



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Aug 8, 2018 – 01:55 AM EDT

PDB ID : 6DR2
EMDB ID: : EMD-7988
Title : Ca²⁺-bound human type 3 1,4,5-inositol trisphosphate receptor
Authors : Hite, R.K.; Paknejad, N.
Deposited on : 2018-06-11
Resolution : 4.33 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031172

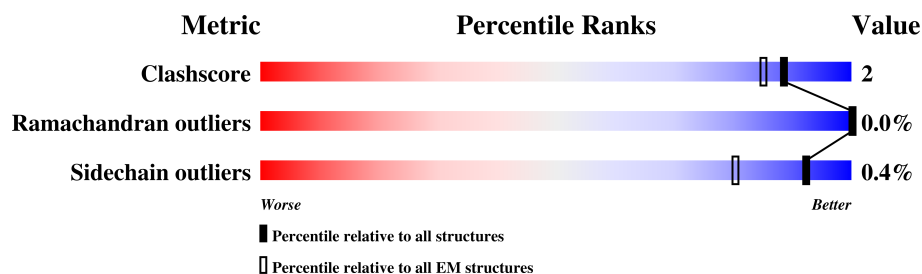
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY





The reported resolution of this entry is 4.33 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	2671	 77% 5% 18%
1	B	2671	 77% 5% 18%
1	C	2671	 76% 5% 18%
1	D	2671	 77% 5% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 139084 atoms, of which 69544 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 3.

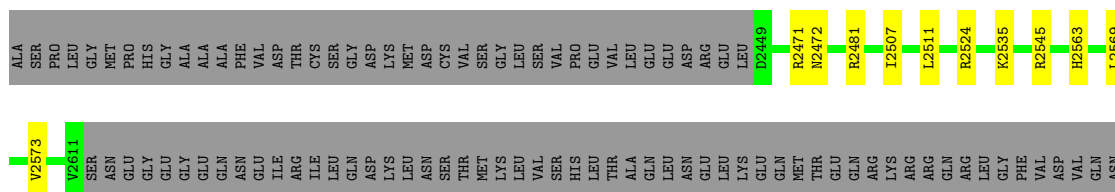
Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2191	Total	C	H	N	O	S	0	0
			34768	11084	17386	2990	3202	106		
1	B	2191	Total	C	H	N	O	S	0	0
			34768	11084	17386	2990	3202	106		
1	C	2191	Total	C	H	N	O	S	0	0
			34768	11084	17386	2990	3202	106		
1	D	2191	Total	C	H	N	O	S	0	0
			34768	11084	17386	2990	3202	106		

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
2	B	1	Total	Zn	0
			1	1	
2	A	1	Total	Zn	0
			1	1	
2	D	1	Total	Zn	0
			1	1	
2	C	1	Total	Zn	0
			1	1	

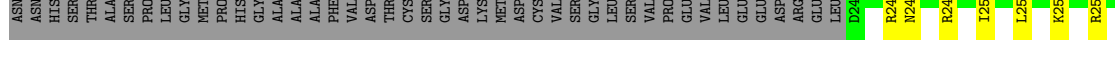
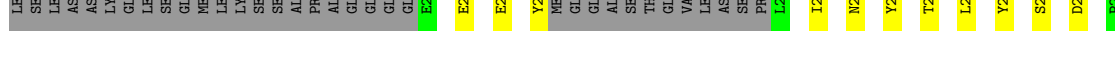
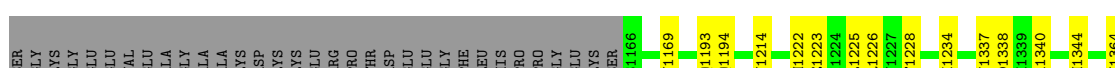
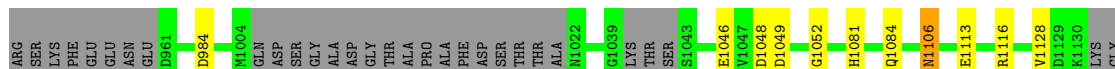
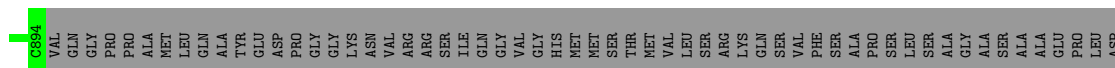
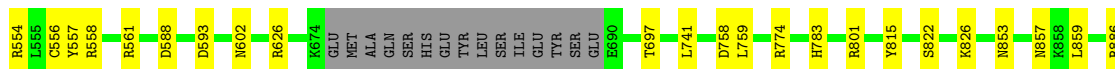
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

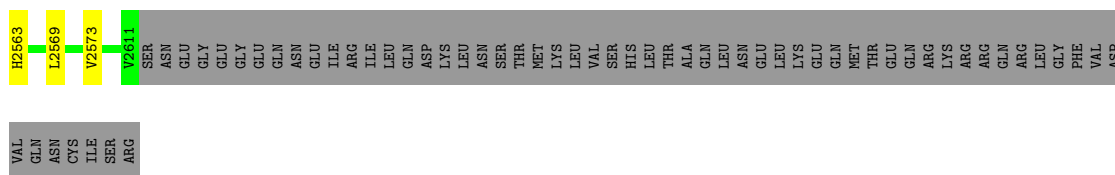
Mol	Chain	Residues	Atoms		AltConf
3	B	2	Total	Ca	0
			2	2	
3	A	2	Total	Ca	0
			2	2	
3	D	2	Total	Ca	0
			2	2	
3	C	2	Total	Ca	0
			2	2	



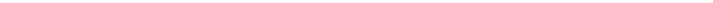
- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

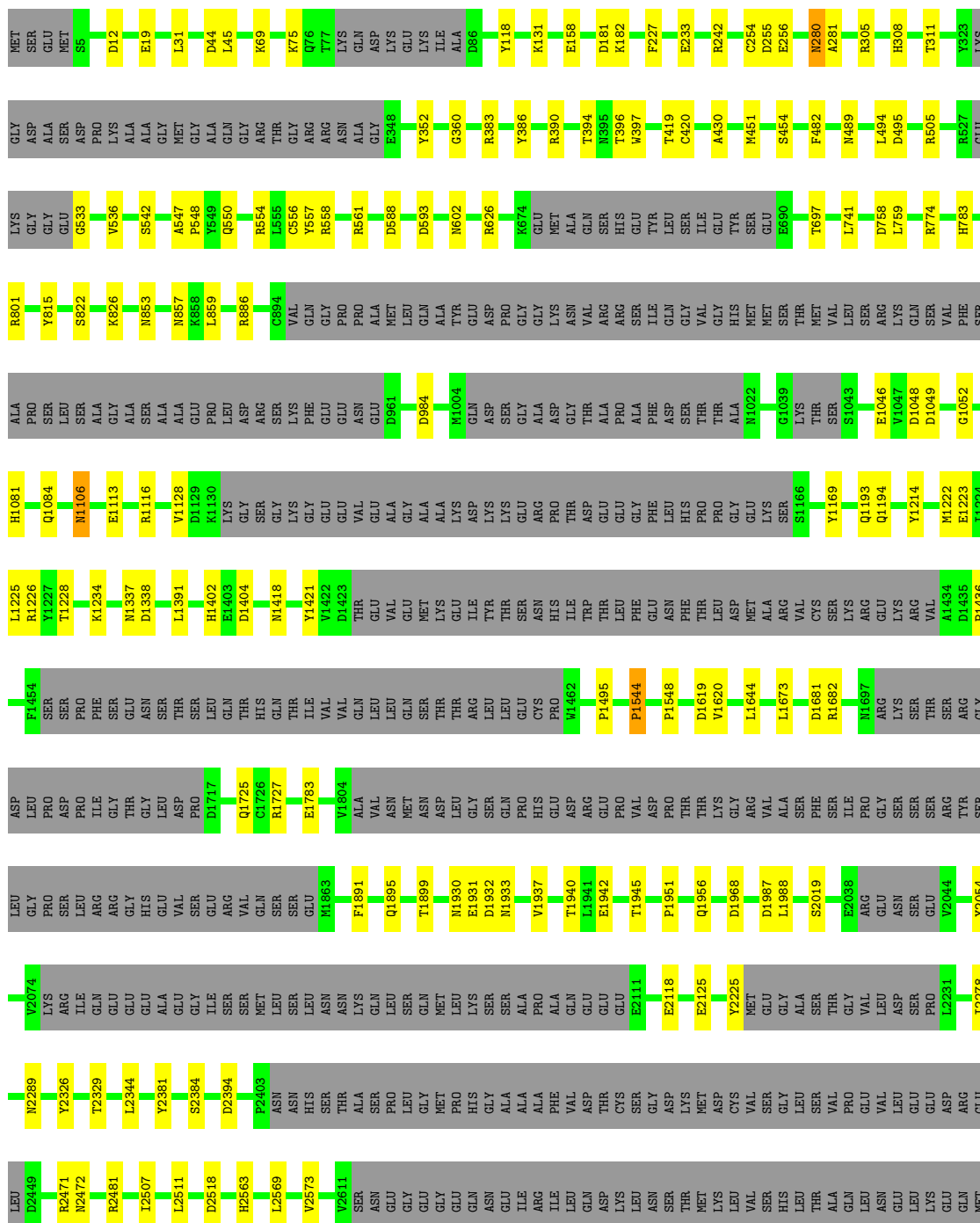
Chain B:






- Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain C:  76% 5% 18%



THR
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GLN
ARG
MET
LYS
ARG
ARG
GLN
LEU
LEU
PHE
VAL
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VAL
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• Molecule 1: Inositol 1,4,5-trisphosphate receptor type 3

Chain D:  77% 5% 18%

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4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	33807	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	61	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	22500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: ZN, CA

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	0.28	0/17689	0.52	5/23903 (0.0%)
1	B	0.28	0/17689	0.52	5/23903 (0.0%)
1	C	0.28	0/17689	0.52	4/23903 (0.0%)
1	D	0.28	0/17689	0.52	5/23903 (0.0%)
All	All	0.28	0/70756	0.52	19/95612 (0.0%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1544	PRO	N-CA-CB	5.67	110.10	103.30
1	A	1544	PRO	N-CA-CB	5.65	110.08	103.30
1	D	1544	PRO	N-CA-CB	5.65	110.08	103.30
1	C	1544	PRO	N-CA-CB	5.64	110.07	103.30
1	B	1495	PRO	N-CA-CB	5.61	110.03	103.30

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	17382	17386	17215	68	0
1	B	17382	17386	17215	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	17382	17386	17215	72	0
1	D	17382	17386	17215	71	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
All	All	69540	69544	68860	275	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 2.

The worst 5 of 275 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:2524:ARG:NE	1:D:2518:ASP:OD2	2.13	0.82
1:A:561:ARG:NH1	1:A:593:ASP:O	2.21	0.74
1:C:561:ARG:NH1	1:C:593:ASP:O	2.21	0.73
1:B:561:ARG:NH1	1:B:593:ASP:O	2.21	0.73
1:D:561:ARG:NH1	1:D:593:ASP:O	2.21	0.73

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 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	2147/2671 (80%)	2055 (96%)	91 (4%)	1 (0%)	100	100
1	B	2147/2671 (80%)	2054 (96%)	92 (4%)	1 (0%)	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	2147/2671 (80%)	2055 (96%)	91 (4%)	1 (0%)	100	100
1	D	2147/2671 (80%)	2053 (96%)	93 (4%)	1 (0%)	100	100
All	All	8588/10684 (80%)	8217 (96%)	367 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1544	PRO
1	B	1544	PRO
1	C	1544	PRO
1	D	1544	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 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	1883/2385 (79%)	1876 (100%)	7 (0%)	92	95
1	B	1883/2385 (79%)	1876 (100%)	7 (0%)	92	95
1	C	1883/2385 (79%)	1875 (100%)	8 (0%)	92	95
1	D	1883/2385 (79%)	1876 (100%)	7 (0%)	92	95
All	All	7532/9540 (79%)	7503 (100%)	29 (0%)	92	95

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2472	ASN
1	C	602	ASN
1	D	2289	ASN
1	C	280	ASN
1	C	1106	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	5
1	A	5
1	D	5
1	C	5

The worst 5 of 20 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1552:GLN	C	1586:TRP	N	55.70
1	B	1552:GLN	C	1586:TRP	N	55.70
1	C	1552:GLN	C	1586:TRP	N	55.70
1	D	1552:GLN	C	1586:TRP	N	55.70
1	A	1533:THR	C	1541:ARG	N	15.48