



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2021 – 07:54 PM EDT

PDB ID : 1T3L
Title : Structural Analysis of the Voltage-Dependent Calcium Channel Beta Subunit
Functional Core in Complex with Alpha1 Interaction Domain
Authors : Opatowsky, Y.; Chen, C.-C.; Campbell, K.P.; Hirsch, J.A.
Deposited on : 2004-04-27
Resolution : 2.20 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
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

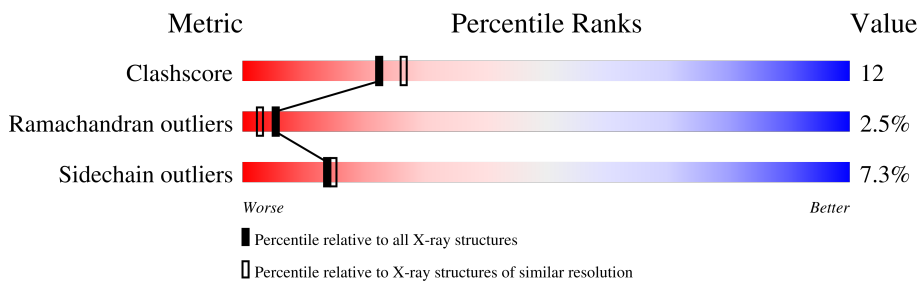
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	337	
2	B	18	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2671 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 Dihydropyridine-sensitive L-type, calcium channel beta-2 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	2409	1526	427	447	9	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	ARG	PRO	engineered mutation	UNP P54288
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 L-type calcium channel alpha-1S subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	17	134	85	20	28	1	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	0	0
			120	120		
3	B	8	Total	O	0	0
			8	8		

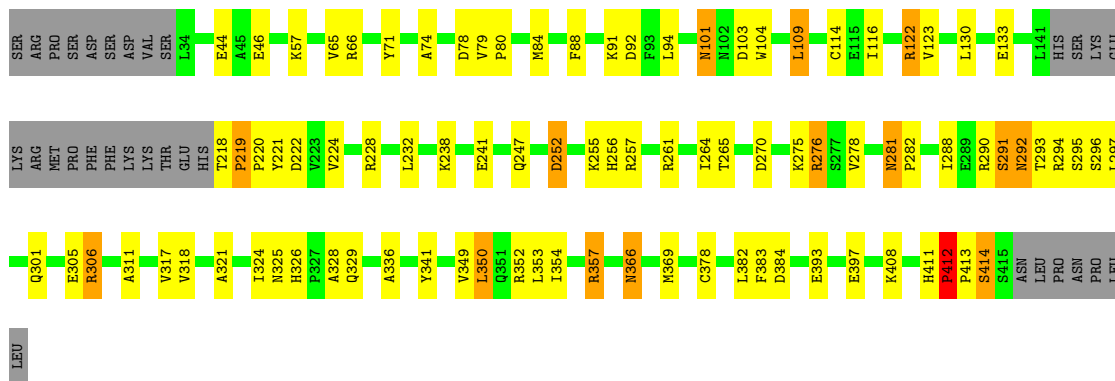
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.


Note EDS was not executed.

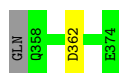
- Molecule 1: Dihydropyridine-sensitive L-type, calcium channel beta-2 subunit

Chain A: 



- Molecule 2: Voltage-dependent L-type calcium channel alpha-1S subunit

Chain B: 



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	72.78Å 168.26Å 34.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.52 – 2.20	Depositor
% Data completeness (in resolution range)	83.8 (84.52-2.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.221 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2671	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.78	0/2456	0.94	9/3328 (0.3%)
2	B	0.85	0/136	0.89	1/183 (0.5%)
All	All	0.79	0/2592	0.94	10/3511 (0.3%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	A	306	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	A	276	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	A	276	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	92	ASP	CB-CG-OD2	6.76	124.38	118.30

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	2409	0	2416	59	1
2	B	134	0	116	0	0
3	A	120	0	0	9	2
3	B	8	0	0	0	0
All	All	2671	0	2532	59	2

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 12.

The worst 5 of 59 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:114:CYS:HB2	3:A:528:HOH:O	1.51	1.10
1:A:326:HIS:HD2	1:A:328:ALA:H	1.36	0.73
1:A:325:ASN:H	1:A:329:GLN:HE22	1.35	0.73
1:A:352:ARG:HB2	3:A:534:HOH:O	1.89	0.72
1:A:412:PRO:HB3	1:A:413:PRO:CD	2.24	0.68

All (2) 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:431:HOH:O	3:A:500:HOH:O[1_554]	1.85	0.35
1:A:292:ASN:OD1	3:A:506:HOH:O[4_556]	2.15	0.05

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	302/337 (90%)	285 (94%)	9 (3%)	8 (3%)	5 3
2	B	15/18 (83%)	15 (100%)	0	0	100 100
All	All	317/355 (89%)	300 (95%)	9 (3%)	8 (2%)	5 3

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	SER
1	A	294	ARG
1	A	411	HIS

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Mol	Chain	Res	Type
1	A	412	PRO
1	A	414	SER

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	261/300 (87%)	241 (92%)	20 (8%)	13	13
2	B	13/16 (81%)	13 (100%)	0	100	100
All	All	274/316 (87%)	254 (93%)	20 (7%)	14	15

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	SER
1	A	366	ASN
1	A	412	PRO
1	A	397	GLU
1	A	224	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	326	HIS
1	A	329	GLN
2	B	358	GLN
1	A	390	ASN
1	A	247	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 monosaccharides 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](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.