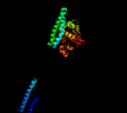
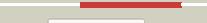
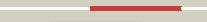


Phyre²

| | |
|---------------|----------------------------------|
| Email | mdejesus@rockefeller.edu |
| Description | RVBD3245c_(mtrB)_3624907_3626610 |
| Date | Thu Aug 8 16:20:45 BST 2019 |
| Unique Job ID | 926c108b1a58c4af |

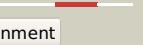
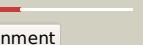
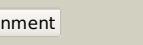
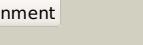
Detailed template information

| # | Template | Alignment Coverage | 3D Model | Confidence | % i.d. | Template Information |
|----|------------------------|---|---|------------|--------|--|
| 1 | c4ew8A |  |  | 100.0 | 28 | PDB header: transferase Chain: A: PDB Molecule: sensor protein divl; PDBTitle: crystal structure of a c-terminal part of tyrosine kinase (divl) from2 caulobacter crescentus cb15 at 2.50 a resolution (psi community3 target, shapiro l.) |
| 2 | c4i5sA |  |  | 100.0 | 33 | PDB header: transferase Chain: A: PDB Molecule: putative histidine kinase covs; vick-like protein; PDBTitle: structure and function of sensor histidine kinase |
| 3 | c3d2rB |  |  | 100.0 | 14 | PDB header: transferase Chain: B: PDB Molecule: [pyruvate dehydrogenase [lipoamide]] kinase isozyme 4; PDBTitle: crystal structure of pyruvate dehydrogenase kinase isoform 4 in2 complex with adp |
| 4 | c2c2aA |  |  | 100.0 | 30 | PDB header: transferase Chain: A: PDB Molecule: sensor histidine kinase; PDBTitle: structure of the entire cytoplasmic portion of a sensor histidine kinase protein |
| 5 | c2q8fA |  |  | 100.0 | 17 | PDB header: transferase Chain: A: PDB Molecule: [pyruvate dehydrogenase [lipoamide]] kinase isozyme 1; PDBTitle: structure of pyruvate dehydrogenase kinase isoform 1 |
| 6 | c4biuB |  |  | 100.0 | 31 | PDB header: transferase Chain: B: PDB Molecule: sensor protein cpxa; PDBTitle: crystal structure of cpxahdc (orthorhombic form 1) |
| 7 | c3d36B |  |  | 100.0 | 21 | PDB header: transferase/transferase inhibitor Chain: B: PDB Molecule: sporulation kinase b; PDBTitle: how to switch off a histidine kinase: crystal structure of2 geobacillus stearothermophilus kinb with the inhibitor sda |
| 8 | c3crlB |  |  | 100.0 | 17 | PDB header: transferase Chain: B: PDB Molecule: pyruvate dehydrogenase [lipoamide] kinase isozyme 2, PDBTitle: crystal structure of the pdhk2-l2 complex. |
| 9 | c6dk8B |  |  | 100.0 | 25 | PDB header: signaling protein Chain: B: PDB Molecule: rets (regulator of exopolysaccharide and type iii PDBTitle: rets kinase region without cobalt |
| 10 | c4kp4B |  |  | 100.0 | 26 | PDB header: transferase/signaling protein Chain: B: PDB Molecule: osmolarity sensor protein envz, histidine kinase; PDBTitle: deciphering cis-trans directionality and visualizing2 autophosphorylation in histidine kinases. |
| 11 | c1y8oA |  |  | 100.0 | 15 | PDB header: transferase Chain: A: PDB Molecule: [pyruvate dehydrogenase [lipoamide]] kinase isozyme 3; PDBTitle: crystal structure of the pdk3-l2 complex |

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|----|-------------------------|--|--------------|-------|----|---|
| 12 | c5idjA | | | 100.0 | 26 | PDB header: transferase Chain: A: PDB Molecule: cell cycle histidine kinase ccka; PDBTitle: bifunctional histidine kinase ccka (domains dhp-ca) in complex with2 adp/mg2+ |
| 13 | c4u7nA | | | 100.0 | 29 | PDB header: transferase Chain: A: PDB Molecule: histidine protein kinase sensor protein; PDBTitle: inactive structure of histidine kinase |
| 14 | c2bu8A | | | 100.0 | 17 | PDB header: transferase Chain: A: PDB Molecule: pyruvate dehydrogenase kinase isoenzyme 2; PDBTitle: crystal structures of human pyruvate dehydrogenase kinase 2 containing2 physiological and synthetic ligands |
| 15 | c1gjvA | | | 100.0 | 14 | PDB header: transferase Chain: A: PDB Molecule: [3-methyl-2-oxobutanoate dehydrogenase [lipoamide]] kinase; PDBTitle: branched-chain alpha-ketoacid dehydrogenase kinase (bck) complexed with2 atp-gamma-s |
| 16 | c3tz5A | | | 100.0 | 13 | PDB header: transferase/transferase inhibitor Chain: A: PDB Molecule: [3-methyl-2-oxobutanoate dehydrogenase [lipoamide]] kinase, PDBTitle: crystal structure of branched-chain alpha-ketoacid dehydrogenase2 kinase/phenylbutyrate complex with adp |
| 17 | c4biyD | | | 100.0 | 30 | PDB header: transferase Chain: D: PDB Molecule: sensor protein cpfa; PDBTitle: crystal structure of cpfa hdc (monoclinic form 2) |
| 18 | c4gczB | | | 100.0 | 22 | PDB header: signaling protein, de novo protein Chain: B: PDB Molecule: blue-light photoreceptor, sensor protein fixl; PDBTitle: structure of a blue-light photoreceptor |
| 19 | c3a0rA | | | 100.0 | 23 | PDB header: transferase Chain: A: PDB Molecule: sensor protein; PDBTitle: crystal structure of histidine kinase thka (tm1359) in complex with2 response regulator protein trra (tm1360) |
| 20 | c1b3qA | | | 100.0 | 18 | PDB header: transferase Chain: A: PDB Molecule: protein (chemotaxis protein chea); PDBTitle: crystal structure of chea-289, a signal transducing histidine kinase |
| 21 | c5idmA | | not modelled | 100.0 | 32 | PDB header: transferase Chain: A: PDB Molecule: cell cycle histidine kinase ccka; PDBTitle: bifunctional histidine kinase ccka (domain, ca) in complex with c-di-2 gmp and amppnp/mg2+ |
| 22 | c6nb0A | | not modelled | 100.0 | 22 | PDB header: transferase Chain: A: PDB Molecule: histidine kinase; PDBTitle: crystal structure of histidine kinase from burkholderia phymatum2 stm815 Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase |
| 23 | d2c2aa2 | | not modelled | 100.0 | 31 | Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: Histidine kinase |
| 24 | c3a0tA | | not modelled | 100.0 | 21 | PDB header: transferase Chain: A: PDB Molecule: sensor protein; PDBTitle: catalytic domain of histidine kinase thka (tm1359) in complex with adp2 and mg ion (trigonal) |
| 25 | c4ctiA | | not modelled | 100.0 | 27 | PDB header: signaling protein Chain: A: PDB Molecule: osmolarity sensor protein envz, af1503; PDBTitle: escherichia coli envz histidine kinase catalytic part fused to2 archaeoglobus fulgidus af1503 hamp domain |
| 26 | d1jm6a2 | | not modelled | 100.0 | 21 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: alpha-ketoacid dehydrogenase kinase, C-terminal domain |
| 27 | c4fmtB | | not modelled | 100.0 | 14 | PDB header: transferase Chain: B: PDB Molecule: chpt protein; PDBTitle: crystal structure of a chpt protein (cc_3470) from caulobacter2 crescentus cb15 at 2.30 a resolution Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase |

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|----|--------------------------|-----------|--------------|-------|----|---|
| 28 | d1id0a_ | Alignment | not modelled | 100.0 | 20 | Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: Histidine kinase |
| 29 | d1bxda_ | Alignment | not modelled | 100.0 | 25 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: Histidine kinase |
| 30 | c6blkB_ | Alignment | not modelled | 100.0 | 28 | PDB header: transferase Chain: B: PDB Molecule: signal transduction histidine-protein kinase/phosphatase PDBTitle: mycobacterial sensor histidine kinase mprb |
| 31 | d1gkza2 | Alignment | not modelled | 100.0 | 20 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: alpha-ketoacid dehydrogenase kinase, C-terminal domain |
| 32 | c4r39A_ | Alignment | not modelled | 100.0 | 16 | PDB header: transferase Chain: A: PDB Molecule: blue-light-activated histidine kinase 2; PDBTitle: histidine kinase domain from erythrobacter litoralis el346 blue-light2 activated histidine kinase |
| 33 | c3sl2A_ | Alignment | not modelled | 99.9 | 29 | PDB header: transferase Chain: A: PDB Molecule: sensor histidine kinase yycg; PDBTitle: atp forms a stable complex with the essential histidine kinase walk2 (yycg) domain |
| 34 | d1ysra1 | Alignment | not modelled | 99.9 | 27 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: Histidine kinase |
| 35 | c4pl9A_ | Alignment | not modelled | 99.9 | 24 | PDB header: transferase Chain: A: PDB Molecule: ethylene receptor 1; PDBTitle: structure of the catalytic domain of etr1 from arabidopsis thaliana |
| 36 | c3jz3B_ | Alignment | not modelled | 99.9 | 28 | PDB header: transferase Chain: B: PDB Molecule: sensor protein qsec; PDBTitle: structure of the cytoplasmic segment of histidine kinase qsec |
| 37 | c2ch4A_ | Alignment | not modelled | 99.9 | 20 | PDB header: transferase/chemotaxis Chain: A: PDB Molecule: chemotaxis protein chea; PDBTitle: complex between bacterial chemotaxis histidine kinase chea2 domains p4 and p5 and receptor-adaptor protein chew |
| 38 | d1i58a_ | Alignment | not modelled | 99.9 | 21 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: Histidine kinase |
| 39 | c4qpkA_ | Alignment | not modelled | 99.9 | 14 | PDB header: signaling protein Chain: A: PDB Molecule: phosphotransferase; PDBTitle: 1.7 angstrom structure of a bacterial phosphotransferase |
| 40 | c5epvB_ | Alignment | not modelled | 99.9 | 13 | PDB header: transferase Chain: B: PDB Molecule: blue-light-activated histidine kinase; PDBTitle: histidine kinase domain from the lov-hk blue-light receptor from2 brucella abortus |
| 41 | c3gieA_ | Alignment | not modelled | 99.9 | 19 | PDB header: transferase Chain: A: PDB Molecule: sensor histidine kinase desk; PDBTitle: crystal structure of deskc_h188e in complex with amppcp |
| 42 | c6e95A_ | Alignment | not modelled | 99.9 | 13 | PDB header: signaling protein Chain: A: PDB Molecule: staphylococcus aureus agrc histidine kinase module fused to PDBTitle: chimeric structure of saccharomyces cerevisiae gcn4 leucine zipper2 fused to staphylococcus aureus agrc cytoplasmic histidine kinase3 module (dataset isotropically truncated by hkl2000) |
| 43 | c4r3aA_ | Alignment | not modelled | 99.9 | 16 | PDB header: signaling protein Chain: A: PDB Molecule: blue-light-activated histidine kinase 2; PDBTitle: erythrobacter litoralis el346 blue-light activated histidine kinase |
| 44 | c4gt8A_ | Alignment | not modelled | 99.9 | 15 | PDB header: transferase Chain: A: PDB Molecule: sensor protein vras; PDBTitle: crystal structure of the catalytic and atp-binding domain from vras in2 complex with adp |
| 45 | d1r62a_ | Alignment | not modelled | 99.8 | 21 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: Histidine kinase |
| 46 | d2hkja3 | Alignment | not modelled | 99.8 | 28 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: DNA gyrase/MutL, N-terminal domain |
| 47 | c3ehgA_ | Alignment | not modelled | 99.8 | 22 | PDB header: transferase Chain: A: PDB Molecule: sensor kinase (yocf protein); PDBTitle: crystal structure of the atp-binding domain of desk in complex with2 atp |
| 48 | c3zxqA_ | Alignment | not modelled | 99.7 | 26 | PDB header: transferase Chain: A: PDB Molecule: hypoxia sensor histidine kinase response regulator dost; PDBTitle: crystal structure of the atp-binding domain of mycobacterium2 tuberculosis dost |
| 49 | c2zbkB_ | Alignment | not modelled | 99.7 | 26 | PDB header: isomerase Chain: B: PDB Molecule: type 2 dna topoisomerase 6 subunit b; PDBTitle: crystal structure of an intact type ii dna topoisomerase:2 insights into dna transfer mechanisms |
| 50 | c1mx0D_ | Alignment | not modelled | 99.7 | 25 | PDB header: isomerase Chain: D: PDB Molecule: type ii dna topoisomerase vi subunit b; PDBTitle: structure of topoisomerase subunit |
| 51 | c4bxiaA_ | Alignment | not modelled | 99.7 | 16 | PDB header: atp-binding protein Chain: A: PDB Molecule: accessory gene regulator protein c; PDBTitle: crystal structure of atp binding domain of agrc from2 staphylococcus aureus |

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|----|-------------------------|--|-----------|--------------|------|----|---|
| 52 | c3xzoB | | Alignment | not modelled | 99.7 | 24 | PDB header: transferase Chain: B; PDB Molecule: redox sensor histidine kinase response regulator devs; PDBTitle: crystal structure of the mutant atp-binding domain of 2 mycobacterium tuberculosis doss |
| 53 | d1ixma | | Alignment | not modelled | 99.6 | 14 | Fold: Sporulation response regulatory protein SpoOB Superfamily: Sporulation response regulatory protein SpoOB Family: Sporulation response regulatory protein SpoOB |
| 54 | c3zrwB | | Alignment | not modelled | 99.6 | 23 | PDB header: signaling protein Chain: B; PDB Molecule: af1503 protein, osmolarity sensor protein envz; PDBTitle: the structure of the dimeric hamp-dhp fusion a291v mutant |
| 55 | c2q2eB | | Alignment | not modelled | 99.6 | 19 | PDB header: isomerase Chain: B; PDB Molecule: type 2 dna topoisomerase 6 subunit b; PDBTitle: crystal structure of the topoisomerase vi holoenzyme from 2 methanosc礼ina mazei |
| 56 | c5jefA | | Alignment | not modelled | 99.5 | 14 | PDB header: transferase Chain: A; PDB Molecule: nitrate/nitrite sensor protein narq; PDBTitle: fragment of nitrate/nitrite sensor histidine kinase narq (wt) in2 asymmetric holo state |
| 57 | d1h7sa2 | | Alignment | not modelled | 99.5 | 17 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: DNA gyrase/MutL, N-terminal domain |
| 58 | d1th8a | | Alignment | not modelled | 99.5 | 22 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: Histidine kinase |
| 59 | d1bkna2 | | Alignment | not modelled | 99.5 | 18 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: DNA gyrase/MutL, N-terminal domain |
| 60 | d1b63a2 | | Alignment | not modelled | 99.4 | 21 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: DNA gyrase/MutL, N-terminal domain |
| 61 | d1y8oa2 | | Alignment | not modelled | 99.4 | 15 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: alpha-ketoacid dehydrogenase kinase, C-terminal domain |
| 62 | d2c2aa1 | | Alignment | not modelled | 99.2 | 32 | Fold: RO-like Superfamily: Homodimeric domain of signal transducing histidine kinase Family: Homodimeric domain of signal transducing histidine kinase |
| 63 | c4mt8A | | Alignment | not modelled | 99.2 | 22 | PDB header: transferase Chain: A; PDB Molecule: ethylene response sensor 1; PDBTitle: structure of the ers1 dimerization and histidine phosphotransfer2 domain from arabidopsis thaliana |
| 64 | c4gn0D | | Alignment | not modelled | 99.1 | 23 | PDB header: signaling protein Chain: D; PDB Molecule: hamp domain of af1503; PDBTitle: de novo phasing of a hamp-complex using an improved arcimboldo method |
| 65 | c5ukvA | | Alignment | not modelled | 99.1 | 32 | PDB header: transferase Chain: A; PDB Molecule: atp-binding protein; PDBTitle: dhp domain of phor of m. tuberculosis - semet |
| 66 | c3lnrA | | Alignment | not modelled | 99.1 | 11 | PDB header: signaling protein Chain: A; PDB Molecule: aerotaxis transducer aer2; PDBTitle: crystal structure of poly-hamp domains from the p. aeruginosa soluble2 receptor aer2 |
| 67 | d1joya | | Alignment | not modelled | 99.0 | 21 | Fold: RO-like Superfamily: Homodimeric domain of signal transducing histidine kinase Family: Homodimeric domain of signal transducing histidine kinase |
| 68 | c3na3A | | Alignment | not modelled | 99.0 | 18 | PDB header: protein binding Chain: A; PDB Molecule: dna mismatch repair protein mlh1; PDBTitle: mutl protein homolog 1 isoform 1 from homo sapiens |
| 69 | c4geeA | | Alignment | not modelled | 98.9 | 16 | PDB header: isomerase/isomerase inhibitor Chain: A; PDB Molecule: dna gyrase subunit b; PDBTitle: pyrrolopyrimidine inhibitors of dna gyrase b and topoisomerase iv,2 part i: structure guided discovery and optimization of dual targeting3 agents with potent, broad-spectrum enzymatic activity. |
| 70 | c4b6cB | | Alignment | not modelled | 98.8 | 18 | PDB header: isomerase Chain: B; PDB Molecule: dna gyrase subunit b,dna gyrase subunit b,dna gyrase PDBTitle: structure of the m. smegmatis gyrb atpase domain in complex with an2 aminopyrazinamide |
| 71 | c3h4IB | | Alignment | not modelled | 98.6 | 16 | PDB header: dna binding protein, protein binding Chain: B; PDB Molecule: dna mismatch repair protein pms1; PDBTitle: crystal structure of n terminal domain of a dna repair protein |
| 72 | c3zx6A | | Alignment | not modelled | 98.6 | 17 | PDB header: signaling Chain: A; PDB Molecule: hamp, methyl-accepting chemotaxis protein i; PDBTitle: structure of hamp(af1503)-tsr fusion - hamp (a291v) mutant |
| 73 | c4emvA | | Alignment | not modelled | 98.5 | 21 | PDB header: isomerase/isomerase inhibitor Chain: A; PDB Molecule: dna topoisomerase iv, b subunit; PDBTitle: crystal structure of a topoisomerase atp inhibitor |
| 74 | d1kija2 | | Alignment | not modelled | 98.4 | 16 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: DNA gyrase/MutL, N-terminal domain |

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|----|-------------------------|---|-----------|--------------|------|----|--|
| 75 | c5j5pB |  | Alignment | not modelled | 98.4 | 24 | PDB header: isomerase/dna Chain: B; PDB Molecule: dna topoisomerase 4 subunit b; PDBTitle: amp-pnp-stabilized atpase domain of topoisomerase iv from streptococcus pneumoniae, complex type i |
| 76 | c1bknA |  | Alignment | not modelled | 98.4 | 24 | PDB header: dna repair Chain: A; PDB Molecule: mutl; PDBTitle: crystal structure of an n-terminal 40kd fragment of e. coli dna mismatch repair protein mutl |
| 77 | c5ix1A |  | Alignment | not modelled | 98.4 | 20 | PDB header: transcription Chain: A; PDB Molecule: morc family cw-type zinc finger protein 3; PDBTitle: crystal structure of mouse morc3 atpase-cw cassette in complex with2 amppnp and h3k4me3 peptide |
| 78 | d1ei1a2 |  | Alignment | not modelled | 98.3 | 25 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: DNA gyrase/MutL, N-terminal domain |
| 79 | d1pvga2 |  | Alignment | not modelled | 98.3 | 15 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: DNA gyrase/MutL, N-terminal domain |
| 80 | d1s16a2 |  | Alignment | not modelled | 98.2 | 18 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: DNA gyrase/MutL, N-terminal domain |
| 81 | d2asxa1 |  | Alignment | not modelled | 98.2 | 25 | Fold: HAMP domain-like Superfamily: HAMP domain-like Family: HAMP domain |
| 82 | c5ofbB |  | Alignment | not modelled | 98.2 | 17 | PDB header: nuclear protein Chain: B; PDB Molecule: morc family cw-type zinc finger protein 2; PDBTitle: crystal structure of human morc2 (residues 1-603) with spinal muscular2 atrophy mutation s871 |
| 83 | c1ei1B |  | Alignment | not modelled | 98.2 | 26 | PDB header: isomerase Chain: B; PDB Molecule: dna gyrase b; PDBTitle: dimerization of e. coli dna gyrase b provides a structural mechanism2 for activating the atpase catalytic center |
| 84 | c1kjB |  | Alignment | not modelled | 98.2 | 21 | PDB header: chaperone Chain: B; PDB Molecule: dna gyrase subunit b; PDBTitle: crystal structure of the 43k atpase domain of thermus thermophilus2 gyrase b in complex with novobiocin |
| 85 | c3iedA |  | Alignment | not modelled | 98.1 | 23 | PDB header: chaperone Chain: A; PDB Molecule: heat shock protein; PDBTitle: crystal structure of n-terminal domain of plasmodium falciparum hsp902 (pf14_0417) in complex with amppn |
| 86 | c3omuB |  | Alignment | not modelled | 98.1 | 26 | PDB header: chaperone Chain: B; PDB Molecule: heat shock protein 83; PDBTitle: crystal structure of the n-terminal domain of an hsp90 from2 trypanosoma brucei, tb10.26.1080 in the presence of a3 thienopyrimidine derivative |
| 87 | c4hymA |  | Alignment | not modelled | 98.1 | 17 | PDB header: isomerase/isomerase inhibitor Chain: A; PDB Molecule: topoisomerase iv, subunit b; PDBTitle: pyrrolopyrimidine inhibitors of dna gyrase b and topoisomerase iv,2 part i: structure guided discovery and optimization of dual targeting3 agents with potent, broad-spectrum enzymatic activity. |
| 88 | c1s16B |  | Alignment | not modelled | 98.1 | 28 | PDB header: isomerase Chain: B; PDB Molecule: topoisomerase iv subunit b; PDBTitle: crystal structure of e. coli topoisomerase iv pare 43kda subunit2 complexed with adpnp |
| 89 | d1uyla |  | Alignment | not modelled | 98.0 | 19 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: Heat shock protein 90, HSP90, N-terminal domain |
| 90 | c1ea6A |  | Alignment | not modelled | 98.0 | 18 | PDB header: dna repair Chain: A; PDB Molecule: pms1 protein homolog 2; PDBTitle: n-terminal 40kda fragment of nhpm2 complexed with adp |
| 91 | c2fwyA |  | Alignment | not modelled | 98.0 | 19 | PDB header: chaperone Chain: A; PDB Molecule: heat shock protein hsp 90-alpha; PDBTitle: structure of human hsp90-alpha bound to the potent water2 soluble inhibitor pu-h64 |
| 92 | c1zxnB |  | Alignment | not modelled | 98.0 | 18 | PDB header: isomerase Chain: B; PDB Molecule: dna topoisomerase ii, alpha isozyme; PDBTitle: human dna topoisomerase iia atpase/adp |
| 93 | c1y4sA |  | Alignment | not modelled | 97.9 | 34 | PDB header: chaperone Chain: A; PDB Molecule: chaperone protein htpg; PDBTitle: conformation rearrangement of heat shock protein 90 upon2 adp binding |
| 94 | c4ipeA |  | Alignment | not modelled | 97.9 | 28 | PDB header: chaperone Chain: A; PDB Molecule: tnf receptor-associated protein 1; PDBTitle: crystal structure of mitochondrial hsp90 (trap1) with amppnp |
| 95 | c3ke6A |  | Alignment | not modelled | 97.9 | 29 | PDB header: unknown function Chain: A; PDB Molecule: protein rv1364c/mt1410; PDBTitle: the crystal structure of the rsbu and rswb domains of rv1364c from2 mycobacterium tuberculosis |
| 96 | c2akpA |  | Alignment | not modelled | 97.8 | 22 | PDB header: chaperone Chain: A; PDB Molecule: atp-dependent molecular chaperone hsp82; PDBTitle: hsp90 delta24-n210 mutant |
| 97 | c5x9yC |  | Alignment | not modelled | 97.8 | 22 | PDB header: dna binding protein Chain: C; PDB Molecule: dna mismatch repair protein mutl; PDBTitle: crystal structure of the atpase domain from bacterial mismatch repair2 endonuclease aquifex aeolicus mutl. |
| 98 | c3zm7E |  | Alignment | not modelled | 97.8 | 23 | PDB header: isomerase Chain: E; PDB Molecule: dna gyrase subunit b; PDBTitle: crystal structure of the atpase region of mycobacterium2 tuberculosis gyrb with amppcp |

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|-----|-------------------------|--|-----------|--------------|------|----|--|
| 99 | c4j0bB_ | | Alignment | not modelled | 97.7 | 29 | PDB header: chaperone Chain: B: PDB Molecule: tnf receptor-associated protein 1; PDBTitle: structure of mitochondrial hsp90 (trap1) with adp-beft3 |
| 100 | d1uyma_ | | Alignment | not modelled | 97.7 | 20 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: Heat shock protein 90, HSP90, N-terminal domain |
| 101 | c1qzrA_ | | Alignment | not modelled | 97.7 | 20 | PDB header: isomerase Chain: A: PDB Molecule: dna topoisomerase ii; PDBTitle: crystal structure of the atpase region of saccharomyces cerevisiae2 topoisomerase ii bound to icrf-187 (dexrazoxane) |
| 102 | c3g7bB_ | | Alignment | not modelled | 97.7 | 19 | PDB header: isomerase/isomerase inhibitor Chain: B: PDB Molecule: dna gyrase subunit b; PDBTitle: staphylococcus aureus gyrase b co-complex with methyl ({5-[4-(4-2 hydroxypiperidin-1-yl)-2-phenyl-1,3-thiazol-5-yl]-1h-pyrazol-3-3 yl}methyl)carbamate inhibitor |
| 103 | d2iwxa1 | | Alignment | not modelled | 97.7 | 22 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: Heat shock protein 90, HSP90, N-terminal domain |
| 104 | c5fwkA_ | | Alignment | not modelled | 97.7 | 25 | PDB header: signaling protein Chain: A: PDB Molecule: heat shock protein hsp 90 beta; PDBTitle: atomic cryoem structure of hsp90-cdc37-cdk4 complex |
| 105 | c1zwhA_ | | Alignment | not modelled | 97.6 | 22 | PDB header: chaperone Chain: A: PDB Molecule: atp-dependent molecular chaperone hsp82; PDBTitle: yeast hsp82 in complex with the novel hsp90 inhibitor radester amine |
| 106 | c3pehB_ | | Alignment | not modelled | 97.6 | 26 | PDB header: chaperone Chain: B: PDB Molecule: endoplasmin homolog; PDBTitle: crystal structure of the n-terminal domain of an hsp90 from plasmodium2 falciparum, pfl1070c in the presence of a thienopyrimidine derivative |
| 107 | c2iorA_ | | Alignment | not modelled | 97.6 | 34 | PDB header: chaperone Chain: A: PDB Molecule: chaperone protein htpg; PDBTitle: crystal structure of the n-terminal domain of htpg, the2 escherichia coli hsp90, bound to adp |
| 108 | d1s14a_ | | Alignment | not modelled | 97.5 | 22 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: DNA gyrase/MutL, N-terminal domain |
| 109 | c2cg9A_ | | Alignment | not modelled | 97.5 | 23 | PDB header: chaperone Chain: A: PDB Molecule: atp-dependent molecular chaperone hsp82; PDBTitle: crystal structure of an hsp90-sba1 closed chaperone complex |
| 110 | c5tthA_ | | Alignment | not modelled | 97.5 | 27 | PDB header: chaperone Chain: A: PDB Molecule: c-terminal spycatcher fusion of wildtype zebrafish tnf PDBTitle: heterodimeric spycatcher/spytag-fused zebrafish trap1 in atp/adp-2 hybrid state |
| 111 | c4gfhA_ | | Alignment | not modelled | 97.4 | 18 | PDB header: isomerase/dna Chain: A: PDB Molecule: dna topoisomerase 2; PDBTitle: topoisomerase ii-dna-amppnp complex |
| 112 | c2rm8A_ | | Alignment | not modelled | 97.4 | 17 | PDB header: signaling protein Chain: A: PDB Molecule: sensory rhodopsin ii transducer; PDBTitle: the solution structure of phototactic transducer protein2 htrii linker region from natronomonas pharaonis |
| 113 | d1qy5a_ | | Alignment | not modelled | 97.4 | 30 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: Heat shock protein 90, HSP90, N-terminal domain |
| 114 | d2gqpa1 | | Alignment | not modelled | 97.3 | 21 | Fold: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Superfamily: ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase Family: Heat shock protein 90, HSP90, N-terminal domain |
| 115 | c2o1wB_ | | Alignment | not modelled | 97.3 | 26 | PDB header: chaperone Chain: B: PDB Molecule: endoplasmin; PDBTitle: structure of n-terminal plus middle domains (n+m) of grp94 |
| 116 | c2iopD_ | | Alignment | not modelled | 97.3 | 37 | PDB header: chaperone Chain: D: PDB Molecule: chaperone protein htpg; PDBTitle: crystal structure of full-length htpg, the escherichia coli2 hsp90, bound to adp |
| 117 | c5ulsA_ | | Alignment | not modelled | 97.2 | 22 | PDB header: chaperone Chain: A: PDB Molecule: endoplasmin; PDBTitle: structure of grp94 in the active conformation |
| 118 | c3lnuA_ | | Alignment | not modelled | 97.1 | 22 | PDB header: isomerase Chain: A: PDB Molecule: topoisomerase iv subunit b; PDBTitle: crystal structure of pare subunit |
| 119 | c2o1uA_ | | Alignment | not modelled | 97.0 | 35 | PDB header: chaperone Chain: A: PDB Molecule: endoplasmin; PDBTitle: structure of full length grp94 with amp-pnp bound |
| 120 | c6gauB_ | | Alignment | not modelled | 96.4 | 26 | PDB header: dna binding protein Chain: B: PDB Molecule: dna gyrase subunit b,dna gyrase subunit a; PDBTitle: extremely 'open' clamp structure of dna gyrase: role of the2 corynebacteriales gyrb specific insert |