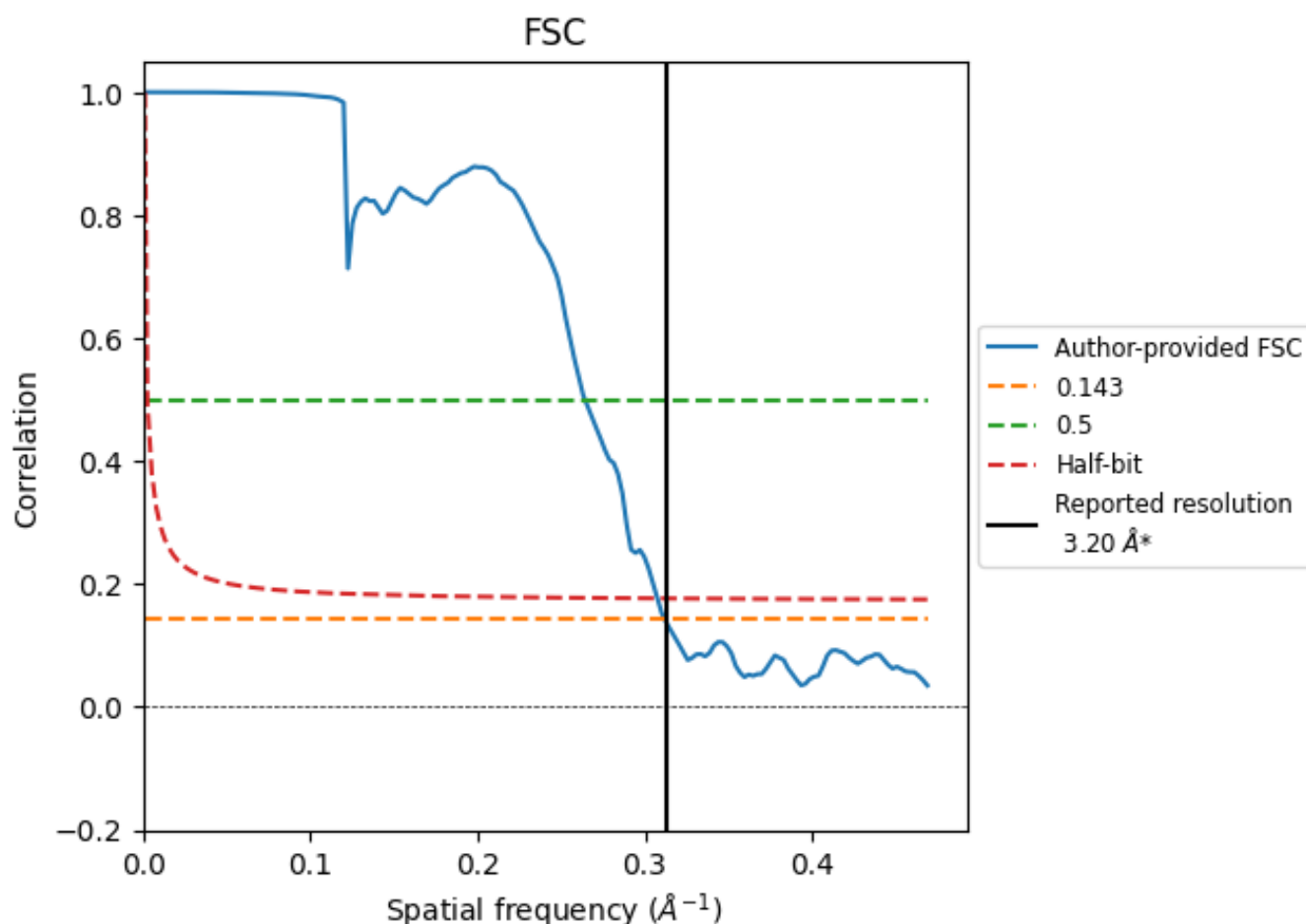


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

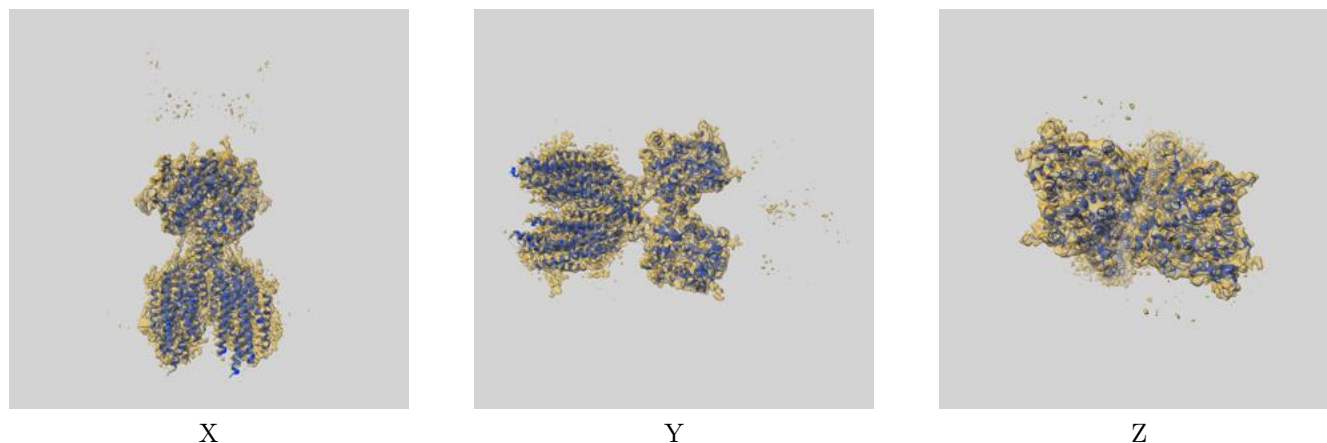
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	3.79	3.25
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

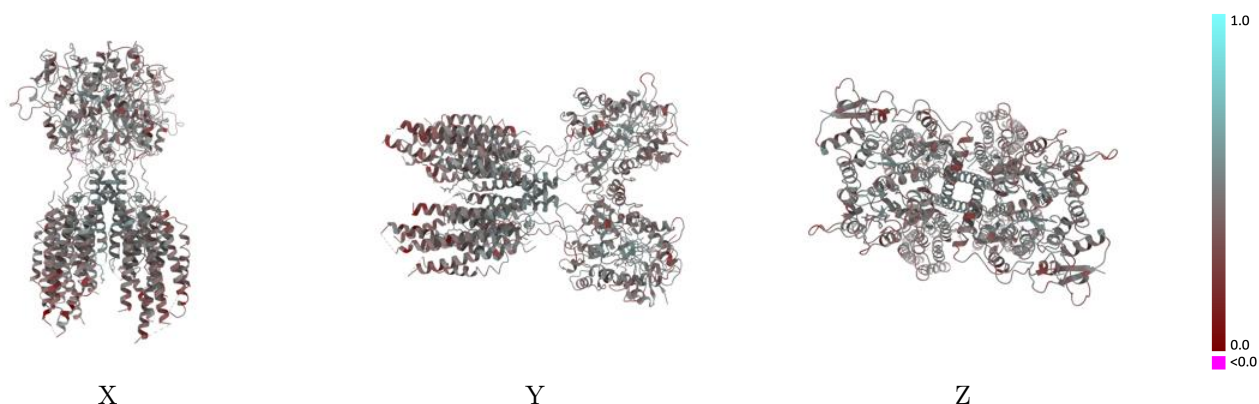
This section contains information regarding the fit between EMDB map EMD-20734 and PDB model 6UD8. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



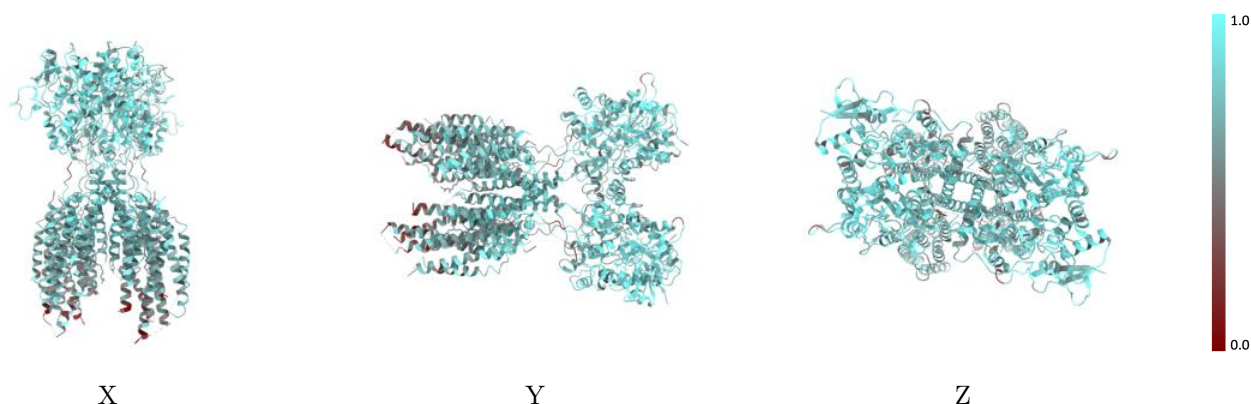
The images above show the 3D surface view of the map at the recommended contour level 0.0218 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



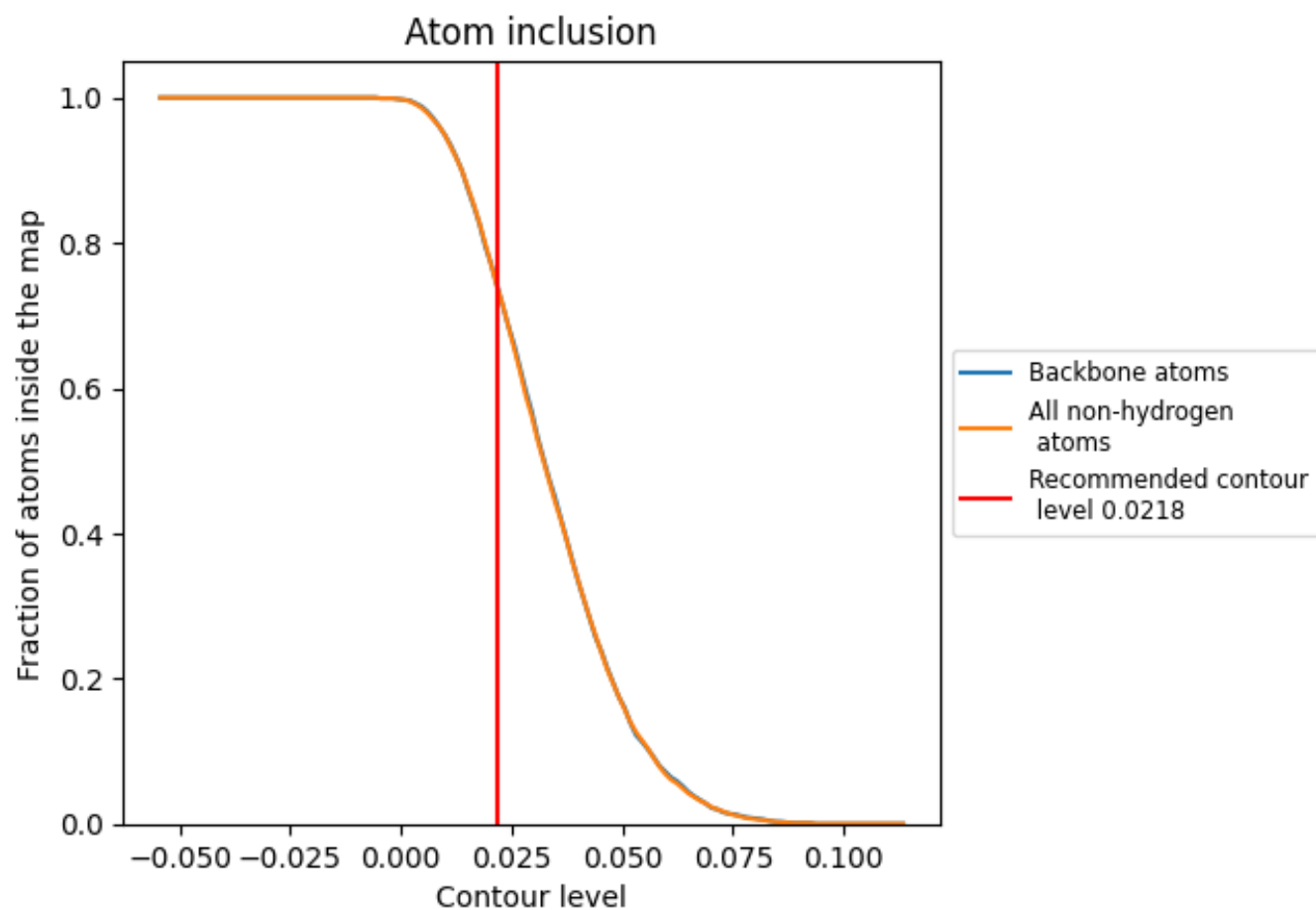
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0218).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 74% 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 (0.0218) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7390	0.4360
A	0.7820	0.4510
B	0.7800	0.4490
C	0.7810	0.4530
D	0.7780	0.4460
E	0.6540	0.3960
F	0.6610	0.4010
G	0.6450	0.4010
H	0.6690	0.4040

