Supporting information for article:

From bacterial to human dihydrouridine synthase: automated structure determination

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**Supplementary Table S1.** Top scoring *phenix.mr_rosetta* placed models and map correlation between 2mFo-DFc maps calculated from placed models and the final refined structure of hDUS2.

| Search model | Phaser TF Z-score/LLG | Map correlation |
|--------------|------------------------|-----------------|
| TtDus (3b0p) | 4.7/39.7               | 0.36            |
| TmDus (1vhn) | 5.2/26.0               | 0.35            |
| EcDusC (4bfa)| 4.8/25.6               | 0.31            |

**Supplementary Table S2.** Comparison of *Buccaneer* automatic model building into maps generated by *phenix.mr_rosetta* starting from structures of TtDus, TmDus and EcDusC; and a comparison of *Buccaneer* built models obtained from *phenix.mr_rosetta* and from Se-SAD phasing.

| Search model | Buccaneer sequenced residues (longest chain) | Buccaneer R/Rfree | Co rmsd(Å) † to Buccaneer model from Se-SAD (no. aligned) |
|--------------|---------------------------------------------|-------------------|----------------------------------------------------------|
| TtDus (3b0p) | 320 (320)                                   | 0.257/0.303       | 0.298 (295)                                              |
| TmDus (1vhn) | 322 (322)                                   | 0.255/0.301       | 0.305 (295)                                              |
| EcDusC (4bfa)| 132 (51)                                    | 0.476/0.551       | N/A                                                      |
| EcDusC (4bfa)*| 330 (330)                                   | 0.249/0.297       | 0.312(295)                                               |

† Phenix-dev-1980/Rosetta-2015_09_57646

† Residues aligned: 7–87, 90–116, 136–188, 194–214, 223–336

**Supplementary Table S3.** Statistics for a conventional molecular replacement approach, showing comparison of search models, 2mFo-DFc map correlation of MR solutions with final refined hDUS2 structure, initial model refinement and *Buccaneer* autobuilding results.

| Search model (catalytic domain) | Co RMSD (Å) to final hDUS2 structure (no. residues aligned) | Sequence identity (after HHpred alignment) | Phaser TF Z-score/LLG | Map correlation | Results of Refmac jelly body refinement | Buccaneer Final R/Rfree |
|---------------------------------|------------------------------------------------------------|------------------------------------------|------------------------|-----------------|----------------------------------------|-------------------------|
| TtDus (3b0p)                    | 1.5 (203)                                                 | 21.2                                     | 8.4/83.4               | 0.37            | 46.4/48.3                              | 0.56                    | 25.9/29.6 |
| TmDus (1vhn)                    | 2.0 (195)                                                 | 21.9                                     | 5.2/25.0               | 0.32            | 47.4/49.2                              | 0.48                    | N/A       |
| EcDusC (4bfa)                   | 1.9 (200)                                                 | 22.7                                     | 4.5/26.9               | 0.30            | 54.0/55.0                              | 0.38                    | N/A       |