



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:19 PM GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at 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.

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

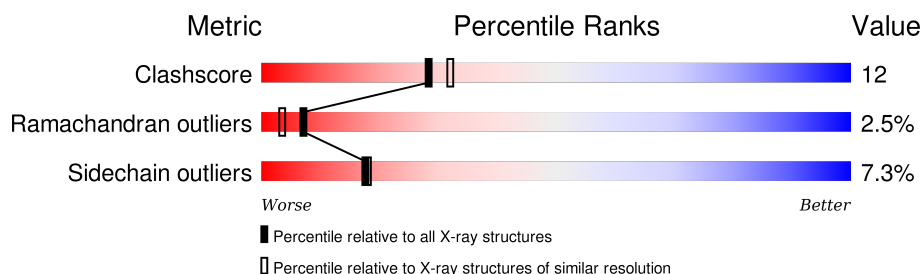
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (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 on the lower 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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	337	 64% 23% • 9%
2	B	18	 89% 6% 6%

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
1	A	306	Total	C	N	O	S	0	0	0
			2409	1526	427	447	9			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	ARG	PRO	ENGINEERED	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.

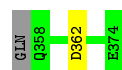
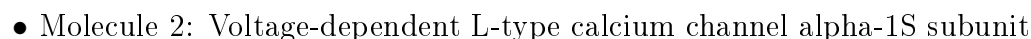
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	17	Total	C	N	O	S	0	0	0
			134	85	20	28	1			

- 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		

Note EDS was not executed.

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



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	72.78 Å 168.26 Å 34.23 Å 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.	Xtriage
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.

All (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
1	A	384	ASP	CB-CG-OD2	6.68	124.31	118.30
1	A	270	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	222	ASP	CB-CG-OD2	5.98	123.69	118.30
2	B	362	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	252	ASP	CB-CG-OD2	5.12	122.91	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
1:A:408:LYS:HA	1:A:412:PRO:CD	2.24	0.68
1:A:278:VAL:HG11	1:A:297:LEU:HD21	1.77	0.66
1:A:101:ASN:HD22	1:A:101:ASN:C	1.99	0.66
1:A:321:ALA:HB1	1:A:324:ILE:HD13	1.80	0.63
1:A:412:PRO:HB3	1:A:413:PRO:HD2	1.82	0.62
1:A:241:GLU:OE1	1:A:357:ARG:HD3	1.99	0.62
1:A:290:ARG:C	1:A:291:SER:O	2.35	0.60
1:A:324:ILE:HD12	1:A:324:ILE:N	2.16	0.60
1:A:408:LYS:HA	1:A:412:PRO:HD2	1.82	0.60
1:A:291:SER:O	1:A:292:ASN:C	2.38	0.60
1:A:255:LYS:HG3	1:A:264:ILE:HD12	1.85	0.58
1:A:261:ARG:HD3	3:A:511:HOH:O	2.03	0.57
1:A:408:LYS:O	1:A:412:PRO:HG2	2.05	0.56
1:A:228:ARG:NH1	1:A:336:ALA:O	2.42	0.53
1:A:57:LYS:HA	1:A:116:ILE:HG13	1.90	0.52
1:A:341:TYR:HB2	1:A:383:PHE:CD2	2.44	0.52
1:A:352:ARG:HD3	3:A:534:HOH:O	2.10	0.51
1:A:325:ASN:H	1:A:329:GLN:NE2	2.07	0.50
1:A:366:ASN:ND2	3:A:454:HOH:O	2.37	0.50
1:A:413:PRO:O	1:A:414:SER:HB2	2.10	0.50
1:A:354:ILE:HD12	1:A:369:MET:CE	2.41	0.49
1:A:281:ASN:HD22	1:A:282:PRO:HD2	1.77	0.49
1:A:278:VAL:CG1	1:A:297:LEU:HD21	2.41	0.49
1:A:66:ARG:HD2	1:A:91:LYS:NZ	2.27	0.49
1:A:228:ARG:HG2	1:A:336:ALA:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ILE:HG12	1:A:318:VAL:HB	1.95	0.48
1:A:44:GLU:HB3	3:A:451:HOH:O	2.13	0.48
1:A:265:THR:OG1	1:A:306:ARG:NH2	2.33	0.47
1:A:412:PRO:CB	1:A:413:PRO:CD	2.90	0.47
1:A:326:HIS:CD2	1:A:328:ALA:H	2.25	0.46
1:A:275:LYS:HB2	1:A:278:VAL:HG23	1.98	0.46
1:A:46:GLU:HB2	3:A:499:HOH:O	2.15	0.45
1:A:101:ASN:ND2	1:A:103:ASP:H	2.14	0.45
1:A:350:LEU:HD13	1:A:369:MET:CE	2.46	0.45
1:A:101:ASN:C	1:A:101:ASN:ND2	2.68	0.44
1:A:378:CYS:SG	1:A:382:LEU:HD12	2.58	0.44
1:A:326:HIS:HE1	3:A:462:HOH:O	2.01	0.43
1:A:412:PRO:HD3	3:A:519:HOH:O	2.18	0.43
1:A:324:ILE:CD1	1:A:324:ILE:N	2.82	0.43
1:A:130:LEU:HA	1:A:133:GLU:OE2	2.19	0.43
1:A:349:VAL:O	1:A:353:LEU:HG	2.19	0.43
1:A:94:LEU:HD23	1:A:109:LEU:HA	2.01	0.43
1:A:65:VAL:HG11	1:A:221:TYR:HB3	2.01	0.43
1:A:122:ARG:HG3	1:A:123:VAL:N	2.32	0.42
1:A:219:PRO:HA	1:A:220:PRO:HD2	1.93	0.42
1:A:252:ASP:O	1:A:256:HIS:HD2	2.02	0.42
1:A:290:ARG:O	1:A:291:SER:O	2.37	0.42
1:A:80:PRO:HD3	1:A:104:TRP:NE1	2.34	0.42
1:A:238:LYS:HE2	1:A:247:GLN:HE22	1.86	0.41
1:A:311:ALA:HB2	1:A:317:VAL:HG21	2.03	0.41
1:A:71:TYR:HB3	1:A:88:PHE:CZ	2.56	0.41
1:A:301:GLN:HG3	1:A:305:GLU:OE2	2.21	0.41
1:A:232:LEU:O	1:A:238:LYS:NZ	2.50	0.40
1:A:393:GLU:CD	1:A:393:GLU:H	2.24	0.40

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%)	7	3
2	B	15/18 (83%)	15 (100%)	0	0	100	100
All	All	317/355 (89%)	300 (95%)	9 (3%)	8 (2%)	7	3

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	291	SER
1	A	294	ARG
1	A	411	HIS
1	A	412	PRO
1	A	414	SER
1	A	78	ASP
1	A	219	PRO
1	A	74	ALA

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%)	16	16
2	B	13/16 (81%)	13 (100%)	0	100	100
All	All	274/316 (87%)	254 (93%)	20 (7%)	17	18

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	VAL
1	A	84	MET
1	A	101	ASN
1	A	109	LEU
1	A	122	ARG
1	A	218	THR
1	A	224	VAL
1	A	257	ARG
1	A	276	ARG
1	A	281	ASN
1	A	288	ILE
1	A	292	ASN
1	A	293	THR
1	A	295	SER
1	A	296	SER
1	A	350	LEU
1	A	357	ARG
1	A	366	ASN
1	A	397	GLU
1	A	412	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	95	HIS
1	A	101	ASN
1	A	127	ASN
1	A	247	GLN
1	A	256	HIS
1	A	281	ASN
1	A	326	HIS
1	A	329	GLN
1	A	390	ASN
2	B	358	GLN

5.3.3 RNA ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.