SWISS-MODEL Homology Modeling Report

Model Building Report

This document lists the results for the homology modeling project "Untitled Project" submitted to SWISS-MODEL workspace on May 5, 2015, 1:39 p.m..The submitted primary amino acid sequence is given in Table T1.

If you use any results in your research, please cite the relevant publications:

Marco Biasini; Stefan Bienert; Andrew Waterhouse; Konstantin Arnold; Gabriel Studer; Tobias Schmidt; Florian Kiefer; Tiziano Gallo Cassarino; Martino Bertoni; Lorenza Bordoli; Torsten Schwede. (2014). SWISS-MODEL: modelling protein tertiary and quaternary structure using evolutionary information. Nucleic Acids Research (1 July 2014) 42 (W1): W252-W258; doi: 10.1093/nar/gku340.
Arnold, K., Bordoli, L., Kopp, J. and Schwede, T. (2006) The SWISS-MODEL workspace: a web-based environment for protein structure homology modelling. Bioinformatics, 22, 195-201.
Benkert, P., Biasini, M. and Schwede, T. (2011) Toward the estimation of the absolute quality of individual protein structure models. Bioinformatics, 27, 343-350

Results

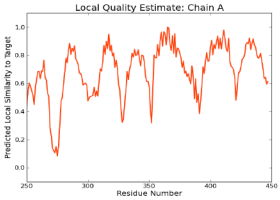
The SWISS-MODEL template library (SMTL version 2015-04-22, PDB release 2015-04-17) was searched with Blast (Altschul et al., 1997) and HHBlits (Remmert, et al., 2011) for evolutionary related structures matching the target sequence in Table T1. For details on the template search, see Materials and Methods. Overall 2484 templates were found (Table T2).

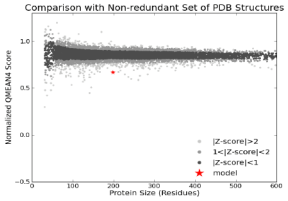
Models

The following models were built (see Materials and Methods "Model Building"):

Model #01	File	Built with	Oligo-State	Ligands	GMQE	QMEAN4
	PDB	ProMod Version 3.70.	MONOMER	None	0.15	-4.56

QMEAN4	-4.56
Cβ	0.62
All Atom	0.86
Solvation	-3.62
Torsion	-3.45





Template	Seq Identity	Oligo-state	Found by	Method	Resolution	Seq Similarity	Range	Coverage	Description
4h5y.1.A	13.76	monomer	HHblits	X-ray	2.10Å	0.28	250 - 447	0.35	LidA protein, substrate of the Dot/Icm system

The template contained no ligands.

```
Target    MTQRSSVTIKSGGTRNFSASSASLLPGCRPGFSSVSVSQSGKSFGGGIGGGFGTRSLHSFGGNKRISIGGGYRSTRASFG
4h5y.1.A  ------------------------------------------------------------------------------

Target    GAACGLGVSGIGYRVGGAYGGYGYGGGMAPGAGGIHEVTVNQSLLTPLHLEIDPSLQRVRKEEKEQIKTLNNKFASFIDK
4h5y.1.A  ------------------------------------------------------------------------------

Target    VRFLEQQNKVLETKWSLLQEHKTTRTNLEPMFEAYITNLRRQLECLGGERSRLETELKSMQDVVEDFKNKYEEEIHRRTA
4h5y.1.A  ------------------------------------------------------------------------------

Target    AENEFVVLKKDVDAAYMNKVELEAKVEALMDEINFLRAFFEAELAQLQAQISETSVVLSMDNNRSLNLDSIIAEVKAQYE
4h5y.1.A  ---------KDVIAELGAQMALQRNINLQNQQ-----DRMEHELFKRRLMAALFLWYLSKKSH----AAEKVKEIIREYN

Target    DIANRSRAE--------------AESWYQTKYEELQRSAGQRGDDL---RTTKMEISELNRAMQRLRSEIDNLKKQCATL
4h5y.1.A  EKAIKNAEKASKPSQQSTSSTSQADKEIQKMLDEYEQAIKRAQENIKKGEELEKKLDKLERQGKDLEDKYKTYEENLEGF

Target    QASIADAEQRGELALKDAKNKLAELEDALQKAKQDMARQLREYQELMNVKLALDIEIATYRKLLEGEECRLTGEGVGAVN
4h5y.1.A  EKLLTDSEELSLSEINEKMKAFSKDSEKLTQLMEKHKGDEKTVQSLQREHHDIKAKLANLQVLH----------------

Target    ISVVSSSGGTGYSGGGGLCVSGGVYSGGGYSGSGLCYGGGGSGGFSSTSGRSVSGSSSSMRIVSKTSSTKKSYRS
4h5y.1.A  ------------------------------------------------------------------------
```