



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:57 PM BST

PDB ID : 3JAV
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 Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

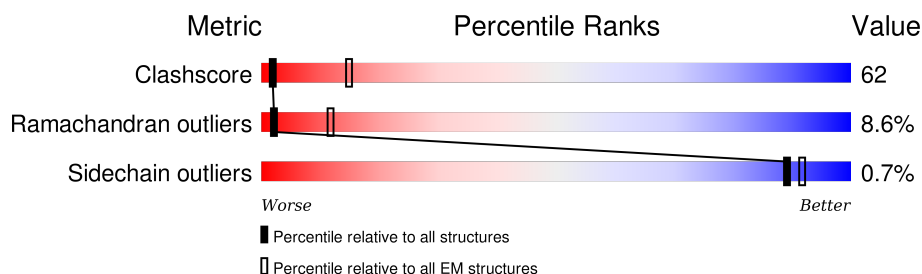
1 Overall quality at a glance

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)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	2750	58% 23% • 15%
1	B	2750	58% 24% • 15%
1	C	2750	58% 24% • 15%
1	D	2750	58% 24% • 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.

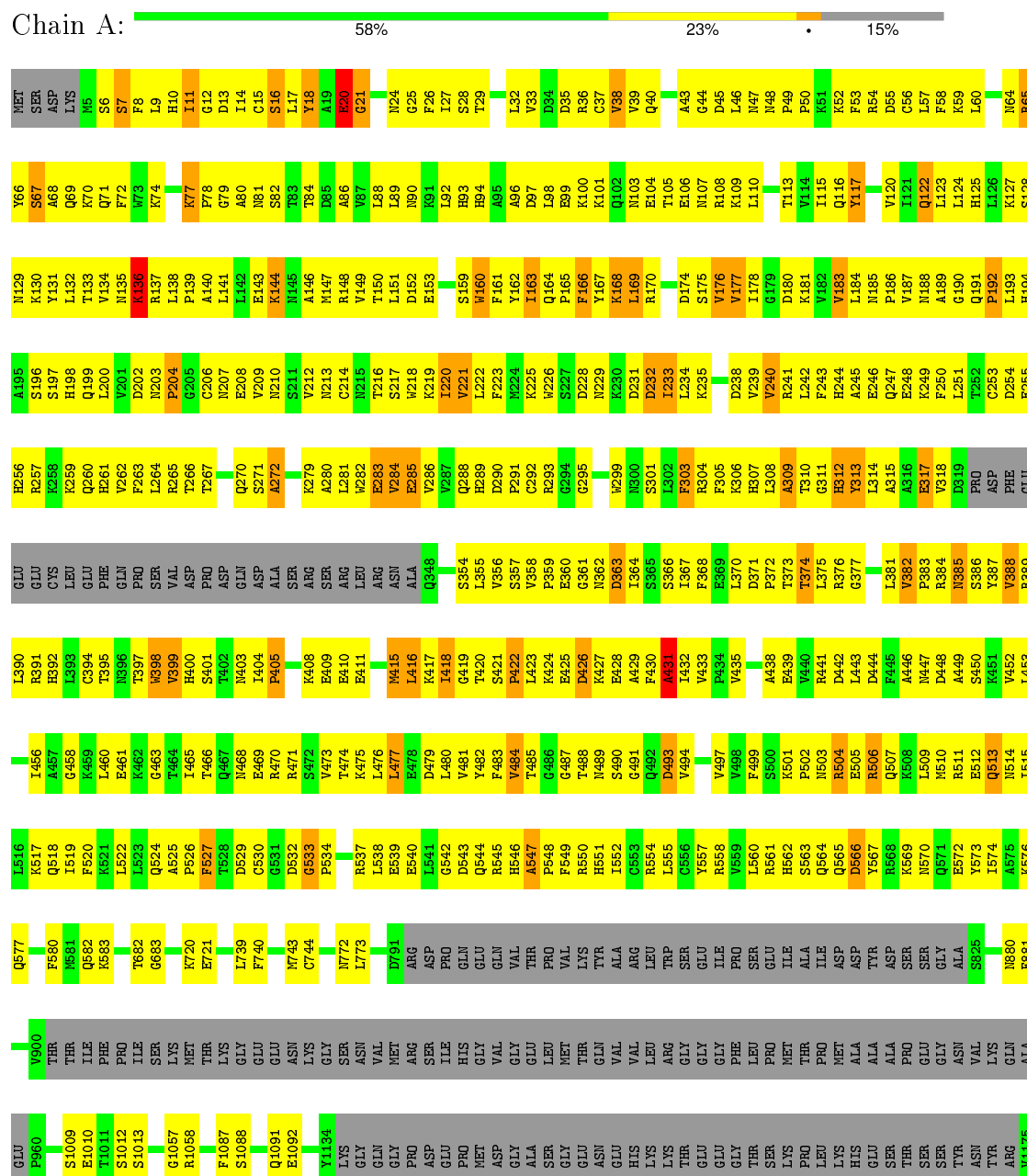
- Molecule 1 is a protein called Inositol 1,4,5-trisphosphate receptor type 1.

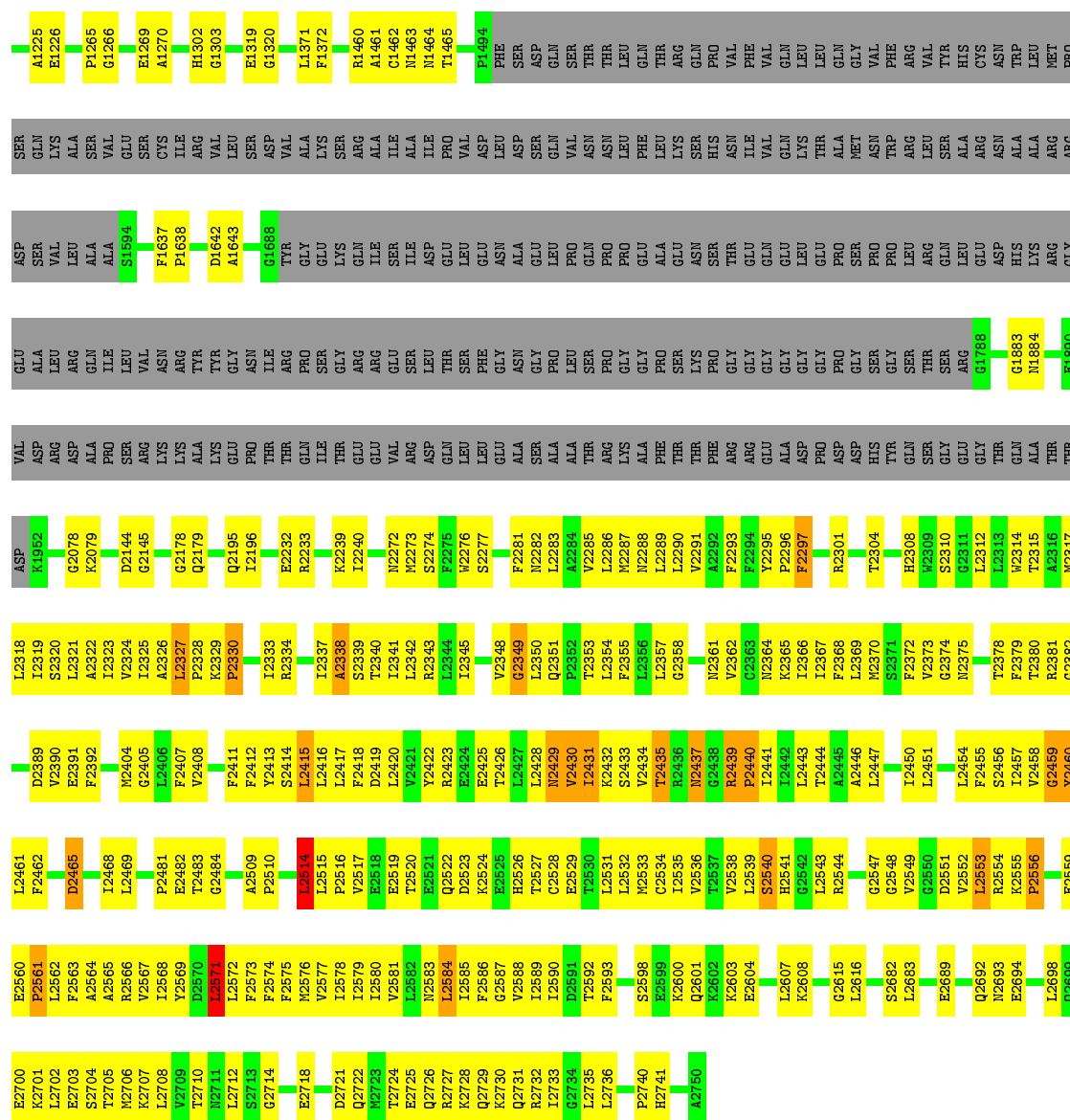
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2327	Total	C	N	O	S	0	1459
			8368	5879	1191	1265	33		
1	B	2327	Total	C	N	O	S	0	1459
			8368	5879	1191	1265	33		
1	C	2327	Total	C	N	O	S	0	1459
			8368	5879	1191	1265	33		
1	D	2327	Total	C	N	O	S	0	1459
			8368	5879	1191	1265	33		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

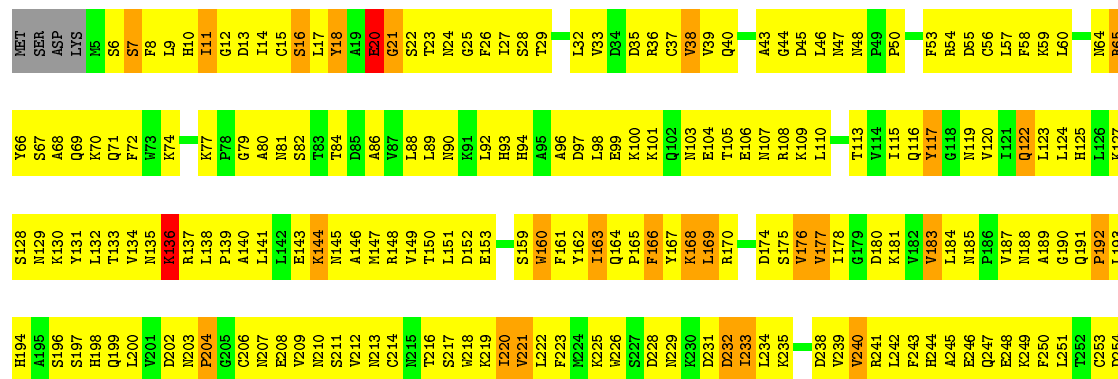
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1



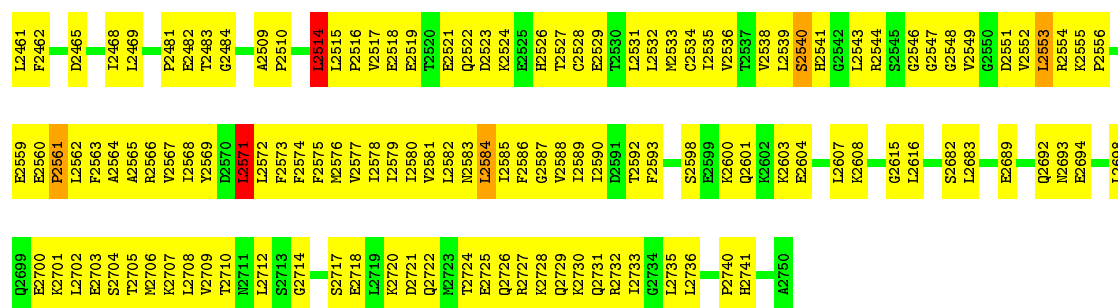


• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 1

Chain B: 58% 24% 15%

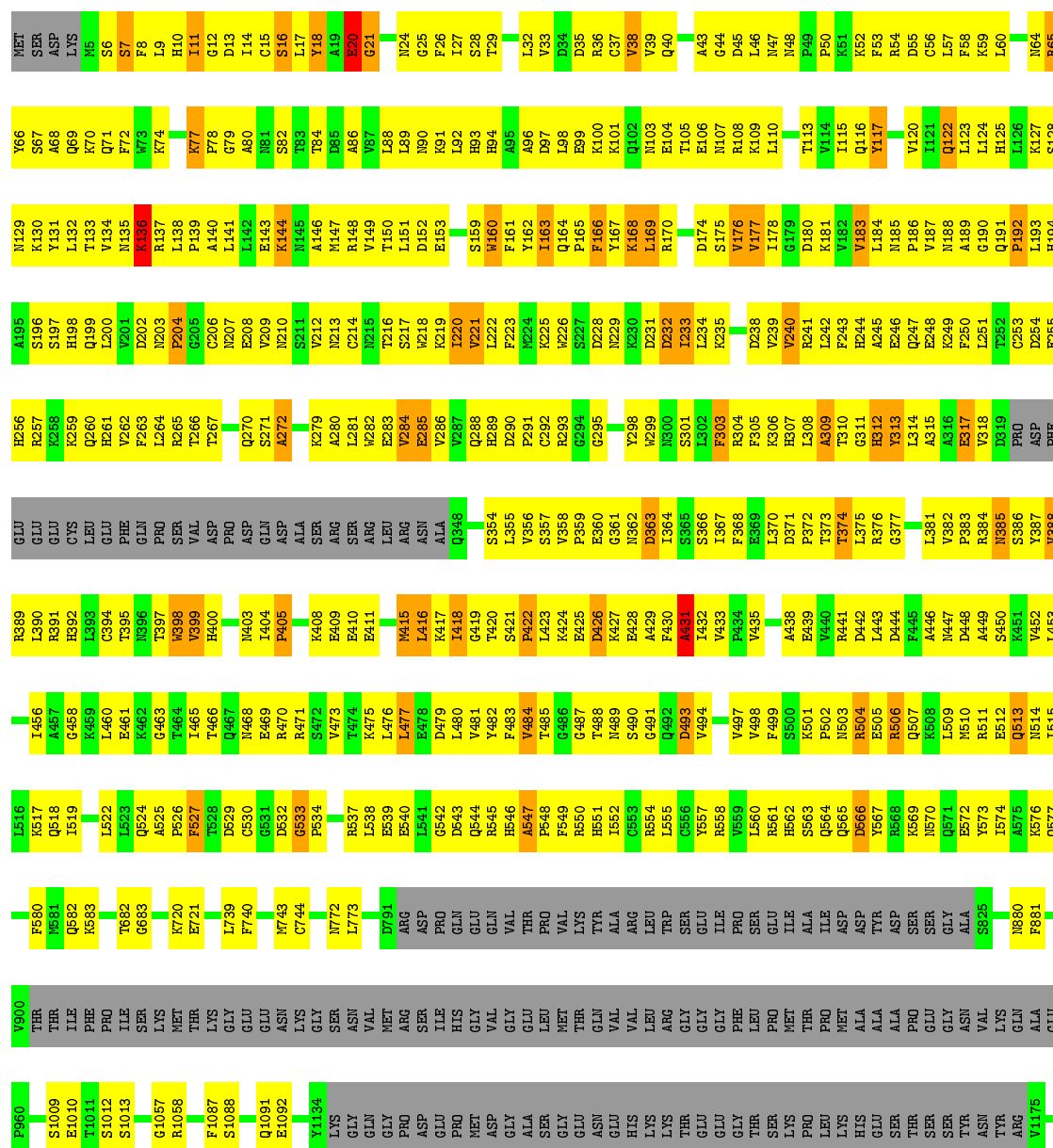


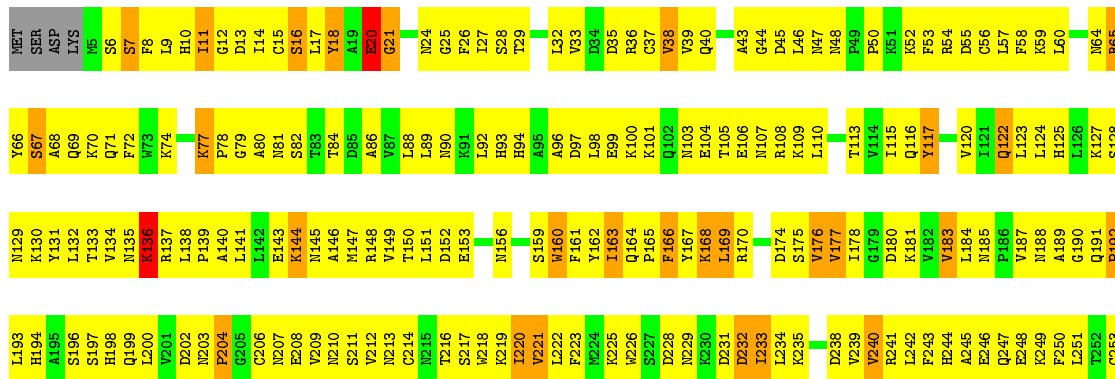
D2389	L2318	THR	E1890	GLY	ARG	PRO	V1475	ALA	P881	K576	H514	V452	R389	GLU	E255
V2390	I2319	ASP	VAL	GLY	ASP	SER	A1225	GLU	P881	Q577	H515	L453	L390	GLU	H256
E2391	S2320	K1952	ASP	ALA	SER	GLN	E1226	P960	V900	F580	L516	I456	H391	CYS	R257
F2392	L2321	VAL	ARG	LEU	VAL	LYS	E1226	S1009	THR	M581	K517	A457	H392	LEU	K258
K2404	A2322	GLN	ALA	ARG	ALA	SER	P1265	E1010	ILE	Q582	H518	G458	L393	LEU	K260
G2405	I2323	PRO	ALA	ILE	ALA	VAL	G1266	T1011	PHE	K583	L519	K459	C394	PHE	H261
L2406	V2324	D2144	SER	LEU	S1594	GLU	G1266	S1012	PRO	T682	L522	L460	T395	GLN	V262
F2407	A2325	G2145	ARG	VAL	ALA	SER	E1269	S1013	ILE	G683	L523	E461	T397	PRO	F263
V2408	L2326	F1637	LYS	ASN	F1637	CYS	A1270	G1057	LYS	K576	A525	G463	H398	SER	L264
V2409	P2328	P1638	ARG	ARG	P1638	ILE	A1270	R1058	THR	K720	P626	T464	H400	VAL	R265
K2329	Q2179	D1642	ALA	TYR	D1642	VAL	H1302	F1087	MET	E721	H527	T465	S401	ASP	T266
P2330	Q2195	A1643	LYS	GLY	A1643	LEU	G1303	F1087	LYS	T682	H528	T466	T402	ASP	T267
F2411	I2333	G1688	GLU	ASN	G1688	SER	E1319	S1088	GLY	F739	D629	Q467	N403	GLN	Q270
F2412	T2334	TYR	THR	ILE	THR	ASP	G1320	Q1091	GLY	F740	C530	N468	N403	ASN	S271
Y2413	R2334	PRO	THR	ARG	GLY	VAL	E1371	E1091	GLU	M743	D532	E469	P405	ALA	A272
S2414	L2337	GLN	GLN	PRO	GLY	ALA	L1371	E1092	LYS	C744	H533	R470	S405	SER	
L2415	I2337	ILE	ILE	ASN	GLY	SER	F1372	Y1134	GLY	N772	H537	S472	K408	ARG	K279
L2416	A2338	GLY	GLY	GLY	GLY	ARG	R1460	LYS	SER	L773	L538	V473	E409	SER	L280
L2417	S2339	LYS	LYS	ILE	LYS	VAL	A1461	GLY	ASN	L773	H540	T474	E410	ARG	L281
F2418	T2340	ARG	GLU	ILE	ILE	ALA	C1462	GLN	VAL	M743	L539	K475	E411	LEU	W282
D2419	I2341	VAL	VAL	GLU	ILE	ALA	C1462	GLY	VAL	D791	H540	K475	E412	ARG	E283
V2420	L2342	SER	ARG	ILE	ILE	ALA	N1463	GLY	MET	D791	H540	L477	ASN	ASN	V284
Y2421	L2343	ASP	ASP	LEU	ILE	ILE	N1464	PRO	ARG	D791	H540	L477	ALA	ALA	E285
Y2422	R2343	LEU	GLN	THR	GLY	PRO	T1465	ASP	SER	ASP	H541	E478	M445	ALA	E286
R2423	I2344	LEU	VAL	THR	GLY	VAL	P1494	PHE	ILE	PRO	H542	D479	L416	Q368	V286
E2424	L2345	LEU	LEU	SER	LEU	ASP	P1494	GLY	ILE	GLU	H543	L480	L417		V287
E2425	V2348	THR	LEU	PHE	GLY	GLY	PHE	PRO	HIS	GLN	H544	L480	L418	S354	Q288
L2426	G2349	GLY	GLY	GLY	GLY	ASN	ASP	GLY	GLY	GLY	H545	V481	G419	L355	H289
L2427	Q2351	GLY	ASN	ASN	GLY	ASP	ASP	ASP	VAL	GLN	H546	Y482	T420	V356	D290
N2429	L2350	PRO	ALA	ASN	GLY	SER	GLN	ALA	GLY	VAL	H547	F483	S421	S357	P291
Y2430	P2352	LEU	ALA	PRO	LEU	GLN	GLN	ALA	GLY	THR	H548	V484	P422	V358	C292
I2431	T2353	LEU	THR	LEU	LEU	VAL	ASP	GLY	LEU	PRO	H549	T485	L423	P359	R293
K2432	L2354	SER	THR	SER	GLN	ASN	THR	GLY	MET	VAL	H550	G486	K424	E360	G294
S2433	F2355	PRO	PRO	PRO	THR	ASN	THR	GLY	THR	LYS	H551	G487	E425	G361	G295
V2434	L2356	GLY	LYS	GLY	PRO	LEU	LEU	ASN	GLN	TYR	H552	T488	D426	N362	
T2435	L2357	PRO	ALA	PRO	ALA	PHE	GLN	GLY	VAL	ALA	H553	N489	K427	D363	V299
R2436	G2358	PRO	PHE	PRO	ALA	LEU	THR	HIS	VAL	ARG	H554	S490	E423	I364	N300
N2437	N2361	THR	THR	SER	GLY	LYS	ARG	LYS	LEU	LEU	H555	G491	A429	S365	S301
R2438	V2362	THR	THR	LYS	ASN	SER	GLN	LYS	ANG	TRP	H556	Q492	F430	S366	L302
R2439	G2363	PHE	PHE	PRO	SER	HIS	GLN	LYS	GLY	SER	H557	D493	I432	I367	F303
P2440	F2294	ARG	ARG	GLY	THR	ASN	VAL	THR	GLY	GLY	H558	V494	I432	F304	R304
I2441	N2364	GLY	GLY	GLY	GLY	ILE	PHE	GLY	PHE	ILE	H559	V497	V433	E369	F305
T2442	K2365	GLY	ALA	GLY	GLY	VAL	VAL	GLY	LEU	PRO	H560	V498	V433	K306	
L2443	I2366	GLY	ALA	GLY	GLY	GLN	GLN	THR	LEU	SER	H561	P499	V435	H307	
T2444	I2367	ASP	ASP	GLY	GLY	LYS	LEU	SER	PRO	GLU	H562	S500	A438	P372	L308
A2445	F2368	GLY	PRO	GLY	GLY	THR	LEU	LYS	MET	ILE	H563	K501	E439	T373	A309
A2446	L2369	PRO	ASP	PRO	PRO	ALA	GLN	PRO	THR	ALA	H564	P502	V440	T374	T310
L2447	M2370	GLY	ASP	GLY	SER	MET	VAL	LEU	PRO	ILE	H565	N503	R441	L375	G311
	S2371	SER	HIS	SER	PRO	ASN	VAL	LYS	MET	ASP	H566	R504	D442	R376	R312
T2450	F2372	THR	TTR	GLY	PRO	TRP	PHE	HIS	ALA	ASP	H567	R505	L443	G377	R313
L2451	V2373	SER	GLN	SER	LEU	ARG	ARG	ALA	ALA	TYR	H568	R506	L444	L381	L314
	G2374	THR	SER	THR	LEU	VAL	VAL	THR	PRO	ASP	H569	Q507	F445	A315	A316
L2454	N2375	GLY	GLY	GLY	GLY	SER	THR	THR	PRO	SER	H570	K508	F445	R382	A317
F2455	L2312	GLY	GLY	ARG	LEU	ALA	HIS	SER	GLY	SER	H571	N509	N447	R384	V318
S2456	L2313	GLY	GLY	GLY	ALA	ARG	CYS	SER	GLY	GLY	H572	M510	D448	N385	P319
I2457	W2314	THR	THR	THR	ASP	ASN	ASN	TTR	ASN	ALA	H573	R511	A449	S386	PRO
V2458	T2380	GLN	GLN	HIS	HIS	ALA	THR	ASN	VAL	S245	H574	E512	S450	Y387	ASP
G2459	R2381	ALA	ALA	LYS	LYS	ALA	LEU	TYR	LYS	N850		Q513	K451	V388	PHE
Y2460	G2382	ARG	THR	THR	ARG	ARG	MET	ARG	GLN						



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

Chain C: 58% 24% 15%








G2459	E2559	L2698
Y2460	E2560	Q2699
L2461	P2561	E2700
F2462	L2562	K2701
	F2563	L2702
	A2564	E2703
D2465	A2565	S2704
	R2566	T2705
L2468	V2567	M2706
L2469	I2568	K2707
P2481	Y2569	L2708
E2482	D2570	V2709
T2483	L2571	T2710
G2484	L2572	E2711
	F2573	L2712
A2509	F2574	S2713
P2510	F2575	G2714
L2514	M2576	
L2515	V2577	S2717
P2516	L2578	E2718
V2517	I2579	L2719
E2518	I2580	K2720
E2519	V2581	D2721
	L2582	Q2722
T2520	M2583	M2723
E2521	L2584	T2724
Q2522	I2585	E2725
D2523	F2586	Q2726
K2524	G2587	R2727
E2525	V2588	K2728
L2526	I2589	Q2729
T2527	I2590	K2730
C2528	D2591	Q2731
E2529	T2592	R2732
T2530	F2593	L2733
L2531	S2598	G2734
L2532	E2599	L2735
M2533	K2600	L2736
C2534	Q2601	P2740
L2535	K2602	H2741
V2536	K2603	
T2537	E2604	A2750
V2538		
L2539		
S2540		
H2541	L2607	
G2542	K2608	
L2543	G2615	
R2544	L2616	
G2547	S2682	
G2548	L2683	
V2549		
G2550	E2689	
D2551		
V2552	Q2692	
L2553	M2693	
R2554	E2694	
K2555		
P2556		

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	96106	Depositor
Resolution determination method	FSC 0.143	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	23000	Depositor
Image detector	GATAN K2 (4k x 4k)	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 >2	RMSZ	# Z >2
1	A	2.33	24/7045 (0.3%)	0.89	25/9516 (0.3%)
1	B	2.33	24/7045 (0.3%)	0.89	25/9516 (0.3%)
1	C	2.34	24/7045 (0.3%)	0.89	25/9516 (0.3%)
1	D	2.34	28/7045 (0.4%)	0.91	29/9516 (0.3%)
All	All	2.34	100/28180 (0.4%)	0.89	104/38064 (0.3%)

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 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	20	GLU	CG-CD	82.22	2.75	1.51
1	D	20	GLU	CG-CD	82.21	2.75	1.51
1	C	20	GLU	CG-CD	82.19	2.75	1.51
1	A	20	GLU	CG-CD	82.13	2.75	1.51
1	D	176	VAL	CA-CB	77.97	3.18	1.54

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	GLU	OE1-CD-OE2	-19.29	100.15	123.30
1	D	20	GLU	OE1-CD-OE2	-19.28	100.16	123.30
1	A	20	GLU	OE1-CD-OE2	-19.28	100.17	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	20	GLU	OE1-CD-OE2	-19.26	100.19	123.30
1	A	285	GLU	O-C-N	-12.35	102.94	122.70

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

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	999	0
1	B	8368	0	6997	1004	0
1	C	8368	0	6997	1004	0
1	D	8368	0	6997	1000	0
All	All	33472	0	27988	3819	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 62.

The worst 5 of 3819 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%)	1	17
1	B	856/2750 (31%)	647 (76%)	135 (16%)	74 (9%)	1	17
1	C	856/2750 (31%)	646 (76%)	137 (16%)	73 (8%)	1	17
1	D	856/2750 (31%)	649 (76%)	133 (16%)	74 (9%)	1	17
All	All	3424/11000 (31%)	2587 (76%)	542 (16%)	295 (9%)	2	17

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%)	764 (99%)	5 (1%)	88	94
1	B	769/2459 (31%)	764 (99%)	5 (1%)	88	94
1	C	769/2459 (31%)	764 (99%)	5 (1%)	88	94
1	D	769/2459 (31%)	764 (99%)	5 (1%)	88	94
All	All	3076/9836 (31%)	3056 (99%)	20 (1%)	89	94

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2571	LEU
1	C	2415	LEU
1	D	2431	ILE
1	B	2435	THR
1	B	2514	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	489	ASN
1	C	94	HIS
1	D	489	ASN
1	B	518	GLN
1	B	2731	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 carbohydrates 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.