

Protein name	RAPDF	Atomic KBP	DFIRE-A	DFIRE-A1.45	DFIRE-A1.70	DFIRE-B	4B OPT POT
<b>4-state reduced</b>							
1ctf	1/3.26b	1/3.53	1/3.86	1/3.33	1/4.01	1/3.03	2/2.32
1r69	1/3.49	1/3.76	1/4.23	1/3.76	1/4.10	1/2.95	2/2.80
1sn3	1/3.26	1/3.50	1/3.79	1/3.83	1/3.13	1/3.40	1/2.69
2cro	1/2.93	1/2.91	1/3.29	1/2.97	1/3.24	2/2.74	1/2.46
3icb	1/2.22	1/2.41	4/2.28c	1/2.15	4/2.29	24/1.68	1/1.99
4pti	1/3.12	1/3.47	1/3.62	1/3.54	1/3.16	1/3.15	1/3.00
4rxn	1/2.79	1/3.12	1/3.33	1/2.78	1/3.42	19/1.88	1/2.67
<b>fisa</b>							
1fc2	497/-2.74	413/-1.05	254/0.23	406/-0.91	60/1.05	1/2.76	496/-2.34
1hdd-C	17/2.00	25/1.78	1/4.50	1/3.77	1/4.45	1/6.76	3/2.10
2cro	14/1.93	24/1.64	1/6.33	1/5.47	1/6.08	1/7.84	62/1.11
4icb	1/3.89	6/2.46	1/6.91	1/6.34	1/6.96	1/8.47	1/3.27
<b>fisa_casp</b>							
1bg8-A	1/4.39	2/2.84	1/5.35	1/5.13	1/4.92	1/3.82	815/-0.46
1bl0	1/3.19	215/0.76	1/4.50	1/4.01	1/4.32	3/2.27	813/-3.20
1jwe	1/4.69	4/2.64	1/6.26	1/5.96	1/5.94	1/4.81	602/0.005
<b>lmds</b>							
1b0n-B	359/-0.45	74/1.03	430/-1.17	398/-0.82	438/-1.33	261/0.03	441/0.18
1bba	501/-11.11	500/-3.51	501/-16.28	501/-18.34	501/-11.78	501/-21.38	470/-1.61
1fc2	501/-7.75	501/-8.86	501/-5.72	501/-6.32	501/-4.19	441/-1.22	501/-3.48
1ctf	1/2.84	1/3.45	1/3.54	1/3.56	1/3.42	1/2.77	70/1.06
1dtk	116/-0.08	31/1.16	1/2.62	62/0.56	1/3.69	5/2.46	99/0.2
1igd	1/4.21	1/4.16	1/5.16	1/5.54	1/4.26	1/4.69	3/2.26
1shf-A	1/5.15	2/2.83	1/6.68	1/6.01	1/6.29	1/5.44	1/2.77
2cro	416/-0.96	175/0.40	1/4.70	109/0.85	1/6.51	1/4.50	5/1.89
2ovo	4/2.76	1/2.86	1/3.21	1/3.27	1/2.92	27/1.48	119/0.48
4pti	157/0.20	13/1.75	1/3.96	5/2.18	1/4.72	1/3.47	157/0.17
<b>lattice_ssfit</b>							
lbco	1/9.79	1/9.47	1/12.09	1/10.80	1/7.36	1/7.95	1/6.37
1ctf	1/6.99	1/7.20	1/10.05	1/7.26	1/8.13	1/6.89	1/4.20
1dkt-A	1/6.78	1/6.78	1/6.87	1/6.38	1/4.50	1/4.92	1/4.28
lfca	1/5.57	1/3.36	1/7.18	1/6.13	1/5.26	1/5.30	1/3.95
1nkl	1/8.33	1/8.16	1/9.29	1/7.15	1/7.15	1/5.83	1/5.64
1pgb	1/8.42	1/6.86	1/11.87	1/8.60	1/9.18	1/9.64	1/3.71
1trl-A	1/4.84	1/5.58	1/6.32	1/4.81	1/5.00	1/3.73	1/4.58
4icb	1/6.68	1/5.65	1/7.81	1/6.12	1/7.06	1/4.25	1/4.96
<b>Summary</b>							
# Correct/Total	22/32	18/32	27/32	25/32	27/32	23/32	15/32
Z- score	0.83	2.87	4.27	3.31	3.91	3.32	1.87

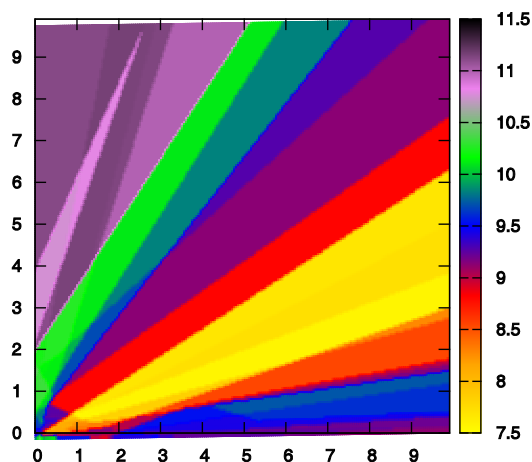
**Table S1.** Native structure rankings and Z-scores for different atomistic potentials and optimized short range and 4-body coarse grained (sequential and non-sequential) potentials, for multiple decoy sets

from Decoys 'R'Us dataset.

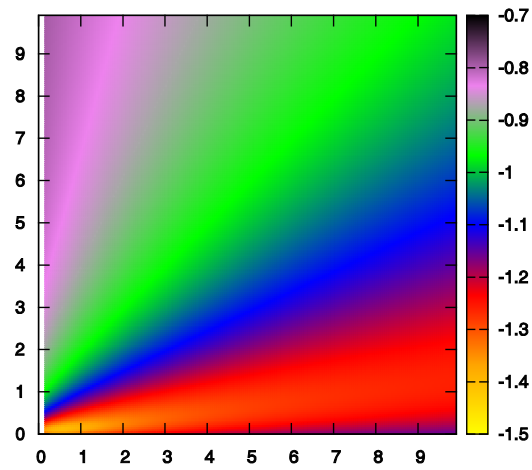
The list of targets for which *four body optimized potential* performed poorly:

1) Small proteins: 1bg8-A (76 aa), 1bba (36 aa), 1fc2 (44 aa), 1ctf (64 aa), 1igd (61 aa), 2cro (66 aa), 1ovo (56 aa), 4pti (58 aa), 1hdd-C (57 aa)

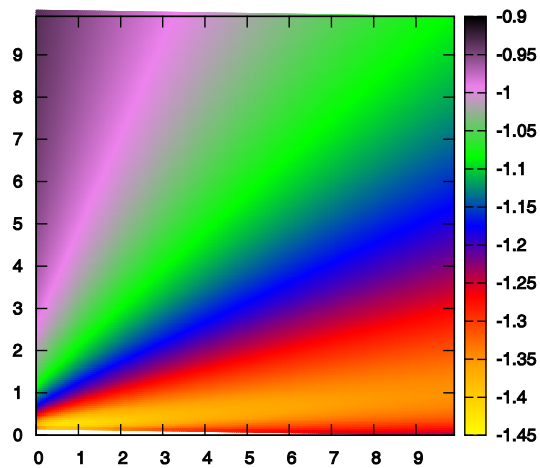
2) Bonded or stabilized by ligands/ions: 1bl0 bound to RNA molecule, 1dtk have (20-30 heavy atoms) ligands bound and 1b0n-B is stabilized by highly charged ions (5 x Zn<sup>2+</sup>)



**Figure S1.** Heat map for the average RMSD for best ranked models, for template-free modeled targets from CASP8, for different weights of the four-body non-sequential and short-range potentials where the color indicates the value of RMSD(Å).



**Figure S2.** Heat map for the average Z-score for best ranked models, for homology modeled targets from CASP8, for different weights of the four-body non-sequential and short-range potentials where the color gives the value of Z-score. The scale for Z-score is negative in contrast to the scale used in the text.



**Figure S3.** Heat map for the average Z-score for best ranked models, for template-free modeled targets from CASP8, for different weights of the four-body non-sequential and short-range potentials where the color gives the value of Z-score. The scale for Z-score is negative in contrast to the scale used in the text.

### CASP8 target data set used

#### Easy targets

T0449      T0388      T0478\_D2    T0417\_D2

T0450	T0389_D1	T0478	T0418_D1
T0451	T0390_old	T0479	T0418
T0452_D2	T0391_D1	T0480	T0419_D2
T0452	T0391_old	T0481	T0419
T0453	T0392	T0483	T0421
T0454_D2	T0393_D1	T0485	T0422_D2
T0454D2	T0393	T0486	T0422
T0454	T0394	T0487_D2	T0423
T0455	T0395	T0487_D3	T0424_D2
T0456_D2	T0396	T0487_D4	T0424_D3
T0456	T0397_D2	T0487_D5	T0424
T0457_D2	T0397	T0487	T0425
T0457	T0398_D2	T0488	T0426
T0459	T0398	T0489	T0427_D2
T0461	T0399	T0490	T0427
T0462_D1	T0400	T0491	T0428
T0462	T0401	T0492	T0429_D2
T0463	T0402	T0493	T0429
T0464	T0404	T0494	T0430_D2
T0466	T0406	T0495	T0430
T0468	T0407_D2	T0496	T0431_D2
T0469	T0407	T0497	T0431
T0470_D2	T0408	T0498	T0432
T0470	T0409_D1	T0499	T0433
T0471	T0409	T0501_D2	T0434
T0472_D2	T0411	T0501	T0435
T0472	T0412	T0502	T0436
T0473	T0413	T0503	T0437
T0474	T0414	T0504_D2	T0438_D2
T0475	T0415	T0504_D3	T0438
T0477	T0416	T0504	T0440
T0509	T0445	T0505_D1	T0441
T0510_D1	T0446_D2	T0505	T0442_D2
T0510	T0446	T0506_D2	T0442
T0511	T0447_D1	T0506	T0443
T0512	T0448	T0507	T0444
T0513	T0514	T0508	T0445_D2

### Hard targets

T0405	T0476
T0416	T0482
T0443_D2	T0496
T0443	T0510
T0460	T0513
T0465	T0405_D2

