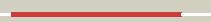
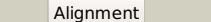
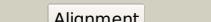
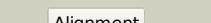


Phyre²

| | |
|---------------|----------------------------------|
| Email | mdejesus@rockefeller.edu |
| Description | RVBD3088 (-) _3454337_3455761 |
| Date | Thu Aug 8 16:20:26 BST 2019 |
| Unique Job ID | 96d5f732e0dfd0c4 |

Detailed template information

| # | Template | Alignment Coverage | 3D Model | Confidence | % i.d. | Template Information |
|----|------------------------|---|---|------------|--------|---|
| 1 | c6chjB |  |  | 100.0 | 29 | PDB header: transferase Chain: B; PDB Molecule: diacylglycerol o-acyltransferase; PDBTitle: wax ester synthase/diacylglycerol acyltransferase from marinobacter2 aquaeolei vt8 |
| 2 | c6n8eA |  |  | 100.0 | 12 | PDB header: hydrolase Chain: A; PDB Molecule: holo-obif1; PDBTitle: crystal structure of holo-obif1, a five domain nonribosomal peptide2 synthetase from burkholderia diffusa |
| 3 | c2vsqA |  |  | 100.0 | 10 | PDB header: ligase Chain: A; PDB Molecule: surfactin synthetase subunit 3; PDBTitle: structure of surfactin a synthetase c (srfa-c), a nonribosomal peptide2 synthetase termination module |
| 4 | c6aefB |  |  | 100.0 | 9 | PDB header: transferase Chain: B; PDB Molecule: polyketide synthase associated protein papa2; PDBTitle: papa2 acyl transferase |
| 5 | c5t81A |  |  | 100.0 | 10 | PDB header: biosynthetic protein Chain: A; PDB Molecule: epob; PDBTitle: rhombohedral crystal form of the epob nrps cyclization-docking2 bidomain from sorangium cellulosum |
| 6 | c5u89A |  |  | 100.0 | 11 | PDB header: hydrolase/inhibitor Chain: A; PDB Molecule: amino acid adenylation domain protein; PDBTitle: crystal structure of a cross-module fragment from the dimodular nrps2 dhhf |
| 7 | c5m6pB |  |  | 100.0 | 14 | PDB header: isomerase Chain: B; PDB Molecule: tyrocidine synthase 2; PDBTitle: crystal structure of the epimerization domain from module 3 of2 tyrocidine synthetase b, tycb3(e) |
| 8 | c5t3eA |  |  | 100.0 | 10 | PDB header: ligase Chain: A; PDB Molecule: bacillamide synthetase heterocyclization domain; PDBTitle: crystal structure of a nonribosomal peptide synthetase2 heterocyclization domain. |
| 9 | c4zxiA |  |  | 100.0 | 13 | PDB header: biosynthetic protein Chain: A; PDB Molecule: tyrocidine synthetase 3; PDBTitle: crystal structure of holo-ab3403 a four domain nonribosomal peptide2 synthetase bound to amp and glycine |
| 10 | c6ad3A |  |  | 100.0 | 9 | PDB header: biosynthetic protein Chain: A; PDB Molecule: lovastatin nonaketide synthase moka; PDBTitle: structural characterization of the condensation domain from monacolin2 k polyketide synthase moka |
| 11 | c2xhgA |  |  | 100.0 | 11 | PDB header: isomerase Chain: A; PDB Molecule: tyrocidine synthetase a; PDBTitle: crystal structure of the epimerization domain from the initiation2 module of tyrocidine biosynthesis |

| | | | | | | |
|----|-------------------------|-----------|---|-------|----|---|
| 12 | c6p1jA | Alignment |  | 100.0 | 13 | PDB header: biosynthetic protein Chain: A: PDB Molecule: txo2; PDBTitle: the structure of condensation and adenylation domains of teixobactin-2 producing nonribosomal peptide synthetase txo2 serine module |
| 13 | c4znmB | Alignment |  | 100.0 | 10 | PDB header: ligase Chain: B: PDB Molecule: c-domain type ii peptide synthetase; PDBTitle: crystal structure of sgcc5 protein from streptomyces globisporus (apo2 form) |
| 14 | c6cg0B | Alignment |  | 100.0 | 11 | PDB header: biosynthetic protein Chain: B: PDB Molecule: condensation domain protein; PDBTitle: molecular basis for condensation domain-mediated chain release from2 the enacyloxin polyketide synthase |
| 15 | c4jn3B | Alignment |  | 100.0 | 15 | PDB header: biosynthetic protein Chain: B: PDB Molecule: cda peptide synthetase i; PDBTitle: crystal structures of the first condensation domain of the cda2 synthetase |
| 16 | c6m7IB | Alignment |  | 100.0 | 10 | PDB header: biosynthetic protein Chain: B: PDB Molecule: putative non-ribosomal peptide synthetase; PDBTitle: complex of oxya with the x-domain from gpa biosynthesis |
| 17 | c4zxjA | Alignment |  | 100.0 | 14 | PDB header: biosynthetic protein Chain: A: PDB Molecule: enterobactin synthase component f; PDBTitle: crystal structure of holo-entf a nonribosomal peptide synthetase in2 the thioester-forming conformation |
| 18 | c2jgpA | Alignment |  | 100.0 | 12 | PDB header: ligase Chain: A: PDB Molecule: tyrocidine synthetase 3; PDBTitle: structure of the tycc5-6 pcp-c bidomain of the tyrocidine synthetase2 tycc |
| 19 | c4tx3B | Alignment |  | 100.0 | 13 | PDB header: oxidoreductase Chain: B: PDB Molecule: peptide synthetase, module 7; PDBTitle: complex of the x-domain and oxyb from teicoplanin biosynthesis |
| 20 | c5ja2A | Alignment |  | 100.0 | 15 | PDB header: ligase Chain: A: PDB Molecule: enterobactin synthase component f; PDBTitle: entf, a terminal nonribosomal peptide synthetase module bound to the2 non-native mbth-like protein pa2412 |
| 21 | c1l5aA | Alignment | not modelled | 100.0 | 10 | PDB header: biosynthetic protein Chain: A: PDB Molecule: amide synthase; PDBTitle: crystal structure of vibh, an nrps condensation enzyme |
| 22 | c6ozvA | Alignment | not modelled | 100.0 | 11 | PDB header: biosynthetic protein Chain: A: PDB Molecule: txo1; PDBTitle: the structure of condensation and adenylation domains of teixobactin-2 producing nonribosomal peptide synthetase txo1 serine module in3 complex with amp |
| 23 | c5dijA | Alignment | not modelled | 100.0 | 8 | PDB header: unknown function Chain: A: PDB Molecule: tqaa; PDBTitle: the crystal structure of ct |
| 24 | c1q9jA | Alignment | not modelled | 100.0 | 15 | PDB header: ligase Chain: A: PDB Molecule: polyketide synthase associated protein 5; PDBTitle: structure of polyketide synthase associated protein 5 from2 mycobacterium tuberculosis |
| 25 | c4hvmC | Alignment | not modelled | 100.0 | 12 | PDB header: biosynthetic protein Chain: C: PDB Molecule: tlmii; PDBTitle: crystal structure of tallysomycin biosynthesis protein tlmii |
| 26 | c3fotA | Alignment | not modelled | 100.0 | 12 | PDB header: transferase Chain: A: PDB Molecule: 15-o-acetyltransferase; PDBTitle: structural and functional characterization of tri trichothecene 15-o-2 acetyltransferase from fusarium sporotrichioides |
| 27 | c6dd2A | Alignment | not modelled | 99.9 | 14 | PDB header: transferase Chain: A: PDB Molecule: probable hydroxycinnamoyl transferase; PDBTitle: crystal structure of selaginina moellendorffii hct |
| 28 | d1l5aa1 | Alignment | not modelled | 99.9 | 8 | Fold: CoA-dependent acyltransferases Superfamily: CoA-dependent acyltransferases Family: NRPS condensation domain (amide synthase) |
| | | | | | | PDB header: transferase |

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|----|-------------------------|-----------|--------------|------|----|--|
| 29 | c4g0bA | Alignment | not modelled | 99.9 | 11 | Chain: A: PDB Molecule: hydroxycinnamoyl-coa shikimate/quinate PDBTitle: structure of native hct from coffeea canephora |
| 30 | d1q9ja1 | Alignment | not modelled | 99.8 | 14 | Fold: CoA-dependent acyltransferases Superfamily: CoA-dependent acyltransferases Family: NRPS condensation domain (amide synthase) |
| 31 | d1l5aa2 | Alignment | not modelled | 99.7 | 13 | Fold: CoA-dependent acyltransferases Superfamily: CoA-dependent acyltransferases Family: NRPS condensation domain (amide synthase) |
| 32 | c2e1ua | Alignment | not modelled | 99.7 | 11 | PDB header: transferase Chain: A: PDB Molecule: acyl transferase; PDBTitle: crystal structure of dendranthema morifolium dmat |
| 33 | d1q9ja2 | Alignment | not modelled | 99.7 | 15 | Fold: CoA-dependent acyltransferases Superfamily: CoA-dependent acyltransferases Family: NRPS condensation domain (amide synthase) |
| 34 | c2bghA | Alignment | not modelled | 99.6 | 11 | PDB header: transferase Chain: A: PDB Molecule: vinorine synthase; PDBTitle: crystal structure of vinorine synthase |
| 35 | c2xr7A | Alignment | not modelled | 99.6 | 8 | PDB header: transferase Chain: A: PDB Molecule: malonyltransferase; PDBTitle: crystal structure of nicotiana tabacum malonyltransferase (ntmat1)2 complexed with malonyl-coa |
| 36 | c4ke4A | Alignment | not modelled | 99.5 | 14 | PDB header: transferase Chain: A: PDB Molecule: hydroxycinnamoyl-coa:shikimate hydroxycinnamoyl PDBTitle: elucidation of the structure and reaction mechanism of sorghum bicolor2 hydroxycinnamoyltransferase and its structural relationship to other3 coa-dependent transferases and synthases |
| 37 | c3b2sA | Alignment | not modelled | 99.2 | 10 | PDB header: transferase Chain: A: PDB Molecule: trichothecene 3-o-acetyltransferase; PDBTitle: crystal structure of f. graminearum tri101 complexed with coenzyme a2 and deoxynivalenol |
| 38 | c2zbaD | Alignment | not modelled | 98.7 | 9 | PDB header: transferase Chain: D: PDB Molecule: trichothecene 3-o-acetyltransferase; PDBTitle: crystal structure of f. sporotrichioides tri101 complexed with2 coenzyme a and t-2 |
| 39 | c6egoB | Alignment | not modelled | 98.2 | 11 | PDB header: oxidoreductase Chain: B: PDB Molecule: acetyl-coenzyme a synthetase; PDBTitle: tri-functional propionyl-coa synthase of erythrobacter sp. nap1 with2 bound nadp+ and phosphomethylphosphonic acid adenylate ester |
| 40 | d1q23a | Alignment | not modelled | 88.2 | 22 | Fold: CoA-dependent acyltransferases Superfamily: CoA-dependent acyltransferases Family: CAT-like |
| 41 | d3claa | Alignment | not modelled | 85.1 | 24 | Fold: CoA-dependent acyltransferases Superfamily: CoA-dependent acyltransferases Family: CAT-like |
| 42 | c5es8A | Alignment | not modelled | 82.0 | 7 | PDB header: ligase Chain: A: PDB Molecule: linear gramicidin synthetase subunit a; PDBTitle: crystal structure of the initiation module of lgra in the thiolation2 state |
| 43 | c3maeA | Alignment | not modelled | 80.7 | 11 | PDB header: transferase Chain: A: PDB Molecule: 2-oxoisovalerate dehydrogenase e2 component, PDBTitle: crystal structure of probable dihydrolipoamide acetyltransferase from2 listeria monocytogenes 4b f2365 |
| 44 | d1ndba2 | Alignment | not modelled | 80.6 | 12 | Fold: CoA-dependent acyltransferases Superfamily: CoA-dependent acyltransferases Family: Choline/Carnitine O-acyltransferase |
| 45 | c3rqcB | Alignment | not modelled | 77.2 | 26 | PDB header: transferase Chain: B: PDB Molecule: probable lipoamide acyltransferase; PDBTitle: crystal structure of the catalytic core of the 2-oxoacid dehydrogenase2 multienzyme complex from thermoplasma acidophilum |
| 46 | c2i9dC | Alignment | not modelled | 77.0 | 23 | PDB header: transferase Chain: C: PDB Molecule: chloramphenicol acetyltransferase; PDBTitle: chloramphenicol acetyltransferase |
| 47 | d1nm8a2 | Alignment | not modelled | 75.7 | 12 | Fold: CoA-dependent acyltransferases Superfamily: CoA-dependent acyltransferases Family: Choline/Carnitine O-acyltransferase |
| 48 | c2h4tB | Alignment | not modelled | 73.5 | 12 | PDB header: transferase Chain: B: PDB Molecule: carnitine o-palmitoyltransferase ii, mitochondrial; PDBTitle: crystal structure of rat carnitine palmitoyltransferase ii |
| 49 | c2fy2A | Alignment | not modelled | 71.3 | 14 | PDB header: transferase Chain: A: PDB Molecule: choline o-acetyltransferase; PDBTitle: structures of ligand bound human choline acetyltransferase provide2 insight into regulation of acetylcholine synthesis |
| 50 | d1scza | Alignment | not modelled | 70.9 | 27 | Fold: CoA-dependent acyltransferases Superfamily: CoA-dependent acyltransferases Family: CAT-like |
| 51 | d1b5sa | Alignment | not modelled | 68.0 | 13 | Fold: CoA-dependent acyltransferases Superfamily: CoA-dependent acyltransferases Family: CAT-like |
| 52 | c1t7qA | Alignment | not modelled | 64.4 | 14 | PDB header: transferase Chain: A: PDB Molecule: carnitine acetyltransferase; PDBTitle: crystal structure of the f565a mutant of murine carnitine2 acetyltransferase in complex with carnitine and coa |
| 53 | c3b8kA | Alignment | not modelled | 62.0 | 14 | PDB header: transferase Chain: A: PDB Molecule: dihydrolipoylysine-residue acetyltransferase; PDBTitle: structure of the truncated human dihydrolipoyl acetyltransferase (e2) |
| | | | | | | Fold: CoA-dependent acyltransferases |

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|----|-------------------------|-----------|--------------|------|----|---|
| 54 | d1dpba | Alignment | not modelled | 61.5 | 12 | Superfamily: CoA-dependent acyltransferases Family: CAT-like |
| 55 | c4n72B | Alignment | not modelled | 54.0 | 11 | PDB header: transferase Chain: B: PDB Molecule: pyruvate dehydrogenase (dihydrolipoyltransacetylase) PDBTitle: catalytic domain from dihydrolipoamide acetyltransferase of pyruvate2 dehydrogenase from escherichia coli |
| 56 | d1xl7a2 | Alignment | not modelled | 50.5 | 11 | Fold: CoA-dependent acyltransferases Superfamily: CoA-dependent acyltransferases Family: Choline/Carnitine O-acyltransferase |
| 57 | c2fyoA | Alignment | not modelled | 49.1 | 12 | PDB header: transferase Chain: A: PDB Molecule: carnitine o-palmitoyltransferase ii, mitochondrial; PDBTitle: crystal structure of rat carnitine palmitoyltransferase 2 in space2 group p43212 |
| 58 | c3I60A | Alignment | not modelled | 37.9 | 13 | PDB header: oxidoreductase Chain: A: PDB Molecule: branched-chain alpha-keto acid dehydrogenase; PDBTitle: crystal structure of branched-chain alpha-keto acid dehydrogenase2 subunit e2 from mycobacterium tuberculosis |
| 59 | c6h60A | Alignment | not modelled | 35.9 | 12 | PDB header: oxidoreductase Chain: A: PDB Molecule: pyruvate dehydrogenase protein x component, mitochondrial; PDBTitle: pseudo-atomic structural model of the e3bp component of the human2 pyruvate dehydrogenase multienzyme complex |
| 60 | c1q6xA | Alignment | not modelled | 34.4 | 17 | PDB header: transferase Chain: A: PDB Molecule: choline o-acetyltransferase; PDBTitle: crystal structure of rat choline acetyltransferase |
| 61 | c2ii4C | Alignment | not modelled | 27.9 | 15 | PDB header: transferase Chain: C: PDB Molecule: lipoamide acyltransferase component of branched-chain PDBTitle: crystal structure of a cubic core of the dihydrolipoamide2 acyltransferase (e2b) component in the branched-chain alpha-ketoacid3 dehydrogenase complex (bckdc), coenzyme a-bound form |
| 62 | c1xl8B | Alignment | not modelled | 24.3 | 16 | PDB header: transferase Chain: B: PDB Molecule: peroxisomal carnitine o-octanoyltransferase; PDBTitle: crystal structure of mouse carnitine octanoyltransferase in2 complex with octanoylcarnitine |
| 63 | d1t1ua2 | Alignment | not modelled | 19.1 | 14 | Fold: CoA-dependent acyltransferases Superfamily: CoA-dependent acyltransferases Family: Choline/Carnitine O-acyltransferase |
| 64 | c5wmmA | Alignment | not modelled | 13.0 | 7 | PDB header: biosynthetic protein Chain: A: PDB Molecule: nmps; PDBTitle: crystal structure of an adenylation domain interrupted by a2 methylation domain (ama4) from nonribosomal peptide synthetase tios |
| 65 | d1ry9a | Alignment | not modelled | 9.9 | 15 | Fold: Secretion chaperone-like Superfamily: Type III secretory system chaperone-like Family: Type III secretory system chaperone |
| 66 | d2fm8a1 | Alignment | not modelled | 8.8 | 10 | Fold: Secretion chaperone-like Superfamily: Type III secretory system chaperone-like Family: Type III secretory system chaperone |
| 67 | d2hh6a1 | Alignment | not modelled | 6.5 | 8 | Fold: Left-handed superhelix Superfamily: BH3980-like Family: BH3980-like |
| 68 | c2k9iB | Alignment | not modelled | 6.0 | 13 | PDB header: dna binding protein Chain: B: PDB Molecule: uncharacterized protein orf56; PDBTitle: nmr structure of plasmid copy control protein orf56 from sulfolobus2 islandicus |
| 69 | c2rrlA | Alignment | not modelled | 5.7 | 5 | PDB header: protein transport Chain: A: PDB Molecule: flagellar hook-length control protein; PDBTitle: solution structure of the c-terminal domain of the flk |
| 70 | c2h0uA | Alignment | not modelled | 5.3 | 11 | PDB header: oxidoreductase Chain: A: PDB Molecule: nadph-flavin oxidoreductase; PDBTitle: crystal structure of nad(p)h-flavin oxidoreductase from helicobacter2 pylori |