



wwPDB EM Validation Summary Report ⓘ

Feb 24, 2025 – 04:45 PM JST

PDB ID : 8X49
EMDB ID : EMD-38043
Title : Cryo-EM structure of Ryanodine receptor 1 (100 nM Ca²⁺)
Authors : Chen, Q.; Hu, H.
Deposited on : 2023-11-15
Resolution : 3.40 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.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.2

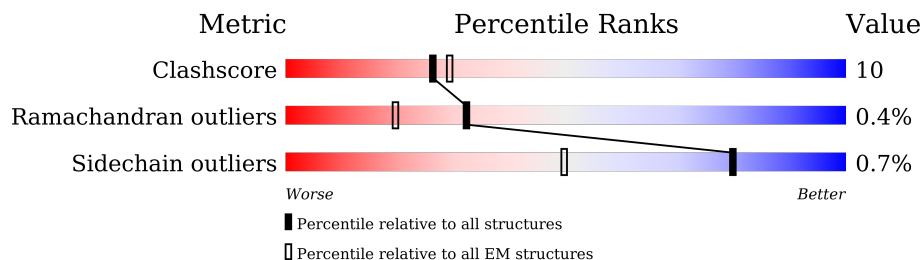
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	5037	 5% 63% 15% 22%
1	B	5037	 5% 63% 15% 22%
1	C	5037	 5% 63% 15% 22%
1	D	5037	 5% 63% 15% 22%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 117356 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 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3952	Total 29337	C 18674	N 5081	O 5394	S 188	0	0
1	B	3952	Total 29337	C 18674	N 5081	O 5394	S 188	0	0
1	C	3952	Total 29337	C 18674	N 5081	O 5394	S 188	0	0
1	D	3952	Total 29337	C 18674	N 5081	O 5394	S 188	0	0

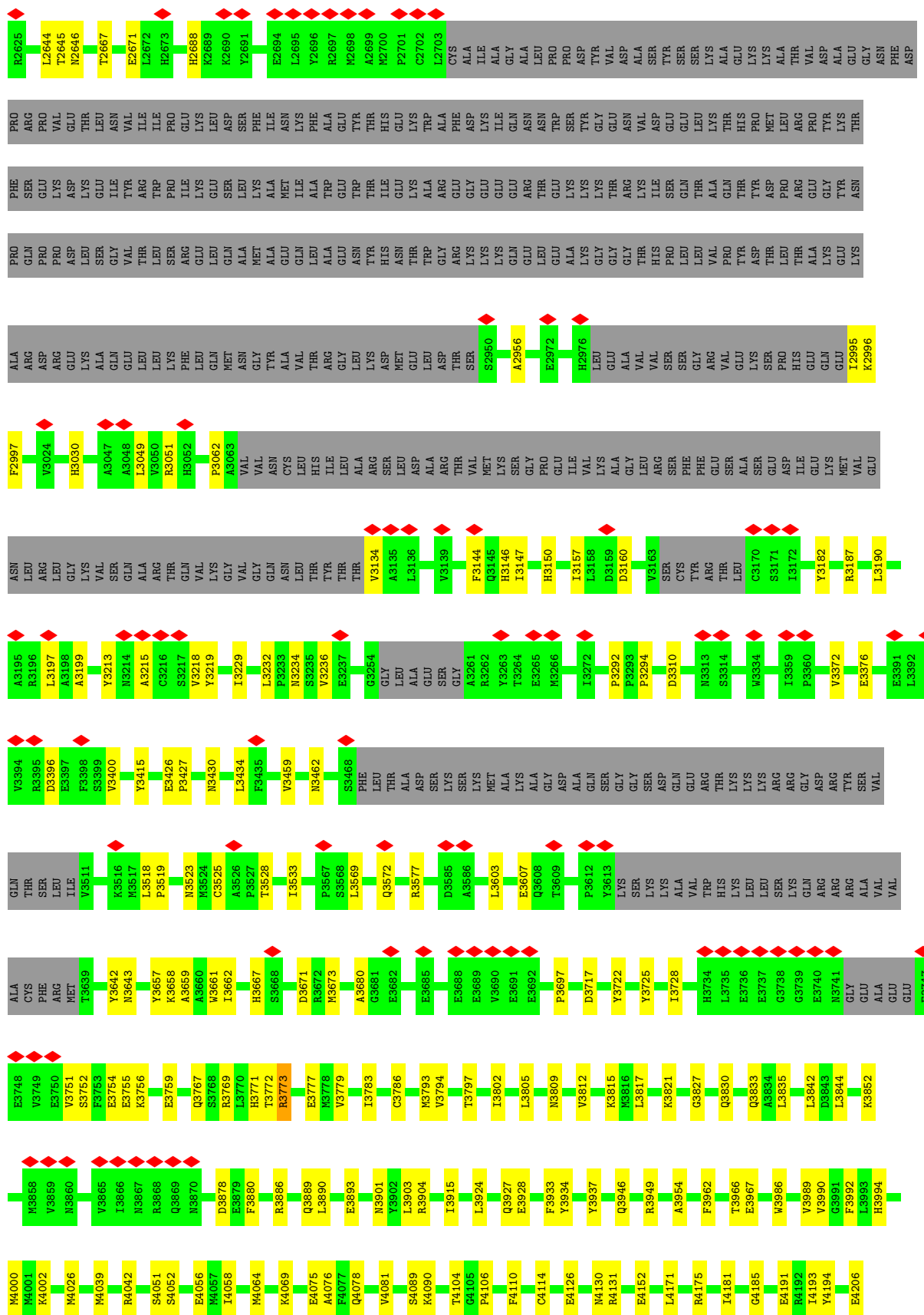
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

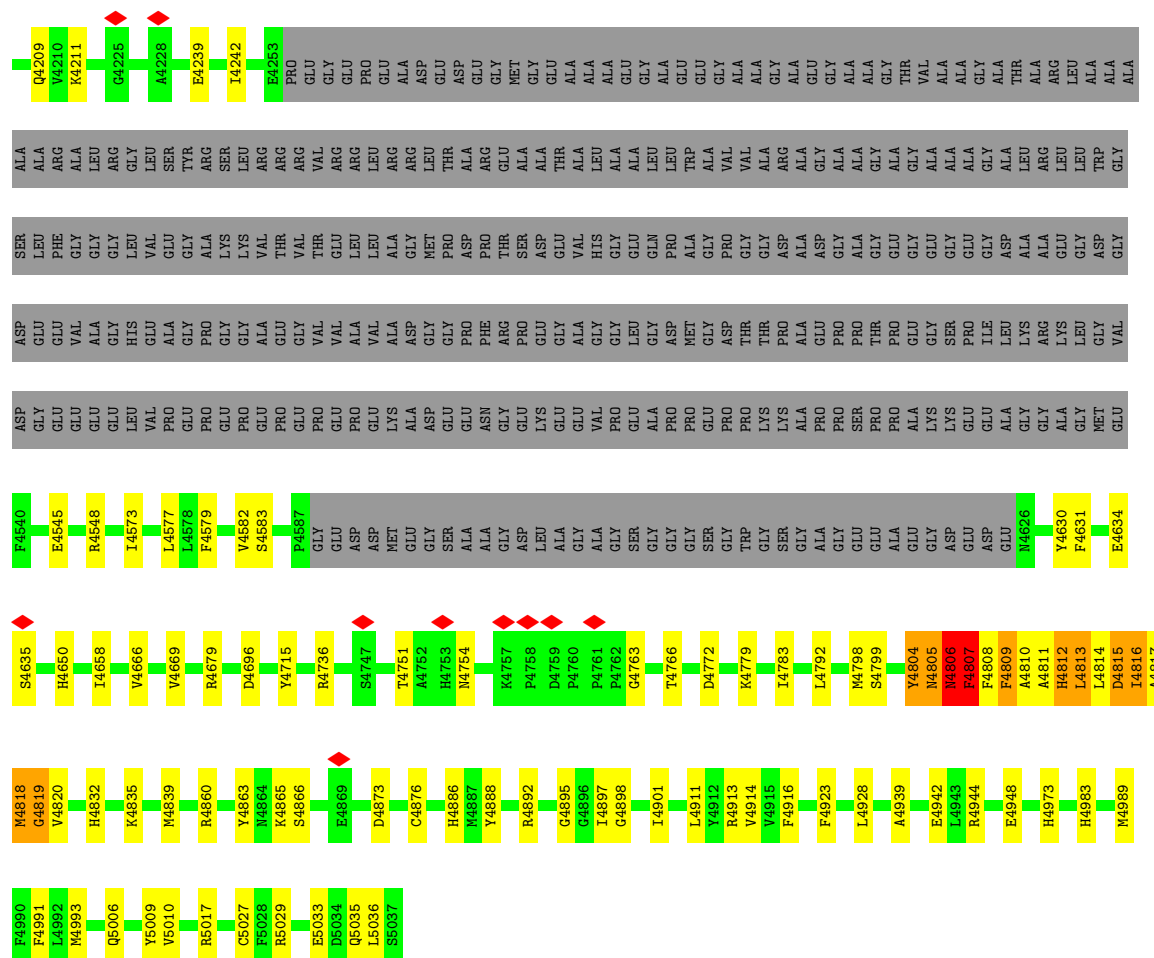
Mol	Chain	Residues	Atoms		AltConf
2	A	1	Total 1	Ca 1	0
2	B	1	Total 1	Ca 1	0
2	C	1	Total 1	Ca 1	0
2	D	1	Total 1	Ca 1	0

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

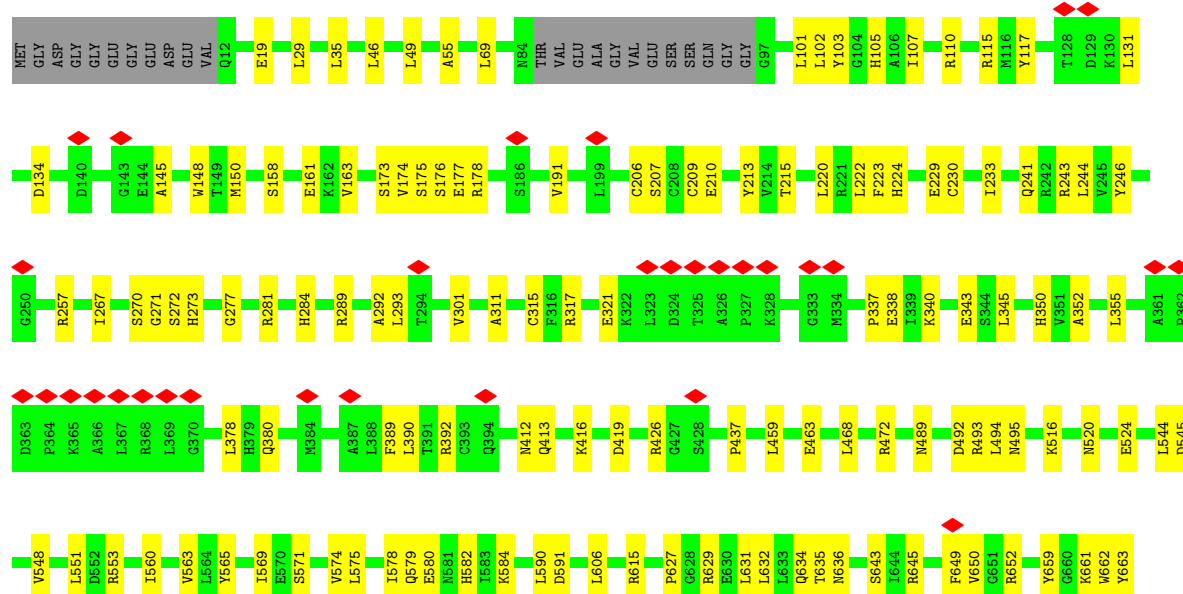
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total 1	Zn 1	0
3	B	1	Total 1	Zn 1	0
3	C	1	Total 1	Zn 1	0
3	D	1	Total 1	Zn 1	0





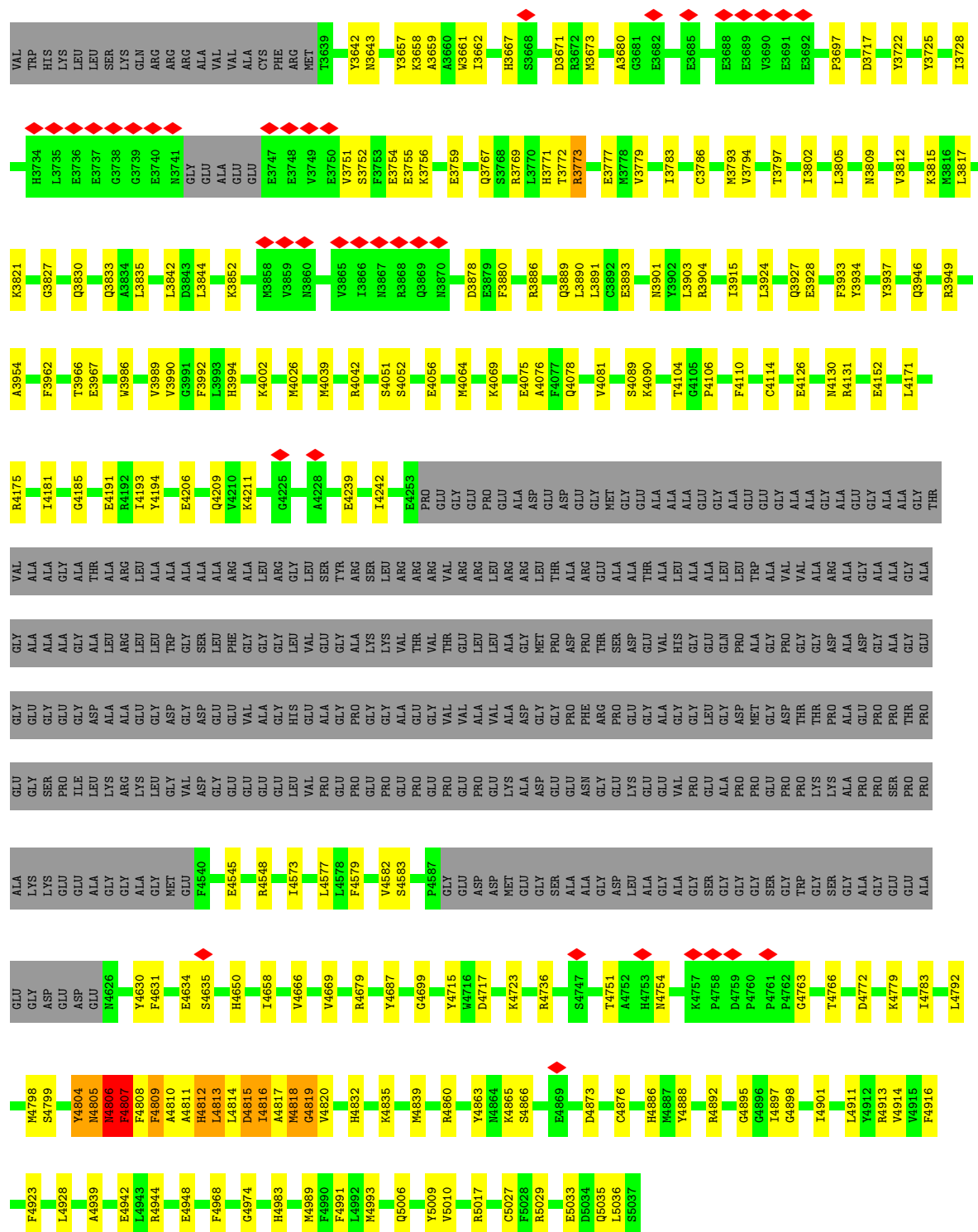


• Molecule 1: Ryanodine receptor 1

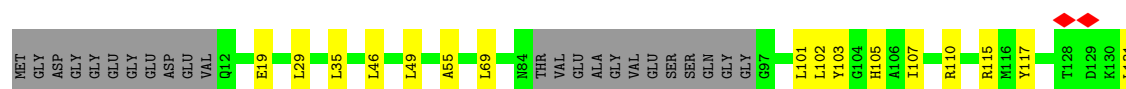


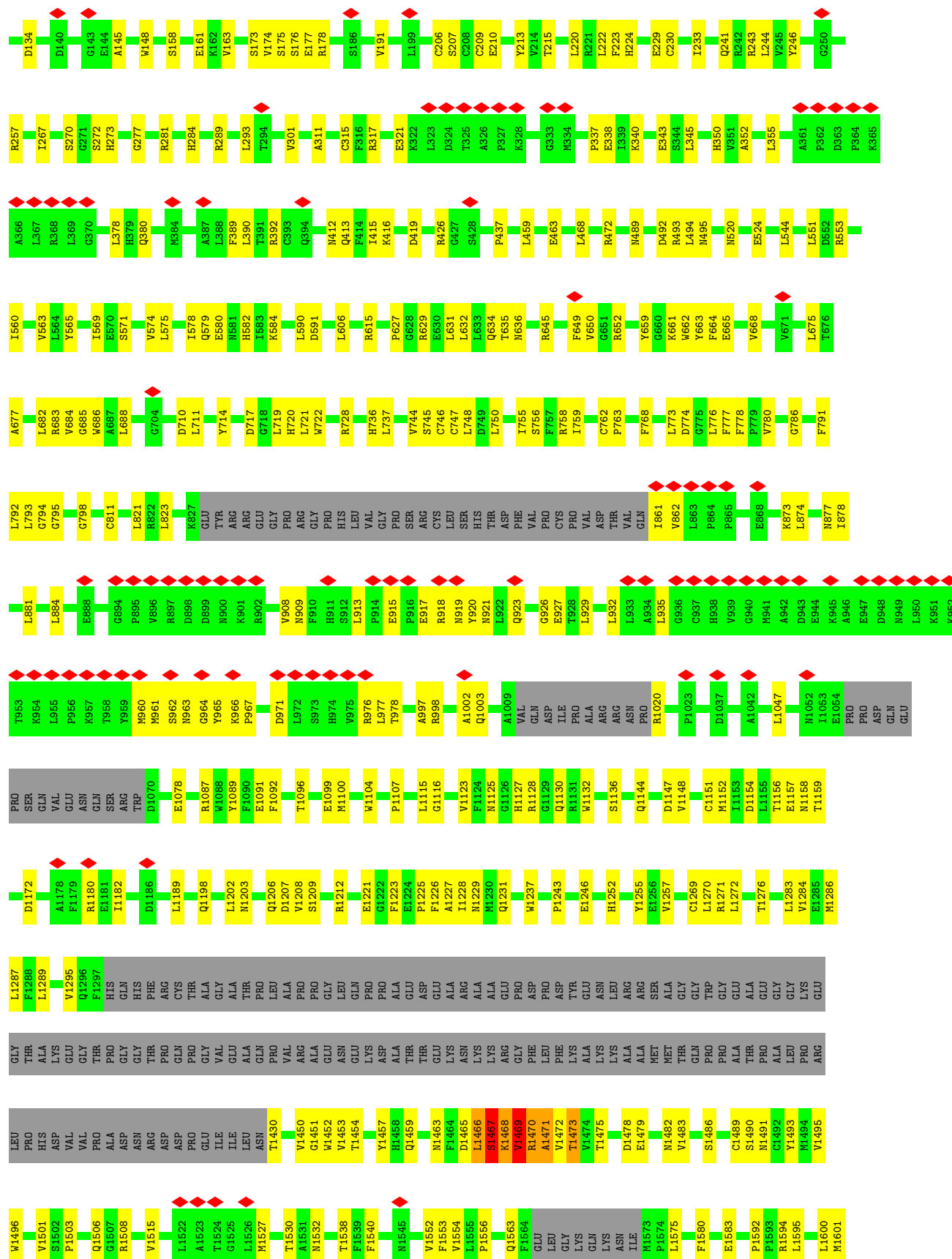






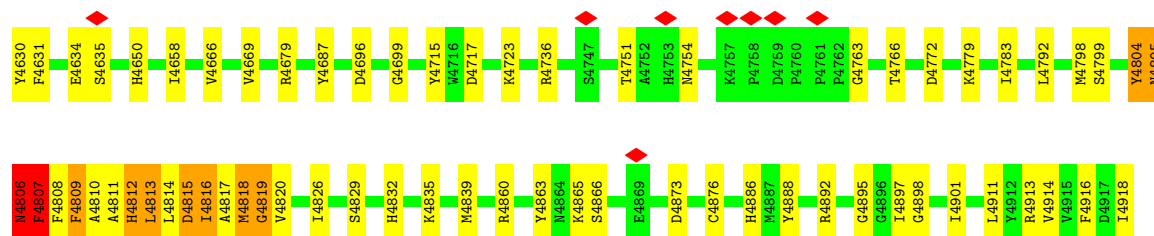
● Molecule 1: Ryanodine receptor 1



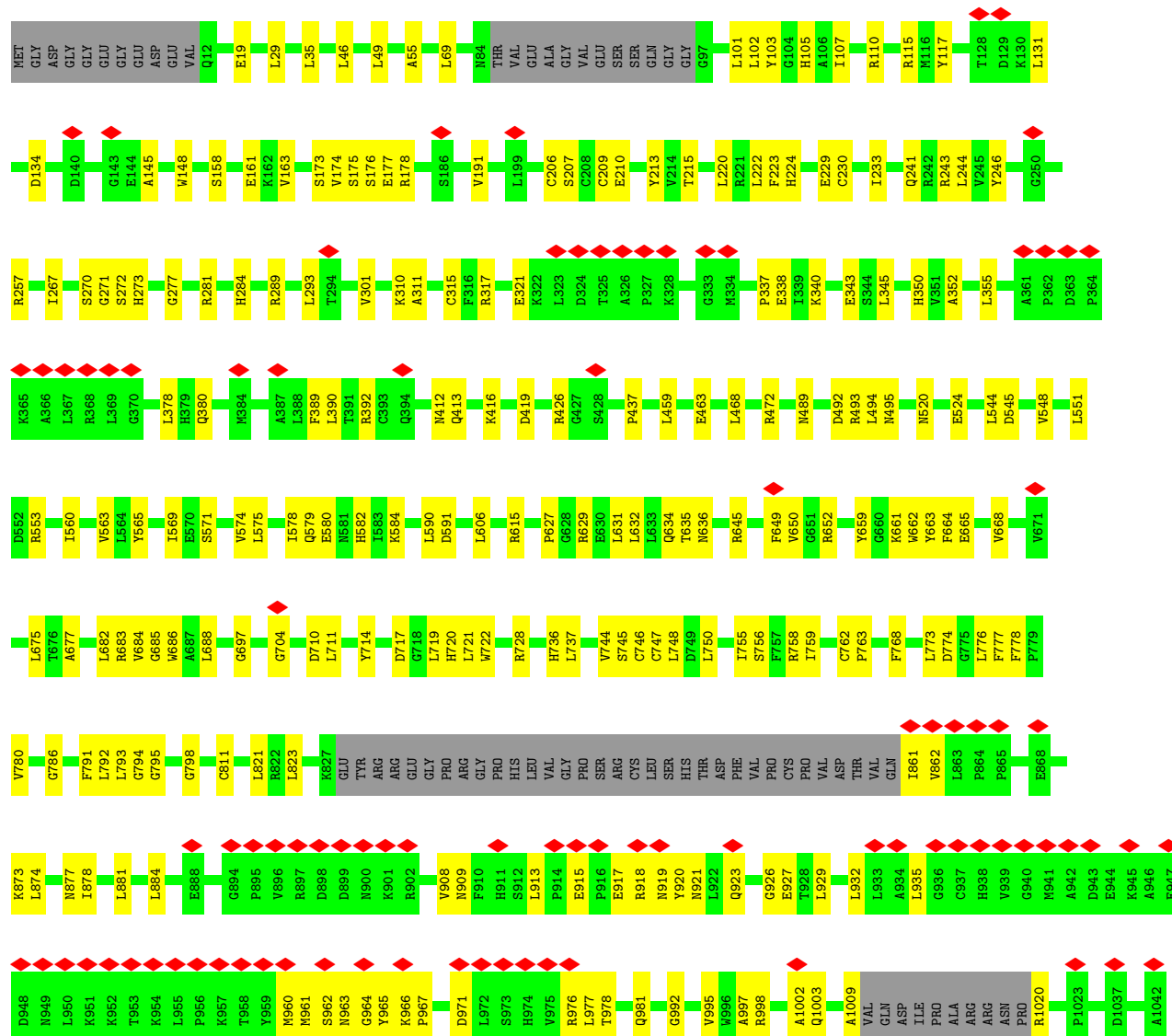








• Molecule 1: Ryanodine receptor 1





A3954	G3827	L3735	HIS	ARG	P3360	R3187	ILE	SER	PRO	THR	GLN	THR	ALA	V2586
F3962	Q3830	E3736	LYS	THR	V3372	L3190	GLU	PRO	TYR	HIS	THR	THR	THR	Y2587
T3966	Q3833	G3738	LEU	LYS	E3376	A3195	VAL	HIS	ASP	MET	PRO	ASP	ALA	S2590
E3967	A3834	G3739	LYS	ARG	E3391	R3196	GLN	GLN	THR	LEU	ARG	GLU	GLY	R2591
W3966	L3835	E3740	GLN	ARG	L3392	L3197	ASN	GLU	THR	ALA	PRO	GLY	GLY	Y2613
L3842	L3842	N3741	ARG	GLY	L3393	A3199	LEU	LYS	TYR	LYS	TYR	ASN	PHE	P2616
V3989	D3843	GLY	ARG	ASP	V3394	A3199	LEU	ALA	ASN	GLY	TYR	ASN	PRO	R2625
V3990	L3844	ALA	VAL	THR	R3395	Y3213	LYS	ASP	GLN	ARG	PRO	ARG	PRO	L2644
G3991	K3852	VAL	VAL	VAL	D3396	N3214	SER	ASP	GLN	SER	GLU	ARG	VAL	T2645
L3953	M3858	GLU	ALA	GLN	E3397	C3216	GLN	ARG	PRO	LYS	LYS	THR	THR	N2646
H3994	V3859	E3747	CYS	THR	F3398	A3047	SER	ALA	ASP	ASP	ASP	GLY	GLY	T2667
M4000	N3860	V3748	THR	SER	S3399	L3049	ALA	GLY	GLU	GLU	LEU	ASN	VAL	E2671
M4001	N3860	V3749	LEU	LEU	V3400	R3051	THR	GLN	VAL	THR	THR	VAL	ILE	L2672
K4002	E3750	E3750	ILE	ILE	Y3415	H3052	VAL	GLN	LEU	ARG	ARG	ILE	ILE	E2673
V3865	V3751	S3751	V3511	K3516	E3426	T3229	LYS	VAL	LEU	THR	THR	THR	PRO	R2688
I3866	S3752	S3752	K3517	M3517	P3427	L3232	GLY	VAL	PHE	ARG	ILE	GLU	PRO	K2689
N3867	F3753	E3754	L3518	P3519	N3430	L3233	GLN	VAL	GLN	LEU	GLY	LEU	LYS	K2690
R3868	K3657	E3755	N3523	N3523	L3434	N3234	ASN	ASN	CYS	GLN	GLU	SER	ASP	Y2691
Q3869	K3658	K3756	M3524	A3526	F3435	N3235	LEU	LEU	LEU	ALA	ALA	ASN	SER	E2694
N3870	A3659	E3759	C3525	P3527	S3446	V3236	THR	ILE	GLY	ALA	ALA	GLU	MET	L2695
D3878	A3660	Q3767	A3526	A3526	H3449	G3254	THR	ALA	VAL	THR	THR	THR	ALA	Y2696
E3879	I3662	R3767	T3528	T3528	V3459	GLY	THR	ARG	THR	ARG	ALA	ALA	TRP	R2697
F3880	I3662	K3768	L3533	L3533	N3462	ALA	ALA	SER	THR	THR	ILE	ILE	ALA	Y2698
R3886	H3667	R3769	P3567	P3567	H3462	SER	GLY	LEU	THR	THR	THR	THR	TRP	R2698
Q3888	S3668	L3770	S3668	S3668	N3462	GLU	V3139	GLU	THR	THR	THR	THR	TRP	A2699
L3890	D3671	R3771	T3528	T3528	S3468	GLU	A3135	LEU	THR	THR	THR	THR	TRP	M2700
C3892	R3672	T3772	L3533	L3533	PHE	ALA	F3144	ASP	THR	THR	THR	THR	TRP	F2701
E3893	M3673	R3773	P3567	P3567	THR	SER	H3146	THR	THR	THR	THR	THR	TRP	C2702
F3899	A3680	E3777	Q3572	Q3572	ALA	ASP	I3147	GLY	THR	THR	THR	THR	TRP	L2703
Q3900	G3681	R3778	R3577	R3577	THR	ASP	H3150	PRO	SER	THR	THR	THR	TRP	CYS
N3901	E3682	V3779	D3585	D3585	LYS	LYS	I3272	GLU	ASP	GLY	GLY	GLY	TRP	ILE
Y3902	E3685	L3783	A3586	A3586	LYS	LYS	P3159	ILE	THR	THR	THR	THR	TRP	ALA
R3904	E3688	C3786	L3603	L3603	MET	LYS	V3163	LYS	GLU	GLY	GLU	GLU	TRP	ALA
I3915	E3689	M3793	Q3607	Q3607	ALA	ALA	SER	VAL	GLN	GLN	GLN	GLN	TRP	ALA
L3924	V3690	V3794	E3608	E3608	ALA	ALA	TYR	VAL	LEU	LEU	LEU	LEU	TRP	ALA
Q3927	E3692	T3797	T3609	T3609	GLY	GLY	CYS	VAL	GLU	GLU	GLU	GLU	TRP	ALA
E3928	P3697	L3802	P3612	P3612	ALA	ALA	ARG	VAL	LEU	LEU	LEU	LEU	TRP	ALA
F3933	D3717	L3805	Y3613	Y3613	ASP	ASP	THR	SER	VAL	VAL	VAL	VAL	TRP	ALA
Y3934	D3722	N3809	LYS	LYS	GLN	GLN	THR	PHE	VAL	VAL	VAL	VAL	TRP	ALA
Y3937	Y3725	V3812	SER	SER	SER	SER	THR	PHE	VAL	VAL	VAL	VAL	TRP	ALA
Q3946	I3728	K3815	LYS	LYS	GLY	GLY	THR	GLU	VAL	VAL	VAL	VAL	TRP	ALA
R3949	H3734	L3817	LYS	LYS	ASP	ASP	THR	SER	VAL	VAL	VAL	VAL	TRP	ALA
		K3821	ALA	ALA	GLN	GLN	THR	GLU	VAL	VAL	VAL	VAL	TRP	ALA
			TRP	TRP	GLU	GLU	THR	GLU	VAL	VAL	VAL	VAL	TRP	ALA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	183859	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	4.737	Depositor
Minimum map value	-2.523	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.130	Depositor
Recommended contour level	0.466	Depositor
Map size (\AA)	516.72003, 516.72003, 516.72003	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0765, 1.0765, 1.0765	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.30	0/29956	0.47	0/40772
1	B	0.30	0/29956	0.47	0/40772
1	C	0.30	0/29956	0.47	0/40772
1	D	0.30	0/29956	0.47	0/40772
All	All	0.30	0/119824	0.47	0/163088

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	29337	0	27528	579	0
1	B	29337	0	27528	585	0
1	C	29337	0	27528	579	0
1	D	29337	0	27528	580	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	117356	0	110112	2250	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 10.

The worst 5 of 2250 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:1965:TYR:CE2	1:C:1969:LEU:HD11	2.12	0.85
1:D:1965:TYR:CE2	1:D:1969:LEU:HD11	2.12	0.84
1:B:1965:TYR:CE2	1:B:1969:LEU:HD11	2.12	0.84
1:A:1965:TYR:CE2	1:A:1969:LEU:HD11	2.12	0.84
1:C:3990:VAL:HG23	1:C:4051:SER:HB3	1.61	0.82

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	3906/5037 (78%)	3513 (90%)	376 (10%)	17 (0%)	30	60
1	B	3906/5037 (78%)	3513 (90%)	376 (10%)	17 (0%)	30	60
1	C	3906/5037 (78%)	3513 (90%)	376 (10%)	17 (0%)	30	60
1	D	3906/5037 (78%)	3513 (90%)	376 (10%)	17 (0%)	30	60
All	All	15624/20148 (78%)	14052 (90%)	1504 (10%)	68 (0%)	32	60

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1469	VAL
1	A	1470	ARG
1	A	1472	VAL
1	A	1836	PHE
1	B	1469	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	2885/4276 (68%)	2865 (99%)	20 (1%)	81	88
1	B	2885/4276 (68%)	2865 (99%)	20 (1%)	81	88
1	C	2885/4276 (68%)	2865 (99%)	20 (1%)	81	88
1	D	2885/4276 (68%)	2865 (99%)	20 (1%)	81	88
All	All	11540/17104 (68%)	11460 (99%)	80 (1%)	80	88

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4813	LEU
1	D	1843	LYS
1	C	4818	MET
1	D	1468	LYS
1	D	4806	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	4201	ASN
1	D	4094	GLN
1	C	3572	GLN
1	D	3998	HIS
1	D	3430	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

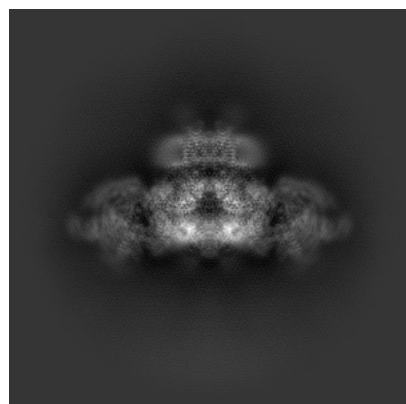
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38043. These allow visual inspection of the internal detail of the map and identification of artifacts.

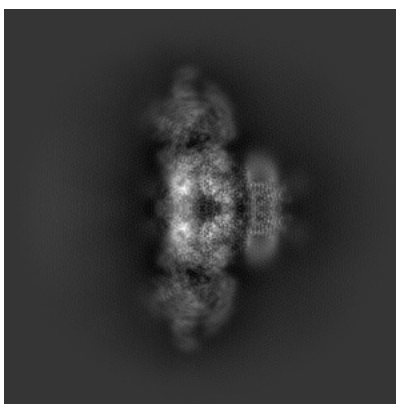
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

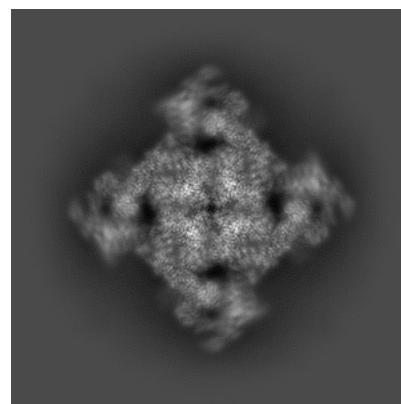
6.1.1 Primary map



X

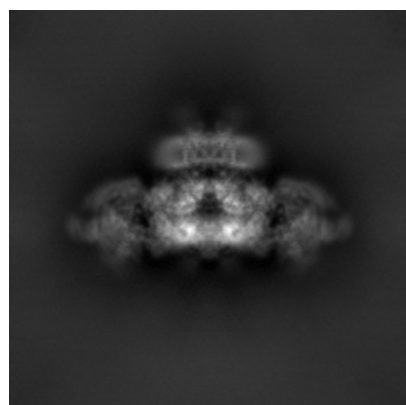


Y

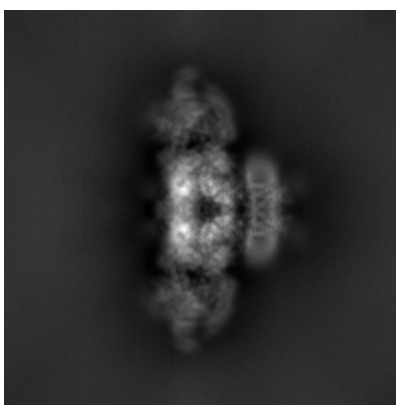


Z

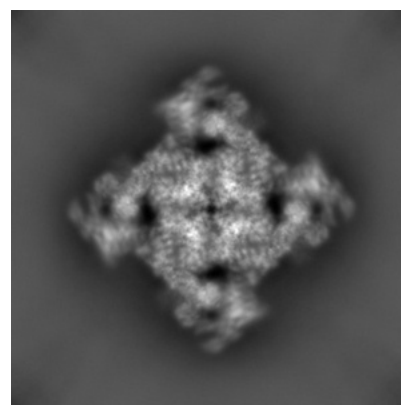
6.1.2 Raw map



X



Y

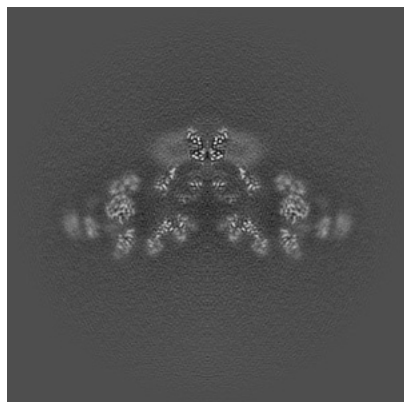


Z

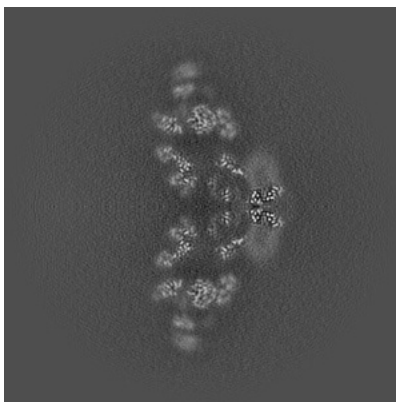
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

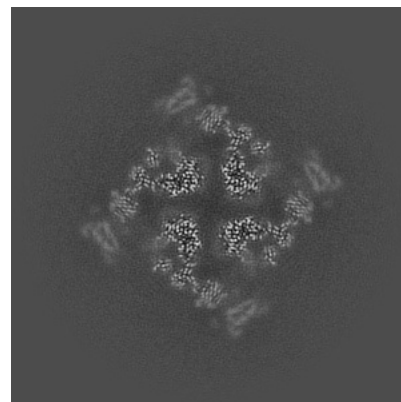
6.2.1 Primary map



X Index: 240

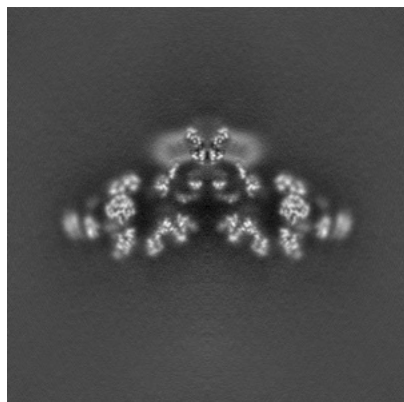


Y Index: 240

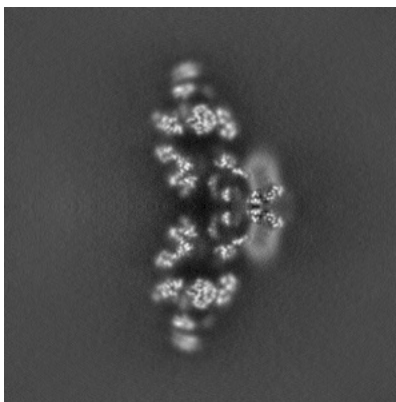


Z Index: 240

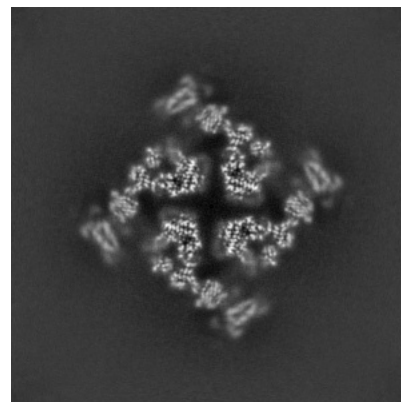
6.2.2 Raw map



X Index: 240



Y Index: 240

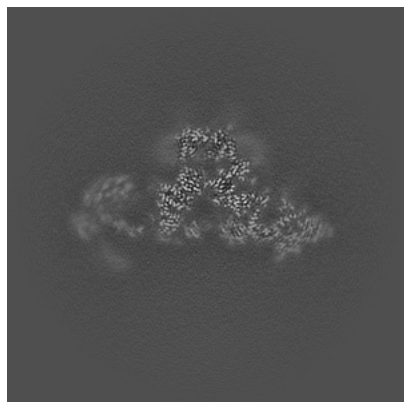


Z Index: 240

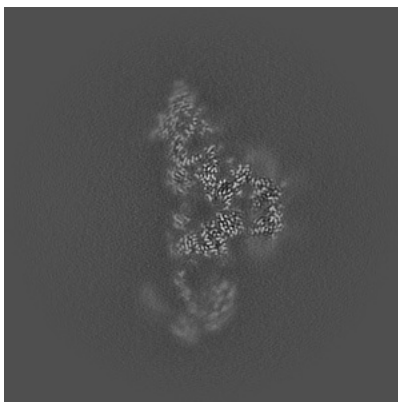
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

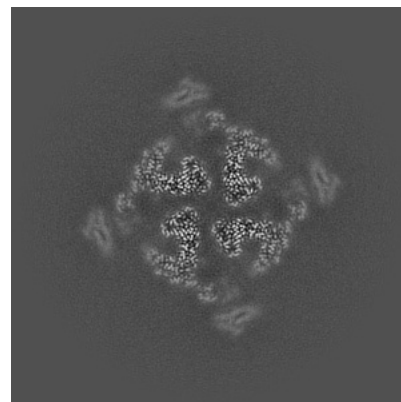
6.3.1 Primary map



X Index: 259

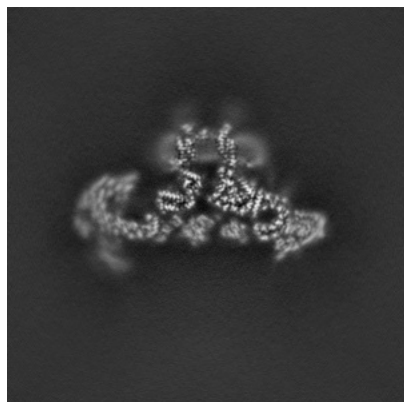


Y Index: 221

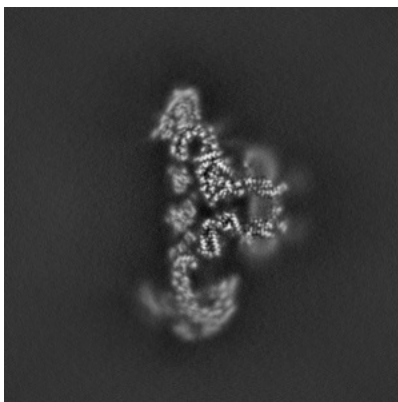


Z Index: 248

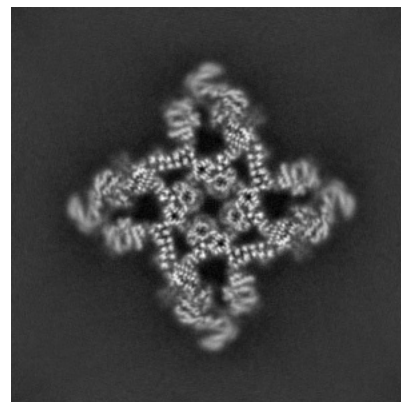
6.3.2 Raw map



X Index: 265



Y Index: 215

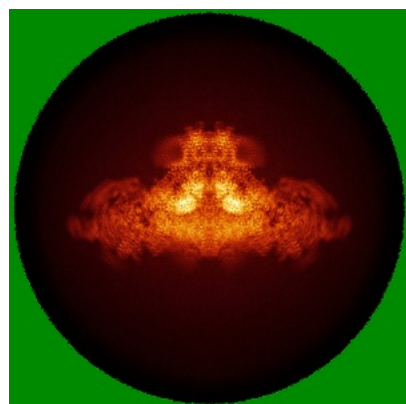


Z Index: 218

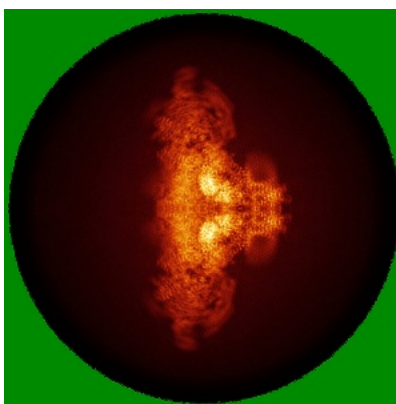
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

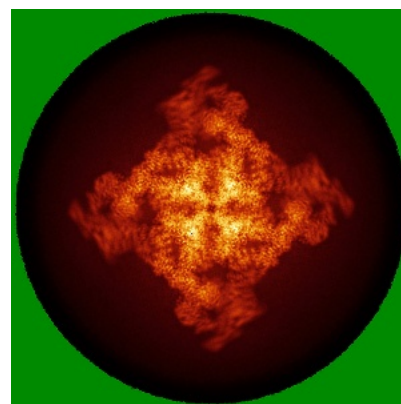
6.4.1 Primary map



X

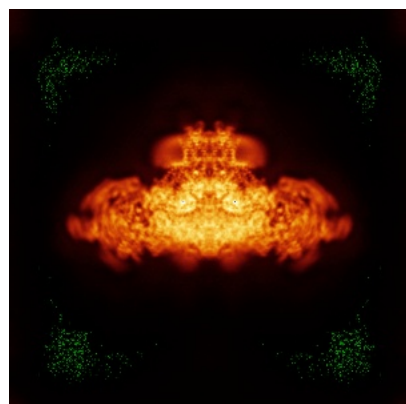


Y

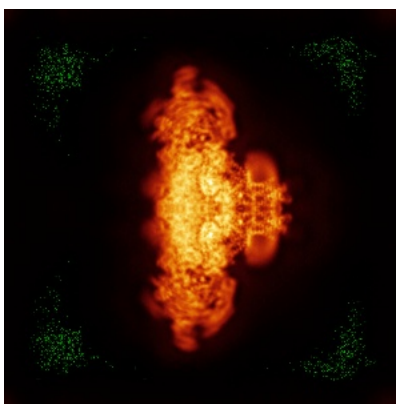


Z

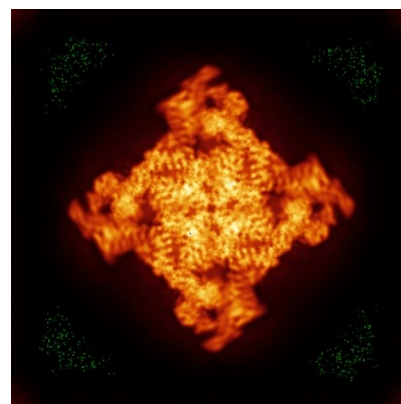
6.4.2 Raw map



X



Y

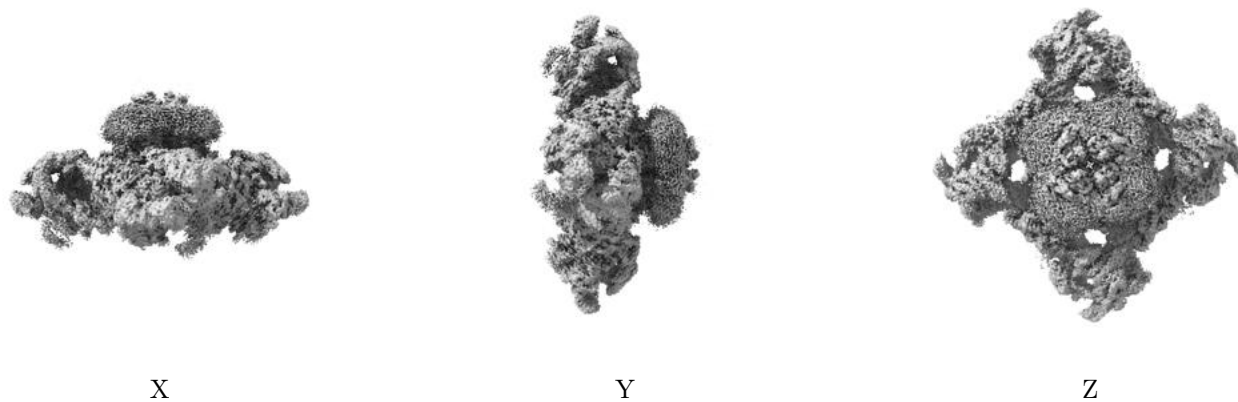


Z

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.

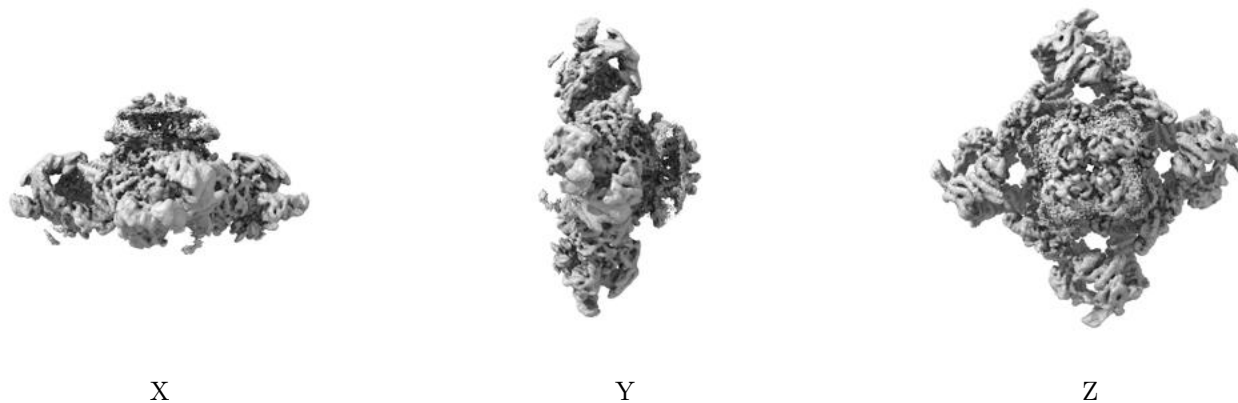
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.466. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

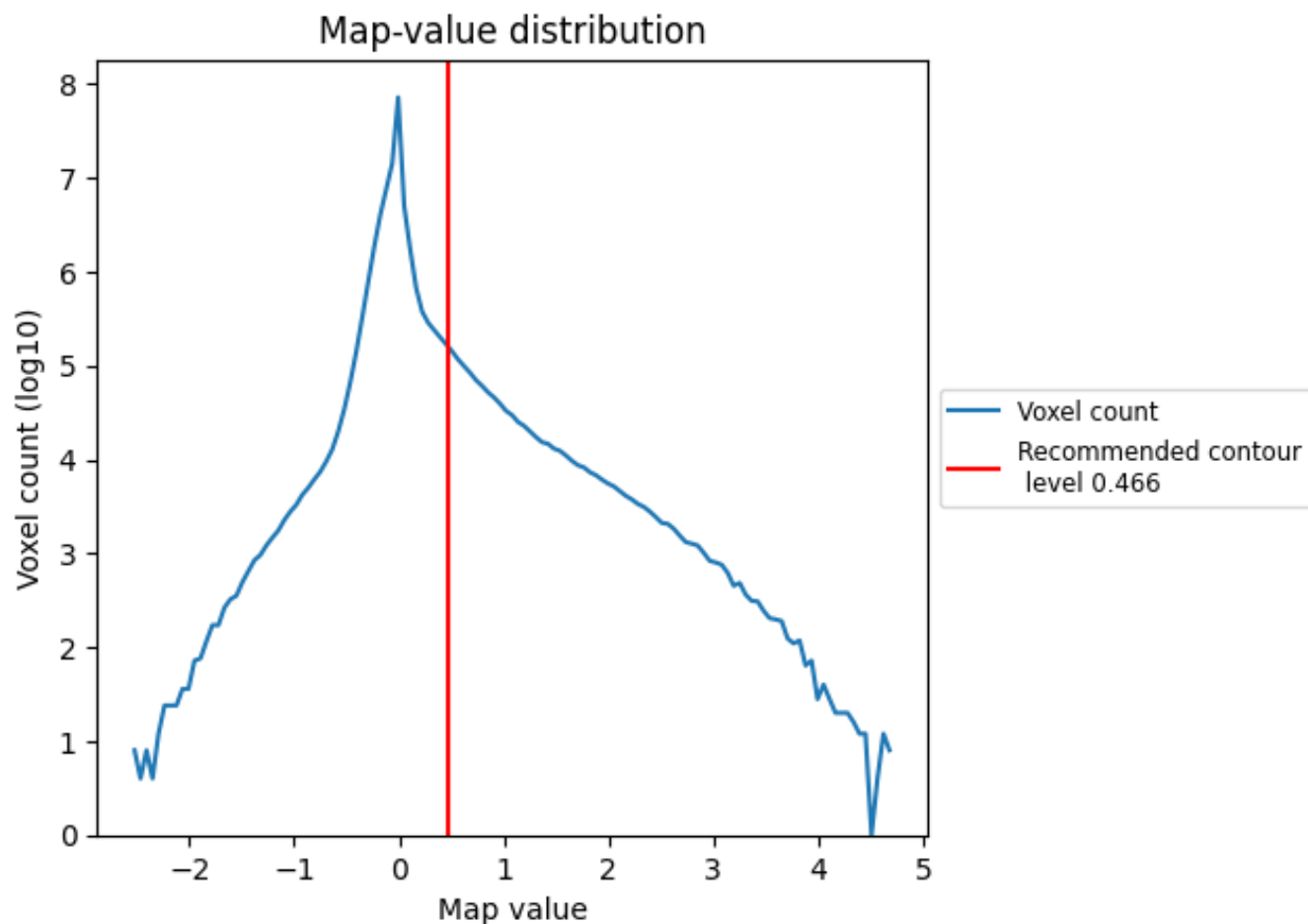
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

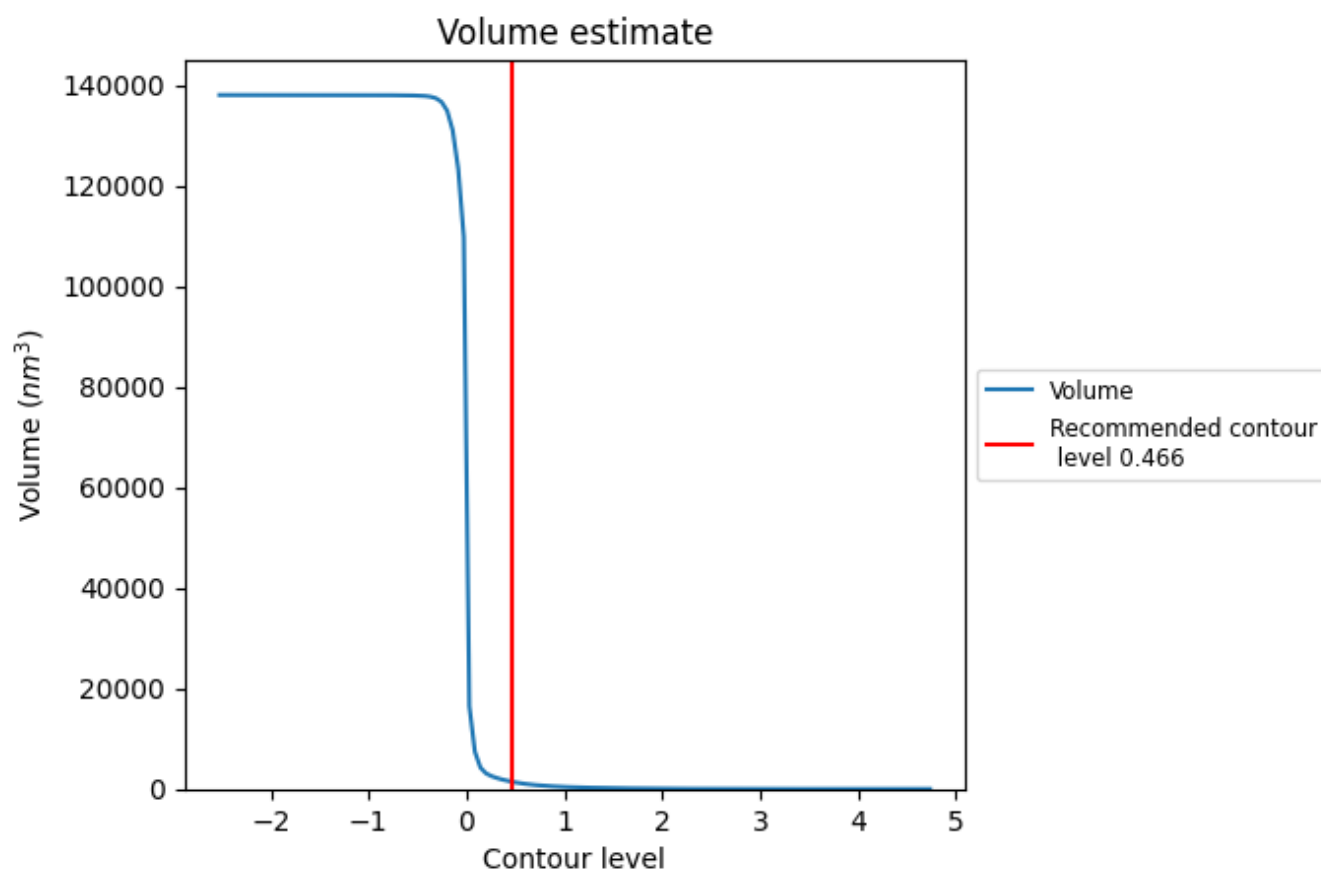
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

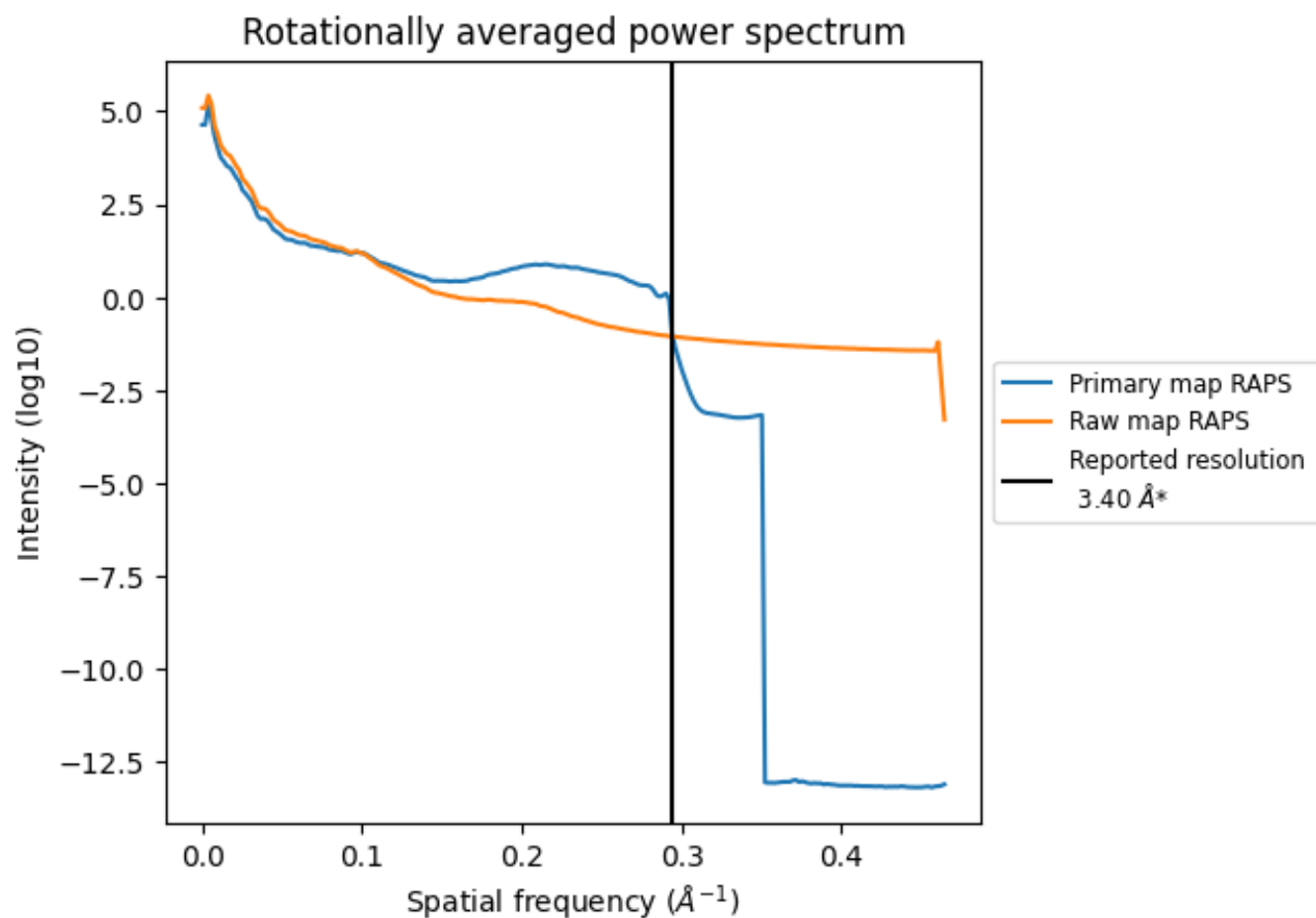
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1425 nm^3 ; this corresponds to an approximate mass of 1287 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

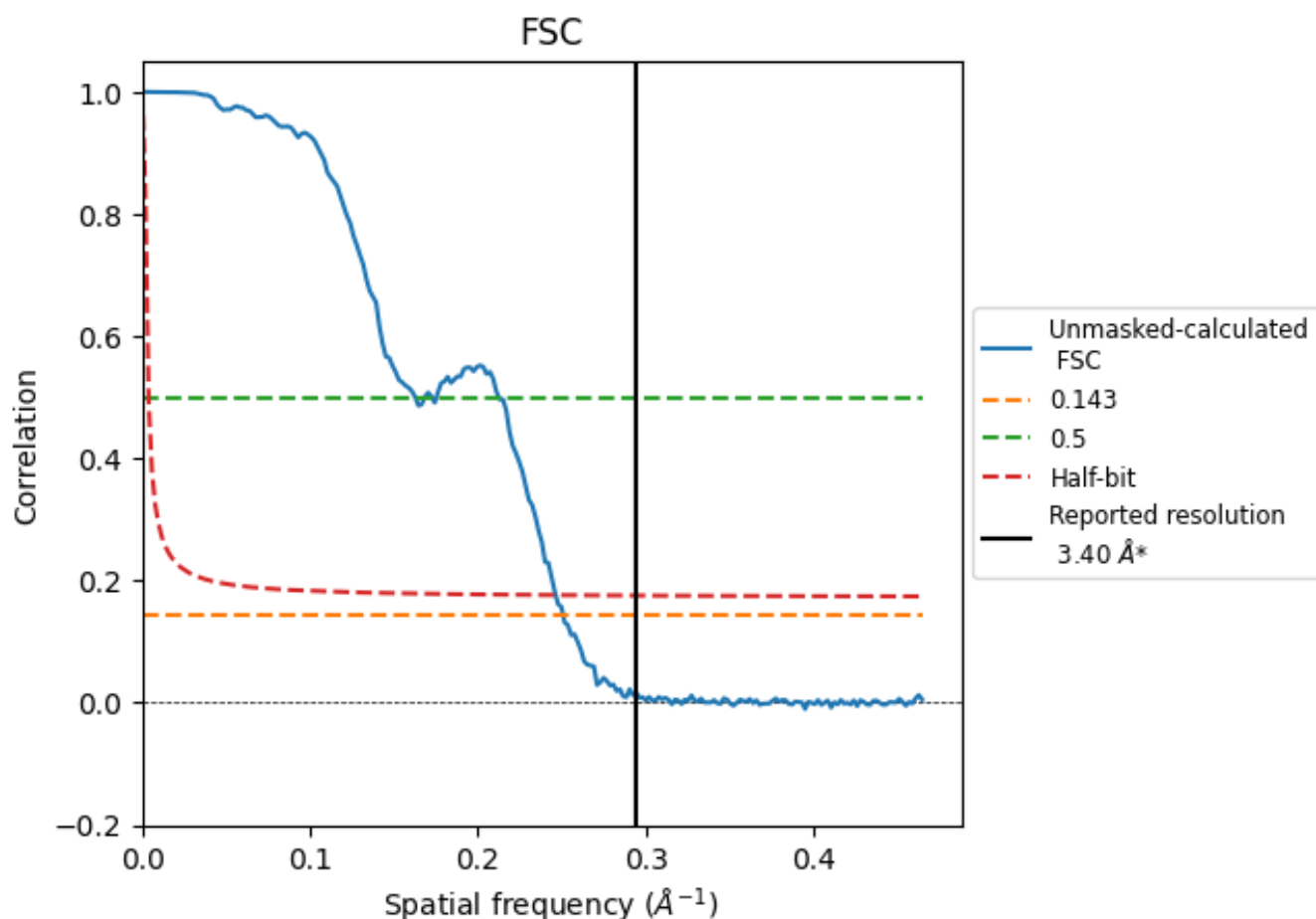


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

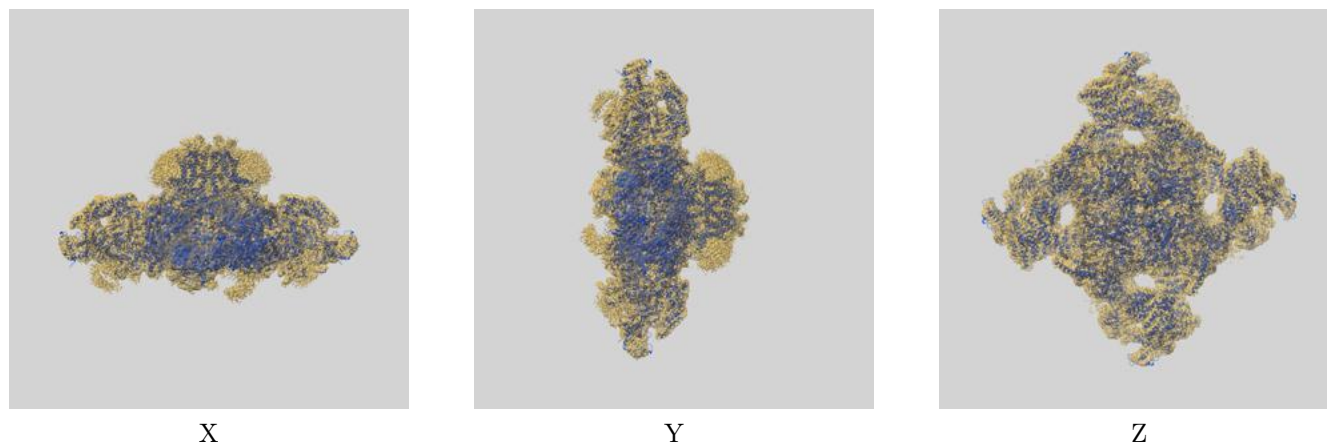
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.99	6.15	4.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.99 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

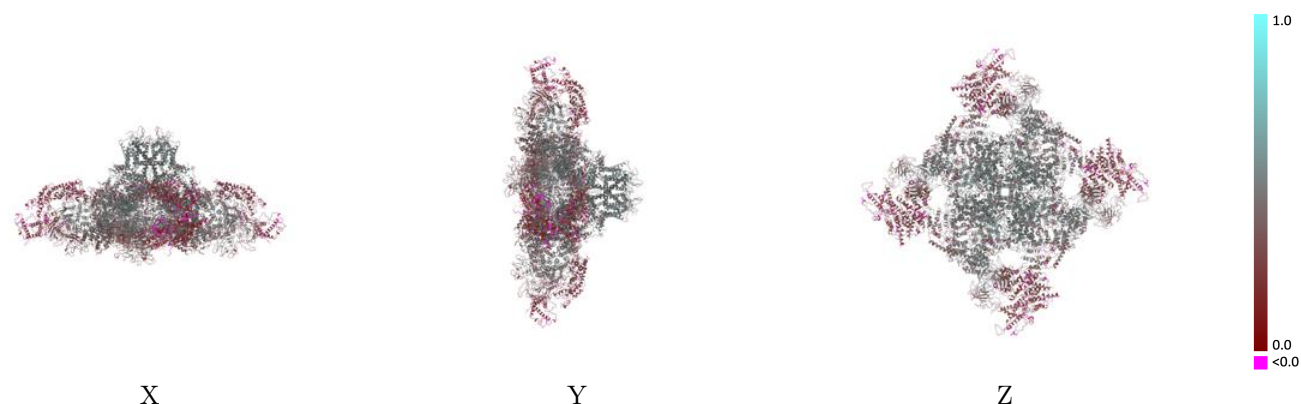
This section contains information regarding the fit between EMDB map EMD-38043 and PDB model 8X49. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



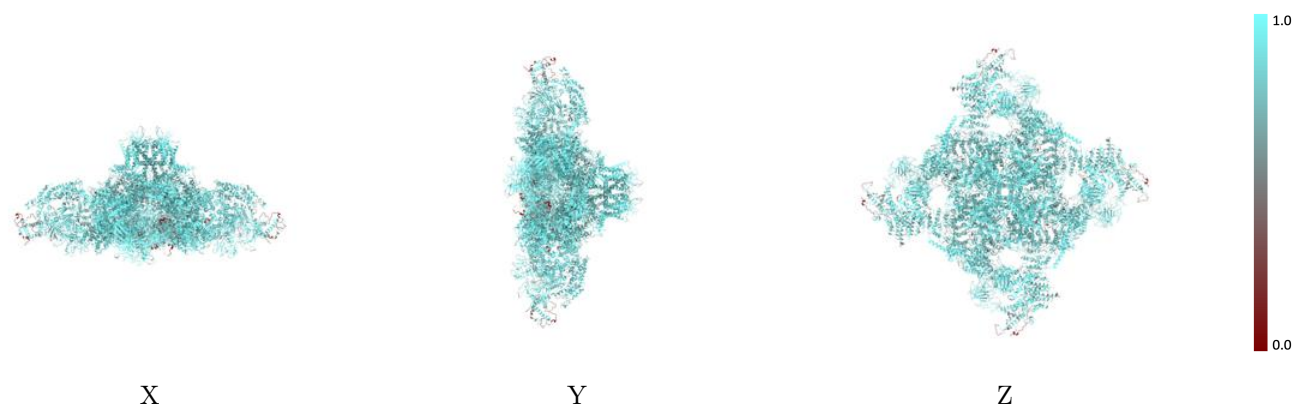
The images above show the 3D surface view of the map at the recommended contour level 0.466 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



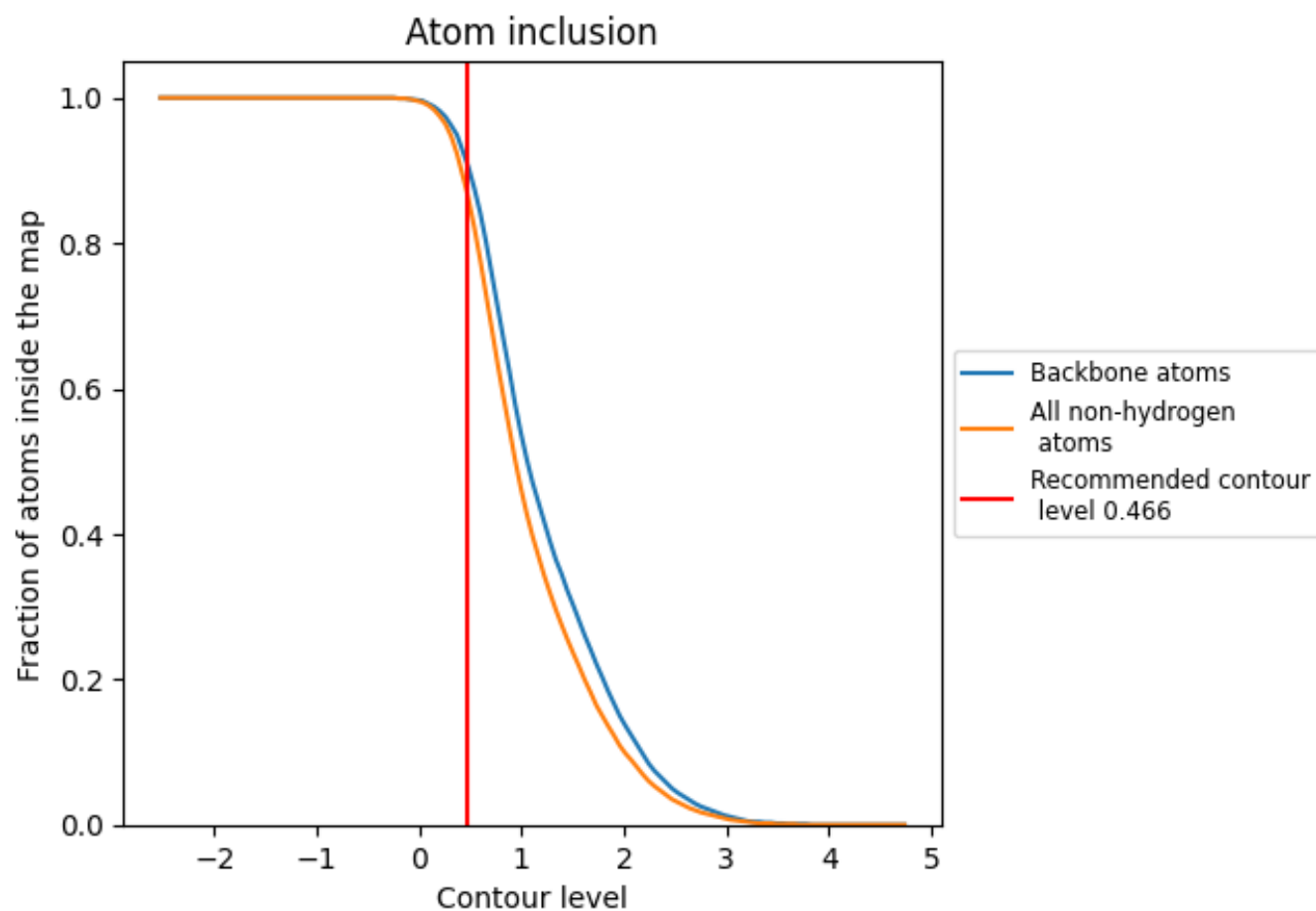
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.466).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.466) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8710	<div></div> 0.3900
A	<div></div> 0.8710	<div></div> 0.3900
B	<div></div> 0.8710	<div></div> 0.3900
C	<div></div> 0.8710	<div></div> 0.3900
D	<div></div> 0.8710	<div></div> 0.3900

