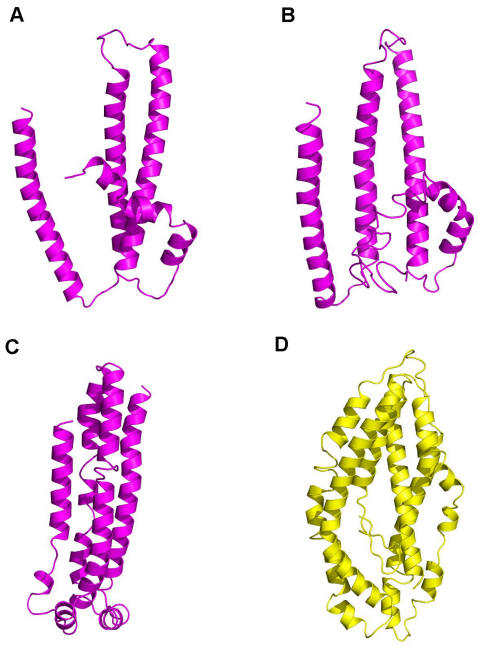


Figure S1. (A) The 3D structures of PF3D7_1372300 obtained by Itasser software. (B) The relaxed structure of PF3D7_1372300 from Itasser's prediction. (C–D) The structures of PF3D7_1372300 and ATS built using Modeller, respectively.

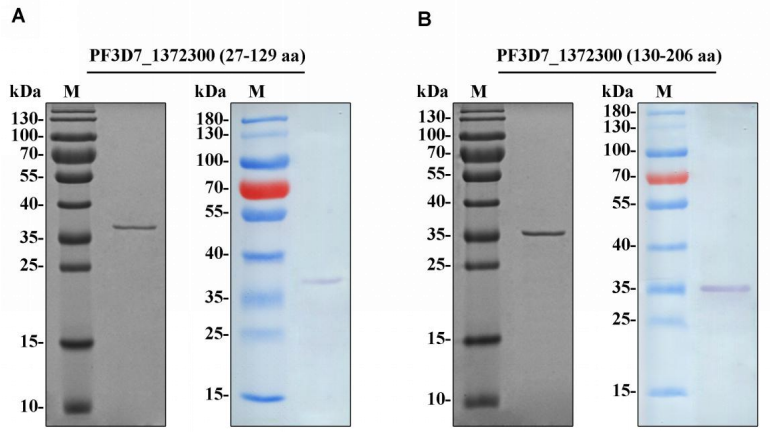


Figure S2. (A – B) Analysis of purified PF3D7_1372300 (residues 27 – 129) and PF3D7_1372300 (residues 130 – 206) by SDS-PAGE (left) and western blotting (right).

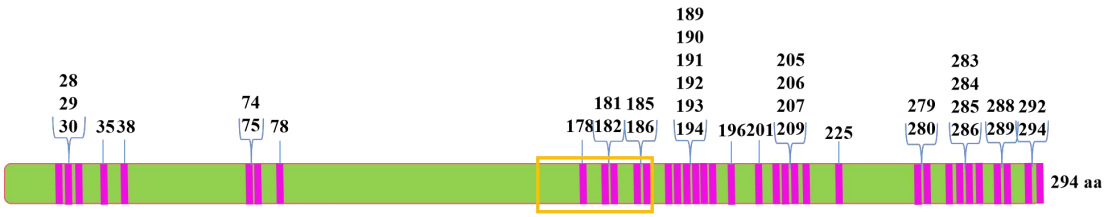


Figure S3. Schematic diagram of interaction sites on ATS. The green bar represents the ATS protein, the deep pink bar represents the amino acids involved in interactions, and the yellow box shows the predicted conserved interaction sites of ATS in previous studies. Five of the residues identified in our MD simulations are located in this predicted conserved interaction region.

Table S1. The primer sequences for cloning the gene fragments encoding the recombinant proteins expressed in *E. coli*.

| Gene name | Primers |
|---|---|
| PF3D7_1372300-His | F:CATGCCATGGGACGAAATGAGATACATAAA<br>R:CCGCTCGAGTTTTTGTTCACTAAATATTTTTTCA |
| PF3D7_1372300-GST | F:CGCGGATCCCGAAATGAGATACATAAAAAT<br>R:CCGCTCGAGCTATTTTTGTTCACTAAATATTTT |
| PF3D7_0800200-His | F:AAACCATGGGAAAGAAAAAACCGAAATCA<br>R:GGGCTCGAGTATATTCCATACATCCGATAT |

Table S2. The primer sequences of RT-qPCR

| Gene name | Primers |
|---|---|
| PF3D7_1372300 | F:ATTCAAGGAATTTGGCACAG<br>R: CTGTTCAGTTACGCTCTCGAA |
| PF3D7_1205100 | F:AAGTAGCAGGTCATCGTGGTT<br>R:TTCGGCACATTCTTCCATAA |

Table S3. Binding kinetics of the PF3D7_1372300-GST and GST-tag to ATS using the ForteBio system.

| Variant | KD(M)[a] | Kon(1/Ms)[b] | Kdis(1/s)[c] | $R^2$ |
|---|---|---|---|---|
| 1372300-GST | 1.19E-07 | 6.33E+03 | 7.56E-04 | 0.9962 |
| GST-tag | <1.0E-12 | 1.00E+04 | <1.0E-07 | 0.1219 |

[a]KD: The equilibrium dissociation constant, calculated as Kdis/Kon.
[b]Kon: The binding rate.
[c]Kdis: The dissociation rate.

Table S4 Molecular dynamics datas of the Positions 1 to Position 5

| Variant | Interaction Energy (kJ/mol) | RMSD (Å) | Number of H-Band | Number of Salt-Bridge |
|---|---|---|---|---|
| Position 1 | -1122.133038 | 12.1089193 | 5.410494852 | 2.081368316 |
| Position 2 | -1230.713395 | 10.2997592 | 7.521641791 | 1.802238806 |
| Position 3 | -1965.027782 | 9.409817975 | 11.95051755 | 5.205251199 |
| Position 4 | -1157.593719 | 13.78770951 | 8.363332591 | 1.959010916 |
| Position 5 | -670.3124425 | 29.76553656 | 3.861900894 | 1.012591389 |

Table S5. Binding kinetics of the PF3D7_1372300-(27-129)-GST and PF3D7_1372300-(130-206)-GST to ATS using the ForteBio system.

| Variant | KD(M)[a] | Kon(1/Ms)[b] | Kdis(1/s)[c] | $R^2$ |
|---|---|---|---|---|
| PF3D7_1372300-(27-129)-GST | 1.27E-07 | 6.63E+03 | 8.44E-04 | 0.9906 |
| PF3D7_1372300-(130-206)-GST | 2.26E-08 | 6.96E+03 | 1.58E-04 | 0.9726 |

[a]KD: The equilibrium dissociation constant, calculated as Kdis/Kon.
[b]Kon: The binding rate.
[c]Kdis: The dissociation rate.
[c]Kdis: The dissociation rate.