



## wwPDB EM Validation Summary Report ⓘ

Nov 29, 2022 – 02:21 AM JST

PDB ID : 7VMS  
EMDB ID : EMD-32037  
Title : Structure of recombinant RyR2 mutant K4593A (Ca<sup>2+</sup> dataset)  
Authors : Kobayashi, T.; Tsutsumi, A.; Kurebayashi, N.; Kodama, M.; Kikkawa, M.;  
Murayama, T.; Ogawa, H.  
Deposited on : 2021-10-09  
Resolution : 3.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

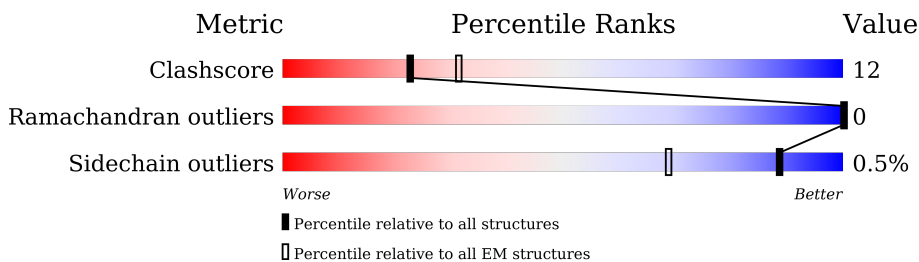
EMDB validation analysis : 0.0.1.dev43  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

# 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 3.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	4966	
1	B	4966	
1	C	4966	
1	D	4966	
2	G	176	
2	H	176	
2	I	176	
2	J	176	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 123552 atoms, of which 0 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 Ryanodine receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4044	30067	19032	5242	5617	176	0	0
1	B	4044	30067	19032	5242	5617	176	0	0
1	C	4044	30067	19032	5242	5617	176	0	0
1	D	4044	30067	19032	5242	5617	176	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4593	ALA	LYS	engineered mutation	UNP E9Q401
B	4593	ALA	LYS	engineered mutation	UNP E9Q401
C	4593	ALA	LYS	engineered mutation	UNP E9Q401
D	4593	ALA	LYS	engineered mutation	UNP E9Q401

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	107	819	516	144	155	4	0	0
2	H	107	819	516	144	155	4	0	0
2	I	107	819	516	144	155	4	0	0
2	J	107	819	516	144	155	4	0	0

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-67	MET	-	initiating methionine	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-66	GLY	-	expression tag	UNP P68106
G	-65	SER	-	expression tag	UNP P68106
G	-64	SER	-	expression tag	UNP P68106
G	-63	HIS	-	expression tag	UNP P68106
G	-62	HIS	-	expression tag	UNP P68106
G	-61	HIS	-	expression tag	UNP P68106
G	-60	HIS	-	expression tag	UNP P68106
G	-59	HIS	-	expression tag	UNP P68106
G	-58	HIS	-	expression tag	UNP P68106
G	-57	SER	-	expression tag	UNP P68106
G	-56	SER	-	expression tag	UNP P68106
G	-55	GLY	-	expression tag	UNP P68106
G	-54	LEU	-	expression tag	UNP P68106
G	-53	VAL	-	expression tag	UNP P68106
G	-52	PRO	-	expression tag	UNP P68106
G	-51	ARG	-	expression tag	UNP P68106
G	-50	GLY	-	expression tag	UNP P68106
G	-49	SER	-	expression tag	UNP P68106
G	-48	HIS	-	expression tag	UNP P68106
G	-47	MET	-	expression tag	UNP P68106
G	-46	ALA	-	expression tag	UNP P68106
G	-45	SER	-	expression tag	UNP P68106
G	-44	MET	-	expression tag	UNP P68106
G	-43	ASP	-	expression tag	UNP P68106
G	-42	GLU	-	expression tag	UNP P68106
G	-41	LYS	-	expression tag	UNP P68106
G	-40	THR	-	expression tag	UNP P68106
G	-39	THR	-	expression tag	UNP P68106
G	-38	GLY	-	expression tag	UNP P68106
G	-37	TRP	-	expression tag	UNP P68106
G	-36	ARG	-	expression tag	UNP P68106
G	-35	GLY	-	expression tag	UNP P68106
G	-34	GLY	-	expression tag	UNP P68106
G	-33	HIS	-	expression tag	UNP P68106
G	-32	VAL	-	expression tag	UNP P68106
G	-31	VAL	-	expression tag	UNP P68106
G	-30	GLU	-	expression tag	UNP P68106
G	-29	GLY	-	expression tag	UNP P68106
G	-28	LEU	-	expression tag	UNP P68106
G	-27	ALA	-	expression tag	UNP P68106
G	-26	GLY	-	expression tag	UNP P68106
G	-25	GLU	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-24	LEU	-	expression tag	UNP P68106
G	-23	GLU	-	expression tag	UNP P68106
G	-22	GLN	-	expression tag	UNP P68106
G	-21	LEU	-	expression tag	UNP P68106
G	-20	ARG	-	expression tag	UNP P68106
G	-19	ALA	-	expression tag	UNP P68106
G	-18	ARG	-	expression tag	UNP P68106
G	-17	LEU	-	expression tag	UNP P68106
G	-16	GLU	-	expression tag	UNP P68106
G	-15	HIS	-	expression tag	UNP P68106
G	-14	HIS	-	expression tag	UNP P68106
G	-13	PRO	-	expression tag	UNP P68106
G	-12	GLN	-	expression tag	UNP P68106
G	-11	GLY	-	expression tag	UNP P68106
G	-10	GLN	-	expression tag	UNP P68106
G	-9	ARG	-	expression tag	UNP P68106
G	-8	GLU	-	expression tag	UNP P68106
G	-7	PRO	-	expression tag	UNP P68106
G	-6	GLY	-	expression tag	UNP P68106
G	-5	SER	-	expression tag	UNP P68106
G	-4	GLY	-	expression tag	UNP P68106
G	-3	GLY	-	expression tag	UNP P68106
G	-2	SER	-	expression tag	UNP P68106
G	-1	GLY	-	expression tag	UNP P68106
G	0	GLY	-	expression tag	UNP P68106
G	1	THR	-	expression tag	UNP P68106
H	-67	MET	-	initiating methionine	UNP P68106
H	-66	GLY	-	expression tag	UNP P68106
H	-65	SER	-	expression tag	UNP P68106
H	-64	SER	-	expression tag	UNP P68106
H	-63	HIS	-	expression tag	UNP P68106
H	-62	HIS	-	expression tag	UNP P68106
H	-61	HIS	-	expression tag	UNP P68106
H	-60	HIS	-	expression tag	UNP P68106
H	-59	HIS	-	expression tag	UNP P68106
H	-58	HIS	-	expression tag	UNP P68106
H	-57	SER	-	expression tag	UNP P68106
H	-56	SER	-	expression tag	UNP P68106
H	-55	GLY	-	expression tag	UNP P68106
H	-54	LEU	-	expression tag	UNP P68106
H	-53	VAL	-	expression tag	UNP P68106
H	-52	PRO	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-51	ARG	-	expression tag	UNP P68106
H	-50	GLY	-	expression tag	UNP P68106
H	-49	SER	-	expression tag	UNP P68106
H	-48	HIS	-	expression tag	UNP P68106
H	-47	MET	-	expression tag	UNP P68106
H	-46	ALA	-	expression tag	UNP P68106
H	-45	SER	-	expression tag	UNP P68106
H	-44	MET	-	expression tag	UNP P68106
H	-43	ASP	-	expression tag	UNP P68106
H	-42	GLU	-	expression tag	UNP P68106
H	-41	LYS	-	expression tag	UNP P68106
H	-40	THR	-	expression tag	UNP P68106
H	-39	THR	-	expression tag	UNP P68106
H	-38	GLY	-	expression tag	UNP P68106
H	-37	TRP	-	expression tag	UNP P68106
H	-36	ARG	-	expression tag	UNP P68106
H	-35	GLY	-	expression tag	UNP P68106
H	-34	GLY	-	expression tag	UNP P68106
H	-33	HIS	-	expression tag	UNP P68106
H	-32	VAL	-	expression tag	UNP P68106
H	-31	VAL	-	expression tag	UNP P68106
H	-30	GLU	-	expression tag	UNP P68106
H	-29	GLY	-	expression tag	UNP P68106
H	-28	LEU	-	expression tag	UNP P68106
H	-27	ALA	-	expression tag	UNP P68106
H	-26	GLY	-	expression tag	UNP P68106
H	-25	GLU	-	expression tag	UNP P68106
H	-24	LEU	-	expression tag	UNP P68106
H	-23	GLU	-	expression tag	UNP P68106
H	-22	GLN	-	expression tag	UNP P68106
H	-21	LEU	-	expression tag	UNP P68106
H	-20	ARG	-	expression tag	UNP P68106
H	-19	ALA	-	expression tag	UNP P68106
H	-18	ARG	-	expression tag	UNP P68106
H	-17	LEU	-	expression tag	UNP P68106
H	-16	GLU	-	expression tag	UNP P68106
H	-15	HIS	-	expression tag	UNP P68106
H	-14	HIS	-	expression tag	UNP P68106
H	-13	PRO	-	expression tag	UNP P68106
H	-12	GLN	-	expression tag	UNP P68106
H	-11	GLY	-	expression tag	UNP P68106
H	-10	GLN	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-9	ARG	-	expression tag	UNP P68106
H	-8	GLU	-	expression tag	UNP P68106
H	-7	PRO	-	expression tag	UNP P68106
H	-6	GLY	-	expression tag	UNP P68106
H	-5	SER	-	expression tag	UNP P68106
H	-4	GLY	-	expression tag	UNP P68106
H	-3	GLY	-	expression tag	UNP P68106
H	-2	SER	-	expression tag	UNP P68106
H	-1	GLY	-	expression tag	UNP P68106
H	0	GLY	-	expression tag	UNP P68106
H	1	THR	-	expression tag	UNP P68106
I	-67	MET	-	initiating methionine	UNP P68106
I	-66	GLY	-	expression tag	UNP P68106
I	-65	SER	-	expression tag	UNP P68106
I	-64	SER	-	expression tag	UNP P68106
I	-63	HIS	-	expression tag	UNP P68106
I	-62	HIS	-	expression tag	UNP P68106
I	-61	HIS	-	expression tag	UNP P68106
I	-60	HIS	-	expression tag	UNP P68106
I	-59	HIS	-	expression tag	UNP P68106
I	-58	HIS	-	expression tag	UNP P68106
I	-57	SER	-	expression tag	UNP P68106
I	-56	SER	-	expression tag	UNP P68106
I	-55	GLY	-	expression tag	UNP P68106
I	-54	LEU	-	expression tag	UNP P68106
I	-53	VAL	-	expression tag	UNP P68106
I	-52	PRO	-	expression tag	UNP P68106
I	-51	ARG	-	expression tag	UNP P68106
I	-50	GLY	-	expression tag	UNP P68106
I	-49	SER	-	expression tag	UNP P68106
I	-48	HIS	-	expression tag	UNP P68106
I	-47	MET	-	expression tag	UNP P68106
I	-46	ALA	-	expression tag	UNP P68106
I	-45	SER	-	expression tag	UNP P68106
I	-44	MET	-	expression tag	UNP P68106
I	-43	ASP	-	expression tag	UNP P68106
I	-42	GLU	-	expression tag	UNP P68106
I	-41	LYS	-	expression tag	UNP P68106
I	-40	THR	-	expression tag	UNP P68106
I	-39	THR	-	expression tag	UNP P68106
I	-38	GLY	-	expression tag	UNP P68106
I	-37	TRP	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-36	ARG	-	expression tag	UNP P68106
I	-35	GLY	-	expression tag	UNP P68106
I	-34	GLY	-	expression tag	UNP P68106
I	-33	HIS	-	expression tag	UNP P68106
I	-32	VAL	-	expression tag	UNP P68106
I	-31	VAL	-	expression tag	UNP P68106
I	-30	GLU	-	expression tag	UNP P68106
I	-29	GLY	-	expression tag	UNP P68106
I	-28	LEU	-	expression tag	UNP P68106
I	-27	ALA	-	expression tag	UNP P68106
I	-26	GLY	-	expression tag	UNP P68106
I	-25	GLU	-	expression tag	UNP P68106
I	-24	LEU	-	expression tag	UNP P68106
I	-23	GLU	-	expression tag	UNP P68106
I	-22	GLN	-	expression tag	UNP P68106
I	-21	LEU	-	expression tag	UNP P68106
I	-20	ARG	-	expression tag	UNP P68106
I	-19	ALA	-	expression tag	UNP P68106
I	-18	ARG	-	expression tag	UNP P68106
I	-17	LEU	-	expression tag	UNP P68106
I	-16	GLU	-	expression tag	UNP P68106
I	-15	HIS	-	expression tag	UNP P68106
I	-14	HIS	-	expression tag	UNP P68106
I	-13	PRO	-	expression tag	UNP P68106
I	-12	GLN	-	expression tag	UNP P68106
I	-11	GLY	-	expression tag	UNP P68106
I	-10	GLN	-	expression tag	UNP P68106
I	-9	ARG	-	expression tag	UNP P68106
I	-8	GLU	-	expression tag	UNP P68106
I	-7	PRO	-	expression tag	UNP P68106
I	-6	GLY	-	expression tag	UNP P68106
I	-5	SER	-	expression tag	UNP P68106
I	-4	GLY	-	expression tag	UNP P68106
I	-3	GLY	-	expression tag	UNP P68106
I	-2	SER	-	expression tag	UNP P68106
I	-1	GLY	-	expression tag	UNP P68106
I	0	GLY	-	expression tag	UNP P68106
I	1	THR	-	expression tag	UNP P68106
J	-67	MET	-	initiating methionine	UNP P68106
J	-66	GLY	-	expression tag	UNP P68106
J	-65	SER	-	expression tag	UNP P68106
J	-64	SER	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-63	HIS	-	expression tag	UNP P68106
J	-62	HIS	-	expression tag	UNP P68106
J	-61	HIS	-	expression tag	UNP P68106
J	-60	HIS	-	expression tag	UNP P68106
J	-59	HIS	-	expression tag	UNP P68106
J	-58	HIS	-	expression tag	UNP P68106
J	-57	SER	-	expression tag	UNP P68106
J	-56	SER	-	expression tag	UNP P68106
J	-55	GLY	-	expression tag	UNP P68106
J	-54	LEU	-	expression tag	UNP P68106
J	-53	VAL	-	expression tag	UNP P68106
J	-52	PRO	-	expression tag	UNP P68106
J	-51	ARG	-	expression tag	UNP P68106
J	-50	GLY	-	expression tag	UNP P68106
J	-49	SER	-	expression tag	UNP P68106
J	-48	HIS	-	expression tag	UNP P68106
J	-47	MET	-	expression tag	UNP P68106
J	-46	ALA	-	expression tag	UNP P68106
J	-45	SER	-	expression tag	UNP P68106
J	-44	MET	-	expression tag	UNP P68106
J	-43	ASP	-	expression tag	UNP P68106
J	-42	GLU	-	expression tag	UNP P68106
J	-41	LYS	-	expression tag	UNP P68106
J	-40	THR	-	expression tag	UNP P68106
J	-39	THR	-	expression tag	UNP P68106
J	-38	GLY	-	expression tag	UNP P68106
J	-37	TRP	-	expression tag	UNP P68106
J	-36	ARG	-	expression tag	UNP P68106
J	-35	GLY	-	expression tag	UNP P68106
J	-34	GLY	-	expression tag	UNP P68106
J	-33	HIS	-	expression tag	UNP P68106
J	-32	VAL	-	expression tag	UNP P68106
J	-31	VAL	-	expression tag	UNP P68106
J	-30	GLU	-	expression tag	UNP P68106
J	-29	GLY	-	expression tag	UNP P68106
J	-28	LEU	-	expression tag	UNP P68106
J	-27	ALA	-	expression tag	UNP P68106
J	-26	GLY	-	expression tag	UNP P68106
J	-25	GLU	-	expression tag	UNP P68106
J	-24	LEU	-	expression tag	UNP P68106
J	-23	GLU	-	expression tag	UNP P68106
J	-22	GLN	-	expression tag	UNP P68106

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-21	LEU	-	expression tag	UNP P68106
J	-20	ARG	-	expression tag	UNP P68106
J	-19	ALA	-	expression tag	UNP P68106
J	-18	ARG	-	expression tag	UNP P68106
J	-17	LEU	-	expression tag	UNP P68106
J	-16	GLU	-	expression tag	UNP P68106
J	-15	HIS	-	expression tag	UNP P68106
J	-14	HIS	-	expression tag	UNP P68106
J	-13	PRO	-	expression tag	UNP P68106
J	-12	GLN	-	expression tag	UNP P68106
J	-11	GLY	-	expression tag	UNP P68106
J	-10	GLN	-	expression tag	UNP P68106
J	-9	ARG	-	expression tag	UNP P68106
J	-8	GLU	-	expression tag	UNP P68106
J	-7	PRO	-	expression tag	UNP P68106
J	-6	GLY	-	expression tag	UNP P68106
J	-5	SER	-	expression tag	UNP P68106
J	-4	GLY	-	expression tag	UNP P68106
J	-3	GLY	-	expression tag	UNP P68106
J	-2	SER	-	expression tag	UNP P68106
J	-1	GLY	-	expression tag	UNP P68106
J	0	GLY	-	expression tag	UNP P68106
J	1	THR	-	expression tag	UNP P68106

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
4	A	1	Total 1	Ca 1	0
4	B	1	Total 1	Ca 1	0
4	C	1	Total 1	Ca 1	0
4	D	1	Total 1	Ca 1	0

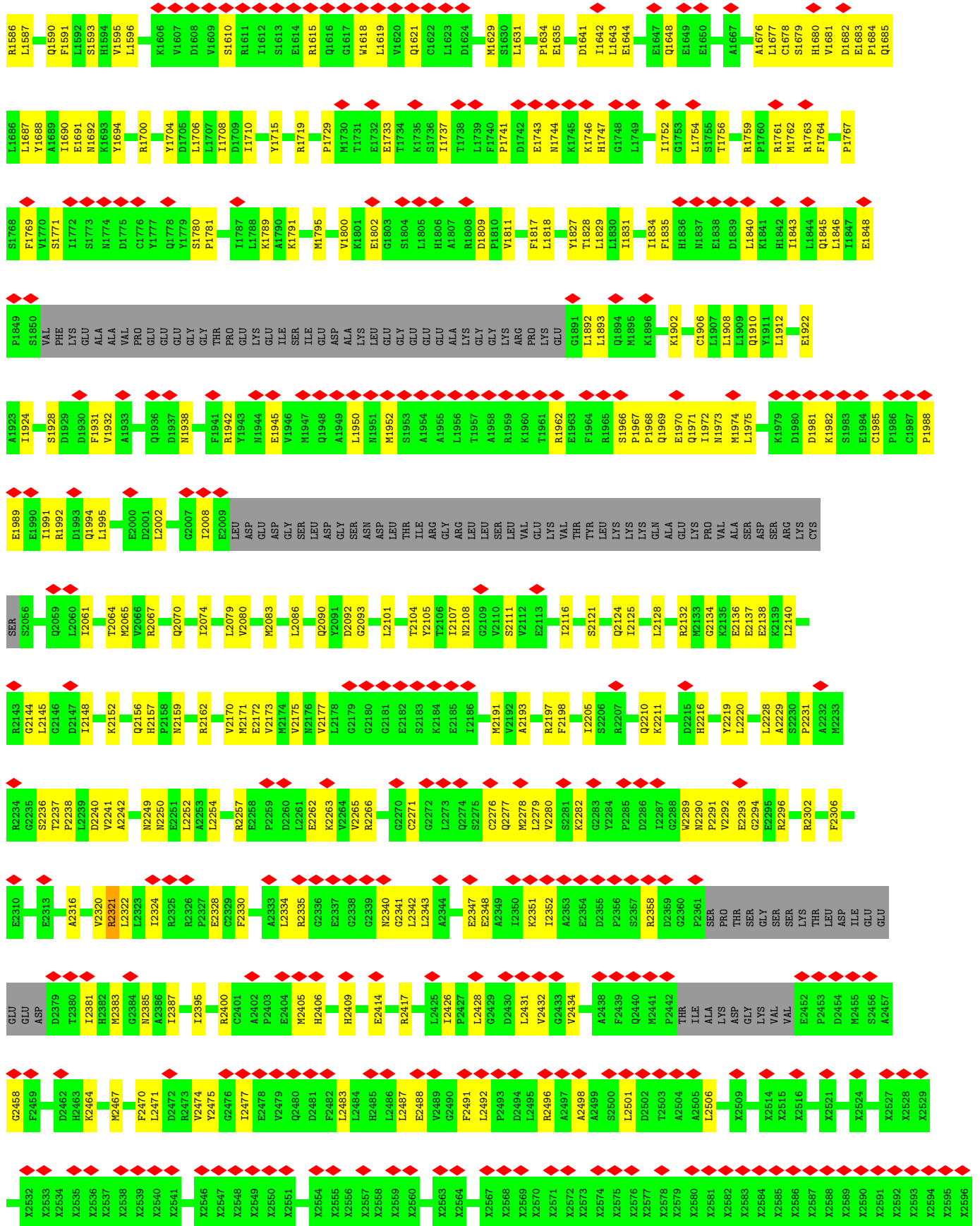
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Ryanodine receptor 2



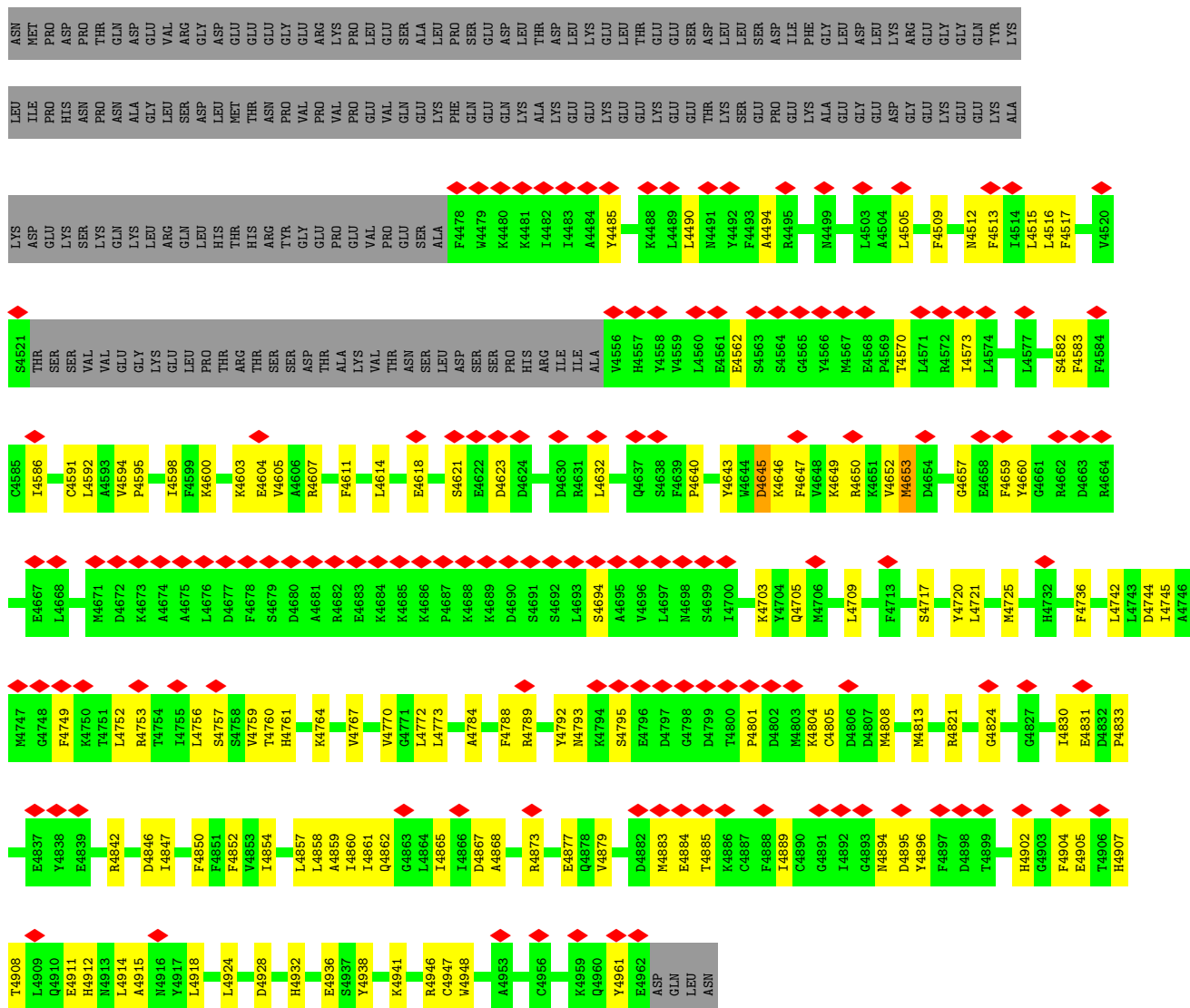




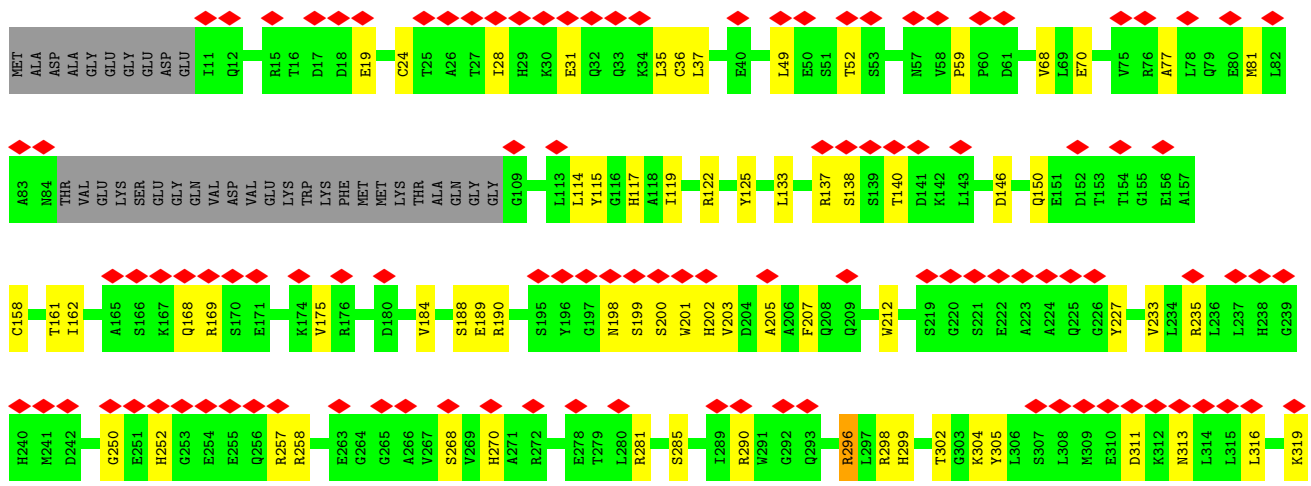
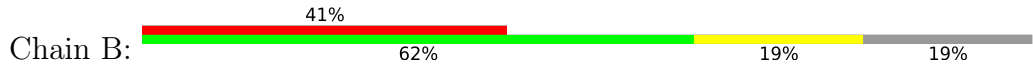
X2597	UNK	12720	T2780	A2840	Y2900	UNK	X3021	UNK	X3141	X3201	X3261	X3321
X2598	UNK	N2721	M2781	E2841	V2901	X2961	X3022	UNK	X3142	X3202	X3262	X3322
X2599	UNK	K2722	L2782	M2842	W2902	X2962	X3023	UNK	X3143	UNK	X3263	X3323
X2600	UNK	Y2723	A2783	M2843	S2903	X2963	X3024	UNK	X3144	UNK	X3264	X3324
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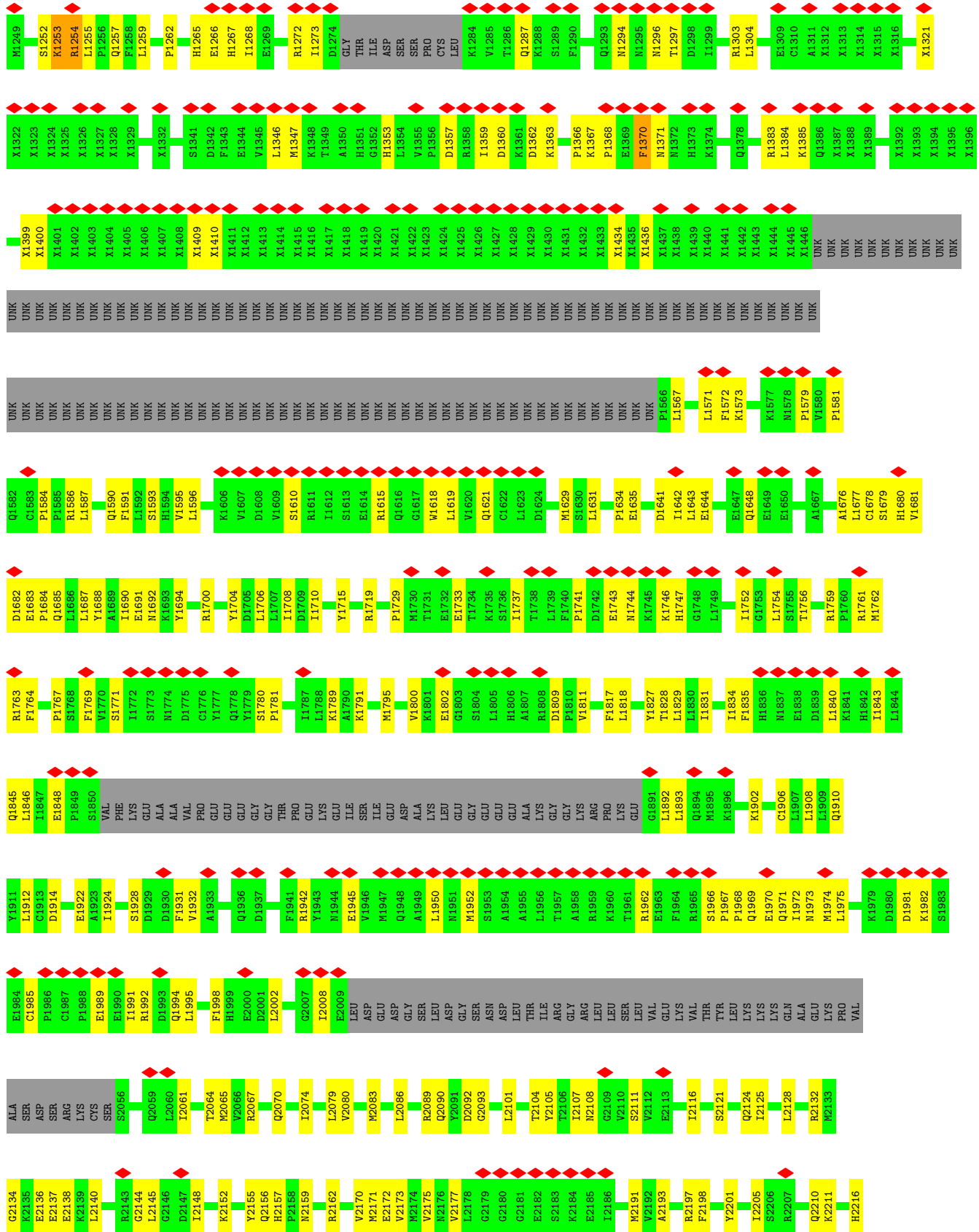




● Molecule 1: Ryanodine receptor 2



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G1179	D1112	L1050	P990	R930	S870	G809	P744	Y674	V778	E459	A382	A322
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D1183	S1118	V1054	A994	Q934	L874	F813	L748	V679	I988	E468	M884	K328
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D1185	P1120	T1056	V996	S936	H876	F815	T751	R750	E591	E473	A330	A320
S1186	G1121	L1057	D997	L937	H877	P816	D752	R750	K595	E473	F331	F329
S1187	C1122	L1058	K998	E938	L878	F817	D753	D753	L600	R478	R332	R332
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A1191	Y1062	N1002	N1002	T942	R882	A821	L759	T691	K603	E491	H995	H995
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F1195	GLU	N1005	N1005	A945	R884	E824	L761	R694	L611	L499	M999	M999
D1196	ALA	V1006	V1006	L946	L885	A825	S762	V695	D612	C501	D400	D400
V1197	PRO	W1007	W1007	G947	A886	W826	A763	M937	V625	I502	G402	G402
G1198	ASP	A1008	A1008	C948	E887	L827	P764	A698	N628	R503	G402	G402
D1199	ASP	R1009	R1009	R949	R888	E828	S765	S699	L631	S509	M403	M403
G1200	HIS	D1010	D1010	Y950	I889	K829	I766	T700	L637	A512	L405	L405
F1201	ALA	I1011	I1011	G951	E890	E830	S767	E701	L637	A512	S406	S406
I1202	ARG	I1012	I1012	I952	E891	K831	F768	G702	L641	A515	R407	R407
P1203	ALA	R1013	R1013	A953	L892	L832	R769	Y703	L642	D516	L406	L406
L1207	VAL	Q1014	Q1014	ASP	W894	K833	I770	Y706	L643	A517	S406	S406
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G1213	TYR	TYR	TYR	ALA	R896	H836	G772	G708	L646	R520	E412	E412
G1214	GLY	GLY	GLY	GLU	K897	S837	Q773	G709	Q645	G523	S413	S413
M1249	ILE	ILE	ILE	LYS	I898	R838	P774	G710	T646	G523	R414	R414
E1250	GLN	GLN	GLN	VAL	E899	E839	W778	E711	H651	E524	R417	R417
H1251	ASP	ASP	ASP	LYS	L900	Y840	F779	W713	V652	E524	V418	V418
Y1252	VAL	VAL	VAL	LYS	G901	K841	E780	W713	S653	I541	T422	T422
S1255	LYS	LYS	LYS	MET	W902	Q842	N781	G714	S654	C548	M427	M427
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G1233	L1032	L1032	L1032	L1032	D909	L850	F723	D722	L661	L558	H366	H366
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Y1226	G975	G975	G975	G975	N911	T854	S793	Y725	S664	L562	D367	D367
F1227	T1036	T1036	T1036	T1036	K912	W854	F794	G726	E665	E563	K438	K438
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M1267	K1043	K1043	K1043	K1043	Y919	ALA	F802	PHE	R802	I445	I445	I445
M1268	K1044	K1044	K1044	K1044	E920	PHE	R802	THR	R802	I446	I446	I446
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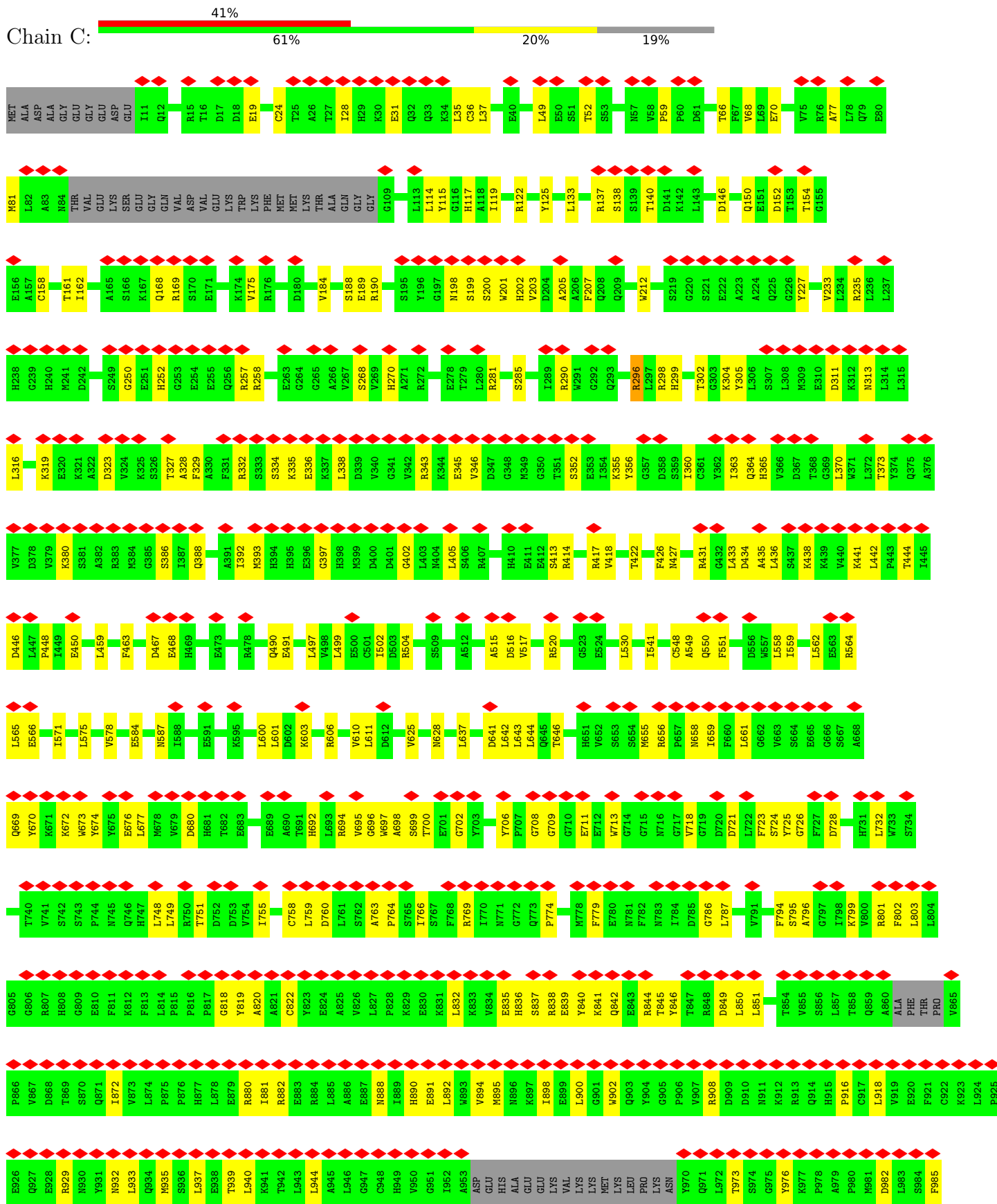








• Molecule 1: Ryanodine receptor 2













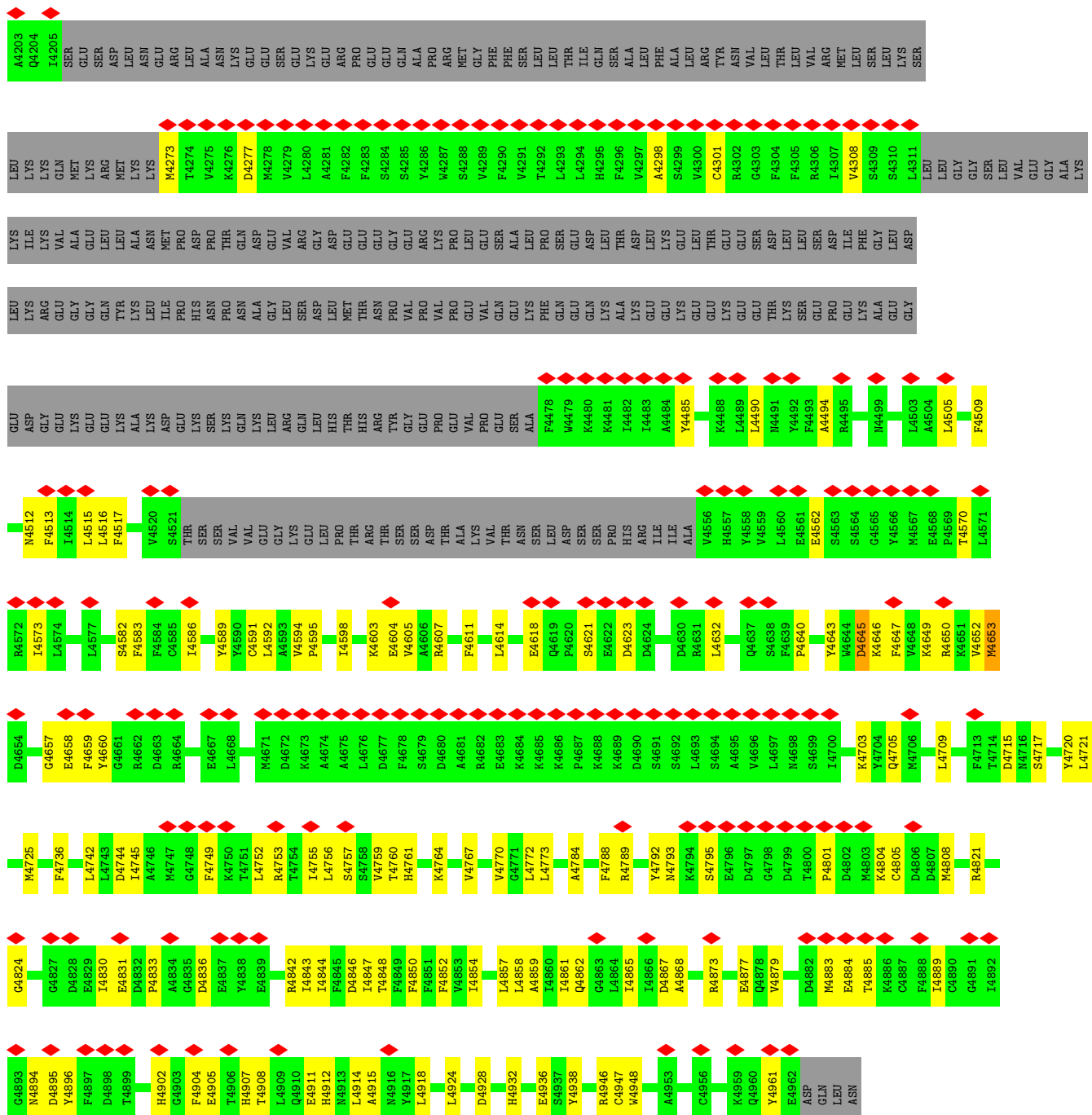
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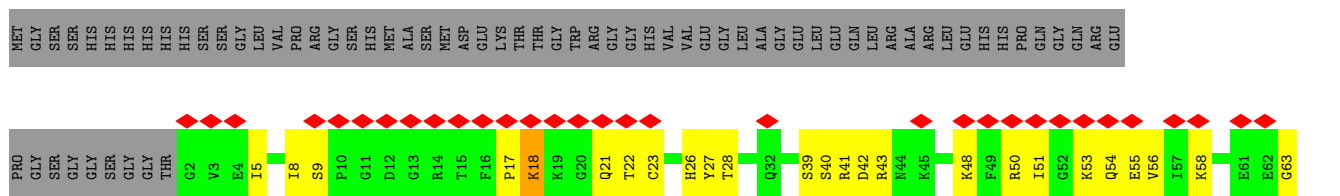


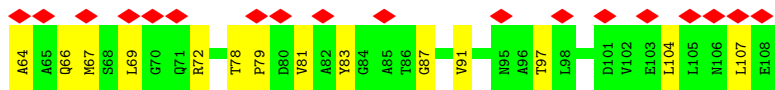
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X3251	X3311	X3371	X3431	X3491	X3551	P3611	V3786	G3883	E3986	H4054	M4126
X3252	X3312	X3372	X3432	X3492	X3552	R3612	Q3790	K3894	G3987	K4055	Q4129
X3253	X3313	X3373	X3433	X3493	X3553	H3613	L3795	D3895	N3988	H4056	L4132
X3254	X3314	X3374	X3434	X3494	X3554	R3614	M3796	I3896	V3989	T4057	R4134
X3255	X3315	X3375	X3434	X3494	X3554	A3616	C3799	I3896	N3991	Y4058	L4135
X3256	X3316	X3376	UNK	X3496	X3556	V3616	C3799	E3899	G3992	Q4059	E4136
X3257	X3317	X3377	UNK	X3497	X3557	F3619	L3802	Q3900	T3993	S4060	C4139
X3258	X3318	X3378	UNK	X3498	X3558	F3620	D3803	G3901	T3993	E4061	R4142
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X3261	X3321	X3381	UNK	X3501	X3561	E3629	R3809	I3909	S4005	F4064	C4139
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X3272	X3332	X3392	UNK	X3512	X3572	I3640	E3821	L3934	M4018	L4077	E4160
X3273	X3333	X3393	UNK	X3513	X3573	E3641	E3822	F4019	F4019	D4078	E4161
X3274	X3334	X3394	UNK	X3514	X3574	D3642	G3823	L3934	L4020	Y4079	R4162
X3275	X3335	X3395	UNK	X3515	X3575	L3643	S3824	R3838	K4021	E4080	R4162
X3276	X3336	X3396	UNK	X3516	X3576	A3644	G3825	L3939	K4023	E4081	K4165
X3277	X3337	X3397	UNK	X3517	X3577	K3645	E3826	W3940	D4024	F4082	E4166
X3278	X3338	X3398	UNK	X3518	X3578	A3648	K3827	D3941	L4025	V4083	S4167
X3279	X3339	X3399	UNK	X3519	X3579	LEU	V3828	A3942	L4026	K4084	R4168
X3280	X3340	X3400	UNK	X3520	UNK	P30	Q3850	F3943	S4027	R4085	R4169
X3281	X3341	X3401	UNK	X3521	UNK	GLU	Q3850	F3950	S4027	F4086	R4169
X3282	X3342	X3402	UNK	X3522	UNK	GLU	D3831	Q3954	S4029	H4087	F4173
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X3284	X3344	X3404	UNK	X3524	UNK	ALA	E3833	Q3964	T4030	K4091	M4177
X3285	X3345	X3405	UNK	X3525	UNK	MET	F3834	S3961	F4031	G4094	E4178
X3286	X3346	X3406	UNK	X3526	UNK	LYS	F3835	I3960	E4032	F4095	G4179
X3287	X3347	X3407	UNK	X3527	UNK	V3660	C3836	D3967	E4033	N4096	G4180
X3288	X3348	X3408	X3477	X3528	UNK	H3664	D3837	I3762	Y4034	V4097	E4181
X3289	X3349	X3409	X3478	X3529	UNK	H3664	R3840	I3764	D4035	A4098	E4182
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X3299	X3359	X3419	X3488	X3539	UNK	I3693	S3883	M3984	D4046	T4112	F4198
X3300	X3360	X3420	X3489	X3540	UNK	UNK	UNK	UNK	H4048	R4113	E4198
X3301	X3361	X3421	X3490	X3541	UNK	UNK	UNK	UNK	K4049	L4114	M4199
X3302	X3362	X3422	X3491	X3542	UNK	UNK	UNK	UNK	A4050	Q4115	A4202
X3303	X3363	X3423	X3492	X3543	UNK	UNK	UNK	UNK	M4051	T4116	UNK
X3304	X3364	X3424	X3493	X3544	UNK	UNK	UNK	UNK	E4052	UNK	UNK
X3305	X3365	X3425	X3494	X3545	UNK	UNK	UNK	UNK	UNK	UNK	UNK
X3306	X3366	X3426	X3495	X3546	UNK	UNK	UNK	UNK	UNK	UNK	UNK
X3307	X3367	X3427	X3496	X3547	UNK	UNK	UNK	UNK	UNK	UNK	UNK
X3308	X3368	X3428	X3497	X3548	UNK	UNK	UNK	UNK	UNK	UNK	UNK

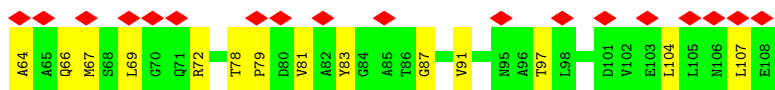
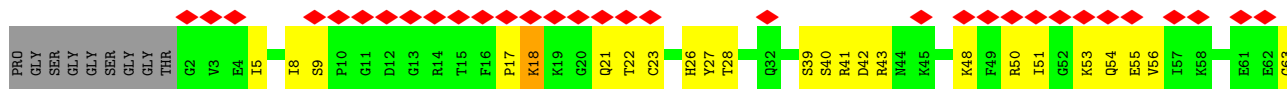


● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

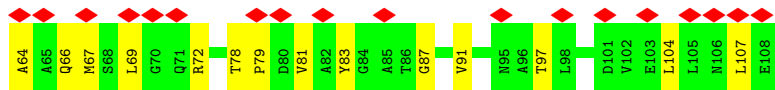
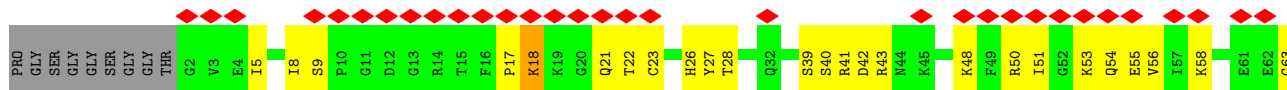




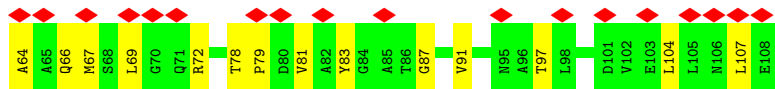
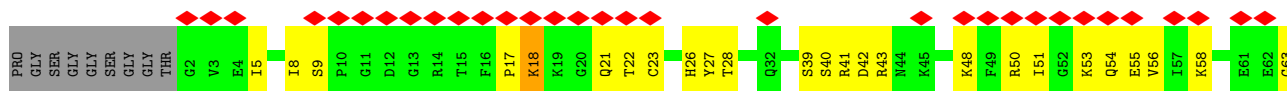
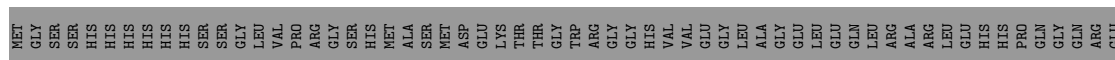
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10879	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)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.123	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.034	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.328, 1.328, 1.328	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.26	0/26891	0.52	3/36312 (0.0%)
1	B	0.27	0/26891	0.52	3/36312 (0.0%)
1	C	0.26	0/26891	0.52	3/36312 (0.0%)
1	D	0.26	0/26891	0.52	3/36312 (0.0%)
2	G	0.27	0/835	0.59	0/1123
2	H	0.27	0/835	0.59	0/1123
2	I	0.27	0/835	0.59	0/1123
2	J	0.27	0/835	0.59	0/1123
All	All	0.27	0/110904	0.52	12/149740 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4653	MET	CA-CB-CG	5.61	122.83	113.30
1	D	4653	MET	CA-CB-CG	5.60	122.81	113.30
1	A	4653	MET	CA-CB-CG	5.58	122.80	113.30
1	B	4653	MET	CA-CB-CG	5.57	122.76	113.30
1	B	4645	ASP	CB-CG-OD1	5.24	123.02	118.30

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	30067	0	26705	711	0
1	B	30067	0	26706	715	0
1	C	30067	0	26705	720	0
1	D	30067	0	26705	719	0
2	G	819	0	821	29	0
2	H	819	0	821	28	0
2	I	819	0	821	31	0
2	J	819	0	821	28	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	123552	0	110105	2918	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 12.

The worst 5 of 2918 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:A:2276:CYS:HB2	1:A:2279:LEU:HD23	1.55	0.88
1:B:1811:VAL:H	1:B:1818:LEU:HD12	1.38	0.88
1:A:4517:PHE:HB3	1:A:4562:GLU:HG3	1.56	0.88
1:C:1811:VAL:H	1:C:1818:LEU:HD12	1.39	0.88
1:B:4517:PHE:HB3	1:B:4562:GLU:HG3	1.56	0.88

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	3255/4966 (66%)	3052 (94%)	203 (6%)	0	100	100
1	B	3255/4966 (66%)	3051 (94%)	204 (6%)	0	100	100
1	C	3255/4966 (66%)	3052 (94%)	203 (6%)	0	100	100
1	D	3255/4966 (66%)	3053 (94%)	202 (6%)	0	100	100
2	G	105/176 (60%)	100 (95%)	5 (5%)	0	100	100
2	H	105/176 (60%)	100 (95%)	5 (5%)	0	100	100
2	I	105/176 (60%)	100 (95%)	5 (5%)	0	100	100
2	J	105/176 (60%)	100 (95%)	5 (5%)	0	100	100
All	All	13440/20568 (65%)	12608 (94%)	832 (6%)	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	2861/3386 (84%)	2847 (100%)	14 (0%)	88	94
1	B	2861/3386 (84%)	2847 (100%)	14 (0%)	88	94
1	C	2861/3386 (84%)	2847 (100%)	14 (0%)	88	94
1	D	2861/3386 (84%)	2847 (100%)	14 (0%)	88	94
2	G	88/140 (63%)	86 (98%)	2 (2%)	50	72
2	H	88/140 (63%)	86 (98%)	2 (2%)	50	72
2	I	88/140 (63%)	86 (98%)	2 (2%)	50	72
2	J	88/140 (63%)	86 (98%)	2 (2%)	50	72
All	All	11796/14104 (84%)	11732 (100%)	64 (0%)	89	94

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2771	ARG
1	D	3924	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	2735	LYS
1	B	2464	LYS
1	D	4049	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3974	GLN
1	D	3860	GLN
1	C	1287	GLN
1	D	3633	HIS
2	J	26	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

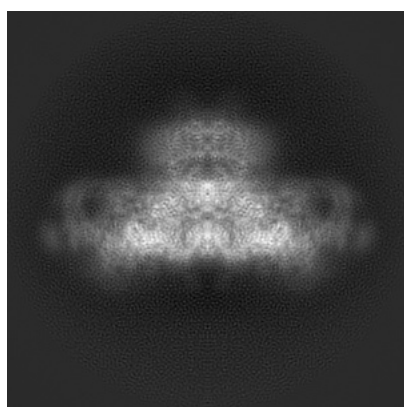
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32037. These allow visual inspection of the internal detail of the map and identification of artifacts.

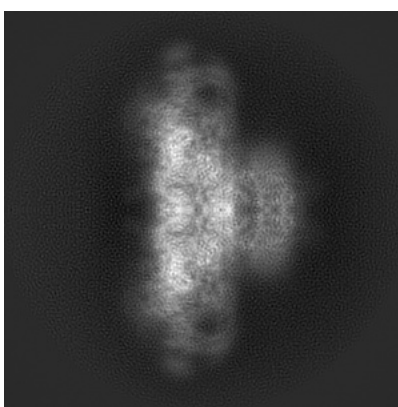
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

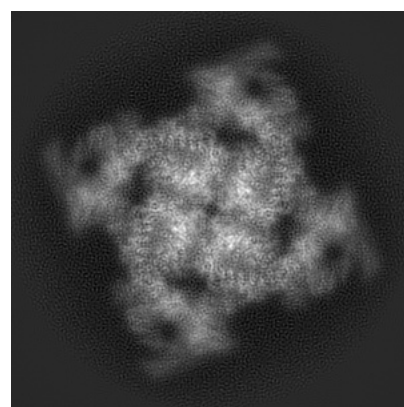
#### 6.1.1 Primary map



X



Y



Z

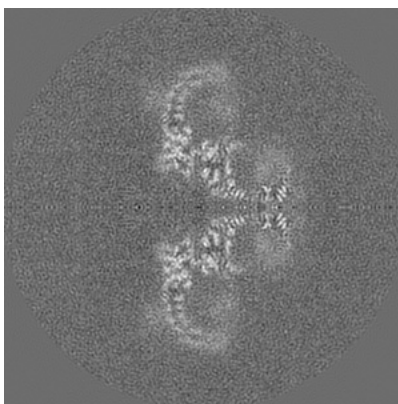
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

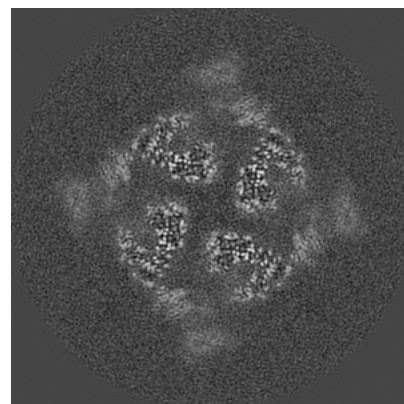
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

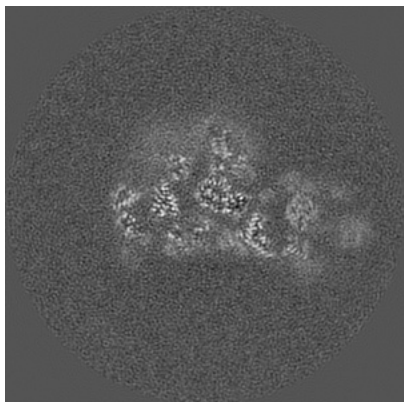


Z Index: 160

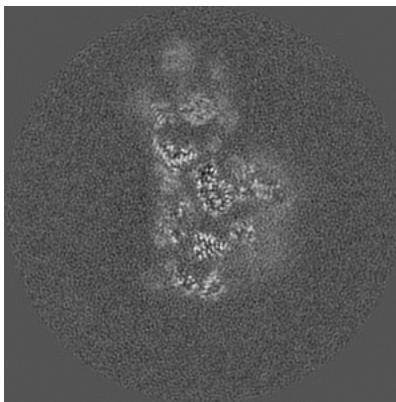
The images above show central slices of the map in three orthogonal directions.

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

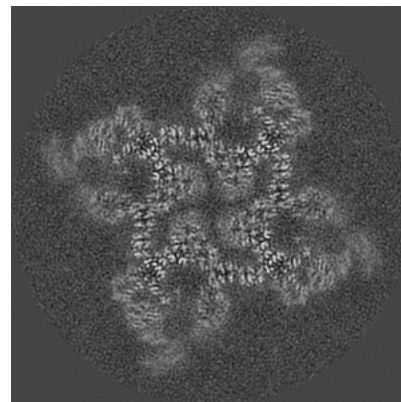
### 6.3.1 Primary map



X Index: 189



Y Index: 131



Z Index: 136

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

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

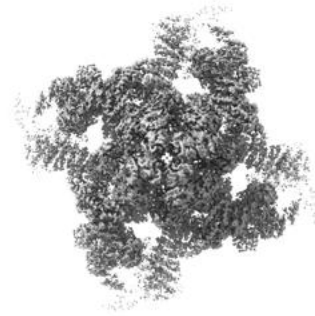
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

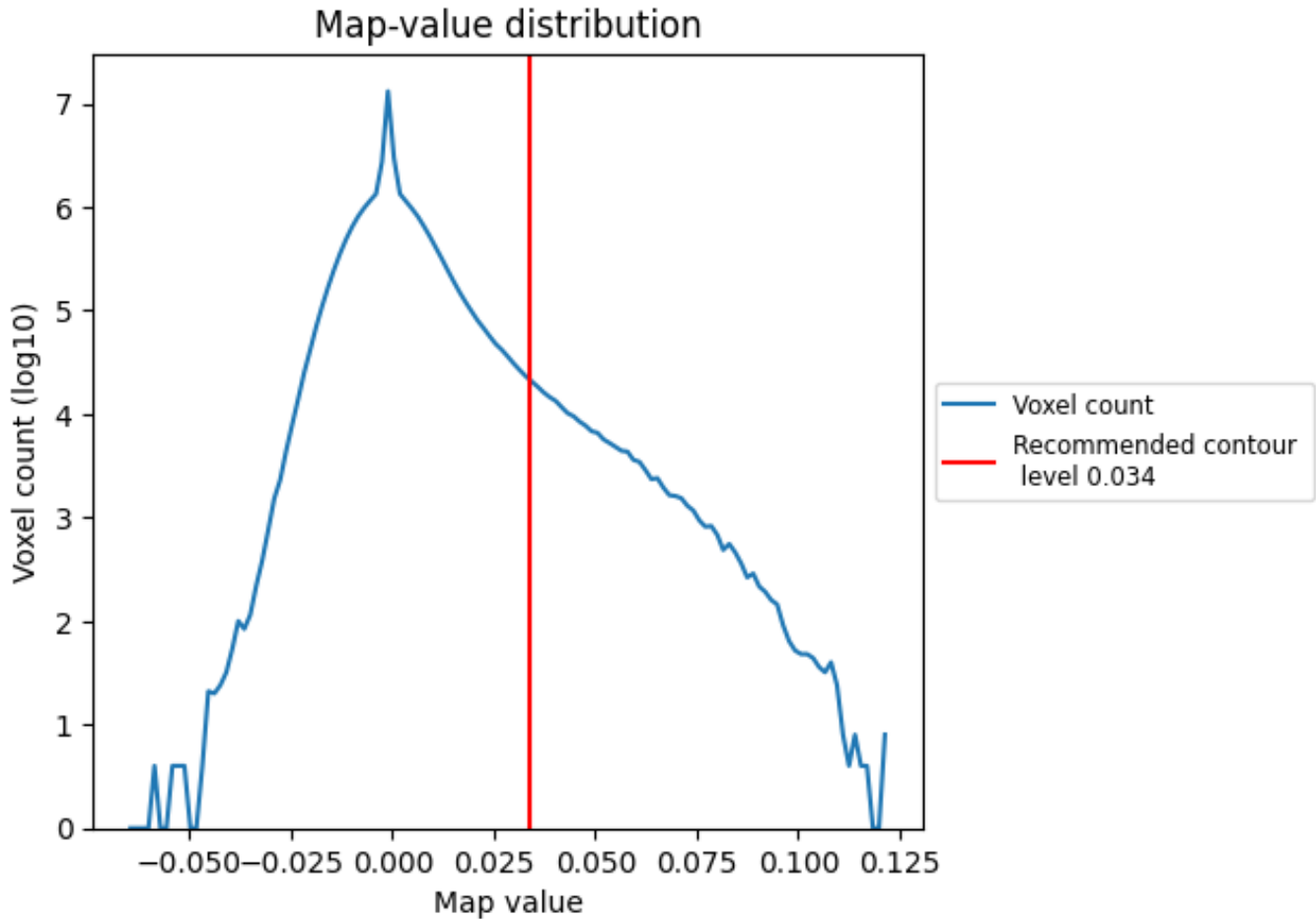
## 6.5 Mask visualisation

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.

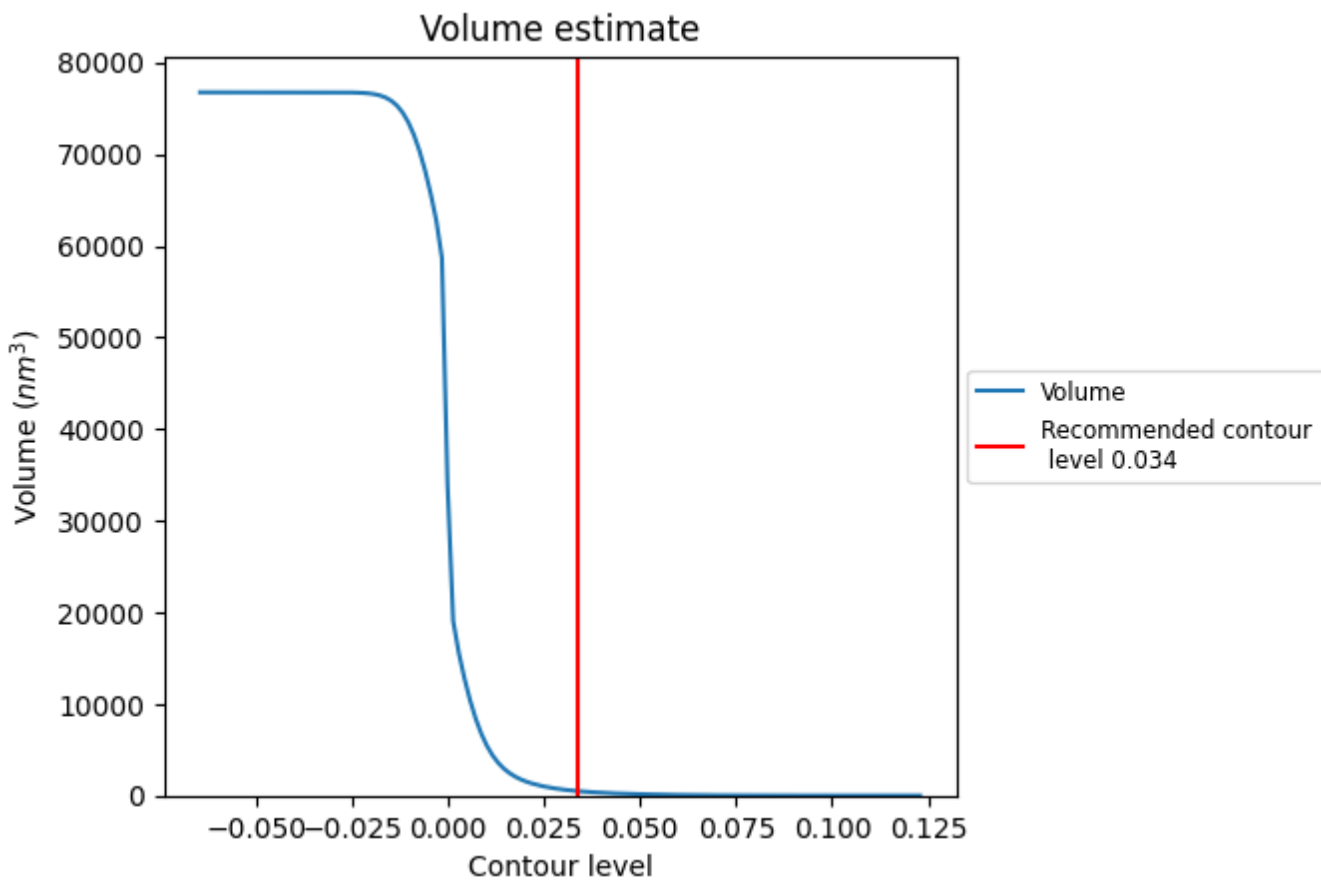
### 7.1 Map-value distribution [i](#)



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.



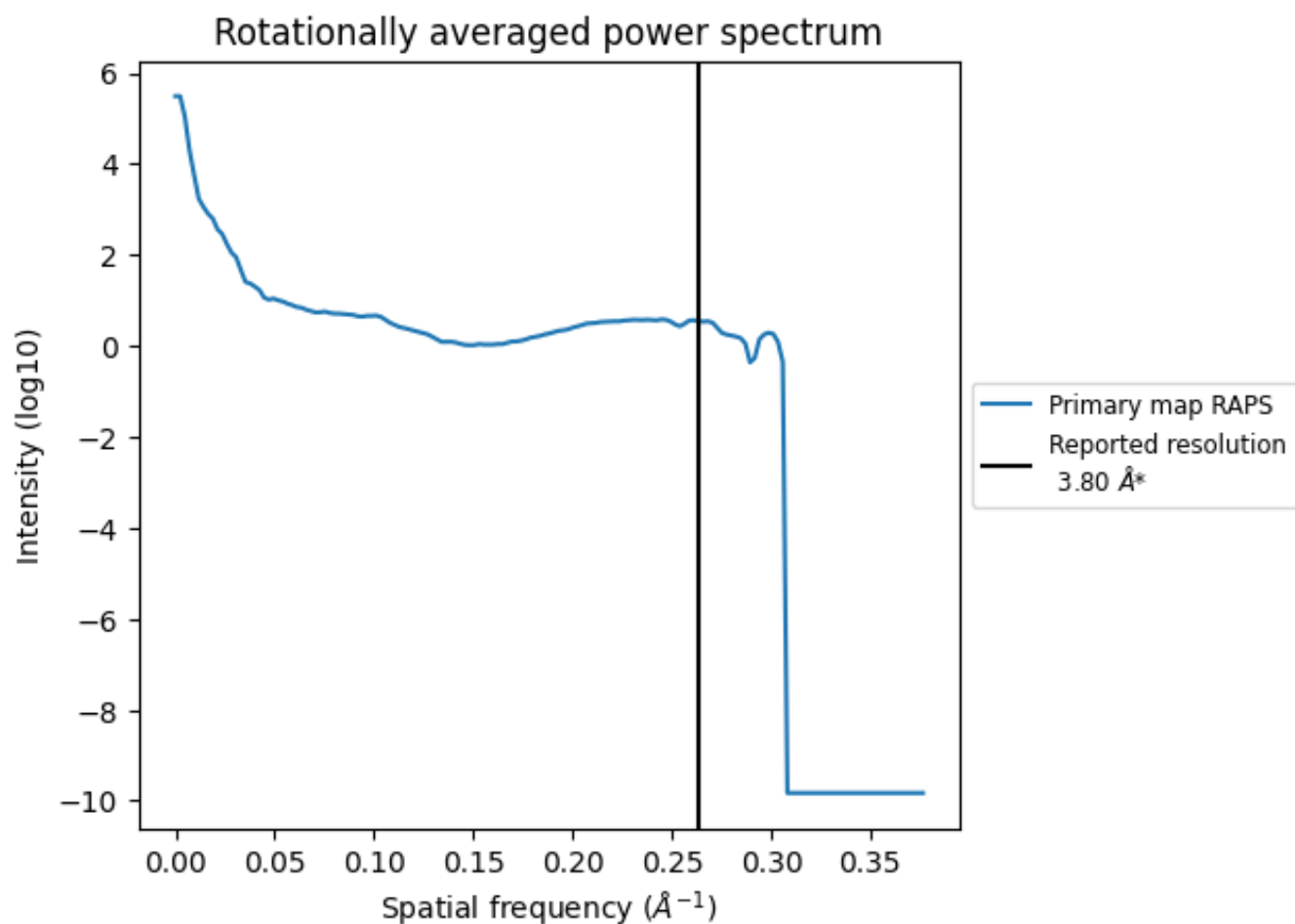
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 478 nm<sup>3</sup>; this corresponds to an approximate mass of 432 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 0.263 Å<sup>-1</sup>

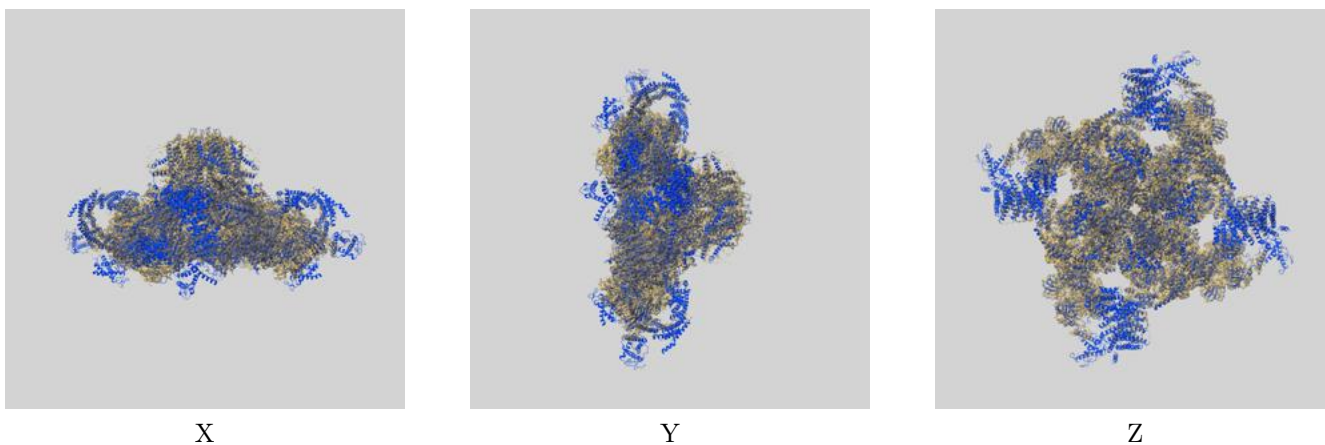
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

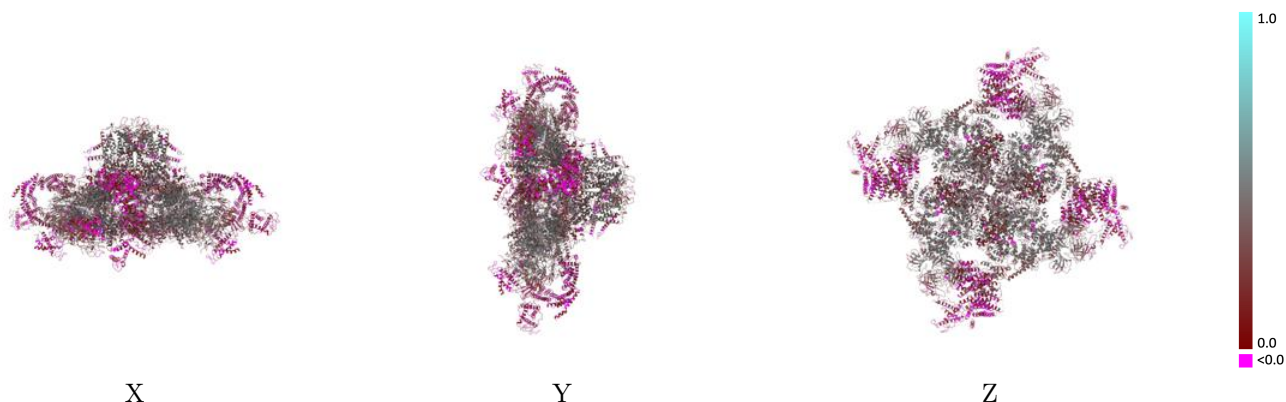
This section contains information regarding the fit between EMDB map EMD-32037 and PDB model 7VMS. Per-residue inclusion information can be found in section 3 on page 12.

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



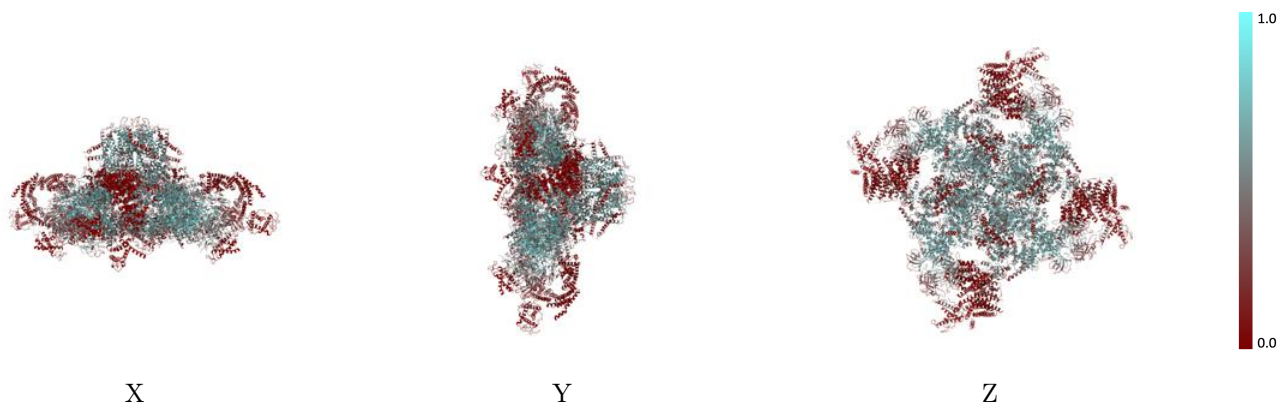
The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



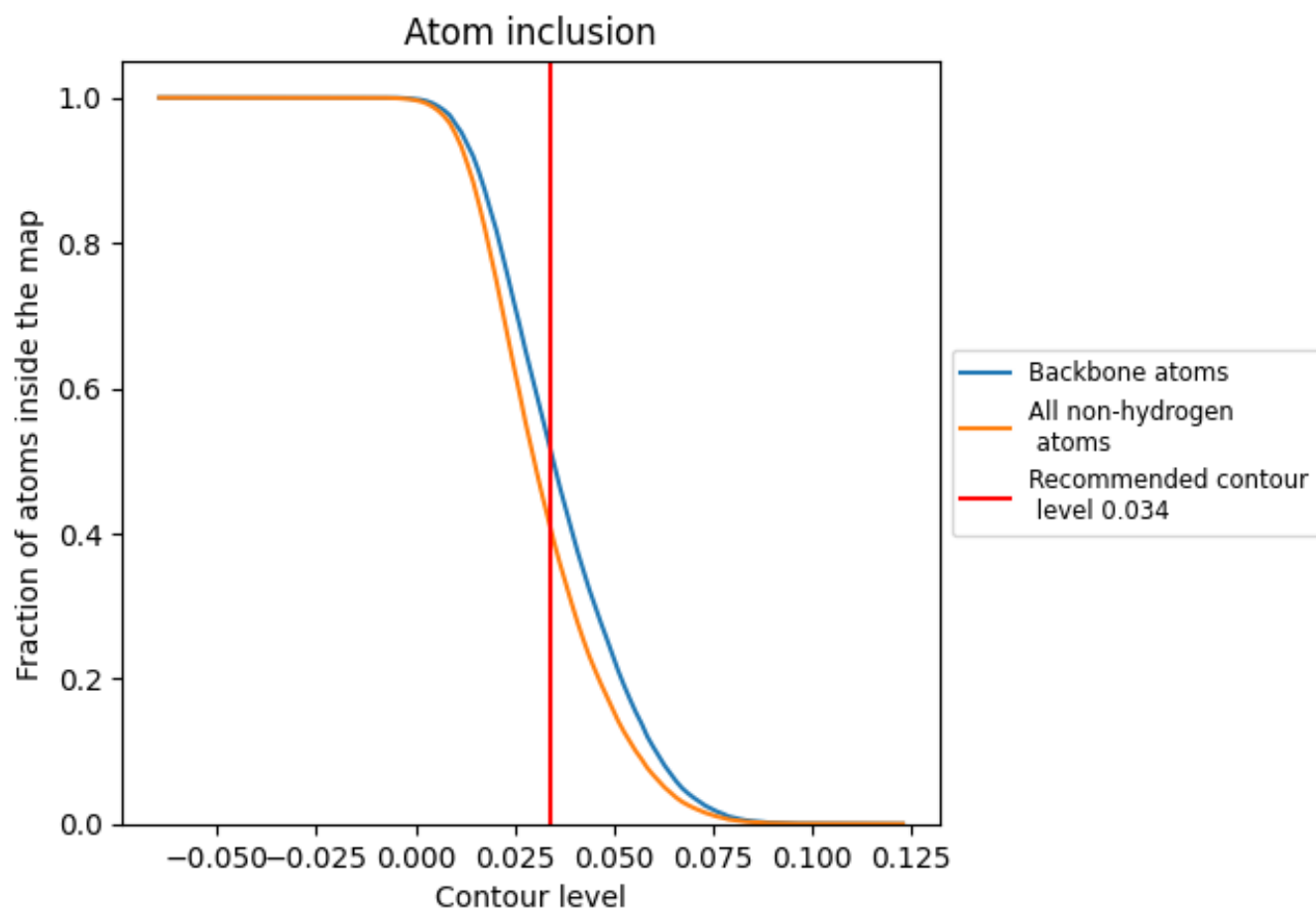
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.034).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 41% 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 (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4073	 0.2990
A	 0.4075	 0.2980
B	 0.4067	 0.2980
C	 0.4071	 0.2970
D	 0.4071	 0.2980
G	 0.4164	 0.3720
H	 0.4176	 0.3690
I	 0.4151	 0.3670
J	 0.4164	 0.3690

