



Full wwPDB EM Validation Report ⓘ

Jun 10, 2024 – 04:03 PM EDT

PDB ID : 8SYG
EMDB ID : EMD-40873
Title : Cryo-EM structure of tetradecameric hub domain of CaMKII alpha
Authors : Chien, C.-T.; Chiu, W.; Khan, S.
Deposited on : 2023-05-25
Resolution : 2.60 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

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.dev92
MolProbity : 4.02b-467
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) : 2.36.2

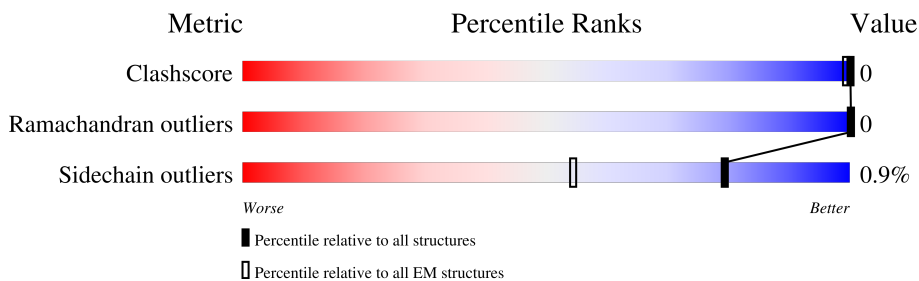
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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	407	31% 67%
1	B	407	31% 67%
1	C	407	31% 67%
1	D	407	31% 67%
1	E	407	31% 67%
1	F	407	31% 67%
1	G	407	31% 67%
1	H	407	31% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	407	 31% 67%
1	J	407	 31% 67%
1	K	407	 31% 67%
1	L	407	 31% 67%
1	M	407	 31% 67%
1	N	407	 31% 67%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 29932 atoms, of which 14714 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 Venus-tagged CaMKII Alpha Association Domain.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	B	134	2138	688	1051	195	199	5	0	0
1	A	134	2138	688	1051	195	199	5	0	0
1	C	134	2138	688	1051	195	199	5	0	0
1	D	134	2138	688	1051	195	199	5	0	0
1	E	134	2138	688	1051	195	199	5	0	0
1	F	134	2138	688	1051	195	199	5	0	0
1	G	134	2138	688	1051	195	199	5	0	0
1	H	134	2138	688	1051	195	199	5	0	0
1	I	134	2138	688	1051	195	199	5	0	0
1	J	134	2138	688	1051	195	199	5	0	0
1	K	134	2138	688	1051	195	199	5	0	0
1	L	134	2138	688	1051	195	199	5	0	0
1	M	134	2138	688	1051	195	199	5	0	0
1	N	134	2138	688	1051	195	199	5	0	0

There are 658 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	72	MET	-	initiating methionine	UNP P42212
B	73	GLY	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	74	SER	-	expression tag	UNP P42212
B	75	SER	-	expression tag	UNP P42212
B	76	HIS	-	expression tag	UNP P42212
B	77	HIS	-	expression tag	UNP P42212
B	78	HIS	-	expression tag	UNP P42212
B	79	HIS	-	expression tag	UNP P42212
B	80	HIS	-	expression tag	UNP P42212
B	81	HIS	-	expression tag	UNP P42212
B	82	SER	-	expression tag	UNP P42212
B	83	SER	-	expression tag	UNP P42212
B	84	GLY	-	expression tag	UNP P42212
B	85	LEU	-	expression tag	UNP P42212
B	86	VAL	-	expression tag	UNP P42212
B	87	PRO	-	expression tag	UNP P42212
B	88	ARG	-	expression tag	UNP P42212
B	89	GLY	-	expression tag	UNP P42212
B	90	SER	-	expression tag	UNP P42212
B	91	HIS	-	expression tag	UNP P42212
B	92	VAL	-	expression tag	UNP P42212
B	137	LEU	PHE	conflict	UNP P42212
B	155	LEU	PHE	conflict	UNP P42212
B	156	GLY	SER	conflict	UNP P42212
B	159	LEU	VAL	conflict	UNP P42212
B	163	ALA	SER	conflict	UNP P42212
B	244	THR	MET	conflict	UNP P42212
B	254	ALA	VAL	conflict	UNP P42212
B	266	GLY	SER	conflict	UNP P42212
B	294	TYR	THR	conflict	UNP P42212
B	297	LYS	ALA	conflict	UNP P42212
B	322	LEU	HIS	conflict	UNP P42212
B	330	SER	-	linker	UNP P42212
B	331	GLY	-	linker	UNP P42212
B	332	LEU	-	linker	UNP P42212
B	333	ARG	-	linker	UNP P42212
B	334	SER	-	linker	UNP P42212
B	335	ARG	-	linker	UNP P42212
B	336	ALA	-	linker	UNP P42212
B	337	GLN	-	linker	UNP P42212
B	338	ALA	-	linker	UNP P42212
B	339	SER	-	linker	UNP P42212
B	340	ASN	-	linker	UNP P42212
B	341	SER	-	linker	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	342	ALA	-	linker	UNP P42212
B	343	VAL	-	linker	UNP P42212
B	344	ASP	-	linker	UNP P42212
A	72	MET	-	initiating methionine	UNP P42212
A	73	GLY	-	expression tag	UNP P42212
A	74	SER	-	expression tag	UNP P42212
A	75	SER	-	expression tag	UNP P42212
A	76	HIS	-	expression tag	UNP P42212
A	77	HIS	-	expression tag	UNP P42212
A	78	HIS	-	expression tag	UNP P42212
A	79	HIS	-	expression tag	UNP P42212
A	80	HIS	-	expression tag	UNP P42212
A	81	HIS	-	expression tag	UNP P42212
A	82	SER	-	expression tag	UNP P42212
A	83	SER	-	expression tag	UNP P42212
A	84	GLY	-	expression tag	UNP P42212
A	85	LEU	-	expression tag	UNP P42212
A	86	VAL	-	expression tag	UNP P42212
A	87	PRO	-	expression tag	UNP P42212
A	88	ARG	-	expression tag	UNP P42212
A	89	GLY	-	expression tag	UNP P42212
A	90	SER	-	expression tag	UNP P42212
A	91	HIS	-	expression tag	UNP P42212
A	92	VAL	-	expression tag	UNP P42212
A	137	LEU	PHE	conflict	UNP P42212
A	155	LEU	PHE	conflict	UNP P42212
A	156	GLY	SER	conflict	UNP P42212
A	159	LEU	VAL	conflict	UNP P42212
A	163	ALA	SER	conflict	UNP P42212
A	244	THR	MET	conflict	UNP P42212
A	254	ALA	VAL	conflict	UNP P42212
A	266	GLY	SER	conflict	UNP P42212
A	294	TYR	THR	conflict	UNP P42212
A	297	LYS	ALA	conflict	UNP P42212
A	322	LEU	HIS	conflict	UNP P42212
A	330	SER	-	linker	UNP P42212
A	331	GLY	-	linker	UNP P42212
A	332	LEU	-	linker	UNP P42212
A	333	ARG	-	linker	UNP P42212
A	334	SER	-	linker	UNP P42212
A	335	ARG	-	linker	UNP P42212
A	336	ALA	-	linker	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	GLN	-	linker	UNP P42212
A	338	ALA	-	linker	UNP P42212
A	339	SER	-	linker	UNP P42212
A	340	ASN	-	linker	UNP P42212
A	341	SER	-	linker	UNP P42212
A	342	ALA	-	linker	UNP P42212
A	343	VAL	-	linker	UNP P42212
A	344	ASP	-	linker	UNP P42212
C	72	MET	-	initiating methionine	UNP P42212
C	73	GLY	-	expression tag	UNP P42212
C	74	SER	-	expression tag	UNP P42212
C	75	SER	-	expression tag	UNP P42212
C	76	HIS	-	expression tag	UNP P42212
C	77	HIS	-	expression tag	UNP P42212
C	78	HIS	-	expression tag	UNP P42212
C	79	HIS	-	expression tag	UNP P42212
C	80	HIS	-	expression tag	UNP P42212
C	81	HIS	-	expression tag	UNP P42212
C	82	SER	-	expression tag	UNP P42212
C	83	SER	-	expression tag	UNP P42212
C	84	GLY	-	expression tag	UNP P42212
C	85	LEU	-	expression tag	UNP P42212
C	86	VAL	-	expression tag	UNP P42212
C	87	PRO	-	expression tag	UNP P42212
C	88	ARG	-	expression tag	UNP P42212
C	89	GLY	-	expression tag	UNP P42212
C	90	SER	-	expression tag	UNP P42212
C	91	HIS	-	expression tag	UNP P42212
C	92	VAL	-	expression tag	UNP P42212
C	137	LEU	PHE	conflict	UNP P42212
C	155	LEU	PHE	conflict	UNP P42212
C	156	GLY	SER	conflict	UNP P42212
C	159	LEU	VAL	conflict	UNP P42212
C	163	ALA	SER	conflict	UNP P42212
C	244	THR	MET	conflict	UNP P42212
C	254	ALA	VAL	conflict	UNP P42212
C	266	GLY	SER	conflict	UNP P42212
C	294	TYR	THR	conflict	UNP P42212
C	297	LYS	ALA	conflict	UNP P42212
C	322	LEU	HIS	conflict	UNP P42212
C	330	SER	-	linker	UNP P42212
C	331	GLY	-	linker	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	332	LEU	-	linker	UNP P42212
C	333	ARG	-	linker	UNP P42212
C	334	SER	-	linker	UNP P42212
C	335	ARG	-	linker	UNP P42212
C	336	ALA	-	linker	UNP P42212
C	337	GLN	-	linker	UNP P42212
C	338	ALA	-	linker	UNP P42212
C	339	SER	-	linker	UNP P42212
C	340	ASN	-	linker	UNP P42212
C	341	SER	-	linker	UNP P42212
C	342	ALA	-	linker	UNP P42212
C	343	VAL	-	linker	UNP P42212
C	344	ASP	-	linker	UNP P42212
D	72	MET	-	initiating methionine	UNP P42212
D	73	GLY	-	expression tag	UNP P42212
D	74	SER	-	expression tag	UNP P42212
D	75	SER	-	expression tag	UNP P42212
D	76	HIS	-	expression tag	UNP P42212
D	77	HIS	-	expression tag	UNP P42212
D	78	HIS	-	expression tag	UNP P42212
D	79	HIS	-	expression tag	UNP P42212
D	80	HIS	-	expression tag	UNP P42212
D	81	HIS	-	expression tag	UNP P42212
D	82	SER	-	expression tag	UNP P42212
D	83	SER	-	expression tag	UNP P42212
D	84	GLY	-	expression tag	UNP P42212
D	85	LEU	-	expression tag	UNP P42212
D	86	VAL	-	expression tag	UNP P42212
D	87	PRO	-	expression tag	UNP P42212
D	88	ARG	-	expression tag	UNP P42212
D	89	GLY	-	expression tag	UNP P42212
D	90	SER	-	expression tag	UNP P42212
D	91	HIS	-	expression tag	UNP P42212
D	92	VAL	-	expression tag	UNP P42212
D	137	LEU	PHE	conflict	UNP P42212
D	155	LEU	PHE	conflict	UNP P42212
D	156	GLY	SER	conflict	UNP P42212
D	159	LEU	VAL	conflict	UNP P42212
D	163	ALA	SER	conflict	UNP P42212
D	244	THR	MET	conflict	UNP P42212
D	254	ALA	VAL	conflict	UNP P42212
D	266	GLY	SER	conflict	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	294	TYR	THR	conflict	UNP P42212
D	297	LYS	ALA	conflict	UNP P42212
D	322	LEU	HIS	conflict	UNP P42212
D	330	SER	-	linker	UNP P42212
D	331	GLY	-	linker	UNP P42212
D	332	LEU	-	linker	UNP P42212
D	333	ARG	-	linker	UNP P42212
D	334	SER	-	linker	UNP P42212
D	335	ARG	-	linker	UNP P42212
D	336	ALA	-	linker	UNP P42212
D	337	GLN	-	linker	UNP P42212
D	338	ALA	-	linker	UNP P42212
D	339	SER	-	linker	UNP P42212
D	340	ASN	-	linker	UNP P42212
D	341	SER	-	linker	UNP P42212
D	342	ALA	-	linker	UNP P42212
D	343	VAL	-	linker	UNP P42212
D	344	ASP	-	linker	UNP P42212
E	72	MET	-	initiating methionine	UNP P42212
E	73	GLY	-	expression tag	UNP P42212
E	74	SER	-	expression tag	UNP P42212
E	75	SER	-	expression tag	UNP P42212
E	76	HIS	-	expression tag	UNP P42212
E	77	HIS	-	expression tag	UNP P42212
E	78	HIS	-	expression tag	UNP P42212
E	79	HIS	-	expression tag	UNP P42212
E	80	HIS	-	expression tag	UNP P42212
E	81	HIS	-	expression tag	UNP P42212
E	82	SER	-	expression tag	UNP P42212
E	83	SER	-	expression tag	UNP P42212
E	84	GLY	-	expression tag	UNP P42212
E	85	LEU	-	expression tag	UNP P42212
E	86	VAL	-	expression tag	UNP P42212
E	87	PRO	-	expression tag	UNP P42212
E	88	ARG	-	expression tag	UNP P42212
E	89	GLY	-	expression tag	UNP P42212
E	90	SER	-	expression tag	UNP P42212
E	91	HIS	-	expression tag	UNP P42212
E	92	VAL	-	expression tag	UNP P42212
E	137	LEU	PHE	conflict	UNP P42212
E	155	LEU	PHE	conflict	UNP P42212
E	156	GLY	SER	conflict	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	159	LEU	VAL	conflict	UNP P42212
E	163	ALA	SER	conflict	UNP P42212
E	244	THR	MET	conflict	UNP P42212
E	254	ALA	VAL	conflict	UNP P42212
E	266	GLY	SER	conflict	UNP P42212
E	294	TYR	THR	conflict	UNP P42212
E	297	LYS	ALA	conflict	UNP P42212
E	322	LEU	HIS	conflict	UNP P42212
E	330	SER	-	linker	UNP P42212
E	331	GLY	-	linker	UNP P42212
E	332	LEU	-	linker	UNP P42212
E	333	ARG	-	linker	UNP P42212
E	334	SER	-	linker	UNP P42212
E	335	ARG	-	linker	UNP P42212
E	336	ALA	-	linker	UNP P42212
E	337	GLN	-	linker	UNP P42212
E	338	ALA	-	linker	UNP P42212
E	339	SER	-	linker	UNP P42212
E	340	ASN	-	linker	UNP P42212
E	341	SER	-	linker	UNP P42212
E	342	ALA	-	linker	UNP P42212
E	343	VAL	-	linker	UNP P42212
E	344	ASP	-	linker	UNP P42212
F	72	MET	-	initiating methionine	UNP P42212
F	73	GLY	-	expression tag	UNP P42212
F	74	SER	-	expression tag	UNP P42212
F	75	SER	-	expression tag	UNP P42212
F	76	HIS	-	expression tag	UNP P42212
F	77	HIS	-	expression tag	UNP P42212
F	78	HIS	-	expression tag	UNP P42212
F	79	HIS	-	expression tag	UNP P42212
F	80	HIS	-	expression tag	UNP P42212
F	81	HIS	-	expression tag	UNP P42212
F	82	SER	-	expression tag	UNP P42212
F	83	SER	-	expression tag	UNP P42212
F	84	GLY	-	expression tag	UNP P42212
F	85	LEU	-	expression tag	UNP P42212
F	86	VAL	-	expression tag	UNP P42212
F	87	PRO	-	expression tag	UNP P42212
F	88	ARG	-	expression tag	UNP P42212
F	89	GLY	-	expression tag	UNP P42212
F	90	SER	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	91	HIS	-	expression tag	UNP P42212
F	92	VAL	-	expression tag	UNP P42212
F	137	LEU	PHE	conflict	UNP P42212
F	155	LEU	PHE	conflict	UNP P42212
F	156	GLY	SER	conflict	UNP P42212
F	159	LEU	VAL	conflict	UNP P42212
F	163	ALA	SER	conflict	UNP P42212
F	244	THR	MET	conflict	UNP P42212
F	254	ALA	VAL	conflict	UNP P42212
F	266	GLY	SER	conflict	UNP P42212
F	294	TYR	THR	conflict	UNP P42212
F	297	LYS	ALA	conflict	UNP P42212
F	322	LEU	HIS	conflict	UNP P42212
F	330	SER	-	linker	UNP P42212
F	331	GLY	-	linker	UNP P42212
F	332	LEU	-	linker	UNP P42212
F	333	ARG	-	linker	UNP P42212
F	334	SER	-	linker	UNP P42212
F	335	ARG	-	linker	UNP P42212
F	336	ALA	-	linker	UNP P42212
F	337	GLN	-	linker	UNP P42212
F	338	ALA	-	linker	UNP P42212
F	339	SER	-	linker	UNP P42212
F	340	ASN	-	linker	UNP P42212
F	341	SER	-	linker	UNP P42212
F	342	ALA	-	linker	UNP P42212
F	343	VAL	-	linker	UNP P42212
F	344	ASP	-	linker	UNP P42212
G	72	MET	-	initiating methionine	UNP P42212
G	73	GLY	-	expression tag	UNP P42212
G	74	SER	-	expression tag	UNP P42212
G	75	SER	-	expression tag	UNP P42212
G	76	HIS	-	expression tag	UNP P42212
G	77	HIS	-	expression tag	UNP P42212
G	78	HIS	-	expression tag	UNP P42212
G	79	HIS	-	expression tag	UNP P42212
G	80	HIS	-	expression tag	UNP P42212
G	81	HIS	-	expression tag	UNP P42212
G	82	SER	-	expression tag	UNP P42212
G	83	SER	-	expression tag	UNP P42212
G	84	GLY	-	expression tag	UNP P42212
G	85	LEU	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	86	VAL	-	expression tag	UNP P42212
G	87	PRO	-	expression tag	UNP P42212
G	88	ARG	-	expression tag	UNP P42212
G	89	GLY	-	expression tag	UNP P42212
G	90	SER	-	expression tag	UNP P42212
G	91	HIS	-	expression tag	UNP P42212
G	92	VAL	-	expression tag	UNP P42212
G	137	LEU	PHE	conflict	UNP P42212
G	155	LEU	PHE	conflict	UNP P42212
G	156	GLY	SER	conflict	UNP P42212
G	159	LEU	VAL	conflict	UNP P42212
G	163	ALA	SER	conflict	UNP P42212
G	244	THR	MET	conflict	UNP P42212
G	254	ALA	VAL	conflict	UNP P42212
G	266	GLY	SER	conflict	UNP P42212
G	294	TYR	THR	conflict	UNP P42212
G	297	LYS	ALA	conflict	UNP P42212
G	322	LEU	HIS	conflict	UNP P42212
G	330	SER	-	linker	UNP P42212
G	331	GLY	-	linker	UNP P42212
G	332	LEU	-	linker	UNP P42212
G	333	ARG	-	linker	UNP P42212
G	334	SER	-	linker	UNP P42212
G	335	ARG	-	linker	UNP P42212
G	336	ALA	-	linker	UNP P42212
G	337	GLN	-	linker	UNP P42212
G	338	ALA	-	linker	UNP P42212
G	339	SER	-	linker	UNP P42212
G	340	ASN	-	linker	UNP P42212
G	341	SER	-	linker	UNP P42212
G	342	ALA	-	linker	UNP P42212
G	343	VAL	-	linker	UNP P42212
G	344	ASP	-	linker	UNP P42212
H	72	MET	-	initiating methionine	UNP P42212
H	73	GLY	-	expression tag	UNP P42212
H	74	SER	-	expression tag	UNP P42212
H	75	SER	-	expression tag	UNP P42212
H	76	HIS	-	expression tag	UNP P42212
H	77	HIS	-	expression tag	UNP P42212
H	78	HIS	-	expression tag	UNP P42212
H	79	HIS	-	expression tag	UNP P42212
H	80	HIS	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	81	HIS	-	expression tag	UNP P42212
H	82	SER	-	expression tag	UNP P42212
H	83	SER	-	expression tag	UNP P42212
H	84	GLY	-	expression tag	UNP P42212
H	85	LEU	-	expression tag	UNP P42212
H	86	VAL	-	expression tag	UNP P42212
H	87	PRO	-	expression tag	UNP P42212
H	88	ARG	-	expression tag	UNP P42212
H	89	GLY	-	expression tag	UNP P42212
H	90	SER	-	expression tag	UNP P42212
H	91	HIS	-	expression tag	UNP P42212
H	92	VAL	-	expression tag	UNP P42212
H	137	LEU	PHE	conflict	UNP P42212
H	155	LEU	PHE	conflict	UNP P42212
H	156	GLY	SER	conflict	UNP P42212
H	159	LEU	VAL	conflict	UNP P42212
H	163	ALA	SER	conflict	UNP P42212
H	244	THR	MET	conflict	UNP P42212
H	254	ALA	VAL	conflict	UNP P42212
H	266	GLY	SER	conflict	UNP P42212
H	294	TYR	THR	conflict	UNP P42212
H	297	LYS	ALA	conflict	UNP P42212
H	322	LEU	HIS	conflict	UNP P42212
H	330	SER	-	linker	UNP P42212
H	331	GLY	-	linker	UNP P42212
H	332	LEU	-	linker	UNP P42212
H	333	ARG	-	linker	UNP P42212
H	334	SER	-	linker	UNP P42212
H	335	ARG	-	linker	UNP P42212
H	336	ALA	-	linker	UNP P42212
H	337	GLN	-	linker	UNP P42212
H	338	ALA	-	linker	UNP P42212
H	339	SER	-	linker	UNP P42212
H	340	ASN	-	linker	UNP P42212
H	341	SER	-	linker	UNP P42212
H	342	ALA	-	linker	UNP P42212
H	343	VAL	-	linker	UNP P42212
H	344	ASP	-	linker	UNP P42212
I	72	MET	-	initiating methionine	UNP P42212
I	73	GLY	-	expression tag	UNP P42212
I	74	SER	-	expression tag	UNP P42212
I	75	SER	-	expression tag	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	76	HIS	-	expression tag	UNP P42212
I	77	HIS	-	expression tag	UNP P42212
I	78	HIS	-	expression tag	UNP P42212
I	79	HIS	-	expression tag	UNP P42212
I	80	HIS	-	expression tag	UNP P42212
I	81	HIS	-	expression tag	UNP P42212
I	82	SER	-	expression tag	UNP P42212
I	83	SER	-	expression tag	UNP P42212
I	84	GLY	-	expression tag	UNP P42212
I	85	LEU	-	expression tag	UNP P42212
I	86	VAL	-	expression tag	UNP P42212
I	87	PRO	-	expression tag	UNP P42212
I	88	ARG	-	expression tag	UNP P42212
I	89	GLY	-	expression tag	UNP P42212
I	90	SER	-	expression tag	UNP P42212
I	91	HIS	-	expression tag	UNP P42212
I	92	VAL	-	expression tag	UNP P42212
I	137	LEU	PHE	conflict	UNP P42212
I	155	LEU	PHE	conflict	UNP P42212
I	156	GLY	SER	conflict	UNP P42212
I	159	LEU	VAL	conflict	UNP P42212
I	163	ALA	SER	conflict	UNP P42212
I	244	THR	MET	conflict	UNP P42212
I	254	ALA	VAL	conflict	UNP P42212
I	266	GLY	SER	conflict	UNP P42212
I	294	TYR	THR	conflict	UNP P42212
I	297	LYS	ALA	conflict	UNP P42212
I	322	LEU	HIS	conflict	UNP P42212
I	330	SER	-	linker	UNP P42212
I	331	GLY	-	linker	UNP P42212
I	332	LEU	-	linker	UNP P42212
I	333	ARG	-	linker	UNP P42212
I	334	SER	-	linker	UNP P42212
I	335	ARG	-	linker	UNP P42212
I	336	ALA	-	linker	UNP P42212
I	337	GLN	-	linker	UNP P42212
I	338	ALA	-	linker	UNP P42212
I	339	SER	-	linker	UNP P42212
I	340	ASN	-	linker	UNP P42212
I	341	SER	-	linker	UNP P42212
I	342	ALA	-	linker	UNP P42212
I	343	VAL	-	linker	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	344	ASP	-	linker	UNP P42212
J	72	MET	-	initiating methionine	UNP P42212
J	73	GLY	-	expression tag	UNP P42212
J	74	SER	-	expression tag	UNP P42212
J	75	SER	-	expression tag	UNP P42212
J	76	HIS	-	expression tag	UNP P42212
J	77	HIS	-	expression tag	UNP P42212
J	78	HIS	-	expression tag	UNP P42212
J	79	HIS	-	expression tag	UNP P42212
J	80	HIS	-	expression tag	UNP P42212
J	81	HIS	-	expression tag	UNP P42212
J	82	SER	-	expression tag	UNP P42212
J	83	SER	-	expression tag	UNP P42212
J	84	GLY	-	expression tag	UNP P42212
J	85	LEU	-	expression tag	UNP P42212
J	86	VAL	-	expression tag	UNP P42212
J	87	PRO	-	expression tag	UNP P42212
J	88	ARG	-	expression tag	UNP P42212
J	89	GLY	-	expression tag	UNP P42212
J	90	SER	-	expression tag	UNP P42212
J	91	HIS	-	expression tag	UNP P42212
J	92	VAL	-	expression tag	UNP P42212
J	137	LEU	PHE	conflict	UNP P42212
J	155	LEU	PHE	conflict	UNP P42212
J	156	GLY	SER	conflict	UNP P42212
J	159	LEU	VAL	conflict	UNP P42212
J	163	ALA	SER	conflict	UNP P42212
J	244	THR	MET	conflict	UNP P42212
J	254	ALA	VAL	conflict	UNP P42212
J	266	GLY	SER	conflict	UNP P42212
J	294	TYR	THR	conflict	UNP P42212
J	297	LYS	ALA	conflict	UNP P42212
J	322	LEU	HIS	conflict	UNP P42212
J	330	SER	-	linker	UNP P42212
J	331	GLY	-	linker	UNP P42212
J	332	LEU	-	linker	UNP P42212
J	333	ARG	-	linker	UNP P42212
J	334	SER	-	linker	UNP P42212
J	335	ARG	-	linker	UNP P42212
J	336	ALA	-	linker	UNP P42212
J	337	GLN	-	linker	UNP P42212
J	338	ALA	-	linker	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	339	SER	-	linker	UNP P42212
J	340	ASN	-	linker	UNP P42212
J	341	SER	-	linker	UNP P42212
J	342	ALA	-	linker	UNP P42212
J	343	VAL	-	linker	UNP P42212
J	344	ASP	-	linker	UNP P42212
K	72	MET	-	initiating methionine	UNP P42212
K	73	GLY	-	expression tag	UNP P42212
K	74	SER	-	expression tag	UNP P42212
K	75	SER	-	expression tag	UNP P42212
K	76	HIS	-	expression tag	UNP P42212
K	77	HIS	-	expression tag	UNP P42212
K	78	HIS	-	expression tag	UNP P42212
K	79	HIS	-	expression tag	UNP P42212
K	80	HIS	-	expression tag	UNP P42212
K	81	HIS	-	expression tag	UNP P42212
K	82	SER	-	expression tag	UNP P42212
K	83	SER	-	expression tag	UNP P42212
K	84	GLY	-	expression tag	UNP P42212
K	85	LEU	-	expression tag	UNP P42212
K	86	VAL	-	expression tag	UNP P42212
K	87	PRO	-	expression tag	UNP P42212
K	88	ARG	-	expression tag	UNP P42212
K	89	GLY	-	expression tag	UNP P42212
K	90	SER	-	expression tag	UNP P42212
K	91	HIS	-	expression tag	UNP P42212
K	92	VAL	-	expression tag	UNP P42212
K	137	LEU	PHE	conflict	UNP P42212
K	155	LEU	PHE	conflict	UNP P42212
K	156	GLY	SER	conflict	UNP P42212
K	159	LEU	VAL	conflict	UNP P42212
K	163	ALA	SER	conflict	UNP P42212
K	244	THR	MET	conflict	UNP P42212
K	254	ALA	VAL	conflict	UNP P42212
K	266	GLY	SER	conflict	UNP P42212
K	294	TYR	THR	conflict	UNP P42212
K	297	LYS	ALA	conflict	UNP P42212
K	322	LEU	HIS	conflict	UNP P42212
K	330	SER	-	linker	UNP P42212
K	331	GLY	-	linker	UNP P42212
K	332	LEU	-	linker	UNP P42212
K	333	ARG	-	linker	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
K	334	SER	-	linker	UNP P42212
K	335	ARG	-	linker	UNP P42212
K	336	ALA	-	linker	UNP P42212
K	337	GLN	-	linker	UNP P42212
K	338	ALA	-	linker	UNP P42212
K	339	SER	-	linker	UNP P42212
K	340	ASN	-	linker	UNP P42212
K	341	SER	-	linker	UNP P42212
K	342	ALA	-	linker	UNP P42212
K	343	VAL	-	linker	UNP P42212
K	344	ASP	-	linker	UNP P42212
L	72	MET	-	initiating methionine	UNP P42212
L	73	GLY	-	expression tag	UNP P42212
L	74	SER	-	expression tag	UNP P42212
L	75	SER	-	expression tag	UNP P42212
L	76	HIS	-	expression tag	UNP P42212
L	77	HIS	-	expression tag	UNP P42212
L	78	HIS	-	expression tag	UNP P42212
L	79	HIS	-	expression tag	UNP P42212
L	80	HIS	-	expression tag	UNP P42212
L	81	HIS	-	expression tag	UNP P42212
L	82	SER	-	expression tag	UNP P42212
L	83	SER	-	expression tag	UNP P42212
L	84	GLY	-	expression tag	UNP P42212
L	85	LEU	-	expression tag	UNP P42212
L	86	VAL	-	expression tag	UNP P42212
L	87	PRO	-	expression tag	UNP P42212
L	88	ARG	-	expression tag	UNP P42212
L	89	GLY	-	expression tag	UNP P42212
L	90	SER	-	expression tag	UNP P42212
L	91	HIS	-	expression tag	UNP P42212
L	92	VAL	-	expression tag	UNP P42212
L	137	LEU	PHE	conflict	UNP P42212
L	155	LEU	PHE	conflict	UNP P42212
L	156	GLY	SER	conflict	UNP P42212
L	159	LEU	VAL	conflict	UNP P42212
L	163	ALA	SER	conflict	UNP P42212
L	244	THR	MET	conflict	UNP P42212
L	254	ALA	VAL	conflict	UNP P42212
L	266	GLY	SER	conflict	UNP P42212
L	294	TYR	THR	conflict	UNP P42212
L	297	LYS	ALA	conflict	UNP P42212

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	322	LEU	HIS	conflict	UNP P42212
L	330	SER	-	linker	UNP P42212
L	331	GLY	-	linker	UNP P42212
L	332	LEU	-	linker	UNP P42212
L	333	ARG	-	linker	UNP P42212
L	334	SER	-	linker	UNP P42212
L	335	ARG	-	linker	UNP P42212
L	336	ALA	-	linker	UNP P42212
L	337	GLN	-	linker	UNP P42212
L	338	ALA	-	linker	UNP P42212
L	339	SER	-	linker	UNP P42212
L	340	ASN	-	linker	UNP P42212
L	341	SER	-	linker	UNP P42212
L	342	ALA	-	linker	UNP P42212
L	343	VAL	-	linker	UNP P42212
L	344	ASP	-	linker	UNP P42212
M	72	MET	-	initiating methionine	UNP P42212
M	73	GLY	-	expression tag	UNP P42212
M	74	SER	-	expression tag	UNP P42212
M	75	SER	-	expression tag	UNP P42212
M	76	HIS	-	expression tag	UNP P42212
M	77	HIS	-	expression tag	UNP P42212
M	78	HIS	-	expression tag	UNP P42212
M	79	HIS	-	expression tag	UNP P42212
M	80	HIS	-	expression tag	UNP P42212
M	81	HIS	-	expression tag	UNP P42212
M	82	SER	-	expression tag	UNP P42212
M	83	SER	-	expression tag	UNP P42212
M	84	GLY	-	expression tag	UNP P42212
M	85	LEU	-	expression tag	UNP P42212
M	86	VAL	-	expression tag	UNP P42212
M	87	PRO	-	expression tag	UNP P42212
M	88	ARG	-	expression tag	UNP P42212
M	89	GLY	-	expression tag	UNP P42212
M	90	SER	-	expression tag	UNP P42212
M	91	HIS	-	expression tag	UNP P42212
M	92	VAL	-	expression tag	UNP P42212
M	137	LEU	PHE	conflict	UNP P42212
M	155	LEU	PHE	conflict	UNP P42212
M	156	GLY	SER	conflict	UNP P42212
M	159	LEU	VAL	conflict	UNP P42212
M	163	ALA	SER	conflict	UNP P42212

Continued on next page...

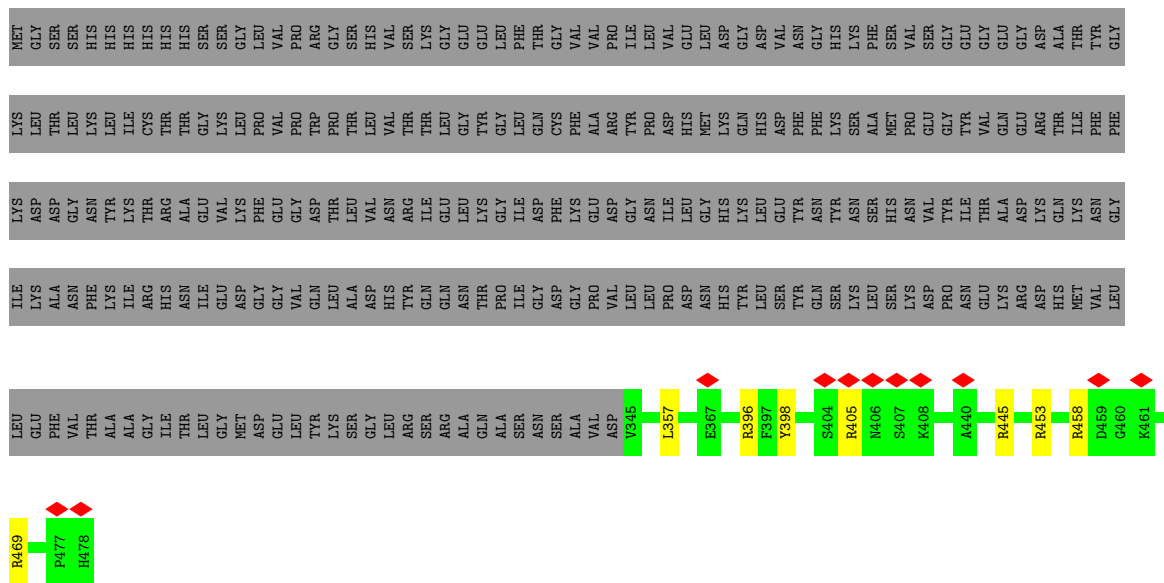
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	244	THR	MET	conflict	UNP P42212
M	254	ALA	VAL	conflict	UNP P42212
M	266	GLY	SER	conflict	UNP P42212
M	294	TYR	THR	conflict	UNP P42212
M	297	LYS	ALA	conflict	UNP P42212
M	322	LEU	HIS	conflict	UNP P42212
M	330	SER	-	linker	UNP P42212
M	331	GLY	-	linker	UNP P42212
M	332	LEU	-	linker	UNP P42212
M	333	ARG	-	linker	UNP P42212
M	334	SER	-	linker	UNP P42212
M	335	ARG	-	linker	UNP P42212
M	336	ALA	-	linker	UNP P42212
M	337	GLN	-	linker	UNP P42212
M	338	ALA	-	linker	UNP P42212
M	339	SER	-	linker	UNP P42212
M	340	ASN	-	linker	UNP P42212
M	341	SER	-	linker	UNP P42212
M	342	ALA	-	linker	UNP P42212
M	343	VAL	-	linker	UNP P42212
M	344	ASP	-	linker	UNP P42212
N	72	MET	-	initiating methionine	UNP P42212
N	73	GLY	-	expression tag	UNP P42212
N	74	SER	-	expression tag	UNP P42212
N	75	SER	-	expression tag	UNP P42212
N	76	HIS	-	expression tag	UNP P42212
N	77	HIS	-	expression tag	UNP P42212
N	78	HIS	-	expression tag	UNP P42212
N	79	HIS	-	expression tag	UNP P42212
N	80	HIS	-	expression tag	UNP P42212
N	81	HIS	-	expression tag	UNP P42212
N	82	SER	-	expression tag	UNP P42212
N	83	SER	-	expression tag	UNP P42212
N	84	GLY	-	expression tag	UNP P42212
N	85	LEU	-	expression tag	UNP P42212
N	86	VAL	-	expression tag	UNP P42212
N	87	PRO	-	expression tag	UNP P42212
N	88	ARG	-	expression tag	UNP P42212
N	89	GLY	-	expression tag	UNP P42212
N	90	SER	-	expression tag	UNP P42212
N	91	HIS	-	expression tag	UNP P42212
N	92	VAL	-	expression tag	UNP P42212

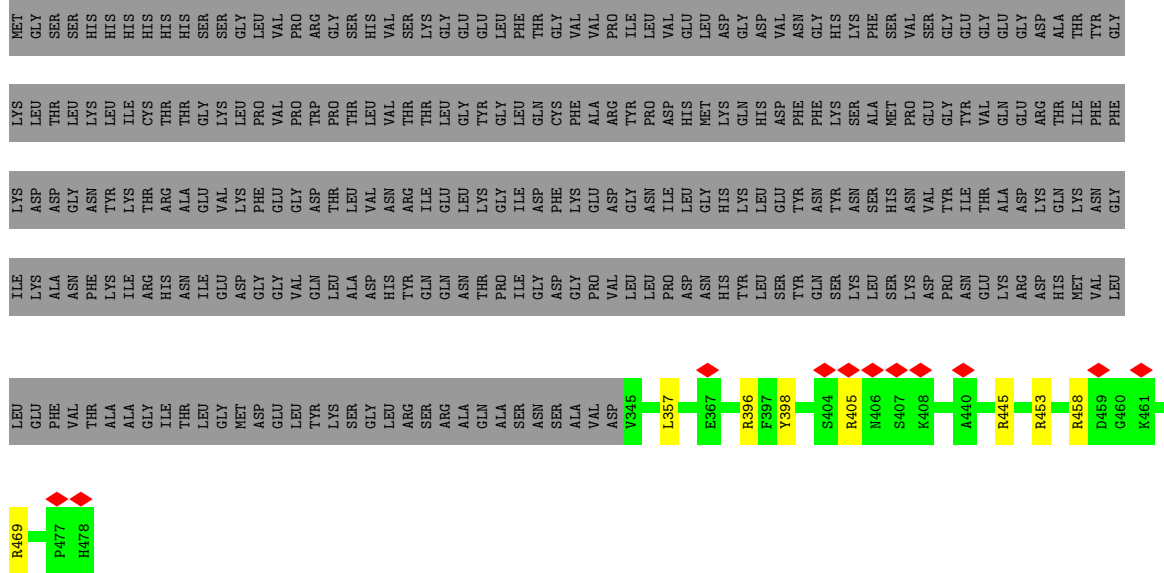
Continued on next page...

Continued from previous page...

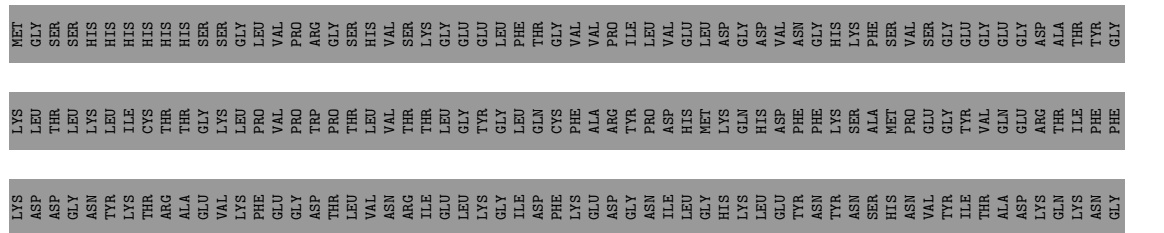
Chain	Residue	Modelled	Actual	Comment	Reference
N	137	LEU	PHE	conflict	UNP P42212
N	155	LEU	PHE	conflict	UNP P42212
N	156	GLY	SER	conflict	UNP P42212
N	159	LEU	VAL	conflict	UNP P42212
N	163	ALA	SER	conflict	UNP P42212
N	244	THR	MET	conflict	UNP P42212
N	254	ALA	VAL	conflict	UNP P42212
N	266	GLY	SER	conflict	UNP P42212
N	294	TYR	THR	conflict	UNP P42212
N	297	LYS	ALA	conflict	UNP P42212
N	322	LEU	HIS	conflict	UNP P42212
N	330	SER	-	linker	UNP P42212
N	331	GLY	-	linker	UNP P42212
N	332	LEU	-	linker	UNP P42212
N	333	ARG	-	linker	UNP P42212
N	334	SER	-	linker	UNP P42212
N	335	ARG	-	linker	UNP P42212
N	336	ALA	-	linker	UNP P42212
N	337	GLN	-	linker	UNP P42212
N	338	ALA	-	linker	UNP P42212
N	339	SER	-	linker	UNP P42212
N	340	ASN	-	linker	UNP P42212
N	341	SER	-	linker	UNP P42212
N	342	ALA	-	linker	UNP P42212
N	343	VAL	-	linker	UNP P42212
N	344	ASP	-	linker	UNP P42212

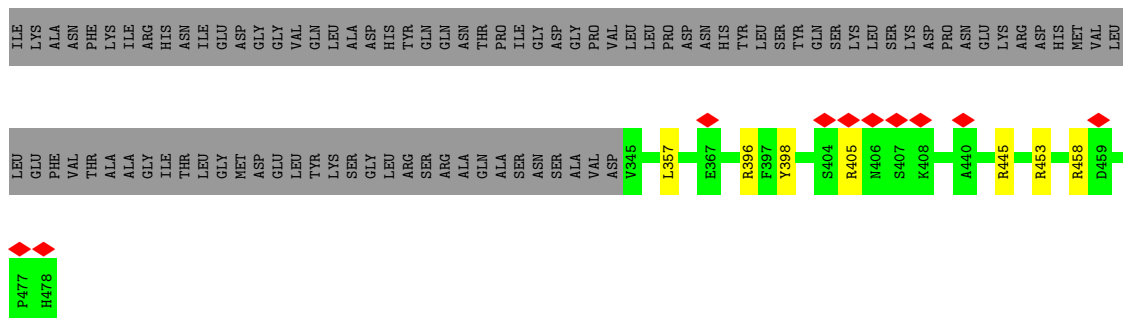


• Molecule 1: Venus-tagged CaMKII Alpha Association Domain

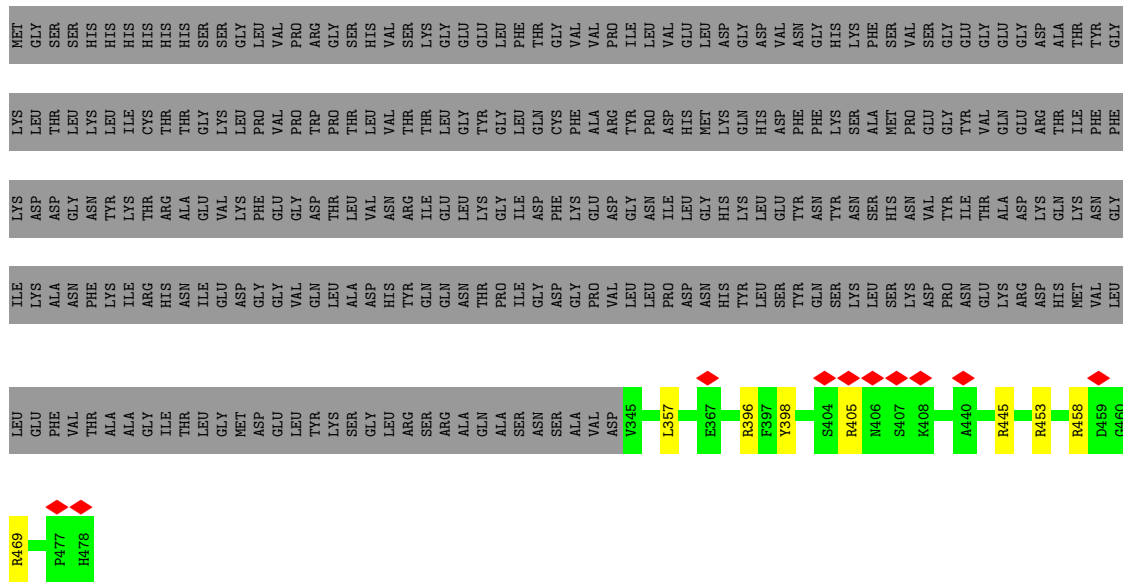


• Molecule 1: Venus-tagged CaMKII Alpha Association Domain

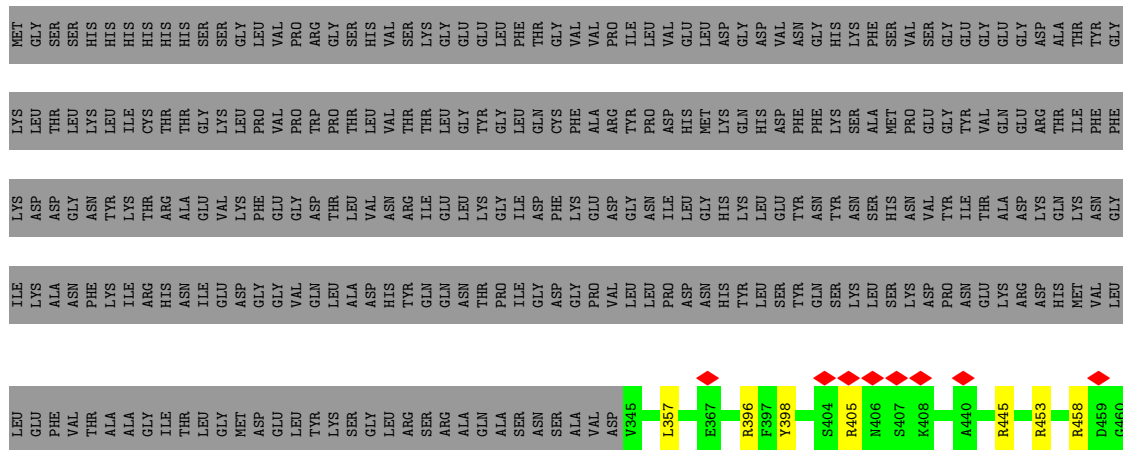


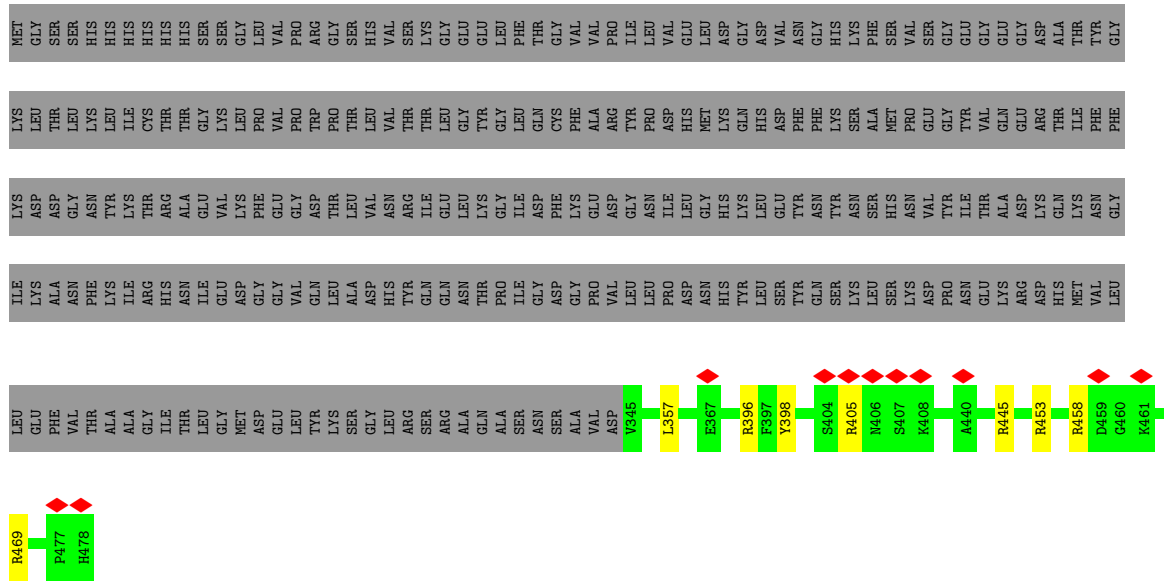


• Molecule 1: Venus-tagged CaMKII Alpha Association Domain

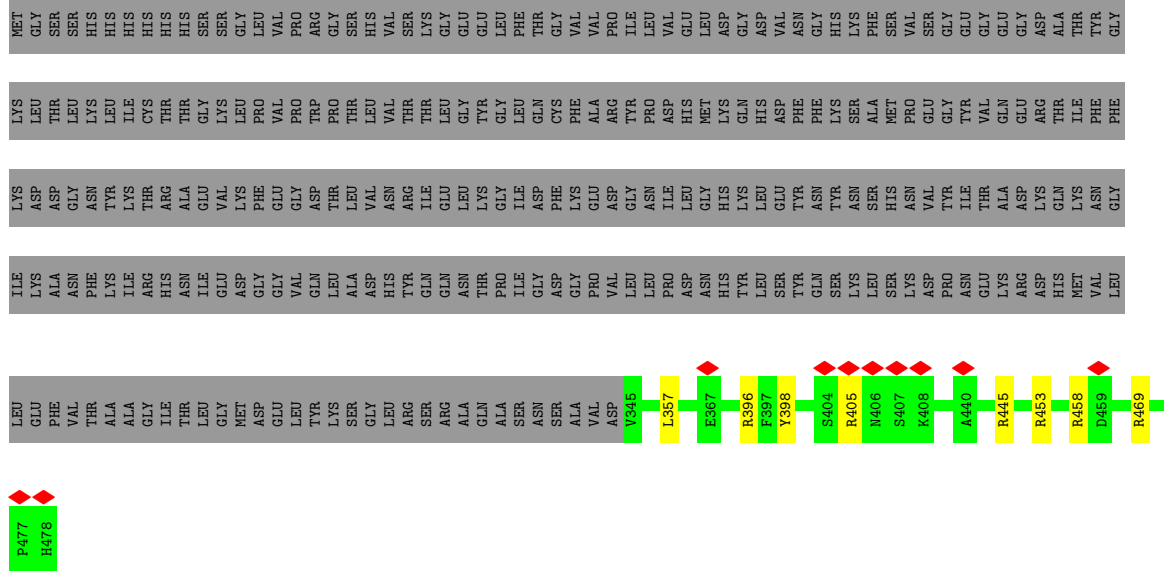


• Molecule 1: Venus-tagged CaMKII Alpha Association Domain

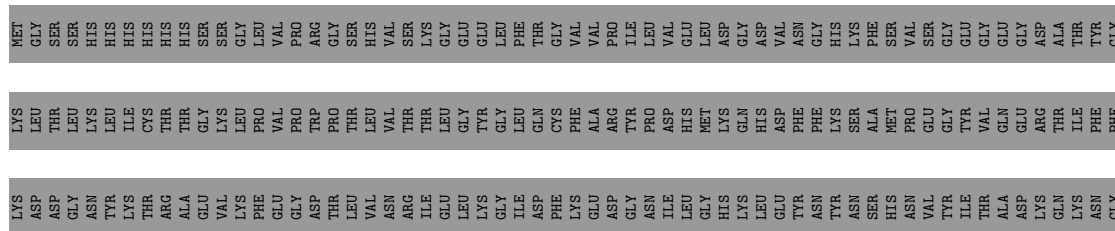




● Molecule 1: Venus-tagged CaMKII Alpha Association Domain



● Molecule 1: Venus-tagged CaMKII Alpha Association Domain



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

LEU
 GLU
 PHE
 VAL
 THR
 ALA
 ALA
 GLY
 ILE
 THR
 LEU
 GLY
 MET
 ASP
 GLU
 LEU
 TYR
 LEU
 SER
 GLY
 LEU
 ARG
 SER
 ARG
 ARG
 ALA
 GLN
 ALA
 SER
 ASN
 SER
 ALA
 VAL
 ASP
 Y345
 L357
 E367
 R396
 F397
 Y398
 S404
 R405
 N406
 S407
 R408
 A440
 R445
 R453
 R458
 D459
 R469

P477
 H478

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	205902	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	7.016	Depositor
Minimum map value	-4.801	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.114	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	284.544, 284.544, 284.544	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.741, 0.741, 0.741	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.67	0/1117	0.99	6/1513 (0.4%)
1	B	0.67	0/1117	0.99	6/1513 (0.4%)
1	C	0.67	0/1117	0.99	6/1513 (0.4%)
1	D	0.67	0/1117	0.99	6/1513 (0.4%)
1	E	0.67	0/1117	0.99	6/1513 (0.4%)
1	F	0.67	0/1117	0.99	6/1513 (0.4%)
1	G	0.67	0/1117	0.99	6/1513 (0.4%)
1	H	0.67	0/1117	0.99	6/1513 (0.4%)
1	I	0.67	0/1117	0.99	6/1513 (0.4%)
1	J	0.67	0/1117	0.99	6/1513 (0.4%)
1	K	0.67	0/1117	0.99	6/1513 (0.4%)
1	L	0.67	0/1117	0.99	6/1513 (0.4%)
1	M	0.67	0/1117	0.99	6/1513 (0.4%)
1	N	0.67	0/1117	0.99	6/1513 (0.4%)
All	All	0.67	0/15638	0.99	84/21182 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	1
1	M	0	1
1	N	0	1
All	All	0	14

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	405	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	I	405	ARG	NE-CZ-NH2	6.83	123.72	120.30
1	D	405	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	E	405	ARG	NE-CZ-NH2	6.80	123.70	120.30
1	L	405	ARG	NE-CZ-NH2	6.79	123.70	120.30
1	G	405	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	A	405	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	B	405	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	H	405	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	C	405	ARG	NE-CZ-NH2	6.77	123.68	120.30
1	K	405	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	M	405	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	F	405	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	N	405	ARG	NE-CZ-NH2	6.71	123.65	120.30
1	E	469	ARG	NE-CZ-NH2	6.51	123.55	120.30
1	L	469	ARG	NE-CZ-NH2	6.51	123.55	120.30
1	K	469	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	G	469	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	I	469	ARG	NE-CZ-NH2	6.41	123.51	120.30
1	A	469	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	C	469	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	B	469	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	H	469	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	N	469	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	J	469	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	D	469	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	F	469	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	M	469	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	G	396	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	A	396	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	L	396	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	C	396	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	I	396	ARG	NE-CZ-NH2	6.23	123.42	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	396	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	J	396	ARG	NE-CZ-NH2	6.21	123.41	120.30
1	B	396	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	H	396	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	F	396	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	N	396	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	M	396	ARG	NE-CZ-NH2	6.15	123.38	120.30
1	K	396	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	D	458	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	K	458	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	E	458	ARG	NE-CZ-NH2	6.11	123.35	120.30
1	L	458	ARG	NE-CZ-NH2	6.11	123.35	120.30
1	J	458	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	B	458	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	H	458	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	458	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	I	458	ARG	NE-CZ-NH2	6.07	123.34	120.30
1	D	396	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	N	458	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	M	458	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	C	458	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	G	458	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	F	458	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	C	445	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	J	445	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	A	445	ARG	NE-CZ-NH2	5.69	123.15	120.30
1	G	445	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	445	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	H	445	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	L	445	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	N	445	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	D	445	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	K	445	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	E	445	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	F	445	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	I	445	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	M	445	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	M	453	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	K	453	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	L	453	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	N	453	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	C	453	ARG	NE-CZ-NH2	5.17	122.89	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	453	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	E	453	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	I	453	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	B	453	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	H	453	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	J	453	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	A	453	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	D	453	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	G	453	ARG	NE-CZ-NH2	5.04	122.82	120.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	TYR	Sidechain
1	B	398	TYR	Sidechain
1	C	398	TYR	Sidechain
1	D	398	TYR	Sidechain
1	E	398	TYR	Sidechain
1	F	398	TYR	Sidechain
1	G	398	TYR	Sidechain
1	H	398	TYR	Sidechain
1	I	398	TYR	Sidechain
1	J	398	TYR	Sidechain
1	K	398	TYR	Sidechain
1	L	398	TYR	Sidechain
1	M	398	TYR	Sidechain
1	N	398	TYR	Sidechain

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	1087	1051	1049	0	0
1	B	1087	1051	1049	0	0
1	C	1087	1051	1049	0	0
1	D	1087	1051	1049	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1087	1051	1049	0	0
1	F	1087	1051	1049	0	0
1	G	1087	1051	1049	0	0
1	H	1087	1051	1049	0	0
1	I	1087	1051	1049	0	0
1	J	1087	1051	1049	0	0
1	K	1087	1051	1049	0	0
1	L	1087	1051	1049	0	0
1	M	1087	1051	1049	0	0
1	N	1087	1051	1049	0	0
All	All	15218	14714	14686	0	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 0.

There are no clashes within the asymmetric unit.

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	132/407 (32%)	129 (98%)	3 (2%)	0	100	100
1	B	132/407 (32%)	129 (98%)	3 (2%)	0	100	100
1	C	132/407 (32%)	129 (98%)	3 (2%)	0	100	100
1	D	132/407 (32%)	129 (98%)	3 (2%)	0	100	100
1	E	132/407 (32%)	129 (98%)	3 (2%)	0	100	100
1	F	132/407 (32%)	129 (98%)	3 (2%)	0	100	100
1	G	132/407 (32%)	129 (98%)	3 (2%)	0	100	100
1	H	132/407 (32%)	129 (98%)	3 (2%)	0	100	100
1	I	132/407 (32%)	129 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	132/407 (32%)	129 (98%)	3 (2%)	0	100	100
1	K	132/407 (32%)	129 (98%)	3 (2%)	0	100	100
1	L	132/407 (32%)	129 (98%)	3 (2%)	0	100	100
1	M	132/407 (32%)	129 (98%)	3 (2%)	0	100	100
1	N	132/407 (32%)	129 (98%)	3 (2%)	0	100	100
All	All	1848/5698 (32%)	1806 (98%)	42 (2%)	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	117/350 (33%)	116 (99%)	1 (1%)	78	91
1	B	117/350 (33%)	116 (99%)	1 (1%)	78	91
1	C	117/350 (33%)	116 (99%)	1 (1%)	78	91
1	D	117/350 (33%)	116 (99%)	1 (1%)	78	91
1	E	117/350 (33%)	116 (99%)	1 (1%)	78	91
1	F	117/350 (33%)	116 (99%)	1 (1%)	78	91
1	G	117/350 (33%)	116 (99%)	1 (1%)	78	91
1	H	117/350 (33%)	116 (99%)	1 (1%)	78	91
1	I	117/350 (33%)	116 (99%)	1 (1%)	78	91
1	J	117/350 (33%)	116 (99%)	1 (1%)	78	91
1	K	117/350 (33%)	116 (99%)	1 (1%)	78	91
1	L	117/350 (33%)	116 (99%)	1 (1%)	78	91
1	M	117/350 (33%)	116 (99%)	1 (1%)	78	91
1	N	117/350 (33%)	116 (99%)	1 (1%)	78	91
All	All	1638/4900 (33%)	1624 (99%)	14 (1%)	79	91

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	357	LEU
1	A	357	LEU
1	C	357	LEU
1	D	357	LEU
1	E	357	LEU
1	F	357	LEU
1	G	357	LEU
1	H	357	LEU
1	I	357	LEU
1	J	357	LEU
1	K	357	LEU
1	L	357	LEU
1	M	357	LEU
1	N	357	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

There are no ligands in this entry.

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.

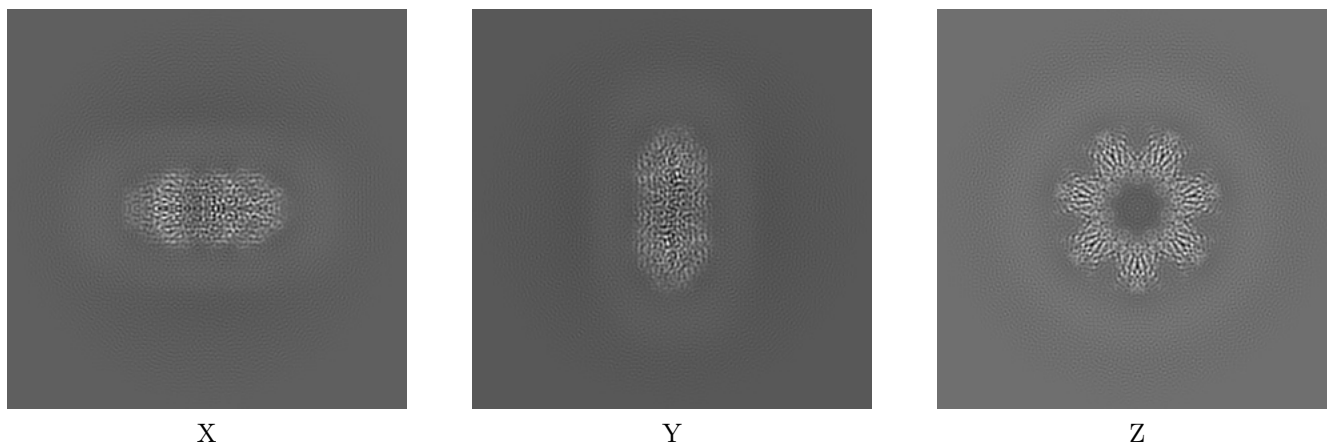
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40873. These allow visual inspection of the internal detail of the map and identification of artifacts.

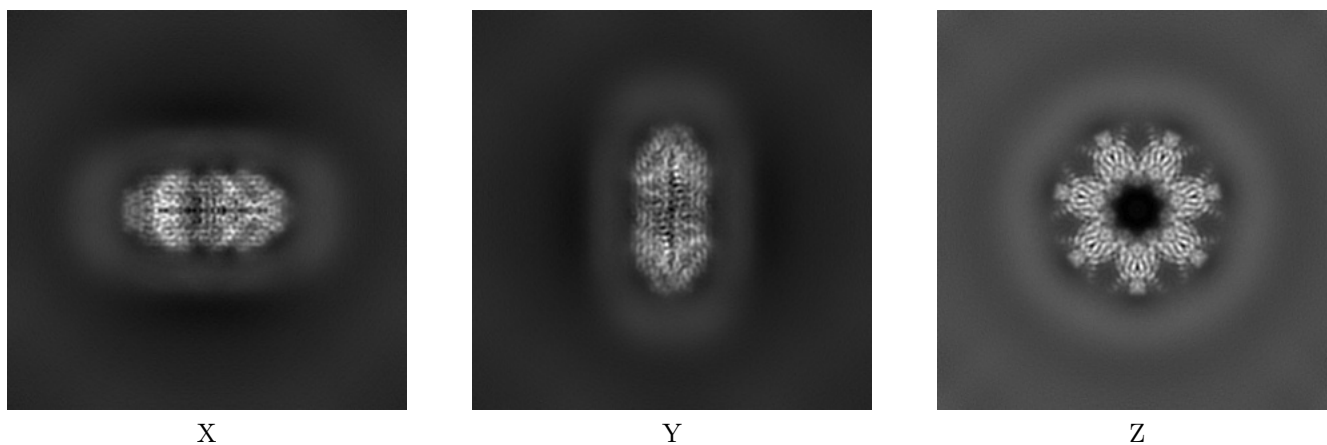
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



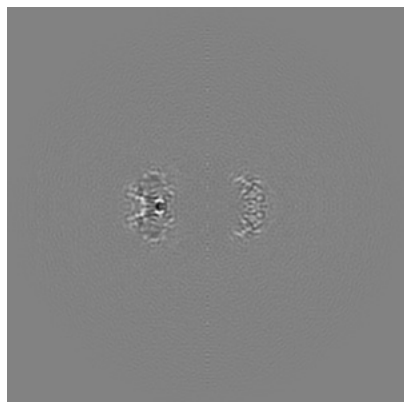
6.1.2 Raw map



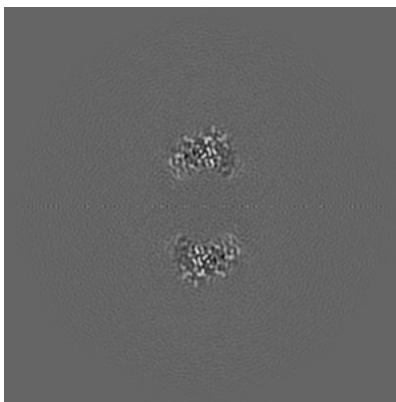
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

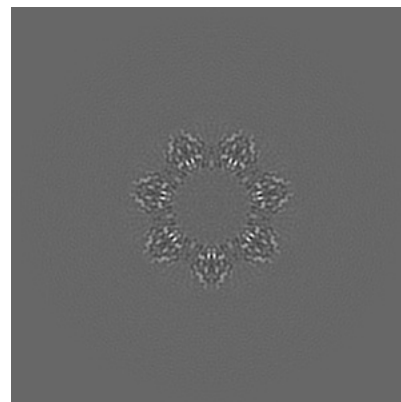
6.2.1 Primary map



X Index: 192

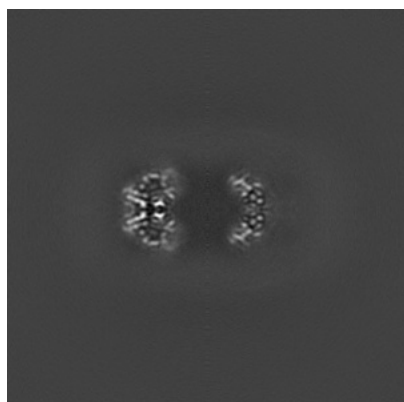


Y Index: 192

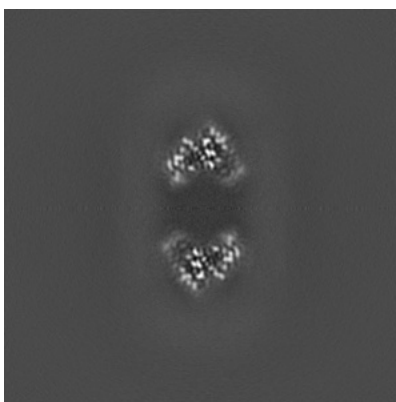


Z Index: 192

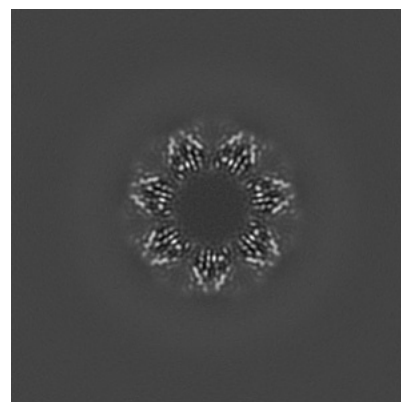
6.2.2 Raw map



X Index: 192



Y Index: 192

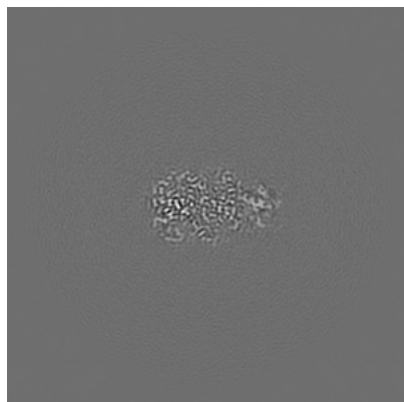


Z Index: 192

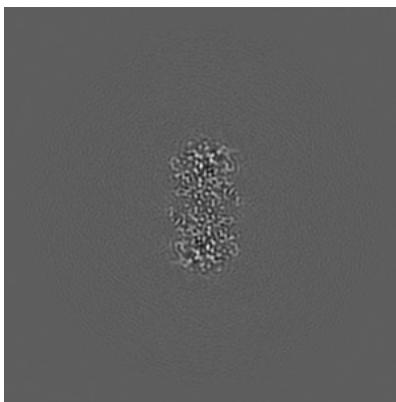
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

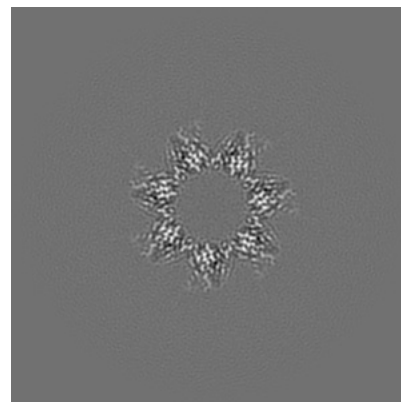
6.3.1 Primary map



X Index: 232

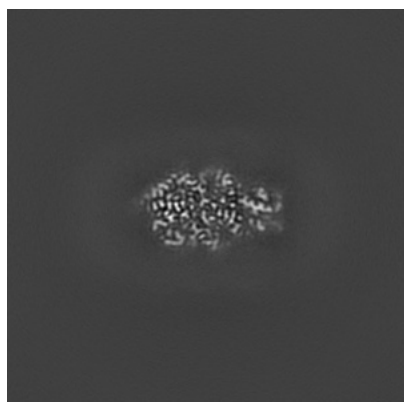


Y Index: 153

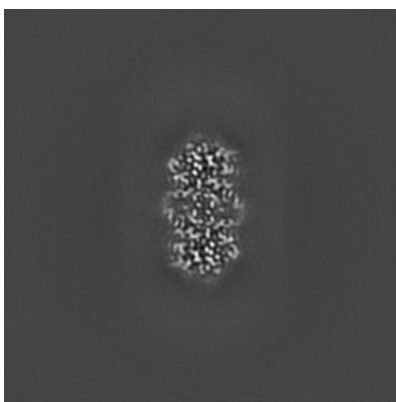


Z Index: 197

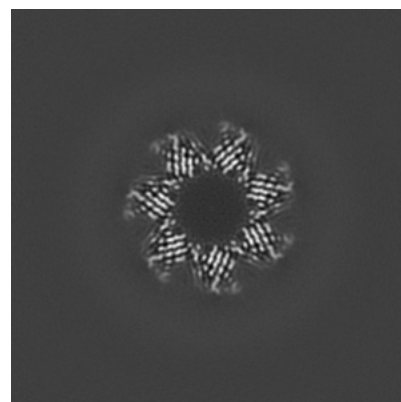
6.3.2 Raw map



X Index: 232



Y Index: 153

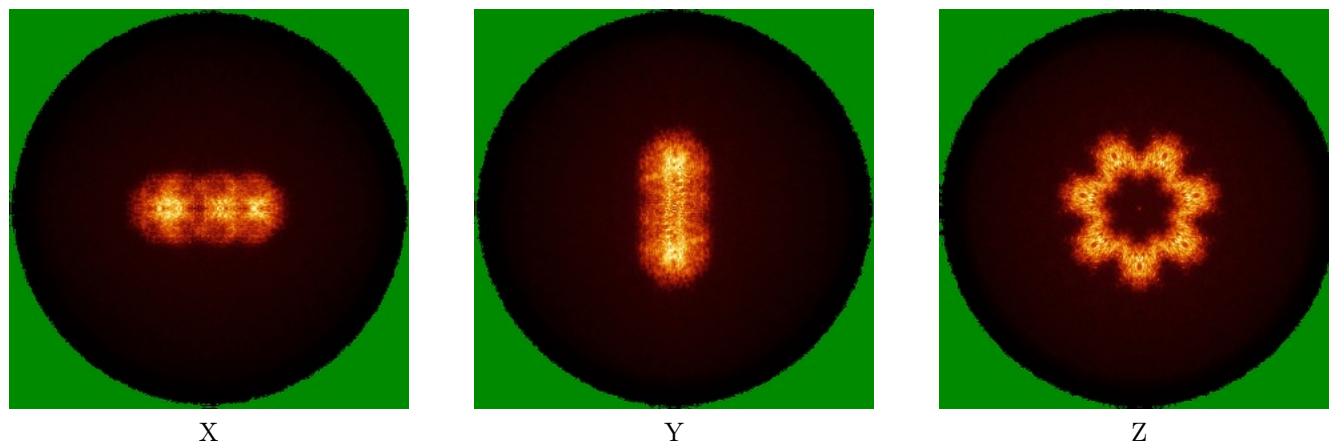


Z Index: 186

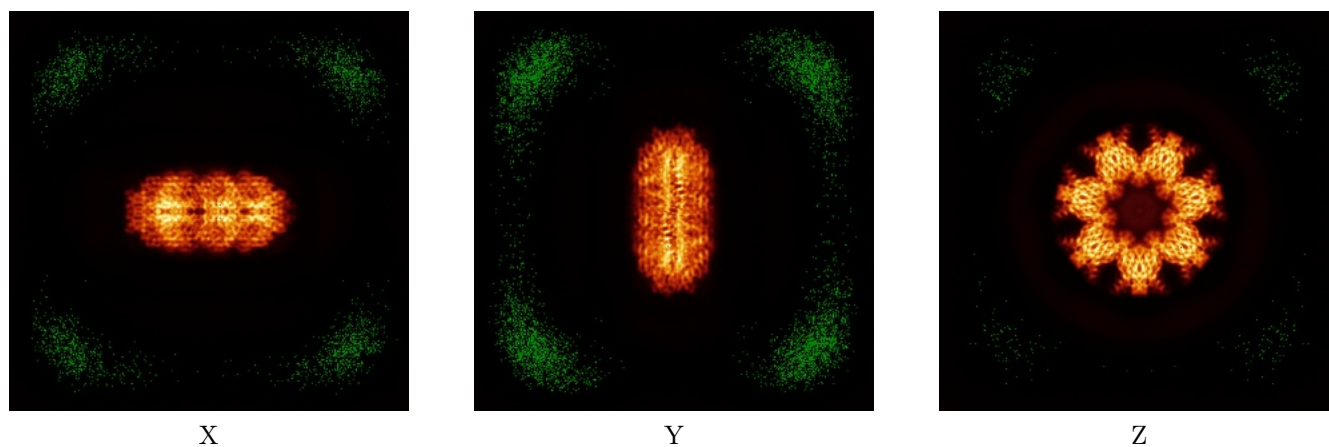
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



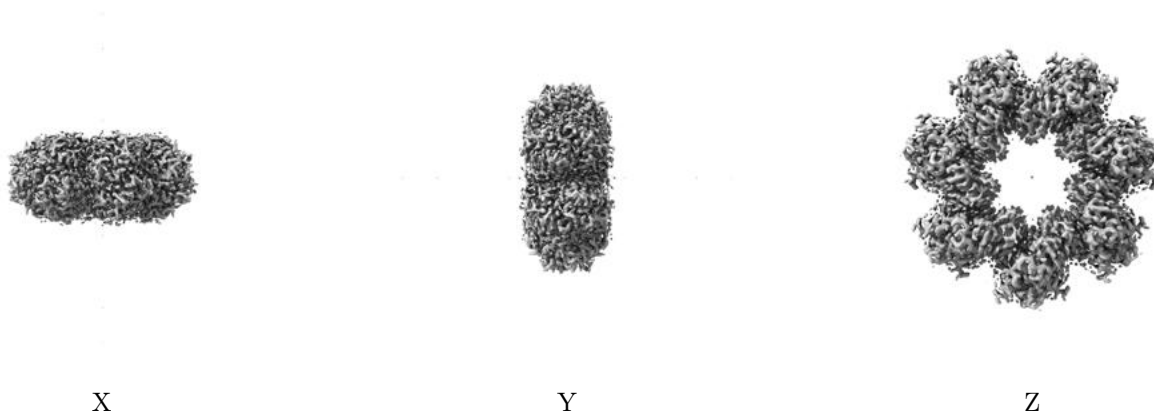
6.4.2 Raw map



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

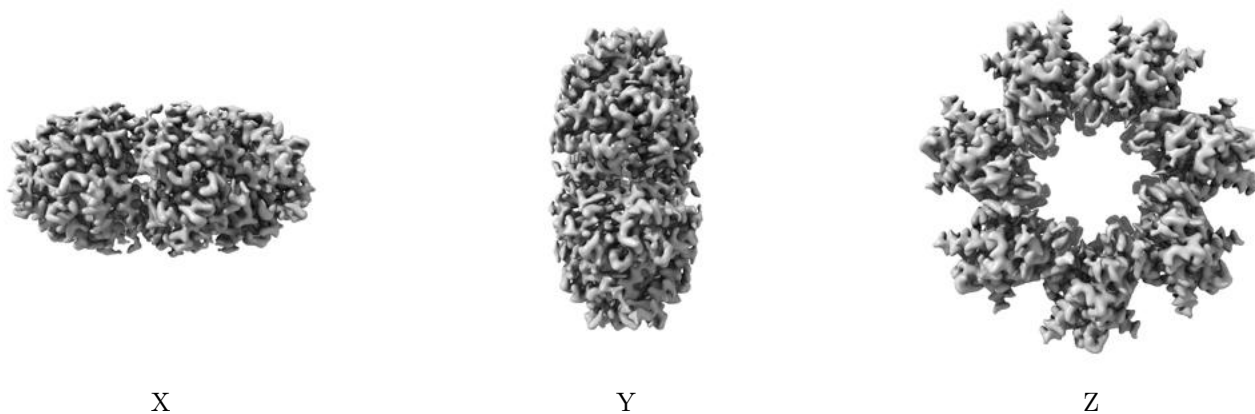
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

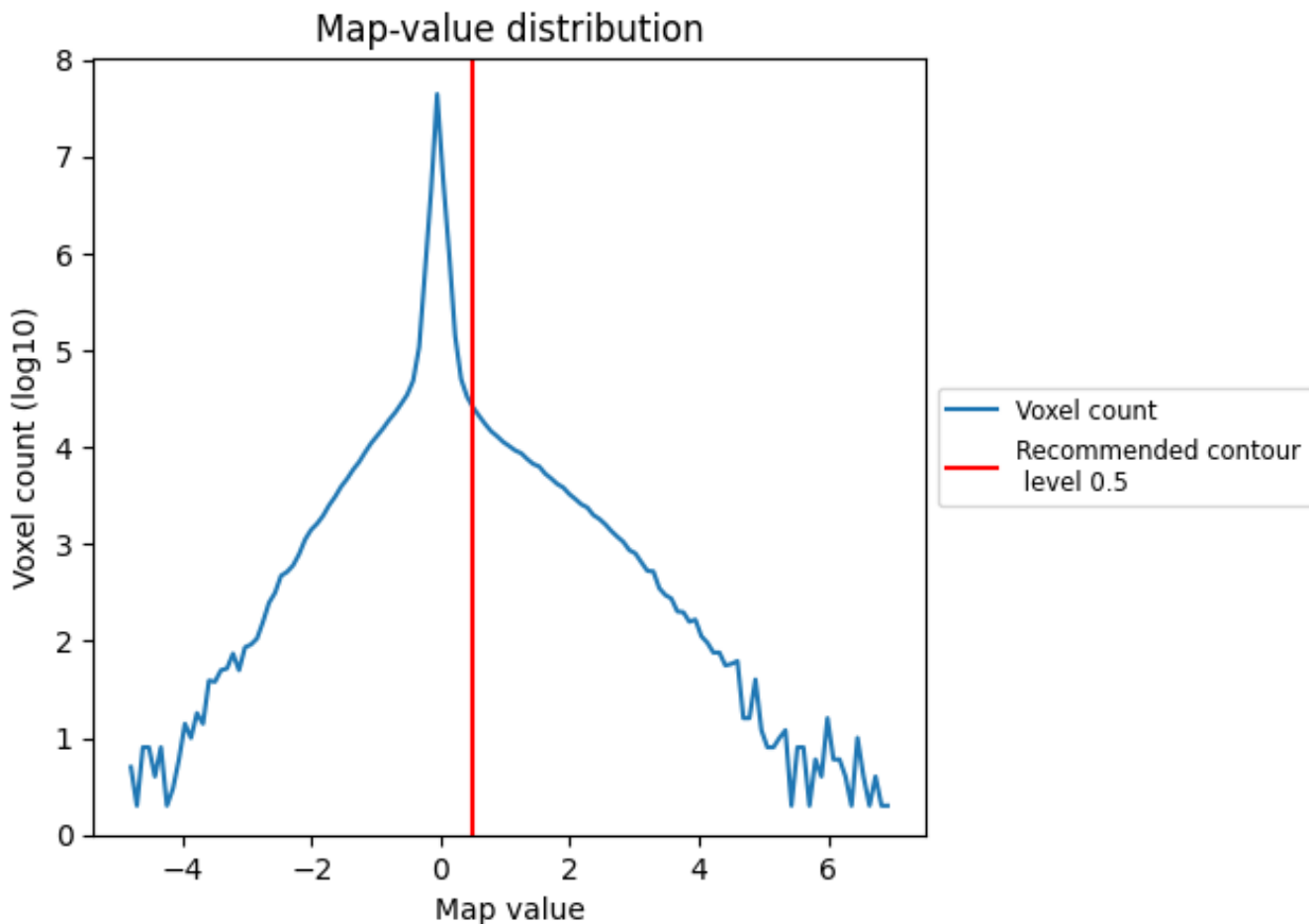
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

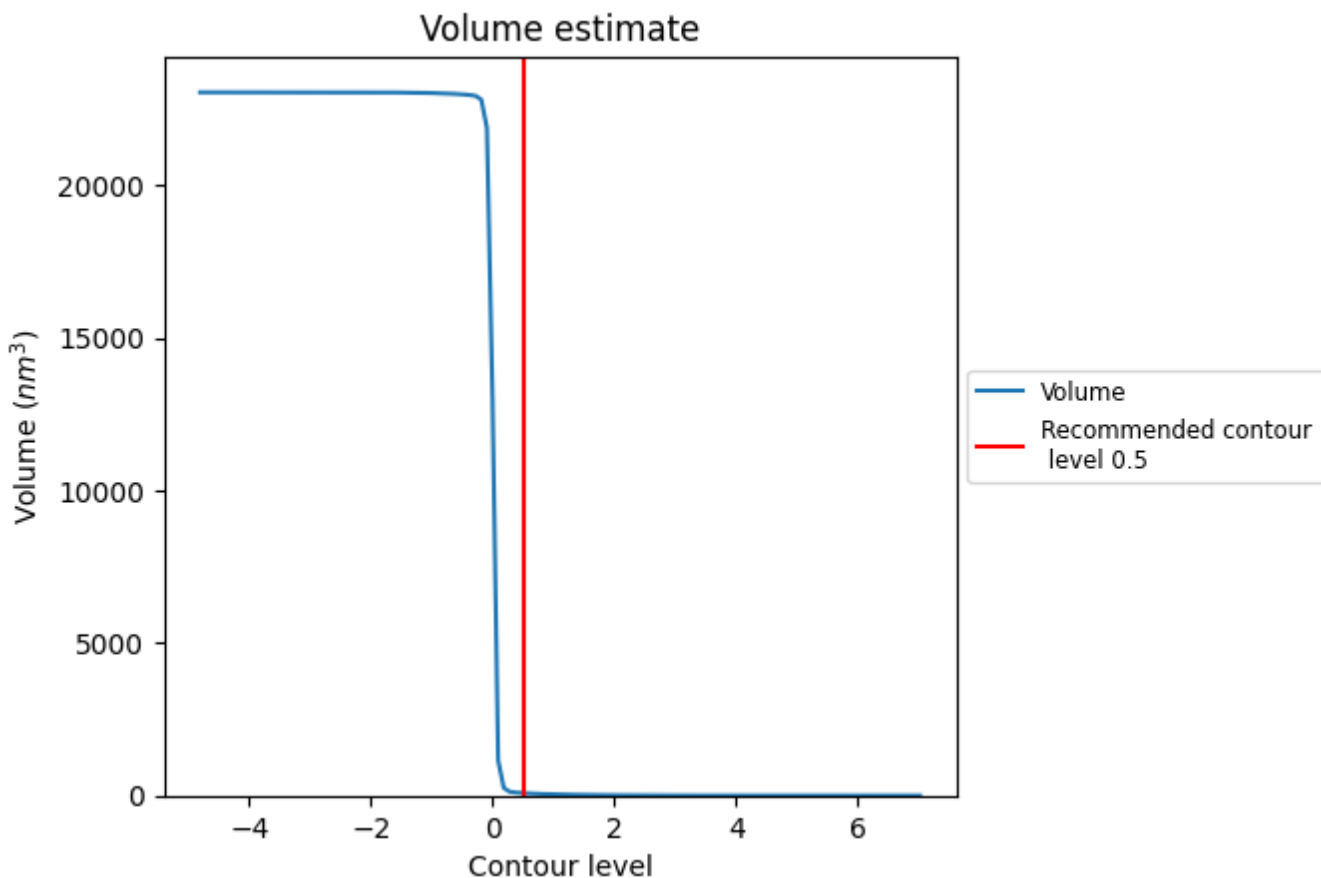
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

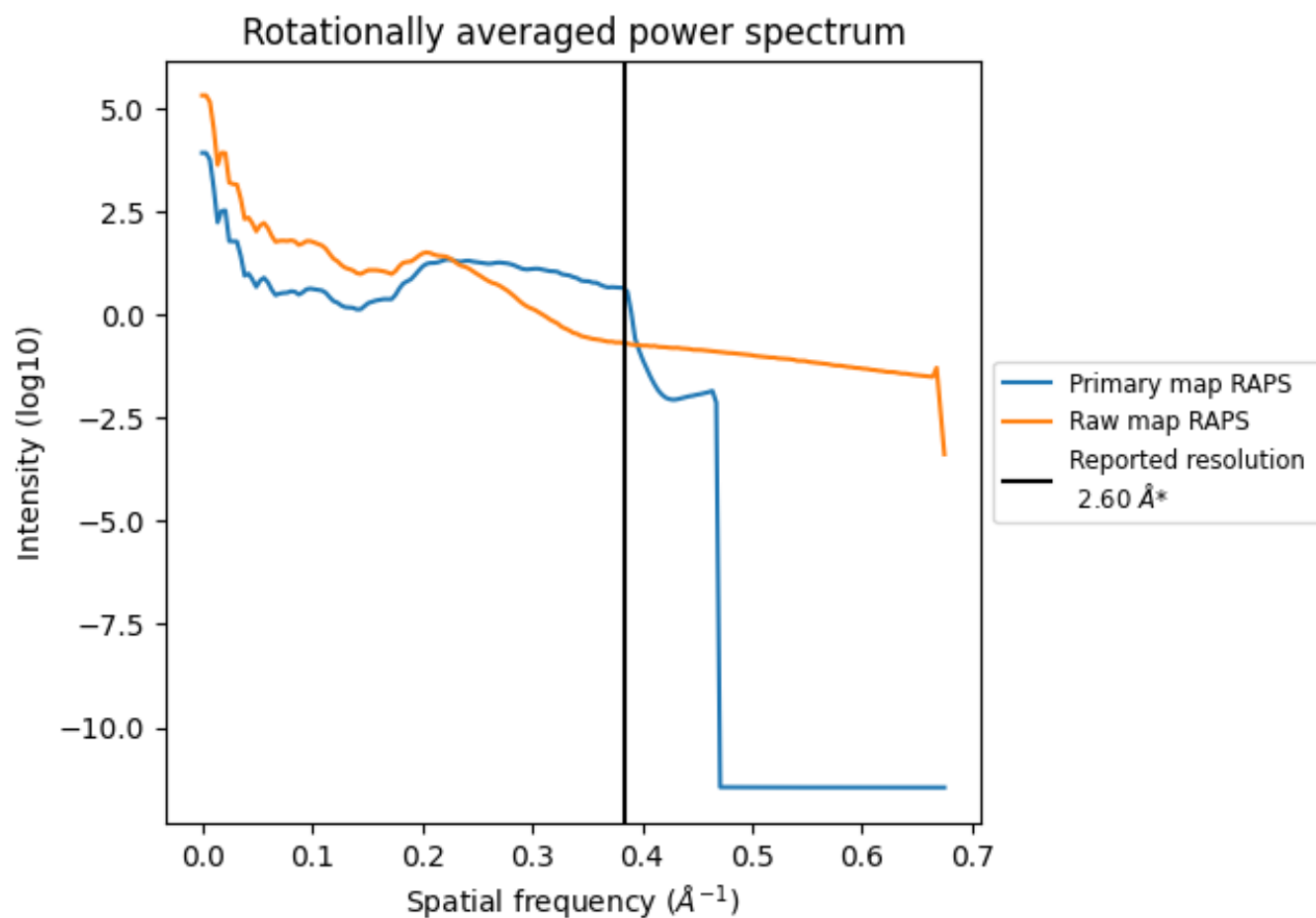
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm^3 ; this corresponds to an approximate mass of 72 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](#)

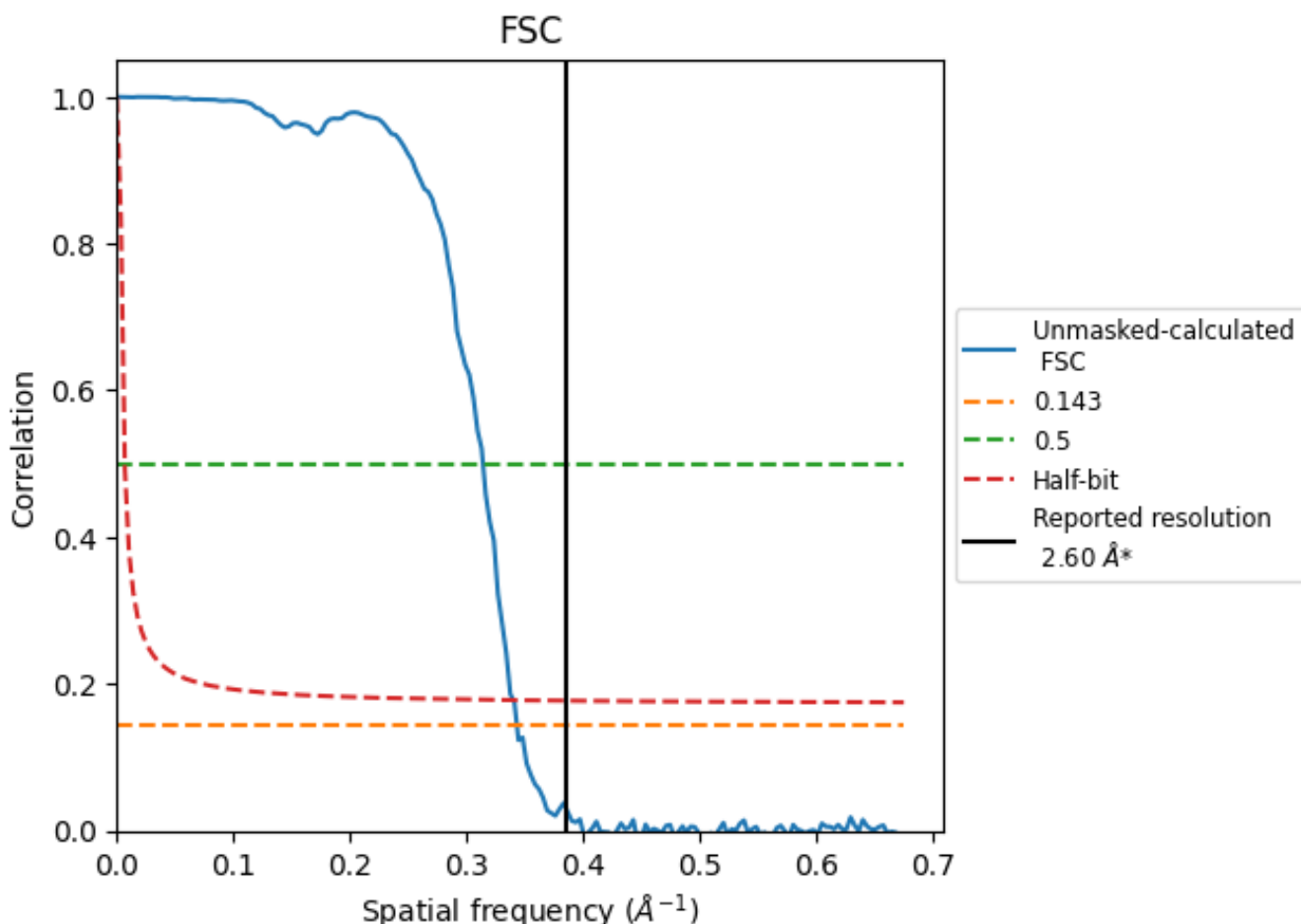


*Reported resolution corresponds to spatial frequency of 0.385 Å⁻¹

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 0.385 \AA^{-1}

8.2 Resolution estimates [i](#)

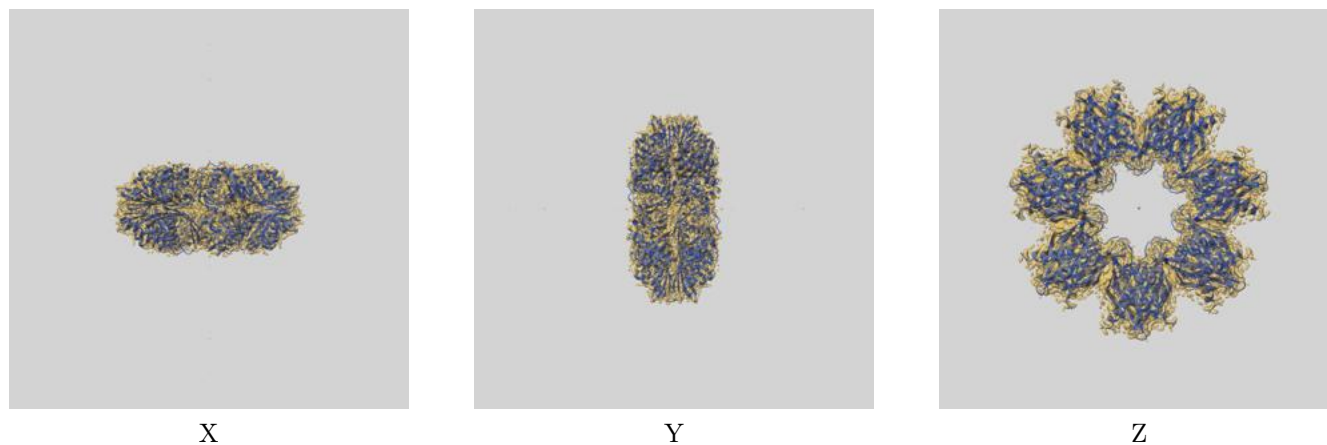
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.91	3.19	2.94

*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 2.91 differs from the reported value 2.6 by more than 10 %

9 Map-model fit [i](#)

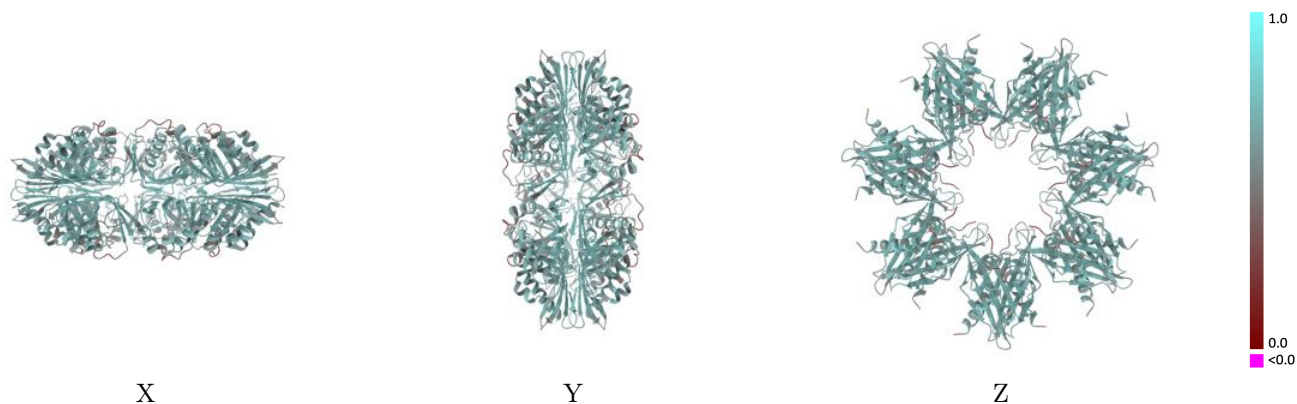
This section contains information regarding the fit between EMDB map EMD-40873 and PDB model 8SYG. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



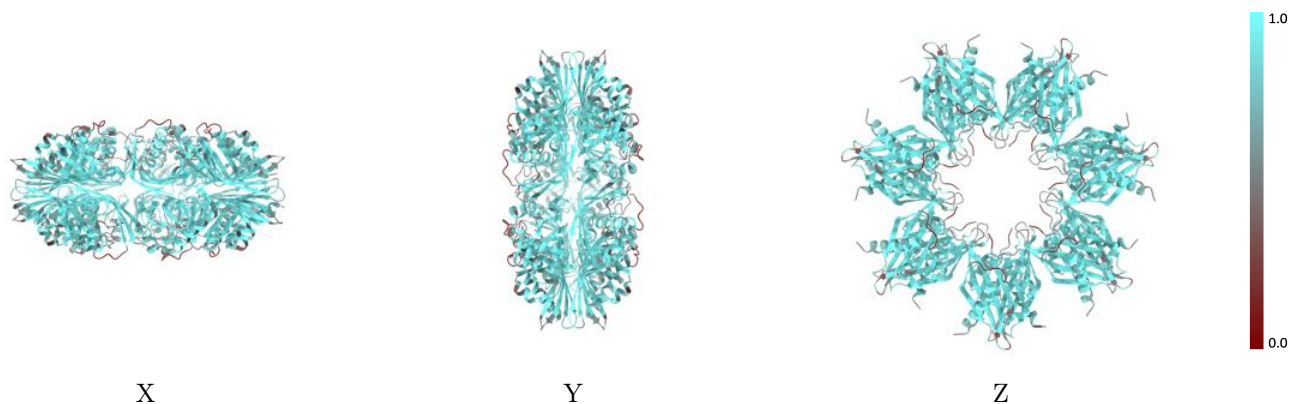
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



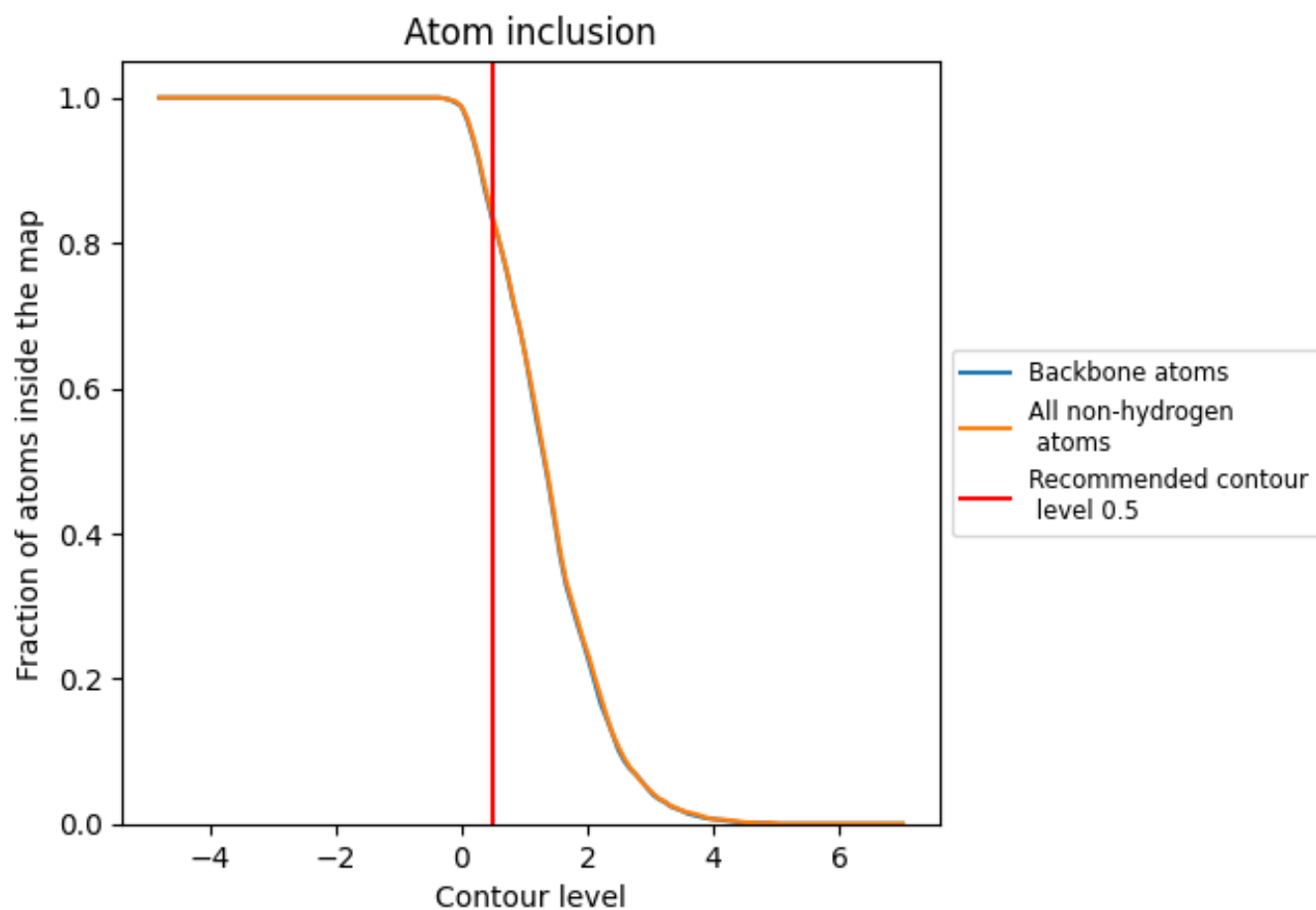
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8340	 0.6140
A	 0.8420	 0.6130
B	 0.8420	 0.6150
C	 0.8410	 0.6130
D	 0.8430	 0.6130
E	 0.8380	 0.6140
F	 0.8390	 0.6150
G	 0.8440	 0.6160
H	 0.8420	 0.6130
I	 0.8420	 0.6140
J	 0.8430	 0.6150
K	 0.8420	 0.6150
L	 0.8390	 0.6150
M	 0.8400	 0.6150
N	 0.8440	 0.6140

