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| --- | --- | --- | --- | --- | --- | --- |
| Rank | PDB ID | Z-score | RMSD (Å) | Seq. Id  (%) | Species | Description (Substrate) |
| 1 | 1JQI | 44.4 | 2.3 | 22 | *Rattus norvegicus* | Short Chain Acyl-CoA Dehydrogenase  (Acetoacetyl-CoA / FAD) |
| 2 | 3MDE | 44.1 | 2.1 | 24 | *Sus scrofa* | Medium chain Acyl-CoA dehydrogenase  (Octanoyl-CoA / FAD) |
| 3 | 2JIF | 44.0 | 2.0 | 22 | *Homo sapiens* | Short/branched chain Acyl-CoA dehydrogenase  (CoA persulfide / FAD) |
| 4 | 2DVL | 43.9 | 1.9 | 27 | *Thermus thermophilus HB8* | TT0160  Acyl-CoA dehydrogenase  (- / FAD) |
| 5 | 1UDY | 43.9 | 2.1 | 24 | *Sus scrofa* | Medium-chain Acyl-CoA dehydrogenase  **(**3-Thiaoctanoyl-CoA **/** FAD**)** |
| 6 | 1T9G | 43.7 | 2.1 | 23 | *Homo sapiens* | Medium-chain Acyl-CoA dehydrogenase: ETF complex  (- / FAD) |
| 7 | 4KCF | 43.6 | 2.4 | 27 | *Actinomadura kijaniata* | KijD3  Flavin-dependent monooxygenase  (dTDP-3-amino-2,3,6-trideoxy-4-keto-3-methyl-D-glucose / FMN) |
| 8 | 4M9A | 43.6 | 2.1 | 23 | *Burkholderia thailandensis* | Acyl-CoA dehydrogenase;  (- / FAD) |
| 9 | 2VIG | 43.4 | 2.2 | 22 | *Homo sapiens* | Short-chain Acyl-CoA dehydrogenase  (CoA persulfide / FAD) |
| 10 | 1IVH | 43.3 | 2.2 | 22 | *Homo sapiens* | Isovaleryl-CoA dehydrogenase  (CoA persulfide / FAD) |
| 11 | 4KTO | 43.3 | 2.2 | 21 | *Sinorhizobium meliloti* | Isovaleryl-CoA dehydrogenase;  (- / FAD) |
| 12 | 3X0Y | 43.2 | 2.1 | 26 | *Rhodococcus erythropolis* | DszC  Flavin-dependent monooxygenase  (dibenzothiophene / FMN) |
| 13 | 5AF7 | 43.2 | 2.5 | 22 | *Advenella mimigardefordensis* | Flavin-dependent monooxygenase  (3SP-CoA / FAD) |
| 14 | 5XDE | 42.9 | 2.2 | 23 | *Paenibacillus sp.* | TdsC  Flavin-dependent monooxygenase  (dibenzothiophene / FMN) |
| 15 | 4IV6 | 42.9 | 2.1 | 26 | *Mycobacterium smegmatis* | Isovaleryl-CoA dehydrogenase;  (- / FAD) |
| 16 | 1BUC | 42.8 | 2.1 | 23 | *Megasphaera elsdenii* | Butyryl-CoA dehydrogenase  (Acetoacetyl-CoA / FAD) |
| 17 | 2D29 | 42.8 | 2.3 | 28 | *Thermus thermophilus* | TT0172  Acyl-CoA dehydrogenase  (- / FAD) |
| 18 | 1RX0 | 42.8 | 2.5 | 20 | *Homo sapiens* | Isobutyryl-CoA dehydrogenase  (Methacrylyl-CoA / FAD) |
| 19 | 3MXL | 42.7 | 2.5 | 26 | *Micromonospora carbonacea* | ORF36  Flavin-dependent monooxygenase  (TDP-l-evernosamine / FAD) |
| 20 | 4ZXV | 42.7 | 2.3 | 25 | *Streptomyces peucetius* | DnmZ  Flavin-dependent monooxygenase  (- / FMN) |