



wwPDB X-ray Structure Validation Summary Report ⓘ

May 12, 2020 – 11:18 pm BST

PDB ID : 5XA0
Title : Crystal structure of inositol 1,4,5-trisphosphate receptor cytosolic domain
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Deposited on : 2017-03-10
Resolution : 5.81 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

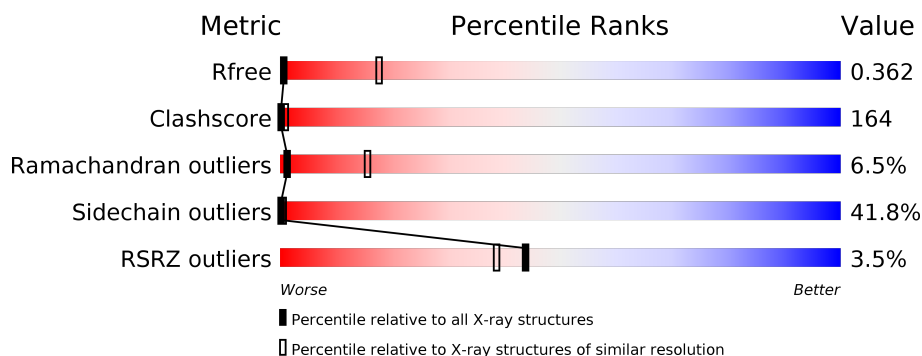
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.81 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}	130704	1009 (7.78-3.86)
Clashscore	141614	1035 (7.70-3.90)
Ramachandran outliers	138981	1004 (7.78-3.86)
Sidechain outliers	138945	1011 (7.82-3.82)
RSRZ outliers	127900	1009 (7.82-3.78)

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 on 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	1581	<div> <div>2%</div> <div> <div></div> <div>36%</div> <div>30%</div> <div>11%</div> <div>•</div> <div>21%</div> </div> </div>
1	B	1581	<div> <div>3%</div> <div> <div></div> <div>36%</div> <div>29%</div> <div>12%</div> <div>•</div> <div>21%</div> </div> </div>

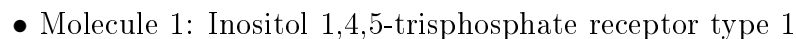
2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17919 atoms, of which 2970 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	1252	Total	C	H	N	O	S	0	0	0
			8949	4595	1485	1410	1444	15			
1	B	1252	Total	C	H	N	O	S	0	0	0
			8970	4610	1485	1412	1447	16			



M1288	M1212	F1030	F876	A686	R558	LEU	V433	T373	H312	E248	V187
M1293	V1213	E1031	Y879	L687	V559	GLU	P434	T374	T313	K249	M188
Q1293	L1214	H1032	E888	A689	V560	VAL	V435	L375	L314	F250	A189
T1301	L1215	I1033	S882	E695	R561	VAL	S436	R376	A315	L251	G190
H1302	E1216	E1034	R883	V696	H562	PHE	P437	G377	A316	T252	Q191
T1309	L1217	E1035	L884	F699	S563	GLU	E439	G378	D254	C253	P192
I1315	L1218	E1036	L885	W700	Q564	VAL	R441	D379	E255	D254	L193
V1316	Q1036	Q1036	T888	Y700	Q565	LYS	D442	S380	E256	H194	A195
K1317	M1047	T1048	T889	S703	Y567	ALA	R443	L381	H257	S196	S197
A1318	P1049	P1049	C897	W704	F580	ARG	D444	P383	K258	H198	H198
E1319	L1058	R1059	R898	I715	M881	LEU	F445	L443	Q260	Q199	Q199
I1323	T1059	T1059	R899	A719	I595	TRP	A446	R384	H261	H200	L200
V1330	F1060	P960	E899	K724	L598	GLY	M447	R385	V262	V201	V201
E1339	L1061	E961	Y898	E725	L599	GLU	D448	R386	F263	D202	D202
D1340	R1062	E962	Y899	R727	M602	ILE	A449	P387	L264	N203	N203
V1343	R1063	E963	Y900	D728	I610	ILE	S455	R388	R265	P204	P204
F1344	R1064	E964	Y901	Y733	T611	ASP	I456	R389	T266	G205	G205
F1345	L1073	P1073	Y902	I737	A612	ASP	A457	R391	T267	C206	C206
H1346	R1078	G1078	Y903	F740	E614	ASP	G458	H392	G268	N207	N207
D1347	R1085	R1085	Y904	L741	I615	GLY	K459	L393	ARG	V209	V209
S1350	R1090	R1090	Y905	Y742	T616	GLU	E461	T395	GLN	N210	N210
I1355	R1093	R1093	Y906	R743	T618	ASN	G463	T402	S271	S211	S211
Q1356	L1094	L1094	Y907	C744	S620	GLY	T464	N403	T276	V212	V212
M1357	A1096	A1096	Y908	L745	S621	PHE	I465	N404	S277	N213	N213
S1360	V1100	S1004	Y909	D746	V622	ASN	T466	N405	S278	C214	C214
E1361	Q1101	Q1101	Y910	R747	V623	THR	E469	P405	K279	N215	N215
R1364	L1102	L1102	Y911	Y749	V624	ASP	R470	N415	A280	T216	T216
S1369	L1107	L1107	Y912	Y750	M625	GLY	E473	N416	L281	S217	S217
P1370	M1111	M1111	Y913	L759	F630	ASP	T473	N417	V287	K218	K218
L1371	D1118	D1118	Y914	D760	F631	GLY	V474	N418	Q288	K219	K219
I1375	L1119	L1119	Y915	V761	V639	LEU	K475	N419	H289	K224	K224
H1376	S1129	S1129	Y916	V762	M654	ARG	L476	N420	D290	K225	K225
V1377	E1130	E1130	Y917	D763	M655	LEU	E477	N421	D291	S227	S227
E1379	L1131	L1131	Y918	S769	M656	GLU	D479	N422	C292	D228	D228
L1380	W1132	W1132	Y919	L773	E667	GLU	L480	N423	R293	N229	N229
L1381	V1133	V1133	Y920	L777	E668	GLU	V481	N424	C294	K230	K230
A1382	L1134	L1134	Y921	S780	E669	GLU	V482	N425	G295	I233	I233
V1383	L1135	L1135	Y922	F781	E670	GLU	V483	N426	A296	L234	L234
T1385	L1136	L1136	Y923	C782	M661	LEU	Y484	N427	G297	K235	K235
N1386	L1137	L1137	Y924	L788	M662	GLY	V485	N428	Y298	G236	G236
N1387	L1138	L1138	Y925	W789	E667	GLY	T485	N429	W299	G237	G237
K1395	L1139	L1139	Y926	V790	E668	GLY	GLY	N430	N300	D238	D238
C1396	L1140	L1140	Y927	D791	E669	GLY	GLY	N431	S301	V239	V239
M1397	L1141	L1141	Y928	ASP	E670	GLY	GLY	N432	L302	V240	V240
	L1142	L1142	Y929	ASP	E671	GLY	GLY	N433	F303	R241	R241
	L1143	L1143	Y930	ASP	E672	GLY	GLY	N434	F304	L242	L242
	L1144	L1144	Y931	ASP	E673	GLY	GLY	N435	F305	F243	F243
	L1145	L1145	Y932	ASP	E674	GLY	GLY	N436	K306	H244	H244
	L1146	L1146	Y933	ASP	E675	GLY	GLY	N437	H307	A245	A245
	L1147	L1147	Y934	ASP	E676	GLY	GLY	N438	L308	E246	E246
	L1148	L1148	Y935	ASP	E677	GLY	GLY	N439	A309	Q247	Q247

ASX	ASX	THR	L1400
LEU	LEU	LEU	P1401
PHE	GLN	THR	L1402
LEU	LEU	ARG	D1403
LYS	ARG	GLN	D1404
SER	SER	PRO	D1413
HIS	ASN	VAL	L1420
ASN	PHE	PHE	A1421
ILE	VAL	GLN	N1424
VAL	LYS	LEU	F1425
GLN	THR	LEU	H1428
LYS	ALA	GLY	D1432
THR	ASN	VAL	T1433
LEU	ARG	ARG	E1434
LEU	LEU	VAL	V1435
ALA	SER	TYR	K1438
ARG	ALA	HIS	E1439
	ARG	ASN	T1440
		TRP	Y1441
		LEU	T1442
		MET	S1443
		PRO	N1444
		SER	N1452
		GLN	F1453
		LYS	L1454
		ALA	G1458
		SER	R1459
		GLU	A1460
		VAL	C1461
		ARG	T1464
		VAL	S1472
		LEU	T1473
		SER	L1474
		ASP	E1475
		VAL	K1476
		ALA	Y1477
		LYS	V1478
		SER	T1488
		ARG	F1489
		ALA	S1491
		ILE	T1492
		PRO	P1493
		VAL	PHE
		ASP	SER
		LEU	ASP
		THR	GLN
		ASN	GLN
		VAL	SER
		THR	THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	128.16Å 128.16Å 369.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 5.81 48.81 – 5.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.81-5.81) 99.9 (48.81-5.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 5.73Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.278 , 0.342 0.300 , 0.362	Depositor DCC
R_{free} test set	818 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	88.0	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 457.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.21$, $\langle L^2 \rangle = 0.07$	Xtriage
Estimated twinning fraction	0.368 for h,-k,-l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	17919	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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	0.66	10/7527 (0.1%)	0.94	41/10362 (0.4%)
1	B	0.67	12/7549 (0.2%)	0.92	39/10390 (0.4%)
All	All	0.66	22/15076 (0.1%)	0.93	80/20752 (0.4%)

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	7
1	B	0	11
All	All	0	18

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	430	PHE	CD1-CE1	8.15	1.55	1.39
1	A	160	TRP	CB-CG	-7.67	1.36	1.50
1	B	218	TRP	CE3-CZ3	-7.18	1.26	1.38
1	B	462	LYS	CD-CE	7.14	1.69	1.51
1	A	459	LYS	CD-CE	6.54	1.67	1.51

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	480	LEU	CB-CG-CD1	-15.76	84.22	111.00
1	B	379	ASP	CB-CG-OD2	12.31	129.38	118.30
1	B	377	GLY	N-CA-C	11.68	142.31	113.10
1	A	416	LEU	CA-CB-CG	11.35	141.40	115.30
1	B	251	LEU	CB-CG-CD2	-10.52	93.12	111.00

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ILE	Peptide
1	A	213	ASN	Peptide
1	A	226	TRP	Peptide
1	A	248	GLU	Peptide
1	A	393	LEU	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	7464	1485	5141	2046	2
1	B	7485	1485	5190	2095	2
All	All	14949	2970	10331	4141	4

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 164.

The worst 5 of 4141 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:263:PHE:HB2	1:A:415:MET:CB	1.50	1.38
1:A:32:LEU:CD1	1:A:445:PHE:HA	1.54	1.35
1:B:18:TYR:O	1:B:181:LYS:NZ	1.59	1.32
1:B:459:LYS:C	1:B:462:LYS:HE3	1.48	1.30
1:A:456:ILE:C	1:A:459:LYS:HD3	1.51	1.30

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ARG:O	1:B:378:GLY:N[2_655]	1.78	0.42
1:A:374:THR:N	1:A:376:ARG:O[2_655]	1.96	0.24
1:B:377:GLY:N	1:B:379:ASP:OD1[2_655]	2.15	0.05
1:A:373:THR:OG1	1:A:376:ARG:O[2_655]	2.16	0.04

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 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	1230/1581 (78%)	1000 (81%)	155 (13%)	75 (6%)	1	16
1	B	1230/1581 (78%)	980 (80%)	165 (13%)	85 (7%)	1	14
All	All	2460/3162 (78%)	1980 (80%)	320 (13%)	160 (6%)	1	15

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	PRO
1	A	50	PRO
1	A	104	GLU
1	A	140	ALA
1	A	192	PRO

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

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	376/1427 (26%)	232 (62%)	144 (38%)	0	0
1	B	384/1427 (27%)	210 (55%)	174 (45%)	0	0
All	All	760/2854 (27%)	442 (58%)	318 (42%)	0	0

5 of 318 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	560	LEU

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Mol	Chain	Res	Type
1	B	108	ARG
1	B	464	THR
1	B	15	CYS
1	B	47	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	400	HIS
1	A	562	HIS
1	B	307	HIS
1	A	507	GLN
1	A	564	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 [i](#)

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	1252/1581 (79%)	-0.31	39 (3%)	49 42	8, 28, 64, 150	0
1	B	1252/1581 (79%)	-0.32	49 (3%)	39 34	8, 27, 65, 120	0
All	All	2504/3162 (79%)	-0.32	88 (3%)	44 38	8, 28, 65, 150	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	899	HIS	6.7
1	B	280	ALA	6.6
1	B	27	ILE	4.5
1	A	267	THR	4.5
1	B	1062	ARG	4.2

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 carbohydrates 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.