












# Phyre2

|               |                                  |
|---------------|----------------------------------|
| Email         | mdejesus@rockefeller.edu         |
| Description   | RVBD3561_(fadD3)_4001816_4003339 |
| Date          | Fri Aug 9 18:20:24 BST 2019      |
| Unique Job ID | 18a4c6c6e5684896                 |

Detailed template information

| #  | Template                | Alignment Coverage                                                                            | 3D Model | Confidence | % i.d. | Template Information                                                                                                                                                                                                                                            |
|----|-------------------------|-----------------------------------------------------------------------------------------------|----------|------------|--------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1  | <a href="#">c6eqoB_</a> |  Alignment   |          | 100.0      | 27     | <b>PDB header:</b> oxidoreductase<br><b>Chain:</b> B: <b>PDB Molecule:</b> acetyl-coenzyme a synthetase;<br><b>PDBTitle:</b> tri-functional propionyl-coa synthase of erythrobacter sp. nap1 with2 bound nadp+ and phosphomethylphosphonic acid adenylate ester |
| 2  | <a href="#">c6p1jA_</a> |  Alignment   |          | 100.0      | 25     | <b>PDB header:</b> biosynthetic protein<br><b>Chain:</b> A: <b>PDB Molecule:</b> txo2;<br><b>PDBTitle:</b> the structure of condensation and adenylation domains of teixobactin-2 producing nonribosomal peptide synthetase txo2 serine module                  |
| 3  | <a href="#">c5es8A_</a> |  Alignment   |          | 100.0      | 23     | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> linear gramicidin synthetase subunit a;<br><b>PDBTitle:</b> crystal structure of the initiation module of lgra in the thiolation2 state                                                      |
| 4  | <a href="#">c5gxdA_</a> |  Alignment   |          | 100.0      | 24     | <b>PDB header:</b> lyase<br><b>Chain:</b> A: <b>PDB Molecule:</b> amp-dependent synthetase and ligase;<br><b>PDBTitle:</b> structure of acryloyl-coa lyase prpe from dinoroseobacter shibae dfi2 12                                                             |
| 5  | <a href="#">c5ifiA_</a> |  Alignment |          | 100.0      | 24     | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> acetyl-coenzyme a synthetase;<br><b>PDBTitle:</b> crystal structure of acetyl-coa synthetase in complex with adenosine-2 5'-propylphosphate from cryptococcus neoformans h99                 |
| 6  | <a href="#">d1pg4a_</a> |  Alignment |          | 100.0      | 23     | <b>Fold:</b> Acetyl-CoA synthetase-like<br><b>Superfamily:</b> Acetyl-CoA synthetase-like<br><b>Family:</b> Acetyl-CoA synthetase-like                                                                                                                          |
| 7  | <a href="#">c5ja2A_</a> |  Alignment |          | 100.0      | 23     | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> enterobactin synthase component f;<br><b>PDBTitle:</b> entf, a terminal nonribosomal peptide synthetase module bound to the2 non-native mbth-like protein pa2412                             |
| 8  | <a href="#">c5u89A_</a> |  Alignment |          | 100.0      | 21     | <b>PDB header:</b> hydrolase/inhibitor<br><b>Chain:</b> A: <b>PDB Molecule:</b> amino acid adenylation domain protein;<br><b>PDBTitle:</b> crystal structure of a cross-module fragment from the dimodular nrps2 dhbf                                           |
| 9  | <a href="#">d1ry2a_</a> |  Alignment |          | 100.0      | 19     | <b>Fold:</b> Acetyl-CoA synthetase-like<br><b>Superfamily:</b> Acetyl-CoA synthetase-like<br><b>Family:</b> Acetyl-CoA synthetase-like                                                                                                                          |
| 10 | <a href="#">c2vsqA_</a> |  Alignment |          | 100.0      | 22     | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> surfactin synthetase subunit 3;<br><b>PDBTitle:</b> structure of surfactin a synthetase c (srfa-c), a nonribosomal peptide2 synthetase termination module                                    |
| 11 | <a href="#">c6n8eA_</a> |  Alignment |          | 100.0      | 23     | <b>PDB header:</b> hydrolase<br><b>Chain:</b> A: <b>PDB Molecule:</b> holo-obif1;<br><b>PDBTitle:</b> crystal structure of holo-obif1, a five domain nonribosomal peptide2 synthetase from burkholderia diffusa                                                 |

|    |                         |           |              |       |    |                                                                                                                                                                                                                                                                                                               |
|----|-------------------------|-----------|--------------|-------|----|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 12 | <a href="#">c5wmmA_</a> | Alignment |              | 100.0 | 23 | <b>PDB header:</b> biosynthetic protein<br><b>Chain:</b> A; <b>PDB Molecule:</b> nrps;<br><b>PDBTitle:</b> crystal structure of an adenylation domain interrupted by a2 methylation domain (ama4) from nonribosomal peptide synthetase tios                                                                   |
| 13 | <a href="#">c3e7wA_</a> | Alignment |              | 100.0 | 19 | <b>PDB header:</b> ligase<br><b>Chain:</b> A; <b>PDB Molecule:</b> d-alanine--poly(phosphoribitol) ligase subunit 1;<br><b>PDBTitle:</b> crystal structure of dlta: implications for the reaction mechanism of 2 non-ribosomal peptide synthetase (nrps) adenylation domains                                  |
| 14 | <a href="#">c5ie2A_</a> | Alignment |              | 100.0 | 29 | <b>PDB header:</b> ligase<br><b>Chain:</b> A; <b>PDB Molecule:</b> oxalate--coa ligase;<br><b>PDBTitle:</b> crystal structure of a plant enzyme                                                                                                                                                               |
| 15 | <a href="#">c3vngA_</a> | Alignment |              | 100.0 | 26 | <b>PDB header:</b> ligase<br><b>Chain:</b> A; <b>PDB Molecule:</b> nrps adenylation protein cytc1;<br><b>PDBTitle:</b> co-crystal structure of nrps adenylation protein cytc1 with atp from 2 streptomyces                                                                                                    |
| 16 | <a href="#">c4wv3A_</a> | Alignment |              | 100.0 | 25 | <b>PDB header:</b> ligase/ligase inhibitor<br><b>Chain:</b> A; <b>PDB Molecule:</b> anthranilate-coa ligase;<br><b>PDBTitle:</b> crystal structure of the anthranilate coa ligase auaeii in complex2 with anthranoyl-amp                                                                                      |
| 17 | <a href="#">c4eatB_</a> | Alignment |              | 100.0 | 25 | <b>PDB header:</b> ligase<br><b>Chain:</b> B; <b>PDB Molecule:</b> benzoate-coenzyme a ligase;<br><b>PDBTitle:</b> crystal structure of a benzoate coenzyme a ligase                                                                                                                                          |
| 18 | <a href="#">d1mdba_</a> | Alignment |              | 100.0 | 25 | <b>Fold:</b> Acetyl-CoA synthetase-like<br><b>Superfamily:</b> Acetyl-CoA synthetase-like<br><b>Family:</b> Acetyl-CoA synthetase-like                                                                                                                                                                        |
| 19 | <a href="#">c5msdA_</a> | Alignment |              | 100.0 | 23 | <b>PDB header:</b> oxidoreductase<br><b>Chain:</b> A; <b>PDB Molecule:</b> carboxylic acid reductase;<br><b>PDBTitle:</b> structure of the a domain of carboxylic acid reductase (car) from 2 nocardia iowensis in complex with amp and benzoic acid                                                          |
| 20 | <a href="#">c4wd1A_</a> | Alignment |              | 100.0 | 20 | <b>PDB header:</b> ligase<br><b>Chain:</b> A; <b>PDB Molecule:</b> acetoacetate-coa ligase;<br><b>PDBTitle:</b> acetoacetyl-coa synthetase from streptomyces lividans                                                                                                                                         |
| 21 | <a href="#">d3cw9a1</a> | Alignment | not modelled | 100.0 | 31 | <b>Fold:</b> Acetyl-CoA synthetase-like<br><b>Superfamily:</b> Acetyl-CoA synthetase-like<br><b>Family:</b> Acetyl-CoA synthetase-like                                                                                                                                                                        |
| 22 | <a href="#">c5wm7A_</a> | Alignment | not modelled | 100.0 | 29 | <b>PDB header:</b> ligase<br><b>Chain:</b> A; <b>PDB Molecule:</b> salicylate-amp ligase;<br><b>PDBTitle:</b> crystal structure of cahj in complex with amp                                                                                                                                                   |
| 23 | <a href="#">c3ni2A_</a> | Alignment | not modelled | 100.0 | 28 | <b>PDB header:</b> ligase<br><b>Chain:</b> A; <b>PDB Molecule:</b> 4-coumarate:coa ligase;<br><b>PDBTitle:</b> crystal structures and enzymatic mechanisms of a populus tomentosa 4-2 coumarate:coa ligase                                                                                                    |
| 24 | <a href="#">c6h1bA_</a> | Alignment | not modelled | 100.0 | 28 | <b>PDB header:</b> ligase<br><b>Chain:</b> A; <b>PDB Molecule:</b> fatty acid coa ligase;<br><b>PDBTitle:</b> structure of amide bond synthetase mcba k483a mutant from 2 marinactinospora thermotolerans                                                                                                     |
| 25 | <a href="#">c6iibA_</a> | Alignment | not modelled | 100.0 | 25 | <b>PDB header:</b> ligase<br><b>Chain:</b> A; <b>PDB Molecule:</b> amp-binding domain protein;<br><b>PDBTitle:</b> structure of 3-methylmercaptopropionate coa ligase mutant k523a in2 complex with amp and mmpa                                                                                              |
| 26 | <a href="#">c4zxiA_</a> | Alignment | not modelled | 100.0 | 23 | <b>PDB header:</b> biosynthetic protein<br><b>Chain:</b> A; <b>PDB Molecule:</b> enterobactin synthase component f;<br><b>PDBTitle:</b> crystal structure of holo-entf a nonribosomal peptide synthetase in2 the thioester-forming conformation                                                               |
| 27 | <a href="#">c4oxiA_</a> | Alignment | not modelled | 100.0 | 19 | <b>PDB header:</b> ligase<br><b>Chain:</b> A; <b>PDB Molecule:</b> enterobactin synthetase component f-related protein;<br><b>PDBTitle:</b> crystal structure of vibrio cholerae adenylation domain alme in2 complex with glycylic-adenosine-5'-phosphate                                                     |
| 28 | <a href="#">c5x8gA_</a> | Alignment | not modelled | 100.0 | 32 | <b>PDB header:</b> ligase<br><b>Chain:</b> A; <b>PDB Molecule:</b> 2-succinylbenzoate--coa ligase;<br><b>PDBTitle:</b> binary complex structure of a double mutant i454ra456k of o-2 succinylbenzoate coa synthetase (mene) from bacillus subtilis bound3 with its product analogue osb-ncoa at 1.90 angstrom |

|    |                         |           |              |       |    |                                                                                                                                                                                                                                                                                                       |
|----|-------------------------|-----------|--------------|-------|----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 29 | <a href="#">c3r44A_</a> | Alignment | not modelled | 100.0 | 31 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> fatty acyl coa synthetase fadd13 (fatty-acyl-coa<br><b>PDBTitle:</b> mycobacterium tuberculosis fatty acyl coa synthetase                                                                                                          |
| 30 | <a href="#">c5u2aA_</a> | Alignment | not modelled | 100.0 | 20 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> amp-dependent synthetase and ligase;<br><b>PDBTitle:</b> crystal structure of brucella canis acyl-coa synthetase                                                                                                                   |
| 31 | <a href="#">c4zxiA_</a> | Alignment | not modelled | 100.0 | 23 | <b>PDB header:</b> biosynthetic protein<br><b>Chain:</b> A: <b>PDB Molecule:</b> tyrocidine synthetase 3;<br><b>PDBTitle:</b> crystal structure of holo-ab3403 a four domain nonribosomal peptide2 synthetase bound to amp and glycine                                                                |
| 32 | <a href="#">c5e7qB_</a> | Alignment | not modelled | 100.0 | 24 | <b>PDB header:</b> transferase<br><b>Chain:</b> B: <b>PDB Molecule:</b> acyl-coa synthetase;<br><b>PDBTitle:</b> acyl-coa synthetase ptma2 from streptomyces platensis                                                                                                                                |
| 33 | <a href="#">c4dg8A_</a> | Alignment | not modelled | 100.0 | 18 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> pa1221;<br><b>PDBTitle:</b> structure of pa1221, an nrps protein containing adenylation and pcp2 domains                                                                                                                           |
| 34 | <a href="#">c5keiA_</a> | Alignment | not modelled | 100.0 | 25 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> 2,3-dihydroxybenzoate-amp ligase;<br><b>PDBTitle:</b> mycobacterium smegmatis mbta apo structure                                                                                                                                   |
| 35 | <a href="#">c5mstA_</a> | Alignment | not modelled | 100.0 | 22 | <b>PDB header:</b> oxidoreductase<br><b>Chain:</b> A: <b>PDB Molecule:</b> thioester reductase domain-containing protein;<br><b>PDBTitle:</b> structure of the a domain of carboxylic acid reductase (car) from2 segniliparus rugosus in complex with amp and a co-purified carboxylic3 acid          |
| 36 | <a href="#">c5aplA_</a> | Alignment | not modelled | 100.0 | 26 | <b>PDB header:</b> transferase<br><b>Chain:</b> A: <b>PDB Molecule:</b> adenylation domain;<br><b>PDBTitle:</b> structure of the adenylation domain thr1 involved in the biosynthesis2 of 4-chlorothreonine in streptomyces sp. oh-5093, apo structure                                                |
| 37 | <a href="#">c5mssA_</a> | Alignment | not modelled | 100.0 | 22 | <b>PDB header:</b> oxidoreductase<br><b>Chain:</b> A: <b>PDB Molecule:</b> thioester reductase domain-containing protein;<br><b>PDBTitle:</b> structure of the a-pcp didomain of carboxylic acid reductase (car)2 from segniliparus rugosus in complex with amp                                       |
| 38 | <a href="#">c6ac3B_</a> | Alignment | not modelled | 100.0 | 24 | <b>PDB header:</b> luminescent protein<br><b>Chain:</b> B: <b>PDB Molecule:</b> red-bioluminescence eliciting luciferase;<br><b>PDBTitle:</b> structure of a natural red emitting luciferase from phrixothrix hirtus2 (p3121 crystal form)                                                            |
| 39 | <a href="#">c2d1tA_</a> | Alignment | not modelled | 100.0 | 25 | <b>PDB header:</b> oxidoreductase<br><b>Chain:</b> A: <b>PDB Molecule:</b> luciferin 4-monooxygenase;<br><b>PDBTitle:</b> crystal structure of the thermostable japanese firefly2 luciferase red-color emission s286n mutant complexed with3 high-energy intermediate analogue                        |
| 40 | <a href="#">d1lcia_</a> | Alignment | not modelled | 100.0 | 23 | <b>Fold:</b> Acetyl-CoA synthetase-like<br><b>Superfamily:</b> Acetyl-CoA synthetase-like<br><b>Family:</b> Acetyl-CoA synthetase-like                                                                                                                                                                |
| 41 | <a href="#">d1amua_</a> | Alignment | not modelled | 100.0 | 19 | <b>Fold:</b> Acetyl-CoA synthetase-like<br><b>Superfamily:</b> Acetyl-CoA synthetase-like<br><b>Family:</b> Acetyl-CoA synthetase-like                                                                                                                                                                |
| 42 | <a href="#">c3eynB_</a> | Alignment | not modelled | 100.0 | 22 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> acyl-coenzyme a synthetase acsm2a;<br><b>PDBTitle:</b> crystal structure of human acyl-coa synthetase medium-chain2 family member 2a (l64p mutation) in a complex with coa                                                         |
| 43 | <a href="#">c4fuqD_</a> | Alignment | not modelled | 100.0 | 32 | <b>PDB header:</b> ligase<br><b>Chain:</b> D: <b>PDB Molecule:</b> malonyl coa synthetase;<br><b>PDBTitle:</b> crystal structure of apo matb from rhodopseudomonas palustris                                                                                                                          |
| 44 | <a href="#">c3etcB_</a> | Alignment | not modelled | 100.0 | 20 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> amp-binding protein;<br><b>PDBTitle:</b> 2.1 a structure of acyl-adenylate synthetase from methanosarcina2 acetivorans containing a link between lys256 and cys298                                                                 |
| 45 | <a href="#">c4dg9A_</a> | Alignment | not modelled | 100.0 | 18 | <b>PDB header:</b> ligase/inhibitor<br><b>Chain:</b> A: <b>PDB Molecule:</b> pa1221;<br><b>PDBTitle:</b> structure of holo-pa1221, an nrps protein containing adenylation and2 pcp domains bound to vinylsulfonamide inhibitor                                                                        |
| 46 | <a href="#">c1amuB_</a> | Alignment | not modelled | 100.0 | 18 | <b>PDB header:</b> peptide synthetase<br><b>Chain:</b> B: <b>PDB Molecule:</b> gramicidin synthetase 1;<br><b>PDBTitle:</b> phenylalanine activating domain of gramicidin synthetase 12 in a complex with amp and phenylalanine                                                                       |
| 47 | <a href="#">c3rg2H_</a> | Alignment | not modelled | 100.0 | 21 | <b>PDB header:</b> ligase<br><b>Chain:</b> H: <b>PDB Molecule:</b> enterobactin synthase component e (ente), 2,3-dihydro-2,3-<br><b>PDBTitle:</b> structure of a two-domain nrps fusion protein containing the ente2 adenylation domain and entb aryl-carrier protein from enterobactin3 biosynthesis |
| 48 | <a href="#">c3dhvA_</a> | Alignment | not modelled | 100.0 | 20 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> d-alanine-poly(phosphoribitol) ligase;<br><b>PDBTitle:</b> crystal structure of dlta protein in complex with d-alanine2 adenylate                                                                                                  |
| 49 | <a href="#">c4ir7A_</a> | Alignment | not modelled | 100.0 | 22 | <b>PDB header:</b> transferase<br><b>Chain:</b> A: <b>PDB Molecule:</b> long chain fatty acid coa ligase fadd10;<br><b>PDBTitle:</b> crystal structure of mtb fadd10 in complex with dodecanoyl-amp                                                                                                   |
| 50 | <a href="#">c6akdA_</a> | Alignment | not modelled | 100.0 | 22 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> amp-dependent synthetase and ligase;<br><b>PDBTitle:</b> crystal structure of idn17                                                                                                                                                |
| 51 | <a href="#">c2v7bB_</a> | Alignment | not modelled | 100.0 | 25 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> benzoate-coenzyme a ligase;<br><b>PDBTitle:</b> crystal structures of a benzoate coa ligase from2 burkholderia xenovorans lb400                                                                                                    |
| 52 | <a href="#">c3gqwB_</a> | Alignment | not modelled | 100.0 | 22 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> fatty acid amp ligase;<br><b>PDBTitle:</b> crystal structure of a fatty acid amp ligase from e. coli with an acyl2 adenylate product bound                                                                                         |

|    |                         |           |              |       |    |                                                                                                                                                                                                                                                                     |
|----|-------------------------|-----------|--------------|-------|----|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 53 | <a href="#">c4d56A_</a> | Alignment | not modelled | 100.0 | 23 | <b>PDB header:</b> hydrolase<br><b>Chain:</b> A: <b>PDB Molecule:</b> apnaa1;<br><b>PDBTitle:</b> understanding bi-specificity of a-domains                                                                                                                         |
| 54 | <a href="#">c5ijqB_</a> | Alignment | not modelled | 100.0 | 24 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> amp-dependent synthetase and ligase;<br><b>PDBTitle:</b> crystal structure of idn11                                                                                                              |
| 55 | <a href="#">c3kxwA_</a> | Alignment | not modelled | 100.0 | 21 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> saframycin mx1 synthetase b;<br><b>PDBTitle:</b> the crystal structure of fatty acid amp ligase from legionella2 pneumophila                                                                     |
| 56 | <a href="#">c5ey8D_</a> | Alignment | not modelled | 100.0 | 23 | <b>PDB header:</b> ligase<br><b>Chain:</b> D: <b>PDB Molecule:</b> acyl-coa synthase;<br><b>PDBTitle:</b> structure of fadd32 from mycobacterium smegmatis complexed to ampc20                                                                                      |
| 57 | <a href="#">c3l8cA_</a> | Alignment | not modelled | 100.0 | 19 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> d-alanine--poly(phosphoribitol) ligase subunit 1;<br><b>PDBTitle:</b> structure of probable d-alanine--poly(phosphoribitol) ligase subunit-12 from streptococcus pyogenes                        |
| 58 | <a href="#">c3iteB_</a> | Alignment | not modelled | 100.0 | 16 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> sidn siderophore synthetase;<br><b>PDBTitle:</b> the third adenylation domain of the fungal sidn non-ribosomal peptide2 synthetase                                                               |
| 59 | <a href="#">c3tsyA_</a> | Alignment | not modelled | 100.0 | 23 | <b>PDB header:</b> ligase, transferase<br><b>Chain:</b> A: <b>PDB Molecule:</b> fusion protein 4-coumarate--coa ligase 1, resveratrol<br><b>PDBTitle:</b> 4-coumaroyl-coa ligase::stilbene synthase fusion protein                                                  |
| 60 | <a href="#">c4r0mB_</a> | Alignment | not modelled | 100.0 | 20 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> mcyg protein;<br><b>PDBTitle:</b> structure of mcyg a-pcp complexed with phenylalanyl-adenylate                                                                                                  |
| 61 | <a href="#">d1v25a_</a> | Alignment | not modelled | 100.0 | 27 | <b>Fold:</b> Acetyl-CoA synthetase-like<br><b>Superfamily:</b> Acetyl-CoA synthetase-like<br><b>Family:</b> Acetyl-CoA synthetase-like                                                                                                                              |
| 62 | <a href="#">c5buqA_</a> | Alignment | not modelled | 100.0 | 29 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> 2-succinylbenzoate--coa ligase;<br><b>PDBTitle:</b> unliganded form of o-succinylbenzoate coenzyme a synthetase (mene)2 from bacillus subtilis, solved at 1.98 angstroms                         |
| 63 | <a href="#">c3nyrA_</a> | Alignment | not modelled | 100.0 | 29 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> malonyl-coa ligase;<br><b>PDBTitle:</b> malonyl-coa ligase ternary product complex with malonyl-coa and amp2 bound                                                                               |
| 64 | <a href="#">c3iplB_</a> | Alignment | not modelled | 100.0 | 26 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> 2-succinylbenzoate--coa ligase;<br><b>PDBTitle:</b> crystal structure of o-succinylbenzoic acid-coa ligase from2 staphylococcus aureus subsp. aureus mu50                                        |
| 65 | <a href="#">c4r0mA_</a> | Alignment | not modelled | 100.0 | 19 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> mcyg protein;<br><b>PDBTitle:</b> structure of mcyg a-pcp complexed with phenylalanyl-adenylate                                                                                                  |
| 66 | <a href="#">c5c5hA_</a> | Alignment | not modelled | 100.0 | 23 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> 2-succinylbenzoate--coa ligase;<br><b>PDBTitle:</b> r195k e. coli mene with bound osb-ams                                                                                                        |
| 67 | <a href="#">c3g7sA_</a> | Alignment | not modelled | 100.0 | 24 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> long-chain-fatty-acid--coa ligase (fadd-1);<br><b>PDBTitle:</b> crystal structure of a long-chain-fatty-acid-coa ligase2 (fadd1) from archaeoglobus fulgidus                                     |
| 68 | <a href="#">c6ozvA_</a> | Alignment | not modelled | 100.0 | 26 | <b>PDB header:</b> biosynthetic protein<br><b>Chain:</b> A: <b>PDB Molecule:</b> txo1;<br><b>PDBTitle:</b> the structure of condensation and adenylation domains of teixobactin-2 producing nonribosomal peptide synthetase txo1 serine module in3 complex with amp |
| 69 | <a href="#">c4gr5B_</a> | Alignment | not modelled | 100.0 | 24 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> non-ribosomal peptide synthetase;<br><b>PDBTitle:</b> crystal structure of slgn1deltaasub in complex with ampcpp                                                                                 |
| 70 | <a href="#">c4w8oA_</a> | Alignment | not modelled | 100.0 | 22 | <b>PDB header:</b> oxidoreductase<br><b>Chain:</b> A: <b>PDB Molecule:</b> luciferase-like enzymeamp-coa-ligase;<br><b>PDBTitle:</b> structure of the luciferase-like enzyme from the nonluminescent2 zophobas morio mealworm                                       |
| 71 | <a href="#">c3o82B_</a> | Alignment | not modelled | 100.0 | 22 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> peptide arylation enzyme;<br><b>PDBTitle:</b> structure of base n-terminal domain from acinetobacter baumannii bound2 to 5'-o-[n-(2,3-dihydroxybenzoyl)sulfamoyl] adenosine                      |
| 72 | <a href="#">c5jipB_</a> | Alignment | not modelled | 100.0 | 25 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> nonribosomal peptide synthase;<br><b>PDBTitle:</b> crystal structure of cmis6                                                                                                                    |
| 73 | <a href="#">c3o82A_</a> | Alignment | not modelled | 100.0 | 22 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> peptide arylation enzyme;<br><b>PDBTitle:</b> structure of base n-terminal domain from acinetobacter baumannii bound2 to 5'-o-[n-(2,3-dihydroxybenzoyl)sulfamoyl] adenosine                      |
| 74 | <a href="#">c3ivrA_</a> | Alignment | not modelled | 100.0 | 25 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> putative long-chain-fatty-acid coa ligase;<br><b>PDBTitle:</b> crystal structure of putative long-chain-fatty-acid coa ligase from2 rhodospseudomonas palustris cga009                           |
| 75 | <a href="#">c3qyaA_</a> | Alignment | not modelled | 100.0 | 22 | <b>PDB header:</b> oxidoreductase<br><b>Chain:</b> A: <b>PDB Molecule:</b> luciferase;<br><b>PDBTitle:</b> crystal structure of a red-emitter mutant of lampyris turkestanicus2 luciferase                                                                          |
| 76 | <a href="#">c5n81B_</a> | Alignment | not modelled | 100.0 | 20 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> tyrocidine synthase 1;<br><b>PDBTitle:</b> crystal structure of an engineered tyca variant in complex with an o-2 propargyl-beta-tyr-amp analog                                                  |
| 77 | <a href="#">c3t5cA_</a> | Alignment | not modelled | 100.0 | 26 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> probable chain-fatty-acid-coa ligase fadd13;<br><b>PDBTitle:</b> crystal structure of n-terminal domain of fac13 from mycobacterium2 tuberculosis in different space group c2                    |

|     |                         |           |              |       |    |                                                                                                                                                                                                                                                                                    |
|-----|-------------------------|-----------|--------------|-------|----|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 78  | <a href="#">c4lqcA</a>  | Alignment | not modelled | 100.0 | 21 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> bile acid-coenzyme a ligase;<br><b>PDBTitle:</b> crystal structure of a bile acid-coenzyme a ligase (baib) from2 clostridium scindens (vpi 12708) at 2.19 a resolution                                          |
| 79  | <a href="#">c5oe3C</a>  | Alignment | not modelled | 100.0 | 20 | <b>PDB header:</b> ligase<br><b>Chain:</b> C: <b>PDB Molecule:</b> anthranilate--coa ligase;<br><b>PDBTitle:</b> crystal structure of the n-terminal domain of pqsa in complex with2 anthraniloyl-amp (crystal form 1)                                                             |
| 80  | <a href="#">c3wv4B</a>  | Alignment | not modelled | 100.0 | 23 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> non-ribosomal peptide synthetase;<br><b>PDBTitle:</b> crystal structure of vinn                                                                                                                                 |
| 81  | <a href="#">c6abhG</a>  | Alignment | not modelled | 100.0 | 22 | <b>PDB header:</b> luminescent protein<br><b>Chain:</b> G: <b>PDB Molecule:</b> red-bioluminescence eliciting luciferase;<br><b>PDBTitle:</b> structure of a natural red emitting luciferase from phrixothrix hirtus2 (p1 crystal form)                                            |
| 82  | <a href="#">c5burB</a>  | Alignment | not modelled | 100.0 | 24 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> 2-succinylbenzoate--coa ligase;<br><b>PDBTitle:</b> o-succinylbenzoate coenzyme a synthetase (mene) from bacillus2 subtilis, in complex with atp and magnesium ion                                              |
| 83  | <a href="#">c5jipC</a>  | Alignment | not modelled | 100.0 | 26 | <b>PDB header:</b> ligase<br><b>Chain:</b> C: <b>PDB Molecule:</b> nonribosomal peptide synthase;<br><b>PDBTitle:</b> crystal structure of cmis6                                                                                                                                   |
| 84  | <a href="#">c3e53A</a>  | Alignment | not modelled | 100.0 | 22 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> fatty-acid-coa ligase fadd28;<br><b>PDBTitle:</b> crystal structure of n-terminal domain of a fatty acyl amp2 ligase faal28 from mycobacterium tuberculosis                                                     |
| 85  | <a href="#">c4gs5A</a>  | Alignment | not modelled | 100.0 | 17 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> acyl-coa synthetase (amp-forming)/amp-acid ligase ii-like<br><b>PDBTitle:</b> the crystal structure of acyl-coa synthetase (amp-forming)/amp-acid2 ligase ii-like protein from dyadobacter fermentans dsm 18053 |
| 86  | <a href="#">c2y4oA</a>  | Alignment | not modelled | 100.0 | 19 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> phenylacetate-coenzyme a ligase;<br><b>PDBTitle:</b> crystal structure of paak2 in complex with phenylacetyl adenylate                                                                                          |
| 87  | <a href="#">c3qovD</a>  | Alignment | not modelled | 100.0 | 15 | <b>PDB header:</b> ligase<br><b>Chain:</b> D: <b>PDB Molecule:</b> phenylacetate-coenzyme a ligase;<br><b>PDBTitle:</b> crystal structure of a hypothetical acyl-coa ligase (bt_0428) from2 bacteroides thetaiotaomicron vpi-5482 at 2.20 a resolution                             |
| 88  | <a href="#">c2y27B</a>  | Alignment | not modelled | 100.0 | 19 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> phenylacetate-coenzyme a ligase;<br><b>PDBTitle:</b> crystal structure of paak1 in complex with atp from burkholderia2 cenocepacia                                                                              |
| 89  | <a href="#">c3laxA</a>  | Alignment | not modelled | 99.5  | 13 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> phenylacetate-coenzyme a ligase;<br><b>PDBTitle:</b> the crystal structure of a domain of phenylacetate-coenzyme2 a ligase from bacteroides vulgatus atcc 8482                                                  |
| 90  | <a href="#">c3hguB</a>  | Alignment | not modelled | 99.3  | 13 | <b>PDB header:</b> biosynthetic protein<br><b>Chain:</b> B: <b>PDB Molecule:</b> ehpf;<br><b>PDBTitle:</b> structure of phenazine antibiotic biosynthesis protein                                                                                                                  |
| 91  | <a href="#">c5kodA</a>  | Alignment | not modelled | 98.2  | 8  | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> indole-3-acetic acid-amido synthetase gh3.5;<br><b>PDBTitle:</b> crystal structure of gh3.5 acyl acid amido synthetase from arabidopsis2 thaliana                                                               |
| 92  | <a href="#">c6avhA</a>  | Alignment | not modelled | 98.0  | 9  | <b>PDB header:</b> ligase, plant protein<br><b>Chain:</b> A: <b>PDB Molecule:</b> gh3.15 acyl acid amido synthetase;<br><b>PDBTitle:</b> gh3.15 acyl acid amido synthetase                                                                                                         |
| 93  | <a href="#">c4ep1A</a>  | Alignment | not modelled | 97.9  | 10 | <b>PDB header:</b> ligase<br><b>Chain:</b> A: <b>PDB Molecule:</b> jasmonic acid-amido synthetase jar1;<br><b>PDBTitle:</b> crystal structure of arabidopsis thaliana gh3.11 (jar1) in complex2 with ja-ile                                                                        |
| 94  | <a href="#">c4b2gB</a>  | Alignment | not modelled | 97.7  | 9  | <b>PDB header:</b> signaling protein<br><b>Chain:</b> B: <b>PDB Molecule:</b> gh3-1 auxin conjugating enzyme;<br><b>PDBTitle:</b> crystal structure of an indole-3-acetic acid amido synthase from vitis2 vinifera involved in auxin homeostasis                                   |
| 95  | <a href="#">c4ewvB</a>  | Alignment | not modelled | 97.0  | 15 | <b>PDB header:</b> ligase<br><b>Chain:</b> B: <b>PDB Molecule:</b> 4-substituted benzoates-glutamate ligase gh3.12;<br><b>PDBTitle:</b> crystal structure of gh3.12 in complex with ampcpp                                                                                         |
| 96  | <a href="#">d2aya1</a>  | Alignment | not modelled | 80.0  | 13 | <b>Fold:</b> Thermophilic metalloprotease-like<br><b>Superfamily:</b> Thermophilic metalloprotease-like<br><b>Family:</b> Thermophilic metalloprotease (M29)                                                                                                                       |
| 97  | <a href="#">c3smaD</a>  | Alignment | not modelled | 63.3  | 27 | <b>PDB header:</b> transferase<br><b>Chain:</b> D: <b>PDB Molecule:</b> frbf;<br><b>PDBTitle:</b> a new n-acetyltransferase fold in the structure and mechanism of the2 phosphonate biosynthetic enzyme frbf                                                                       |
| 98  | <a href="#">d1piwa2</a> | Alignment | not modelled | 61.9  | 13 | <b>Fold:</b> NAD(P)-binding Rossmann-fold domains<br><b>Superfamily:</b> NAD(P)-binding Rossmann-fold domains<br><b>Family:</b> Alcohol dehydrogenase-like, C-terminal domain                                                                                                      |
| 99  | <a href="#">d1z7wa1</a> | Alignment | not modelled | 59.9  | 14 | <b>Fold:</b> Tryptophan synthase beta subunit-like PLP-dependent enzymes<br><b>Superfamily:</b> Tryptophan synthase beta subunit-like PLP-dependent enzymes<br><b>Family:</b> Tryptophan synthase beta subunit-like PLP-dependent enzymes                                          |
| 100 | <a href="#">d1e3ja2</a> | Alignment | not modelled | 57.9  | 15 | <b>Fold:</b> NAD(P)-binding Rossmann-fold domains<br><b>Superfamily:</b> NAD(P)-binding Rossmann-fold domains<br><b>Family:</b> Alcohol dehydrogenase-like, C-terminal domain                                                                                                      |
| 101 | <a href="#">d1pl8a2</a> | Alignment | not modelled | 56.9  | 17 | <b>Fold:</b> NAD(P)-binding Rossmann-fold domains<br><b>Superfamily:</b> NAD(P)-binding Rossmann-fold domains<br><b>Family:</b> Alcohol dehydrogenase-like, C-terminal domain                                                                                                      |
| 102 | <a href="#">d1kola2</a> | Alignment | not modelled | 56.6  | 15 | <b>Fold:</b> NAD(P)-binding Rossmann-fold domains<br><b>Superfamily:</b> NAD(P)-binding Rossmann-fold domains<br><b>Family:</b> Alcohol dehydrogenase-like, C-terminal domain<br><b>PDB header:</b> transferase                                                                    |



|     |                         |           |              |      |    |                                                                                                                                                                                                                                                                                                       |
|-----|-------------------------|-----------|--------------|------|----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 103 | <a href="#">c4k2bA_</a> | Alignment | not modelled | 56.2 | 20 | <b>Chain:</b> A; <b>PDB Molecule:</b> ntd biosynthesis operon protein ntda;<br><b>PDBTitle:</b> crystal structure of ntda from bacillus subtilis in complex with the2 internal aldimine                                                                                                               |
| 104 | <a href="#">c6mb6A_</a> | Alignment | not modelled | 55.4 | 23 | <b>PDB header:</b> transferase<br><b>Chain:</b> A; <b>PDB Molecule:</b> aac(3)-iiib protein;<br><b>PDBTitle:</b> aac-iiib binary with coash                                                                                                                                                           |
| 105 | <a href="#">c6bc3A_</a> | Alignment | not modelled | 53.6 | 20 | <b>PDB header:</b> transferase/antibiotic<br><b>Chain:</b> A; <b>PDB Molecule:</b> aac 3-vi protein;<br><b>PDBTitle:</b> cryo x-ray structure of sisomicin bound aac-via                                                                                                                              |
| 106 | <a href="#">c5ht0B_</a> | Alignment | not modelled | 53.4 | 18 | <b>PDB header:</b> transferase<br><b>Chain:</b> B; <b>PDB Molecule:</b> aminoglycoside acetyltransferase hmb0005;<br><b>PDBTitle:</b> crystal structure of an antibiotic_nat family aminoglycoside2 acetyltransferase hmb0038 from an uncultured soil metagenomic sample3 in complex with coenzyme a  |
| 107 | <a href="#">c4lmaA_</a> | Alignment | not modelled | 51.7 | 11 | <b>PDB header:</b> transferase<br><b>Chain:</b> A; <b>PDB Molecule:</b> cysteine synthase;<br><b>PDBTitle:</b> crystal structure analysis of o-acetylserine sulfhydrylase cysk1 from2 microcystis aeruginosa 7806                                                                                     |
| 108 | <a href="#">d1rjwa2</a> | Alignment | not modelled | 50.5 | 18 | <b>Fold:</b> NAD(P)-binding Rossmann-fold domains<br><b>Superfamily:</b> NAD(P)-binding Rossmann-fold domains<br><b>Family:</b> Alcohol dehydrogenase-like, C-terminal domain                                                                                                                         |
| 109 | <a href="#">c3ewbX_</a> | Alignment | not modelled | 49.9 | 12 | <b>PDB header:</b> transferase<br><b>Chain:</b> X; <b>PDB Molecule:</b> 2-isopropylmalate synthase;<br><b>PDBTitle:</b> crystal structure of n-terminal domain of putative 2-isopropylmalate2 synthase from listeria monocytogenes                                                                    |
| 110 | <a href="#">c4z1oB_</a> | Alignment | not modelled | 49.1 | 26 | <b>PDB header:</b> transferase<br><b>Chain:</b> B; <b>PDB Molecule:</b> phosphoribosyltransferase;<br><b>PDBTitle:</b> hypoxanthine-guanine-xanthine phosphoribosyltransferase (hgxprrt) from2 sulfobolus sulfataricus in complex with alpha-3 phosphoribosylpyrophosphoric acid (prpp) and magnesium |
| 111 | <a href="#">c3e4fB_</a> | Alignment | not modelled | 47.2 | 20 | <b>PDB header:</b> transferase<br><b>Chain:</b> B; <b>PDB Molecule:</b> aminoglycoside n3-acetyltransferase;<br><b>PDBTitle:</b> crystal structure of ba2930- a putative aminoglycoside n3-2 acetyltransferase from bacillus anthracis                                                                |
| 112 | <a href="#">c6mn5A_</a> | Alignment | not modelled | 46.7 | 26 | <b>PDB header:</b> transferase/antibiotic<br><b>Chain:</b> A; <b>PDB Molecule:</b> aminoglycoside n(3)-acetyltransferase, aac(3)-iva;<br><b>PDBTitle:</b> crystal structure of aminoglycoside acetyltransferase aac(3)-iva,2 h154a mutant, in complex with gentamicin c1a                             |
| 113 | <a href="#">d2nyga1</a> | Alignment | not modelled | 44.6 | 27 | <b>Fold:</b> TTHA0583/YokD-like<br><b>Superfamily:</b> TTHA0583/YokD-like<br><b>Family:</b> Aminoglycoside 3-N-acetyltransferase-like                                                                                                                                                                 |
| 114 | <a href="#">c5i7wA_</a> | Alignment | not modelled | 44.3 | 12 | <b>PDB header:</b> transferase<br><b>Chain:</b> A; <b>PDB Molecule:</b> cysteine synthase a;<br><b>PDBTitle:</b> crystal structure of a cysteine synthase from brucella suis                                                                                                                          |
| 115 | <a href="#">d1iz0a2</a> | Alignment | not modelled | 42.7 | 16 | <b>Fold:</b> NAD(P)-binding Rossmann-fold domains<br><b>Superfamily:</b> NAD(P)-binding Rossmann-fold domains<br><b>Family:</b> Alcohol dehydrogenase-like, C-terminal domain                                                                                                                         |
| 116 | <a href="#">c3eegB_</a> | Alignment | not modelled | 38.7 | 9  | <b>PDB header:</b> transferase<br><b>Chain:</b> B; <b>PDB Molecule:</b> 2-isopropylmalate synthase;<br><b>PDBTitle:</b> crystal structure of a 2-isopropylmalate synthase from2 cytophaga hutchinsonii                                                                                                |
| 117 | <a href="#">c2cw6B_</a> | Alignment | not modelled | 37.6 | 17 | <b>PDB header:</b> lyase<br><b>Chain:</b> B; <b>PDB Molecule:</b> hydroxymethylglutaryl-coa lyase, mitochondrial;<br><b>PDBTitle:</b> crystal structure of human hmg-coa lyase: insights into2 catalysis and the molecular basis for3 hydroxymethylglutaric aciduria                                  |
| 118 | <a href="#">d1d1ta2</a> | Alignment | not modelled | 36.9 | 12 | <b>Fold:</b> NAD(P)-binding Rossmann-fold domains<br><b>Superfamily:</b> NAD(P)-binding Rossmann-fold domains<br><b>Family:</b> Alcohol dehydrogenase-like, C-terminal domain                                                                                                                         |
| 119 | <a href="#">c5u18A_</a> | Alignment | not modelled | 35.9 | 33 | <b>PDB header:</b> transferase<br><b>Chain:</b> A; <b>PDB Molecule:</b> n-3'' methyltransferase;<br><b>PDBTitle:</b> crystal structure of a methyltransferase involved in the biosynthesis2 of gentamicin in complex with the geneticin                                                               |
| 120 | <a href="#">c1uarA_</a> | Alignment | not modelled | 35.3 | 10 | <b>PDB header:</b> transferase<br><b>Chain:</b> A; <b>PDB Molecule:</b> rhodanese;<br><b>PDBTitle:</b> crystal structure of rhodanese from thermus thermophilus hb8                                                                                                                                   |