

Integration of QUARK and I-TASSER for *ab initio* protein structure prediction in CASP11

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SUPPLEMENTARY INFORMATION

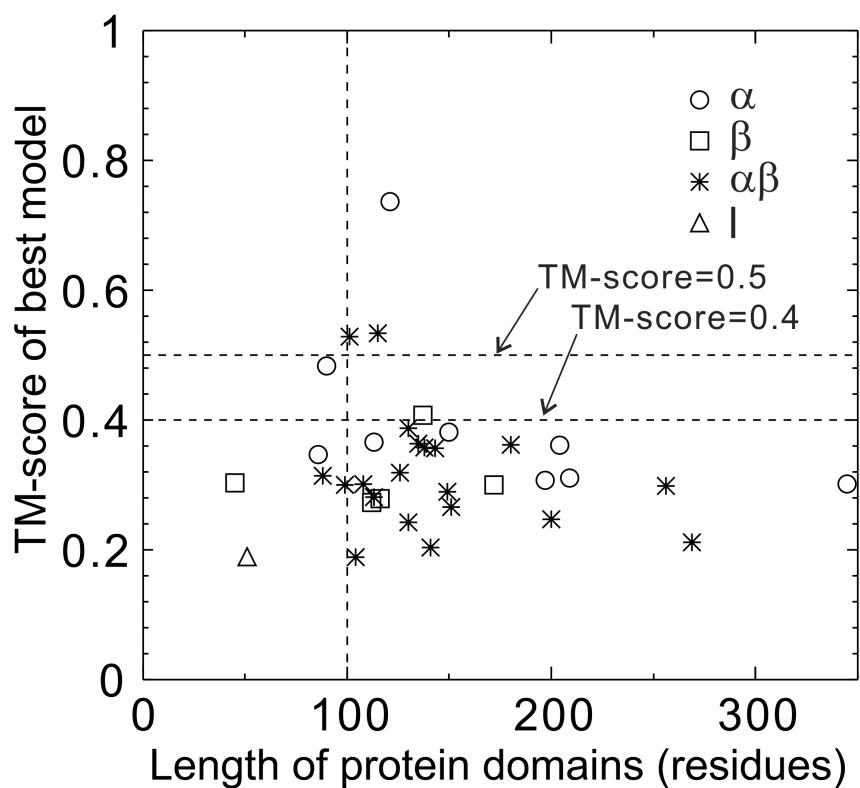


Figure S1. TM-score of the best QUARK models for 35 FM domains versus protein length.

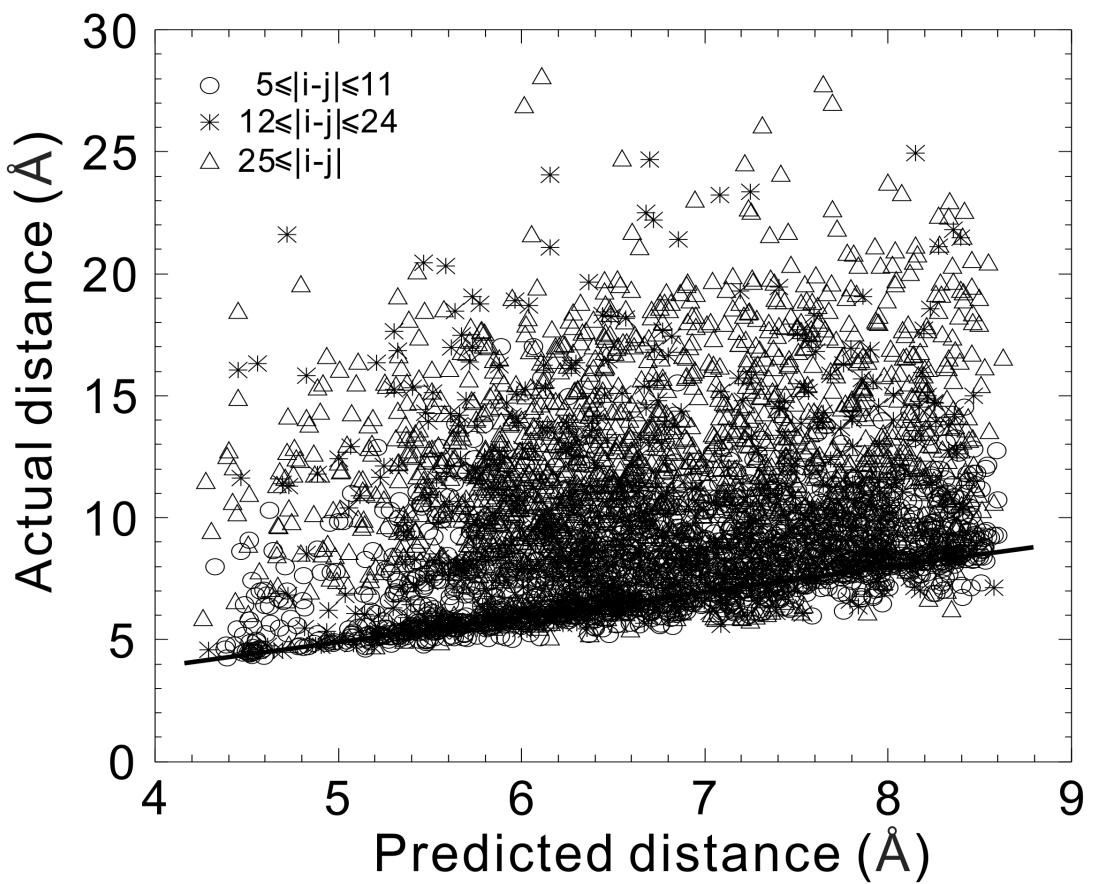


Figure S2. Predicted distance of the residue pairs by QUARK as in contact versus the actual distance of the residue pairs in the native structure. Points in different shapes indicate data from residue pairs of different contact order. The solid line shows the position with identical distances to guide the eye.

Table S1. RMSD of the fragments identified by QUARK for T0837-D1. The ten best fragments are counted at each position and the average RMSD is calculated along the positions for a given fragment size.

| Size of fragments (residues) | Average RMSD (Å) | Standard deviation (Å) |
|------------------------------|------------------|------------------------|
| 2 | 0.011 | 0.010 |
| 3 | 0.113 | 0.078 |
| 4 | 0.789 | 0.226 |
| 5 | 1.372 | 0.303 |
| 6 | 1.470 | 0.310 |
| 7 | 1.548 | 0.298 |
| 8 | 1.612 | 0.296 |
| 9 | 1.729 | 0.300 |
| 10 | 1.803 | 0.346 |
| 11 | 1.874 | 0.376 |
| 12 | 1.948 | 0.393 |
| 13 | 2.031 | 0.415 |
| 14 | 2.103 | 0.425 |
| 15 | 2.181 | 0.441 |
| 16 | 2.259 | 0.446 |
| 17 | 2.341 | 0.454 |
| 18 | 2.436 | 0.450 |
| 19 | 2.530 | 0.437 |
| 20 | 2.637 | 0.421 |

Table S2. Contact prediction results using fragment-based distance profile by QUARK for T0837-D1.

| # | i | j | i-j | d _{pred} (Å) ^a | d _{exp} (Å) ^b | d _{pred} -d _{exp} (Å) |
|---------|-----|-----|-----|------------------------------------|-----------------------------------|---|
| 1 | 7 | 18 | 11 | 7.923 | 6.150 | 1.773 |
| 2 | 8 | 17 | 9 | 8.435 | 9.035 | 0.600 |
| 3 | 10 | 15 | 5 | 8.201 | 8.143 | 0.058 |
| 4 | 10 | 16 | 6 | 8.350 | 8.636 | 0.286 |
| 5 | 11 | 18 | 7 | 6.708 | 5.498 | 1.210 |
| 6 | 11 | 17 | 6 | 6.255 | 6.220 | 0.035 |
| 7 | 11 | 16 | 5 | 5.072 | 5.360 | 0.288 |
| 8 | 12 | 18 | 6 | 7.996 | 8.540 | 0.544 |
| 9 | 12 | 17 | 5 | 7.969 | 8.391 | 0.422 |
| 10 | 19 | 24 | 5 | 7.319 | 8.555 | 1.236 |
| 11 | 20 | 56 | 36 | 7.942 | 10.250 | 2.308 |
| 12 | 20 | 52 | 32 | 8.224 | 11.178 | 2.954 |
| 13 | 24 | 55 | 31 | 6.921 | 7.102 | 0.181 |
| 14 | 24 | 59 | 35 | 7.542 | 8.047 | 0.505 |
| 15 | 38 | 43 | 5 | 8.419 | 8.117 | 0.302 |
| 16 | 39 | 44 | 5 | 6.097 | 8.835 | 2.738 |
| 17 | 40 | 45 | 5 | 7.980 | 8.856 | 0.876 |
| 18 | 42 | 47 | 5 | 8.052 | 8.455 | 0.403 |
| 19 | 43 | 48 | 5 | 6.650 | 6.687 | 0.037 |
| 20 | 64 | 70 | 6 | 8.067 | 7.862 | 0.205 |
| 21 | 64 | 69 | 5 | 6.915 | 6.665 | 0.250 |
| 22 | 65 | 70 | 5 | 6.773 | 6.108 | 0.665 |
| 23 | 77 | 83 | 6 | 8.136 | 6.806 | 1.330 |
| 24 | 77 | 82 | 5 | 5.544 | 5.231 | 0.313 |
| 25 | 78 | 83 | 5 | 6.206 | 6.340 | 0.134 |
| 26 | 78 | 84 | 6 | 7.299 | 6.294 | 1.005 |
| 27 | 86 | 91 | 5 | 6.463 | 7.956 | 1.493 |
| 28 | 92 | 97 | 5 | 8.528 | 9.030 | 0.502 |
| 29 | 98 | 103 | 5 | 7.908 | 7.326 | 0.582 |
| 30 | 99 | 104 | 5 | 7.595 | 9.826 | 2.231 |
| 31 | 102 | 107 | 5 | 7.834 | 11.721 | 3.887 |
| 32 | 103 | 108 | 5 | 7.359 | 7.724 | 0.365 |
| 33 | 115 | 120 | 5 | 7.809 | 7.523 | 0.286 |
| 34 | 116 | 121 | 5 | 7.361 | 8.190 | 0.829 |
| Average | | | | | | 0.934 |

^ad_{pred}: predicted distance by QUARK.

^bd_{exp}: actual distance in experimental structure.