



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 09:57 PM EDT

PDB ID : 5X9Z / pdb_00005x9z
Title : Crystal structure of inositol 1,4,5-trisphosphate receptor large cytosolic domain
Authors : Hamada, K.; Miyatake, H.; Terauchi, A.; Mikoshiba, K.
Deposited on : 2017-03-10
Resolution : 7.31 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

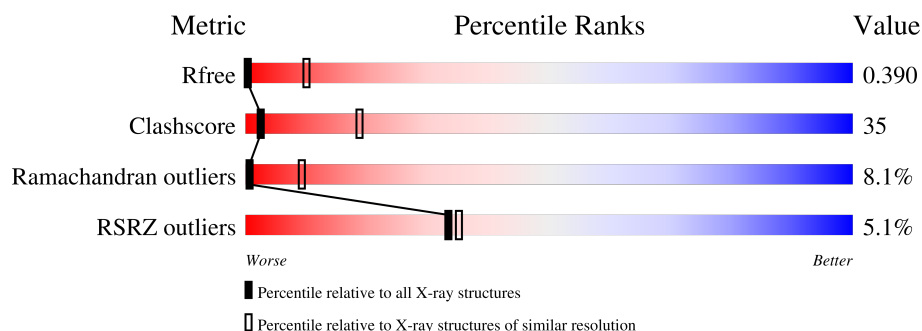
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.31 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1167 (10.00-4.00)
Clashscore	190562	1000 (10.00-4.06)
Ramachandran outliers	187476	1054 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2217	
1	B	2217	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16948 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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				ZeroOcc	AltConf	Trace
1	A	1710	Total	C	N	O	0	0	0
			8479	5059	1710	1710			
1	B	1708	Total	C	N	O	0	0	0
			8469	5053	1708	1708			

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

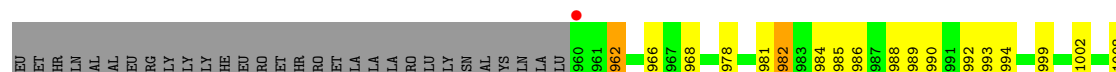
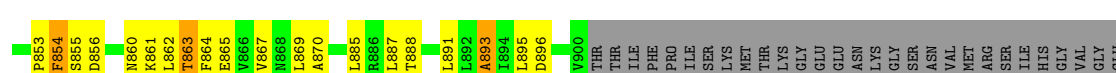
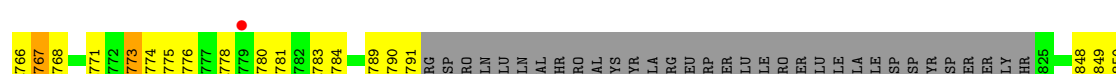
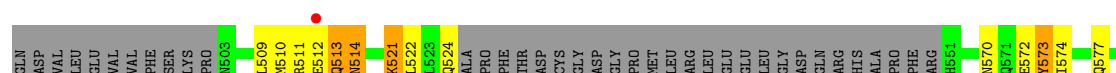
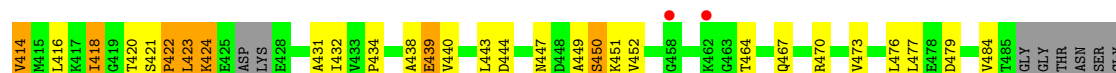
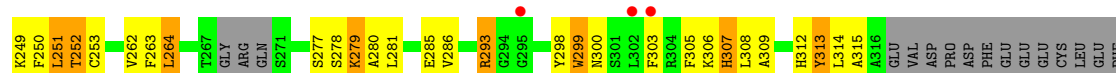
- Chain A: 

Position	Residue	Conservation (%)
1	LEU	100
2	TRP	100
3	ASP	100
4	GLU	100
5	ILE	100
6	PRO	100
7	SER	100
8	GLU	100
9	ILE	100
10	ALA	100
11	ALA	0
12	ASP	0
13	PRO	0
14	ILE	0
15	ASP	0
16	ASP	0
17	GLY	0
18	THR	0
19	SER	0
20	ASP	0
21	LEU	0
22	TRP	0
23	ASP	0
24	GLU	0
25	ILE	0
26	PRO	0
27	SER	0
28	GLU	0
29	ILE	0
30	ALA	0
31	ASP	0
32	PRO	0
33	ILE	0
34	ASP	0
35	ASP	0
36	GLU	0
37	ILE	0
38	PRO	0
39	SER	0
40	GLU	0
41	ILE	0
42	ALA	0
43	ASP	0
44	PRO	0
45	ILE	0
46	ASP	0
47	ASP	0
48	GLU	0
49	ILE	0
50	ALA	0
51	ASP	0
52	PRO	0
53	ILE	0
54	ASP	0
55	ASP	0
56	GLU	0
57	ILE	0
58	PRO	0
59	SER	0
60	GLU	0
61	ILE	0
62	ALA	0
63	ASP	0
64	PRO	0
65	ILE	0
66	ASP	0
67	ASP	0
68	GLU	0
69	ILE	0
70	ALA	0
71	ASP	0
72	PRO	0
73	ILE	0
74	ASP	0
75	ASP	0
76	GLU	0
77	ILE	0
78	PRO	0
79	SER	0
80	GLU	0
81	ILE	0
82	ALA	0
83	ASP	0
84	PRO	0
85	ILE	0
86	ASP	0
87	ASP	0
88	GLU	0
89	ILE	0
90	PRO	0
91	SER	0
92	GLU	0
93	ILE	0
94	ALA	0
95	ASP	0
96	PRO	0
97	ILE	0
98	ASP	0
99	ASP	0
100	GLU	0
101	ILE	0
102	PRO	0
103	SER	0
104	GLU	0
105	ILE	0
106	ALA	0
107	ASP	0
108	PRO	0
109	ILE	0
110	ASP	0
111	ASP	0
112	GLU	0
113	ILE	0
114	PRO	0
115	SER	0
116	GLU	0
117	ILE	0
118	PRO	0
119	SER	0
120	GLU	0
121	ILE	0
122	ALA	0
123	ASP	0
124	PRO	0
125	ILE	0
126	ASP	0
127	ASP	0
128	GLU	0
129	ILE	0
130	PRO	0
131	SER	0
132	GLU	0
133	ILE	0
134	ALA	0
135	ASP	0
136	PRO	0
137	ILE	0
138	ASP	0
139	ASP	0
140	GLU	0
141	ILE	0
142	PRO	0
143	SER	0
144	GLU	0
145	ILE	0
146	ALA	0
147	ASP	0
148	PRO	0
149	ILE	0
150	ASP	0
151	ASP	0
152	GLU	0
153	ILE	0
154	PRO	0
155	SER	0
156	GLU	0
157	ILE	0
158	ALA	0
159		

L2022	L2023	L2036	L2037	L2038	L2039	T2040	C2043	G2044	G2045	P2046	C2047	W2050	Q2051	W2052	C2053	G2060	G2061	I2062	L2068	W2071	D2072	L2076	R2080	L2083	L2087	K2088	S2092	A2097	I2098	H2103	D2104	S2105	F2106	W2107	K2108	W2114	R2115	F2117	L2118	E2119	L2120											
GLU	GLY	THR	GLN	ALA	THR	THR	ASP	A1951	A1952	K1953	D1954	D1955	Q1966	P1967	R1970	Q1973	L1974	L1975	C1976	N1980	R1981	D1982	L1983	Q1984	N1985	F1986	L1987	R1988	C1989	Q1990	N1991	N1992	T1994	L1998	V1999	C2000	L2003	D2007	C2008	I2009	C2010	G2011	S2012	T2013	G2016	L2017	C2018	L2019	R2020	G2021		
PRO	GLY	SER	SER	SER	THR	SER	THR	M1789	A1792	E1793	V1794	Q1795	C1796	H1797	L1798	D1799	G1802	A1803	S1804	A1814	S1815	F1820	G1834	N1835	T1836	T1837	I1838	Q1839	E1848	D1849	K1850	E1853	D1861	R1862	M1863	K1864	V1865	A1866	Q1867	Q1868	A1872	T1873	V1874	L1875	V1876	L1881	G1882					
N1883	K1884	K1885	K1886	D1887	D1888	E1889	V1890	ASP	ARG	ASP	ALA	PRO	SER	ARG	LYS	LYS	ALA	GLN	ILE	GLU	GLU	VAL	ARG	ASP	GLN	L1987	R1988	GLU	GLU	ALA	ALA	THR	ARG	LYS	PHE	THR	THR	PHE	ARG	ARG	GLU	ALA	PRO	ASP	ASP	HIS	TVR	GLN	GLY			
PRO	SER	PRO	PRO	LEU	ARG	GLN	LEU	GLY	GLY	HIS	LYS	ARG	GLY	ALA	LEU	ARG	GLN	ASN	THR	THR	GLY	ASN	ILE	SER	GLY	THR	SER	PHE	GLY	THR	THR	THR	GLY	ASN	ALA	PRO	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR					
VAL	LEU	ALA	ALA	S1593	D1605	A1609	H1630	R1631	F1636	P1637	E1638	N1639	S1648	Q1676	E1680	M1681	M1682	D1685	R1686	G1687	TYR	GLY	GLY	LYS	GLN	ASN	GLY	GLY	SER	GLY	GLY	GLY	ASN	ALA	GLY	PRO	LEU	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR					
LYS	ALA	SER	VAL	GLU	SER	CYS	ILE	ARG	VAL	ALA	ALA	LYS	ASP	VAL	ALA	PRO	ASP	GLN	ASP	GLN	VAL	VAL	VAL	VAL	VAL	GLN	VAL	ILE	ASN	GLY	GLY	GLY	GLN	LEU	LEU	VAL	TRP	ALA	ARG	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
Y1441	E1332	E1333	L1334	I1457	M1336	V1341	F1344	N1463	T1464	M1346	S1465	R1466	A1349	S1369	P1370	L1371	M1372	Y1373	H1374	I1375	H1376	L1377	V1378	E1379	L1380	A1381	A1382	V1383	C1384	T1385	E1386	G1387	C1396	M1397	S1398	L1399	L1400	T1410	H1411	E1412	E1417	V1418	K1419	I1420	A1421	N1424	F1425	L1426	M1427	A1318	E1319	V1435
V1213	V1214	L1215	P1221	K1224	M1230	Q1231	R1235	H1238	E1239	F1240	C1245	M1261	Q1262	L1265	H1266	M1264	I1267	A1270	V1271	T1272	M1273	Q1274	H1275	M1279	L1283	C1284	S1285	M1288	V1291	H1294	F1295	V1296	H1297	C1298	I1299	T1301	K1317	A1318	E1319	I1323	Y1134	F1030										
GLY	GLN	GLY	PRO	GLU	PRO	MET	ALA	SER	GLY	GLY	ASN	HIS	LYS	THR	THR	SER	LYS	LEU	ASP	GLN	GLN	THR	THR	THR	VAL	VAL	GLN	LEU	LEU	GLN	GLY	VAL	TRP	ALA	SER	THR	ALA	ALA	ARG	ASN	ASN	CYS	TRP	LEU	MET	PRO	ASP	GLN				
I1033	E1034	E1035	Q1036	I1040	G1043	S1044	T1048	P1049	L1050	D1053	D1054	Q1055	L1061	R1062	H1066	R1085	H1086	F1087	S1088	Q1089	L1094	Q1095	A1096	Q1101	D1102	E1103	Q1107	S1108	Y1112	I1115	K1116	Q1117	D1118	L1119	Q1121	L1122	I1125	V1126	S1129	E1130	L1131	W1132	Y1133	Y1134	F1030							
THR	THR	ILE	PHE	PRO	ILE	SER	LYS	MET	THR	LYS	GLY	GLU	ASN	LYS	GLY	ASN	GLY	LEU	ASN	VAL	VAL	ARG	SER	ILE	GLY	VAL	GLY	THR	GLN	VAL	VAL	ARG	SER	GLY	GLY	PHE	LEU	PRO	MET	THR	PRO	MET	ALA	ALA								
L891	L892	A893	I894	L895	D896	C897	V898	H899	V900	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR					



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.50Å 221.73Å 318.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 7.31 49.15 – 7.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.15-7.31) 88.5 (49.15-7.31)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 7.37Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.317 , 0.394 0.316 , 0.390	Depositor DCC
R_{free} test set	536 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	209.8	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 406.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.25$, $\langle L^2 \rangle = 0.10$	Xtriage
Estimated twinning fraction	0.219 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.68	EDS
Total number of atoms	16948	wwPDB-VP
Average B, all atoms (Å ²)	170.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.65	3/8465 (0.0%)	1.00	25/11786 (0.2%)
1	B	0.69	7/8455 (0.1%)	1.02	22/11772 (0.2%)
All	All	0.67	10/16920 (0.1%)	1.01	47/23558 (0.2%)

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	25
1	B	0	22
All	All	0	47

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	178	ILE	C-O	10.83	1.36	1.24
1	A	554	ARG	CA-C	8.30	1.63	1.52
1	B	1445	HIS	CA-C	-8.05	1.42	1.52
1	B	1445	HIS	N-CA	7.73	1.51	1.46
1	B	177	VAL	N-CA	-6.53	1.38	1.46

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	VAL	N-CA-C	9.47	129.03	109.34
1	A	999	ARG	N-CA-C	-8.87	91.92	110.80
1	B	8	PHE	N-CA-C	8.22	122.44	110.28
1	A	554	ARG	CA-C-O	-8.03	109.02	120.51
1	B	743	MET	CA-C-N	7.86	135.84	121.70

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	GLY	Peptide
1	A	15	CYS	Peptide
1	A	176	VAL	Peptide
1	A	73	TRP	Peptide
1	A	8	PHE	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	8479	0	3697	432	0
1	B	8469	0	3697	414	0
All	All	16948	0	7394	845	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 35.

The worst 5 of 845 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1208:MET:O	1:A:1212:ALA:HB3	1.49	1.10
1:A:162:TYR:O	1:A:184:LEU:C	1.97	1.07
1:A:405:PRO:HA	1:A:416:LEU:HA	1.39	1.04
1:B:1682:MET:O	1:B:1686:ARG:N	1.93	1.01
1:A:1472:SER:O	1:A:1476:LYS:CB	2.10	1.00

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1682/2217 (76%)	1265 (75%)	296 (18%)	121 (7%)	1	11
1	B	1680/2217 (76%)	1193 (71%)	337 (20%)	150 (9%)	0	8
All	All	3362/4434 (76%)	2458 (73%)	633 (19%)	271 (8%)	1	9

5 of 271 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	ALA
1	A	87	VAL
1	A	213	ASN
1	A	222	LEU
1	A	226	TRP

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1710/2217 (77%)	-0.13	78 (4%) 37 37	0, 157, 428, 888	0
1	B	1708/2217 (77%)	-0.08	97 (5%) 29 33	0, 136, 432, 776	0
All	All	3418/4434 (77%)	-0.11	175 (5%) 33 35	0, 147, 430, 888	0

The worst 5 of 175 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1429	CYS	11.3
1	B	1432	ASP	9.8
1	B	1428	HIS	7.8
1	B	2164	ARG	6.6
1	A	1888	ASP	6.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.