Supporting material for: ProQ3: Improved model quality assessments using Rosetta energy terms

Karolis Uziela, Nanjiang Shu, Björn Wallner and Arne Elofsson

Table S1: **Wilcoxon test p-values for significance of differences in per target correlations between ProQ3 and other methods.** P-values lower than 0.05 are marked in bold.

	ProQ2	**ProQ-RosFA**	**ProQ-RosCen**	**QMEAN**	**QPROB**	**SMOQ**	**DOPE**	**DDFIRE**
PROQ3, CASP11	0.485	0.498	0.153	**3.91E-04**	**0.018**	**3.35E-09**	**8.25E-13**	**2.81E-09**
PROQ3, CAMEO	0.12	0.232	**0.011**	**9.13E-12**	**0.028**	**5.18E-46**	0.104	**0.019**

Table S2: **Method performance on CASP11 free modelling targets (15 targets).** Only targets that have all domains classified as free modeling domains according to the official CASP classification are considered.

	Global whole data set correlation	**Global per target correlation**	**Local whole data set correlation**	**Local per model correlation**	**Average first ranked GDT_TS**
ProQ3	0.520	0.492	0.334	0.285	21.9
ProQRosFA	0.475	0.471	0.305	0.272	21.9
ProQRosCen	0.470	0.482	0.279	0.206	20.5
ProQ2	0.507	0.506	0.298	0.244	21.9
QMEAN	0.446	0.474	0.231	0.206	21.8
QPROB	0.420	0.514	-	-	22.3
SMOQ	0.238	0.465	0.165	0.157	21.4
DOPE	0.224	0.371	0.037	0.082	22.5
DDFIRE	-0.366	0.383	-	-	17.7

Table S3: **Method performance on CASP11 template-based targets (52 targets).** Only targets that have all domains classified as template-based domains according to the official CASP classification are considered.

	Global whole data set correlation	**Global per target correlation**	**Local whole data set correlation**	**Local per model correlation**	**Average first ranked GDT_TS**
ProQ3	0.804	0.581	0.702	0.548	62.7
ProQRosFA	0.775	0.564	0.674	0.530	61.7
ProQRosCen	0.732	0.529	0.638	0.461	59.3
ProQ2	0.794	0.558	0.688	0.523	62.3
QMEAN	0.689	0.479	0.580	0.468	59.3
QPROB	0.717	0.483	-	-	60.1
SMOQ	0.501	0.329	0.394	0.295	57
DOPE	0.491	0.305	0.211	0.189	59.5
DDFIRE	0.306	0.369	-	-	57.2

Table S4: **ProQ3 performance with and without side-chain repacking.**

	Global whole data set correlation	**Global per target correlation**	**Local whole data set correlation**	**Local per model correlation**	**Average first ranked GDT_TS**
ProQ3-no-repack, CASP11	0.849	0.467	0.730	0.471	51.2
ProQ3-repack, CASP11	0.865	0.548	0.739	0.476	51.5
ProQ3-no-repack, CAMEO	0.725	0.322	0.600	0.503	69.6
ProQ3-repack, CAMEO	0.737	0.529	0.615	0.511	70.9

Table S5: **Average GDT_TS1 for each method before and after re-ranking for all prediction groups.** Targets column denotes on how many targets each group was evaluated. Groups that submitted only 1 model per target were excluded.

	Original GDT_TS1	**ProQ3 GDT_TS1**	**ProQ2 GDT_TS1**	**Optimal GDT_TS1**	**Targets**
QUARK	51.0	50.7	50.8	53.2	83
Zhang-Server	50.7	51.5	50.7	53.4	83
nns	49.7	49.7	49.8	51.7	83
myprotein-me	49.4	50.0	49.6	52.6	83
BAKER-ROSETTASERVER	49.2	50.8	50.7	53.2	83
MULTICOM-CONSTRUCT	48.9	48.4	48.5	50.5	83
MULTICOM-CLUSTER	48.8	49.3	49.2	50.2	83
MULTICOM-NOVEL	47.9	48.2	48.1	50.7	83
RaptorX	47.5	47.8	47.7	48.5	82
HHPredA	47.2	47.2	47.2	47.2	83
HHPredX	47.1	47.1	47.1	47.1	83
FALCON_MANUAL_X	47.0	47.2	47.3	48.1	83
TASSER-VMT	47.0	47.6	47.4	49.7	83
FALCON_MANUAL	47.0	47.0	47.2	48.2	83
FALCON_TOPO	46.9	47.0	46.9	48.0	83
FALCON_EnvFold	46.9	47.3	47.3	48.4	83
Pcons-net	46.3	46.8	46.2	48.4	83
FFAS-3D	46.3	46.8	46.7	47.7	83
MULTICOM-REFINE	46.2	46.0	46.1	47.5	83
raghavagps-tsppred	45.5	44.6	45.2	46.0	83
PhyreX	45.4	45.8	45.8	46.6	83
BioSerf	45.4	45.3	45.1	48.0	80
Seok-server	44.7	44.7	44.7	44.9	83
chuo-fams-server	43.5	43.7	44.0	45.3	83
FLOUDAS_SERVER	42.8	42.7	42.7	44.4	81
FFAS03	42.6	43.0	43.0	43.9	83
eThread	42.5	43.4	42.9	46.0	83
slbio	42.3	43.0	42.8	45.1	82
Distill	42.2	42.4	42.4	44.5	81
3D-Jigsaw-V5_1	42.1	42.2	42.2	43.9	82
STRINGS	42.0	43.6	42.8	46.3	81
ZHOU-SPARKS-X	41.7	42.2	42.3	44.9	83
Atome2_CBS	41.7	43.6	43.7	46.3	82
RBO_Aleph	41.4	42.0	41.9	44.3	81
MUFOLD-Server	41.2	41.2	41.2	42.5	83
Alpha-Gelly-Server	40.7	44.1	44.0	45.6	83
BhageerathH	38.7	40.7	40.6	41.7	83
FUSION	34.1	35.0	34.7	37.3	83
BioShell-server	32.9	34.3	34.6	36.9	81
SAM-T08-server	29.0	28.6	28.7	45.7	54
PSF	20.3	20.3	20.3	33.1	51
MATRIX	18.7	18.7	18.5	30.7	52
IntFOLD3	15.3	15.3	15.3	35.4	36
RaptorX-FM	8.0	8.3	8.4	23.2	32