



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:18 PM GMT

PDB ID : 1T0J  
Title : Crystal structure of a complex between voltage-gated calcium channel beta2a subunit and a peptide of the alpha1c subunit  
Authors : Van Petegem, F.; Clark, K.; Chatelain, F.; Minor Jr., D.  
Deposited on : 2004-04-09  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

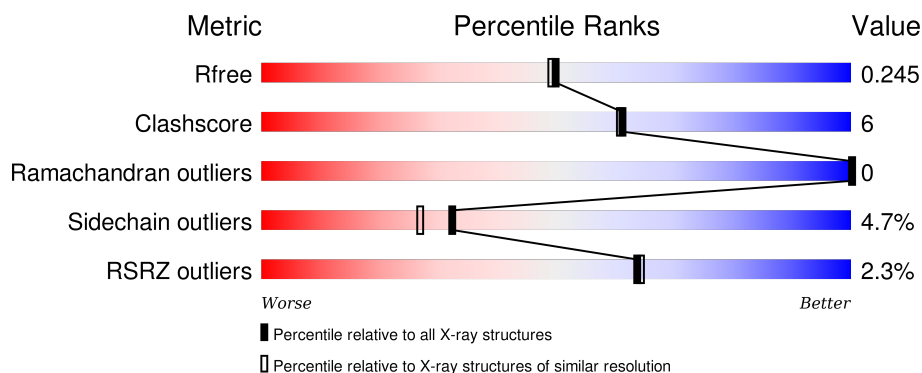
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	132	<div> <div>61%</div> <div>10%</div> <div>27%</div> </div>
2	B	224	<div> <div>73%</div> <div>10%</div> <div>17%</div> </div>
3	C	20	<div> <div>65%</div> <div>15%</div> <div>20%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2506 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 voltage-gated calcium channel subunit beta2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	96	Total	C	N	O	S	0	0	0
			760	481	137	139	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLY	-	CLONING ARTIFACT	UNP Q8VGC3
A	15	HIS	-	CLONING ARTIFACT	UNP Q8VGC3
A	16	MET	-	CLONING ARTIFACT	UNP Q8VGC3

- Molecule 2 is a protein called voltage-gated calcium channel subunit beta2a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	187	Total	C	N	O	S	0	0	0
			1468	934	253	275	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	201	MET	-	CLONING ARTIFACT	UNP Q8VGC3

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel alpha-1C subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	16	Total	C	N	O	0	0	0
			139	89	21	29			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	426	GLY	-	CLONING ARTIFACT	UNP Q13936
C	427	ALA	-	CLONING ARTIFACT	UNP Q13936

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0

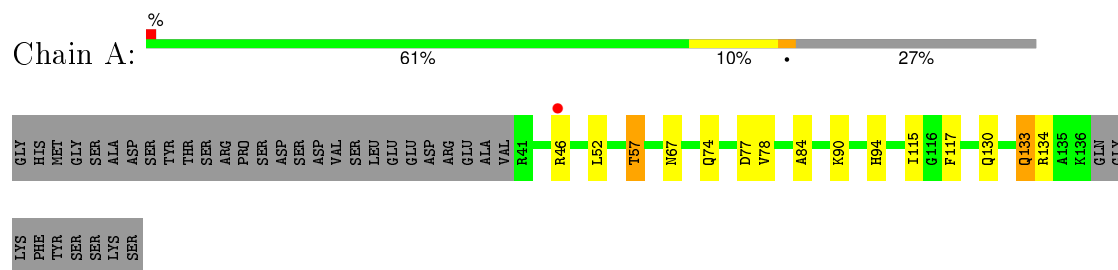
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	55	Total 55	O 55	0	0
5	B	77	Total 77	O 77	0	0
5	C	6	Total 6	O 6	0	0

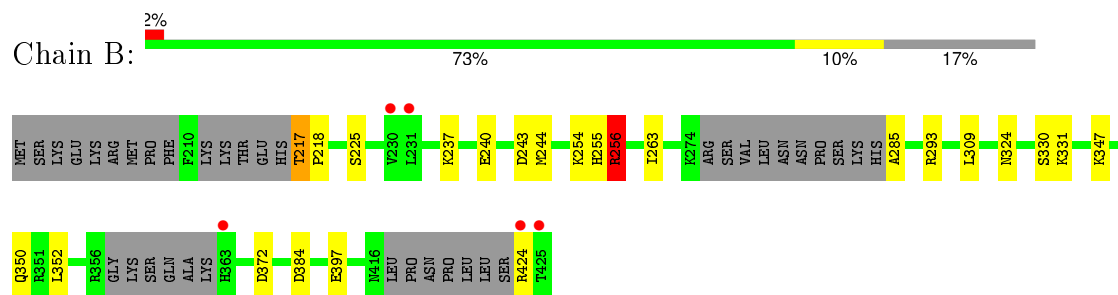
### 3 Residue-property plots [i](#)

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 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.

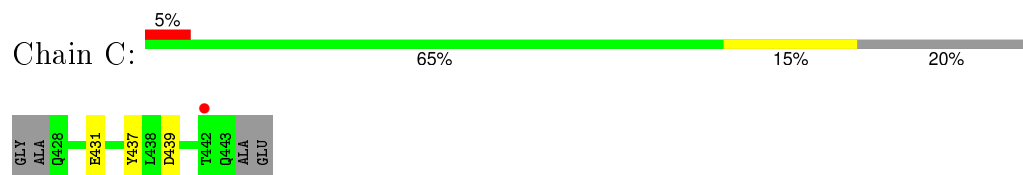
- Molecule 1: voltage-gated calcium channel subunit beta2a



- Molecule 2: voltage-gated calcium channel subunit beta2a



- Molecule 3: Voltage-dependent L-type calcium channel alpha-1C subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.76Å 45.33Å 60.65Å 96.81° 102.46° 98.53°	Depositor
Resolution (Å)	30.00 – 2.00 29.25 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-2.00) 91.9 (29.25-1.98)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.61 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.200 , 0.242 0.208 , 0.245	Depositor DCC
$R_{free}$ test set	1266 reflections (5.43%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 24889 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2506	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.94	0/776	0.91	1/1047 (0.1%)
2	B	0.82	0/1493	0.92	5/2025 (0.2%)
3	C	0.96	0/141	0.98	1/190 (0.5%)
All	All	0.87	0/2410	0.92	7/3262 (0.2%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	384	ASP	CB-CG-OD2	7.93	125.43	118.30
2	B	256	ARG	NE-CZ-NH1	-6.98	116.81	120.30
2	B	372	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	77	ASP	CB-CG-OD2	5.37	123.13	118.30
2	B	309	LEU	CA-CB-CG	5.25	127.37	115.30
3	C	439	ASP	CB-CG-OD2	5.18	122.96	118.30
2	B	293	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	760	0	742	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1468	0	1485	14	0
3	C	139	0	129	1	0
4	B	1	0	0	0	0
5	A	55	0	0	3	0
5	B	77	0	0	2	0
5	C	6	0	0	0	0
All	All	2506	0	2356	26	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.

All (26) 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)
2:B:244:MET:CE	2:B:244:MET:SD	2.01	1.48
2:B:255:HIS:ND1	5:B:46:HOH:O	2.11	0.84
2:B:244:MET:CE	2:B:244:MET:CG	2.77	0.62
1:A:90:LYS:HA	1:A:90:LYS:HE3	1.79	0.62
1:A:67:ASN:HD22	1:A:90:LYS:NZ	1.97	0.62
2:B:237:LYS:H	2:B:324:ASN:HD21	1.50	0.57
2:B:217:THR:N	2:B:218:PRO:HD2	2.20	0.57
1:A:78:VAL:HG21	1:A:84:ALA:HB2	1.91	0.51
1:A:94:HIS:HD2	5:A:149:HOH:O	1.96	0.49
1:A:67:ASN:HD22	1:A:90:LYS:HZ2	1.61	0.48
2:B:352:LEU:HD11	3:C:437:TYR:HB3	1.96	0.47
1:A:67:ASN:ND2	1:A:90:LYS:NZ	2.63	0.47
2:B:237:LYS:H	2:B:324:ASN:ND2	2.13	0.47
2:B:240:GLU:O	2:B:244:MET:HG3	2.15	0.47
1:A:94:HIS:HE1	2:B:225:SER:O	1.99	0.46
2:B:217:THR:N	2:B:218:PRO:CD	2.80	0.45
1:A:67:ASN:ND2	1:A:90:LYS:HZ1	2.15	0.45
1:A:133:GLN:HG3	1:A:134:ARG:N	2.32	0.44
1:A:130:GLN:HG2	1:A:134:ARG:HD2	1.99	0.43
2:B:256:ARG:NH1	2:B:397:GLU:OE1	2.52	0.42
2:B:285:ALA:N	5:B:115:HOH:O	2.52	0.42
2:B:254:LYS:HG3	2:B:263:ILE:HD12	2.02	0.42
2:B:243:ASP:OD1	2:B:424:ARG:NE	2.52	0.41
1:A:52:LEU:HD13	1:A:117:PHE:CZ	2.55	0.41
1:A:57:THR:HB	5:A:179:HOH:O	2.21	0.41
1:A:67:ASN:ND2	5:A:162:HOH:O	2.54	0.40



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	94/132 (71%)	93 (99%)	1 (1%)	0	100	100
2	B	178/224 (80%)	176 (99%)	2 (1%)	0	100	100
3	C	14/20 (70%)	14 (100%)	0	0	100	100
All	All	286/376 (76%)	283 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	77/112 (69%)	72 (94%)	5 (6%)	21	15
2	B	165/203 (81%)	159 (96%)	6 (4%)	42	39
3	C	15/16 (94%)	14 (93%)	1 (7%)	20	14
All	All	257/331 (78%)	245 (95%)	12 (5%)	32	27

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	ARG
1	A	57	THR

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Mol	Chain	Res	Type
1	A	74	GLN
1	A	115	ILE
1	A	133	GLN
2	B	217	THR
2	B	256	ARG
2	B	330	SER
2	B	331	LYS
2	B	347	LYS
2	B	350	GLN
3	C	431	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	94	HIS
2	B	291	ASN
2	B	324	ASN
3	C	443	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](#)

Of 1 ligands modelled in this entry, 1 is 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

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	96/132 (72%)	-0.19	1 (1%) 84 84	11, 19, 35, 43	0
2	B	187/224 (83%)	-0.02	5 (2%) 58 58	12, 21, 33, 68	0
3	C	16/20 (80%)	0.12	1 (6%) 23 24	28, 32, 42, 47	0
All	All	299/376 (79%)	-0.07	7 (2%) 64 64	11, 21, 36, 68	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	425	THR	5.1
3	C	442	THR	2.8
2	B	230	VAL	2.7
2	B	231	LEU	2.4
2	B	363	HIS	2.3
2	B	424	ARG	2.3
1	A	46	ARG	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CL	B	426	1/1	0.97	0.05	-	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.