



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:57 PM GMT

PDB ID : 1VYU
Title : BETA3 SUBUNIT OF VOLTAGE-GATED CA2+-CHANNEL
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Deposited on : 2004-05-07
Resolution : 2.30 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) : 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

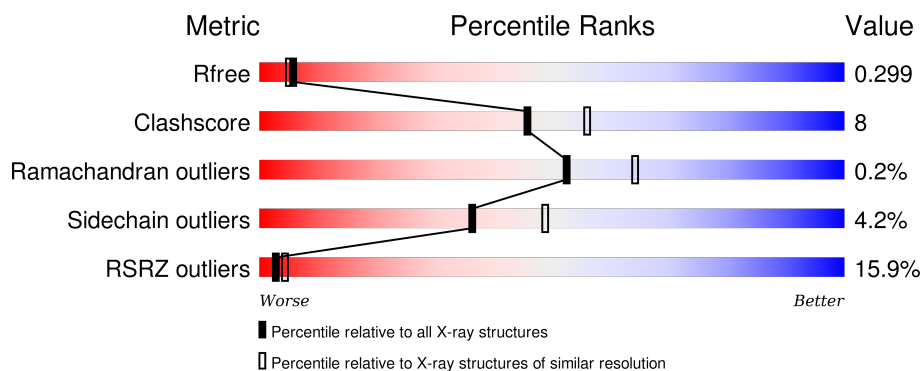
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	A	351	
1	B	351	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4851 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 CALCIUM CHANNEL BETA-3 SUBUNIT.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	Se	0	0	1
			2168	1378	380	400	4	6			
1	B	287	Total	C	N	O	S	Se	0	0	1
			2286	1444	405	427	4	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	234	Total	O	0	0
			234	234		
2	B	163	Total	O	0	0
			163	163		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.30Å 66.40Å 90.00Å 90.00° 103.10° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.22 – 2.27	Depositor EDS
% Data completeness (in resolution range)	93.8 (30.00-2.30) 91.7 (29.22-2.27)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.97 (at 2.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.248 0.275 , 0.299	Depositor DCC
R_{free} test set	2745 reflections (9.93%)	DCC
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 27952 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4851	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.42	0/2204	0.66	0/2969
1	B	0.33	0/2322	0.59	0/3126
All	All	0.38	0/4526	0.63	0/6095

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	2168	0	2193	33	1
1	B	2286	0	2302	36	0
2	A	234	0	0	4	0
2	B	163	0	0	1	0
All	All	4851	0	4495	69	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 8.

All (69) 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:B:73:VAL:HG13	1:B:86:ASN:HD21	1.28	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:LYS:HG3	1:A:214:ILE:HD12	1.53	0.90
1:A:168:VAL:HG13	1:A:169:PRO:HD3	1.54	0.89
1:B:257:ILE:HD11	1:B:285:LEU:HD22	1.65	0.79
1:A:54:ARG:O	2:A:2010:HOH:O	2.03	0.75
1:A:198:LYS:NZ	2:A:2137:HOH:O	2.20	0.75
1:A:276:HIS:HD2	1:A:278:ALA:H	1.36	0.71
1:A:57:HIS:O	2:A:2016:HOH:O	2.11	0.68
1:A:300:LEU:HG	1:A:319:MSE:HE1	1.77	0.66
1:B:225:LYS:H	1:B:225:LYS:HD3	1.61	0.65
1:B:211:ARG:HB2	1:B:357:TRP:CH2	2.31	0.65
1:A:215:THR:OG1	1:A:256:ARG:NH2	2.27	0.65
1:B:316:THR:HG22	1:B:320:MSE:HE2	1.79	0.64
1:A:39:SER:HB2	1:A:42:ARG:HG2	1.80	0.64
1:B:315:LEU:HD12	1:B:319:MSE:HE3	1.80	0.63
1:A:214:ILE:HG12	1:A:268:VAL:HB	1.81	0.63
1:A:304:ILE:HD12	1:A:319:MSE:CE	2.28	0.63
1:B:73:VAL:HG13	1:B:86:ASN:ND2	2.07	0.62
1:A:128:ARG:O	1:A:132:GLU:HB2	1.99	0.62
1:A:107:ARG:HD2	1:A:113:GLY:O	2.04	0.58
1:A:224:ALA:HB3	1:A:283:THR:HG22	1.85	0.58
1:B:110:LYS:HA	1:B:359:ALA:HB1	1.87	0.57
1:B:250:VAL:O	1:B:254:ILE:HG12	2.06	0.56
1:A:76:GLU:H	1:A:76:GLU:CD	2.08	0.55
1:B:304:ILE:HD12	1:B:319:MSE:HE1	1.89	0.53
1:A:302:ARG:HE	1:A:305:ARG:HH21	1.54	0.53
1:B:89:ALA:O	1:B:90:LYS:HB2	2.07	0.53
1:B:286:ALA:N	1:B:287:PRO:HD3	2.23	0.53
1:A:212:ILE:HD11	1:A:268:VAL:HG21	1.90	0.53
1:B:83:SER:O	1:B:116:ALA:HB1	2.09	0.53
1:A:205:LYS:CG	1:A:214:ILE:HD12	2.35	0.52
1:A:276:HIS:CD2	1:A:278:ALA:H	2.22	0.52
1:B:255:GLU:O	1:B:259:GLU:HG2	2.10	0.52
1:B:207:ARG:NH1	1:B:350:ALA:HB1	2.26	0.51
1:A:168:VAL:CG1	1:A:169:PRO:HD3	2.35	0.50
1:A:191:GLU:OE2	1:A:307:ARG:HD3	2.12	0.50
1:B:196:MSE:HG3	1:B:342:LEU:HD21	1.94	0.49
1:B:253:GLU:O	1:B:257:ILE:HG23	2.12	0.49
1:B:107:ARG:HD2	1:B:113:GLY:O	2.13	0.48
1:B:246:SER:O	1:B:250:VAL:HG23	2.15	0.47
1:B:291:PHE:HB2	1:B:333:PHE:CD2	2.51	0.46
1:B:207:ARG:HD2	2:B:2118:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ARG:HH11	1:B:358:ARG:HB2	1.80	0.46
1:A:348:HIS:HE1	2:A:2116:HOH:O	1.99	0.46
1:A:276:HIS:CD2	1:A:277:PRO:HD2	2.51	0.45
1:B:339:GLU:CD	1:B:339:GLU:H	2.18	0.45
1:A:304:ILE:HD12	1:A:319:MSE:HE3	1.98	0.45
1:A:95:ILE:N	1:A:95:ILE:HD12	2.31	0.45
1:B:322:TYR:O	1:B:326:VAL:HG23	2.18	0.44
1:A:89:ALA:O	1:A:90:LYS:HB2	2.17	0.43
1:A:70:TYR:HB3	1:A:87:PHE:CE1	2.53	0.43
1:B:87:PHE:HB3	1:B:108:LEU:HD21	2.00	0.43
1:B:315:LEU:CD1	1:B:319:MSE:HE3	2.47	0.43
1:B:225:LYS:NZ	1:B:251:GLN:HE21	2.18	0.42
1:A:212:ILE:HD11	1:A:268:VAL:CG2	2.50	0.42
1:B:207:ARG:HH11	1:B:350:ALA:HB1	1.83	0.42
1:B:169:PRO:HA	1:B:170:PRO:HD3	1.88	0.41
1:A:297:PRO:HG3	1:A:322:TYR:CE2	2.55	0.41
1:B:351:GLU:HG3	1:B:352:TYR:N	2.36	0.41
1:B:43:GLU:O	1:B:47:GLN:HG2	2.20	0.41
1:A:55:ALA:O	1:A:96:LYS:HD3	2.21	0.41
1:B:358:ARG:HB2	1:B:358:ARG:NH1	2.36	0.41
1:A:125:GLU:O	1:A:129:LEU:HB2	2.21	0.41
1:B:93:LEU:HD23	1:B:108:LEU:HD23	2.03	0.41
1:A:300:LEU:HG	1:A:319:MSE:CE	2.49	0.41
1:A:302:ARG:NH2	1:A:305:ARG:HE	2.18	0.41
1:B:282:LYS:HD2	1:B:282:LYS:N	2.36	0.41
1:B:179:PRO:HG2	1:B:257:ILE:CD1	2.51	0.40
1:B:331:GLU:CD	1:B:331:GLU:H	2.24	0.40

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)
1:A:57:HIS:ND1	1:A:256:ARG:NH2[2_456]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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	266/351 (76%)	256 (96%)	10 (4%)	0	100	100
1	B	279/351 (80%)	273 (98%)	5 (2%)	1 (0%)	39	48
All	All	545/702 (78%)	529 (97%)	15 (3%)	1 (0%)	52	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	139	GLY

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	241/304 (79%)	230 (95%)	11 (5%)	33	44
1	B	254/304 (84%)	244 (96%)	10 (4%)	39	53
All	All	495/608 (81%)	474 (96%)	21 (4%)	36	49

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	51	GLN
1	A	76	GLU
1	A	102	ASP
1	A	133	GLN
1	A	168	VAL
1	A	207	ARG
1	A	225	LYS
1	A	249	GLU
1	A	348	HIS
1	A	351	GLU

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Mol	Chain	Res	Type
1	B	90	LYS
1	B	110	LYS
1	B	125	GLU
1	B	129	LEU
1	B	136	ARG
1	B	225	LYS
1	B	257	ILE
1	B	331	GLU
1	B	343	ASP
1	B	348	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	265	GLN
1	A	276	HIS
1	A	361	HIS
1	B	206	HIS
1	B	251	GLN
1	B	265	GLN
1	B	301	GLN
1	B	327	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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, 95th 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 ²)	Q<0.9
1	A	266/351 (75%)	1.30	46 (17%) 2 3	14, 30, 72, 112	0
1	B	281/351 (80%)	1.08	41 (14%) 3 5	22, 43, 71, 98	0
All	All	547/702 (77%)	1.19	87 (15%) 3 4	14, 37, 73, 112	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	PRO	14.0
1	B	362	HIS	11.2
1	A	40	ALA	8.9
1	A	225	LYS	7.3
1	B	167	HIS	6.9
1	B	31	VAL	5.3
1	B	342	LEU	5.0
1	B	245	SER	4.7
1	A	42	ARG	4.4
1	A	247	ILE	4.3
1	A	133	GLN	4.3
1	A	310	SER	4.3
1	B	224	ALA	4.2
1	A	206	HIS	4.1
1	A	39	SER	3.9
1	A	313	LYS	3.8
1	B	57	HIS	3.8
1	A	129	LEU	3.7
1	A	43	GLU	3.7
1	B	223	LEU	3.6
1	B	140	ASN	3.6
1	A	246	SER	3.5
1	A	44	VAL	3.5
1	A	343	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	35	GLU	3.4
1	A	55	ALA	3.3
1	B	331	GLU	3.3
1	B	225	LYS	3.3
1	B	168	VAL	3.3
1	A	132	GLU	3.2
1	B	181	VAL	3.2
1	A	362	HIS	3.1
1	A	199	ALA	3.1
1	B	32	SER	3.1
1	A	268	VAL	3.0
1	B	114	ASP	3.0
1	A	260	LEU	3.0
1	B	345	ALA	3.0
1	A	113	GLY	2.9
1	B	282	LYS	2.9
1	B	358	ARG	2.9
1	A	266	LEU	2.9
1	A	131	GLN	2.9
1	B	249	GLU	2.8
1	A	134	LYS	2.8
1	B	139	GLY	2.7
1	A	309	LYS	2.7
1	A	181	VAL	2.7
1	A	214	ILE	2.7
1	A	290	VAL	2.6
1	A	201	PHE	2.6
1	B	207	ARG	2.6
1	A	41	ARG	2.6
1	B	81	GLN	2.6
1	B	288	ILE	2.5
1	B	328	CYS	2.5
1	A	71	CYS	2.5
1	A	183	VAL	2.5
1	A	224	ALA	2.5
1	B	76	GLU	2.4
1	B	341	GLN	2.4
1	B	180	VAL	2.4
1	B	206	HIS	2.4
1	A	351	GLU	2.4
1	B	353	LEU	2.3
1	A	353	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	343	ASP	2.3
1	B	59	PRO	2.3
1	A	264	LEU	2.3
1	A	106	GLY	2.2
1	B	79	PRO	2.2
1	B	290	VAL	2.2
1	A	168	VAL	2.2
1	B	83	SER	2.2
1	B	39	SER	2.1
1	A	308	GLY	2.1
1	A	361	HIS	2.1
1	B	337	LEU	2.1
1	B	179	PRO	2.1
1	B	210	GLY	2.1
1	B	36	ASP	2.1
1	A	282	LYS	2.1
1	A	302	ARG	2.0
1	A	300	LEU	2.0
1	B	268	VAL	2.0
1	A	249	GLU	2.0
1	A	127	ILE	2.0

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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.