

Supplementary Material for "On the Evolution of Structure in the  
Aminoacyl-tRNA Synthetases"

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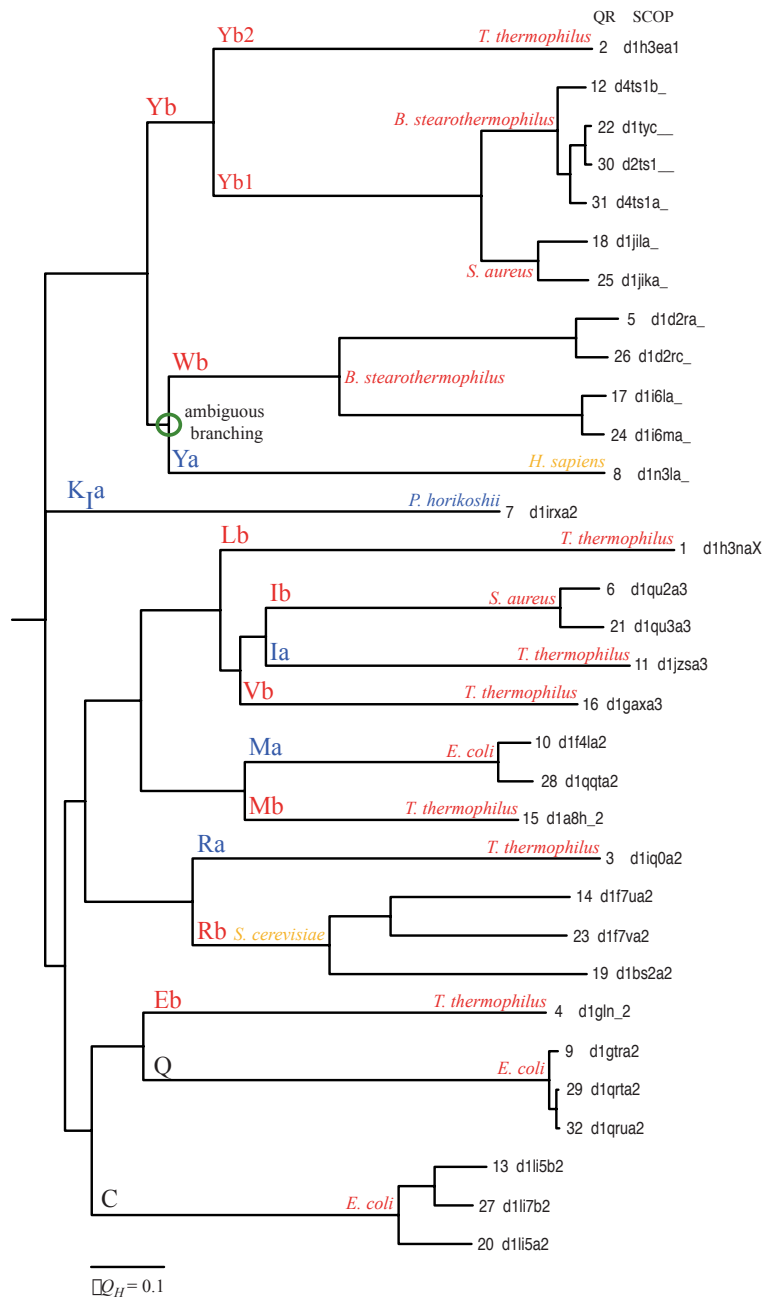
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Protein Name	PDB name	SCOP domain name	residue index	PDB numbering
GlnRS	1gtr chain A	d1gtra2	1-331	8-338
AsnRS*	–	d11sca2	1-331	108-438

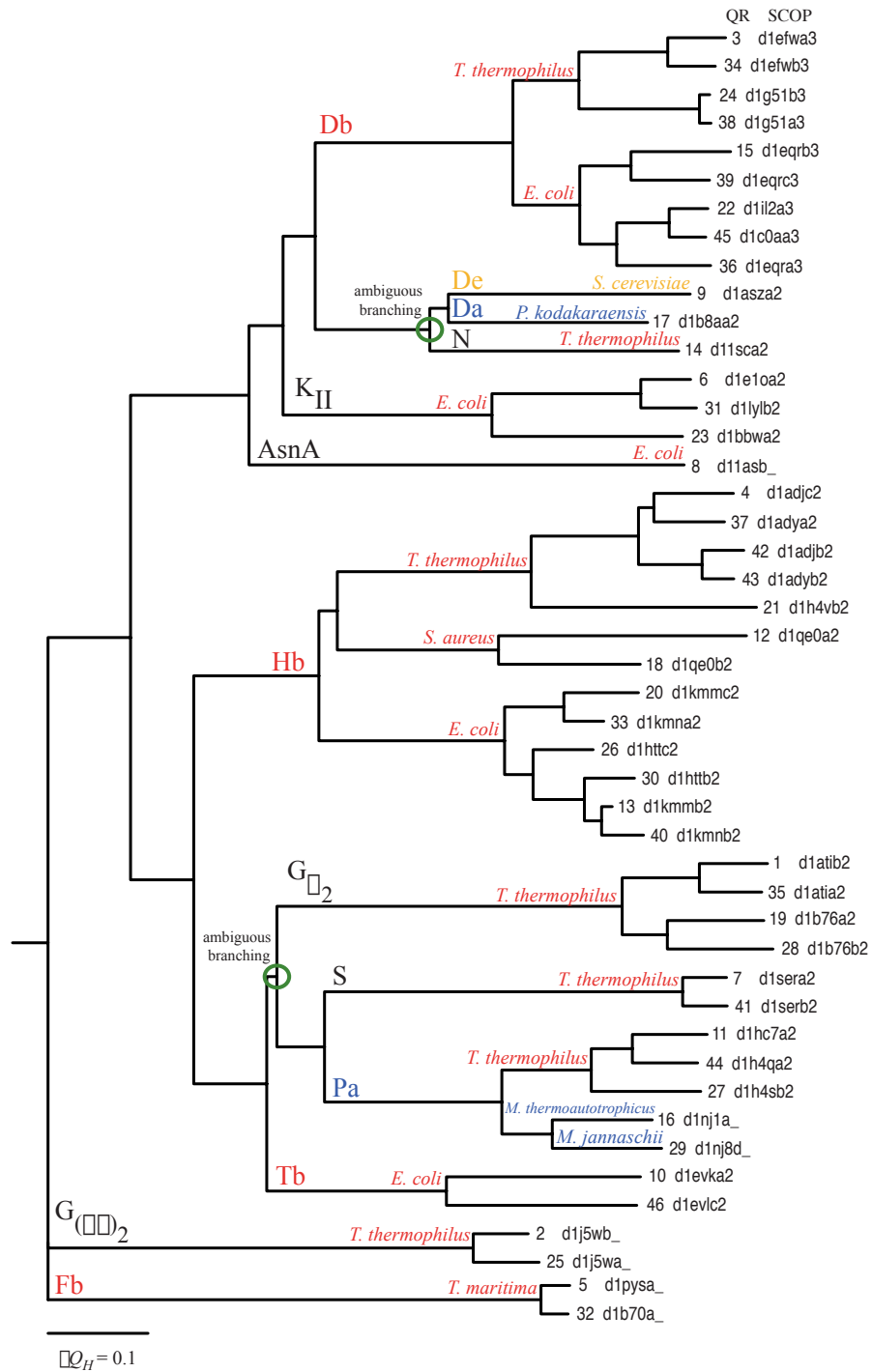
Supplementary Table 1: Definition of residue indices in Figure 13. \* – There is no PDB entry for AsnRS from *T. thermophilus* [Berthet-Colominas et al. (1998) *EMBO J.*, **17**, 2947.] which is identified by the fictitious SCOP domain name d11sca2. Coordinates were provided by Stephen Cusack, personal communication.

Protein Name	PDB name	SCOP domain name	residue index	PDB numbering
TyrRS	4ts1 chain B	d4ts1b_	1-16	34 36 37 38 68 70 73 78 82
				123 169 173 176 189 195 198
AspRS	1c0a chain A	d1c0aa3	1-17	192 193 195 198 231 233 234 235
				448 449 485 486 487 489 530 531 532
			18-31	217 224 225 226 227 229 482
				483 484 533 534 536 537 548
			32-54	107 108 109 110 111 113 114
				115 116 117 118 119 120 122 223
				547 549 556 557 558 559 561 563
			55-75	169 170 171 172 173
				174 192 193 195 196 217 219 220
				221 222 225 448 449 450 451 514

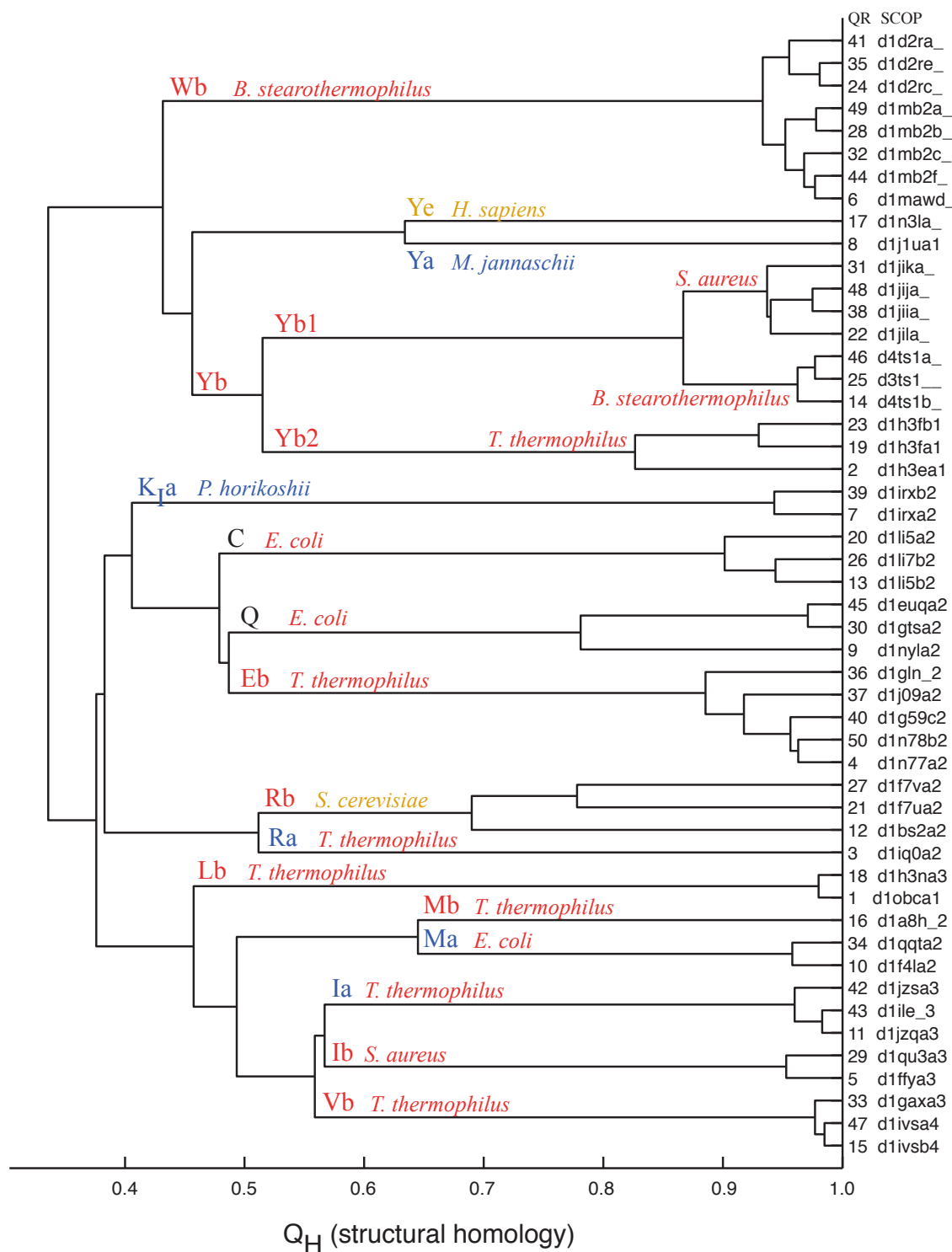
Supplementary Table 2: Definition of residue indices in Figure 16.



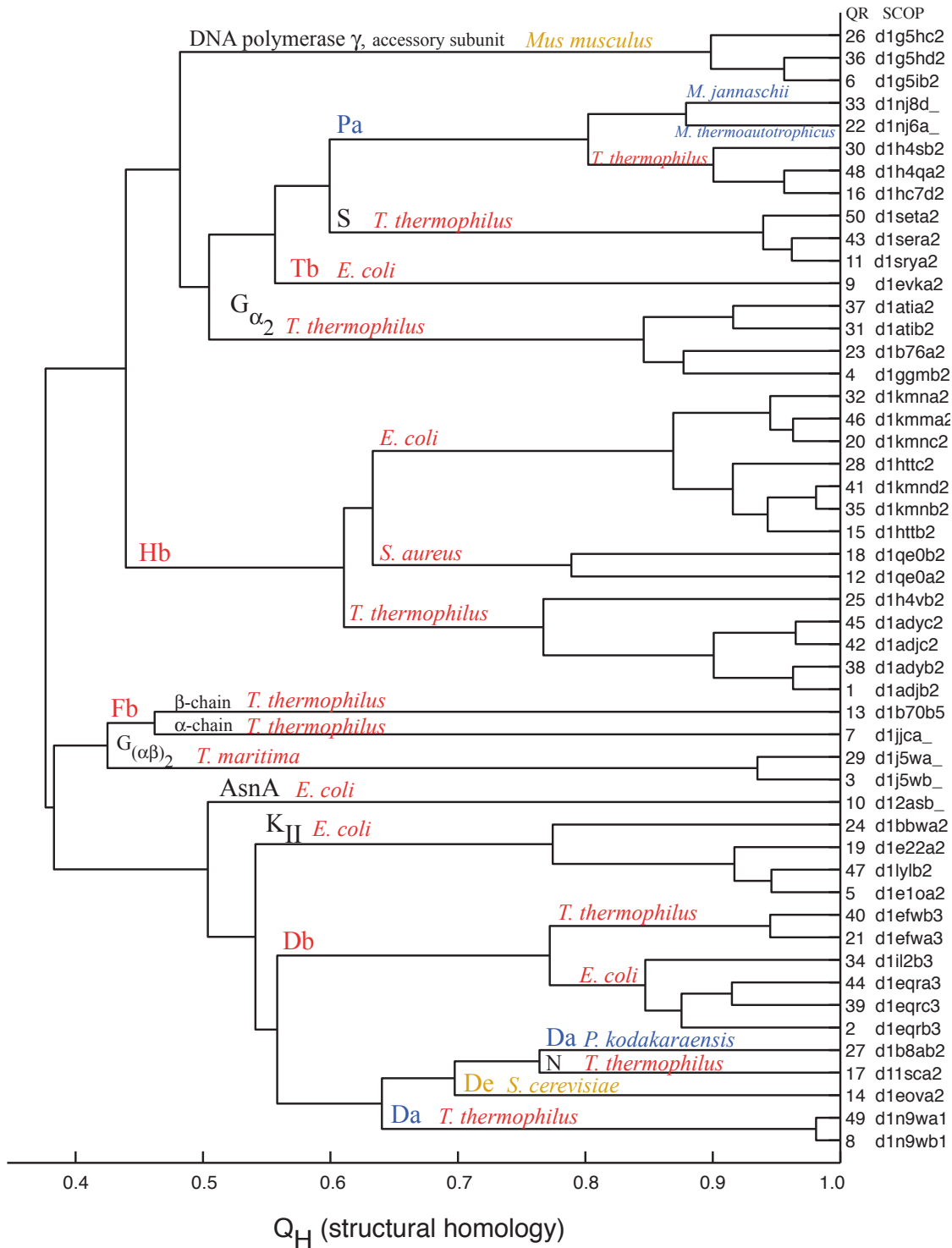
Supplementary Figure 1: Full neighbor joining tree of the Class I aminoacyl-tRNA synthetase catalytic domains. Crystal structures with high sequence identity, i.e., ~100%, have been omitted (see Computational Methods). The ordering according to the QR transformation and the SCOP domain codes are listed on the right. Ambiguous branchings, those that are different from the UPGMA branchings in Figures 9-12, are marked with a green circle. This ambiguity is partially lifted with the inclusion of the new archaeal structure for TyrRS (Ya, see Supplementary Figure 3), but complete removal of the conflict will require a structure of the archaeal type TrpRS (Wa). Other labeling is as defined in Figures 9 and 11. Neighbor joining tree constructed with defaults settings of the Phylip package [Felsenstein, J. (1989) *Cladistics* 5, 164.] using our measure of structural homology,  $Q_H$ , see Computational Methods. The tree was rooted with the K1a structure (d1irxa2).



Supplementary Figure 2: Full neighbor joining tree of the Class II aminoacyl-tRNA synthetase catalytic domains. Other notes same as in Supplementary Figure 1. The tree was rooted with  $G_{(\alpha\beta)_2}$  (d1j5wb) and Fb (d1pysa) structures.



Supplementary Figure 3: Full structural dendrogram of the class I aminoacyl-tRNA synthetase catalytic domains. Recently, a crystal structure of TyrRS from the archaeon *M. jannaschii* (Ya) [T. Kobayashi et al. (2003) *Nature Struct. Biol.* **10**, 425.] has become available which now allows us to verify the full canonical pattern structurally for this synthetase. Crystal structures with high sequence identity, i.e., ~100%, have been omitted (see Computational Methods). The ordering according to the QR transformation and the SCOP domain codes are listed on the right. In general the features of the structural dendrogram agree with the sequence-based phylogenetic analysis of Woese et al. [Woese et al. (2000) *Micro. Mol. Biol. Rev.* **64**, 202.]. The organism names are color coded according to the domain of life: red (Bacteria), blue (Archaea), gold (Eucarya). The AARSs are labeled by their one letter code for specificity and genre. Whenever an organism and enzyme differ in color, a horizontal transfer has occurred except in the cases of non-canonically distributed AARSs, black.



Supplementary Figure 4: Full structural dendrogram of the class II synthetases. A structure of the non-discriminating archaeal type AspRS (Da) from *T. thermophilus* [C. Charron et al. (2003) *EMBO J.* **22**, 1632.] has also become recently available. *T. thermophilus* has two AspRS synthetases, a discriminating bacterial type, and a non-discriminating archaeal type. The structural phylogeny shows that the bacterial type groups with the other bacterial type AspRS, and the archaeal type AspRS from *T. thermophilus* groups with the other AspRS of the archaeal genus. *T. thermophilus* acquired this archaeal type AspRS via horizontal gene transfer. See Supplementary Figure 3 for other the details.