Sequence co-evolution gives 3D contacts and structures of protein complexes


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Supplementary Figure Legends

Supplementary Figure 1. Genomic distance of concatenated sequence pairs. For all candidates in the benchmark set, the cumulative number of concatenated sequence pairs below a certain genomic distance threshold is plotted. Sequence numbers are normalized by the length of the concatenated alignment.

Supplementary Figure 2. Comparison of Interface RMSD to HADDOCK score. The HADDOCK scores of docked models are plotted against their iRMSDs to the bound complex crystal. Color-coding of data points according to the number of top ranked inter-ECs used for docking: none (grey), 5 (red), 10 (purple). HADDOCK score outliers with scores > 150 are not shown, and any model with an iRMSD > 20Å is displayed as iRMSD=20Å for visualization purposes.

Supplementary Figure 3. Complex contact maps for benchmark set. For all complexes in the benchmark set, increasing numbers of the highest-ranked predicted coevolving residue pairs are visualized in complex contact maps (red stars, all inter-ECs and all intra-ECs until the 5th/10th/15th/20th top ranked inter-EC). Top left and bottom right quadrants: intra-ECs; top right and bottom left quadrants: inter-ECs. Inter- and intra-protein crystal structure contacts at minimum atom distance cutoffs of 5/6/7 Å are shown as dark/middle/light grey dots, respectively; missing data in the crystal structure as shaded blue rectangles.

Supplementary Figure 4. Inter-EC strength as a quality measure for contacts. The number of intra-ECs for each subunit (normalized by subunit length; blue and green solid lines) in the EC pair list down to the occurrence of a given number of inter-ECs is shown as a measure of the relative strength of inter- vs. intra-ECs. The subset of true positive (minimum atom distance < 8 Å) intra-ECs is indicated by dotted lines.

Supplementary Figure 5. Precision of evolutionary couplings on benchmark complexes. The percentage of true positive ECs (minimum atom distance in crystal structure < 8 Å; inter-ECs: red, intra-ECs for both subunits: blue, green) is shown as a function of inter-EC rank. For any data point on the intra-EC curves, all intra-ECs in the EC pair list down to the occurrence of a given number of inter-ECs were evaluated. EC pairs missing in the crystal structure are not excluded in the analysis.
Supplementary Figure 2

**ATPCAINT**

**BTUC-BTJD**

**BTUC-BTUF**

**CLPS-CLFA**

**HGRA**

**METI-METN**

**MOAD-MOAE**

Legend:
- no ECs
- 5 ECs
- 10 ECs
Supplementary Figure 3

atpeg_hammer_e2: ATPE_ECOLI and ATPG_ECOLI

Top 5 inter ECs, plm, theta 0.3

Top 10 inter ECs, plm, theta 0.3

Top 15 inter ECs, plm, theta 0.3

Top 20 inter ECs, plm, theta 0.3
btucf_hmmer_e10_e5: BTUC_ECOLI and BTUF_ECOLI

Top 5 inter ECs, plm, theta 0.3

Top 10 inter ECs, plm, theta 0.3

Top 15 inter ECs, plm, theta 0.3

Top 20 inter ECs, plm, theta 0.3
btucf_hmmer_e10_e5_BF: BTUC_ECOLI and BTUF_ECOLI

Top 5 inter ECs, plm, theta 0.3

Top 10 inter ECs, plm, theta 0.3

Top 15 inter ECs, plm, theta 0.3

Top 20 inter ECs, plm, theta 0.3
moade_hammer_e1: MOAD_ECOLI and MOAE_ECOLI

Top 5 inter ECs, plm, theta 0.3

Top 10 inter ECs, plm, theta 0.3

Top 15 inter ECs, plm, theta 0.3

Top 20 inter ECs, plm, theta 0.3
hk_rr_hmmer_e25: Q9WZV7_THEMA and Q9WYT9_THEMA

Top 5 inter ECs, plm, theta 0.3

Top 10 inter ECs, plm, theta 0.3

Top 15 inter ECs, plm, theta 0.3

Top 20 inter ECs, plm, theta 0.3
Top 5 inter ECs, plm, theta 0.3

Top 10 inter ECs, plm, theta 0.3

Top 15 inter ECs, plm, theta 0.3

Top 20 inter ECs, plm, theta 0.3
trxb_thio_hmmer_e45_e30_noDistfilter: TRXB_ECOLI and THIO_ECOLI

Top 5 inter ECs, plm, theta 0.3

Top 10 inter ECs, plm, theta 0.3

Top 15 inter ECs, plm, theta 0.3

Top 20 inter ECs, plm, theta 0.3
hisfh_hammer_e15_e10: HIS6_THEMA and HIS5_THEMA

Top 5 inter ECs, plm, theta 0.3

Top 10 inter ECs, plm, theta 0.3

Top 15 inter ECs, plm, theta 0.3

Top 20 inter ECs, plm, theta 0.3
Supplementary Figure 5