



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:47 PM GMT

PDB ID : 4DEX  
Title : Crystal structure of the Voltage Dependent Calcium Channel beta-2 Subunit in Complex With The CaV2.2 I-II Linker.  
Authors : Almagor, L.; Hirsch, J.A.  
Deposited on : 2012-01-22  
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

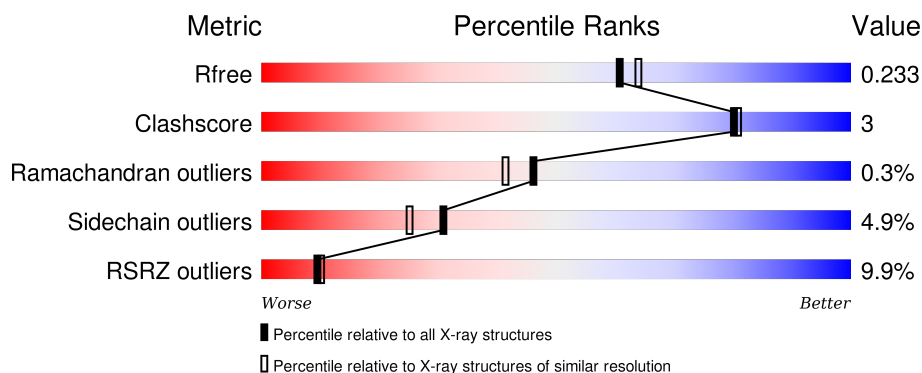
# 1 Overall quality at a glance

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	339	<div> <div>9%</div> <div>74%</div> <div>11%</div> <div>•</div> <div>15%</div> </div>
2	B	113	<div> <div>%</div> <div>36%</div> <div>•</div> <div>60%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2826 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-dependent L-type calcium channel subunit beta-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2284	1453	398	424	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	GLU	-	SEE REMARK 999	UNP P54288
A	139	PHE	-	SEE REMARK 999	UNP P54288
A	140	LYS	-	SEE REMARK 999	UNP P54288
A	141	LEU	-	SEE REMARK 999	UNP P54288

- Molecule 2 is a protein called Voltage-dependent N-type calcium channel subunit alpha-1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	45	Total	C	N	O	S	0	0	0
			380	237	72	70	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	356	GLY	-	EXPRESSION TAG	UNP Q02294
B	357	SER	-	EXPRESSION TAG	UNP Q02294

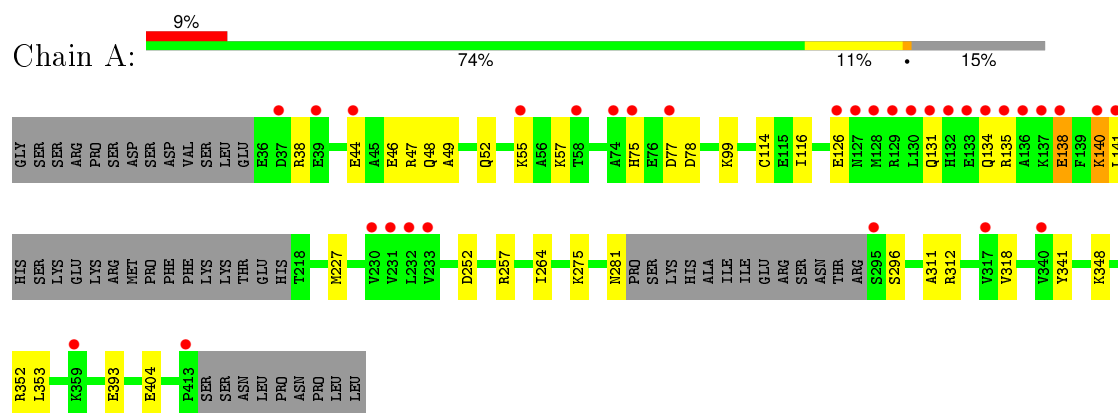
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	147	Total	O	0	0
			147	147		
3	B	15	Total	O	0	0
			15	15		

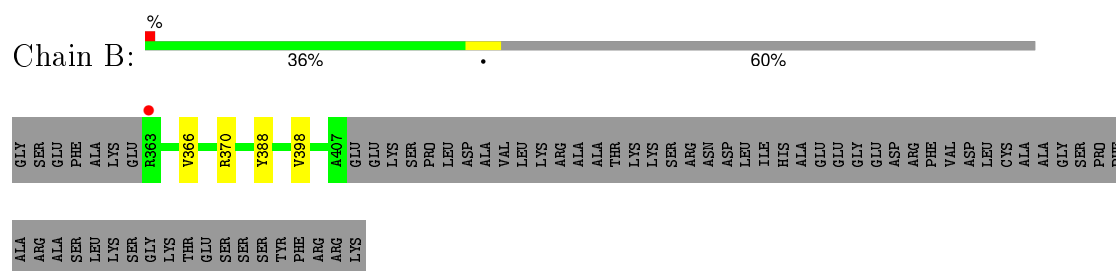
### 3 Residue-property plots

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-dependent L-type calcium channel subunit beta-2



- Molecule 2: Voltage-dependent N-type calcium channel subunit alpha-1B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.91Å 68.66Å 79.16Å 90.00° 102.55° 90.00°	Depositor
Resolution (Å)	27.31 – 2.00 27.31 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.9 (27.31-2.00) 91.0 (27.31-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 1.99Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.198 , 0.238 0.194 , 0.233	Depositor DCC
$R_{free}$ test set	1235 reflections (5.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 63.5	EDS
Estimated twinning fraction	0.045 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23830 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	2826	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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

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	0.40	0/2329	0.52	0/3153
2	B	0.36	0/384	0.43	0/513
All	All	0.39	0/2713	0.51	0/3666

There are no bond length outliers.

There are no bond angle outliers.

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	2284	0	2301	17	0
2	B	380	0	367	3	0
3	A	147	0	0	3	1
3	B	15	0	0	0	0
All	All	2826	0	2668	18	1

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 3.

All (18) 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:257:ARG:NH1	1:A:404:GLU:OE1	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:CYS:SG	3:A:639:HOH:O	2.42	0.78
1:A:281:ASN:O	3:A:638:HOH:O	2.05	0.73
1:A:252:ASP:OD2	2:B:398:VAL:HG21	1.93	0.68
1:A:140:LYS:HB2	1:A:141:LEU:HA	1.78	0.65
1:A:44:GLU:OE1	1:A:47:ARG:NH2	2.33	0.59
1:A:281:ASN:O	3:A:614:HOH:O	2.18	0.54
1:A:78:ASP:N	1:A:78:ASP:OD1	2.42	0.53
1:A:348:LYS:NZ	1:A:352:ARG:HD2	2.25	0.52
1:A:134:GLN:NE2	1:A:138:GLU:OE2	2.44	0.49
1:A:393:GLU:H	1:A:393:GLU:CD	2.16	0.48
1:A:227:MET:H	1:A:311:ALA:HB1	1.80	0.47
1:A:49:ALA:O	1:A:52:GLN:HB2	2.18	0.44
1:A:353:LEU:HD11	2:B:388:TYR:HB3	2.00	0.43
1:A:57:LYS:HG3	1:A:116:ILE:HG21	2.01	0.43
1:A:44:GLU:OE2	1:A:48:GLN:NE2	2.52	0.43
1:A:264:ILE:HG12	1:A:318:VAL:HB	2.01	0.41
2:B:366:VAL:O	2:B:370:ARG:HG3	2.20	0.41

All (1) 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)
3:A:523:HOH:O	3:A:635:HOH:O[2_545]	2.18	0.02

## 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	283/339 (84%)	279 (99%)	3 (1%)	1 (0%)	39	33
2	B	43/113 (38%)	43 (100%)	0	0	100	100
All	All	326/452 (72%)	322 (99%)	3 (1%)	1 (0%)	46	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ARG

### 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	249/301 (83%)	235 (94%)	14 (6%)	26	20
2	B	37/95 (39%)	37 (100%)	0	100	100
All	All	286/396 (72%)	272 (95%)	14 (5%)	31	25

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	55	LYS
1	A	75	HIS
1	A	77	ASP
1	A	99	LYS
1	A	126	GLU
1	A	131	GLN
1	A	135	ARG
1	A	138	GLU
1	A	140	LYS
1	A	275	LYS
1	A	296	SER
1	A	312	ARG
1	A	341	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	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

### 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	289/339 (85%)	0.48	32 (11%) <b>7</b> <b>8</b>	26, 41, 94, 117	0
2	B	45/113 (39%)	0.15	1 (2%) 65 66	30, 57, 101, 118	0
All	All	334/452 (73%)	0.43	33 (9%) <b>9</b> <b>10</b>	26, 43, 96, 118	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	HIS	5.7
1	A	130	LEU	5.6
1	A	134	GLN	5.1
1	A	126	GLU	4.8
1	A	138	GLU	4.6
1	A	137	LYS	4.1
1	A	141	LEU	4.0
1	A	129	ARG	3.9
1	A	132	HIS	3.9
1	A	232	LEU	3.7
1	A	136	ALA	3.4
1	A	37	ASP	3.3
1	A	133	GLU	3.3
1	A	128	MET	3.3
1	A	230	VAL	3.2
1	A	77	ASP	3.1
1	A	295	SER	3.1
1	A	39	GLU	3.0
1	A	44	GLU	2.9
1	A	135	ARG	2.9
1	A	231	VAL	2.7
1	A	55	LYS	2.7
1	A	340	VAL	2.6
1	A	140	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	359	LYS	2.5
1	A	317	VAL	2.5
1	A	131	GLN	2.5
2	B	363	ARG	2.4
1	A	58	THR	2.4
1	A	127	ASN	2.4
1	A	233	VAL	2.3
1	A	413	PRO	2.3
1	A	74	ALA	2.3

## 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 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.