



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 03:44 AM UTC

PDB ID : 3JAV / pdb_00003jav
EMDB ID : EMD-6369
Title : Structure of full-length IP3R1 channel in the apo-state determined by single particle cryo-EM
Authors : Fan, G.; Baker, M.L.; Wang, Z.; Baker, M.R.; Sinyagovskiy, P.A.; Chiu, W.; Ludtke, S.J.; Serysheva, I.I.
Deposited on : 2015-06-30
Resolution : 4.70 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:

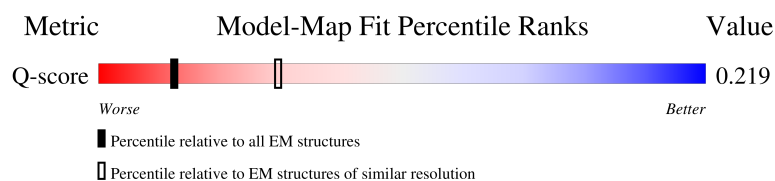
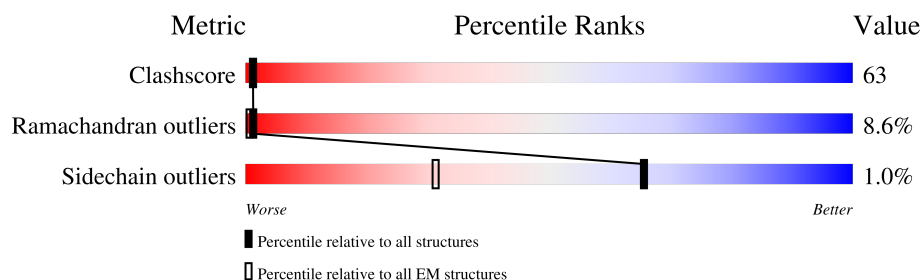
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.70 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	1989 (4.20 - 5.20)

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	2750	 12% 58% 22% • 15%
1	B	2750	 12% 57% 23% • 15%
1	C	2750	 12% 58% 23% • 15%
1	D	2750	 12% 57% 23% • 15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 33472 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.

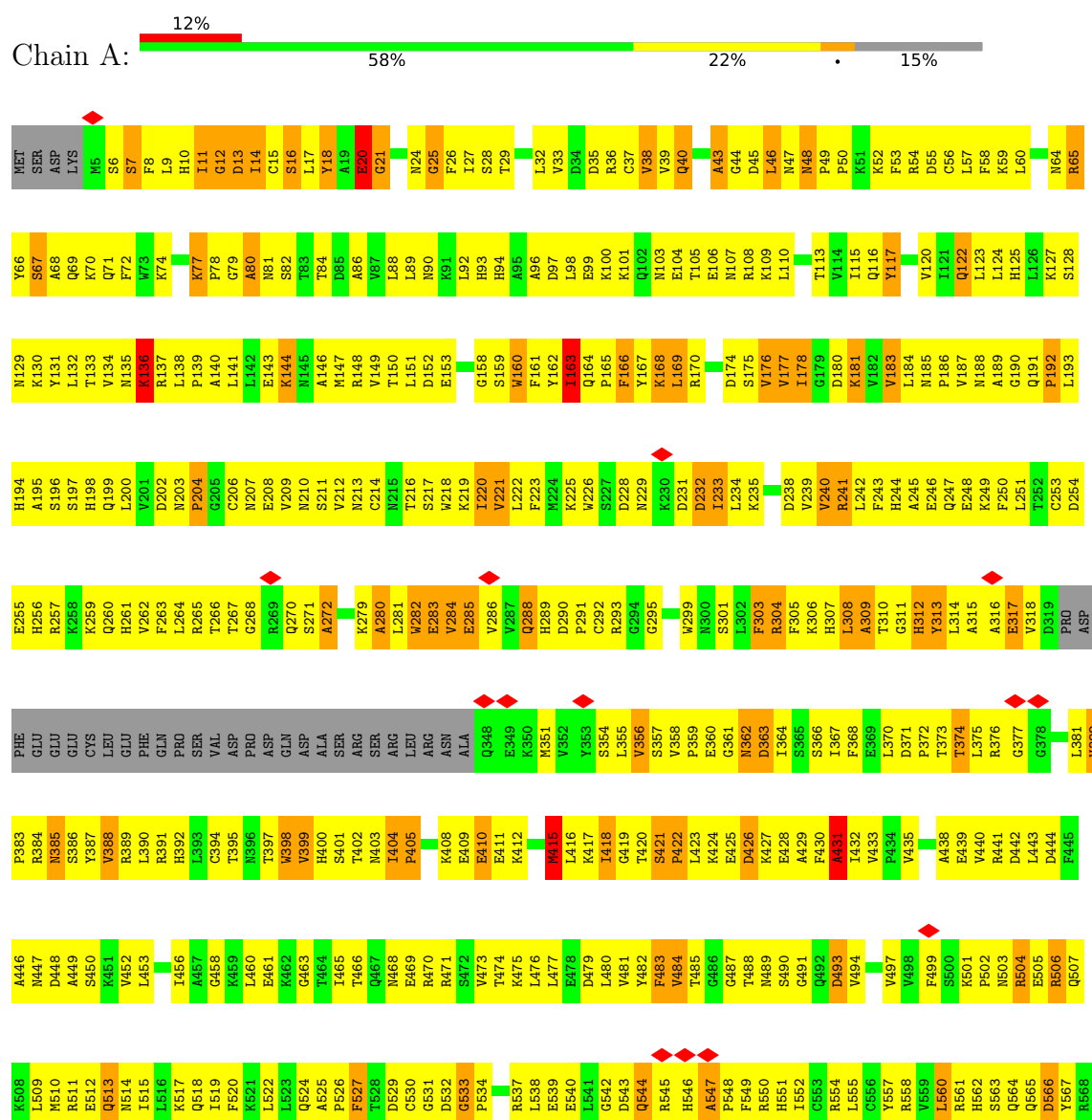
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 1.

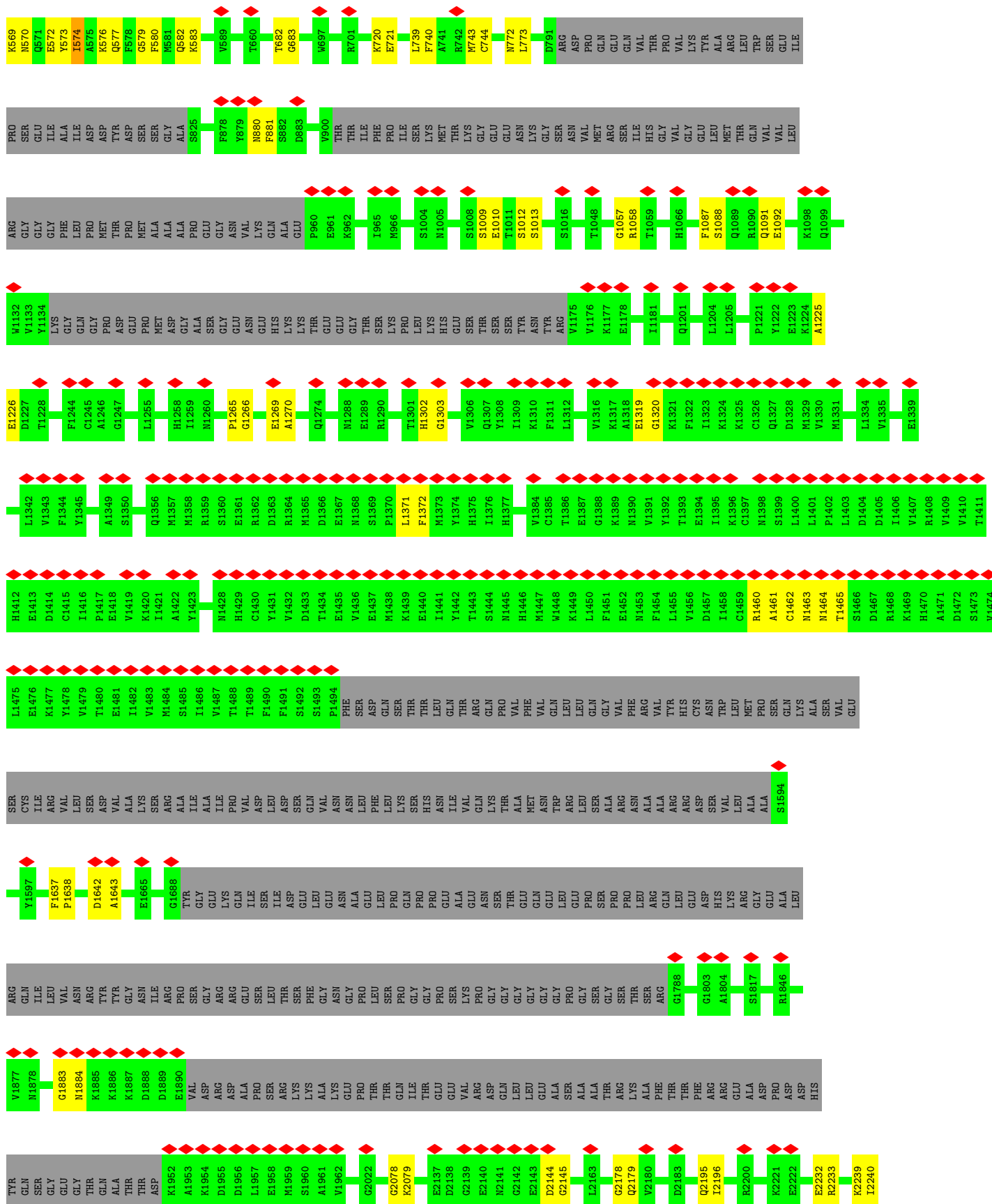
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2327	Total	C	N	O	S	0	1459
			8368	5879	1191	1265	33		
1	B	2327	Total	C	N	O	S	0	1459
			8368	5879	1191	1265	33		
1	C	2327	Total	C	N	O	S	0	1459
			8368	5879	1191	1265	33		
1	D	2327	Total	C	N	O	S	0	1459
			8368	5879	1191	1265	33		

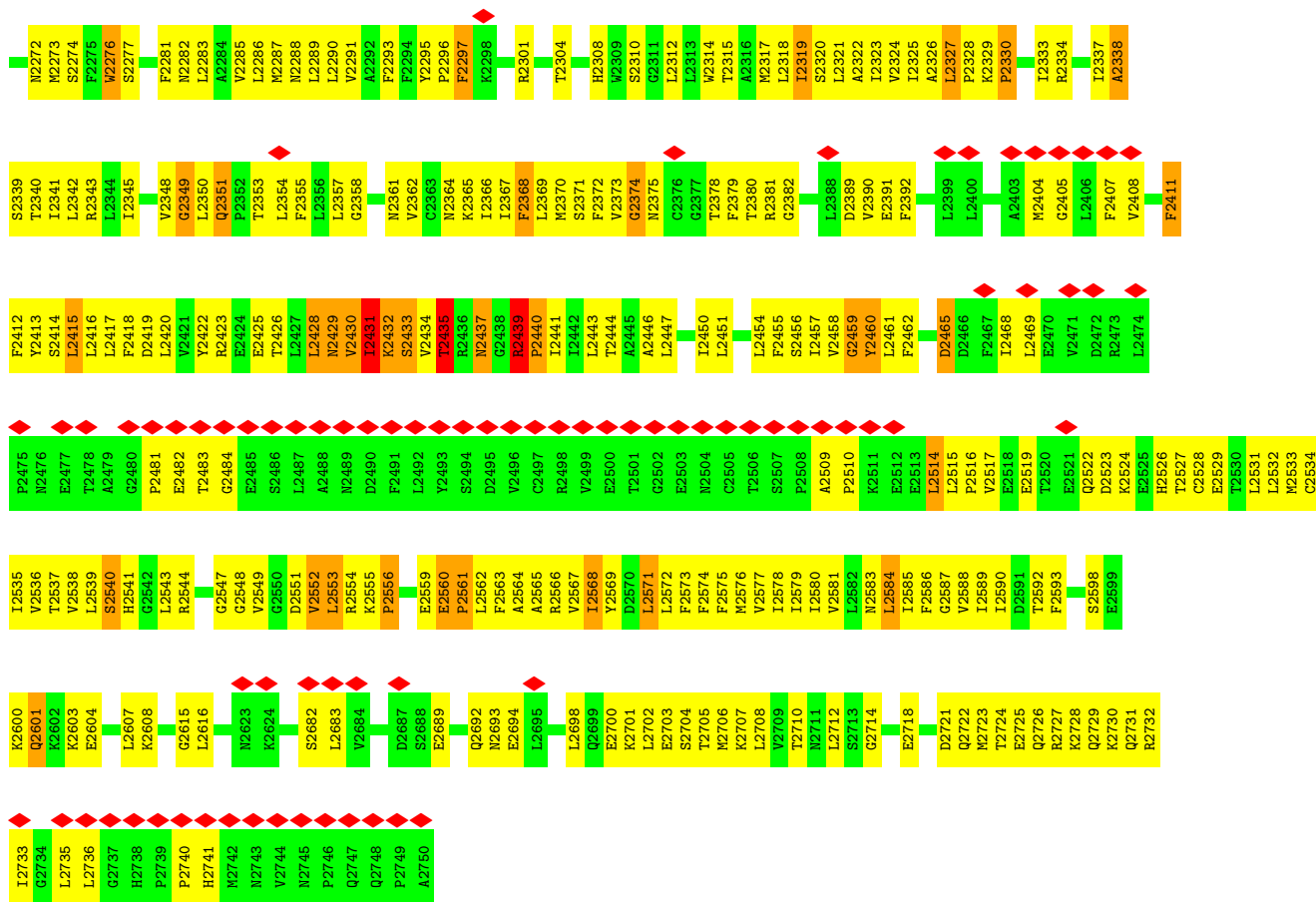
3 Residue-property plots [i](#)

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.

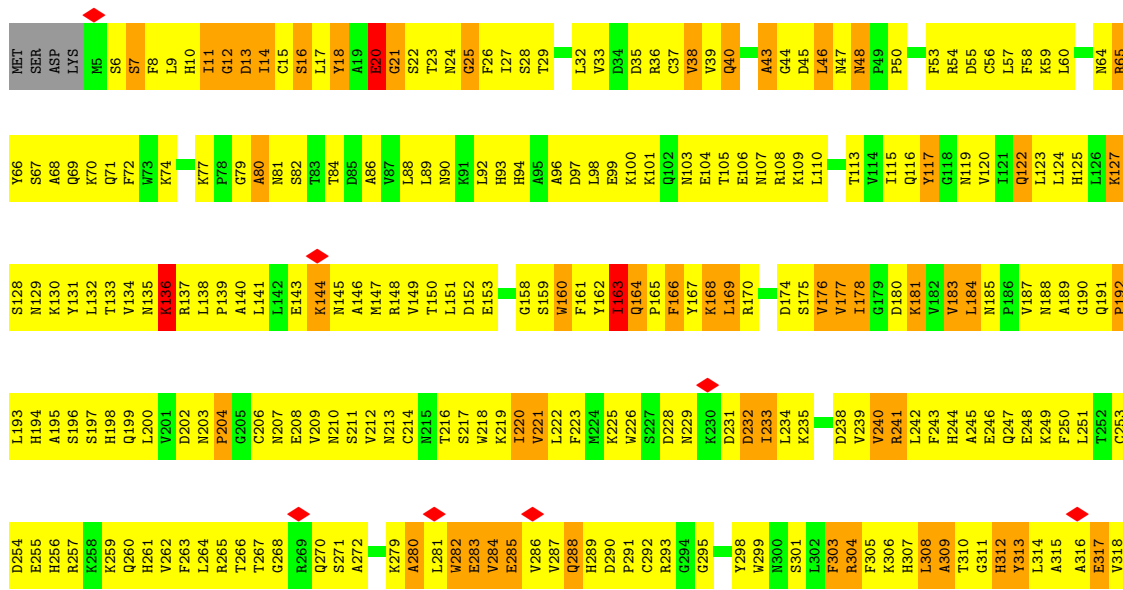
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

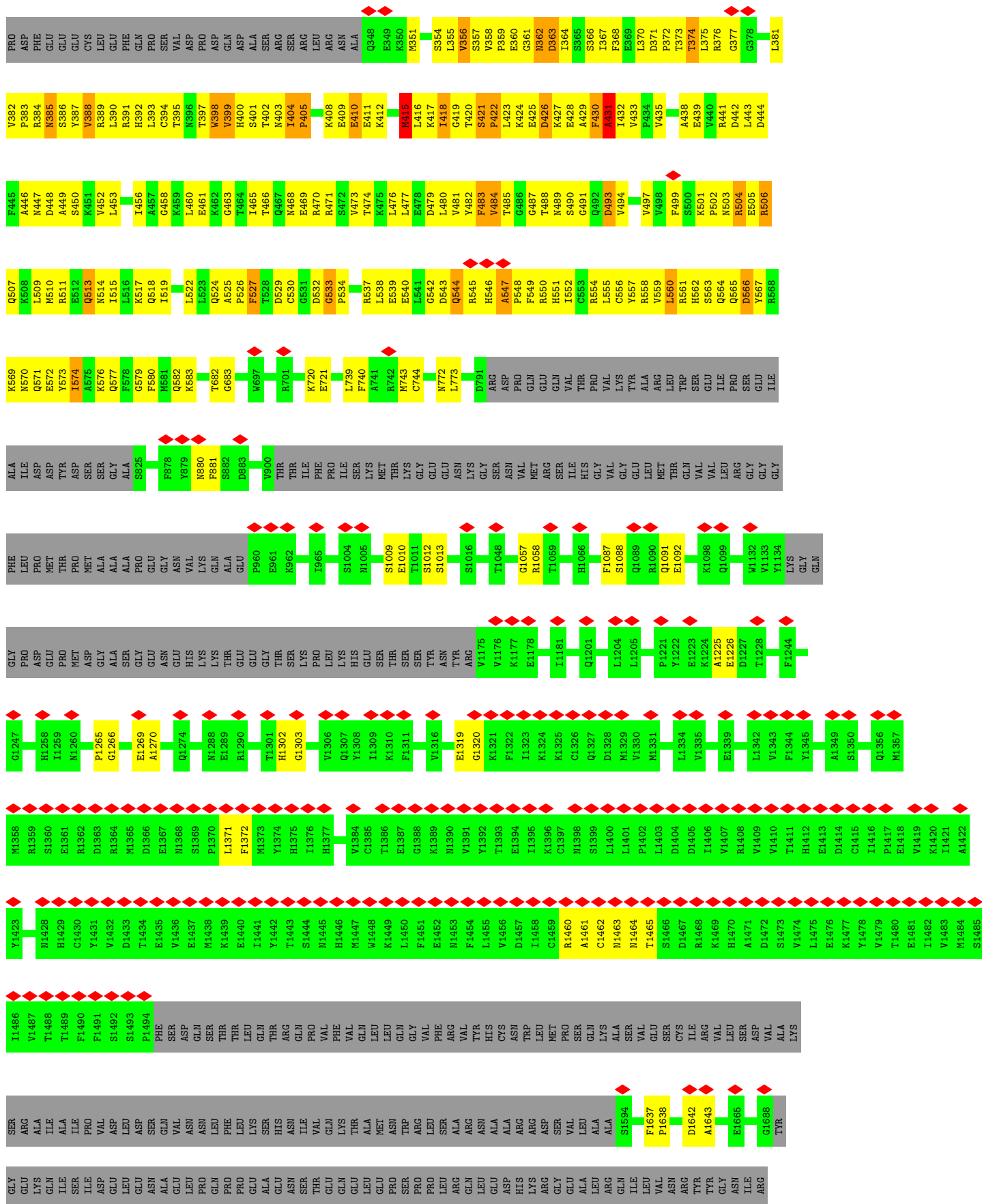


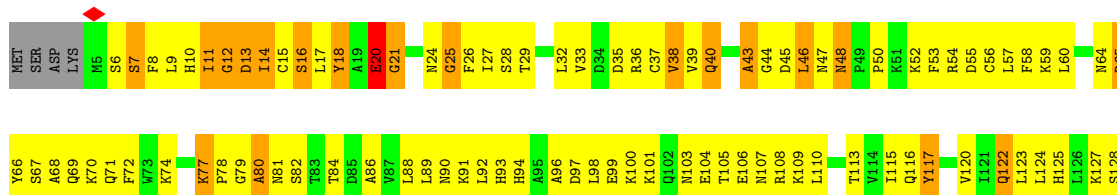
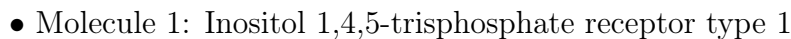


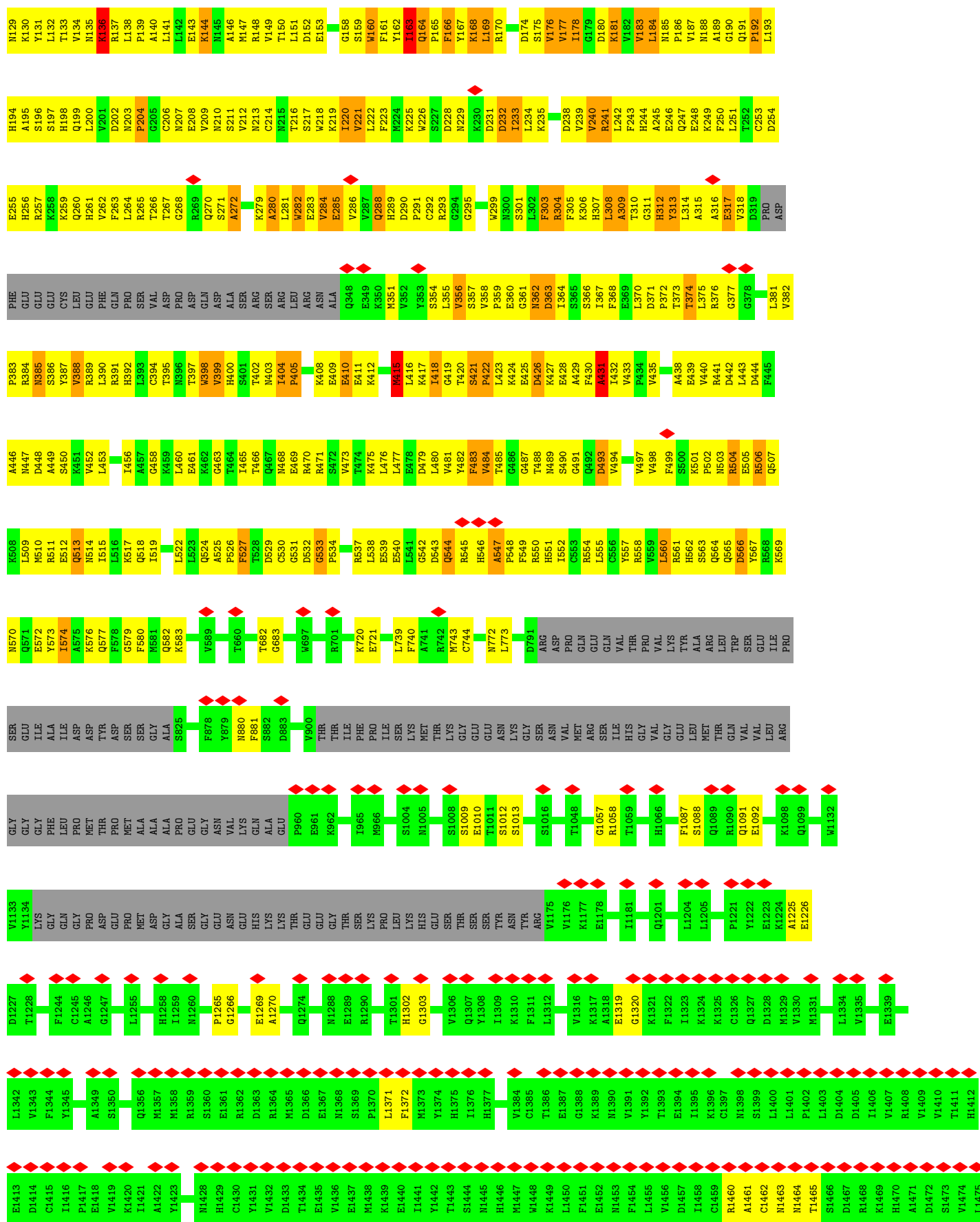


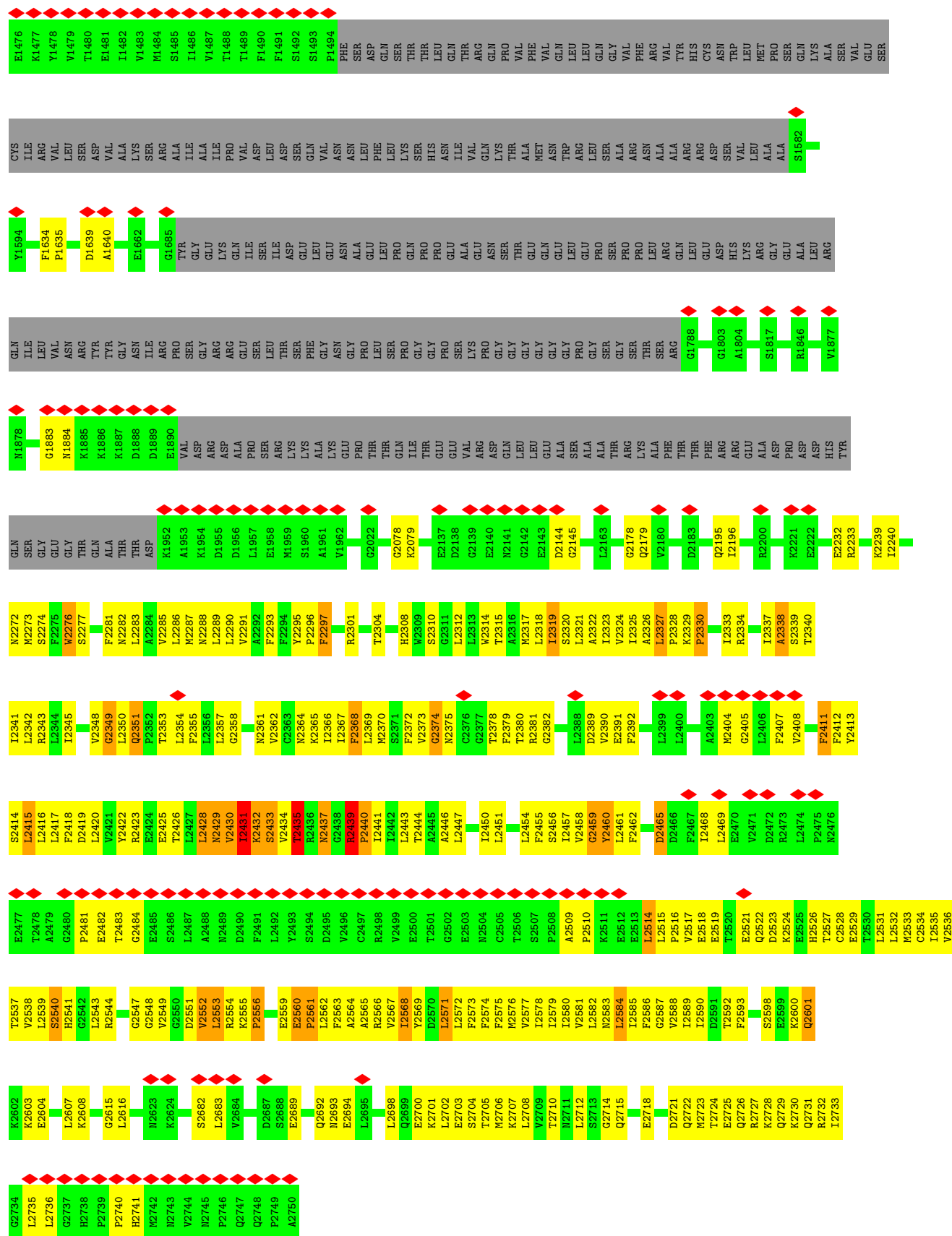
• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1











- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1



T2426	N2489	F2355	N2287	ARG	TYR	LYS	A1422	M1357	G1247
L2427	D2490	L2356	N2288	PRO	GLY	SER	Y1423	M1358	H1258
N2428	F2491	L2357	L2289	GLY	GLU	ARG		R1359	I1259
N2429	L2492	L2290	L2290	ARG	GLN	ILE	N1428	E1360	N1260
L2430	L2493	L2291	D1956	ARG	ILE	ALA	H1429	R1362	
L2431	L2494	L2292	L1957	GLU	SER	ILE	T1488	D1363	P1265
L2432	S2494	L2293	E1958	SER	ILE	PRO	F1490	R1364	G1266
S2433	D2495	L2294	M1959	LEU	ASP	VAL	Y1431	D1365	E1269
L2434	L2496	L2295	L1959	THR	GLU	ASP	C1430	R1366	A1270
L2435	L2497	L2296	S1960	SER	LEU	LEU	D1433	M1367	
L2436	C2497	L2366	A1961	SER	GLU	ASP	T1434	E1367	
L2437	R2498	L2367	V1962	PHE	ASN	GLN	E1435	Q1274	
L2438	L2499	L2368		GLY	ALA	VAL	E1436	N1288	
L2439	E2500	L2369	G2022	ASN	GLU	GLN	Y1437	E1289	
L2440	E2501	M2370	G2078	PRO	LEU	ASN	E1438	N1290	
L2441	T2502	S2371	K2079	LEU	PRO	ASN	M1438	T1301	
L2442	G2503	F2372		THR	GLN	PRO	P1370	H1302	
L2443	E2504	V2373		GLU	GLN	LEU	K1439	G1303	
L2444	N2505	G2374		GLU	PRO	PHE	E1440		
L2445	C2506	N2375		VAL	PRO	ILE	I1441	F1372	
A2446	T2507	C2376		GLY	GLU	LEU	E1442	M1373	
L2447	L2508	T2377		GLY	GLU	GLN	Y1443	Y1374	
		G2378		SER	ALA	THR	Y1444	H1375	
L2450	L2509	F2379		LYS	ASN	ARG	T1443	I1376	
L2451	P2510	T2380		PRO	SER	ILE	N1445		
L2452	K2511	R2381		GLY	THR	VAL	N1446		
L2453	K2512	G2382		GLY	GLU	GLN	H1446		
L2454	L2513			GLY	GLU	THR	M1447		
F2455	E2514	L2388		GLY	LEU	ALA	W1448		
S2456	L2515	L2389		GLY	LEU	ALA	W1449		
L2457	P2516	D2390		GLY	LEU	ALA	K1449		
L2458	V2517	V2391		GLY	LEU	ALA	L1450		
L2459	L2518	E2392		GLY	LEU	ALA	F1451		
L2460	L2519	F2392		GLY	LEU	ALA	E1452		
L2461	L2520			GLY	LEU	ALA	N1453		
L2462	L2521	L2399		GLY	LEU	ALA	F1454		
L2463	L2522	L2400		GLY	LEU	ALA	N1455		
L2464	L2523	L2401		GLY	LEU	ALA	L1455		
L2465	L2524	L2402		GLY	LEU	ALA	Y1456		
L2466	L2525	A2403		GLY	LEU	ALA	D1457		
L2467	L2526	M2404		GLY	LEU	ALA	T1458		
L2468	L2527	G2405		GLY	LEU	ALA	C1459		
L2469	L2528	L2406		GLY	LEU	ALA	R1460		
L2470	L2529	L2407		GLY	LEU	ALA	A1461		
L2471	L2530	L2408		GLY	LEU	ALA	C1462		
L2472	L2531	L2409		GLY	LEU	ALA	N1463		
L2473	L2532	Y2412		GLY	LEU	ALA	SER		
L2474	L2533	Y2413		GLY	LEU	ALA	T1465		
L2475	L2534	L2415		GLY	LEU	ALA	N1466		
L2476	L2535	L2416		GLY	LEU	ALA	S1466		
L2477	L2536	L2417		GLY	LEU	ALA	D1467		
L2478	L2537	L2418		GLY	LEU	ALA	C1468		
L2479	L2538	L2419		GLY	LEU	ALA	R1469		
L2480	L2539	L2420		GLY	LEU	ALA	K1469		
L2481	L2540	L2421		GLY	LEU	ALA	H1470		
L2482	L2541	Y2422		GLY	LEU	ALA	A1471		
L2483	L2542	R2423		GLY	LEU	ALA	D1472		
L2484	L2543	E2424		GLY	LEU	ALA	S1473		
L2485	L2544	E2425		GLY	LEU	ALA	V1474		
L2486	L2545			GLY	LEU	ALA	L1475		
L2487	L2546			GLY	LEU	ALA	V1476		
L2488	L2547			GLY	LEU	ALA	L1477		
	L2548			GLY	LEU	ALA	Y1478		
	L2549			GLY	LEU	ALA	Y1479		
				GLY	LEU	ALA	T1480		
				GLY	LEU	ALA	E1481		
				GLY	LEU	ALA	I1482		
				GLY	LEU	ALA	V1483		
				GLY	LEU	ALA	M1484		



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	96106	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	CTFFIND3	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	22	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	30886	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	16.272	Depositor
Minimum map value	-6.215	Depositor
Average map value	0.030	Depositor
Map value standard deviation	0.385	Depositor
Recommended contour level	0.7	Depositor
Map size ($\text{\AA}$)	414.72, 414.72, 414.72	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.62, 1.62, 1.62	Depositor

5 Model quality

5.1 Standard geometry

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	2.29	27/7045 (0.4%)	1.25	77/9516 (0.8%)
1	B	2.29	27/7045 (0.4%)	1.25	79/9516 (0.8%)
1	C	2.29	27/7045 (0.4%)	1.25	79/9516 (0.8%)
1	D	2.32	34/7045 (0.5%)	1.31	85/9516 (0.9%)
All	All	2.30	115/28180 (0.4%)	1.26	320/38064 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	8
1	C	0	8
1	D	0	8
All	All	0	32

The worst 5 of 115 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	176	VAL	CA-CB	139.10	3.18	1.54
1	B	176	VAL	CA-CB	139.03	3.18	1.54
1	C	176	VAL	CA-CB	138.98	3.18	1.54
1	A	176	VAL	CA-CB	138.94	3.18	1.54
1	B	285	GLU	CA-C	68.45	2.44	1.52

The worst 5 of 320 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2429	ASN	N-CA-C	20.73	133.25	111.07
1	D	2428	LEU	N-CA-C	20.44	140.11	109.24
1	A	285	GLU	O-C-N	-14.78	102.94	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	285	GLU	O-C-N	-14.77	102.94	122.59
1	D	285	GLU	O-C-N	-14.76	102.96	122.59

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	GLY	Peptide
1	A	136	LYS	Peptide
1	A	163	ILE	Peptide
1	A	169	LEU	Peptide
1	A	240	VAL	Peptide

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	8368	0	6997	1017	0
1	B	8368	0	6997	1024	0
1	C	8368	0	6997	1020	0
1	D	8368	0	6997	1026	0
All	All	33472	0	27988	3892	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 63.

The worst 5 of 3892 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:D:303:PHE:CG	1:D:303:PHE:CD1	1.75	1.72
1:B:303:PHE:CD1	1:B:303:PHE:CG	1.75	1.71
1:D:117:TYR:CE1	1:D:117:TYR:CZ	1.80	1.70
1:A:117:TYR:CE2	1:A:117:TYR:CZ	1.78	1.70
1:B:18:TYR:CZ	1:B:18:TYR:CE2	1.80	1.69

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	856/2750 (31%)	645 (75%)	137 (16%)	74 (9%)	0	9
1	B	856/2750 (31%)	647 (76%)	135 (16%)	74 (9%)	0	9
1	C	856/2750 (31%)	646 (76%)	137 (16%)	73 (8%)	0	9
1	D	856/2750 (31%)	649 (76%)	133 (16%)	74 (9%)	0	9
All	All	3424/11000 (31%)	2587 (76%)	542 (16%)	295 (9%)	1	9

5 of 295 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	20	GLU
1	A	144	LYS
1	A	165	PRO
1	A	166	PHE

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	769/2459 (31%)	761 (99%)	8 (1%)	68	76
1	B	769/2459 (31%)	761 (99%)	8 (1%)	68	76
1	C	769/2459 (31%)	761 (99%)	8 (1%)	68	76
1	D	769/2459 (31%)	762 (99%)	7 (1%)	70	77
All	All	3076/9836 (31%)	3045 (99%)	31 (1%)	65	76

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2514	LEU
1	D	2431	ILE
1	C	178	ILE
1	D	2514	LEU
1	D	14	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	188	ASN
1	C	518	GLN
1	D	2731	GLN
1	C	213	ASN
1	C	289	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

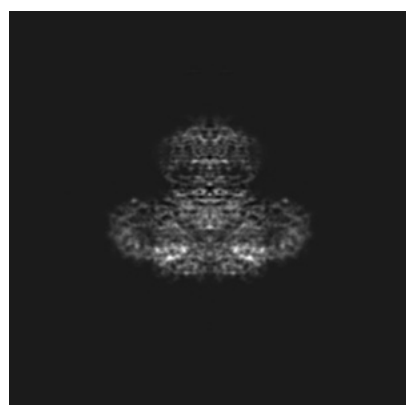
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6369. These allow visual inspection of the internal detail of the map and identification of artifacts.

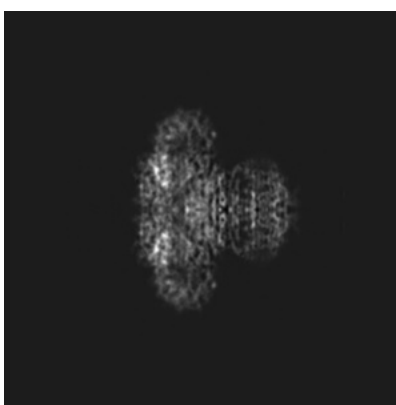
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

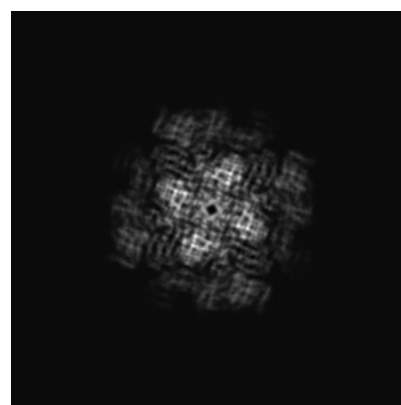
6.1.1 Primary map



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: 128



Y Index: 128

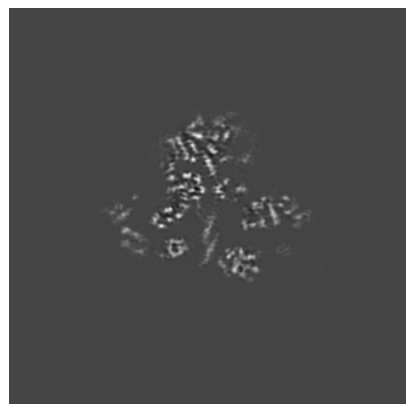


Z Index: 128

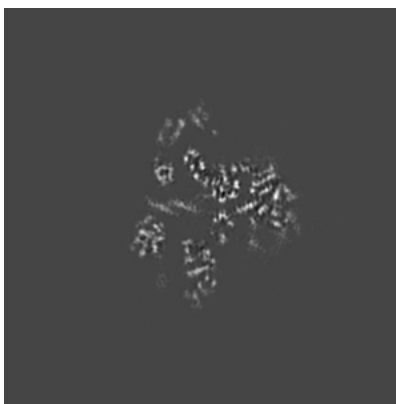
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

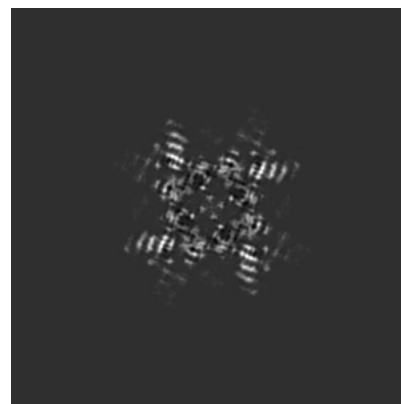
6.3.1 Primary map



X Index: 123



Y Index: 123

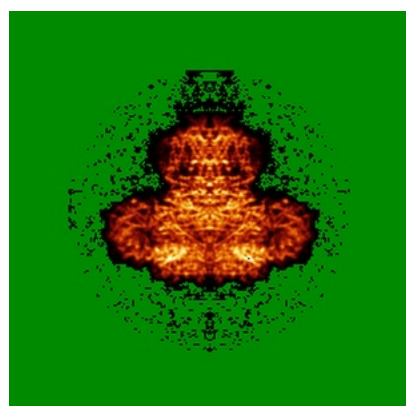


Z Index: 97

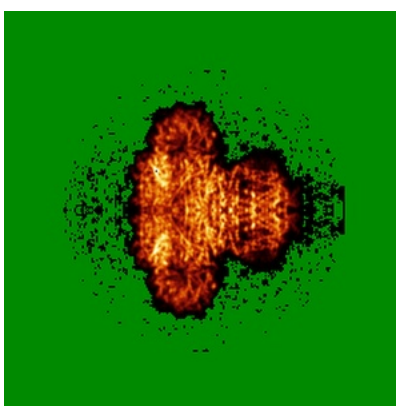
The images above show the largest variance slices of the map in three orthogonal directions.

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

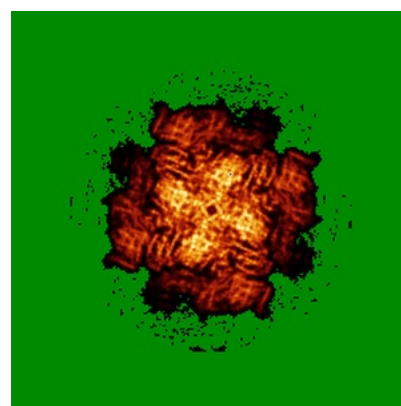
6.4.1 Primary map



X



Y

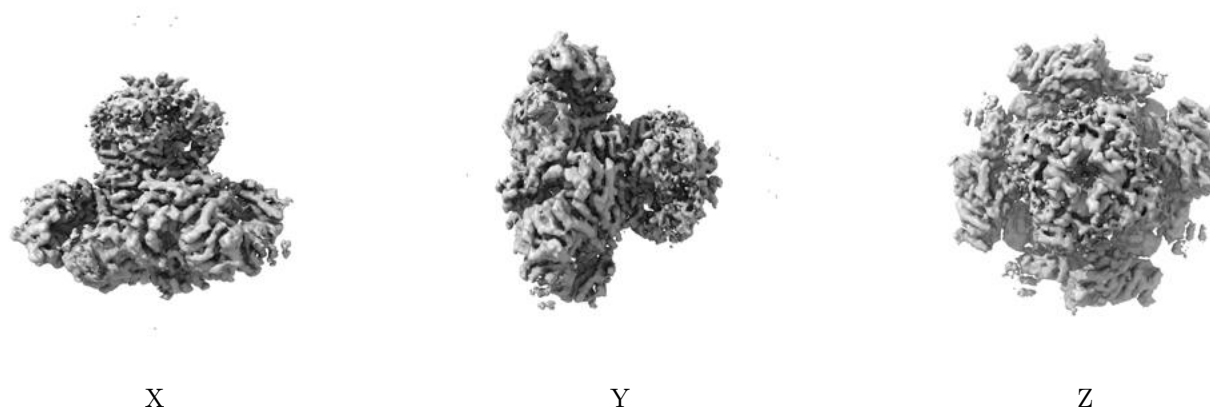


Z

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

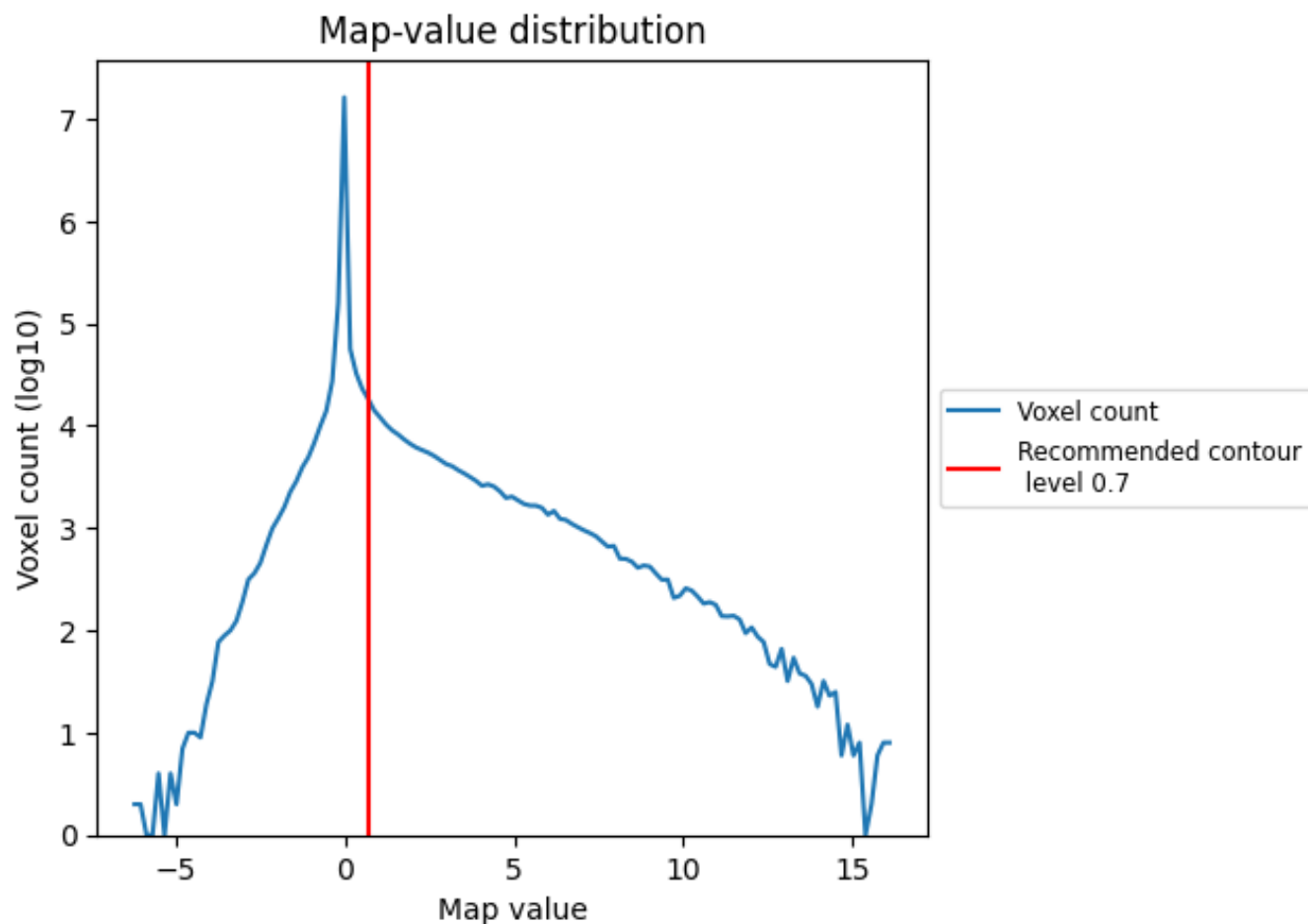
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

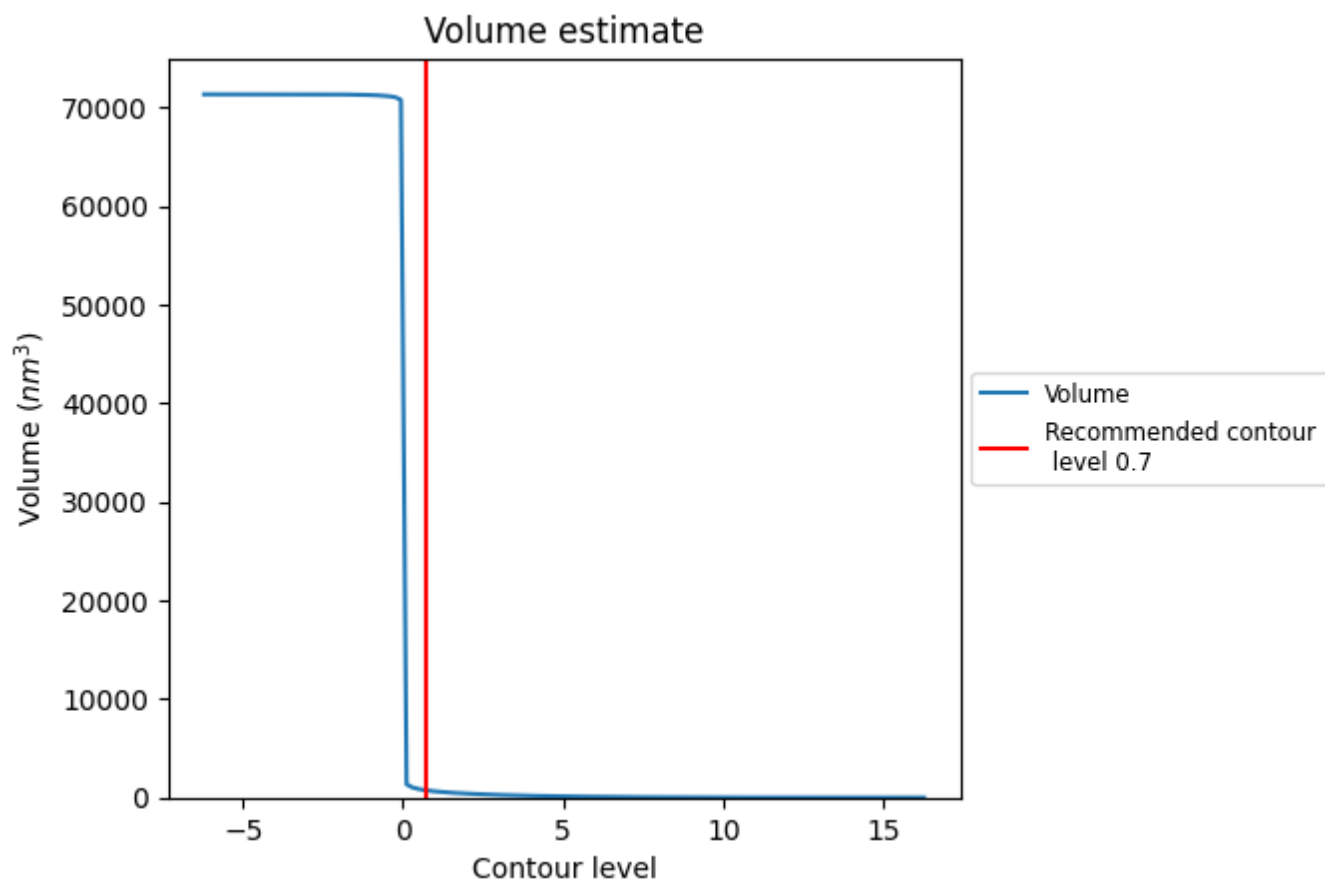
This section contains the results of statistical analysis of the map.

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.

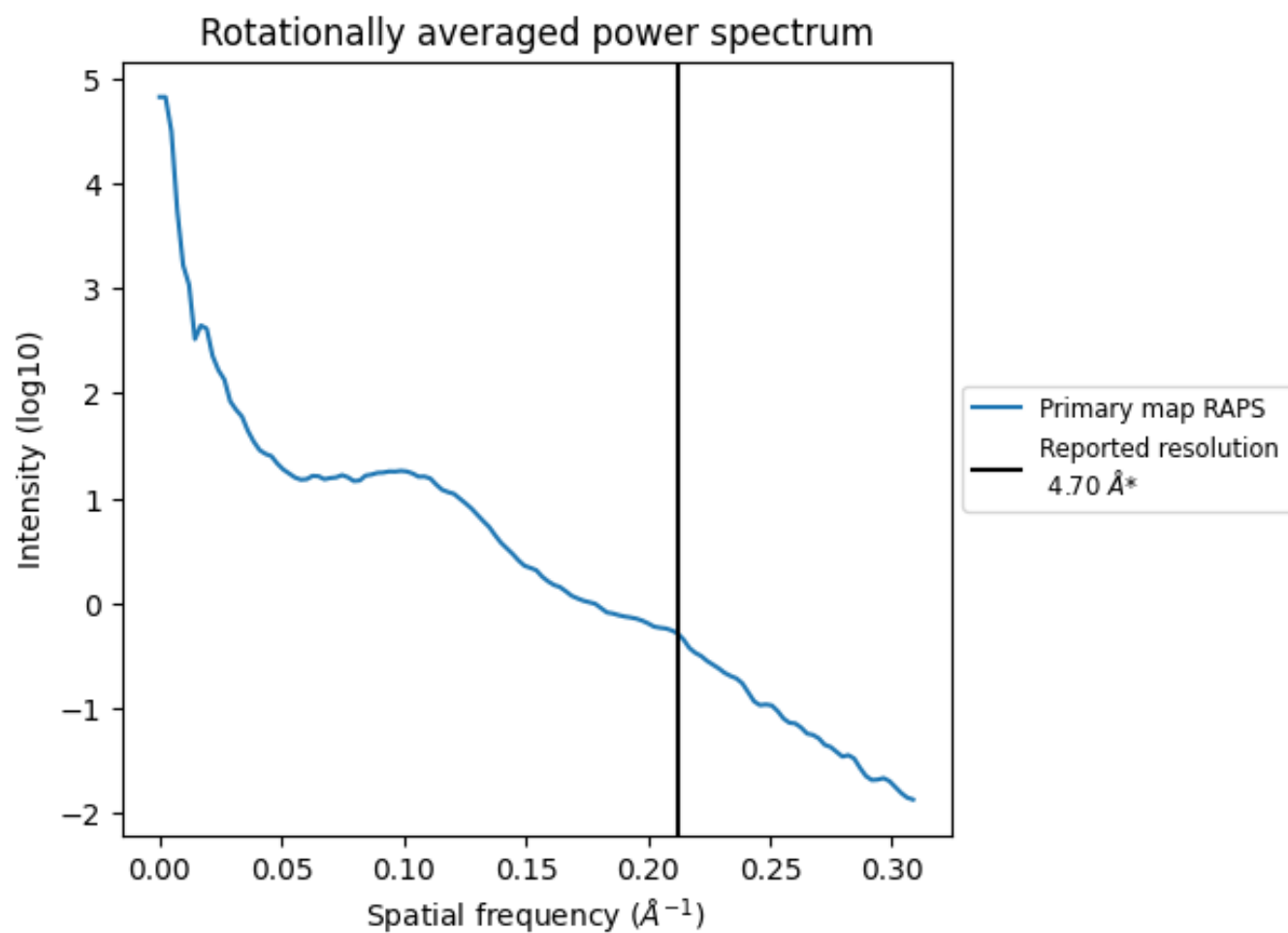
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 745 nm^3 ; this corresponds to an approximate mass of 673 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 0.213 Å⁻¹

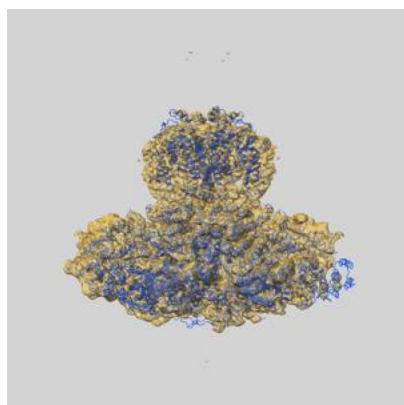
8 Fourier-Shell correlation

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

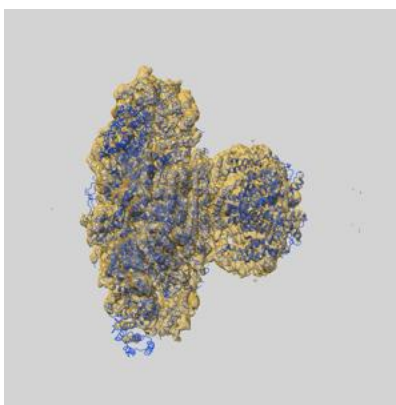
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6369 and PDB model 3JAV. Per-residue inclusion information can be found in section [3](#) on page [4](#).

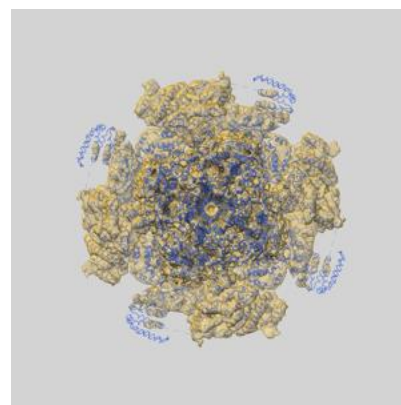
9.1 Map-model overlay [i](#)



X



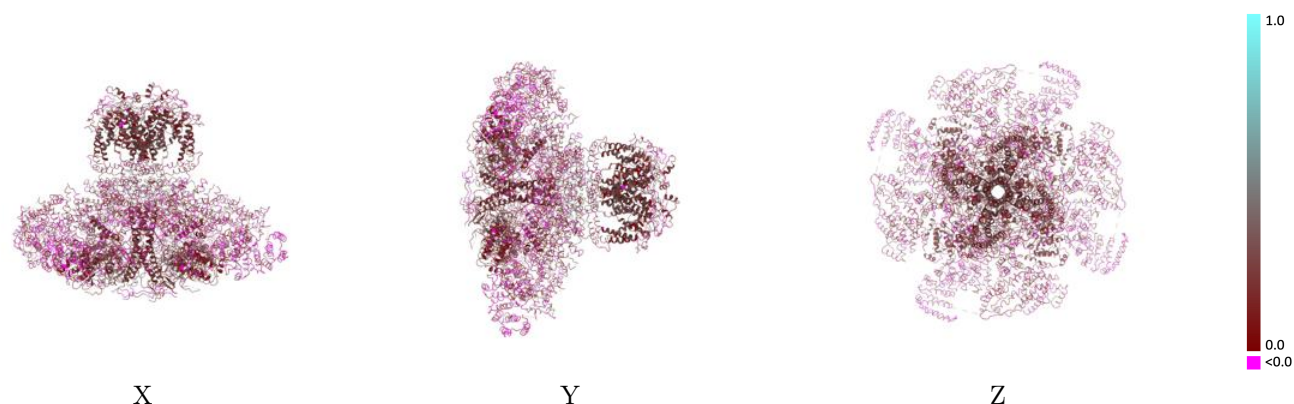
Y



Z

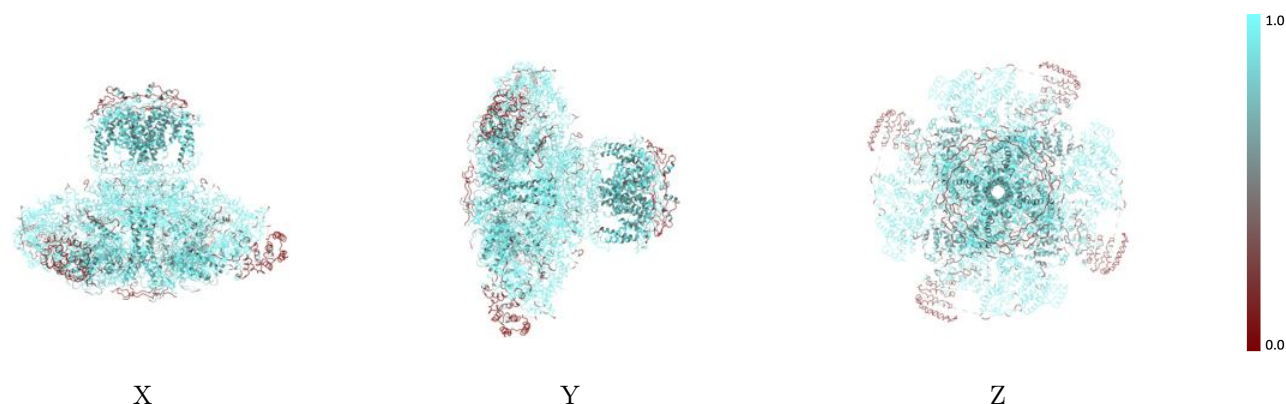
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



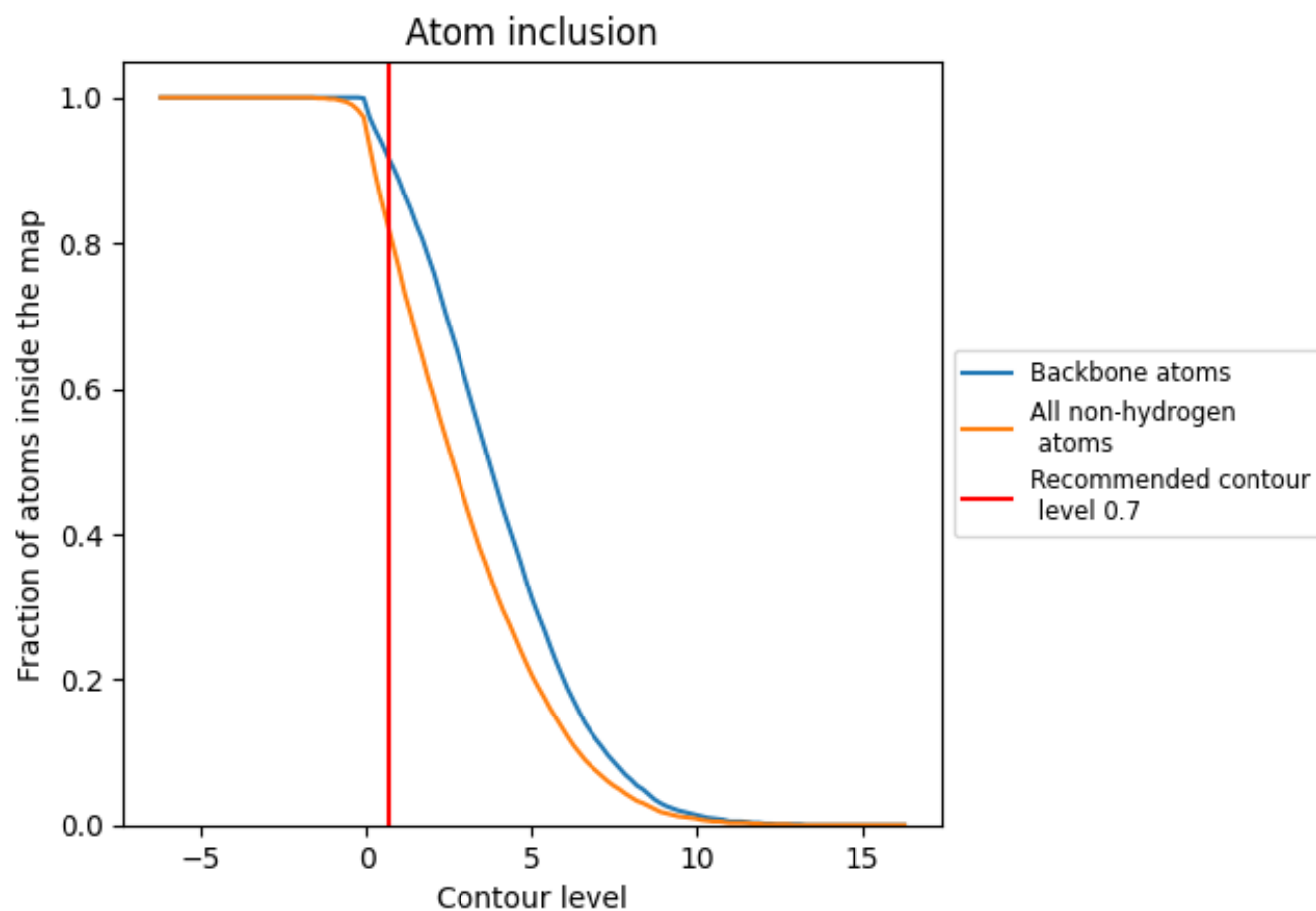
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 82% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8170	0.2190
A	0.8170	0.2180
B	0.8190	0.2190
C	0.8170	0.2180
D	0.8180	0.2190

