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PRISM-EM: template interface-based modelling of multi-protein complexes guided by cryo-electron microscopy density maps. Corrigendum

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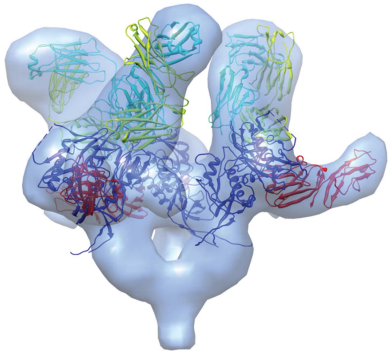
A revised Table 6 and Supporting Information are provided for the article by Kuzu *et al.* [(2016), *Acta Cryst.* D**72**, 1137–1148].

After the online publication of the article by Kuzu *et al.* (2016), Drs Sjoer de Vries and Alexandre Bonvin noticed an apparent anomaly in the i.r.m.s.d. values in Table 6. Indeed, there were erroneous and duplicate entries in this table. (i) The values in the old Table 6 were computed using a definition which is different from that used in *CAPRI*. In the paper, the superposition was performed for the entire protein, and the r.m.s.d. was then computed only for the interface residues. We have revised Table 6 by recalculating i.r.m.s.d.

Table 6
Performance of our method on the *HADDOCK-EM* set (van Zundert *et al.*, 2015) where cases were selected from the ZDOCK benchmark set.

Models were compared with the PDB structures and the results are presented with i.r.m.s.d. values. The first column gives the PDB code of the complex. The second column indicates the difficulty level assigned as in the benchmark data set. The third column lists the *HADDOCK-EM* results using unbound structures (listed in the benchmark). The fourth column gives the *PRISM-EM* results using the same set of unbound structures. Note that for equal comparison, columns 3 and 4 should be used. The fifth column lists the i.r.m.s.d. values of *PRISM-EM* using the alternative structures of the same proteins available in the PDB. The sixth column lists the i.r.m.s.d. values when the individual proteins are from the bound complex structures. A dash indicates a case where *PRISM-EM* could not find a model. Asterisks indicate use of the self-template interfaces of bound structures.

		I.r.m.s.d. (Å)			
		HADDOCK-EM (itw)	*PRISM-EM*		
Complex	Difficulty	Query (unbound) proteins	Query (unbound) proteins	Query proteins and their alternatives	Bound proteins
1avx	Easy	0.67	1.72	1.01	0.51
2oul	Easy	0.63	0.83	0.83	0.55
1ay7	Easy	0.66	1.25	1.19	0.75
4cpa	Easy	0.94	—	—	—
1ahw	Easy	0.91	1.23	1.23	0.47*
7cei	Easy	0.78	0.90	0.90	0.53
2oob	Easy	0.97	7.43	7.43	0.73*
2fd6	Easy	1.13	1.43	0.94	0.45
1ak4	Easy	1.22	1.40	1.40	1.01
1b6c	Easy	1.88	2.22	2.22	0.74
1bgx	Medium	4.85	7.18*	7.18*	0.53*
1r6q	Medium	1.26	9.38	0.95	0.72
1m10	Medium	2.82	2.59	0.93	0.47
1acb	Medium	2.43	9.24	0.68	0.59*
1jk9	Hard	2.32	3.11	3.11	0.49
1bkd	Hard	3.62	4.61	0.92	0.49
1jmo	Hard	4.23	15.62	15.62	3.43*



values as described in *CAPRI* evaluations (Mendez *et al.*, 2003) using the script `irsmd.py` (Viswanath *et al.*, 2013), considering only the interface backbone atoms. (ii) The results for alternative conformations were compared with the rigid-body docking of *HADDOCK-EM* (it0) in the old table. We now compare these results with their explicit solvent docking results (itw), which are their best generated complexes among the top 400 solutions, with our results for both unbound and alternative structures. We have revised Table 6 accordingly. Using only unbound structures, *HADDOCK-EM* (itw) models all 17 cases, where 15 of them have i.r.m.s.d. values less than 4 Å. *PRISM-EM* models ten of the 17 cases using unbound structures, where only one model has a better i.r.m.s.d. (1m10) than *HADDOCK-EM* models. Therefore, using unbound structures, *HADDOCK-EM* outperforms *PRISM-EM* (comparison of columns 3 and 4). When *PRISM-EM* considers alternative structures, the following cases additionally become better than *HADDOCK-EM*: 2fd6 (easy), 1r6q (medium), 1acb (medium) and 1bkd (hard). The supplementary tables have been revised to provide the alternative structures which have been used in the calculations. All of the models of Table 6 are also provided in the Supporting Information.

The authors apologize for any inconvenience that this has caused.

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