



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 12, 2024 – 09:59 PM EDT

PDB ID : 3UJ4
Title : Crystal structure of the apo-inositol 1,4,5-trisphosphate receptor
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Deposited on : 2011-11-07
Resolution : 3.00 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
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)	:	2.36.2

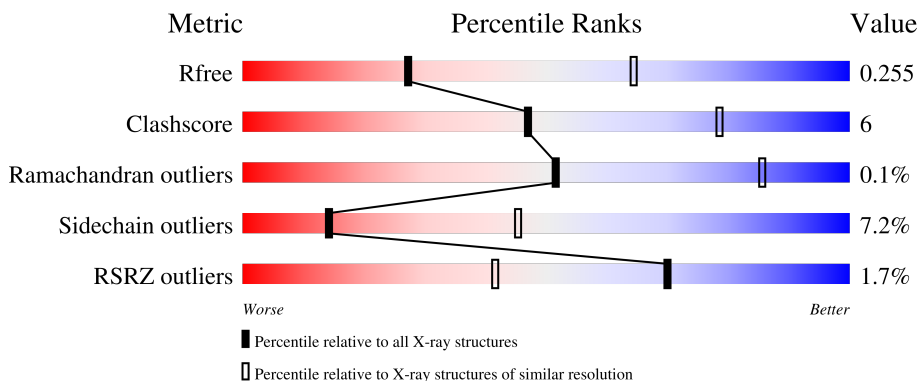
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	604	 2% 67% 12% 20%
1	B	604	 2% 65% 15% 19%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7454 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	486	Total	C	N	O	S	0	0	0
			3721	2372	656	688	5			
1	B	490	Total	C	N	O	S	0	0	0
			3700	2351	646	698	5			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	ALA	CYS	engineered mutation	UNP P29994
A	37	ALA	CYS	engineered mutation	UNP P29994
A	56	ALA	CYS	engineered mutation	UNP P29994
A	61	ALA	CYS	engineered mutation	UNP P29994
A	206	ALA	CYS	engineered mutation	UNP P29994
A	214	ALA	CYS	engineered mutation	UNP P29994
A	253	ALA	CYS	engineered mutation	UNP P29994
A	292	ALA	CYS	engineered mutation	UNP P29994
A	326	ALA	CYS	engineered mutation	UNP P29994
A	394	ALA	CYS	engineered mutation	UNP P29994
A	530	ALA	CYS	engineered mutation	UNP P29994
A	553	ALA	CYS	engineered mutation	UNP P29994
A	556	ALA	CYS	engineered mutation	UNP P29994
B	15	ALA	CYS	engineered mutation	UNP P29994
B	37	ALA	CYS	engineered mutation	UNP P29994
B	56	ALA	CYS	engineered mutation	UNP P29994
B	61	ALA	CYS	engineered mutation	UNP P29994
B	206	ALA	CYS	engineered mutation	UNP P29994
B	214	ALA	CYS	engineered mutation	UNP P29994
B	253	ALA	CYS	engineered mutation	UNP P29994
B	292	ALA	CYS	engineered mutation	UNP P29994
B	326	ALA	CYS	engineered mutation	UNP P29994
B	394	ALA	CYS	engineered mutation	UNP P29994
B	530	ALA	CYS	engineered mutation	UNP P29994
B	553	ALA	CYS	engineered mutation	UNP P29994

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Chain	Residue	Modelled	Actual	Comment	Reference
B	556	ALA	CYS	engineered mutation	UNP P29994

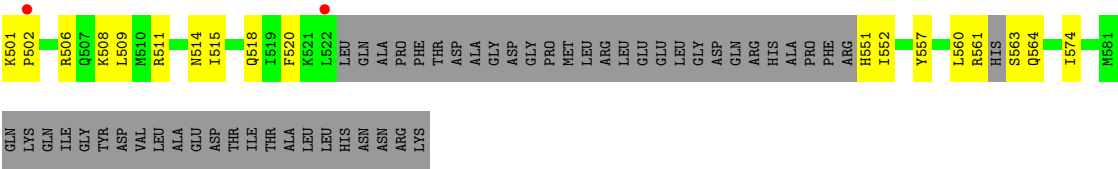
- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	14	Total	O	0	0
			14	14		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.11Å 77.19Å 101.51Å 105.36° 99.98° 101.04°	Depositor
Resolution (Å)	50.00 – 3.00 46.79 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-3.00) 98.6 (46.79-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.208 , 0.256 0.208 , 0.255	Depositor DCC
R_{free} test set	1746 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7454	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.50	2/3794 (0.1%)	0.59	0/5153
1	B	0.49	3/3771 (0.1%)	0.57	0/5129
All	All	0.49	5/7565 (0.1%)	0.58	0/10282

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	TRP	CD2-CE2	5.19	1.47	1.41
1	B	226	TRP	CD2-CE2	5.17	1.47	1.41
1	B	299	TRP	CD2-CE2	5.08	1.47	1.41
1	B	73	TRP	CD2-CE2	5.04	1.47	1.41
1	A	160	TRP	CD2-CE2	5.02	1.47	1.41

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	3721	0	3629	39	0
1	B	3700	0	3531	53	0
2	B	5	0	0	0	0
3	A	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	0	2	0
All	All	7454	0	7160	90	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 6.

The worst 5 of 90 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:251:LEU:HD12	1:A:418:ILE:HD13	1.59	0.83
1:B:204:PRO:HA	3:B:611:HOH:O	1.80	0.82
1:A:251:LEU:HD12	1:A:418:ILE:CD1	2.12	0.79
1:B:64:ASN:H	1:B:122:GLN:NE2	1.86	0.72
1:B:293:ARG:CG	1:B:293:ARG:HH11	2.02	0.72

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	472/604 (78%)	447 (95%)	25 (5%)	0	100	100
1	B	472/604 (78%)	443 (94%)	28 (6%)	1 (0%)	47	82
All	All	944/1208 (78%)	890 (94%)	53 (6%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	PRO

5.3.2 Protein sidechains [i](#)

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	384/520 (74%)	354 (92%)	30 (8%)	12	42
1	B	377/520 (72%)	352 (93%)	25 (7%)	16	49
All	All	761/1040 (73%)	706 (93%)	55 (7%)	14	45

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	567	TYR
1	B	210	ASN
1	B	509	LEU
1	B	396	ASN
1	A	568	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	185	ASN
1	B	307	HIS
1	B	564	GLN
1	B	312	HIS
1	B	261	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	605	-	4,4,4	0.38	0	6,6,6	0.17	0

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 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	486/604 (80%)	-0.33	5 (1%) 82 59	47, 71, 149, 226	0
1	B	490/604 (81%)	-0.22	12 (2%) 59 30	51, 88, 154, 189	0
All	All	976/1208 (80%)	-0.27	17 (1%) 70 41	47, 78, 153, 226	0

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	464	THR	4.6
1	B	88	LEU	4.3
1	B	463	GLY	3.8
1	A	91	LYS	3.4
1	A	87	VAL	3.3

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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	B	605	5/5	0.97	0.11	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.