**Table S3. Comparative analysis of *P. furiosus* MoaB, *A. aeolicus* MogA and *T. thermophilus* MogA**

|  |  |  |  |
| --- | --- | --- | --- |
| **Domain** | Archaea | Bacteria | Bacteria |
| **Species** | *Pyrococcus furiosus* | *Aquifex aeolicus* | *Thermus thermophilus* |
| **Max. living temperature,°C** | 103 | 95 | 85 |
| **MPT-adenylyl-transferase** | MoaB | MogA | MogA |
| **Oligomerization state** | hexamer | trimer | trimer |
| **Crystal structure (RCSB PDB)** | 4LHB | 3MCI | 3MCH |
| **Resolution, Å** | 2.6 | 1.9 | 1.6 |
| **N° of residues** | 169 | 178 | 164 |
| **N° of residues in structure** | 159 | 177 | 159 |
|  |  |  |  |
| **Proline content1, %** | 2.96 | 7.30 | 7.93 |
|  |  |  |  |
| **Non α-helical, β-sheet regions2, %** | 22.0 | 33.3 | 28.3 |
|  |  |  |  |
| **N° of hydrogen bonds3** |  |  |  |
| within monomer | 271 | 322 | 296 |
| at trimerization interface | 80 | 31 | 31 |
| at hexamerization interface | 55 | - | - |
|  |  |  |  |
| **N° of salt bridges3** |  |  |  |
| within monomer | 5 | 11 | 10 |
| at trimerization interface | 6 | 38 | 4 |
| at hexamerization interface | 12 | - | - |
|  |  |  |  |
| **Interface area4, Å** |  |  |  |
| trimerization interface | 1800 | 1476 | 1566 |
| hexamerization interface | 1938 | - | - |
|  |  |  |  |
| **Non-polar interface area5, Å** |  |  |  |
| trimerization interface | 1094 | 1098 | 1106 |
| hexamerization interface | 1297 | - | - |

1calculated based on the number of residues in sequence.

2calculated based on the number of residues in structure.

3values given for the interfaces are totals for all subunits of the respective interface.

4total interface area determined for two subunits involved in the interaction at the corresponding interface.

5total non-polar interface area determined for two subunits involved in the interaction at the corresponding interface.