PREDICTED BONDS	SEQUENCE	SCORE
α_2 5 – 962 δ	XMAAGCLLALT - LSKQSCITEQT	0.01037
α_2 303 – 354 α_2	AQDVSCFQHLV - VSRANCNKIIM	0.99715
α_2 404 – 1047 δ	**IQWMACENKGY - KGPDVCFDNNV**	**0.99862**
α_2 507 – 987 δ	PRFTLCPNGYY - LDCGNCSRIFH	0.87141
α_2 655 – 822 α_2	APREYCNDLKP - SIRDPCAGPVC	0.50051
α_2 685 – 1012 δ	PNNPSCNTDLI - ESKGTCPCDTR	0.83708
α_2 827 – 838 α_2	CAGPVCDCKRN - SDVMDCVILDD	0.0104
α_2 829 – 984 δ	GPVCDCKRNSD - SGLLDCGNCSR	0.99568
α_2 892 – 1014 δ	DYQSVCDPGAA - KGTCPCDTRLL	0.99536
δ 1032 – 1059 δ	DGPDPCMVKQ - EDYTDCGGVSG	0.01047

Aida Calderón-Rivera, Arturo Andrade, Oscar Hernández-Hernández, Ricardo González-Ramírez, Alejandro Sandoval, Manuel Rivera, Juan Carlos Gomora, Ricardo Felix

Identification of a disulfide bridge essential for structure and function of the voltage-gated Ca2+ channel α2δ-1 auxiliary subunit

Cell Calcium, Volume 51, Issue 1, 2012, 22–30

http://dx.doi.org/10.1016/j.ceca.2011.10.002

Algorithm	Parameter	α_2	δ	$\alpha_2\delta$
PROCHECK[1]	All-atom pairwise energy	-3.67	-3.26	-3.68
	Solvation energy	-4.14	-5.28	-4.93
	Torsion angle energy	-5.86	-3.5	-5.15
	Secondary structure agreement	-3.76	-0.59	-3.9
	Solvent accessibility agreement	-3.45	-1.56	-3.56
Structure Z-scores[2]	2nd generation packing quality	-4.072	-3.491	-4.052
	Ramachandran plot appearance	-6.298	-1.766	-5.69
	chi-1/chi-2 rotamer normality	0.559	5.566	1.257
	Backbone conformation	-16.585	-8.516	-15.73
RMS Z-scores[2]	Bond lengths	1.678	0.896	1.631
	Bond angles	2.305	0.568	2.156
	Omega angle restraints	3.824	0.989	3.588
	Side chain planarity	3.62	2.209	3.467
	Improper dihedral distribution	2.883	1.023	2.713
	Inside/Outside distribution	1.242	1.224	1.255
Ramachandran plot residues[2]	Core	57%	86.80%	61%
	Allowed region	26.40%	12.40%	24.50%
	Generously Allowed Region	9.80%	0.80%	8.60%
	Total	93.20%	100.00%	94.10%

The quality of the models was evaluated using the Protein Structure & Model Assessment Tool available at http://swissmodel.expasy.org/workspace/index.php func=tools_structureassessment1. Though the sequence of the full-length protein is unusual long (1091 aa) for this analysis, the parameters maintained acceptable or medium scores as the initial template structures.

[1] Laskowski RA, MacArthur MW, Moss DS, Thornton JM (1993) PROCHECK: A program to check the stereochemical quality of protein structures. J Appl Cryst 26: 283-291.

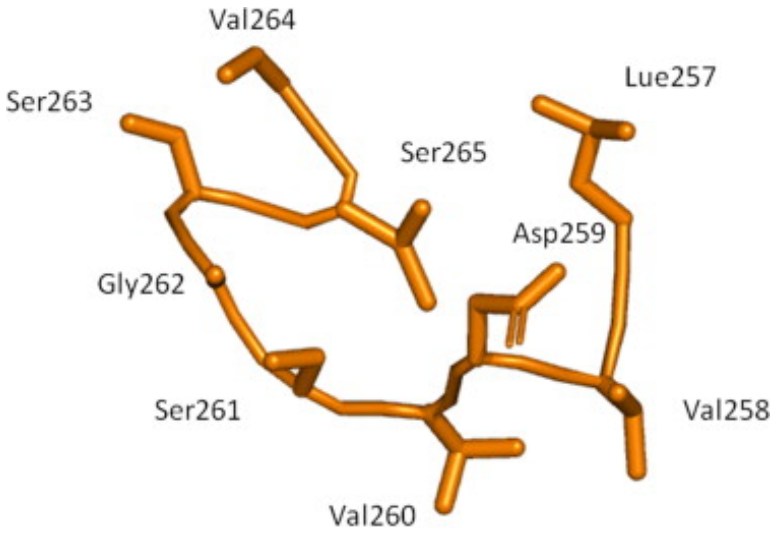
[2] Hooft RW, Vriend G, Sander C, Abola EE. (1996) Errors in protein structures. Nature 381(6580): 272.

Aida Calderón-Rivera, Arturo Andrade, Oscar Hernández-Hernández, Ricardo González-Ramírez, Alejandro Sandoval, Manuel Rivera, Juan Carlos Gomora, Ricardo Felix

Identification of a disulfide bridge essential for structure and function of the voltage-gated Ca2+ channel α2δ-1 auxiliary subunit

Cell Calcium, Volume 51, Issue 1, 2012, 22–30

http://dx.doi.org/10.1016/j.ceca.2011.10.002



MIDAS motif
LV**DVSGS**VS

Aida Calderón-Rivera, Arturo Andrade, Oscar Hernández-Hernández, Ricardo González-Ramírez, Alejandro Sandoval, Manuel Rivera, Juan Carlos Gomora, Ricardo Felix

Identification of a disulfide bridge essential for structure and function of the voltage-gated Ca2+ channel α2δ-1 auxiliary subunit

Cell Calcium, Volume 51, Issue 1, 2012, 22–30

http://dx.doi.org/10.1016/j.ceca.2011.10.002

vWFA motif

DMLILVDVSGSVSGLTLKLIRTSVSEMLETLSDDDFVNVASFNSNAQDVSCFQHLVQANV
RNKKVLKDAVNNITAKGITDYKKGFSFAFEQLLNYNVSRANCNKIIMLFTDGGEERAQEI
FAKYNKDKKVRVFTFSVGQHNYDRGPIQWMACENKGYYYEIPSIGAIRINTQEYLDVL

Rossman fold: 259 **LVDVSGSVS** 265

Aida Calderón-Rivera, Arturo Andrade, Oscar Hernández-Hernández, Ricardo González-Ramírez, Alejandro Sandoval, Manuel Rivera, Juan Carlos Gomora, Ricardo Felix

Identification of a disulfide bridge essential for structure and function of the voltage-gated Ca2+ channel α2δ-1 auxiliary subunit

Cell Calcium, Volume 51, Issue 1, 2012, 22–30

http://dx.doi.org/10.1016/j.ceca.2011.10.002

Cache motif

WTNVYLDALELGLVITGTLPVFNVTGQSENKTNLKNQLILGVMGV
DVSLEDIKRLTPRFTLCPNGYYFAIDPNGYVLLHPNLQPKPIGVGIP

Aida Calderón-Rivera, Arturo Andrade, Oscar Hernández-Hernández, Ricardo González-Ramírez, Alejandro Sandoval, Manuel Rivera, Juan Carlos Gomora, Ricardo Felix

Identification of a disulfide bridge essential for structure and function of the voltage-gated Ca2+ channel α2δ-1 auxiliary subunit

Cell Calcium, Volume 51, Issue 1, 2012, 22–30

http://dx.doi.org/10.1016/j.ceca.2011.10.002