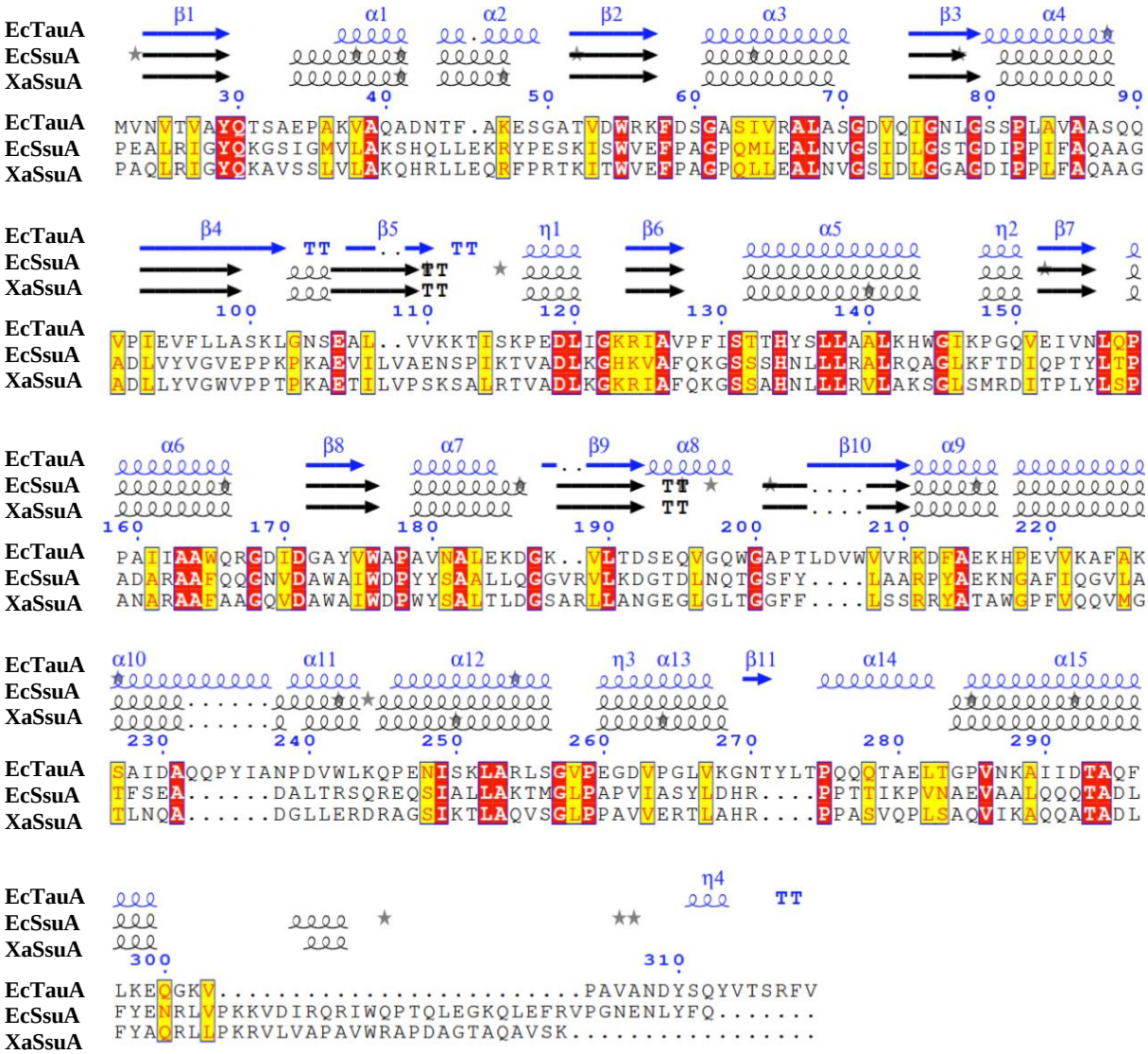
**Table S1.** Data collection and refinement statistics. Values in parentheses are for the highest-resolution shell.

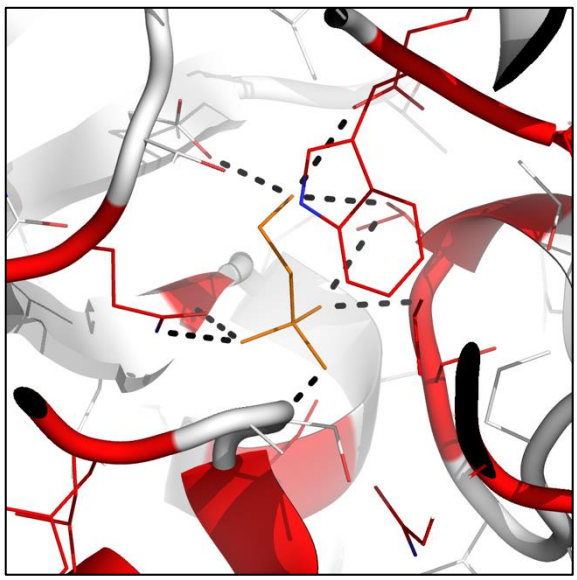
| | **TauA-taurine (phasing)** | **TauA-taurine (refinement)** | **TauA-2-AEP** | **TauA-ACES** | **TauA-MES** |
|---|---|---|---|---|---|
| **Data collection** | | | | | |
| Beamline | DLS-I23 | DLS-I03 | DLS-I24 | DLS-I24 | DLS-I24 |
| Wavelength (Å) | 2.3751 | 0.9763 | 0.9686 | 0.9686 | 0.9686 |
| Resolution (Å) | 65.47-1.77 (1.81-1.77) | 67.53-1.30 (1.33-1.30) | 65.68-1.62 (1.65-1.62) | 35.9-1.50 (1.53-1.50) | 40.97-1.55 (1.59 – 1.55) |
| Space group | $P2_12_12_1$ | $P2_12_12_1$ | $P2_12_12_1$ | $P2_12_12_1$ | $P2_12_12_1$ |
| Cell dimensions | | | | | |
| a,b,c (Å) | 45.01, 71.32, 165.03 | 44.96, 74.09, 164.11 | 45.1, 71.64, 164.55 | 45.16, 71.8, 164.78 | 45.22, 73.0, 163.90 |
| α, β, γ (°) | 90, 90, 90 | 90, 90, 90 | 90, 90, 90 | 90, 90, 90 | 90, 90, 90 |
| Total reflections | 873204 (39274) | 417657 (20677) | 433767 (19645) | 330516 (14581) | 362377 (24578) |
| Unique reflections | 45258 (2202) | 130542 (6414) | 68655 (3375) | 85811 (4180) | 77044 (5553) |
| Completeness (%) | 86.0 (74.0) | 97.5 (96.9) | 99.8 (99.9) | 98.9 (97.8) | 97.0 (95.3) |
| Anomalous Completeness (%) | 85.2 (72.8) | - | - | - | - |
| Redundancy | 19.3 (17.8) | 3.2 (3.2) | 6.3 (5.8) | 3.9 (3.5) | 4.7 (4.4) |
| Anomalous Redundancy | 9.9 (9.1) | - | - | - | - |
| Rmerge | 0.12 (0.83) | 0.056 (0.43) | 0.1 (0.86) | 0.072 (0.8) | 0.09 (1.22) |
| I/sig(I) | 15.9 (3.1) | 11 (2.5) | 10.9 (1.9) | 11.9 (1.7) | 8 (1) |
| CC1/2 | 1 (0.8) | 1 (0.8) | 1 (0.6) | 1 (0.5) | 1 (0.5) |
| | | | | | |
| **Refinement** | | | | | |
| $R_{work}/R_{free}$ (%) | - | 14.5/18.3 | 16.8/20.3 | 15.6/22.2 | 19.3/23.1 |
| Average B-factors ($Å^2$) | - | 16.6 | 20.8 | 20.9 | 24.9 |
| protein | - | 15.1 | 20.1 | 19.8 | 24.1 |
| taurine | - | 18.3 | 26.7 | 22.7 | 31.3 |
| Ramachandran (%) | | | | | |
| Favoured | - | 98.48 | 98.48 | 98.65 | 97.8 |
| Allowed | - | 1.18 | 1.18 | 1.02 | 1.86 |
| Outliers | - | 0.34 | 0.34 | 0.00 | 0.34 |

R-free was calculated using 5% of data excluded from refinement.

**(A)**


EcTauA
EcSsuA
XaSsuA
β1 α1 α2 β2 α3 β3 α4
30 40 50 60 70 80 90
MVNVTVAYQTSAEPAKVAQADNTF.AKESGATVDWRKFDSCASIVRALASGDVQIGNLGSSPLAVAASQQ
PEALRIGYQKGSIGMVLAKSHQLLEKRYPESKISWVEFPAGPQMLEALNVGSIDLGSTGDIPPIFAQAAG
PAQLRIGYQKAVSSLVLAKQHRLLEQRFPRTKITWVEFPAGPQLLEALNVGSIDLGGAGDIPPLFAQAAG
β4 β5 η1 β6 α5 η2 β7
100 110 120 130 140 150
VPIEVFLLASKLGNSEAL..VVKKTISKPEDIIGKRIAVPFISTTHYSLLAALKHWGIKPGQVEIVNLQP
ADLVYVGVEPPKPKAEVILVAENSPIKTVADLKGHKVAFQKGSSSHNLLRALRQAGLKFTDIQPTYLTP
ADLLYVGWVPPTPKAETILVPSKSALRTVADLKGKRIAFQKGSSAHNLLRVLAKSGLSMRDITPLYLSP
α6 β8 α7 β9 α8 β10 α9
160 170 180 190 200 210 220
PAIIAAWQRGDIDGAYVWAPAVNALEKDGK..VLTDSEQVGQWGAPTLDVWVVRKDFAEKHPEVVKAFAK
ADARAAFQQGNVDAWAIWDPYYSAALLQGGVRVLKDGTDLNQTGSFY....LAARPYAEKNGAFIQGVLA
ANARAAFAAGQVDAWAIWDPWYSALTLDGSARLLANGEGLGLTGGFF....LSSRRYATAWGPFVQQVMG
α10 α11 α12 η3 α13 β11 α14 α15
230 240 250 260 270 280 290
SAIDAQQPYIANPDVWLKQPENISKLARLSGVPEGDVPGLVKGNTYLTPQQQTAELTGPVNKAIIDTAQF
TFSEA......DALTRSQREQSIALLAKTMGLPAPVIASYLDHR....PPTTIKPVNAEVAALQQQTADL
TLNQA......DGLLERDRAGSIKTLAQVSGLPPAVVERTLAHR....PPASVQPLSAQVIKAQQATADL
η4
300 310
LKEQGKV.........................PAVANDYSQYVTSRFV
FYENRLVPKKVDIRQRIWQPTQLEGKQLEFRVPGNENLYFQ.....
FYAQRLLPKRVLVAPAVWRAPDAGTAQAVSK................

**(B)**



**(C)** **(D)**

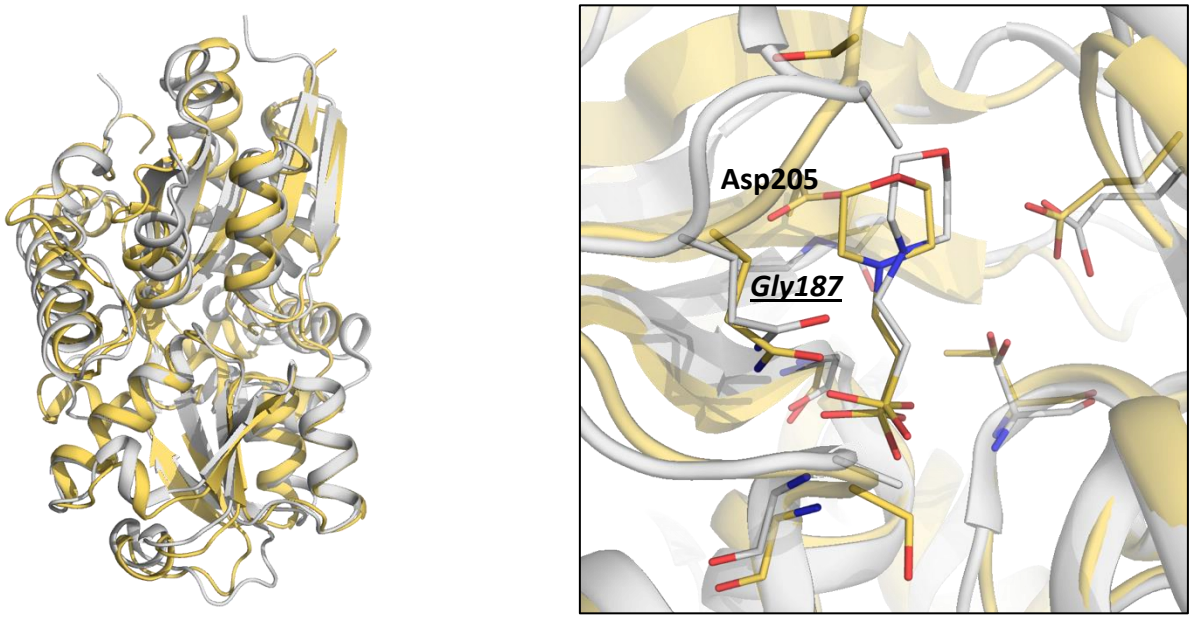



**Figure S1.** Sequence and structural comparison of TauA and SsuA. (A) Sequence alignment of *E. coli* TauA with *E. coli* and *X. axonopodis* SsuA, respectively. Conserved amino acids are shown in red boxes. Sequence alignment was performed with Clustal Omega. (B) Close-up of the *E. coli* TauA bidning site with the conserved residues from the sequence alignment mapped onto the TauA-taurine structure. Conserved residues are shown in red and non-conserved in grey. The taurine is coordinated by conserved and non-conserved residues. (C) Superimposition of *E. coli* TauA (shown in yellow cartoon) and *X. axonopodis* SsuA (shown in grey cartoon) structures display a high degree of structural similarity. (D) A close-up of the binding site of the *E. coli* TauA and *X. axonopodis* SsuA bound to MES show conserved interactions. Asp205 is absent in *X. axonopodis* SsuA and it is the key determinant to taurine binding. The equivalent residue in SsuA is Gly187 (shown in italic and underlined). Although Asp205 is not involved in MES coordination, it shown for clarity.

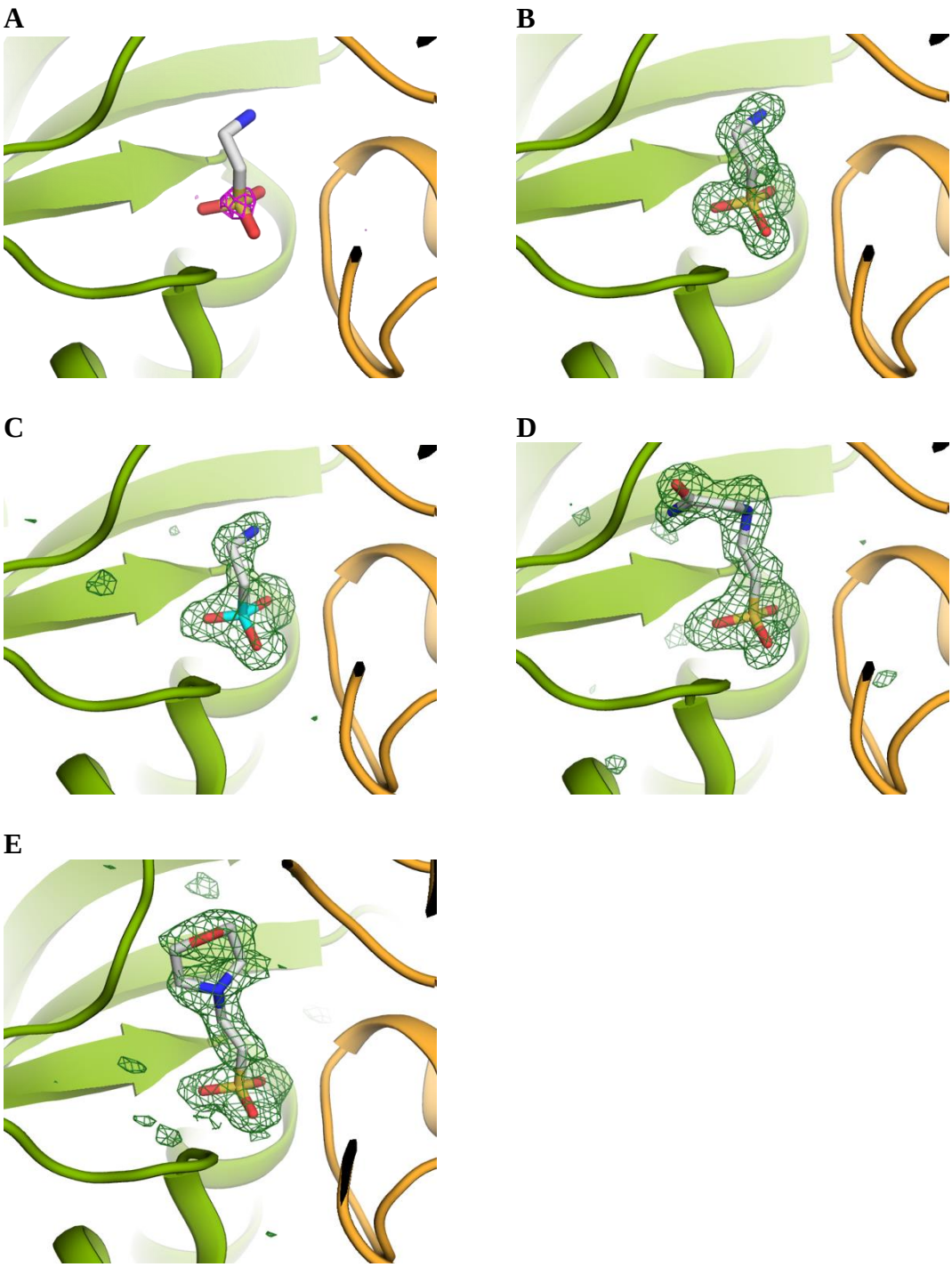



**Figure S2.** Electron density maps. (A) Anomalous difference map (magenta mesh) contoured at 8 σ, is shown for taurine from the long-wavelength data set, λ=2.37 Å. (B-E) Positive Fo-Fc electron density maps (green mesh) contoured at 3 σ, for (B) taurine, (C) 2-AEP, (D) ACES and (E) MES after molecular replacement. The molecules have not been included in the refinement but are shown for reference. Same colour scheme as Figure 1.

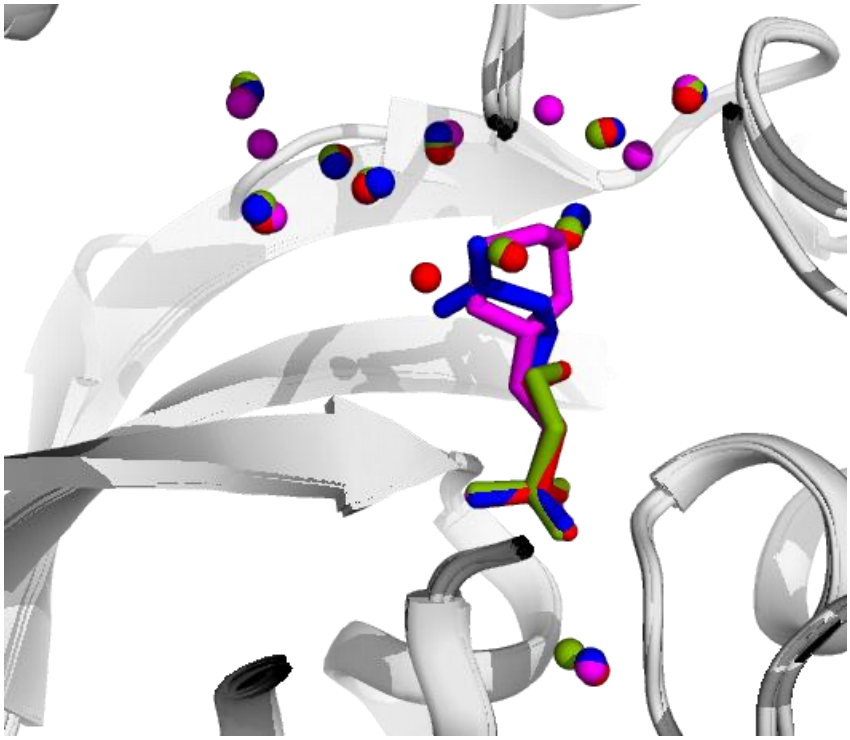


**Figure S3.** Water analysis from the crystal structures. All the ligand-bound TauA structures have been superimposed. There are 'conserved' water molecules at the proximity of the ligands, but displacement of water molecules occurs relative to the taurine structure (shown in red). Binding of ACES (shown in blue) and MES (shown in purple) results in significant water molecule displacement. Most of the waters are conserved between the taurine and 2-AEP (shown in green).