SWISS-MODEL Homology Modeling Report

Model Building Report

This document lists the results for the homology modeling project "Yeast_YHL021C" submitted to SWISS-MODEL workspace on April 1, 2015, 11:22 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:

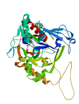
Marco Biasini; Stefan Bienert; Andrew Waterhouse; Konstantin Arnold; Gabriel Studer; Tobias Schmidt; Florian Kiefer; Tiziano Gallo Cassarino; Martino Bertoni; Lorenza Bordoli; Torsten Schwede. (2014). SWISS-MODEL: modelling protein tertiary and quaternary structure using evolutionary information. Nucleic 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

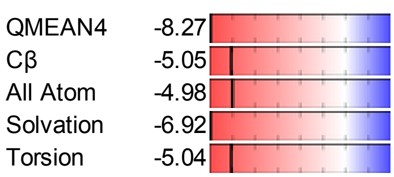
Results

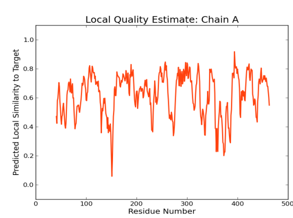
The SWISS-MODEL template library (SMTL version 2015-03-25, PDB release 2015-04-03) was searched with Blast (Altschul et al., 1997) and HHBlits (Remmert, et al., 2011) for evolutionary related structures matching the target sequence in Table T1. For details on the template search, see Materials and Methods. Overall 117 templates were found (Table T2).

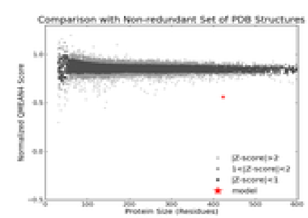
Models

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 (matching prediction)	None	0.49	-8.27







Template	Seq Identity	Oligo-state	Found by	Method	Resolution	Seq Similarity	Range	Coverage	Description
3o2g.1.A	20.00	homo-dimer	HHblits	X-ray	1.78Å	0.31	41 - 463	0.76	Gamma-butyrobetaine dioxygenase

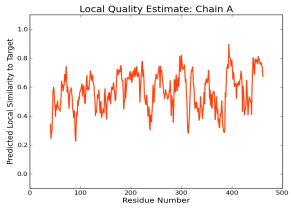
Ligand	Added to Model	Description
EDO	✕ - Not biologically relevant.	1,2-ETHANEDIOL
EDO	✕ - Not biologically relevant.	1,2-ETHANEDIOL
EDO	✕ - Not biologically relevant.	1,2-ETHANEDIOL
EDO	✕ - Not biologically relevant.	1,2-ETHANEDIOL
EDO	✕ - Not biologically relevant.	1,2-ETHANEDIOL
EDO	✕ - Not biologically relevant.	1,2-ETHANEDIOL
EDO	✕ - Not biologically relevant.	1,2-ETHANEDIOL
EDO	✕ - Not biologically relevant.	1,2-ETHANEDIOL
EDO	✕ - Not biologically relevant.	1,2-ETHANEDIOL
EDO	✕ - Not biologically relevant.	1,2-ETHANEDIOL
NM2	✕ - Binding site not conserved.	3-CARBOXY-N,N,N-TRIMETHYLPROPAN-1-AMINIUM
NM2	✕ - Binding site not conserved.	3-CARBOXY-N,N,N-TRIMETHYLPROPAN-1-AMINIUM
OGA	✕ - Binding site not conserved.	N-OXALYLGLYCINE

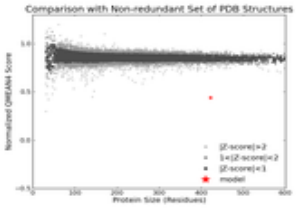
OGA	× - Binding site not conserved.	N-OXALYLGLYCINE
ZN	× - Binding site not conserved.	ZINC ION
ZN	× - Binding site not conserved.	ZINC ION
ZN	× - Binding site not conserved.	ZINC ION
ZN	× - Binding site not conserved.	ZINC ION

```
Target    MLRSNLCRGSRILARLTTTPRTYTSAATAAAANRGHIIKTYFNRDSTTITFSMEESSKPVSVCFNNVFLRDASHSAK---
3o2g.1.A  ----------------------------------------LDGAHLMQILWY---DEEE--SLYPAVWLRDNCPCSDCYL

Target    ------LVTTGELYHNEKLTAPQDIQISEDGKSLVVKWKDGGHHQFPLQFFIDYKGSSFVSPATRKQES-----RYRPQL
3o2g.1.A  DSAKARKLLVEALDVNIG---IKGLIFDRK--KVYITWPDEHYSEFQADWLKKRCFS-----KQARAKLQRELFFPECQY

Target    WNKRILKDNVKDLLSVSYNEFIDPKDDSKLFQTLVNLQKFGIAFISGTPSSSSEGLTIQKICERIGPIRSTVHGEGTFDV
3o2g.1.A  WGSE---LQLP---TLDFEDVLR--YDEHAYKWLSTLKKVGIVRLTGASDKPGE---VSKLGKRMGFLYLTFYGH-TWQV

Target    NASQATSVNAHYANKDLPLHTDLPFLENVPGFQILQSLPATEGEDPNTRPMNYFVDAFYATRNVRESDFEAYEALQIVPV
3o2g.1.A  QD-KIDANNVAYTTGKLSFHTDYPALHHPPGVQLLHCIKQTV---TGG--DSEIVDGFNVCQKLKKNNPQAFQILSSTFV

Target    NYIYENGDK---RYYQSKPLIEHHDINEDNTLLGNYEALIKCINYSPPYQAPF-TFGIYDKPSDLNNNLDLNLITTPAKL
3o2g.1.A  DFTDIGVDYCDFSVQSKHKIIELDDKGQ-----------VVRINFNNATRDTIFDV-------PV---------------

Target    TERFLFKSFIRGLNLFESHINDFNNQFRLQLPENCCVIFNNRRILHANSLTS----SNQQWLKGCYFDSDTFKSKLKFLE
3o2g.1.A  ---ERVQPFYAALKEFVDLMNSKESKFTFKMNPGDVITFDNWRLLHGRRSYEAGTEIS-RHLEGAYADWDVVMSRLRILR

Target    EKFPHDK
3o2g.1.A  QRVENGN
```

Model #03	File	Built with	Oligo-State	Ligands	GMQE	QMEAN4
	PDB	ProMod Version 3.70.	MONOMER (matching prediction)	None	0.47	-11.69

QMEAN4	-11.69
Cβ	-11.34
All Atom	-6.96
Solvation	-11.25
Torsion	-5.06





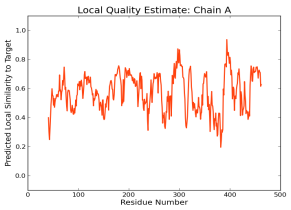
Template	Seq Identity	Oligo-state	Found by	Method	Resolution	Seq Similarity	Range	Coverage	Description
4c8r.2.A	20.00	homo-dimer	HHblits	X-ray	2.82Å	0.31	41 - 462	0.76	GAMMA-BUTYROBETAINE DIOXYGENASE

Ligand	Added to Model	Description
6YT	× - Binding site not conserved.	N-(3-HYDROXYPICOLINOYL)-S-(PYRIDIN-2-YLMETHYL)-L-CYSTEINE
6YT	× - Binding site not conserved.	N-(3-HYDROXYPICOLINOYL)-S-(PYRIDIN-2-YLMETHYL)-L-CYSTEINE
EDO	× - Not biologically relevant.	1,2-ETHANEDIOL
EDO	× - Not biologically relevant.	1,2-ETHANEDIOL
EDO	× - Not biologically relevant.	1,2-ETHANEDIOL
EDO	× - Not biologically relevant.	1,2-ETHANEDIOL
NI	× - Binding site not conserved.	NICKEL (II) ION
NI	× - Binding site not conserved.	NICKEL (II) ION
ZN	× - Binding site not conserved.	ZINC ION
ZN	× - Binding site not conserved.	ZINC ION

```
Target    MLRSNLCRGSRILARLTTTPRTYTSAATAAAANRGHIIKTYFNRDSTTITFSMEESSKPVSVCFNNVFLRDASHSAK---
4c8r.2.A  ----------------------------------------LDGAHLMQILWY---DEEE--SLYPAVWLRDNCPCSDCYL

Target    ------LVTTGELYHNEKLTAPQDIQISEDGKSLVVKWKDGGHHQFPLQFFIDYKGSSFVSPATRKQES-----RYRPQL
4c8r.2.A  DSAKARKLLVEALDVNIG---IKGLIFDRK--KVYITWPDEHYSEFQADWLKKRCFS-----KQARAKLQRELFFPECQY

Target    WNKRILKDNVKDLLSVSYNEFIDPKDDSKLFQTLVNLQKFGIAFISGTPSSSSEGLTIQKICERIGPIRSTVHGEGTFDV
4c8r.2.A  WGSE---LQLP---TLDFEDVLR--YDEHAYKWLSTLKKVGIVRLTGASDKPGE---VSKLGKRMGFLYLTFYGH-TWQV

Target    NASQATSVNAHYANKDLPLHTDLPFLENVPGFQILQSLPATEGEDPNTRPMNYFVDAFYATRNVRESDFEAYEALQIVPV
4c8r.2.A  QD-KIDANNVAYTTGKLSFHTDYPALHHPPGVQLLHCIKQTV---TGG--DSEIVDGFNVCQKLKKNNPQAFQILSSTFV

Target    NYIYENGDK---RYYQSKPLIEHHDINEDNTLLGNYEALIKCINYSPPYQAPF-TFGIYDKPSDLNNNLDLNLITTPAKL
4c8r.2.A  DFTDIGVDYCDFSVQSKHKIIELDDKGQ-----------VVRINFNNATRDTIFDV-------PV---------------

Target    TERFLFKSFIRGLNLFESHINDFNNQFRLQLPENCCVIFNNRRILHANSLTS----SNQQWLKGCYFDSDTFKSKLKFLE
4c8r.2.A  ---ERVQPFYAALKEFVDLMNSKESKFTFKMNPGDVITFDNWRLLHGRRSYEAGTEIS-RHLEGAYADWDVVMSRLRILR

Target    EKFPHDK
4c8r.2.A  QRVENGN
```

Model #02	File	Built with	Oligo-State	Ligands	GMQE	QMEAN4
	PDB	ProMod Version 3.70.	MONOMER (matching prediction)	None	0.47	-12.19

QMEAN4	-12.19
Cβ	-10.28
All Atom	-6.77
Solvation	-11.76
Torsion	-5.71



Template	Seq Identity	Oligo-state	Found by	Method	Resolution	Seq Similarity	Range	Coverage	Description
4c8r.3.B	20.00	homo-dimer	HHblits	X-ray	2.82Å	0.31		0.76	GAMMA-BUTYROBETAINE DIOXYGENASE

Ligand	Added to Model	Description
6YT	× - Binding site not conserved.	N-(3-HYDROXYPICOLINOYL)-S-(PYRIDIN-2-YLMETHYL)-L-CYSTEINE
6YT	× - Binding site not conserved.	N-(3-HYDROXYPICOLINOYL)-S-(PYRIDIN-2-YLMETHYL)-L-CYSTEINE
EDO	× - Not biologically relevant.	1,2-ETHANEDIOL
EDO	× - Not biologically relevant.	1,2-ETHANEDIOL
EDO	× - Not biologically relevant.	1,2-ETHANEDIOL
EDO	× - Not biologically relevant.	1,2-ETHANEDIOL
EDO	× - Not biologically relevant.	1,2-ETHANEDIOL
NI	× - Binding site not conserved.	NICKEL (II) ION
NI	× - Binding site not conserved.	NICKEL (II) ION
ZN	× - Binding site not conserved.	ZINC ION
ZN	× - Binding site not conserved.	ZINC ION

```
Target    MLRSNLCRGSRILARLTTTPRTYTSAATAAAANRGHIIKTYFNRDSTTITFSMEESSKPVSVCFNNVFLRDASHSAK---
4c8r.3.B  ----------------------------------------LDGAHLMQILWY---DEEE--SLYPAVWLRDNCPCSDCYL

Target    ------LVTTGELYHNEKLTAPQDIQISEDGKSLVVKWKDGGHHQFPLQFFIDYKGSSFVSPATRKQES-----RYRPQL
4c8r.3.B  DSAKARKLLVEALDVNIG---IKGLIFDRK--KVYITWPDEHYSEFQADWLKKRCFS-----KQARAKLQRELFFPECQY

Target    WNKRILKDNVKDLLSVSYNEFIDPKDDSKLFQTLVNLQKFGIAFISGTPSSSSEGLTIQKICERIGPIRSTVHGEGTFDV
4c8r.3.B  WGSE---LQLP---TLDFEDVLR--YDEHAYKWLSTLKKVGIVRLTGASDKPGE---VSKLGKRMGFLYLTFYGH-TWQV

Target    NASQATSVNAHYANKDLPLHTDLPFLENVPGFQILQSLPATEGEDPNTRPMNYFVDAFYATRNVRESDFEAYEALQIVPV
4c8r.3.B  QD-KIDANNVAYTTGKLSFHTDYPALHHPPGVQLLHCIKQTV---TGG--DSEIVDGFNVCQKLKKNNPQAFQILSSTFV

Target    NYIYENGDK---RYYQSKPLIEHHDINEDNTLLGNYEALIKCINYSPPYQAPF-TFGIYDKPSDLNNNLDLNLITTPAKL
4c8r.3.B  DFTDIGVDYCDFSVQSKHKIIELDDKGQ-----------VVRINFNNATRDTIFDV-------PV---------------

Target    TERFLFKSFIRGLNLFESHINDFNNQFRLQLPENCCVIFNNRRILHANSLTS----SNQQWLKGCYFDSDTFKSKLKFLE
4c8r.3.B  ---ERVQPFYAALKEFVDLMNSKESKFTFKMNPGDVITFDNWRLLHGRRSYEAGTEIS-RHLEGAYADWDVVMSRLRILR

Target    EKFPHDK
4c8r.3.B  QRVENGN
```

Materials and Methods

Template Search

Template search with Blast and HHBlits has been performed against the SWISS-MODEL template library (SMTL, last update: 2015-03-25, last included PDB release: 2015-04-03).

The target sequence was searched with BLAST (Altschul et al., 1997) against the primary amino acid sequence contained in the SMTL. A total of 16 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 65 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 Promod-II. Coordinates which are conserved between the target and the template are copied from the template to the model. Insertions and deletions are remodeled 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 ProMod-II (Guex, et al., 1997) does not give satisfactory results, an alternative model is built with MODELLER (Sali, et al., 1993).

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 Modeling

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 polypetide 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.

```
MLRSNLCRGSRILARLTTTPRTYTSAATAAAANRGHIIKTYFNRDSTTITFSMEESSKPVSVCFNNVFLRDASHSAKLVTTGELYHNEKLTAPQDIQISE
DGKSLVVKWKDGGHHQFPLQFFIDYKGSSFVSPATRKQESRYRPQLWNKRILKDNVKDLLSVSYNEFIDPKDDSKLFQTLVNLQKFGIAFISGTPSSSSE
GLTIQKICERIGPIRSTVHGEGTFDVNASQATSVNAHYANKDLPLHTDLPFLENVPGFQILQSLPATEGEDPNTRPMNYFVDAFYATRNVRESDFEAYEA
LQIVPVNYIYENGDKRYYQSKPLIEHHDINEDNTLLGNYEALIKCINYSPPYQAPFTFGIYDKPSDLNNNLDLNLITTPAKLTERFLFKSFIRGLNLFES
HINDFNNQFRLQLPENCCVIFNNRRILHANSLTSSNQQWLKGCYFDSDTFKSKLKFLEEKFPHDK
```

Table T2:

Template	Seq Identity	Oligo-state	Found by	Method	Resolution	Seq Similarity	Coverage	Description
3o2g.1.A	20.00	homo-dimer	HHblits	X-ray	1.78Å	0.31	0.76	Gamma-butyrobetaine dioxygenase
4c8r.2.B	20.00	homo-dimer	HHblits	X-ray	2.82Å	0.31	0.76	GAMMA-BUTYROBETAINE DIOXYGENASE
4c8r.2.A	20.00	homo-dimer	HHblits	X-ray	2.82Å	0.31	0.76	GAMMA-BUTYROBETAINE DIOXYGENASE
4c8r.3.B	20.00	homo-dimer	HHblits	X-ray	2.82Å	0.31	0.76	GAMMA-BUTYROBETAINE DIOXYGENASE
4bg1.1.A	20.11	homo-dimer	HHblits	X-ray	1.89Å	0.31	0.76	GAMMA-BUTYROBETAINE DIOXYGENASE
3n6w.1.A	20.11	homo-dimer	HHblits	X-ray	2.00Å	0.31	0.76	Gamma-butyrobetaine dioxygenase
2r6s.1.A	13.22	homo-octamer	HHblits	X-ray	2.10Å	0.28	0.52	Gab protein
1jr7.1.A	13.69	homo-tetramer	HHblits	X-ray	2.00Å	0.28	0.52	HYPOTHETICAL 37.4 KDA PROTEIN IN ILEY-GABD INTERGENIC REGION
1oik.1.A	15.09	homo-tetramer	HHblits	X-ray	2.06Å	0.29	0.50	PUTATIVE ALKYLSULFATASE ATSK
3eat.1.A	16.02	homo-trimer	HHblits	X-ray	2.50Å	0.29	0.50	Pyoverdine biosynthesis protein PvcB
3r1j.1.A	15.52	homo-tetramer	HHblits	X-ray	2.05Å	0.28	0.50	Alpha-ketoglutarate-dependent taurine dioxygenase
1oij.3.A	15.15	monomer	HHblits	X-ray	2.10Å	0.28	0.50	PUTATIVE ALKYLSULFATASE ATSK
1gqw.1.A	12.39	homo-tetramer	HHblits	X-ray	3.00Å	0.27	0.50	ALPHA-KETOGLUTARATE-DEPENDENT TAURINE DIOXYGENASE
1otj.1.B	12.39	homo-dimer	HHblits	X-ray	1.90Å	0.27	0.50	Alpha-Ketoglutarate-Dependent Taurine Dioxygenase
1otj.2.A	12.39	homo-dimer	HHblits	X-ray	1.90Å	0.27	0.50	Alpha-Ketoglutarate-Dependent Taurine Dioxygenase
1vz4.1.A	15.28	homo-tetramer	HHblits	X-ray	2.50Å	0.28	0.49	PUTATIVE ALKYLSULFATASE ATSK
4j5i.1.A	14.78	homo-tetramer	HHblits	X-ray	2.60Å	0.28	0.49	Alpha-ketoglutarate-dependent taurine dioxygenase
		homo-						

1y0z.1.A	11.02	dimer	HHblits	X-ray	2.40Å	0.26	0.51	protein product of AT3G21360
1y0z.1.B	11.02	homo-dimer	HHblits	X-ray	2.40Å	0.26	0.51	protein product of AT3G21360
4cvy.1.A	14.91	homo-dimer	HHblits	X-ray	2.00Å	0.28	0.49	DIOXYGENASE RV3406/MT3514
4ffa.1.A	14.91	homo-tetramer	HHblits	X-ray	2.50Å	0.28	0.49	Rv3406 alkyl sulfatase
3v15.1.C	13.91	homo-tetramer	HHblits	X-ray	2.60Å	0.27	0.49	Alpha-ketoglutarate-dependent taurine dioxygenase
3v17.1.C	13.91	homo-tetramer	HHblits	X-ray	2.57Å	0.27	0.49	Alpha-ketoglutarate-dependent taurine dioxygenase
3v17.1.A	13.91	homo-tetramer	HHblits	X-ray	2.57Å	0.27	0.49	Alpha-ketoglutarate-dependent taurine dioxygenase
3v15.1.B	13.91	homo-tetramer	HHblits	X-ray	2.60Å	0.27	0.49	Alpha-ketoglutarate-dependent taurine dioxygenase
3v15.1.A	13.91	homo-tetramer	HHblits	X-ray	2.60Å	0.27	0.49	Alpha-ketoglutarate-dependent taurine dioxygenase
3v17.1.D	13.91	homo-tetramer	HHblits	X-ray	2.57Å	0.27	0.49	Alpha-ketoglutarate-dependent taurine dioxygenase
3v15.1.D	13.91	homo-tetramer	HHblits	X-ray	2.60Å	0.27	0.49	Alpha-ketoglutarate-dependent taurine dioxygenase
3pvj.1.B	13.91	homo-tetramer	HHblits	X-ray	1.85Å	0.27	0.49	Alpha-ketoglutarate-dependent taurine dioxygenase
3pvj.1.A	13.91	homo-tetramer	HHblits	X-ray	1.85Å	0.27	0.49	Alpha-ketoglutarate-dependent taurine dioxygenase
1ds1.1.A	15.72	monomer	HHblits	X-ray	1.08Å	0.27	0.49	CLAVAMINATE SYNTHASE 1
2wbq.1.A	13.48	monomer	HHblits	X-ray	1.10Å	0.27	0.49	L-ARGININE BETA-HYDROXYLASE
3swt.1.A	16.30	monomer	HHblits	X-ray	2.05Å	0.28	0.49	Taurine catabolism dioxygenase, TauD
2wbo.1.A	13.04	monomer	HHblits	X-ray	1.30Å	0.27	0.49	L-ARGININE BETA-HYDROXYLASE
1nx4.1.A	12.07	homo-hexamer	HHblits	X-ray	2.40Å	0.25	0.50	Carbapenem synthase
4oj8.1.A	12.07	homo-hexamer	HHblits	X-ray	2.10Å	0.25	0.50	(5R)-carbapenem-3-carboxylate synthase
4oj8.1.B	12.07	homo-hexamer	HHblits	X-ray	2.10Å	0.25	0.50	(5R)-carbapenem-3-carboxylate synthase
4ne0.2.A	14.22	homo-dimer	HHblits	X-ray	2.17Å	0.26	0.48	L-arginine beta-hydroxylase
4ne0.1.A	14.22	homo-dimer	HHblits	X-ray	2.17Å	0.26	0.48	L-arginine beta-hydroxylase
4ne0.1.B	14.22	homo-dimer	HHblits	X-ray	2.17Å	0.26	0.48	L-arginine beta-hydroxylase
4m23.1.A	14.22	homo-dimer	HHblits	X-ray	1.76Å	0.26	0.48	L-arginine beta-hydroxylase
4m2i.1.B	14.22	homo-dimer	HHblits	X-ray	2.53Å	0.26	0.48	L-arginine beta-hydroxylase
4m2c.1.B	14.22	homo-dimer	HHblits	X-ray	2.35Å	0.26	0.48	L-arginine beta-hydroxylase
4m2i.2.B	14.22	homo-dimer	HHblits	X-ray	2.53Å	0.26	0.48	L-arginine beta-hydroxylase
4m2i.2.A	14.22	homo-dimer	HHblits	X-ray	2.53Å	0.26	0.48	L-arginine beta-hydroxylase
4m26.2.B	14.22	homo-dimer	HHblits	X-ray	2.02Å	0.26	0.48	L-arginine beta-hydroxylase
4m26.1.B	14.22	homo-dimer	HHblits	X-ray	2.02Å	0.26	0.48	L-arginine beta-hydroxylase
4m2f.2.A	14.22	homo-dimer	HHblits	X-ray	1.92Å	0.26	0.48	L-arginine beta-hydroxylase
4m2c.2.A	14.22	homo-dimer	HHblits	X-ray	2.35Å	0.26	0.48	L-arginine beta-hydroxylase
		homo-						

4m25.1.B	14.22	dimer	HHblits	X-ray	1.84Å	0.26	0.48	L-arginine beta-hydroxylase
4m2c.2.B	14.22	homo-dimer	HHblits	X-ray	2.35Å	0.26	0.48	L-arginine beta-hydroxylase
4m2g.1.B	14.22	homo-dimer	HHblits	X-ray	2.39Å	0.26	0.48	L-arginine beta-hydroxylase
4m2f.1.B	14.22	homo-dimer	HHblits	X-ray	1.92Å	0.26	0.48	L-arginine beta-hydroxylase
4m23.2.A	14.22	homo-dimer	HHblits	X-ray	1.76Å	0.26	0.48	L-arginine beta-hydroxylase
4m23.1.B	14.22	homo-dimer	HHblits	X-ray	1.76Å	0.26	0.48	L-arginine beta-hydroxylase
2og7.1.A	14.35	monomer	HHblits	X-ray	1.66Å	0.27	0.48	asparagine oxygenase
2og6.1.A	14.35	monomer	HHblits	X-ray	1.92Å	0.27	0.48	asparagine oxygenase
4bg1.1.A	26.20	homo-dimer	BLAST	X-ray	1.89Å	0.35	0.40	GAMMA-BUTYROBETAINE DIOXYGENASE
3n6w.1.A	26.20	homo-dimer	BLAST	X-ray	2.00Å	0.35	0.40	Gamma-butyrobetaine dioxygenase
3o2g.1.A	26.20	homo-dimer	BLAST	X-ray	1.78Å	0.35	0.40	Gamma-butyrobetaine dioxygenase
4c8r.2.B	26.20	homo-dimer	BLAST	X-ray	2.82Å	0.35	0.40	GAMMA-BUTYROBETAINE DIOXYGENASE
4c8r.2.A	26.20	homo-dimer	BLAST	X-ray	2.82Å	0.35	0.40	GAMMA-BUTYROBETAINE DIOXYGENASE
4c8r.3.B	26.20	homo-dimer	BLAST	X-ray	2.82Å	0.35	0.40	GAMMA-BUTYROBETAINE DIOXYGENASE
2l6p.1.A	16.67	monomer	HHblits	NMR	NA	0.27	0.17	PhaC1, phaC2 and phaD genes
2l6n.1.A	16.88	monomer	HHblits	NMR	NA	0.28	0.17	uncharacterized protein YP_001092504.1
3luu.1.A	8.86	monomer	HHblits	X-ray	1.93Å	0.24	0.17	Uncharacterized protein
3w21.1.B	14.04	homo-dimer	HHblits	X-ray	1.98Å	0.27	0.12	Putative uncharacterized protein
3w20.1.A	14.04	homo-dimer	HHblits	X-ray	1.77Å	0.27	0.12	Putative uncharacterized protein
2dbi.1.A	10.53	monomer	HHblits	X-ray	2.05Å	0.25	0.12	Hypothetical protein ybiU
2fcu.2.A	18.60	monomer	HHblits	X-ray	1.60Å	0.30	0.09	syringomycin biosynthesis enzyme 2
2fcu.1.A	18.60	monomer	HHblits	X-ray	1.60Å	0.30	0.09	syringomycin biosynthesis enzyme 2
2fcv.1.A	18.60	monomer	HHblits	X-ray	1.80Å	0.30	0.09	syringomycin biosynthesis enzyme 2
3gja.1.A	16.28	monomer	HHblits	X-ray	2.20Å	0.29	0.09	CytC3
3emr.1.A	9.30	monomer	HHblits	X-ray	1.85Å	0.25	0.09	EctD
4rgk.1.A	12.20	homo-dimer	HHblits	X-ray	2.15Å	0.28	0.09	Uncharacterized protein
2csg.1.A	14.63	monomer	HHblits	X-ray	2.90Å	0.27	0.09	putative cytoplasmic protein
2opw.1.A	4.88	monomer	HHblits	X-ray	1.90Å	0.26	0.09	PHYHD1 protein
2l6p.1.A	22.22	monomer	HHblits	NMR	NA	0.34	0.08	PhaC1, phaC2 and phaD genes
4j25.8.A	13.16	monomer	HHblits	X-ray	1.97Å	0.28	0.08	Putative uncharacterized protein
4j25.5.A	13.16	monomer	HHblits	X-ray	1.97Å	0.28	0.08	Putative uncharacterized protein
4iw3.1.A	13.16	hetero-oligomer	HHblits	X-ray	2.70Å	0.28	0.08	Putative uncharacterized protein
4j25.1.A	13.16	monomer	HHblits	X-ray	1.97Å	0.28	0.08	Putative uncharacterized protein
2l6n.1.A	11.11	monomer	HHblits	NMR	NA	0.29	0.08	uncharacterized protein YP_001092504.1
3luu.1.A	16.67	monomer	HHblits	X-ray	1.93Å	0.29	0.08	Uncharacterized protein
4nao.1.A	14.29	homo-dimer	HHblits	X-ray	1.65Å	0.27	0.08	Putative oxygenase
4bg1.1.A	14.29	homo-dimer	HHblits	X-ray	1.89Å	0.29	0.06	GAMMA-BUTYROBETAINE DIOXYGENASE
3o2g.1.A	14.29	homo-dimer	HHblits	X-ray	1.78Å	0.29	0.06	Gamma-butyrobetaine dioxygenase
3n6w.1.A	14.29	homo-dimer	HHblits	X-ray	2.00Å	0.29	0.06	Gamma-butyrobetaine dioxygenase

4c8r.2.B	14.29	homo-dimer	HHblits	X-ray	2.82Å	0.29	0.06	GAMMA-BUTYROBETAINE DIOXYGENASE
4c8r.2.A	14.29	homo-dimer	HHblits	X-ray	2.82Å	0.29	0.06	GAMMA-BUTYROBETAINE DIOXYGENASE
4c8r.3.B	14.29	homo-dimer	HHblits	X-ray	2.82Å	0.29	0.06	GAMMA-BUTYROBETAINE DIOXYGENASE
1wdi.1.A	22.73	monomer	HHblits	X-ray	2.10Å	0.32	0.05	hypothetical protein TT0907
1yy3.1.A	35.00	monomer	HHblits	X-ray	2.88Å	0.37	0.04	S-adenosylmethionine:tRNA ribosyltransferase-isomerase
1tz5.1.A	4.35	monomer	HHblits	NMR	NA	0.23	0.05	Chimera of Pancreatic hormone and Neuropeptide Y
1ljv.1.A	4.35	monomer	HHblits	NMR	NA	0.22	0.05	PANCREATIC HORMONE
1vky.1.A	14.29	homo-dimer	HHblits	X-ray	2.00Å	0.29	0.05	S-adenosylmethionine:tRNA ribosyltransferase-isomerase
2h4b.1.A	9.09	homo-dimer	HHblits	NMR	NA	0.24	0.05	Pancreatic hormone
2h3t.1.A	9.09	monomer	HHblits	NMR	NA	0.24	0.05	Pancreatic hormone
2h3s.1.A	9.09	monomer	HHblits	NMR	NA	0.24	0.05	Pancreatic hormone
1qbf.1.A	4.55	monomer	HHblits	NMR	NA	0.23	0.05	PEPTIDE YY
2dez.1.A	4.55	monomer	HHblits	NMR	NA	0.23	0.05	Peptide YY
2df0.1.A	4.55	monomer	HHblits	NMR	NA	0.23	0.05	Peptide YY
2oon.1.A	4.55	monomer	HHblits	NMR	NA	0.23	0.05	Peptide YY
2oop.1.A	4.55	monomer	HHblits	NMR	NA	0.23	0.05	Peptide YY
2l60.1.A	4.55	monomer	HHblits	NMR	NA	0.23	0.05	Peptide YY
1ruu.1.A	4.55	monomer	HHblits	NMR	NA	0.23	0.05	Peptide YY
2rlk.1.A	4.55	monomer	HHblits	NMR	NA	0.23	0.05	Peptide YY
1ru5.1.A	4.55	monomer	HHblits	NMR	NA	0.23	0.05	Peptide YY
1ron.1.A	9.09	monomer	HHblits	NMR	NA	0.23	0.05	NEUROPEPTIDE Y
1f8p.1.A	9.09	monomer	HHblits	NMR	NA	0.23	0.05	NEUROPEPTIDE Y (PNPY)
1tz4.1.A	9.09	monomer	HHblits	NMR	NA	0.23	0.05	Chimera of Neuropeptide Y and Pancreatic hormone
1fvn.1.A	4.55	monomer	HHblits	NMR	NA	0.21	0.05	NEUROPEPTIDE Y
1icy.1.A	4.55	monomer	HHblits	NMR	NA	0.21	0.05	NEUROPEPTIDE Y
2bf9.1.A	9.52	homo-dimer	HHblits	X-ray	0.99Å	0.24	0.05	PANCREATIC HORMONE
1ppt.1.A	9.52	homo-dimer	HHblits	X-ray	1.37Å	0.24	0.05	AVIAN PANCREATIC POLYPEPTIDE
1bba.1.A	4.76	monomer	HHblits	NMR	NA	0.23	0.05	BOVINE PANCREATIC POLYPEPTIDE
2k76.1.A	11.76	monomer	HHblits	NMR	NA	0.25	0.04	pGolemi