



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 08:32 AM UTC

PDB ID : 7VMS / pdb_00007vms
EMDB ID : EMD-32037
Title : Structure of recombinant RyR2 mutant K4593A (Ca²⁺ 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

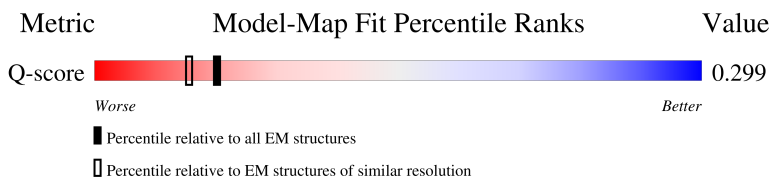
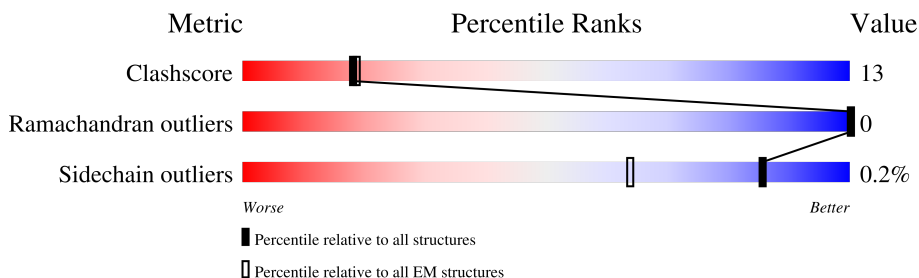
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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.



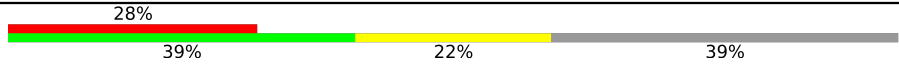
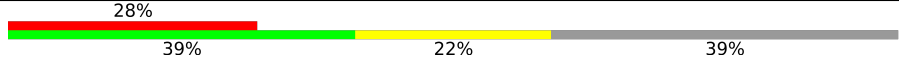
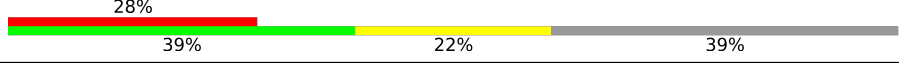
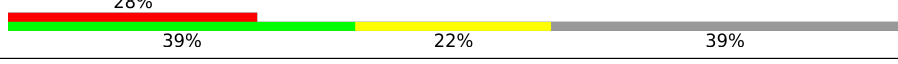
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	4966	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">41%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">61%</div> <div style="text-align: center;">20%</div> <div style="text-align: center;">19%</div> </div>
1	B	4966	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">41%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">61%</div> <div style="text-align: center;">20%</div> <div style="text-align: center;">19%</div> </div>
1	C	4966	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">41%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">61%</div> <div style="text-align: center;">20%</div> <div style="text-align: center;">19%</div> </div>
1	D	4966	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">41%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: center;">61%</div> <div style="text-align: center;">20%</div> <div style="text-align: center;">19%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (CCD ID: 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 (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
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

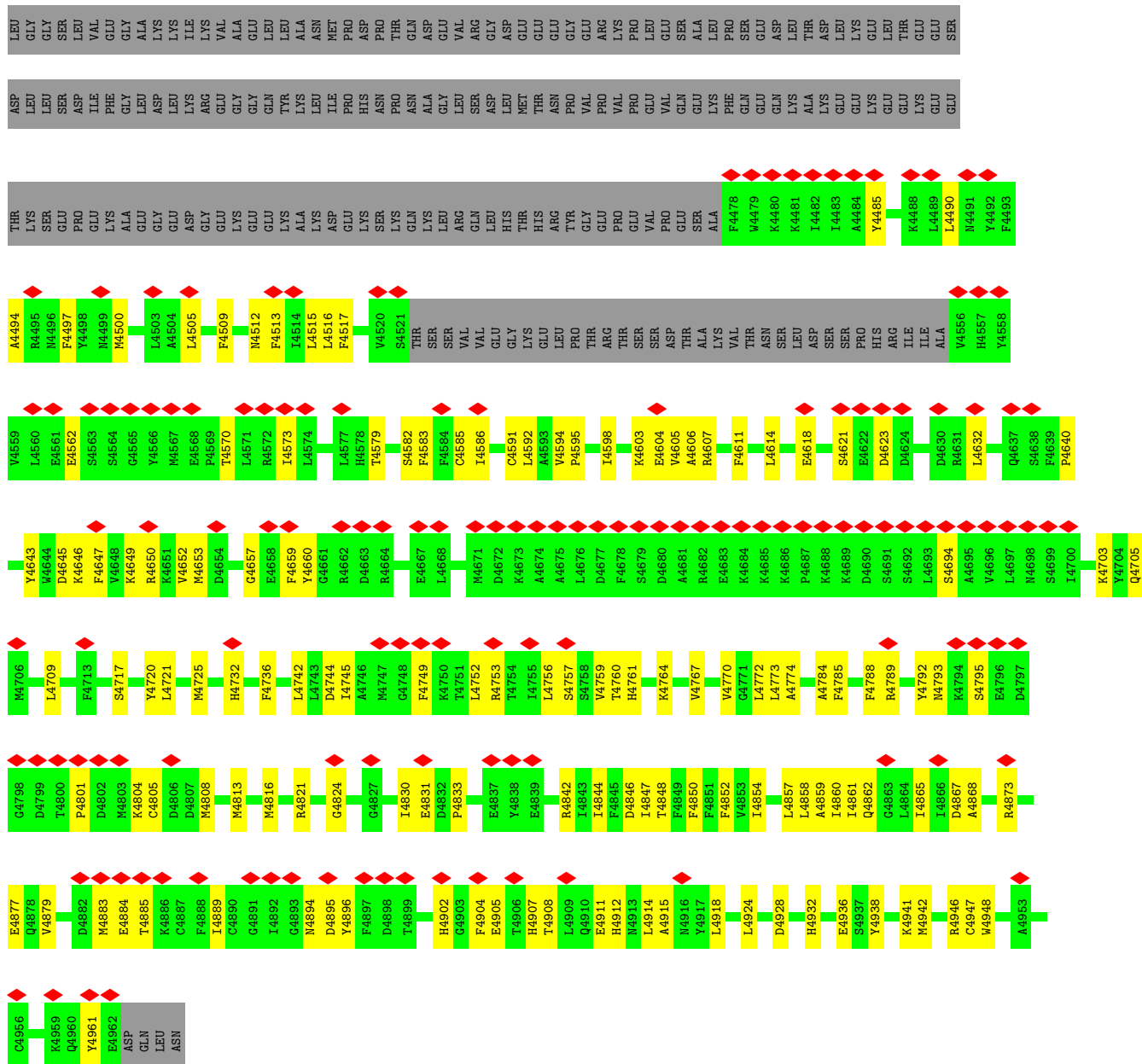
3 Residue-property plots

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.

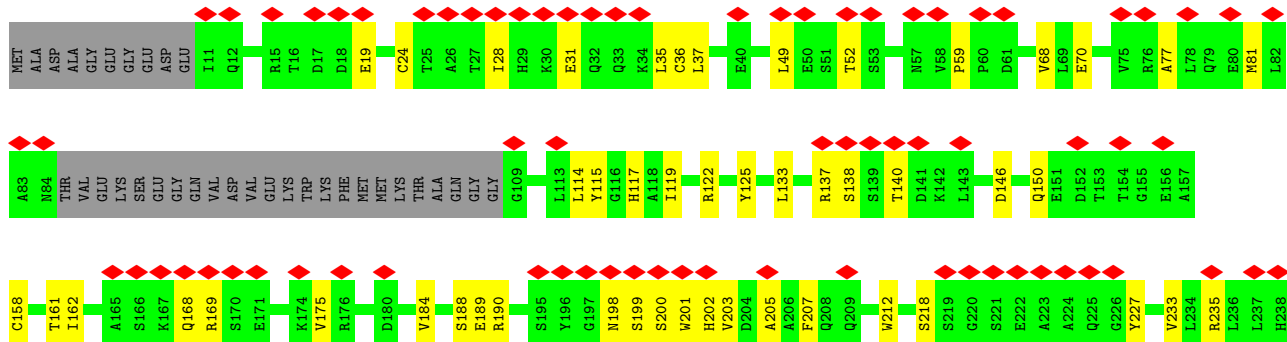
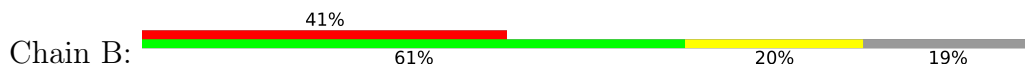
• Molecule 1: Ryanodine receptor 2



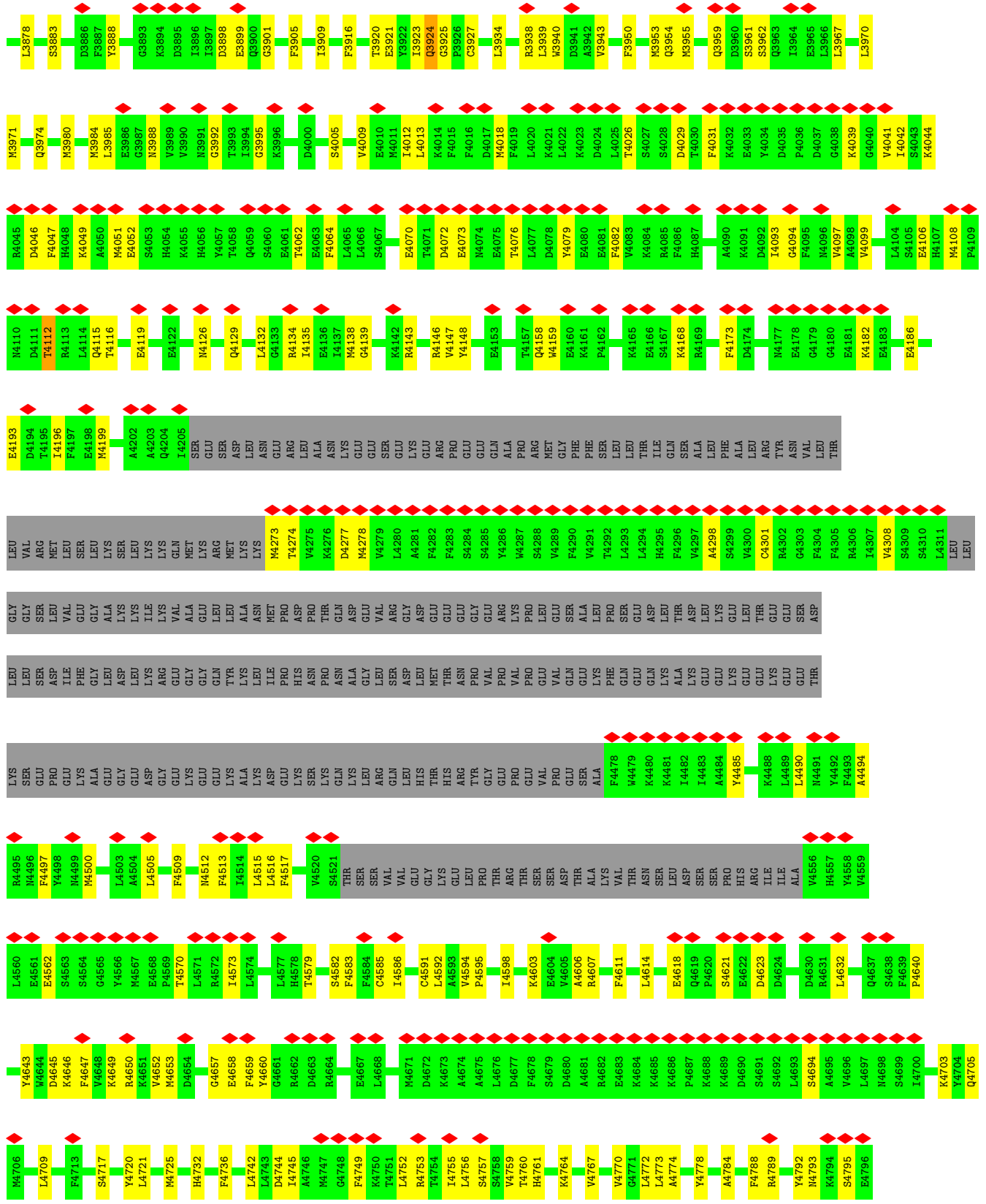
THR	M4110	R4045	M3971	L3878	E3782	K3696	X3552	X3492	X3432	X3372
LEU	D4111	D4046	Q3974	S3883	E3783	K3697	X3553	X3493	X3433	X3373
VAL	T4112	F4047	M3930	D3886	K3784	C3698	X3554	X3494	X3434	X3374
ARG	R4113	H4048	M3984	F3887	D3785	H3699	X3555	X3495	UNK	X3375
MET	L4114	K4049	K3984	Y3888	V3786	ASP	X3556	X3496	UNK	X3376
LEU	Q4115	A4050	L3985	Y3887	Q3790	GLU	X3557	X3497	UNK	X3377
LEU	T4116	E3986	L3986	F3887	Q3790	GLU	X3558	X3498	UNK	X3378
LYS	E4119	S4052	G3993	G3993	L3795	ASP	X3559	X3499	UNK	X3379
SER	A4202	S4053	K3894	K3894	M3796	ASP	X3560	X3500	UNK	X3380
SER	A4203	H4054	V3989	D3895	M3796	ASP	X3561	X3501	UNK	X3381
GLN	Q4204	H4055	V3990	I3896	GLY	GLY	X3562	X3502	UNK	X3382
SER	I4205	H4056	K3991	C3799	GLU	GLU	X3563	X3503	UNK	X3383
LYS	A4202	Y4057	G3992	L3802	GLU	GLU	X3564	X3504	UNK	X3384
LYS	Q4129	T4058	G3990	D3803	VAL	VAL	X3565	X3505	UNK	X3385
ARG	L4132	Q4059	I3991	A3806	LYS	SS712	X3566	X3506	UNK	X3386
GLU	G4133	S4060	F3905	R3809	E3714	F3634	X3567	X3507	UNK	X3387
GLU	R4134	E4061	I3909	A3813	E3715	F3635	X3568	X3508	UNK	X3388
ALA	I4135	F4063	F3905	A3814	E3716	K3645	X3569	X3509	UNK	X3389
ALA	E4136	F4064	I3909	E3814	K3716	E3636	X3570	X3510	UNK	X3390
LYS	I4137	L4066	F3916	G3815	E3717	L3639	X3571	X3511	UNK	X3391
GLU	M4138	L4066	T3920	G3816	E3718	I3640	X3572	X3512	UNK	X3392
GLU	G4139	S4067	Y3922	R3817	E3719	E3641	X3573	X3513	UNK	X3393
SER	K4142	E4070	I3923	M3818	L3723	D3642	X3574	X3514	UNK	X3394
GLU	R4143	T4071	Q3924	M3818	Q3726	L3643	X3575	X3515	UNK	X3395
LYS	R4146	T4071	Q3925	V3819	Q3727	A3644	X3576	X3516	UNK	X3396
GLU	V4147	D4072	F3926	T3820	A3728	K3645	X3577	X3517	UNK	X3397
ARG	V4148	F4073	C3927	E3821	R3729	A3648	X3578	X3518	UNK	X3398
PRO	E4153	M4074	M3930	E3822	L3730	GLU	X3579	X3519	UNK	X3399
GLU	E4157	E4075	L3934	G3823	D3732	LEU	UNK	X3520	UNK	X3400
GLN	T4157	T4076	M4018	S3824	R3731	PRO	UNK	X3521	UNK	X3401
ALA	T4157	L4076	F4019	E3826	H3740	GLU	UNK	X3522	UNK	X3402
PRO	Q4158	D4077	R3938	E3826	L3740	GLU	UNK	X3523	UNK	X3403
ARG	W4159	D4078	L3939	V3827	G3748	ASP	UNK	X3524	UNK	X3404
MET	W4159	Y4079	V3940	V3827	K3827	GLU	UNK	X3525	UNK	X3405
GLY	E4160	Y4079	D3941	V3828	V3828	ALA	UNK	X3526	UNK	X3406
PHE	K4161	E4080	A3942	L3829	P3752	LYS	UNK	X3527	UNK	X3407
PHE	P4162	E4081	V3943	Q3830	K3753	R3659	UNK	X3528	UNK	X3408
SER	K4165	F4082	F3950	R3831	I3754	V3660	UNK	X3529	UNK	X3409
LEU	E4166	V4083	F3950	D3832	T3757	H3664	UNK	X3530	UNK	X3410
LEU	S4167	K4084	M3953	E3833	L3758	H3664	UNK	X3531	UNK	X3411
THR	S4167	R4085	L3939	F3834	K3759	H3664	UNK	X3532	UNK	X3412
ILE	K4168	F4086	V3954	T3835	L3760	L3668	UNK	X3533	UNK	X3413
GLN	R4169	H4087	M3955	C3836	G3761	L3669	UNK	X3534	UNK	X3414
SER	R4169	H4087	M3955	C3837	I3762	L3669	UNK	X3535	UNK	X3415
ALA	F4173	A4090	Q3959	D3837	I3762	T3676	UNK	X3536	UNK	X3416
LEU	D4174	K4091	D3960	R3840	A3763	E3677	UNK	X3537	UNK	X3417
PHE	D4174	E4033	S3961	R3840	L3764	E3677	UNK	X3538	UNK	X3418
ALA	M4177	D4092	S3962	Q3843	I3769	K3678	UNK	X3539	UNK	X3419
LEU	M4177	I4093	S3963	Q3843	I3769	K3678	UNK	X3540	UNK	X3420
ARG	E4178	G4094	Q3963	H3849	K3776	L3681	UNK	X3541	UNK	X3421
TYR	G4179	F4095	I3964	H3849	K3776	L3681	UNK	X3542	UNK	X3422
ASN	G4179	M4096	E3965	Q3860	D3778	E3682	UNK	X3543	UNK	X3423
VAL	G4180	M4096	L3966	Q3860	D3778	E3683	UNK	X3544	UNK	X3424
LEU	E4181	V4097	L3967	Q3860	D3778	D3684	UNK	X3545	UNK	X3425
LEU	K4182	A4098	K4039	M3864	X3779	D3684	UNK	X3546	UNK	X3426
LEU	E4183	V4099	G4040	T3866	X3779	D3684	UNK	X3547	UNK	X3427
LEU	L4104	L4104	V4041	T3866	X3779	D3684	UNK	X3548	UNK	X3428
LEU	E4106	S4105	I4042	T3867	X3779	D3684	UNK	X3549	UNK	X3429
LEU	H4107	H4107	S4043	V3867	X3779	D3684	UNK	X3550	UNK	X3430
LEU	M4108	M4108	K4044	V3867	X3779	D3684	UNK	X3551	UNK	X3431
LEU	P4109	P4109	K4044	V3867	X3779	D3684	UNK	X3551	UNK	X3431

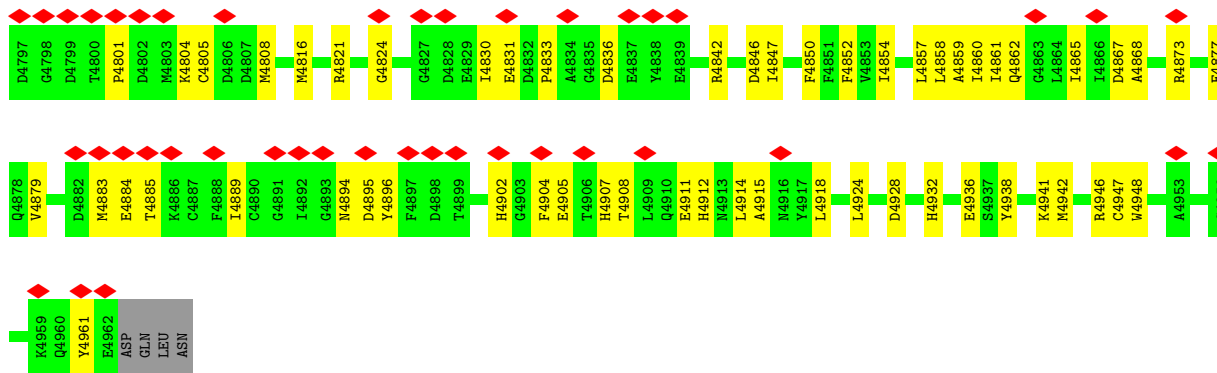


• Molecule 1: Ryanodine receptor 2

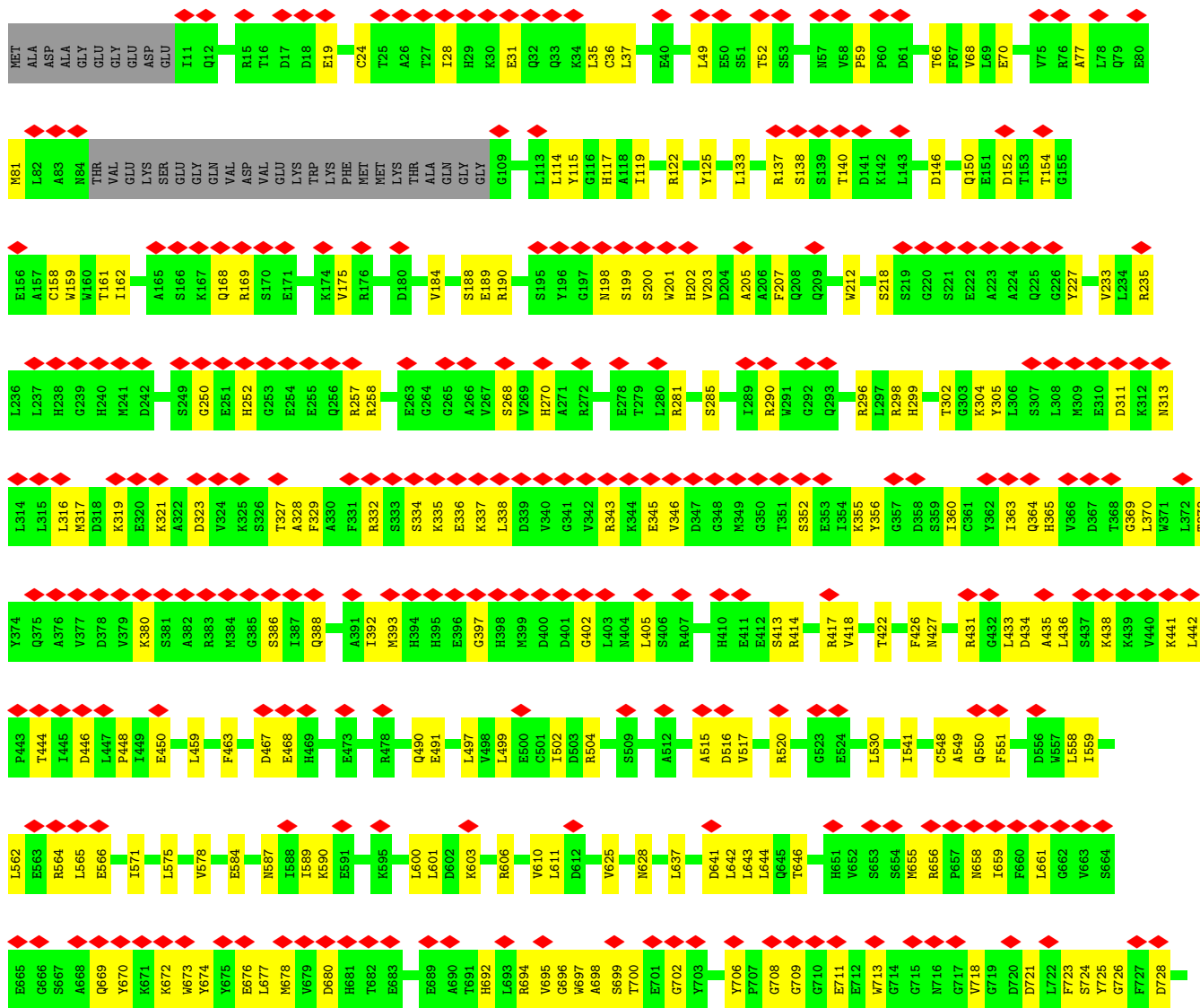
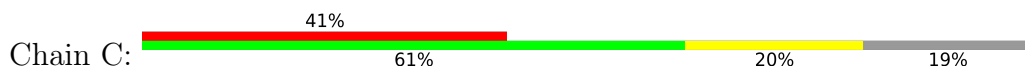


G239	H240	M241	D242	G250	E251	H252	G253	E254	E255	Q256	R257	F258	E263	G264	G265	A266	V267	S268	V269	H270	A271	R272	E278	T279	L280	R281	S285	I289	R290	W291	G292	Q293	R296	L297	R298	H299	T302	G303	K304	Y305	L306	S307	L308	M309	E310	D311	K312	N313	L314	L315	L316	M317										
D318	K319	E320	K321	A322	D323	V324	K325	S326	T327	A328	F329	A330	F331	R332	S333	S334	K335	E336	K337	G337	L338	D339	V340	G341	V342	R343	K344	E345	L346	V347	D347	G348	M349	G350	T351	S352	E353	I354	K355	Y356	G357	D358	S359	I360	Y362	I363	Q364	H365	V366	D367	T368	G369	L370	W371	L372	T373	Y374	Q375	A376	V377		
D378	V379	K380	S381	A382	R383	M384	G385	S386	E387	I388	Q388	A391	I392	M393	H394	H395	E396	H398	M399	D400	D401	G402	L403	M404	L405	S406	L407	H410	E411	E412	S413	R414	R417	V418	T422	F426	M427	R431	G432	L433	D434	A435	L436	S437	K438	K439	V440	L441	L442	P443	T444	I445	D446									
L447	P448	I449	E450	L459	F463	D467	E468	H469	E473	R478	Q490	E491	L497	V498	L499	E500	C501	I502	D503	R504	S509	A512	A515	D516	V517	R520	G523	E524	I541	C548	A549	Q550	F551	D556	W557	L558	I559	L562	E563	R564	L565	E566																				
I571	Q669	Y670	R671	K672	W673	Y674	Y675	E676	I677	M678	V679	D680	H681	T682	E683	E689	A690	T691	H692	L693	R694	V695	G696	W697	A698	S699	T700	E701	G702	Y703	Y706	T707	L708	L709	L710	L711	L712	L713	G714	G715	N716	G717	V718	G719	D720	D721	L722	F723	S724	Y725	G726	E727	D728	H731	L732	W733	S734					
T740	W741	S742	S743	P744	W745	G746	H747	L748	L749	R750	T751	D752	D753	W754	I755	C758	L759	D760	L761	S762	A763	P764	S765	T766	F768	R769	I770	W771	G772	G773	P774	W778	F779	E780	N781	F782	M783	I784	D785	G786	L787	W791	V792	S793	F794	S795	A796	G797	I798	K799	W800	R801	F802	L803								
L804	G805	G806	R807	H808	G809	E810	F811	K812	F813	L814	F815	F816	C818	Y819	A820	A821	C822	T823	E824	A825	H826	L827	P828	K829	E830	K831	L832	K833	H834	E835	H836	R837	R838	E839	Y840	K841	Q842	E843	R844	T845	Y846	T847	H848	D849	L850	L851	T854	W855	S856	L857	T858	Q859	A860	ALA	PHE	THR	PRO					
W865	P866	Y867	D868	T869	S870	Q871	L872	W873	L874	P875	P876	H877	E879	R880	L881	R882	E883	R884	L885	A886	E887	R888	I889	H890	E891	L892	W893	Y894	M895	H896	K897	L898	E899	L900	G901	W902	Q903	R904	G905	P906	Y907	R908	D909	D910	H911	K912	R913	Q914	H915	P916	C917	L918	Y919	E920	F921	C922	K923	L924				
P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	L943	L944	A945	L946	G947	C948	H949	V950	G951	I952	A953	ASP	GLU	TRP	THR	GLY	TYR	GLY	ILE	GLN	GLN	ASP	VAL	LYS	ASN	R1027	R1028	N1029	P1030	R1031	L1032	V1033	P1034	Y1035	T1036	K977	Q914	P978	A979	P980	M981	D982	L983	S984		
F985	I986	K987	L988	T989	P990	S991	Q992	E993	A994	M995	V996	D997	K998	L999	A1000	E1001	N1002	A1003	H1004	N1005	V1006	W1007	A1008	D1010	I1011	R1012	Y1013	Q1014	GLY	CYS	THR	GLY	THR	GLY	ILE	GLN	GLN	ASP	VAL	LYS	ASN	R1027	R1028	N1029	P1030	R1031	L1032	V1033	P1034	Y1035	T1036	K977	Q914	P978	A979	P980	M981	D982	L983	S984		
S1045	M1046	K1047	D1048	S1049	L1050	R1051	E1052	A1053	V1054	R1055	T1056	L1057	L1058	G1059	Y1060	G1061	HIS	LEU	GLU	ALA	PRO	ASP	GLN	ASP	HIS	ALA	SER	ARG	ALA	GLU	VAL	CYS	THR	GLY	THR	GLY	ILE	GLN	GLN	ASP	VAL	LYS	ASN	R1027	R1028	N1029	P1030	R1031	L1032	V1033	P1034	Y1035	T1036	K977	Q914	P978	A979	P980	M981	D982	L983	S984
F1087	F1088	R1089	A1090	E1091	Y1094	A1095	V1096	K1097	A1098	G1099	R1100	W1101	Y1102	F1103	E1104	F1105	E1106	D1131	D1132	R1133	A1134	F1137	D1138	G1139	F1140	K1141	A1142	Q1143	R1144	Q1147	G1148	N1149	E1150	H1151	Y1152	S1155	W1156	Q1157	A1158	G1159	D1160	V1161	L1162	G1163	CH164	M1165	V1166	D1167	M1168	N1169	E1170	M1173										



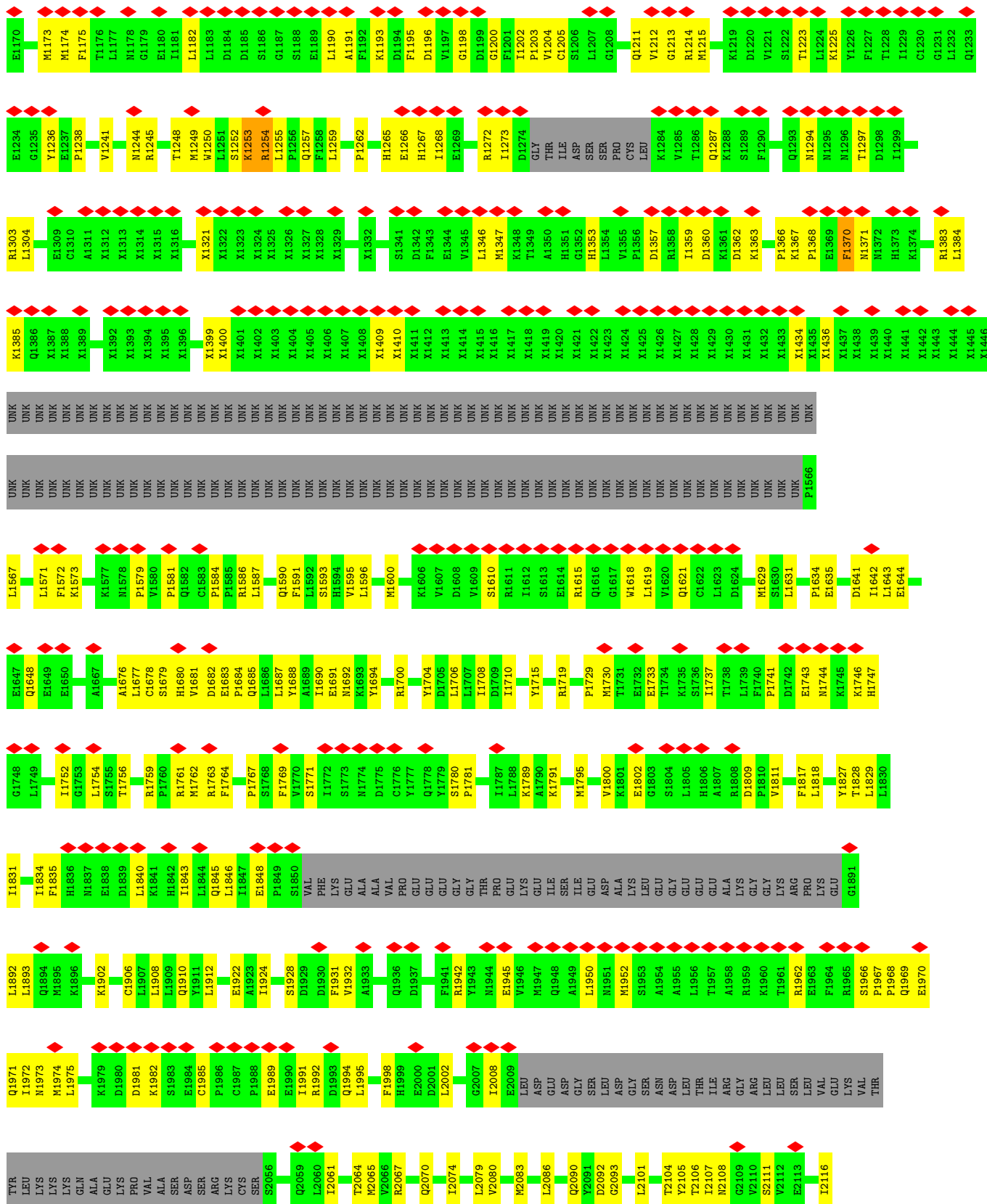


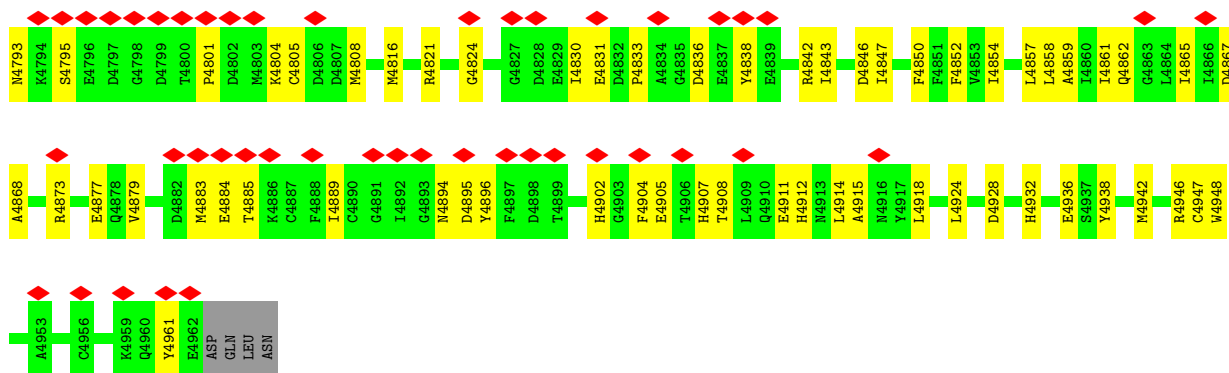
• Molecule 1: Ryanodine receptor 2



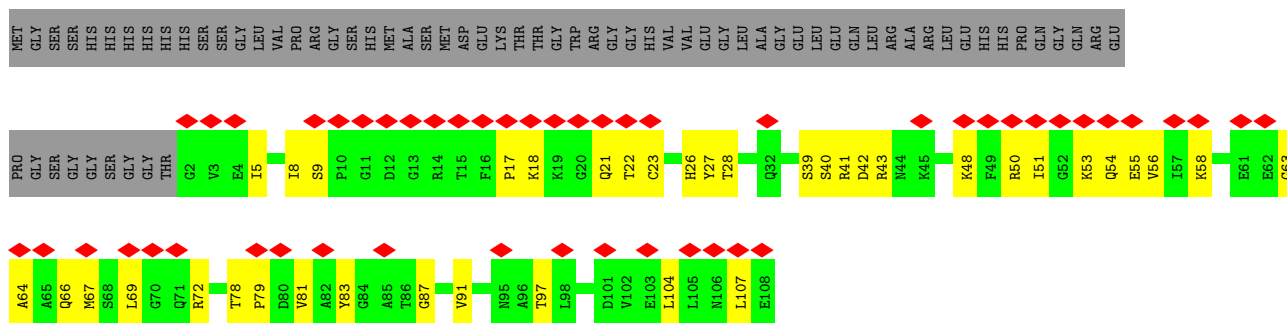
L2506	X2509	X2514	X2515	X2516	X2521	X2524	X2527	X2528	X2529	X2532	X2533	X2534	X2535	X2536	X2537	X2538	X2539	X2540	X2541	X2546	X2547	X2548	X2549	X2550	X2551	X2554	X2555	X2556	X2557	X2558	X2559	X2563	X2564	X2567	X2568	X2569	X2570	X2571	X2572	X2573	X2574	X2575	X2576	X2577	X2578	X2579	X2580	X2581	X2582							
M2441	P2442	THR	ILE	ALA	LYS	ASP	GLY	LYS	VAL	VAL	E2452	P2453	D2454	M2455	S2456	A2457	G2458	F2459	D2462	M2467	F2470	L2471	D2472	R2473	Y2474	Y2475	G2476	I2477	E2478	V2479	Q2480	F2481	F2482	L2483	L2484	H2485	L2486	L2487	E2488	V2489	G2490	F2491	L2492	P2493	D2494	L2495	R2496	A2497	A2498	A2499	S2500	L2501	D2502	T2503	A2504	A2505
L2279	V2280	K2281	K2282	G2283	Y2284	P2285	PRO	D2286	I2287	G2288	N2289	N2290	P2291	V2292	E2293	G2294	E2295	R2296	E2310	E2313	A2316	V2320	R2321	L2322	L2323	I2324	R2325	R2326	P2327	E2328	G2329	F2330	A2333	L2334	R2335	G2336	E2337	G2338	G2339	N2340	G2341	L2342	L2343	A2344	E2347	E2348	D2349	L2350	K2351	I2352	A2353	D2354	P2355	P2356		
C2196	R2197	F2198	I2205	S2206	R2207	Q2210	K2211	D2215	H2216	Y2219	L2220	L2228	S2230	P2231	A2232	M2233	R2234	G2235	S2236	T2237	P2238	D2240	L2241	A2242	N2249	M2250	E2251	L2252	A2253	L2254	R2257	E2258	P2259	D2260	L2261	E2262	V2264	R2265	G2270	C2271	G2272	Q2274	S2275	C2276	M2278											
L2119	A2120	S2121	Q2124	L2125	L2128	R2132	H2133	G2134	K2135	E2136	E2137	E2138	E2139	L2140	R2143	G2144	L2145	G2146	D2147	I2148	K2152	Q2156	H2157	P2158	L2160	M2161	R2162	V2170	M2171	E2172	V2173	M2174	V2175	D2092	N2176	V2177	L2178	G2179	K2180	G2181	E2182	S2183	K2184	E2185	L2186	M2191	V2192	A2193	N2194	C2195						
L1893	Q1894	M1895	K1896	K1902	C1906	L1907	L1908	L1909	Q1910	Y1911	L1912	C1913	D1914	E1922	A1923	I1924	S1928	D1929	D1930	F1931	M1932	A1933	Q1936	D1937	F1941	R1942	Y1943	M1944	E1945	V1946	M1947	Q1948	A1949	L1950	M1951	M1952	S1953	A1954	A1955	L1956	T1957	A1958	R1959	K1960	T1961	R1962	E1963	F1964	R1965	S1966	P1967	P1968	Q1969			
E1970	Q1971	I1972	M1973	M1974	L1975	K1979	D1980	D1981	K1982	S1983	E1984	C1985	P1986	C1987	E1988	E1989	E1990	I1991	R1992	D1993	Q1994	E2000	D2001	L2002	G2007	L2008	E2009	LEU	ASP	GLU	ASP	GLY	SER	LEU	ASP	GLY	ASN	ASP	GLY	THR	ILE	M2108	G2109	S2111	E2112	V2113	L2116									
LEU	LYS	LYS	LYS	GLN	ALA	LYS	PRO	VAL	ALA	SER	ASP	ARG	LYS	CYS	SER	S2056	Q2059	L2060	I2061	T2064	M2065	V2066	R2067	Q2070	I2074	L2079	V2080	M2083	L2086	R2089	Q2090	D2091	D2092	G2093	L2101	T2104	Y2105	I2107	M2108	G2109	S2111	E2112	V2113	L2116												
L1884	F1885	H1836	M1837	E1838	D1839	L1840	K1841	H1842	L1843	L1844	Q1845	L1846	I1847	E1848	P1849	S1850	VAL	PHE	LYS	GLU	ALA	ALA	VAL	PRO	GLU	GLU	GLU	GLY	GLY	THR	PRO	GLU	LYS	GLU	ILE	SER	ILE	GLY	ASP	ALA	LEU	GLY	GLY	GLY	ARG	PRO	LYS	GLU	G1891	L1892						
L1749	I1752	G1753	L1754	S1755	T1756	R1759	P1760	R1761	M1762	R1763	F1764	P1767	S1768	A1769	V1770	S1771	I1772	S1773	M1774	D1775	C1776	Y1777	Q1778	Y1779	S1780	P1781	I1787	L1788	K1789	A1790	K1791	M1795	P1729	M1730	T1731	E1732	E1733	T1734	K1735	S1736	I1737	T1738	L1739	F1740	P1741	D1742	E1743	M1744	K1745	K1746	H1747	G1748				
F1572	K1573	K1577	M1578	P1579	L1580	P1581	Q1582	C1583	P1584	E1585	R1586	L1587	Q1590	Y1591	L1592	S1593	H1594	V1595	L1596	M1600	K1606	D1607	D1608	L1609	S1610	R1611	I1612	S1613	E1614	R1615	Q1616	G1617	M1618	L1619	V1620	Q1621	C1622	L1623	D1624	M1629	S1630	L1631	P1634	E1635	D1641	I1642	L1643	E1644	E1647	Q1648	E1649					

L237	H238	G239	H240	M241	D242	S249	G250	E251	H252	G253	E254	E255	Q256	R257	R258	E263	G264	G265	A266	V267	S268	V269	S268	E278	T279	L280	R281	S285	I289	R290	V291	G292	Q293	R296	L297	R298	H299	T302	G303	Y304	Y305	L306	L307	S307	L308	M309	E310	D311	K312	N313	L314																																																																																																																																																			
L315	L316	M317	D318	K319	E320	K321	A322	D323	V324	K325	S326	T327	A328	F329	A330	F331	R332	S333	S334	K335	E336	K337	L338	D339	V340	D400	G341	R342	R343	K344	E345	V346	D347	G348	M349	G350	T351	S352	E353	I354	K355	Y356	G357	D358	S359	I360	G361	Y362	I363	Q364	D434	H365	S366	M367	T368	G369	L370	N371	L372	T373	Y374																																																																																																																																									
Q375	A376	V377	D378	V379	K380	S381	A382	R383	M384	G385	S386	I387	Q388	A391	I392	M393	H394	H395	E396	G397	H398	M399	D400	D401	C402	L403	M404	L405	S406	R407	H410	E411	E412	S413	R414	R417	V418	T422	F426	N427	R431	G432	L433	D434	A435	L436	S437	K438	V439	V440	K441	L442	P443																																																																																																																																																	
T444	I445	D446	L447	P448	I449	E450	L459	F463	D467	E468	H469	E473	R478	Q490	E491	L497	V498	L499	E500	C501	I502	D503	R504	S509	A512	A515	D516	V517	R520	G523	E524	L530	I541	C548	A549	Q550	F551	D556	H557	L558	I559	L562	E563	R564	L565	E566	I571	L575	V578	E584	N587	I588	I589	K590	E591	K595	L600	L601	D602	K603	R606	V610	L611	D612	V625	N628	L637	D641	L642	L643	L644	Q645	T646	H651	V652	S653	S654	M655	R656	P657	M658	G659	F660	L661	G662	S664	E665	G666	S667	A668	Q669	V670	K671	K672	M673	Y674	Y675	E676	L677	M678	V679	D680	H681	T682	E683	E689	A690	D692	T691	H692	L693	R694	V695	G696	M697	A698	S699	T700	E701	G702	Y703	D706	Y707	G708	G709	G710	E711	E712	M713	G714	G715	N716	G717	V718	G719	D720	L721	F723	S724	Y725	G726	F727	D728	H731	L732	M733	S734	T740	V741	S742	P744	N745	O746	H747	L748	L749	R750	T751	D752	D753	V754	I755	S756	C757	C758	L759	D760	L761	S762	A763	P764	S765	T766	F768	R769	I770	M771	G772	Q773	P774	M778	F779	E780	N781	F782	N783	I784	D785	G786	L787	V791	F794	S795	A796	G797	L798	K799	V800
R801	F802	L803	L804	G805	G806	R807	H808	G809	E810	F811	K812	F813	L814	P815	F816	C818	Y819	A820	A821	C822	Y823	E824	A825	Y826	L827	R828	E830	K831	L832	K833	H834	E835	H836	S837	R838	E839	K841	R842	F843	R844	T845	Y846	T847	R848	D849	L850	L851	T854	V855	S856	L857	T858	R859	ALA	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	E883	R884	A885	A886	E887	R888	H889	E891	L892	H893	V894	M895	H896	E897	ALA	GLY	THR	THR	ALA	GLY	GLY	ILE	LYS	VAL	LYS	LYS	LYS	LYS	LYS	LEU	PRO	PRO	ASN	Y970	Q971	L972	T973	S974	G975	Y976	K977	P978	A979	P980	M981																																																																													
PHE	THR	PRO	V865	P866	V867	D868	T869	S870	O871	I872	V873	L874	P875	H876	H877	L878	E879	R880	I881	R882	E883	R884	L885	A886	E887	R888	H889	E891	L892	H893	V894	M895	H896	E897	ALA	GLY	THR	THR	ALA	GLY	GLY	ILE	LYS	VAL	LYS	LYS	LYS	LYS	LEU	PRO	PRO	ASN	Y970	Q971	L972	T973	S974	G975	Y976	K977	P978	A979	P980	M981																																																																																																																																						
C922	K923	L924	P925	E926	Q927	E928	R929	N930	Y931	N932	L933	Q934	M935	S936	L937	E938	T939	L940	K941	T942	L943	L944	A945	L946	G947	C948	H949	V950	G951	L952	A953	ASP	GLY	GLU	HIS	THR	THR	ALA	GLY	GLY	ILE	LYS	VAL	LYS	LYS	LYS	LEU	PRO	PRO	ASN	Y970	Q971	L972	T973	S974	G975	Y976	K977	P978	A979	P980	M981																																																																																																																																								
D982	L983	S984	F985	I986	K987	L988	T989	P990	S991	Q992	E993	A994	M995	V996	D997	K998	L999	A1000	E1001	N1002	HIS	A1003	LEU	LEU	ALA	ALA	PRO	ASP	ASP	ASP	HIS	ALA	ALA	ARG	ALA	GLU	VAL	CYS	TRP	THR	THR	GLY	GLY	ILE	LYS	GLN	GLN	ASP	VAL	LYS	LYS	LYS	ASN	R1027	R1028	P1030	Y1094	A1095	V1096	K1097	V1098	G1099	R1100	H1101	Y1102	F1103																																																																																																																																				
T1042	K1043	K1044	S1045	M1046	K1047	D1048	S1049	L1050	R1051	E1052	A1053	V1054	M1055	T1056	L1057	L1058	G1059	Y1060	G1061	Y1062	HIS	A1003	LEU	LEU	ALA	ALA	PRO	ASP	ASP	ASP	HIS	ALA	ALA	ARG	ALA	GLU	VAL	CYS	TRP	THR	THR	GLY	GLY	ILE	LYS	GLN	GLN	ASP	VAL	LYS	LYS	LYS	ASN	R1027	R1028	P1030	Y1094	A1095	V1096	K1097	V1098	G1099	R1100	H1101	Y1102	F1103																																																																																																																																				
E1104	F1105	E1106	A1107	V1108	T1109	A1110	G1111	D1112	M1113	G1116	S1118	L1119	P1120	G1121	C1122	Q1123	P1124	D1125	L1126	E1127	D1131	D1132	R1133	A1134	F1137	D1138	G1139	F1140	K1141	A1142	Q1143	R1144	Q1147	G1148	N1149	E1150	H1151	Y1152	S1155	V1156	Q1157	A1158	G1159	D1160	V1161	V1162	G1163	C1164	M1165	V1166	D1167	M1168	N1169																																																																																																																																																	

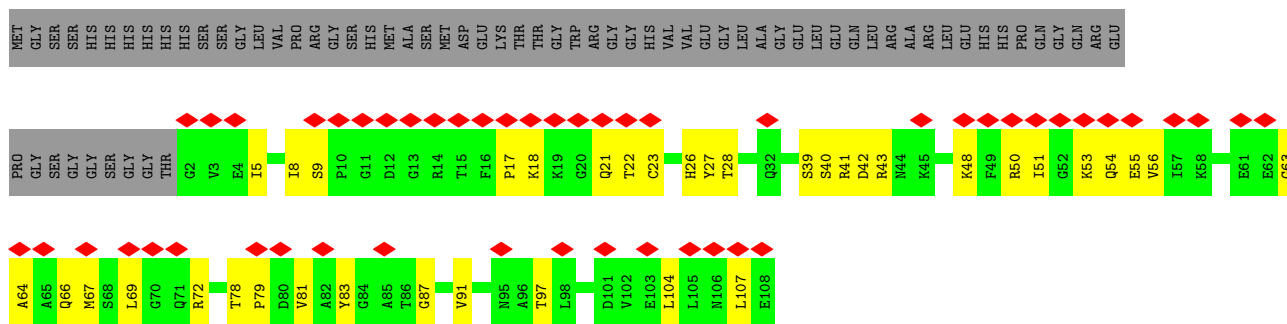




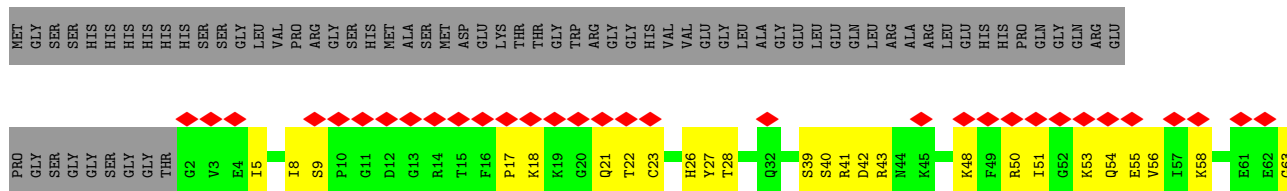
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• 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 (\AA)	424.96, 424.96, 424.96	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	0.14	1/26891 (0.0%)	0.37	0/36312
1	B	0.15	1/26891 (0.0%)	0.38	0/36312
1	C	0.15	1/26891 (0.0%)	0.38	0/36312
1	D	0.15	1/26891 (0.0%)	0.38	0/36312
2	G	0.13	0/835	0.41	0/1123
2	H	0.13	0/835	0.42	0/1123
2	I	0.13	0/835	0.42	0/1123
2	J	0.13	0/835	0.41	0/1123
All	All	0.15	4/110904 (0.0%)	0.38	0/149740

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4606	ALA	C-N	5.67	1.41	1.33
1	A	4606	ALA	C-N	5.64	1.41	1.33
1	D	4606	ALA	C-N	5.64	1.41	1.33
1	B	4606	ALA	C-N	5.60	1.41	1.33

There are no bond angle outliers.

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	756	0
1	B	30067	0	26706	754	0
1	C	30067	0	26705	759	0
1	D	30067	0	26705	760	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	29	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	3081	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 13.

The worst 5 of 3081 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:C:1629:MET:HE3	1:C:1685:GLN:HE21	1.35	0.92
1:D:1629:MET:HE3	1:D:1685:GLN:HE21	1.34	0.92
1:B:1629:MET:HE3	1:B:1685:GLN:HE21	1.35	0.92
1:A:1629:MET:HE3	1:A:1685:GLN:HE21	1.35	0.90
1:A:2276:CYS:HB2	1:A:2279:LEU:HD23	1.55	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%)	2856 (100%)	5 (0%)	87	87
1	B	2861/3386 (84%)	2856 (100%)	5 (0%)	87	87
1	C	2861/3386 (84%)	2856 (100%)	5 (0%)	87	87
1	D	2861/3386 (84%)	2856 (100%)	5 (0%)	87	87
2	G	88/140 (63%)	87 (99%)	1 (1%)	65	73
2	H	88/140 (63%)	87 (99%)	1 (1%)	65	73
2	I	88/140 (63%)	87 (99%)	1 (1%)	65	73
2	J	88/140 (63%)	87 (99%)	1 (1%)	65	73
All	All	11796/14104 (84%)	11772 (100%)	24 (0%)	85	87

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1370	PHE
2	I	9	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	4112	THR
1	D	1253	LYS
1	B	1253	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 156 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	26	HIS
1	D	2308	ASN
1	D	150	GLN
1	D	1265	HIS
1	D	3954	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

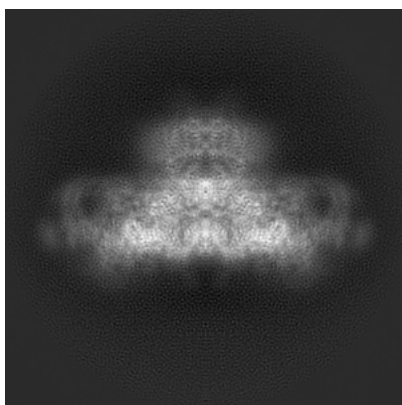
6 Map visualisation [i](#)

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.

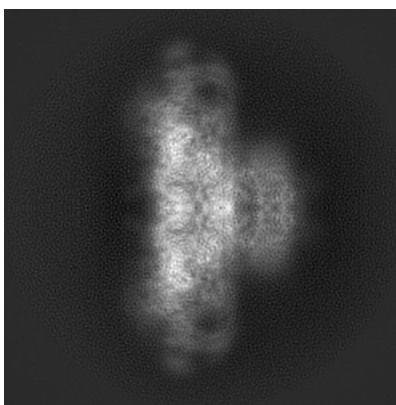
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

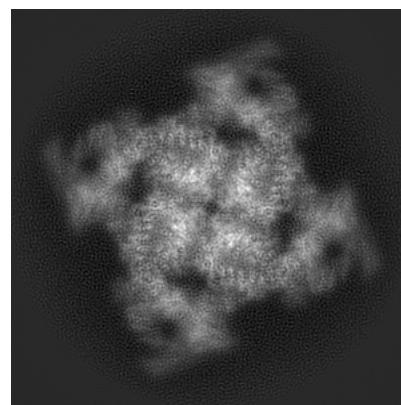
6.1.1 Primary map



X



Y



Z

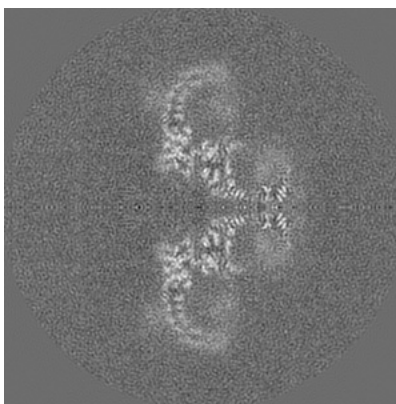
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

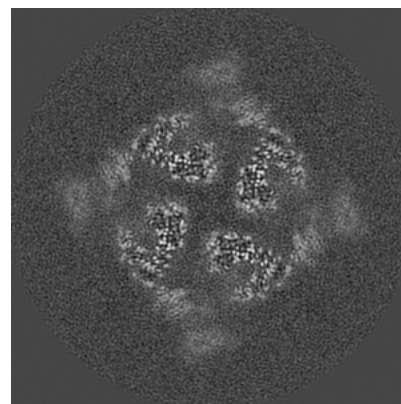
6.2.1 Primary map



X Index: 160



Y Index: 160

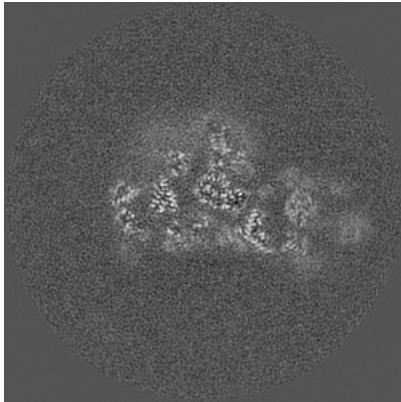


Z Index: 160

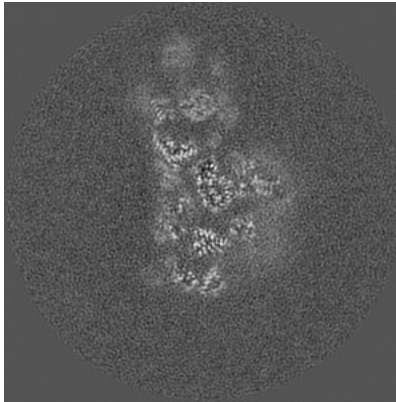
The images above show central slices of the map in three orthogonal directions.

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

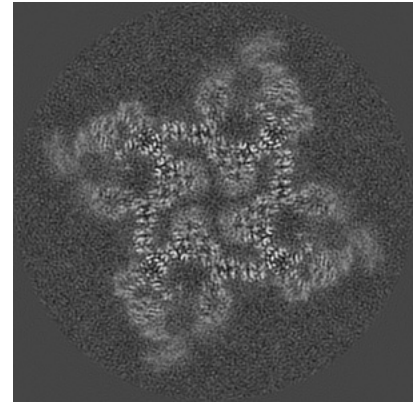
6.3.1 Primary map



X Index: 189



Y Index: 131

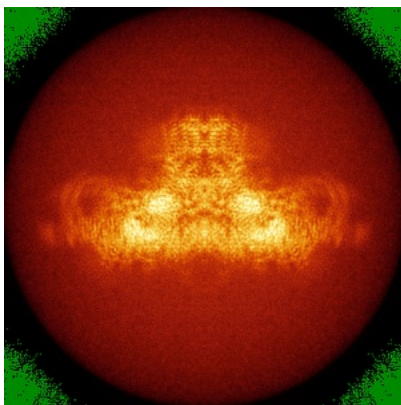


Z Index: 136

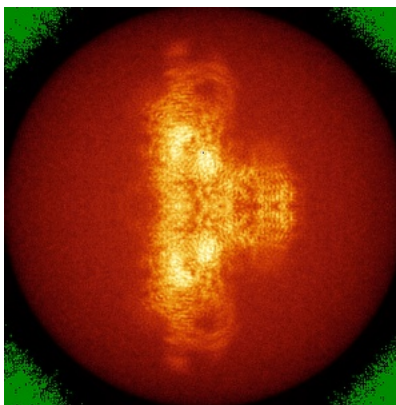
The images above show the largest variance slices of the map in three orthogonal directions.

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

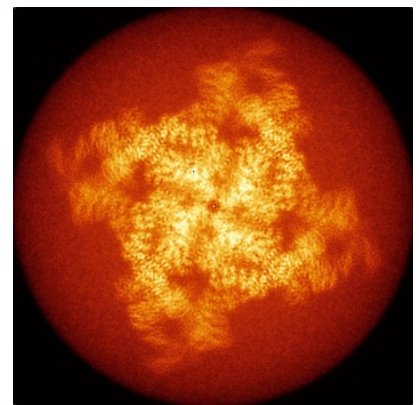
6.4.1 Primary map



X



Y

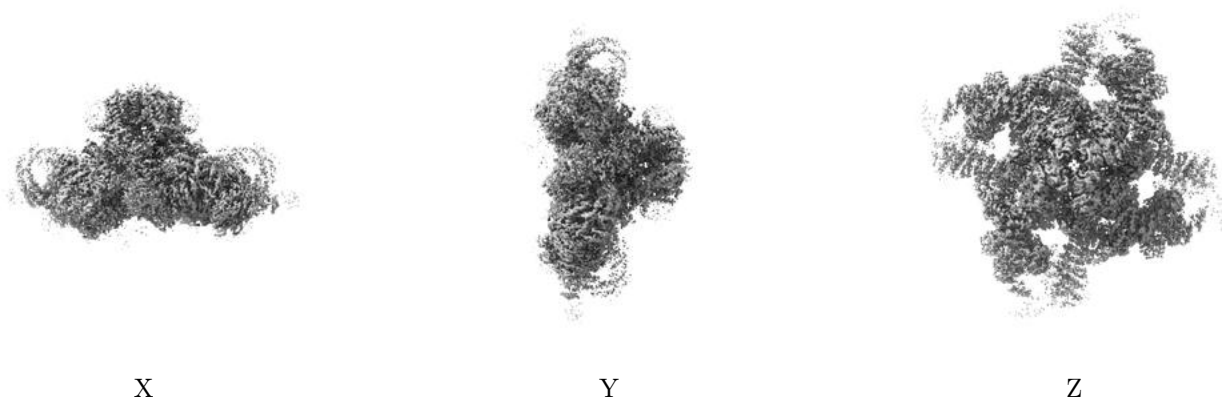


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

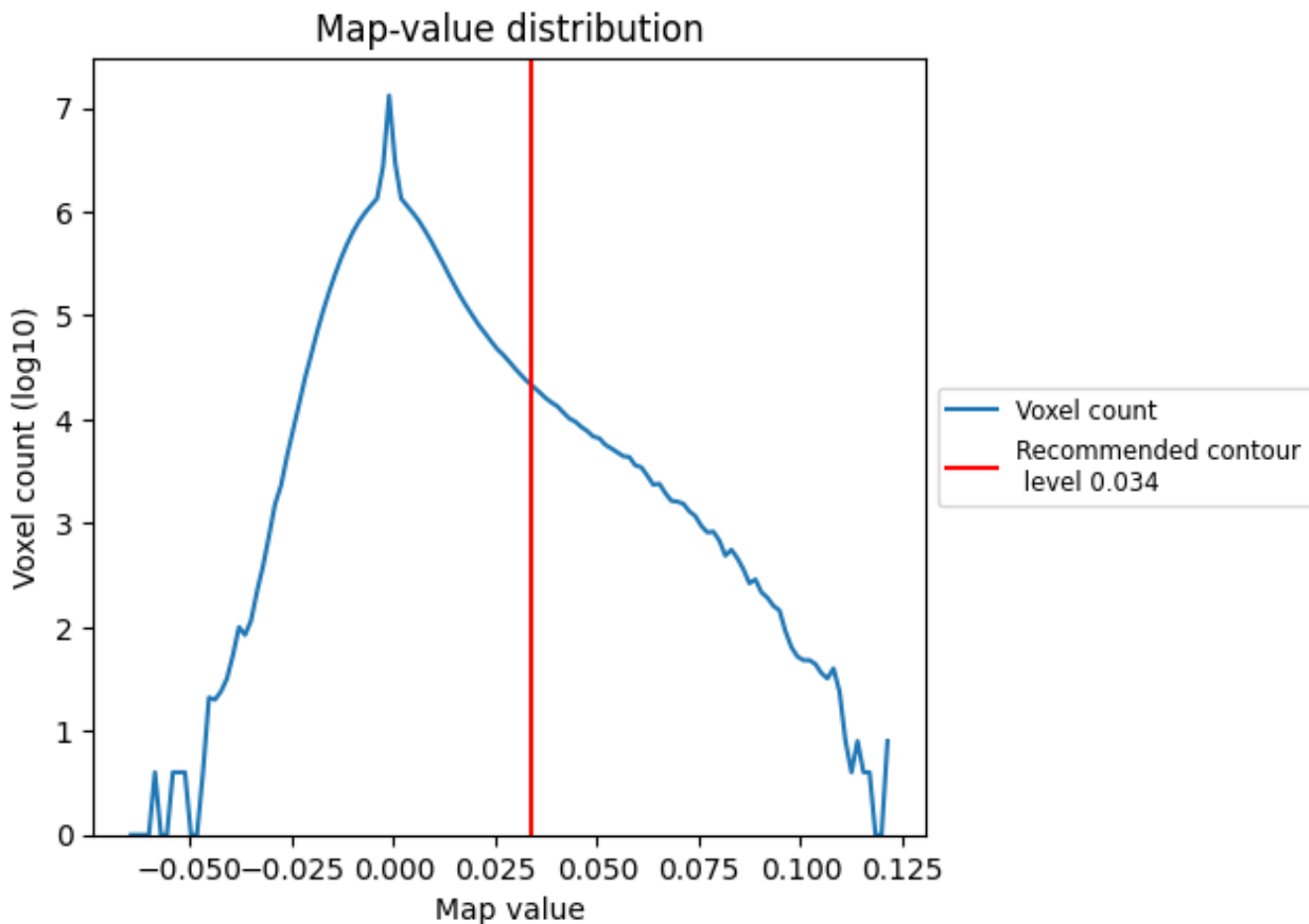
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

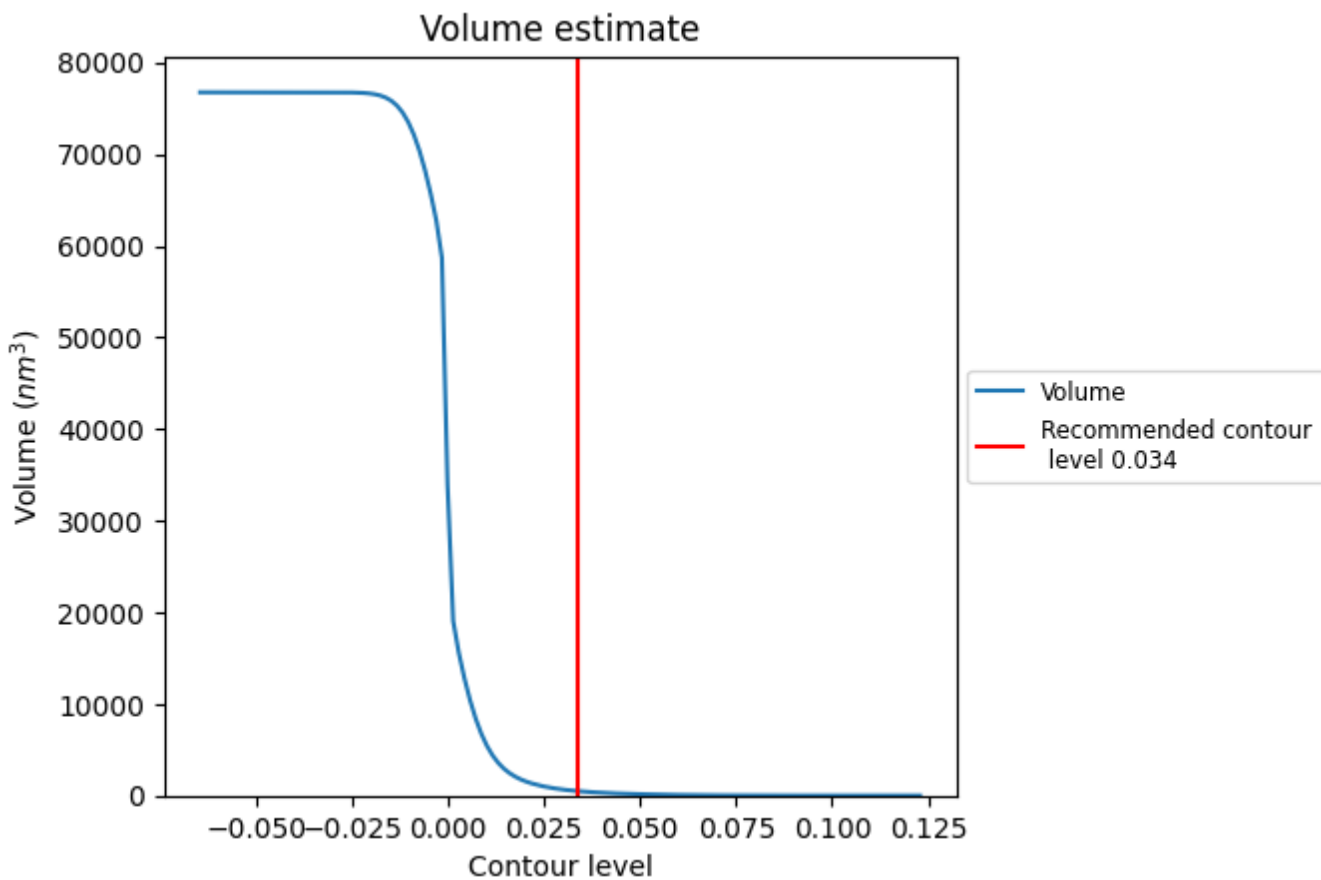
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

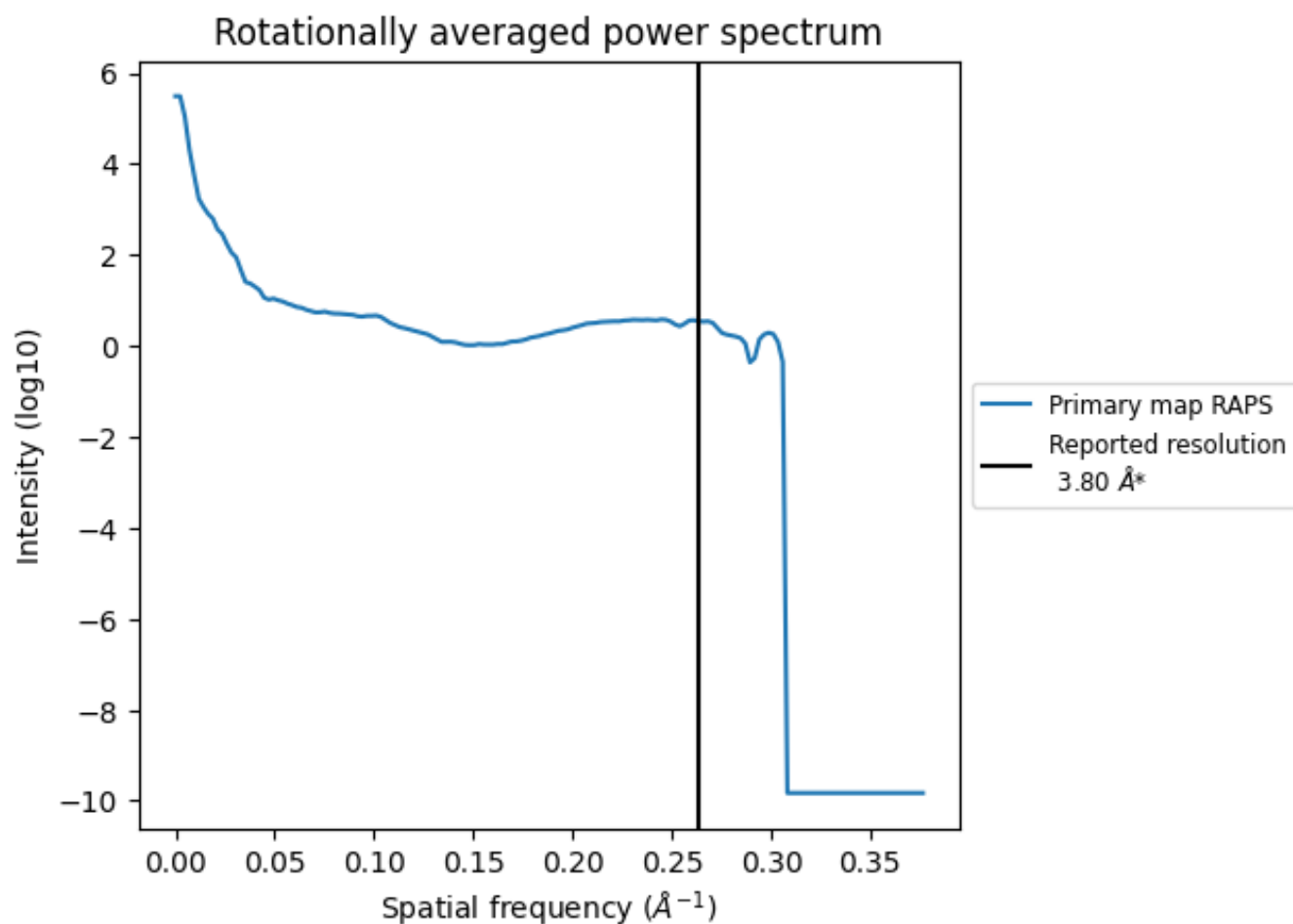
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 478 nm³; 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⁻¹

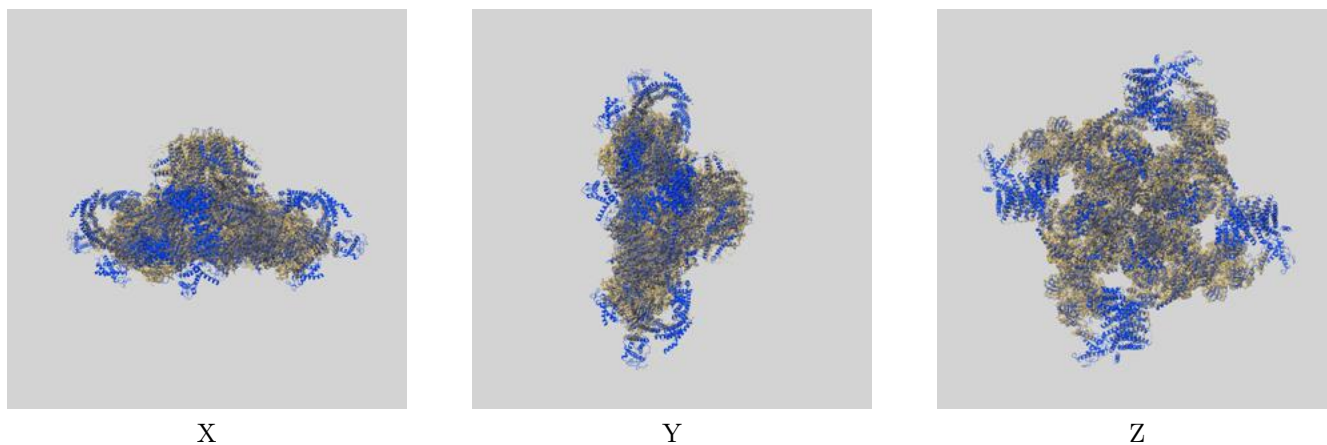
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

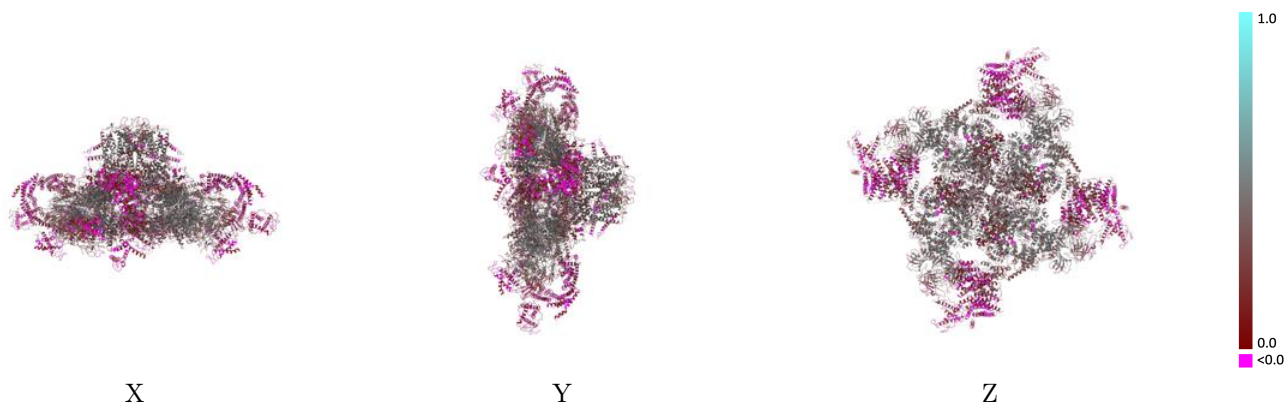
This section contains information regarding the fit between EMDB map EMD-32037 and PDB model 7VMS. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



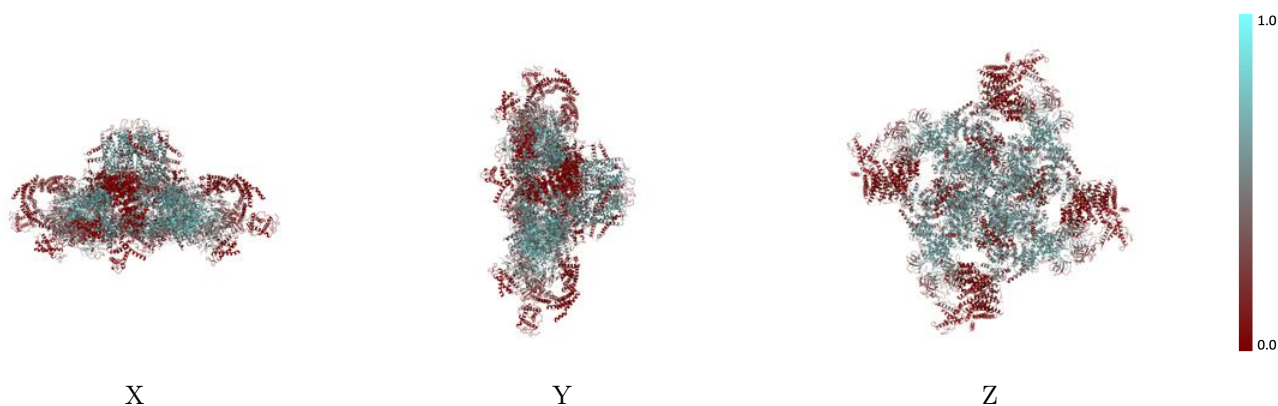
The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



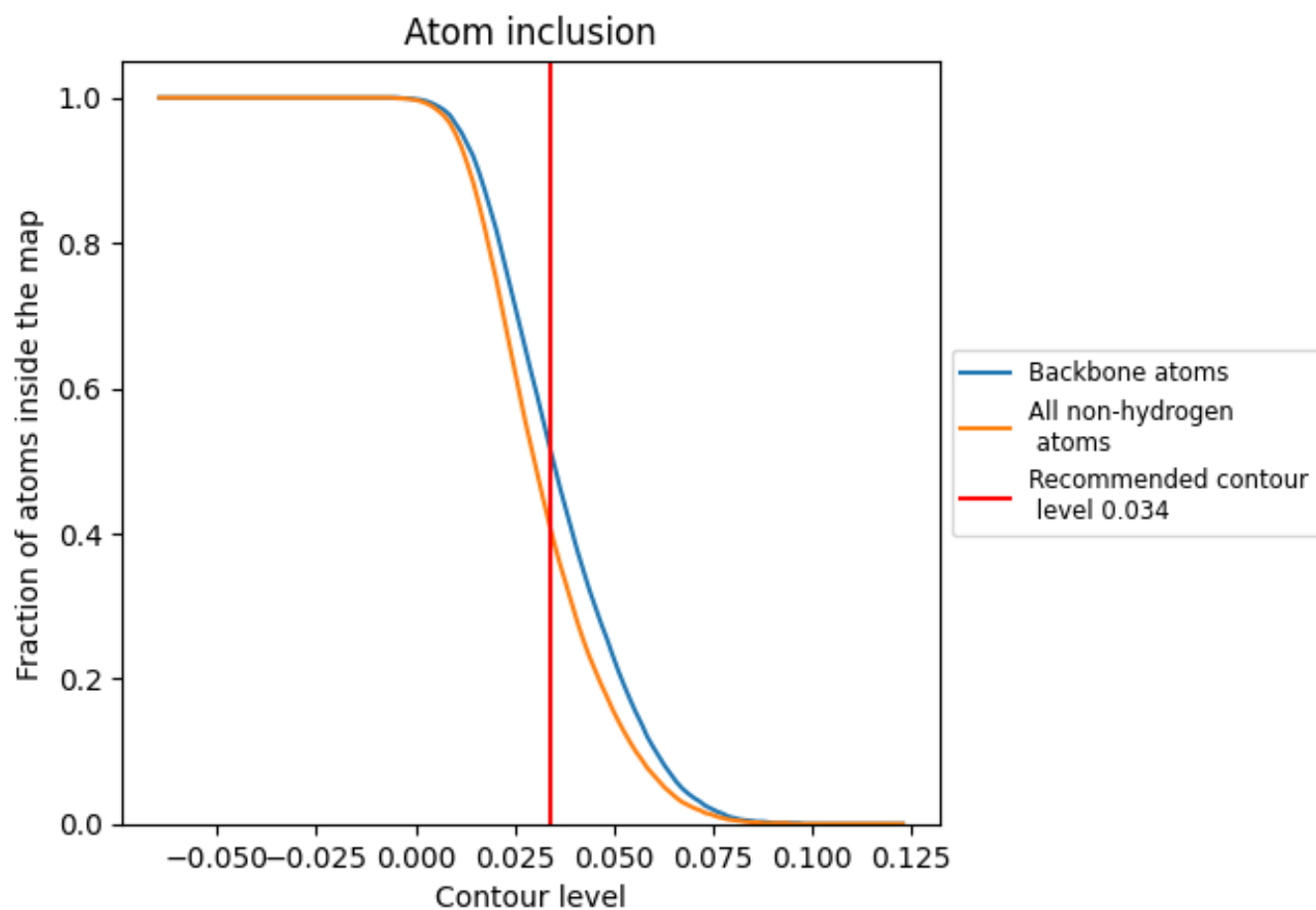
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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 [i](#)

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	0.4070	0.2990
A	0.4070	0.2980
B	0.4070	0.2980
C	0.4070	0.2970
D	0.4070	0.2980
G	0.4160	0.3720
H	0.4180	0.3690
I	0.4150	0.3670
J	0.4160	0.3690

