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Table 4: The Lowest rmsd Value in Top Five Complexes Selected by Various Energy Functions, Compared with the Lowest Possible rmsd Value in the Decoy Sets

PDB ID ^a	$\Gamma(^{\circ})^b$	DDNA ^c	FIRE ^d	vFIRE ^e	cFIRE ^f	vcFIRE ^g	RV ^h	Lowest ⁱ
1qna	35.70	1.43	1.24	6.38	1.05	1.05	1.05	0.49
1d02	13.62	1.23	1.44	1.44	0.43	0.43	0.43	0.43
1eon	13.41	0.73	0.42	0.42	0.42	0.42	0.42	0.42
1ckq	12.29	0.82	0.61	0.61	0.61	0.41	0.61	0.39
1dmu	9.12	0.25	0.25	25.66	0.25	0.25	0.25	0.25
1qpz	8.53	0.72	1.10	0.20	0.20	0.20	0.20	0.20
1au7	8.48	1.18	0.50	0.50	0.50	0.50	0.50	0.50
1je8	8.15	0.41	0.35	0.41	0.35	0.35	0.35	0.35
2cgp	7.84	1.28	0.45	0.58	0.31	0.31	0.31	0.31
1b3t	7.74	0.90	0.62	25.07	0.88	0.70	0.88	0.51
1tc3	7.30	1.54	12.99	12.71	1.00	0.69	2.38	0.59
1g9z	7.17	1.16	0.41	0.41	0.41	0.41	0.49	0.41
1zme	6.84	0.72	0.96	20.80	0.90	0.90	0.90	0.50
1a73	6.56	0.80	0.45	0.45	0.45	0.45	0.45	0.45
1jko	6.55	0.92	0.66	0.66	0.66	0.66	1.27	0.38
1bdt	6.41	1.01	0.90	0.90	0.46	0.54	0.54	0.46
2bop	6.28	1.10	0.50	0.50	0.58	0.50	0.58	0.50
1ali	6.21	1.74	0.17	0.17	0.17	0.17	0.17	0.17
1bc8	6.10	1.20	0.33	0.33	0.87	0.33	0.87	0.33
1pdn	6.04	0.80	4.63	4.63	1.01	0.54	1.01	0.54
1skn	5.96	1.23	0.50	0.62	0.50	0.50	0.50	0.50
1mjo	5.94	0.78	0.37	0.37	0.37	0.37	0.37	0.37
1bl0	5.88	1.13	0.47	0.47	0.35	0.40	0.35	0.35
2dgc	5.75	2.01	0.06	0.06	0.06	0.06	0.06	0.06
3pvi	5.71	0.78	0.63	0.58	0.61	0.64	0.61	0.58
2hdd	5.61	1.24	0.75	0.55	0.77	0.41	0.52	0.41
1ign	5.19	1.04	0.66	0.51	0.51	0.51	0.51	0.51
1qpi	5.09	1.13	0.59	0.59	0.59	0.59	0.59	0.59
1a3q	5.08	0.87	0.42	0.42	0.42	0.42	0.42	0.42
1dfm	5.05	1.40	0.40	0.40	0.40	0.40	0.40	0.40
1lql	5.04	0.89	0.42	0.42	0.42	0.42	0.42	0.42
1tro	5.02	1.13	0.63	0.63	0.55	0.55	0.55	0.55
1fjl	4.95	0.51	0.51	0.46	0.50	0.46	0.50	0.46
1h8a_b	4.82	2.71	0.75	0.75	0.80	0.67	0.80	0.53
1h8a_a	4.82	3.51	0.11	0.11	0.11	0.11	0.11	0.11
1f4k	4.80	1.94	0.45	0.45	0.45	0.45	0.45	0.44
6pax	4.73	0.97	2.13	8.00	0.63	0.44	0.63	0.44
1hlv	4.53	0.86	0.48	0.34	0.34	0.34	0.34	0.34
1mn	4.46	1.14	0.73	0.73	0.83	0.56	0.74	0.56
1dsz	4.38	0.72	0.40	0.24	0.24	0.24	0.40	0.24
1hwt	4.13	0.89	1.64	7.35	1.64	1.35	1.09	0.55
1per	4.09	0.69	0.54	0.54	0.54	0.54	0.54	0.54
1l3l	4.02	1.61	0.67	0.67	0.64	0.64	0.64	0.64
3hts	3.87	1.74	0.69	0.69	0.69	0.69	0.69	0.69
3bam	3.77	1.03	0.47	24.45	0.44	0.42	0.44	0.42
Median		1.04	0.51	0.55	0.50	0.45	0.50	0.44

^aProtein databank identification code.

^bThe degree of overall DNA deformation.²⁶

^cDDNA [DFIRE with 19-atomic types acted on interfacial atoms only].³⁵

^dFIRE with residue/base-specific atom types and 10 Å^o cutoff without distance scaling.

^eVolume-fraction correction added to FIRE (vFIRE).

^fLow-count correction with Dirichlet pseudo counts added to FIRE (cFIRE).

^gVolume-fraction correction added to cFIRE (vcFIRE).

^hRobertson and Varani²⁶ energy function that was trained by the same 167 complexes as FIRE-based energy functions.

ⁱThe lowest rmsd structure in decoys.

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