

# SWISS-MODEL Homology Modelling Report

# **Model Building Report**

This document lists the results for the homology modelling project "TPH2\_GG" submitted to SWISS-MODEL workspace on Oct. 20, 2017, 10:14 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

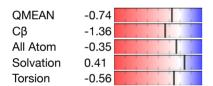
#### Results

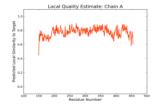
The SWISS-MODEL template library (SMTL version 2017-10-11, PDB release 2017-10-06) was searched with Blast (Altschul et al., 1997) and HHBlits (Remmert, et al., 2011) for evolutionary related structures matching the target sequence in Table T1. For details on the template search, see Materials and Methods. Overall 277 templates were found (Table T2).

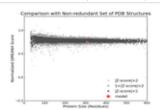
## **Models**

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

Model #02	File	Built with	Oligo-State	Ligands	GMQE	QMEAN
	PDB	ProMod3 Version 1.1.0.	MONOMER	1 x FE: FE (III) ION; 1 x IMD: IMIDAZOLE; 1 x TRP: TRYPTOPHAN;	0.64	-0.74







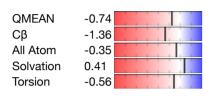
Template	Seq Identity	Oligo- state	Found by	Method	Resolution	Seq Similar		Range	Coverage	Description		
3e2t.1.A	83.71	monomer	BLAST	X-ray	1.90Å	0.57		149 - 455	0.64	Tryptophan 5-hydroxylase 1		
Ligand Added to Model							Description					
FE		✓							FE (III) ION			
IMD		✓							IMIDA	ZOLE		
TRP		✓							TRYPTO	PHAN		
PGE	PGE X - Not biolog			gically rel	evant.	TRIETHYLENE GLYCOL						
PGE		× -	Not biolo	gically rel	evant.		TRIETHYLENE GLYCOL					
SO4	SO4 X - Not bi			gically rel	evant.		SULFATE ION					

Target 3e2t.1.A	MQPAMMMFSSKYWARRGFSLDSALPEERPGGLTINRSSSGKNEDKKGNKGNGKGESVSEGGKTAVVFSLKNEVGGLVKAL
Target 3e2t.1.A	RLFQEKHVSMVHIESRKSKRRNSEVEIFVDCDCSKKEFNELIQLLKFQTNIVSLNPPENIWTDEEDLDCVPWFPRKISEL
Target 3e2t.1.A	DKCSQRVLMYGSELDADHPGFKDNVYRQRRKYFVDVAMSYKYGQPIPRVEYTAEEIKTWGVVFRELSKLYPTHACREYLK DKCANRVLMYGSDLDADHPGFKDNVYRKRRKYFADLAMNYKHGDPIPEIEFTEEEIKTWGTVYRELNKLYPTHACREYLK
Target 3e2t.1.A	${\tt NFPLLTKYCGYREDNVPQLEDVSIFLKERSGFTVRPVAGYLSPRDFLAGLAYRVFHCTQYVRHGSDPLYTPEPDTCHELL}\\ {\tt NLPLLTKYCGYREDNIPQLEDVSRFLKERTGFTIRPVAGYLSPRDFLAGLAFRVFHCTQYVRHSSDPLYTPEPDTCHELL}\\ {\tt NLPLLTKYCGYREDNIPQLAGYLSPRDFLAGLAFRVFHCTQYVRHSSDPLYTPEPDTCHELL}\\ {\tt NLPLLTKYCGYREDNIPQLAGYLSPRDFLAGLAFRVFHCTQYVRHSSDPLYTPEPDTCHELL}\\ {\tt NLPLLTKYCGYREDNIPQLAGYLSPRDFLAGATATATATATATATATATATATATATATATATATATA$
Target 3e2t.1.A	${\tt GHVPLLADPKFAQFSQEIGLASLGASDEDVQKLATCYFFTIEFGLCKQEGQLRAYGAGLLSSIGELKHALSDKAKVKTFD}\\ {\tt GHVPLLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFFTVEFGLCKQEGQLRVYGAGLLSSISELKHSLSGSAKVKPFD}\\ {\tt CHVPLLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFFTVEFGLCKQEGQLRVYGAGLLSSISELKHSLSGSAKVKPFD}\\ {\tt CHVPLLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFFTVEFGLCKQEGQLRVYGAGLLSSISELKHSLSGSAKVKPFD}\\ {\tt CHVPLLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFFTVEFGLCKQEGQLRVYGAGLLSSISELKHSLSGSAKVKPFD}\\ {\tt CHVPLLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFFTVEFGLCKQEGQLRVYGAGLLSSISELKHSLSGSAKVKPFD}\\ {\tt CHVPLLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFFTVEFGLCKQEGQLRVYGAGLLSSISELKHSLSGSAKVKPFD}\\ {\tt CHVPLLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFFTVEFGLCKQEGQLRVYGAGLLSSISELKHSLSGSAKVKPFD}\\ {\tt CHVPLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFFTVEFGLCKQEGQLRVYGAGLLSSISELKHSLSGSAKVKPFD}\\ {\tt CHVPLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFFTVEFGLCKQEGQLRVYGAGLLSSISELKHSLSGSAKVKPFD}\\ {\tt CHVPLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFFTVEFGLCKQEGQLRVYGAGLLSSISELKHSLSGSAKVKPFD}\\ {\tt CHVPLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFFTVEFGLCKQEGQLRVYGAGLLSSISELKHSLSGSAKVKPFD}\\ {\tt CHVPLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFTVEFGLCKQEGQLRVYGAGLLSSISELKHSLSGSAKVKPFD}\\ {\tt CHVPLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFTVEFGLCKQEGQLRVYGAGLASLGASDEAVQKLATCYFTVEFGLCKQEGQLRVYGAGLASLGASDEAVQKLATCYFTVEFGLCKQEGQLRVYGAGLASLGASDEAVQKLATCYFTVEFGLCKQEGQLRVYGAGLASLGASDEAVQKLATCYFTVEFGLCKQEGQLRVYGAGATCYFTVEFGLCKQEGQLRVYGAGATCYFTVEFGLCKQEGQLRVYGAGATCYFTVEFGLCKQEGQLRVYGAGATCYFTVEFGLCKQEGQLRVYGAGATCYFTVEFGLCKQEGQLRVYGAGATCYFTVEFGLCKQEGQLRVYGAGATCYFTVEFGLCKQUATCYFTVEFGLCKQUATCYFTVEFGLCKQUATCYFTVEFGLCKQUATCYFTVEFGLCKQUATCYFTVEFGLCKQUATCYFTVEFGLCKQUATCYFTVATCYFTTVEFGLCKQUATCYFTVATCYFTTVEFGLCKQUATCYFTVATCYFTTTVATCYFTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT$
Target	PKTTCLQECLITTFQEAYFVSESFEEAKEKMRDFAKSINRPFSVYFNPYTQSIEILKDTRSIENVVQDLRSDLNTVCDAL

# 3e2t.1.A PKVTCKQECLITTFQEVYFVSESFEEAKEKMREFAKTIKRPFGVKYNPYTQSVQILKD------

Target SKMNRYLGI 3e2t.1.A

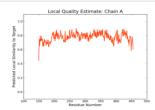
Model #04	File	Built with	Oligo-State	Ligands	GMQE	QMEAN
	PDB	ProMod3 Version 1.1.0.	MONOMER	1 x FE: FE (III) ION; 1 x IMD: IMIDAZOLE; 1 x TRP: TRYPTOPHAN;	0.64	-0.74

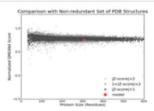


Seq

Oligo-

**Found** 





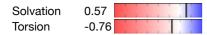
Template	Seq Identit	Oligo- y state	Found by	Method	Resolution	Seq Similar	ity	Range Coverage Desc	
3e2t.1.A	83.71	monomer	BLAST	X-ray	1.90Å	0.57	149 - 455	0.64	
Ligand Added to Model						Description			
FE				✓		FE (III) ION			
IMD		✓						IMIDA	ZOLE
TRP	TRP ✓						TRYPTO	PHAN	
PGE		×-	X - Not biologically relevant.  TRIETHYLENE GLYCOL						NE GLYCOL
PGE		×-	Not biolo	gically rel	evant.	TRIETHYLENE GLYCOL			
SO4	SO4 X - Not biologically relevant. SULFATE ION				SULFATE ION				

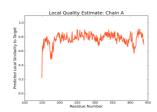
Seq

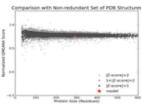
Target 3e2t.1.A	MQPAMMMFSSKYWARRGFSLDSALPEERPGGLTINRSSSGKNEDKKGNKGNGKGESVSEGGKTAVVFSLKNEVGGLVKAL
Target 3e2t.1.A	RLFQEKHVSMVHIESRKSKRRNSEVEIFVDCDCSKKEFNELIQLLKFQTNIVSLNPPENIWTDEEDLDCVPWFPRKISEL
Target	DKCSQRVLMYGSELDADHPGFKDNVYRQRRKYFVDVAMSYKYGQPIPRVEYTAEEIKTWGVVFRELSKLYPTHACREYLK
3e2t.1.A	DKCANRVLMYGSDLDADHPGFKDNVYRKRRKYFADLAMNYKHGDPIPEIEFTEEEIKTWGTVYRELNKLYPTHACREYLK
Target 3e2t.1.A	NFPLLTKYCGYREDNVPQLEDVSIFLKERSGFTVRPVAGYLSPRDFLAGLAYRVFHCTQYVRHGSDPLYTPEPDTCHELL NLPLLTKYCGYREDNIPQLEDVSRFLKERTGFTIRPVAGYLSPRDFLAGLAFRVFHCTQYVRHSSDPLYTPEPDTCHELL
Target	GHVPLLADPKFAQFSQEIGLASLGASDEDVQKLATCYFFTIEFGLCKQEGQLRAYGAGLLSSIGELKHALSDKAKVKTFD
3e2t.1.A	GHVPLLAEPSFAQFSQEIGLASLGASDEAVQKLATCYFFTVEFGLCKQEGQLRVYGAGLLSSISELKHSLSGSAKVKPFD
Target	PKTTCLQECLITTFQEAYFVSESFEEAKEKMRDFAKSINRPFSVYFNPYTQSIEILKDTRSIENVVQDLRSDLNTVCDAL
3e2t.1.A	PKVTCKQECLITTFQEVYFVSESFEEAKEKMREFAKTIKRPFGVKYNPYTQSVQILKD
Target	SKMNRYLGI
3e2t.1.A	

Model #03	File	Built with	Oligo- State	GMQE	QMEAN	
	PDB	ProMod3 Version 1.1.0.	MONOMER	1 x 6Z4: (3~{S})-8-[2-azanyl-6-[(1~{R}))-1-(4- chloranyl-2-phenyl-phenyl)-2,2,2- tris(fluoranyl)ethoxy]pyrimidin-4-yl]-2,8- diazaspiro[4.5]decane-3-carboxylic acid; 1 x FE: FE (III) ION;	0.59	-0.82

QMEAN	-0.82
Сβ	-0.92
All Atom	-0.48







Template	Seq Identity	Oligo- state	Found by	Method	Resolution	Seq Similarity	Range	Coverage	Description
5l01.1.A	73.33	monomer	HHblits	X-ray	1.90Å	0.53	149 - 439	0.89	Tryptophan 5-hydroxylase 1

Ligand	Added to Model	Description
6Z4	✓	(3~{S})-8-[2-azanyl-6-[(1~{R})-1-(4-chloranyl-2-phenyl-phenyl)-2,2,2-tris(fluoranyl)ethoxy]pyrimidin-4-yl]-2,8-diazaspiro[4.5]decane-3-carboxylic acid
FE	✓	FE (III) ION

Target MQPAMMMFSSKYWARRGFSLDSALPEERPGGLTINRSSSGKNEDKKGNKGNGKGESVSEGGKTAVVFSLKNEVGGLVKAL 5101.1.A -------KDHSLERGRASLIFSLKNEVGGLIKAL

Target RLFQEKHVSMVHIESRKSKRRNSEVEIFVDCDCSKKEFNELIQLLKFQTNIVSLNPPENIWTDEEDLDCVPWFPRKISEL 5101.1.A KIFQEKHVNLLHIESRKSKRRNSEFEIFVDCDINREQLNDIFHLLKSHTNVLSVNLPDNFTLKEDGMETVPWFPKKISDL

Target DKCSQRVLMYGSELDADHPGFKDNVYRQRRKYFVDVAMSYKYGQPIPRVEYTAEEIKTWGVVFRELSKLYPTHACREYLK 5101.1.A DHCANRVLMYGSELDADHPGFKDNVYRKRRKYFADLAMNYKHGDPIPKVEFTEEEIKTWGTVFQELNKLYPTHACREYLK

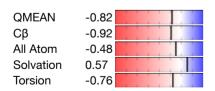
Target NFPLLTKYCGYREDNVPQLEDVSIFLKERSGFTVRPVAGYLSPRDFLAGLAYRVFHCTQYVRHGSDPLYTPEPDTCHELL 5101.1.A NLPLLSKYCGYREDNIPQLEDVSNFLKERTGFSIRPVAGYLSPRDFLSGLAFRVFHCTQYVRHSSDPFYTPEPDTCHELL

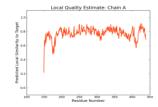
Target GHVPLLADPKFAQFSQEIGLASLGASDEDVQKLATCYFFTIEFGLCKQEGQLRAYGAGLLSSIGELKHALSDKAKVKTFD 5101.1.A GHVPLLAEPSFAQFSQEIGLASLGASEEAVQKLATCYFFTVEFGLCKQDGQLRVFGAGLLSSISELKHALSGHAKVKPFD

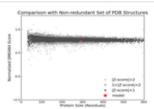
Target PKTTCLQECLITTFQEAYFVSESFEEAKEKMRDFAKSINRPFSVYFNPYTQSIEILKDTRSIENVVQDLRSDLNTVCDAL 5101.1.A PKITCKQECLITTFQDVYFVSESFEDAKEKMREFTKTIKRPFGVKYNPYTRSIQILKDTKSITSAMNELQHDLDVVSDAL

Target SKMNRYLGI 5101.1.A AKVSRKPS-

Model #01	File	Built with	Oligo- State	ligands				
	PDB	ProMod3 Version 1.1.0.	MONOMER	1 x 6Z4: (3~{S})-8-[2-azanyl-6-[(1~{R})-1-(4- chloranyl-2-phenyl-phenyl)-2,2,2- tris(fluoranyl)ethoxy]pyrimidin-4-yl]-2,8- diazaspiro[4.5]decane-3-carboxylic acid; 1 x FE: FE (III) ION;	0.59	-0.82		







Template	Seq Identity	Oligo- state	Found by	Method	Resolution	Seq Similarity	Range	Coverage	Description
5l01.1.A	73.33	monomer	HHblits	X-ray	1.90Å	0.53	149 - 439	0.89	Tryptophan 5-hydroxylase 1

Ligand	Added to Model	Description
6Z4	✓	$(3~\{S\})-8-[2-azanyl-6-[(1~\{R\})-1-(4-chloranyl-2-phenyl-phenyl)-2,2,2-tris(fluoranyl)ethoxy]pyrimidin-4-yl]-2,8-diazaspiro[4.5]decane-3-carboxylic acid$
FE	✓	FE (III) ION
Ligand	Added to	Description

Model

Target 5101.1.A	MQPAMMMFSSKYWARRGFSLDSALPEERPGGLTINRSSSGKNEDKKGNKGNGKGESVSEGGKTAVVFSLKNEVGGLVKAL
Target	RLFQEKHVSMVHIESRKSKRRNSEVEIFVDCDCSKKEFNELIQLLKFQTNIVSLNPPENIWTDEEDLDCVPWFPRKISEL
5101.1.A	KIFQEKHVNLLHIESRKSKRRNSEFEIFVDCDINREQLNDIFHLLKSHTNVLSVNLPDNFTLKEDGMETVPWFPKKISDL
Target	DKCSQRVLMYGSELDADHPGFKDNVYRQRRKYFVDVAMSYKYGQPIPRVEYTAEEIKTWGVVFRELSKLYPTHACREYLK
5101.1.A	DHCANRVLMYGSELDADHPGFKDNVYRKRRKYFADLAMNYKHGDPIPKVEFTEEEIKTWGTVFQELNKLYPTHACREYLK
Target 5101.1.A	${\tt NFPLLTKYCGYREDNVPQLEDVSIFLKERSGFTVRPVAGYLSPRDFLAGLAYRVFHCTQYVRHGSDPLYTPEPDTCHELL}\\ {\tt NLPLLSKYCGYREDNIPQLEDVSNFLKERTGFSIRPVAGYLSPRDFLSGLAFRVFHCTQYVRHSSDPFYTPEPDTCHELL}\\ {\tt NLPLLSKYCGYREDNIPQLSGLAFRVFHCTQYVRHSSDPFYTPEPDTCHELL}\\ {\tt NLPLLSKYCGYREDNIPQLSGLAFRVFHCTQYVRHSSDPFYTPEPDTCHELL}\\ {\tt NLPLLSKYCGYREDNIPQLSGLAFRVFHCTQYVRHSSDPFYTPEPDTCHELL}\\ {\tt NLPLLSKYCGYREDNIPQLSGLAFRVFHCTQYVRHSSDPFYTPEPDTCHELL}\\ {\tt NLPLLSKYCGYREDNIPQLSGLAFRVFHCTQYVRHSSDPFYTPEPDTCHELL}\\ {\tt NLPLLSKYCGYREDNIPQLSGLAFRVFHCTQYVRHSSDPFYTPEPDTCHELL}\\ {\tt NLPLLSKYCGYREDNIPQLSGLAFTYPTPTPTPTPTPTPTPTPTPTPTPTPTPTPTPTPTPTP$
Target 5101.1.A	$ \texttt{GHVPLLADPKFAQFSQEIGLASLGASDEDVQKLATCYFFTIEFGLCKQEGQLRAYGAGLLSSIGELKHALSDKAKVKTFD} \\ \texttt{GHVPLLAEPSFAQFSQEIGLASLGASEEAVQKLATCYFFTVEFGLCKQDGQLRVFGAGLLSSISELKHALSGHAKVKPFD} \\ $
Target	PKTTCLQECLITTFQEAYFVSESFEEAKEKMRDFAKSINRPFSVYFNPYTQSIEILKDTRSIENVVQDLRSDLNTVCDAL
5101.1.A	PKITCKQECLITTFQDVYFVSESFEDAKEKMREFTKTIKRPFGVKYNPYTRSIQILKDTKSITSAMNELQHDLDVVSDAL
Target	SKMNRYLGI
5101.1.A	AKVSRKPS-

#### Materials and Methods

#### **Template Search**

Template search with Blast and HHBlits has been performed against the SWISS-MODEL template library (SMTL, last update: 2017-10-11, last included PDB release: 2017-10-06).

The target sequence was searched with BLAST (Altschul et al., 1997) against the primary amino acid sequence contained in the SMTL. A total of 49 templates were found.

An initial HHblits profile has been built using the procedure outlined in (Remmert, et al., 2011), followed by 1 iteration of HHblits against NR20. The obtained profile has then be searched against all profiles of the SMTL. A total of 232 templates were found.

#### **Template Selection**

For each identified template, the template's quality has been predicted from features of the target-template alignment. The templates with the highest quality have then been selected for model building.

#### **Model Building**

Models are built based on the target-template alignment using ProMod3. Coordinates which are conserved between the target and the template are copied from the template to the model. Insertions and deletions are remodelled using a fragment library. Side chains are then rebuilt. Finally, the geometry of the resulting model is regularized by using a force field. In case loop modelling with ProMod3 fails, an alternative model is built with PROMOD-II (Guex, et al., 1997).

## **Model Quality Estimation**

The global and per-residue model quality has been assessed using the QMEAN scoring function (Benkert, et al., 2011). For improved performance, weights of the individual QMEAN terms have been trained specifically for SWISS-MODEL.

#### Ligand Modelling

Ligands present in the template structure are transferred by homology to the model when the following criteria are met (Gallo - Casserino, to be published): (a) The ligands are annotated as biologically relevant in the template library, (b) the ligand is in contact with the model, (c) the ligand is not clashing with the protein, (d) the residues in contact with the ligand are conserved between the target and the template. If any of these four criteria is not satisfied, a certain ligand will not be included in the model. The model summary includes information on why and which ligand has not been included.

# **Oligomeric State Conservation**

Homo-oligomeric structure of the target protein is predicted based on the analysis of pairwise interfaces of the identified template structures. For each relevant interface between polypeptide chains (interfaces with more than 10 residue-residue interactions), the QscoreOligomer (Mariani et al., 2011) is predicted from features such as similarity to target and frequency of observing this interface in the identified templates (Kiefer, Bertoni, Biasini, to be published). The prediction is performed with a random forest regressor using these features as input parameters to predict the probability of conservation for each interface. The QscoreOligomer of the whole complex is then calculated as the weight-averaged QscoreOligomer of the interfaces. The oligomeric state of the target is predicted to be the same as in the template when QscoreOligomer is predicted to be higher or equal to 0.5.

#### References

Altschul, S.F., Madden, T.L., Schaffer, A.A., Zhang, J., Zhang, Z., Miller, W. and Lipman, D.J. (1997) Gapped BLAST and PSI-BLAST: a new generation of protein database search programs. Nucleic Acids Res, 25, 3389-3402.

Remmert, M., Biegert, A., Hauser, A. and Soding, J. (2012) HHblits: lightning-fast iterative protein sequence searching by HMM-HMM alignment. Nat Methods, 9, 173-175.

Guex, N. and Peitsch, M.C. (1997) SWISS-MODEL and the Swiss-PdbViewer: an environment for comparative protein modeling. Electrophoresis, 18, 2714-2723.

Sali, A. and Blundell, T.L. (1993) Comparative protein modelling by satisfaction of spatial restraints. J Mol Biol, 234, 779-815. Benkert, P., Biasini, M. and Schwede, T. (2011) Toward the estimation of the absolute quality of individual protein structure models. Bioinformatics, 27, 343-350.

Mariani, V., Kiefer, F., Schmidt, T., Haas, J. and Schwede, T. (2011) Assessment of template based protein structure predictions in CASP9. Proteins, 79 Suppl 10, 37-58.

#### Table T1:

Primary amino acid sequence for which templates were searched and models were built.

 $\label{thm:permodes} $$ MQPAMMMFSSKYWARRGFSLDSALPEERPGGLTINRSSSGKNEDKKGNKGNGKGESVSEGGKTAVVFSLKNEVGGLVKALRLFQEKHVSMVHIESRKSKR RNSEVEIFVDCDCSKKEFNELIQLLKFQTNIVSLNPPENIWTDEEDLDCVPWFPRKISELDKCSQRVLMYGSELDADHPGFKDNVYRQRRKYFVDVAMSY KYGQPIPRVEYTAEEIKTWGVVFRELSKLYPTHACREYLKNFPLLTKYCGYREDNVPQLEDVSIFLKERSGFTVRPVAGYLSPRDFLAGLAYRVFHCTQY VRHGSDPLYTPEPDTCHELLGHVPLLADPKFAQFSQEIGLASLGASDEDVQKLATCYFFTIEFGLCKQEGQLRAYGAGLLSSIGELKHALSDKAKVKTFD PKTTCLOECLITTFOEAYFVSESFEEAKEKMRDFAKSINRPFSVYFNPYTOSIEILKDTRSIENVVODLRSDLNTVCDALSKMNRYLGI$ 

## Table T2:

Template	Seq Identity	Oligo- state	Found by	Method	Resolution	Seq Similarity	Coverage	Description
5l01.1.A	73.33	monomer	HHblits	X-ray	1.90Å	0.53	0.89	Tryptophan 5-hydroxylase 1
5l01.1.A	74.71	monomer	BLAST	X-ray	1.90Å	0.54	0.87	Tryptophan 5-hydroxylase 1
5den.1.B	53.79	homo- tetramer	HHblits	X-ray	2.90Å	0.45	0.92	Phenylalanine-4-hydroxylase
5den.1.A	53.79	homo- tetramer	HHblits	X-ray	2.90Å	0.45	0.92	Phenylalanine-4-hydroxylase
5fgj.1.A	53.79	homo- tetramer	HHblits	X-ray	3.60Å	0.45	0.92	Phenylalanine-4-hydroxylase
5fgj.1.B	53.79	homo- tetramer	HHblits	X-ray	3.60Å	0.45	0.92	Phenylalanine-4-hydroxylase
5egq.1.A	53.57	homo- tetramer	HHblits	X-ray	2.50Å	0.45	0.92	Phenylalanine-4-hydroxylase
5egq.1.B	53.57	homo- tetramer	HHblits	X-ray	2.50Å	0.45	0.92	Phenylalanine-4-hydroxylase
5egq.1.C	53.57	homo- tetramer	HHblits	X-ray	2.50Å	0.45	0.92	Phenylalanine-4-hydroxylase
5egq.1.D	53.57	homo- tetramer	HHblits	X-ray	2.50Å	0.45	0.92	Phenylalanine-4-hydroxylase
5den.1.B	57.01	homo- tetramer	BLAST	X-ray	2.90Å	0.47	0.86	Phenylalanine-4-hydroxylase
5den.1.A	57.01	homo- tetramer	BLAST	X-ray	2.90Å	0.47	0.86	Phenylalanine-4-hydroxylase
5fgj.1.A	57.01	homo- tetramer	BLAST	X-ray	3.60Å	0.47	0.86	Phenylalanine-4-hydroxylase
5fgj.1.B	57.01	homo- tetramer	BLAST	X-ray	3.60Å	0.47	0.86	Phenylalanine-4-hydroxylase
5egq.1.A	56.77	homo- tetramer	BLAST	X-ray	2.50Å	0.47	0.86	Phenylalanine-4-hydroxylase
5egq.1.B	56.77	homo- tetramer	BLAST	X-ray	2.50Å	0.47	0.86	Phenylalanine-4-hydroxylase
5egq.1.C	56.77	homo- tetramer	BLAST	X-ray	2.50Å	0.47	0.86	Phenylalanine-4-hydroxylase
5egq.1.D	56.77	homo- tetramer	BLAST	X-ray	2.50Å	0.47	0.86	Phenylalanine-4-hydroxylase
2phm.1.A	55.53	homo- dimer	HHblits	X-ray	2.60Å	0.46	0.87	PROTEIN (PHENYLALANINE-4- HYDROXYLASE)
4v06.1.A	96.21	monomer	BLAST	X-ray	2.63Å	0.60	0.70	TRYPTOPHAN 5-HYDROXYLASE 2
4v06.1.A	96.19	monomer	HHblits	X-ray	2.63Å	0.60	0.70	TRYPTOPHAN 5-HYDROXYLASE 2
2phm.1.A	59.05	homo- dimer	BLAST	X-ray	2.60Å	0.47	0.81	PROTEIN (PHENYLALANINE-4- HYDROXYLASE)
5jk5.1.B	53.67	homo- dimer	HHblits	X-ray	2.07Å	0.46	0.81	Phenylalanine-4-hydroxylase

Template	Seq Identity	Oligo- state	Found by	Method	Resolution	Seq Similarity	Coverage	Description
5jk5.1.A	53.67	homo- dimer	HHblits	X-ray	2.07Å	0.46	0.81	Phenylalanine-4-hydroxylase
5jk8.1.A	53.67	homo- dimer	HHblits	X-ray	2.39Å	0.46	0.81	Phenylalanine-4-hydroxylase
5jk5.1.B	53.44	homo- dimer	BLAST	X-ray	2.07Å	0.46	0.80	Phenylalanine-4-hydroxylase
5jk5.1.A	53.44	homo- dimer	BLAST	X-ray	2.07Å	0.46	0.80	Phenylalanine-4-hydroxylase
5jk8.1.A	53.44	homo- dimer	BLAST	X-ray	2.39Å	0.46	0.80	Phenylalanine-4-hydroxylase
3e2t.1.A	83.71	monomer	BLAST	X-ray	1.90Å	0.57	0.64	Tryptophan 5-hydroxylase 1
3e2t.1.A	83.65	monomer	HHblits	X-ray	1.90Å	0.57	0.64	Tryptophan 5-hydroxylase 1
1toh.1.A	61.72	homo- tetramer	HHblits	X-ray	2.30Å	0.49	0.69	TYROSINE HYDROXYLASE
2toh.1.A	61.42	homo- tetramer	HHblits	X-ray	2.30Å	0.49	0.69	TYROSINE 3-MONOOXYGENASE
2pah.1.A	62.39	homo- tetramer	HHblits	X-ray	3.10Å	0.49	0.69	PROTEIN (PHENYLALANINE HYDROXYLASE)
2pah.1.B	62.39	homo- tetramer	HHblits	X-ray	3.10Å	0.49	0.69	PROTEIN (PHENYLALANINE HYDROXYLASE)
2pah.1.A	62.57	homo- tetramer	BLAST	X-ray	3.10Å	0.49	0.68	PROTEIN (PHENYLALANINE HYDROXYLASE)
2pah.1.B	62.57	homo- tetramer	BLAST	X-ray	3.10Å	0.49	0.68	PROTEIN (PHENYLALANINE HYDROXYLASE)
2xsn.1.A	60.00	homo- tetramer	HHblits	X-ray	2.68Å	0.48	0.69	TYROSINE 3-MONOOXYGENASE
1mlw.1.A	82.06	monomer	BLAST	X-ray	1.71Å	0.57	0.62	Tryptophan 5-monooxygenase
5j6d.1.A	81.73	monomer	BLAST	X-ray	1.90Å	0.57	0.62	Tryptophan 5-hydroxylase 1
1mlw.1.A	82.33	monomer	HHblits	X-ray	1.71Å	0.57	0.61	Tryptophan 5-monooxygenase
5j6d.1.A	82.00	monomer	HHblits	X-ray	1.90Å	0.57	0.61	Tryptophan 5-hydroxylase 1
5tpg.1.A	82.27	monomer		X-ray	1.50Å	0.57	0.61	Tryptophan 5-hydroxylase 1
5tpg.1.A	82.55	monomer	BLAST	X-ray	1.50Å	0.57	0.61	Tryptophan 5-hydroxylase 1
1mmk.1.A	63.58	homo- dimer	HHblits	X-ray	2.00Å	0.49	0.66	Phenylalanine-4-hydroxylase
1lrm.1.A	63.58	homo- dimer	HHblits	X-ray	2.10Å	0.49	0.66	Phenylalanine-4-hydroxylase
4anp.1.A	63.78	monomer	HHblits	X-ray	2.11Å	0.49	0.66	PHENYLALANINE-4-HYDROXYLASE
3hfb.1.A	83.45	monomer	HHblits	X-ray	1.92Å	0.57	0.59	Tryptophan 5-hydroxylase 1
3hfb.1.A	83.74	monomer	BLAST	X-ray	1.92Å	0.57	0.59	Tryptophan 5-hydroxylase 1
1mmk.1.A	65.71	homo- dimer	BLAST	X-ray	2.00Å	0.50	0.64	Phenylalanine-4-hydroxylase
1lrm.1.A	65.71	homo- dimer	BLAST	X-ray	2.10Å	0.50	0.64	Phenylalanine-4-hydroxylase
4anp.1.A	65.71	monomer	BLAST	X-ray	2.11Å	0.50	0.64	PHENYLALANINE-4-HYDROXYLASE
1pah.1.A	65.91	monomer	HHblits	X-ray	2.00Å	0.50	0.63	PHENYLALANINE HYDROXYLASE
1tdw.1.A	65.58	monomer		X-ray	2.10Å	0.50	0.63	Phenylalanine-4-hydroxylase
1dmw.1.A		monomer		X-ray	2.00Å	0.50	0.63	PHENYLALANINE HYDROXYLASE
1pah.1.A	66.12	monomer		X-ray	2.00Å	0.50	0.63	PHENYLALANINE HYDROXYLASE
1tdw.1.A	65.80	monomer		X-ray	2.10Å	0.50	0.63	Phenylalanine-4-hydroxylase
4q3w.1.A	30.83	monomer		X-ray	1.40Å	0.34	0.52	Phenylalanine-4-hydroxylase
4etl.1.A	30.43	monomer		X-ray	1.49Å	0.34	0.52	Phenylalanine-4-hydroxylase
3tcy.1.A	30.43	monomer		X-ray	1.55Å	0.34	0.52	Phenylalanine-4-hydroxylase
3tk2.1.A	30.04	monomer		X-ray	1.35Å	0.34	0.52	Phenylalanine-4-hydroxylase
1ltu.1.A	30.43	monomer		X-ray	1.74Å	0.34	0.52	PHENYLALANINE-4-HYDROXYLASE
4jpy.1.A	30.43	monomer		X-ray	2.13Å	0.34	0.52	Phenylalanine-4-hydroxylase
4q3z.1.A	30.43	monomer		X-ray	1.35Å	0.34	0.52	Phenylalanine-4-hydroxylase
4q3x.1.A	30.43	monomer		X-ray	1.35Å	0.34	0.52	Phenylalanine-4-hydroxylase
4q3y.1.A	30.43	monomer	HHblits	X-ray	1.40Å	0.34	0.52	Phenylalanine-4-hydroxylase

Template	Seq Identity	Oligo- state	Found by	Method	Resolution	Seq Similarity	Coverage	Description
4jpx.1.A	30.04	monomer	HHblits	X-ray	1.55Å	0.34	0.52	Phenylalanine-4-hydroxylase
4esm.1.A	30.43	monomer	HHblits	X-ray	1.35Å	0.34	0.52	Phenylalanine-4-hydroxylase
4bpt.1.A	35.15	monomer	HHblits	X-ray	2.50Å	0.37	0.49	PHENYLALANINE-4-HYDROXYLASE (PAH) (PHE-4-MONOOXYGENASE)
4bpt.1.A	35.96	monomer	BLAST	X-ray	2.50Å	0.38	0.47	PHENYLALANINE-4-HYDROXYLASE (PAH) (PHE-4-MONOOXYGENASE)
2v28.1.A	31.03	homo- dimer	HHblits	X-ray	1.95Å	0.35	0.47	PHENYLALANINE-4-HYDROXYLASE
2v28.1.B	31.03	homo- dimer	HHblits	X-ray	1.95Å	0.35	0.47	PHENYLALANINE-4-HYDROXYLASE
2v27.1.A	31.03	homo- dimer	HHblits	X-ray	1.50Å	0.35	0.47	PHENYLALANINE HYDROXYLASE
2v27.1.B	31.03	homo- dimer	HHblits	X-ray	1.50Å	0.35	0.47	PHENYLALANINE HYDROXYLASE
4q3w.1.A	36.36	monomer	BLAST	X-ray	1.40Å	0.37	0.45	Phenylalanine-4-hydroxylase
1ltu.1.A	35.91	monomer	BLAST	X-ray	1.74Å	0.37	0.45	PHENYLALANINE-4-HYDROXYLASE
4jpy.1.A	35.91	monomer	BLAST	X-ray	2.13Å	0.37	0.45	Phenylalanine-4-hydroxylase
3tcy.1.A	35.91	monomer	BLAST	X-ray	1.55Å	0.37	0.45	Phenylalanine-4-hydroxylase
4etl.1.A	35.91	monomer	BLAST	X-ray	1.49Å	0.37	0.45	Phenylalanine-4-hydroxylase
3tk2.1.A	35.45	monomer	BLAST	X-ray	1.35Å	0.37	0.45	Phenylalanine-4-hydroxylase
4q3z.1.A	35.91	monomer	BLAST	X-ray	1.35Å	0.37	0.45	Phenylalanine-4-hydroxylase
4q3x.1.A	35.91	monomer	BLAST	X-ray	1.35Å	0.37	0.45	Phenylalanine-4-hydroxylase
4q3y.1.A	35.91	monomer	BLAST	X-ray	1.40Å	0.37	0.45	Phenylalanine-4-hydroxylase
4jpx.1.A	35.45	monomer	BLAST	X-ray	1.55Å	0.37	0.45	Phenylalanine-4-hydroxylase
4esm.1.A	35.91	monomer	BLAST	X-ray	1.35Å	0.37	0.45	Phenylalanine-4-hydroxylase
2v28.1.A	34.72	homo- dimer	BLAST	X-ray	1.95Å	0.37	0.39	PHENYLALANINE-4-HYDROXYLASE
2v28.1.B	34.72	homo- dimer	BLAST	X-ray	1.95Å	0.37	0.39	PHENYLALANINE-4-HYDROXYLASE
2v27.1.A	34.72	homo- dimer	BLAST	X-ray	1.50Å	0.37	0.39	PHENYLALANINE HYDROXYLASE
2v27.1.B	34.72	homo- dimer	BLAST	X-ray	1.50Å	0.37	0.39	PHENYLALANINE HYDROXYLASE
3tvi.1.A	21.62	homo- dimer	HHblits	X-ray	3.00Å	0.30	0.23	Aspartokinase
3tvi.1.B	21.62	homo- dimer	HHblits	X-ray	3.00Å	0.30	0.23	Aspartokinase
3tvi.2.A	21.62	homo- dimer	HHblits	X-ray	3.00Å	0.30	0.23	Aspartokinase
3tvi.2.B	21.62	homo- dimer	HHblits	X-ray	3.00Å	0.30	0.23	Aspartokinase
3tvi.3.A	21.62	homo- dimer	HHblits	X-ray	3.00Å	0.30	0.23	Aspartokinase
3tvi.3.B	21.62	homo- dimer	HHblits	X-ray	3.00Å	0.30	0.23	Aspartokinase
3tvi.4.B	21.62	homo- dimer	HHblits	X-ray	3.00Å	0.30	0.23	Aspartokinase
3tvi.5.A	21.62	homo- dimer	HHblits	X-ray	3.00Å	0.30	0.23	Aspartokinase
3tvi.5.B	21.62	homo- dimer	HHblits	X-ray	3.00Å	0.30	0.23	Aspartokinase
3tvi.6.A	21.62	homo- dimer	HHblits	X-ray	3.00Å	0.30	0.23	Aspartokinase
3tvi.6.B	21.62	homo- dimer homo-	HHblits	X-ray	3.00Å	0.30	0.23	Aspartokinase
3mwb.1.A		tetramer	HHblits	X-ray	2.00Å	0.28	0.23	Prephenate dehydratase
3mwb.1.B	17.86	tetramer	HHblits	X-ray	2.00Å	0.28	0.23	Prephenate dehydratase

Template	Seq Identity	Oligo- state	Found by	Method	Resolution	Seq Similarity	Coverage	Description
3luy.1.A	15.96	homo- dimer	HHblits	X-ray	2.00Å	0.28	0.19	Probable chorismate mutase
5fii.1.B	37.33	homo- dimer	HHblits	X-ray	1.80Å	0.39	0.15	PHENYLALANINE-4-HYDROXYLASE
5fii.1.A	37.33	homo- dimer	HHblits	X-ray	1.80Å	0.39	0.15	PHENYLALANINE-4-HYDROXYLASE
5fii.2.B	37.33	homo- dimer	HHblits	X-ray	1.80Å	0.39	0.15	PHENYLALANINE-4-HYDROXYLASE
2qmx.1.A	26.92	homo- dimer	HHblits	X-ray	2.30Å	0.33	0.16	Prephenate dehydratase
2qmx.1.B	26.92	homo- dimer	HHblits	X-ray	2.30Å	0.33	0.16	Prephenate dehydratase
2mda.1.A	19.23	homo- dimer	HHblits	NMR	NA	0.31	0.16	Tyrosine 3-monooxygenase
5fii.1.B	43.28	homo- dimer	BLAST	X-ray	1.80Å	0.41	0.14	PHENYLALANINE-4-HYDROXYLASE
5fii.1.A	43.28	homo- dimer	BLAST	X-ray	1.80Å	0.41	0.14	PHENYLALANINE-4-HYDROXYLASE
5fii.2.B	43.28	homo- dimer	BLAST	X-ray	1.80Å	0.41	0.14	PHENYLALANINE-4-HYDROXYLASE
4lub.1.A	23.68	homo- dimer	HHblits	X-ray	2.10Å	0.30	0.16	Putative prephenate dehydratase
4lub.1.B	23.68	homo- dimer	HHblits	X-ray	2.10Å	0.30	0.16	Putative prephenate dehydratase
2qmw.1.A	20.00	homo- tetramer	HHblits	X-ray	2.30Å	0.30	0.15	Prephenate dehydratase
2qmw.1.B	20.00	homo- tetramer	HHblits	X-ray	2.30Å	0.30	0.15	Prephenate dehydratase
1tdj.1.A	20.55	homo- dimer	HHblits	X-ray	2.80Å	0.29	0.15	BIOSYNTHETIC THREONINE DEAMINASE
2fgc.1.A	13.70	homo- dimer	HHblits	X-ray	2.30Å	0.28	0.15	acetolactate synthase, small subunit
2lvw.1.A	9.59	homo- dimer	HHblits	NMR	NA	0.27	0.15	Acetolactate synthase isozyme 1 small subunit
5kps.1.A	11.11	hetero- oligomer	HHblits	EM	NA	0.28	0.15	GTP pyrophosphokinase
5kpv.1.w	11.11	hetero- oligomer	HHblits	EM	NA	0.28	0.15	GTP pyrophosphokinase
5kpw.1.w	11.11	hetero- oligomer	HHblits	EM	NA	0.28	0.15	GTP pyrophosphokinase
5kpx.1.w	11.11	hetero- oligomer	HHblits	EM	NA	0.28	0.15	GTP pyrophosphokinase
5iqr.1.w	9.72	hetero- oligomer	HHblits	EM	3.00Å	0.28	0.15	GTP pyrophosphokinase
2pc6.1.A	12.50	homo- dimer	HHblits	X-ray	2.50Å	0.28	0.15	Probable acetolactate synthase isozyme III (Small subunit)
2pc6.1.B	12.50	homo- dimer	HHblits	X-ray	2.50Å	0.28	0.15	Probable acetolactate synthase isozyme III (Small subunit)
2pc6.2.B	12.50	homo- dimer	HHblits	X-ray	2.50Å	0.28	0.15	Probable acetolactate synthase isozyme III (Small subunit)
5l3p.1.t	11.27	hetero- oligomer	HHblits	EM	NA	0.28	0.15	GTP pyrophosphokinase,GTP pyrophosphokinase
2f1f.1.A	12.86	homo- dimer	HHblits	X-ray	1.75Å	0.28	0.14	Acetolactate synthase isozyme III small subunit
2f1f.1.B	12.86	homo- dimer	HHblits	X-ray	1.75Å	0.28	0.14	Acetolactate synthase isozyme III small subunit
1y7p.2.A	13.24	homo- dimer	HHblits	X-ray	1.90Å	0.29	0.14	Hypothetical protein AF1403
1y7p.1.B	13.24	homo- dimer	HHblits	X-ray	1.90Å	0.29	0.14	Hypothetical protein AF1403
1y7p.1.A	13.24	homo- dimer	HHblits	X-ray	1.90Å	0.29	0.14	Hypothetical protein AF1403

Template	Seq Identity	Oligo- state	Found by	Method	Resolution	Seq Similarity	Coverage	Description
5it4.1.A	8.45	homo- dimer	HHblits	X-ray	2.10Å	0.24	0.15	Phosphoserine phosphatase
5t41.1.A	8.57	monomer	HHblits	X-ray	3.15Å	0.24	0.14	Phosphoserine phosphatase
5uyy.1.B	7.35	homo- dimer	HHblits	X-ray	2.60Å	0.26	0.14	Prephenate dehydrogenase
5uyy.1.A	7.35	homo- dimer	HHblits	X-ray	2.60Å	0.26	0.14	Prephenate dehydrogenase
5uyy.2.A	7.35	homo- dimer	HHblits	X-ray	2.60Å	0.26	0.14	Prephenate dehydrogenase
1sc6.1.A	13.85	homo- tetramer	HHblits	X-ray	2.09Å	0.28	0.13	D-3-phosphoglycerate dehydrogenase
1sc6.1.B	13.85	homo- tetramer	HHblits	X-ray	2.09Å	0.28	0.13	D-3-phosphoglycerate dehydrogenase
1sc6.1.C	13.85	homo- tetramer	HHblits	X-ray	2.09Å	0.28	0.13	D-3-phosphoglycerate dehydrogenase
1sc6.1.D	13.85	homo- tetramer	HHblits	X-ray	2.09Å	0.28	0.13	D-3-phosphoglycerate dehydrogenase
2p9g.1.A	14.06	homo- tetramer	HHblits	X-ray	2.80Å	0.29	0.13	D-3-phosphoglycerate dehydrogenase
2p9g.1.B	14.06	homo- tetramer	HHblits	X-ray	2.80Å	0.29	0.13	D-3-phosphoglycerate dehydrogenase
1psd.1.A	14.06	homo- tetramer	HHblits	X-ray	2.75Å	0.28	0.13	D-3-PHOSPHOGLYCERATE DEHYDROGENASE (PHOSPHOGLYCERATE DEHYDROGENASE)
1psd.1.B	14.06	homo- tetramer	HHblits	X-ray	2.75Å	0.28	0.13	D-3-PHOSPHOGLYCERATE DEHYDROGENASE (PHOSPHOGLYCERATE DEHYDROGENASE)
2f06.1.A	22.58	homo- tetramer	HHblits	X-ray	2.10Å	0.31	0.13	conserved hypothetical protein
2f06.1.B	22.58	homo- tetramer	HHblits	X-ray	2.10Å	0.31	0.13	conserved hypothetical protein
3nrb.1.A	15.63	homo- tetramer	HHblits	X-ray	2.05Å	0.28	0.13	Formyltetrahydrofolate deformylase
3p96.1.A	10.94	homo- dimer	HHblits	X-ray	2.05Å	0.28	0.13	Phosphoserine phosphatase SerB
1zpv.1.A	10.61	homo- trimer	HHblits	X-ray	1.90Å	0.25	0.13	ACT domain protein
1zpv.1.B	10.61	homo- trimer	HHblits	X-ray	1.90Å	0.25	0.13	ACT domain protein
5jjb.1.A	10.94	homo- dimer	HHblits	X-ray	2.31Å	0.28	0.13	Phosphoserine phosphatase
1yba.1.A	14.29	homo- tetramer	HHblits	X-ray	2.24Å	0.29	0.13	D-3-phosphoglycerate dehydrogenase
1yba.1.C	14.29	homo- tetramer	HHblits	X-ray	2.24Å	0.29	0.13	D-3-phosphoglycerate dehydrogenase
1yba.1.D	14.29	homo- tetramer	HHblits	X-ray	2.24Å	0.29	0.13	D-3-phosphoglycerate dehydrogenase
2p9c.1.A	14.29	homo- tetramer	HHblits	X-ray	2.46Å	0.28	0.13	D-3-phosphoglycerate dehydrogenase
2p9e.1.B	14.29	homo- tetramer	HHblits	X-ray	2.60Å	0.28	0.13	D-3-phosphoglycerate dehydrogenase
2p9e.1.C	14.29	homo- tetramer	HHblits	X-ray	2.60Å	0.28	0.13	D-3-phosphoglycerate dehydrogenase
2p9e.1.D	14.29	homo- tetramer	HHblits	X-ray	2.60Å	0.28	0.13	D-3-phosphoglycerate dehydrogenase
2p9e.1.A	14.29	homo- tetramer	HHblits	X-ray	2.60Å	0.28	0.13	D-3-phosphoglycerate dehydrogenase
2p9c.1.B	14.29	homo- tetramer	HHblits	X-ray	2.46Å	0.28	0.13	D-3-phosphoglycerate dehydrogenase
5it0.1.A	9.09	homo- dimer	HHblits	X-ray	1.97Å	0.24	0.13	Phosphoserine phosphatase

Template	Seq Identity	Oligo- state	Found by	Method	Resolution	Seq Similarity	Coverage	Description
3n0v.1.A	10.77	homo- tetramer	HHblits	X-ray	2.25Å	0.25	0.13	Formyltetrahydrofolate deformylase
5it4.1.A	9.52	homo- dimer	HHblits	X-ray	2.10Å	0.27	0.13	Phosphoserine phosphatase
3mtj.1.A	11.11	homo- tetramer	HHblits	X-ray	2.15Å	0.27	0.13	Homoserine dehydrogenase
3p96.1.A	9.23	homo- dimer	HHblits	X-ray	2.05Å	0.24	0.13	Phosphoserine phosphatase SerB
3k5p.1.A	12.90	homo- tetramer	HHblits	X-ray	2.15Å	0.28	0.13	D-3-phosphoglycerate dehydrogenase
2ko1.1.A	7.69	homo- dimer	HHblits	NMR	NA	0.24	0.13	GTP pyrophosphokinase
2ko1.1.B	7.69	homo- dimer	HHblits	NMR	NA	0.24	0.13	GTP pyrophosphokinase
3ibw.1.A	7.69	homo- dimer	HHblits	X-ray	1.93Å	0.24	0.13	GTP pyrophosphokinase
3ibw.1.B	7.69	homo- dimer	HHblits	X-ray	1.93Å	0.24	0.13	GTP pyrophosphokinase
5t41.1.A	7.94	monomer	HHblits	X-ray	3.15Å	0.26	0.13	Phosphoserine phosphatase
3obi.1.A	7.81	homo- tetramer	HHblits	X-ray	1.95Å	0.25	0.13	Formyltetrahydrofolate deformylase
3o1l.1.A	7.81	homo- dimer	HHblits	X-ray	2.20Å	0.25	0.13	Formyltetrahydrofolate deformylase
5it0.1.A	9.68	homo- dimer	HHblits	X-ray	1.97Å	0.27	0.13	Phosphoserine phosphatase
5is2.1.A	9.68	homo- dimer	HHblits	X-ray	1.88Å	0.27	0.13	Phosphoserine phosphatase
5v0s.1.A	8.06	homo- dimer	HHblits	X-ray	2.01Å	0.27	0.13	Prephenate dehydrogenase
2jhe.1.A	13.11	homo- dimer	HHblits	X-ray	2.30Å	0.27	0.12	TRANSCRIPTION REGULATOR TYRR
2jhe.1.B	13.11	homo- dimer	HHblits	X-ray	2.30Å	0.27	0.12	TRANSCRIPTION REGULATOR TYRR
2jhe.2.A	13.11	homo- dimer	HHblits	X-ray	2.30Å	0.27	0.12	TRANSCRIPTION REGULATOR TYRR
2jhe.2.B	13.11	homo- dimer	HHblits	X-ray	2.30Å	0.27	0.12	TRANSCRIPTION REGULATOR TYRR
2re1.1.A	18.97	homo- dimer	HHblits	X-ray	2.75Å	0.31	0.12	Aspartokinase, alpha and beta subunits
2re1.1.B	18.97	homo- dimer	HHblits	X-ray	2.75Å	0.31	0.12	Aspartokinase, alpha and beta subunits
2zho.1.B	8.20	homo- dimer	HHblits	X-ray	2.98Å	0.26	0.12	Aspartokinase
2zho.1.A	8.20	homo- dimer	HHblits	X-ray	2.98Å	0.26	0.12	Aspartokinase
2zho.2.B	8.20	homo- dimer	HHblits	X-ray	2.98Å	0.26	0.12	Aspartokinase
2zho.3.A	8.20	homo- dimer	HHblits	X-ray	2.98Å	0.26	0.12	Aspartokinase
2zho.3.B	8.20	homo- dimer	HHblits	X-ray	2.98Å	0.26	0.12	Aspartokinase
2dt9.1.A	8.20	homo- dimer	HHblits	X-ray	2.15Å	0.26	0.12	Aspartokinase
2dt9.1.B	8.20	homo- dimer	HHblits	X-ray	2.15Å	0.26	0.12	Aspartokinase
3aaw.1.B	13.79	hetero- oligomer	HHblits	X-ray	2.50Å	0.30	0.12	Aspartokinase LysC beta subunit
3ab2.1.B	13.79	hetero- oligomer	HHblits	X-ray	2.59Å	0.30	0.12	Aspartokinase
2dtj.1.A	13.79	homo- dimer	HHblits	X-ray	1.58Å	0.30	0.12	Aspartokinase

Template	Seq Identity	Oligo- state	Found by	Method	Resolution	Seq Similarity	Coverage	Description
2dtj.1.B	13.79	homo- dimer	HHblits	X-ray	1.58Å	0.30	0.12	Aspartokinase
1ygy.1.A	11.48	homo- tetramer	HHblits	X-ray	2.30Å	0.26	0.12	D-3-phosphoglycerate dehydrogenase
1ygy.1.B	11.48	homo- tetramer	HHblits	X-ray	2.30Å	0.26	0.12	D-3-phosphoglycerate dehydrogenase
3ddn.1.A	11.48	homo- tetramer	HHblits	X-ray	2.40Å	0.26	0.12	D-3-phosphoglycerate dehydrogenase
3ddn.1.B	11.48	homo- tetramer	HHblits	X-ray	2.40Å	0.26	0.12	D-3-phosphoglycerate dehydrogenase
5jjb.1.A	7.94	homo- dimer	HHblits	X-ray	2.31Å	0.24	0.13	Phosphoserine phosphatase
5is2.1.A	7.94	homo- dimer	HHblits	X-ray	1.88Å	0.23	0.13	Phosphoserine phosphatase
3s1t.1.A	11.86	hetero- oligomer	HHblits	X-ray	1.63Å	0.28	0.12	Aspartokinase
3ab4.3.C	10.17	hetero- oligomer	HHblits	X-ray	2.47Å	0.28	0.12	Aspartokinase
3ab4.1.C	10.17	hetero- oligomer	HHblits	X-ray	2.47Å	0.28	0.12	Aspartokinase
3ab4.2.A	10.17	hetero- oligomer	HHblits	X-ray	2.47Å	0.28	0.12	Aspartokinase
3ab4.2.C	10.17	hetero- oligomer	HHblits	X-ray	2.47Å	0.28	0.12	Aspartokinase
3ab4.3.A	10.17	hetero- oligomer	HHblits	X-ray	2.47Å	0.28	0.12	Aspartokinase
3ab4.1.A	10.17	hetero- oligomer	HHblits	X-ray	2.47Å	0.28	0.12	Aspartokinase
3ab4.4.C	10.17	hetero- oligomer	HHblits	X-ray	2.47Å	0.28	0.12	Aspartokinase
4go5.1.A	15.25	homo- dimer	HHblits	X-ray	2.60Å	0.28	0.12	Aspartokinase
4go7.1.A	15.25	homo- dimer	HHblits	X-ray	2.00Å	0.28	0.12	Aspartokinase
2zho.1.B	13.56	homo- dimer	HHblits	X-ray	2.98Å	0.28	0.12	Aspartokinase
2zho.1.A	13.56	homo- dimer	HHblits	X-ray	2.98Å	0.28	0.12	Aspartokinase
2zho.2.B	13.56	homo- dimer	HHblits	X-ray	2.98Å	0.28	0.12	Aspartokinase
2zho.3.A	13.56	homo- dimer	HHblits	X-ray	2.98Å	0.28	0.12	Aspartokinase
2zho.3.B	13.56	homo- dimer	HHblits	X-ray	2.98Å	0.28	0.12	Aspartokinase
2dt9.1.A	13.56	homo- dimer	HHblits	X-ray	2.15Å	0.28	0.12	Aspartokinase
2dt9.1.B	13.56	homo- dimer	HHblits	X-ray	2.15Å	0.28	0.12	Aspartokinase
3l76.1.A	11.67	homo- dimer	HHblits	X-ray	2.54Å	0.26	0.12	Aspartokinase
3l76.1.B	11.67	homo- dimer	HHblits	X-ray	2.54Å	0.26	0.12	Aspartokinase
1tdj.1.A	11.67	homo- dimer	HHblits	X-ray	2.80Å	0.26	0.12	BIOSYNTHETIC THREONINE DEAMINASE
3ab2.1.C	12.07	hetero- oligomer	HHblits	X-ray	2.59Å	0.29	0.12	Aspartokinase
3aaw.1.C	12.07	hetero- oligomer	HHblits	X-ray	2.50Å	0.29	0.12	Aspartokinase
3ab2.1.A	12.07	hetero- oligomer	HHblits	X-ray	2.59Å	0.29	0.12	Aspartokinase
3aaw.1.A	12.07	hetero- oligomer	HHblits	X-ray	2.50Å	0.29	0.12	Aspartokinase

Template	Seq Identity	Oligo- state	Found by	Method	Resolution	Seq Similarity	Coverage	Description
3ab2.3.A	12.07	hetero- oligomer	HHblits	X-ray	2.59Å	0.29	0.12	Aspartokinase
3ab2.4.C	12.07	hetero- oligomer	HHblits	X-ray	2.59Å	0.29	0.12	Aspartokinase
2nyi.1.A	8.33	homo- dimer	HHblits	X-ray	1.80Å	0.25	0.12	unknown protein
2nyi.1.B	8.33	homo- dimer	HHblits	X-ray	1.80Å	0.25	0.12	unknown protein
4go5.1.A	10.34	homo- dimer	HHblits	X-ray	2.60Å	0.28	0.12	Aspartokinase
4go7.1.A	10.34	homo- dimer	HHblits	X-ray	2.00Å	0.28	0.12	Aspartokinase
3s1t.1.A	13.79	hetero- oligomer	HHblits	X-ray	1.63Å	0.27	0.12	Aspartokinase
3aaw.1.B	10.53	hetero- oligomer	HHblits	X-ray	2.50Å	0.28	0.12	Aspartokinase LysC beta subunit
3ab2.1.B	10.53	hetero- oligomer	HHblits	X-ray	2.59Å	0.28	0.12	Aspartokinase
2dtj.1.A	10.53	homo- dimer	HHblits	X-ray	1.58Å	0.28	0.12	Aspartokinase
2dtj.1.B	10.53	homo- dimer	HHblits	X-ray	1.58Å	0.28	0.12	Aspartokinase
2re1.1.A	10.34	homo- dimer	HHblits	X-ray	2.75Å	0.26	0.12	Aspartokinase, alpha and beta subunits
2re1.1.B	10.34	homo- dimer	HHblits	X-ray	2.75Å	0.26	0.12	Aspartokinase, alpha and beta subunits
3ab4.1.B	8.77	hetero- oligomer	HHblits	X-ray	2.47Å	0.27	0.12	Aspartokinase
3ab4.1.D	8.77	hetero- oligomer	HHblits	X-ray	2.47Å	0.27	0.12	Aspartokinase
3ab4.2.D	8.77	hetero- oligomer	HHblits	X-ray	2.47Å	0.27	0.12	Aspartokinase
3ab4.3.B	8.77	hetero- oligomer	HHblits	X-ray	2.47Å	0.27	0.12	Aspartokinase
3ab4.3.D	8.77	hetero- oligomer	HHblits	X-ray	2.47Å	0.27	0.12	Aspartokinase
3ab4.4.D	8.77	hetero- oligomer	HHblits	X-ray	2.47Å	0.27	0.12	Aspartokinase
3l76.1.A	12.07	homo- dimer	HHblits	X-ray	2.54Å	0.26	0.12	Aspartokinase
3l76.1.B	12.07	homo- dimer	HHblits	X-ray	2.54Å	0.26	0.12	Aspartokinase
3ab4.1.B	12.00	hetero- oligomer	HHblits	X-ray	2.47Å	0.29	0.10	Aspartokinase
3ab4.1.D	12.00	hetero- oligomer	HHblits	X-ray	2.47Å	0.29	0.10	Aspartokinase
3ab4.2.D	12.00	hetero- oligomer	HHblits	X-ray	2.47Å	0.29	0.10	Aspartokinase
3ab4.3.B	12.00	hetero- oligomer	HHblits	X-ray	2.47Å	0.29	0.10	Aspartokinase
3ab4.3.D	12.00	hetero- oligomer	HHblits	X-ray	2.47Å	0.29	0.10	Aspartokinase
3ab4.4.D	12.00	hetero- oligomer	HHblits	X-ray	2.47Å	0.29	0.10	Aspartokinase
2ktr.1.B	5.88	hetero- oligomer	HHblits	NMR	NA	0.27	0.10	Sequestosome-1
2nyi.1.A	7.69	homo- dimer	HHblits	X-ray	1.80Å	0.25	0.11	unknown protein
2nyi.1.B	7.69	homo- dimer	HHblits	X-ray	1.80Å	0.25	0.11	unknown protein
4mjs.2.B	3.92	hetero- oligomer	HHblits	X-ray	2.50Å	0.26	0.10	Sequestosome-1

Template	Seq Identity	Oligo- state	Found by	Method	Resolution	Seq Similarity	Coverage	Description
4mjs.1.B	3.92	hetero- oligomer	HHblits		2.50Å	0.26	0.10	Sequestosome-1
4mjs.3.B	3.92	hetero- oligomer	HHblits	X-ray	2.50Å	0.26	0.10	Sequestosome-1
4mjs.4.B	3.92	hetero- oligomer	HHblits	X-ray	2.50Å	0.26	0.10	Sequestosome-1
4mjs.5.B	3.92	hetero- oligomer	HHblits	X-ray	2.50Å	0.26	0.10	Sequestosome-1
4mjs.8.B	3.92	hetero- oligomer	HHblits	X-ray	2.50Å	0.26	0.10	Sequestosome-1
4mjs.10.B	3.92	hetero- oligomer	HHblits	X-ray	2.50Å	0.26	0.10	Sequestosome-1
4mjs.11.B	3.92	hetero- oligomer	HHblits	X-ray	2.50Å	0.26	0.10	Sequestosome-1
4mjs.12.B	3.92	hetero- oligomer	HHblits	X-ray	2.50Å	0.26	0.10	Sequestosome-1
4uf9.1.A	3.92	homo- 60-mer	HHblits	EM	10.30Å	0.26	0.10	SEQUESTOSOME-1
4uf8.1.A	3.92	homo- tetramer	HHblits	EM	10.90Å	0.26	0.10	SEQUESTOSOME-1
2kkc.1.A	4.00	monomer	HHblits	NMR	NA	0.26	0.10	Sequestosome-1
3lou.1.A	8.33	homo- tetramer	HHblits	X-ray	1.90Å	0.25	0.10	Formyltetrahydrofolate deformylase
3lou.1.B	8.33	homo- tetramer	HHblits	X-ray	1.90Å	0.25	0.10	Formyltetrahydrofolate deformylase
1u8s.1.A	13.89	homo- dimer	HHblits	X-ray	2.45Å	0.31	0.07	glycine cleavage system transcriptional repressor, putative
1u8s.1.B	13.89	homo- dimer	HHblits	X-ray	2.45Å	0.31	0.07	glycine cleavage system transcriptional repressor, putative
2f06.1.A	11.76	homo- tetramer	HHblits	X-ray	2.10Å	0.30	0.07	conserved hypothetical protein
2f06.1.B	11.76	homo- tetramer	HHblits	X-ray	2.10Å	0.30	0.07	conserved hypothetical protein
1u8s.1.A	8.57	homo- dimer	HHblits	X-ray	2.45Å	0.26	0.07	glycine cleavage system transcriptional repressor, putative
1u8s.1.B	8.57	homo- dimer	HHblits	X-ray	2.45Å	0.26	0.07	glycine cleavage system transcriptional repressor, putative
3w7b.1.A	3.23	homo- tetramer	HHblits	X-ray	2.71Å	0.26	0.06	Formyltetrahydrofolate deformylase
3lw6.1.A	10.71	monomer	HHblits	X-ray	1.81Å	0.26	0.06	Beta-4-galactosyltransferase 7
4lw3.1.A	10.71	monomer	HHblits	X-ray	2.00Å	0.26	0.06	Beta-4-galactosyltransferase 7