**Table S1.** **Coordination and distance of Mg2+ with corresponding residues as predicted in *Pam*Tps1 structure**

|  |  |  |
| --- | --- | --- |
| **Mg2+ no.** | **Residue** | **Distance** |
| Mg2+A | D296 | 2.74 Å |
| D300 | 2.18 Å |
| Mg2+B | D440 | 2.37 Å |
| T444 | 2.25 Å |
| E448 | 2.17 Å |
| Mg2+C | D296 | 2.40 Å |
| D300 | 2.10 Å |

Table S2. Coordination and distance of GPP and FPP with *Pam*Tps1 residues and Mg2+

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Substrate** | **Docking score** | **Full Fitness** | **Hydrogen bond** | **Atom** | **Residue/Cofactor** | **Distance** |
| **GPP** | -106.157 | -2937.4248 | 4 | Oδ3 | R259 | 2.18 Å |
| Oδ5  Oδ6 | R437 | 3.10 Å  3.08 Å |
| Oδ7 | K456 | 3.24 Å |
|  | Oδ5 | Mg2+ A | 2.27 Å |
| Oδ2  Oδ7 | Mg2+ B | 2.48 Å  2.15 Å |
| Oδ5 | Mg2+ C | 1.94 Å |
| **FPP** | -102.248 | -2917.827 | 4 | Oδ3 | R259 | 2.16 Å |
| Oδ5  Oδ6 | R437 | 3.07 Å  3.07 Å |
| Oδ6 | K456 | 3.07 Å |
|  | Oδ4  Oδ7 | Mg2+ A | 2.24 Å  2.30 Å |
| Oδ2  Oδ6 | Mg2+ B | 2.14 Å  2.43 Å |
| Oδ7 | Mg2+ C | 1.92 Å |

**Table S3:** **Comparison of *Pam*Tps1 3D model structure evaluation with BPPS (1N24) template**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Validation** | **Analysis** | **Threshold values** | **BPPS (1N24)** | ***Pam*Tps1** |
| SWISS-MODEL | Sequence identity |  | 67.04 % | |
| GMQE | 0-1 | 0.82 | |
| QMEAN | 0 | -1.32 | |
| Chimera | RMSD | Superimposition | 0.203 Å | |
| PROCHECK | Ramachandran plot | Favored region | 92.8 % | 92.8 % |
| Additional allowed | 7.0 % | 6.6 % |
| Generously allowed | 0.2 % | 0.2 % |
| Disallowed region | 0.0 % | 0.4 % |
| PROVE | Z-score mean |  | n/a | 0.487 |
| Z-score RMS | 1-3.9 Å | n/a | 1.421 |
| Outliers |  | 2.8 % | 4.7 % |
| ERRAT | Quality factor | ≥ 95 % | 100 % | 95.88 % |
| Verify3D | 3D/1D profile | ≥ 80 | 73.14 % | 95.73 % |
| ProSA | Z-score | Close to template value | -10.92 | - 12 |