Supplemental data, scripts, and RosettaScripts for Fleishman et al. 2011

the colons (::::::::::) delineate different files. See comments within colons
for details on each file

::::::::::::::
The data used to produce Figs 2 and S1
data/GroupSubmission.txt
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****
Group 1s-
Raw scores are given in units of kcal/mol

	Raw score	normalized
design_1	0.660	3
design_2	7.681	5
design_3	0.851	3
design_4	-0.270	2
design_5	0.558	3
design_6	-0.621	2
design_7	-0.013	2
design_8	-0.813	2
design_9	1.371	4
design_10	1.975	4
design_11	1.948	4
design_12	3.578	5
design_13	0.059	3
design_14	0.211	3
design_15	1.342	4
design_16	1.335	4
design_17	-7.022	1
design_18	1.945	4
design_19	0.112	3
design_20	0.838	3
design_21	2.101	5
design_22	-1.026	1
design_23	0.441	3
design_24	-0.373	2
design_25	-0.616	2
design_26	-2.165	1
design_27	0.606	3
design_28	2.006	5
design_29	-0.737	2
design_30	1.341	4
design_31	1.733	4
design_32	-2.772	1

design_33	0.260	3
design_34	0.267	3
design_35	2.559	5
design_36	2.716	5
design_37	-1.230	1
design_38	-0.630	2
design_39	2.214	5
design_40	13.284	5
design_41	3.465	5
design_42	0.154	3
design_43	-2.013	1
design_44	2.654	5
design_45	0.938	3
design_46	-0.296	2
design_47	0.180	3
design_48	5.867	5
design_49	0.756	3
design_50	-0.419	2
design_51	-0.438	2
design_52	1.509	4
design_53	1.841	4
design_54	1.973	4
design_55	-0.419	2
design_56	2.527	5
design_57	0.993	3
design_58	-4.139	1
design_59	0.840	3
design_60	0.675	3
design_61	-1.976	1
design_62	0.067	3
design_63	-1.950	1
design_64	2.907	5
design_65	-1.190	1
design_66	-0.361	2
design_67	3.298	5
design_68	0.055	3
design_69	-1.472	1
design_70	0.431	3
design_71	-0.087	2
design_72	-0.833	2
design_73	-0.268	2
design_74	2.325	5
design_75	-0.288	2
design_76	-0.063	2
design_77	-3.094	1
design_78	0.050	3

design_79	1.005	4
design_80	0.223	3
design_81	-0.417	2
design_82	-0.085	2
design_83	-0.126	2
design_84	0.037	3
design_85	-0.500	2
design_86	3.683	5
design_87	0.700	3
1A2K	-1.601	1
1ACB	-0.323	2
1AHW	-3.182	1
1AK4	-1.000	2
1AKJ	-2.298	1
1AVX	-0.953	2
1AY7	-0.422	2
1AZS	-1.747	1
1B6C	1.285	4
1BGX	-1.731	1
1BJ1	-8.934	1
1BKD	-0.690	2
1BUH	-0.482	2
1BVK	0.812	3
1BVN	0.631	3
1CGI	0.466	3
1D6R	0.165	3
1DE4	-7.190	1
1DFJ	-3.309	1
1DQJ	2.064	5
1E4K	-0.027	2
1E6J	-1.902	1
1E96	-0.765	2
1EAW	-1.476	1
1EER	-8.048	1
1EFN	-2.064	1
1EWY	-1.078	1
1EZU	1.674	4
1F34	5.090	5
1F51	2.175	5
1FAK	1.985	4
1FC2	0.904	3
1FQ1	-1.812	1
1FQJ	-2.862	1
1FSK	-4.625	1
1GCQ	0.438	3
1GHQ	1.920	4

1GLA	-7.982	1
1GP2	-4.221	1
1GPW	-6.309	1
1GRN	-1.393	1
1H1V	3.796	5
1HE1	-0.381	2
1HE8	2.214	5
1HIA	-1.525	1
1I2M	-7.028	1
1I4D	0.695	3
1I9R	-3.302	1
1IB1	0.870	3
1IBR	-7.444	1
1IJK	-7.494	1
1IQD	-2.529	1
1IRA	0.571	3
1J2J	-0.810	2
1JMO	-4.288	1
1JPS	-5.017	1
1K4C	-2.062	1
1K5D	-8.320	1
1K74	-3.891	1
1KAC	-1.123	1
1KKL	3.700	5
1KLU	-1.855	1
1KTZ	-2.377	1
1KXP	-0.853	2
1KXQ	-0.974	2
1M10	-5.628	1
1MAH	-3.736	1
1ML0	-13.882	1
1MLC	-2.617	1
1N2C	-25.490	1
1N8O	0.470	3
1NCA	-0.843	2
1NSN	6.128	5
1NW9	0.885	3
1OPH	-2.697	1
1PPE	0.261	3
1PXV	-1.320	1
1QA9	-2.488	1
1QFW	-1.933	1
1R0R	0.169	3
1R8S	-0.857	2
1RLB	-0.697	2
1S1Q	0.051	3

1SBB	-0.124	2
1T6B	2.533	5
1UDI	-5.223	1
1VFB	0.524	3
1WEJ	-8.803	1
1WQ1	-1.764	1
1XD3	-1.162	1
1XQS	-8.718	1
1Y64	0.371	3
1YVB	-1.888	1
1Z0K	-2.029	1
1Z5Y	0.018	3
1ZHI	-2.936	1
2AJF	0.591	3
2B42	0.291	3
2C0L	0.845	3
2CFH	0.732	3
2FD6	2.552	5
2H7V	1.629	4
2HLE	-2.175	1
2HMI	12.227	5
2HQS	0.104	3
2HRK	-0.828	2
2I25	0.081	3
2JEL	-3.692	1
2MTA	0.408	3
2NZ8	-0.319	2
2O8V	0.182	3
2OOB	0.041	3
2OT3	-1.537	1
2PCC	-8.250	1
2QFW	-1.068	1
2SIC	-0.131	2
2SNI	0.289	3
2UUY	0.191	3
2VIS	-1.518	1
7CEI	-10.742	1

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Group 4s-

Raw scores are given in units of average likelihood scores for surface contact point pairs (sorry, best I can do)

	Raw score	normalized score
design_1	-1.252	1
design_2	-0.664	3

design_3	-0.033	4
design_4	-0.970	2
design_5	-0.315	4
design_6	-0.868	2
design_7	-0.932	2
design_8	-0.726	3
design_9	-0.970	2
design_10	-1.000	1
design_11	-0.925	2
design_12	-1.209	1
design_13	-0.675	3
design_14	-0.118	4
design_15	-0.781	2
design_16	-0.281	4
design_17	-0.071	4
design_18	-0.323	4
design_19	-0.691	3
design_20	-0.862	2
design_21	-1.150	1
design_22	-1.024	1
design_23	0.234	4
design_24	-0.875	2
design_25	-0.677	3
design_26	-0.298	4
design_27	-0.373	4
design_28	-0.472	4
design_29	-0.767	2
design_30	-0.190	4
design_31	-0.418	4
design_32	-0.399	4
design_33	-0.349	4
design_34	-0.017	4
design_35	-0.291	4
design_36	-0.801	2
design_37	-1.222	1
design_38	-0.807	2
design_39	-0.549	3
design_40	-1.038	1
design_41	-0.436	4
design_42	-0.860	2
design_43	-0.852	2
design_44	-0.332	4
design_45	-0.829	2
design_46	-0.467	4
design_47	-0.966	2
design_48	-0.759	2

design_49	-0.137	4
design_50	-0.383	4
design_51	-0.153	4
design_52	-1.063	1
design_53	-0.880	2
design_54	0.302	4
design_55	-1.075	1
design_56	-0.770	2
design_57	-0.393	4
design_58	-0.767	2
design_59	-0.341	4
design_60	-0.320	4
design_61	-0.783	2
design_62	-0.815	2
design_63	-1.468	1
design_64	-0.863	2
design_65	-1.216	1
design_66	-1.393	1
design_67	-0.775	2
design_68	-0.457	4
design_69	-0.944	2
design_70	-0.205	4
design_71	-0.976	2
design_72	-0.569	3
design_73	-0.803	2
design_74	-0.610	3
design_75	-1.219	1
design_76	-0.804	2
design_77	-0.914	2
design_78	-0.923	2
design_79	-0.720	3
design_80	-0.612	3
design_81	-0.734	3
design_82	-0.895	2
design_83	-0.749	3
design_84	-0.651	3
design_85	-0.880	2
design_86	-0.790	2
design_87	-0.287	4
1A2K	-1.113	1
1ACB	-0.209	4
1AHW	-1.256	1
1AK4	-1.297	1
1AKJ	-1.342	1
1AVX	-0.132	4
1AY7	-0.603	3

1AZS	-0.158	4
1B6C	-0.638	3
1BGX	-0.435	4
1BJ1	0.649	4
1BKD	-1.208	1
1BUH	-0.787	2
1BVK	-0.680	3
1BVN	-0.673	3
1CGI	-0.060	4
1D6R	-0.412	4
1DE4	-0.680	3
1DFJ	-0.748	3
1DQJ	-0.641	3
1E4K	-0.784	2
1E6J	-1.166	1
1E96	-0.988	2
1EAW	-0.391	4
1EER	-1.429	1
1EFN	-1.011	1
1EWY	-1.002	1
1EZU	-0.178	4
1F34	-0.199	4
1F51	-0.801	2
1FAK	-1.005	1
1FC2	-0.399	4
1FQ1	-0.754	2
1FQJ	-0.823	2
1FSK	-0.276	4
1GCQ	-1.203	1
1GHQ	-0.431	4
1GLA	-1.650	1
1GP2	-1.258	1
1GPW	-0.291	4
1GRN	-1.274	1
1H1V	-1.101	1
1HE1	-1.097	1
1HE8	-1.167	1
1HIA	0.091	4
1I2M	-1.429	1
1I4D	-0.933	2
1I9R	-0.700	3
1IB1	-1.327	1
1IBR	-1.239	1
1IJK	-1.518	1
1IRA	-0.775	2
1J2J	-1.177	1

1JMO	-0.469	4
1JPS	-1.196	1
1K4C	-0.683	3
1K5D	-0.904	2
1K74	-1.446	1
1KAC	-1.397	1
1KKL	-0.982	2
1KLU	-0.816	2
1KTZ	-0.902	2
1KXP	-1.313	1
1KXQ	-0.607	3
1M10	-1.270	1
1MAH	-0.718	3
1ML0	-0.964	2
1MLC	-0.628	3
1N2C	-1.327	1
1N8O	-0.351	4
1NCA	-0.913	2
1NSN	-1.014	1
1NW9	-0.247	4
1OPH	-0.212	4
1PPE	0.248	4
1PXV	-0.838	2
1QA9	-1.800	1
1QFW	-1.110	1
1R0R	-0.690	3
1R8S	-1.122	1
1RLB	-0.860	2
1S1Q	-0.530	3
1SBB	-0.647	3
1T6B	-0.851	2
1UDI	-1.415	1
1VFB	-0.879	2
1WEJ	-0.686	3
1WQ1	-0.914	2
1XD3	-0.982	2
1XQS	-1.207	1
1Y64	-1.195	1
1YVB	-0.272	4
1Z0K	-1.133	1
1Z5Y	-1.066	1
1ZHI	-0.640	3
2AJF	-0.935	2
2B42	-0.563	3
2C0L	-1.443	1
2CFH	-1.649	1

2H7V -1.607 1
2HLE -0.772 2
2HMI -0.033 4
2HQS -1.132 1
2HRK -1.043 1
2I25 -0.878 2
2JEL -0.780 2
2MTA -0.513 3
2NZ8 -1.080 1
2O8V -0.195 4
2OOB -0.412 4
2OT3 -0.481 4
2PCC -1.508 1
2QFW -0.449 4
2SIC -0.329 4
2SNI -0.662 3
2UUY -0.216 4
2VIS -0.876 2
7CEI -1.383 1

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Group 5s-
1A2K 4.958 1
1ACB 5.213 1
1AHW 4.541 1
1AK4 4.081 1
1AKJ 3.431 1
1AVX 4.811 1
1AY7 3.356 1
1AZS 3.412 1
1B6C 4.625 1
1BGX 6.778 1
1BJ1 3.900 1
1BKD 6.343 1
1BUH 2.962 2
1BVK 2.320 2
1BVN 5.423 1
1CGI 4.525 1
1D6R 1.100 3
1DFJ 3.702 1
1DQJ 4.910 1
1E4K 2.494 2
1E6J 4.655 1
1E96 2.290 2
1EAW 2.823 2

1EER 6.672 1
1EFN 3.538 1
1EWY 1.989 3
1EZU 5.288 1
1F34 5.466 1
1F51 4.728 1
1FAK 6.095 1
1FC2 3.840 1
1FQ1 3.308 1
1FQJ 1.595 3
1FSK 5.042 1
1GCQ 3.826 1
1GHQ -0.279 4
1GLA 3.014 1
1GP2 4.036 1
1GPW 3.972 1
1GRN 5.748 1
1H1V 4.782 1
1HE1 5.359 1
1HE8 2.542 2
1HIA 3.153 1
1I2M 6.383 1
1I4D 3.261 1
1I9R 1.526 3
1IB1 5.013 1
1IBR 5.980 1
1IJK 4.880 1
1IQD 6.625 1
1IRA 6.263 1
1J2J 3.682 1
1JMO 6.118 1
1JPS 5.054 1
1K4C 3.985 1
1K5D 4.758 1
1K74 5.496 1
1KAC 4.126 1
1KKL 2.860 2
1KLU 2.860 2
1KTZ 0.971 4
1KXP 6.098 1
1KXQ 6.225 1
1M10 4.323 1
1MAH 4.412 1
1ML0 4.255 1
1MLC 4.703 1
1N2C 6.272 1

1N8O 3.478 1
1NCA 3.751 1
1NSN 3.516 1
1NW9 3.459 1
1OPH 3.423 1
1PPE 3.942 1
1PXV 5.159 1
1QA9 1.813 3
1QFW 3.231 1
1R0R 4.690 1
1R8S 5.895 1
1RLB 2.274 2
1S1Q 2.420 2
1SBB 1.540 3
1T6B 5.510 1
1UDI 4.711 1
1VFB 3.405 1
1WEJ 3.905 1
1WQ1 4.629 1
1XD3 6.122 1
1XQS 4.343 1
1Y64 2.086 2
1YVB 4.179 1
1Z0K 5.462 1
1Z5Y 4.093 1
1ZHI 2.495 2
2AJF 4.587 1
2B42 5.636 1
2C0L 6.465 1
2CFH 5.631 1
2FD6 2.472 2
2H7V 5.005 1
2HLE 4.029 1
2HQS 4.863 1
2HRK 3.805 1
2I25 4.328 1
2JEL 1.963 3
2MTA 1.817 3
2NZ8 4.697 1
2O8V 4.074 1
2OOB 1.112 3
2OT3 6.061 1
2PCC 1.679 3
2QFW 2.828 2
2SIC 2.217 2
2SNI 5.063 1

2UUY 2.609 2
2VIS 3.199 1
7CEI 6.004 1
design_1 1.789 3
design_10 2.418 2
design_11 1.649 3
design_12 3.078 1
design_13 1.482 3
design_14 0.502 4
design_15 2.937 2
design_16 1.593 3
design_17 0.527 4
design_18 1.782 3
design_19 3.362 1
design_2 1.914 3
design_20 4.460 1
design_21 2.845 2
design_22 5.558 1
design_23 0.843 4
design_24 5.216 1
design_25 1.010 3
design_26 0.119 4
design_27 1.635 3
design_28 2.254 2
design_29 2.353 2
design_3 2.367 2
design_30 2.650 2
design_31 0.492 4
design_32 -0.539 4
design_33 3.391 1
design_34 2.674 2
design_35 2.632 2
design_36 2.195 2
design_37 4.719 1
design_38 4.285 1
design_39 1.023 3
design_4 1.489 3
design_40 1.520 3
design_41 2.040 2
design_42 0.927 4
design_43 1.867 3
design_44 3.287 1
design_45 2.754 2
design_46 1.849 3
design_47 2.157 2
design_48 2.663 2

design_49 2.055 2
design_5 0.983 4
design_50 1.062 3
design_51 1.757 3
design_52 3.048 1
design_53 1.900 3
design_54 0.174 4
design_55 4.509 1
design_56 1.494 3
design_57 1.498 3
design_58 1.928 3
design_59 0.857 4
design_6 5.277 1
design_60 0.342 4
design_61 1.723 3
design_62 1.769 3
design_63 2.672 2
design_64 1.332 3
design_65 1.509 3
design_66 4.178 1
design_67 1.767 3
design_68 3.958 1
design_69 1.230 3
design_7 1.621 3
design_70 1.002 3
design_71 4.417 1
design_72 2.472 2
design_73 1.140 3
design_74 -0.789 4
design_75 4.101 1
design_77 3.115 1
design_78 1.297 3
design_79 0.303 4
design_8 3.577 1
design_80 0.842 4
design_81 2.026 2
design_82 4.704 1
design_83 3.047 1
design_84 4.070 1
design_85 3.140 1
design_86 1.662 3
design_87 1.207 3
design_9 1.656 3
design_76 0 5
2HMI 0 5
1DE4 0 5

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Group 6s-
The methodology used is as follows:

All 207 structures were redocked, globally with SwarmDock [1], and locally with PyRosetta [2]. Encounter complex formation and dissociation was simulated with BioSimz [1]. A number of metrics which characterise the results of these computations were derived. Numerous interface descriptors and binding energy terms were also calculated: the analytical continuum solvent (ACE) potential terms [3], DComplex [4], Rosetta energy terms [2], interface packing and surface complementarity scores [5], and generalised Born (GBSW) electrostatic and non-polar solvation energy [6]. Further parameters, describing interface flexibility and flexibility differences of core and periphery interface residues, were calculated using elastic network normal mode analysis [7], as well as counts of the number of residues with binding energies below various energy thresholds and the number of buried H-bond donors and acceptors. The distribution of these parameter values indicates that, compared to the designed, the benchmark complexes have a lower H-bond binding energy, fewer unsatisfied buried H-bond donors and acceptors, a more favourable change in ACE energy upon binding, and more favourable encounter complex formation dynamics. These parameters are sufficient to distinguish the benchmark and designed complexes, as a parameter set capable of binomial classification at 97.6% accuracy (95.7% accuracy with leave-one-out cross validation) was found, using a support vector machine with an analysis of variance kernal and a population-based forward greedy feature selection algorithm. However, as the designed complexes are not to be used in the discrimination of the two categories, the parameters were used in linear combination, in an energy function trained on empirically derived binding free energy values.

Dissociation constants for 95 complexes in the Benchmark 3.0 were manually amalgamated from the literature and empirical binding free energies were calculated. Linear regression of a number of parameter sets were performed, for which thresholds could be found to discriminate the benchmark complexes from the designed with between 70% and 90% accuracy. Values shown, in kcal/mol, correspond to an energy function composed of the following parameters, along with their relative importance (derived from normalised weights), where the first two parameters are boolean: Is SwarmDock top ranked structure under 5√Ö rmsd to bound? (0.076), does the biggest SwarmDock cluster correspond to the bound? (0.009), Rosetta fine-grained pair potential (0.299), Rosetta coarse-grained pair potential (0.122), Van der Waals (0.192), BioSimz predicted kon constant (0.027), interface packing (0.181), surface complementarity (0.176), ACE self-solvation energy (0.780) and GBSW solvation energy (0.071). The regression has a RMS error of 2.76 and a correlation of 0.414, has an area-under-ROC

of 91.2% and can be used to correctly classify 88.4% of the complexes with a threshold of -9.55kcal/mol. Bins are chosen such that the 'binds' category contains complexes with predicted binding energies below -9.8 kcal/mol, and the cutoffs for the higher bins, likely to bind, uncertain, likely not to bind and don't bind, are chosen at intervals of 0.2 kcal/mol.

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[2] S. Chaudhury, S. Lyskov, and J.J. Gray, 'PyRosetta: a script-based interface for implementing custom molecular modeling algorithms using Rosetta.' Bioinformatics, 26(5):689-691 (2010).
[3] M. Schaefer, and M. Karplus. 'A Comprehensive Analytical Treatment of Continuum Electrostatics.' J. Phys. Chem. 100:1578-1599 (1996).
[4] S. Liu, C. Zhang, H. Zhou, and Y. Zhou, 'A physical reference state unifies the structure-derived potential of mean force for protein folding and binding.' Proteins 56, 93-101 (2004).
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[6] W. Im, M.S. Lee, and C.L. Brooks III, 'Generalized Born Model with a Simple Smoothing Function.' J. Comput. Chem. 24:1691-1702 (2003).
[7] K. Suhre, and Y. H. Sanejouand, 'ElNemo: a normal mode web server for protein movement analysis and the generation of templates for molecular replacement.' Nucleic Acids Res. 32:610-614 (2004)
AUTHOR Iain Moal, Xiofan Li and Paul Bates
REMARK Binding scores for benchmark and designed protein-protein complexes.
REMARK
REMARK Scores are calculated using an energy function derived by linear regression of parameter values to 95 empirical binding free energies.
REMARK
REMARK Parameters used in regression (normalised relative weight):
REMARK 1) Is SwarmDock top ranked structure under 5√Ö rmsd to bound? (0.076) - Boolean, 1 for true 0 for false
REMARK 2) Does the biggest SwarmDock cluster correspond to the bound? (0.009) - Boolean, 1 for true 0 for false
REMARK 3) Rosetta fine-grained pair potential (0.299)
REMARK 4) Rosetta coarse-grained pair potential (0.122)
REMARK 5) Van der Waals (0.192)
REMARK 6) BioSimz predicted kon constant (0.027)
REMARK 7) Interface packing (0.181)
REMARK 8) Surface complementarity (0.176)
REMARK 9) ACE self-solvation energy (0.780)
REMARK 10)GBSW solvation energy (0.071)
REMARK

REMARK Normalised scores are categorised as follows:
REMARK 1) E <= -9.8
REMARK 2) -9.8 < E <= -9.6
REMARK 5) -9.6 < E <= -9.4
REMARK 3) -9.4 < E <= -9.2
REMARK 4) E > -9.2
REMARK
REMARK NB) Only approximate BioSimz predicted kon constant are used for design_81 to design_87, however, as this is the parameter with
REMARK NB) the second least weight, the results are not expected to change significantly.

Raw scores are given in units of kcal/mol

	Raw score	normalized score
design_1	-9.18847791452	4
design_2	-8.90359639623	4
design_3	-9.53346129658	5
design_4	-8.99509329802	4
design_5	-11.1160282123	1
design_6	-8.03409371939	4
design_7	-8.38165944955	4
design_8	-9.02092503814	4
design_9	-8.4490811097	4
design_10	-8.7060972057	4
design_11	-8.69127425161	4
design_12	-9.43344956353	5
design_13	-9.46993229462	5
design_14	-8.3584442799	4
design_15	-9.1694760495	4
design_16	-9.01192198793	4
design_17	-7.97547194152	4
design_18	-8.9952521212	4
design_19	-9.35145292258	3
design_20	-9.50758680655	5
design_21	-9.29596879779	3
design_22	-9.05564697222	4
design_23	-8.80975493305	4
design_24	-9.75745007701	2
design_25	-8.19016971131	4
design_26	-8.97891832583	4
design_27	-8.71806843924	4
design_28	-9.08174636748	4
design_29	-8.66389305593	4
design_30	-8.89682585848	4
design_31	-9.3026178676	3
design_32	-9.19555060366	4

design_33 -8.95650861444 4
design_34 -9.15368481371 4
design_35 -8.97918368259 4
design_36 -9.4144038019 5
design_37 -9.46949466746 5
design_38 -9.07520631389 4
design_39 -8.60218399906 4
design_40 -9.32934161874 3
design_41 -8.71829504275 4
design_42 -9.00796015877 4
design_43 -8.20184781052 4
design_44 -9.47362184972 5
design_45 -9.09725518196 4
design_46 -8.90703349036 4
design_47 -9.00416910934 4
design_48 -8.42842829621 4
design_49 -7.79288107894 4
design_50 -8.49343245768 4
design_51 -8.82258900294 4
design_52 -8.55742439894 4
design_53 -8.48849308328 4
design_54 -8.01766134472 4
design_55 -8.71583845797 4
design_56 -8.64055336191 4
design_57 -9.4958680998 5
design_58 -9.20406749431 3
design_59 -8.96353222894 4
design_60 -9.11214229127 4
design_61 -8.86588904814 4
design_62 -8.71325025569 4
design_63 -9.25605667347 3
design_64 -8.56009756485 4
design_65 -8.08101953667 4
design_66 -8.97932930684 4
design_67 -8.56774802284 4
design_68 -9.25258583588 3
design_69 -8.33096156597 4
design_70 -9.32575008386 3
design_71 -9.05941459633 4
design_72 -9.24587238012 3
design_73 -8.85849303889 4
design_74 -8.6452449847 4
design_75 -9.01997121624 4
design_76 -8.89013182734 4
design_77 -9.33254682959 3
design_78 -9.01071452693 4

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design_79 -8.69159256039      4
design_80 -8.39631598169      4
design_81 -8.89020746203      4
design_82 -9.19795167366      4
design_83 -8.93775736642      4
design_84 -9.15586042072      4
design_85 -8.49634235468      4
design_86 -8.16075244609      4
design_87 -8.87452852255      4
1A2K -10.275063058      1
1ACB -10.2183654111      1
1AHW -11.2102666632      1
1AK4 -9.0828343192      4
1AKJ -10.5226412477      1
1AVX -10.5818443789      1
1AY7 -10.1136271661      1
1AZS -8.34178999      4
1B6C -10.5623682722      1
1BGX -14.9875754209      1
1BJ1 -9.98239458041      1
1BKD -10.7497003629      1
1BUH -9.66568201645      2
1BVK -10.3673967854      1
1BVN -13.7372119384      1
1CGI -11.4321081499      1
1D6R -10.8573208625      1
1DE4 -10.0201579214      1
1DFJ -11.5751848188      1
1DQJ -11.3408099821      1
1E4K -9.06570648749      4
1E6J -10.4161197065      1
1E96 -9.71066077559      2
1EAW -11.6090827615      1
1EER -12.6126903129      1
1EFN -9.17730136508      4
1EWY -9.84730782703      1
1EZU -11.0558805055      1
1F34 -12.4945874221      1
1F51 -10.9471529362      1
1FAK -11.2166354672      1
1FC2 -8.79094254088      4
1FQ1 -8.96748278164      4
1FQJ -11.0958967428      1
1FSK -10.5638670331      1
1GCQ -10.5283409126      1
1GHQ -8.52154556383      4
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1GLA -10.072399939 1
1GP2 -10.1699546314 1
1GPW -12.1809193139 1
1GRN -10.7050797955 1
1H1V -10.3078549362 1
1HE1 -11.7284419433 1
1HE8 -8.94531312806 4
1HIA -11.1127406596 1
1I2M -12.97461115 1
1I4D -9.60927236477 2
1I9R -10.6727705624 1
1IB1 -10.1453398424 1
1IBR -10.6473631407 1
1IJK -9.19708093907 4
1IQD -10.8649328652 1
1IRA -13.0884686573 1
1J2J -8.64093297969 4
1JMO -11.8910036468 1
1JPS -12.048482704 1
1K4C -10.5874132993 1
1K5D -12.2964912957 1
1K74 -11.1923539505 1
1KAC -10.0662375724 1
1KKL -11.2978511503 1
1KLU -9.76258421132 2
1KTZ -8.90017335603 4
1KXP -12.0068833669 1
1KXQ -9.78420358877 2
1M10 -10.3440294196 1
1MAH -11.0898577128 1
1ML0 -10.505824502 1
1MLC -11.7047339005 1
1N2C -10.7023203807 1
1N8O -10.6544013178 1
1NCA -10.3557025951 1
1NSN -10.6317893406 1
1NW9 -10.1455202765 1
1OPH -11.0950020934 1
1PPE -11.9646632573 1
1PXV -11.0822465619 1
1QA9 -9.04209226259 4
1QFW -10.7161145683 1
1R0R -10.1215092768 1
1R8S -10.0877977653 1
1RLB -9.58593521567 5
1S1Q -9.7322508746 2

1SBB -8.92111030215 4
1T6B -11.2784602799 1
1UDI -10.375196373 1
1VFB -10.9874227752 1
1WEJ -10.9501315928 1
1WQ1 -13.2807760786 1
1XD3 -10.7690797672 1
1XQS -11.3118271685 1
1Y64 -9.51011400679 5
1YVB -10.200387327 1
1Z0K -12.1231810162 1
1Z5Y -9.75884887025 2
1ZHI -9.08620707229 4
2AJF -9.2991494347 3
2B42 -12.330913126 1
2C0L -10.8380933877 1
2CFH -10.4758544886 1
2FD6 -9.98429762422 1
2H7V -9.42807159427 5
2HLE -11.4682202574 1
2HMI -9.10639175212 4
2HQS -12.3529566062 1
2HRK -9.69236170356 2
2I25 -9.01165053107 4
2JEL -10.6200361831 1
2MTA -9.58760960782 5
2NZ8 -12.2353126859 1
2O8V -9.88539273253 1
2OOB -7.76601892709 4
2OT3 -11.3961113128 1
2PCC -8.90654115711 4
2QFW -9.92255933423 1
2SIC -10.2127631578 1
2SNI -10.2857777957 1
2UUY -11.5157152076 1
2VIS -9.48880947591 5
7CEI -10.8595097025 1

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Group 7s -
REMARK Please use this file to submit your results for both designs and the docking benchmark
REMARK SCORING and DOCKING based on the Attract program (Zacharias, 2003) and the latest parameter set
REMARK
The raw score is a composite score in RT units (however, in principle an

arbitrary scale).
It is an "ad hoc" score (see comments below)
with the following 3 equally weighted contributions (each 33%):

1. Attract score of the energy minimized complex (in rotational and translational coordinates)
2. RMSD of the minimized complex from the start structure multiplied by 1 RT.
3. RANK of the solution closest to the "native" provided complex in a systematic search,
if rank within top 10: 0 RT; if rank within 10-100: 6 RT: if rank within 100-1000: 12 RT;
if rank > 1000: 18 RT.

Explanation of the composite raw score:
contribution 1:
Typically the Attract score for the minimized complex gives already an impression if the complex is favorable or not. However, often the score alone is not sufficient.
contribution 2:
For experimental complex structures the docking minimization typically yields an Rmsd (ligand)
of < 1-3 Angstrom. Larger deviations indicate that the complex may not be stable.
This explains contribution 2 which increases with the Rmsd deviation of the minimized
complex from the provided "native" structure.
contribution 3:
For experimental complex structures (bound partners) a systematic ATTRACT search
typically gives the docking minimum closest to experiment as top ranking solution
or within the 10 best solutions.
If this is not the case it indicates that the complex is probably unrealistic.
To translate this into a score the rules given above (see 3.) were used.
The weights on this and the other contributions were not optimized.

Explanation of the normalized score:
Based on the score for the zdock-structures the following normalized score was derived.

1. raw score < -6 RT : normalized score: 1
2. -6 RT < raw score < -3 RT: normailized score: 2
3. -3 RT < raw score < 0 RT: normalized score: 3
4. raw score > 0 RT : normalized score: 4

(normailized score 5 was not needed)

For 90% of the ZdockRos-structures the raw score was better than -6, therefore a score better -6 was selected as best score(1). For very few Zdock-cases a score above zero was found, therefore 0 RT was chosen as the limit to distinguish non-binders (score 4). The -3 value (in between 0 and -6) was then chosen to distinguish between likely binders and likely non-binders.

Name	Score	normalized score
design_1	-2.747	3
design_2	-0.399	3
design_3	-5.449	2
design_4	0.541	4
design_5	-2.272	3
design_6	-4.624	2
design_7	-5.836	2
design_8	-4.434	2
design_9	4.227	4
design_10	-2.460	3
design_11	0.400	4
design_12	5.986	4
design_13	-0.235	3
design_14	-0.059	3
design_15	-1.867	3
design_16	-6.147	1
design_17	0.270	4
design_18	-2.451	3
design_19	-0.570	3
design_20	-7.385	1
design_21	-6.819	1
design_22	1.427	4
design_23	0.609	4
design_24	-2.746	3
design_25	4.826	4
design_26	4.015	4
design_27	0.139	4
design_28	-1.989	3
design_29	-4.418	2
design_30	-6.494	1
design_31	-0.850	3
design_32	4.619	4
design_33	-6.507	1
design_34	-6.983	1
design_35	-7.183	1

design_36	-3.854	2
design_37	-6.227	1
design_38	-1.205	3
design_39	-5.414	2
design_40	-0.287	3
design_41	-0.204	3
design_42	0.979	4
design_43	3.251	4
design_44	-6.527	1
design_45	-2.642	3
design_46	-2.341	3
design_47	4.405	4
design_48	0.738	4
design_49	1.390	4
design_50	-4.900	2
design_51	-3.394	2
design_52	-5.853	2
design_53	-4.270	2
design_54	0.294	4
design_55	1.463	4
design_56	3.490	4
design_57	-6.050	1
design_58	-2.374	3
design_59	1.077	4
design_60	-0.656	3
design_61	-6.335	1
design_62	-1.966	3
design_63	-0.563	3
design_64	0.488	4
design_65	-2.261	3
design_66	-2.292	3
design_67	-2.381	3
design_68	1.357	4
design_69	1.180	4
design_70	1.207	4
design_71	-2.962	3
design_72	-0.009	3
design_73	4.079	4
design_74	0.346	4
design_75	0.833	4
design_76	2.575	4
design_77	-8.187	1
design_78	3.876	4
design_79	1.079	4
design_80	-1.987	3
design_81	-5.605	2

design_82	-4.595	2
design_83	-3.283	2
design_84	-2.882	3
design_85	-5.220	2
design_86	4.174	4
design_87	0.101	4
1A2K	-6.321	1
1ACB	-6.996	1
1AHW	-4.976	2
1AK4	-5.454	2
1AKJ	-5.448	2
1AVX	-8.259	1
1AY7	-6.477	1
1B6C	-8.575	1
1BGX	10.935	4
1BJ1	-9.213	1
1BUH	-5.946	2
1BVK	-4.811	2
1BVN	-10.123	1
1CGI	-9.999	1
1D6R	-6.012	1
1DFJ	-9.378	1
1DQJ	-2.670	3
1E6J	-6.204	1
1E96	-5.402	2
1EAW	-8.036	1
1EER	-10.104	1
1EWY	-2.547	3
1EZU	-9.034	1
1F34	-10.301	1
1F51	-8.284	1
1FAK	-9.558	1
1FC2	-6.888	1
1FQ1	-7.326	1
1FQJ	-6.584	1
1FSK	-9.068	1
1GCQ	-6.152	1
1GHQ	4.752	4
1GP2	8.600	4
1GRN	-5.536	2
1H1V	-6.606	1
1HE1	-7.709	1
1HE8	-4.742	2
1HIA	-8.009	1
1I2M	-11.764	1
1I4D	-5.437	2

1I9R	-5.219	2
1IB1	-6.463	1
1IBR	-8.702	1
1IJK	-8.250	1
1IQD	-8.894	1
1JPS	-6.587	1
1K4C	-9.340	1
1K5D	-8.850	1
1KAC	-2.987	3
1KKL	-3.923	2
1KLU	-6.556	1
1KTZ	0.150	4
1KXP	-10.275	1
1KXQ	-8.892	1
1M10	-7.046	1
1MAH	-5.416	2
1ML0	-8.528	1
1MLC	-7.011	1
1NCA	-6.676	1
1NSN	-6.175	1
1PPE	-7.949	1
1QA9	-5.620	2
1QFW	-6.474	1
1RLB	-5.003	2
1SBB	-6.689	1
1UDI	-8.005	1
1VFB	-5.916	2
1WEJ	-6.251	1
1WQ1	-8.203	1
2HMI	1.205	4
2JEL	-2.858	3
2MTA	-5.381	2
2PCC	-4.399	2
2QFW	-4.939	2
2SIC	-6.522	1
2SNI	-6.936	1
2VIS	-6.881	1
7CEI	-7.346	1
1J2J	-6.502	1
1IRA	-7.371	1
1GPW	-8.412	1
1GLA	-5.672	2
1EFN	-6.669	1
1E4K	-9.030	1
1BKD	-12.488	1
1AZS	-5.541	2

1Y64 -1.486 3
1XQS -9.550 1
1XD3 -9.347 1
1T6B -8.539 1
1S1Q -4.546 2
1R8S -11.162 1
1R0R -7.745 1
1PXV -9.064 1
1OPH -7.386 1
1NW9 -8.139 1
1N8O -8.008 1
1K74 -9.422 1
1JMO -11.997 1
2CFH -11.982 1
2C0L -7.075 1
2B42 -10.218 1
2AJF -6.726 1
1ZHI -5.657 2
1Z5Y -6.606 1
1Z0K -7.493 1
1YVB -5.075 2
2UUY -6.285 1
2OT3 -6.230 1
2OOB -4.744 2
2O8V -7.387 1
2NZ8 -9.034 1
2I25 -7.277 1
2HRK -5.792 2
2HQS -8.530 1
2HLE -4.988 2
2H7V -5.725 2
2FD6 -6.011 1
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Group 8s-
Description of binding affinity prediction by Seok group

We used the summation of seven energy terms to predict binding affinities for target complexes. These terms are : 1) DFIRE, 2) Van der Waals (CHARMM19), 3) Electrostatics (CHARMM19), 4) Solvation term described by Atomic Solvation Parameter, 5) Hydrogen bonding, 6) Sequence conservation score derived from psi-BLAST search, and 7) sidechain entropy. Among the seven terms, majorly contributing terms are 6) and 7). We optimized the weights and decided the cut for binding status by training on 107 training targets. The training set consists of 74 protein-protein complexes with known binding affinity values, and 33 complexes from CAPRI round 20.

1A2K	-18.747	1
1ACB	-23.776	1
1AHW	-3.555	3
1AK4	-27.775	1
1AKJ	-8.133	1
1AVX	-28.542	1
1AY7	-10.276	1
1B6C	-16.927	1
1BJ1	-0.770	4
1BUH	-13.678	1
1BVK	-2.393	3
1BVN	-4.387	3
1CGI	-30.534	1
1D6R	-28.268	1
1DFJ	-11.772	1
1DQJ	-0.909	4
1E6J	-6.281	2
1E96	-4.803	3
1EAW	-35.873	1
1EER	-9.400	1
1EWY	-9.480	1
1EZU	-47.098	1
1F34	-14.319	1
1F51	-20.290	1
1FAK	-13.375	1
1FC2	3.715	5
1FQ1	-22.194	1
1FQJ	-4.032	3
1FSK	-3.166	3
1GCQ	-17.096	1
1GHQ	3.574	5
1GP2	-15.658	1
1GRN	-37.985	1
1H1V	-6.732	2
1HE1	-14.631	1
1HE8	-7.116	2
1HIA	-22.160	1
1I4D	-9.660	1
1I9R	2.201	5
1IB1	-11.395	1
1IBR	-13.157	1
1IJK	-2.784	3
1IQD	4.438	5
1JPS	-2.501	3
1K4C	4.928	5
1K5D	-19.666	1

1KAC	-0.542	4
1KKL	-11.932	1
1KLU	4.555	5
1KTZ	-2.760	3
1KXQ	-15.266	1
1MAH	-0.213	4
1ML0	-6.801	2
1MLC	-0.867	4
1NCA	-3.634	3
1NSN	-0.525	4
1PPE	-34.648	1
1QA9	2.092	5
1QFW	-6.720	2
1RLB	2.108	5
1SBB	2.632	5
1UDI	-12.733	1
1VFB	-2.439	3
1WEJ	0.894	5
1WQ1	-14.811	1
2JEL	-4.656	3
2MTA	-3.463	3
2PCC	-3.600	3
2QFW	0.231	5
2SIC	-35.559	1
2SNI	-36.302	1
2VIS	-3.171	3
7CEI	-12.489	1
1AZS	2.298	5
1BKD	-22.274	1
1E4K	2.566	5
1EFN	-15.374	1
1GLA	-2.936	3
1GPW	-37.691	1
1IRA	-1.699	3
1J2J	-8.149	1
1JMO	-28.669	1
1N8O	-28.536	1
1NW9	-11.036	1
1OPH	-27.931	1
1PXV	-4.253	3
1R0R	-39.597	1
1S1Q	-10.807	1
1T6B	-2.305	3
1XD3	-19.724	1
1XQS	-22.027	1
1Y64	-16.096	1

1YVB	-20.774	1
1Z0K	-23.489	1
1Z5Y	-8.574	1
1ZHI	4.822	5
2AJF	3.424	5
2B42	-13.184	1
2C0L	-1.373	3
2CFH	-17.249	1
2FD6	-2.016	3
2H7V	-13.479	1
2HLE	-6.383	2
2HQS	-1.341	3
2HRK	-5.000	3
2NZ8	-25.642	1
2O8V	-26.730	1
2OOB	-14.595	1
2OT3	-30.039	1
2UUY	-25.015	1
design_1	-5.951	3
design_2	-2.747	3
design_3	2.804	5
design_4	-2.453	3
design_5	-1.898	3
design_6	-2.740	3
design_7	-0.840	4
design_8	-----	3
design_9	-0.289	4
design_10	-0.097	4
design_11	-7.228	2
design_12	-5.822	3
design_13	-3.284	3
design_14	-0.361	4
design_15	-4.008	3
design_16	0.977	5
design_17	-0.797	4
design_18	-2.915	3
design_19	-4.126	3
design_20	-----	3
design_21	-2.755	3
design_22	-6.543	2
design_23	2.045	5
design_24	-3.027	3
design_25	-0.494	4
design_26	-1.734	3
design_27	-0.596	4
design_28	-3.114	3

design_29	-----	3
design_30	-2.867	3
design_31	-2.742	3
design_32	1.620	5
design_33	-2.496	3
design_34	-10.118	1
design_35	-2.371	3
design_36	-0.820	4
design_37	-9.623	1
design_38	-----	3
design_39	-0.238	4
design_40	3.098	5
design_41	0.348	5
design_42	0.761	5
design_43	-7.267	2
design_44	-0.847	4
design_45	-3.267	3
design_46	1.378	5
design_47	-1.712	3
design_48	-1.785	3
design_49	-0.850	4
design_50	-1.417	3
design_51	-2.579	3
design_52	0.941	5
design_53	-4.495	3
design_54	3.175	5
design_55	-----	3
design_56	-2.146	3
design_57	2.247	5
design_58	-2.937	3
design_59	1.588	5
design_60	-2.037	3
design_61	-1.541	3
design_62	-----	3
design_63	-2.148	3
design_64	-1.893	3
design_65	-7.947	2
design_66	-2.607	3
design_67	1.125	5
design_68	-----	3
design_69	-0.890	4
design_70	-1.757	3
design_71	-2.584	3
design_72	-6.317	2
design_73	-4.915	3
design_74	0.623	5

```
design_75     -5.499 3
design_76     -1.998 3
design_77     -7.990 2
design_78     -0.173 4
design_79      0.779 5
design_80     -1.398 3
design_81     -2.353 3
design_82     -0.473 4
design_83      ----- 3
design_84     -2.562 3
design_85     -4.046 3
design_86      2.629 5
design_87     -1.741 3
*************************
Group 9s-
design_1        1328.472248    2
design_2        1699.993332    1
design_3        1053.0764395   5
design_4        1559.4020535   1
design_5        893.4992255    3
design_6        249.5758305    4
design_7        1216.90549     2
design_8        112.7288585    4
design_9        1430.0492485   1
design_10       1464.363524    1
design_11       1223.0122015   2
design_12       1493.826892    1
design_13       1259.1848265   2
design_14       280.3333175    4
design_15       -36.6327865    4
design_16       1620.8225525   1
design_17       963.168257     3
design_18       1768.8445685   1
design_19       1032.6960525   3
design_20       1080.209282    5
design_21       2018.5712855   1
design_22       1193.295454    2
design_23       -244.314628    4
design_24       579.629499     4
design_25       1340.718613    2
design_26       1725.329886    1
design_27       1340.742324    2
design_28       372.000453     4
design_29       1315.6461785   2
design_30       1223.930668    2
design_31       1619.4905515   1
```

design_32	1140.4131215	2
design_33	538.5939025	4
design_34	1416.1282385	1
design_35	1168.370939	2
design_36	2192.7292525	1
design_37	493.8319465	4
design_38	481.976658	4
design_39	1356.5584235	2
design_40	1686.3124085	1
design_41	1870.5353675	1
design_42	1623.995228	1
design_43	837.58206	3
design_44	1784.554693	1
design_45	1277.607559	2
design_46	1761.273977	1
design_47	1087.553829	5
design_48	1291.976514	2
design_49	676.582184	4
design_50	1790.314023	1
design_51	1277.819837	2
design_52	1488.459639	1
design_53	1751.588266	1
design_54	1045.3972085	3
design_55	874.91772	3
design_56	967.895314	3
design_57	1192.93213	2
design_58	1243.3860185	2
design_59	1027.834711	3
design_60	666.080163	4
design_61	701.789183	4
design_62	-453.710239	4
design_63	1061.2640785	5
design_64	1095.798401	5
design_65	1861.4412405	1
design_66	1046.177019	3
design_67	687.3474515	4
design_68	562.14345	4
design_69	1438.1867145	1
design_70	1991.779078	1
design_71	544.4980855	4
design_72	1200.5068885	2
design_73	1540.2511645	1
design_74	882.2291155	3
design_75	526.3083165	4
design_76	1737.931004	1
design_77	1261.7450775	2

design_78	324.6881045	4
design_79	1352.357525	2
design_80	1145.883502	2
design_81	1261.180428	2
design_82	424.3608515	4
design_83	616.1022775	4
design_84	936.61514	3
design_85	1714.6203865	1
design_86	1085.606216	5
design_87	1269.10754	2
1A2K	1335.437024	2
1ACB	604.647362	4
1AHW	1622.7856285	1
1AK4	695.493178	4
1AKJ	1062.0314255	5
1AVX	1222.9661515	2
1AY7	711.4922745	4
1B6C	1270.1634225	2
1BGX	1301.4810185	2
1BJ1	1310.6502635	2
1BUH	989.000633	3
1BVK	359.3838785	4
1BVN	1211.214479	2
1CGI	1051.46922	5
1D6R	1143.3531575	2
1DE4	1076.3951315	5
1DFJ	1430.2921935	1
1DQJ	35.50468	4
1E6J	351.2199145	4
1E96	840.3110935	3
1EAW	-58.5760055	4
1EER	1452.606524	1
1EWY	578.811475	4
1EZU	1775.4820425	1
1F34	1081.874449	5
1F51	1146.480521	2
1FAK	1374.7883325	2
1FC2	1820.2148725	1
1FQ1	1205.5096705	2
1FQJ	1506.4572585	1
1FSK	835.0396205	3
1GCQ	995.3567515	3
1GHQ	226.475282	4
1GP2	1659.612069	1
1GRN	1280.439304	2
1H1V	1459.651467	1

1HE1	1372.215343	2
1HE8	1503.1912055	1
1HIA	814.492202	3
1I2M	1471.383521	1
1I4D	1243.923859	2
1I9R	1434.146759	1
1IB1	1200.050316	2
1IBR	2182.189563	1
1IJK	1880.3918955	1
1IQD	1343.294609	2
1JPS	1634.441768	1
1K4C	625.090973	4
1K5D	1139.4431365	2
1KAC	295.3325785	4
1KKL	1666.900958	1
1KLU	1491.609623	1
1KTZ	404.674222	4
1KXP	1473.2530195	1
1KXQ	1093.750023	5
1M10	1599.9807525	1
1MAH	1043.569863	3
1ML0	1340.537023	2
1MLC	-191.178702	4
1N2C	2036.059859	1
1NCA	1137.4558835	2
1NSN	1433.5818825	1
1PPE	1140.3962415	2
1QA9	474.6158225	4
1QFW	1017.656891	3
1RLB	1517.3591	1
1SBB	696.839352	4
1UDI	791.5695545	4
1VFB	188.5126445	4
1WEJ	112.654061	4
1WQ1	741.2637235	4
2HMI	1118.004212	5
2JEL	256.0743985	4
2MTA	1497.6760665	1
2PCC	1018.1470635	3
2QFW	75.026882	4
2SIC	95.0830075	4
2SNI	384.5356275	4
2VIS	946.3250525	3
7CEI	1148.89921	2
1AZS	696.150993	4
1BKD	1388.759769	1

```
1E4K    534.4921685     4
1EFN    913.18677       3
1GLA    852.858011      3
1GPW    1576.253632     1
1IRA    1404.301882     1
1J2J    951.824363      3
1JMO    1387.9643415    1
1K74    1015.4459045    3
1N8O    1253.980597     2
1NW9    1266.5824785    2
1OPH    1285.4560355    2
1PXV    1206.5204185    2
1R0R    1065.608054     5
1R8S    762.5862205     4
1S1Q    1095.34908      5
1T6B    753.39242       4
1XD3    1125.987736     2
1XQS    1228.974929     2
1Y64    1165.3553045    2
1YVB    1432.0895365    1
1Z0K    985.529208      3
1Z5Y    1195.432284     2
1ZHI    1374.6161765    2
2AJF    1469.6154555    1
2B42    1047.832506     5
2C0L    1151.207707     2
2CFH    810.2423385     3
2FD6    936.4258805     3
2H7V    164.3794945     4
2HLE    949.8513385     3
2HQS    876.4077885     3
2HRK    1106.100849     5
2I25    765.8729325     4
2NZ8    1388.590404     1
2O8V    83.6445115      4
2OOB    1002.5640695    3
2OT3    1230.8058315    2
2UUY    921.4620505     3

*************************
Group 10s-
Raw Scores are given in units of : DiffColl
               diffColl normalized score
design_1   -0.2581 3
design_2   -0.5671 4
design_3   -0.4627 4
```

```
design_4   -0.2946 3
design_5   -0.3527 4
design_6   -0.3215 3
design_7   -0.3447 3
design_8    0.1557 1
design_9   -0.6527 4
design_10  -0.5841 4
design_11  -0.6399 4
design_12   0.2263 1
design_13  -0.2262 2
design_14  -0.2295 2
design_15   0.3292 1
design_16  -0.4214 4
design_17  -0.1543 2
design_18  -0.7460 4
design_19  -0.3719 4
design_20   0.3056 1
design_21  -0.6873 4
design_22   0.0409 1
design_23  -0.5125 4
design_24  -0.3215 3
design_25  -0.6884 4
design_26  -0.6986 4
design_27  -0.6514 4
design_28   0.3845 1
design_29  -0.4209 4
design_30  -0.2556 3
design_31  -0.7648 4
design_32   0.4645 1
design_33   0.1052 1
design_34  -0.5747 4
design_35  -0.7767 4
design_36  -0.6654 4
design_37  -0.1153 2
design_38  -0.3244 3
design_39  -0.2495 3
design_40  -0.7164 4
design_41  -0.2802 3
design_42   0.0344 1
design_43  -0.2816 3
design_44  -0.2960 3
design_45  -0.5713 4
design_46  -0.2371 2
design_47  -0.7723 4
design_48  -0.6787 4
design_49  -0.4731 4
```

design_50	-0.7051	4
design_51	-0.1828	2
design_52	-0.4572	4
design_53	-0.5726	4
design_54	-0.3768	4
design_55	0.3509	1
design_56	-0.3345	3
design_57	-0.7325	4
design_58	-0.2749	3
design_59	-0.6231	4
design_60	-0.6599	4
design_61	-0.7143	4
design_62	0.1569	1
design_63	-0.3797	4
design_64	-0.1134	2
design_65	-0.7274	4
design_66	-0.7278	4
design_67	-0.8605	4
design_68	-0.8605	4
design_69	-0.3513	4
design_70	-0.6295	4
design_71	0.4496	1
design_72	-0.7738	4
design_73	-0.7418	4
design_74	-0.4251	4
design_75	0.0083	1
design_76	0.0639	1
design_77	-0.7267	4
design_78	-0.7178	4
design_79	-0.3277	3
design_80	-0.6533	4
design_81	-0.6808	4
design_82	-0.0582	2
design_83	0.3695	1
design_84	0.1804	1
design_85	-0.4932	4
design_86	-0.3001	3
design_87	-0.0561	2
1A2K	-0.1070	2
1ACB	0.0476	1
1AHW	0.1762	1
1AK4	0.1611	1
1AKJ	0.1474	1
1AVX	0.0054	1
1AY7	0.1313	1
1AZS	-0.0705	2

```
1B6C       -0.3083 3
1BGX       -0.6450 4
1BJ1        0.1561 1
1BKD        0.6381 1
1BUH       -0.2183 2
1BVK       -0.0572 2
1BVN        0.3466 1
1CGI        0.2104 1
1D6R        0.3639 1
1DE4       -0.3896 4
1DFJ        0.5268 1
1DQJ       -0.5251 4
1E4K        0.2389 1
1E6J        0.0998 1
1E96        0.4086 1
1EAW        0.5646 1
1EER        0.9570 1
1EFN        0.1434 1
1EWY       -0.4846 4
1EZU        0.9044 1
1F34        0.0774 1
1F51       -0.9179 4
1FAK        0.4781 1
1FC2        0.4703 1
1FQ1        0.2499 1
1FQJ        0.2027 1
1FSK       -0.4218 4
1GCQ        0.3377 1
1GHQ        0.4767 1
1GLA        0.0429 1
1GP2        0.0848 1
1GPW        0.3260 1
1GRN       -0.0098 2
1H1V       -0.1782 2
1HE1        0.0360 1
1HE8        0.4661 1
1HIA        0.9399 1
1I2M       -0.2378 2
1I4D        0.9621 1
1I9R       -0.8740 4
1IB1       -0.5439 4
1IBR        0.9775 1
1IJK        0.6027 1
1IQD       -0.6046 4
1IRA       -0.7545 4
1J2J        0.9250 1
```

```
1JMO       -0.7572 4
1JPS        0.1550 1
1K4C        0.3124 1
1K5D       -0.2643 3
1K74        0.1774 1
1KAC        0.0020 1
1KKL       -0.7306 4
1KLU       -0.1641 2
1KTZ       -0.8458 4
1KXP        0.2787 1
1KXQ       -0.2590 3
1M10       -0.0412 2
1MAH       -0.1772 2
1ML0       -0.6593 4
1MLC       -0.2901 3
1N2C       -0.5412 4
1N8O       -0.0511 2
1NCA       -0.2901 3
1NSN       -0.7584 4
1NW9        0.1182 1
1OPH       -0.2333 2
1PPE        0.2557 1
1QA9       -0.1077 2
1QFW        0.2771 1
1R0R        0.4411 1
1R8S        0.7085 1
1RLB       -0.4888 4
1S1Q       -0.0182 2
1SBB       -0.1263 2
1T6B       -0.2251 2
1UDI       -0.7893 4
1VFB       -0.1141 2
1WEJ       -0.3876 4
1WQ1        0.5558 1
1XD3        0.5558 1
1XQS       -0.0023 2
1Y64        0.4917 1
1Z0K        0.8917 1
1Z5Y       -0.1241 2
1ZHI        0.0293 1
2AJF        0.1165 1
2B42       -0.1636 2
2C0L       -0.5353 4
2CFH       -0.4809 4
2FD6       -0.2532 3
2H7V        0.8083 1
```

2HLE -0.6566 4
2HMI -0.4904 4
2HQS 0.1366 1
2HRK -0.4207 4
2I25 0.1233 1
2JEL -0.6368 4
2MTA -0.7297 4
2NZ8 0.5242 1
2O8V 0.2178 1
2OOB -0.0836 2
2OT3 0.7544 1
2PCC -0.3792 4
2QFW -0.0103 2
2SIC 0.0941 1
2SNI 0.2394 1
2UUY 0.1264 1
2VIS 0.1285 1
7CEI 0.2995 1

****
Group 11s-
has pdf file with explanation in email from Thom.Vreven@umassmed.edu

short explanation -
We applied the ZRANK scoring function from our lab, which has been developed to re-rank docking results [1]. Hydrogens were added using the Rosetta package [2]. The area-under-curve (AUC) of the receiver-operator curve is 0.75, indicating that ZRANK is a reasonable predictor. Investigating the behavior further, we noticed that the attractive vdW term, which is a component of ZRANK, gives an AUC of 0.82. Since the vdW term depends primarily on the size on the interface, we speculate that the performance of ZRANK is related to the particular interface sizes of the set of designed complexes. This is supported when using the number of atom contacts (with 6√Ö cutoff) between the binding partners as predictor, which gives an AUC of 0.81 .

[1] Pierce B, Weng Z. ZRANK: Reranking protein docking predictions with an optimized energy function. Proteins-Structure Function and Bioinformatics 2007;67(4):1078-1086.

[2] Gray JJ, Moughon S, Wang C, Schueler-Furman O, Kuhlman B, Rohl CA, Baker D. Protein-protein docking with simultaneous optimization of rigid-body displacement and side-chain conformations. Journal of Molecular Biology 2003;331(1):281-299.

design_1	-54.2095	4
design_2	-43.5998	4
design_3	-88.834	2
design_4	-59.3188	3
design_5	-54.1076	4
design_6	-84.3031	2
design_7	-97.9103	2
design_8	-77.8305	5
design_9	-65.2979	3
design_10	-64.7104	3
design_11	-51.5924	4
design_12	-70.6903	5
design_13	-53.8173	4
design_14	-57.3189	4
design_15	-68.9639	5
design_16	-82.0901	2
design_17	-67.8039	5
design_18	-68.3127	5
design_19	-93.6504	2
design_20	-104.292	1
design_21	-83.4195	2
design_22	-80.1347	2
design_23	-65.7007	3
design_24	-78.682	2
design_25	-52.7295	4
design_26	-62.6116	3
design_27	-69.7417	5
design_28	-62.6114	3
design_29	-103.997	1
design_30	-96.5717	2
design_31	-48.9536	4
design_32	-60.2272	3
design_33	-85.8795	2
design_34	-89.8833	2
design_35	-94.8501	2
design_36	-67.3013	3
design_37	-94.6139	2
design_38	-102.694	2
design_39	-60.1389	3
design_40	-61.3133	3
design_41	-66.332	3
design_42	-82.2422	2
design_43	-88.5778	2
design_44	-74.6762	5

design_45	-75.2205	5
design_46	-50.1028	4
design_47	-71.0536	5
design_48	-68.5784	5
design_49	-63.7671	3
design_50	-66.5286	3
design_51	-86.1967	2
design_52	-75.6866	5
design_53	-81.5766	2
design_54	-54.7056	4
design_55	-72.1243	5
design_56	-42.732	4
design_57	-83.5235	2
design_58	-80.5635	2
design_59	-67.7435	3
design_60	-58.0489	4
design_61	-92.1201	2
design_62	-92.1178	2
design_63	-72.8509	5
design_64	-50.4813	4
design_65	-74.1867	5
design_66	-88.358	2
design_67	-40.9544	4
design_68	-78.1151	2
design_69	-89.1319	2
design_70	-59.188	3
design_71	-91.2671	2
design_72	-85.654	2
design_73	-51.757	4
design_74	-53.5563	4
design_75	-67.2955	3
design_76	-88.07	2
design_77	-80.415	2
design_78	-48.702	4
design_79	-37.237	4
design_80	-54.1086	4
design_81	-74.3524	5
design_82	-79.0958	2
design_83	-113.253	1
design_84	-80.0213	2
design_85	-97.0714	2
design_86	-53.7501	4
design_87	-83.4547	2
1A2K	-98.1066	2
1ACB	-116.525	1
1AHW	-91.7122	2

1AK4	-50.3709	4
1AKJ	-93.5625	2
1AVX	-121.666	1
1AY7	-80.4904	2
1AZS	-99.4465	2
1B6C	-105.795	1
1BGX	-223.762	1
1BJ1	-109.787	1
1BKD	-157.818	1
1BUH	-66.3244	3
1BVK	-56.6103	4
1BVN	-134.322	1
1CGI	-155.963	1
1D6R	-83.2146	2
1DE4	-102.732	1
1DFJ	-129.096	1
1DQJ	-77.6184	5
1E4K	-85.5908	2
1E6J	-77.094 5	
1E96	-76.3037	5
1EAW	-114.713	1
1EER	-234.116	1
1EFN	-80.2186	2
1EWY	-80.9605	2
1EZU	-142.524	1
1F34	-127.597	1
1F51	-114.449	1
1FAK	-131.15 1	
1FC2	-66.1225	3
1FQ1	-105.098	1
1FQJ	-71.0644	5
1FSK	-104.887	1
1GCQ	-68.8924	5
1GHQ	-14.5526	4
1GLA	-87.0095	2
1GP2	-137.092	1
1GPW	-135.199	1
1GRN	-101.28 2	
1H1V	-46.9424	4
1HE1	-114.324	1
1HE8	-76.7497	5
1HIA	-113.557	1
1I2M	-161.798	1
1I4D	-68.1423	5
1I9R	-77.6153	5
1IB1	-123.498	1

```
1IBR    -200.365        1
1IJK    -129.2  1
1IQD    -151.759        1
1IRA    -155.789        1
1J2J    -59.723 3
1JMO    -233.246        1
1JPS    -100.755        2
1K4C    -111.516        1
1K5D    -184.779        1
1K74    -121.555        1
1KAC    -70.446 5
1KKL    -76.0651        5
1KLU    -60.1236        3
1KTZ    -62.3266        3
1KXP    -180.994        1
1KXQ    -97.396 2
1M10    -135.17 1
1MAH    -121.641        1
1ML0    -170.592        1
1MLC    -86.2662        2
1N2C    -229.189        1
1N8O    -120.44 1
1NCA    -102.858        1
1NSN    -59.9277        3
1NW9    -122.698        1
1OPH    -86.2429        2
1PPE    -121.923        1
1PXV    -147.675        1
1QA9    -65.4071        3
1QFW    -80.5551        2
1R0R    -82.7869        2
1R8S    -172.229        1
1RLB    -62.3366        3
1S1Q    -40.3317        4
1SBB    -41.4878        4
1T6B    -80.7864        2
1UDI    -119.633        1
1VFB    -58.4516        4
1WEJ    -68.1119        5
1WQ1    -146.643        1
1XD3    -141.185        1
1XQS    -187.368        1
1Y64    -96.9998        2
1YVB    -96.111 2
1Z0K    -104.395        1
1Z5Y    -84.4071        2
```

1ZHI	-74.1985	5
2AJF	-52.0478	4
2B42	-108.103	1
2C0L	-104.234	1
2CFH	-145.227	1
2FD6	-61.7296	3
2H7V	-85.2176	2
2HLE	-143.859	1
2HMI	-60.814	3
2HQS	-103.003	1
2HRK	-68.171	5
2I25	-84.3263	2
2JEL	-67.543	3
2MTA	-60.6691	3
2NZ8	-109.871	1
2O8V	-102.027	2
2OOB	-41.3815	4
2OT3	-157.188	1
2PCC	-71.4377	5
2QFW	-86.6897	2
2SIC	-98.1362	2
2SNI	-105.602	1
2UUY	-91.7453	2
2VIS	-64.0717	3
7CEI	-120.386	1

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Group 12s -

The "Raw score" values are based on our pyDock energy-based function, with a new weight for desolvation as derived from fitting to the Bonvin experimental data set. The units are technically in kcal/mol but in practice they can be considered as arbitrary units. Based solely on the correlation with the experimental data, we decided to make the following "normalized score" categories:

1 - binds E < -15.0
2 - likely to bind -15.0 < E < -5.0
3 - likely not to bind +5.0 < E < +15.0
4 - does not bind E > +15.0
5 - uncertain -5.0 < E < +5.0

	Raw score	normalized score
design_1	11.047	3
design_2	4.225	5
design_3	3.437	5

design_4	-3.713	5
design_5	0.699	5
design_6	3.582	5
design_7	-14.170	2
design_8	24.219	4
design_9	-1.500	5
design_10	32.957	4
design_11	1.207	5
design_12	24.288	4
design_13	4.568	5
design_14	26.951	4
design_15	16.783	4
design_16	12.015	3
design_17	18.035	4
design_18	11.938	3
design_19	14.356	3
design_20	25.292	4
design_21	16.421	4
design_22	13.682	3
design_23	15.113	4
design_24	-0.641	5
design_25	-2.845	5
design_26	-6.937	2
design_27	3.316	5
design_28	18.686	4
design_29	-1.470	5
design_30	8.509	3
design_31	11.975	3
design_32	10.868	3
design_33	12.887	3
design_34	25.664	4
design_35	38.980	4
design_36	2.343	5
design_37	9.054	3
design_38	14.981	3
design_39	14.426	3
design_40	8.342	3
design_41	13.410	3
design_42	1.532	5
design_43	-2.976	5
design_44	17.499	4
design_45	23.829	4
design_46	11.558	3
design_47	13.307	3
design_48	49.070	4
design_49	54.258	4

design_50	3.208	5
design_51	20.453	4
design_52	-20.885	1
design_53	-2.585	5
design_54	7.930	3
design_55	25.470	4
design_56	12.656	3
design_57	-7.382	2
design_58	6.464	3
design_59	-4.003	5
design_60	4.070	5
design_61	-4.092	5
design_62	22.112	4
design_63	-1.503	5
design_64	7.957	3
design_65	-14.033	2
design_66	22.479	4
design_67	-6.901	2
design_68	-1.015	5
design_69	6.419	3
design_70	9.082	3
design_71	20.235	4
design_72	-14.626	2
design_73	-14.580	2
design_74	21.350	4
design_75	16.779	4
design_76	-7.390	2
design_77	-0.183	5
design_78	4.386	5
design_79	-10.709	2
design_80	8.564	3
design_81	-3.531	5
design_82	14.806	3
design_83	37.252	4
design_84	16.634	4
design_85	29.577	4
design_86	15.579	4
design_87	15.024	4
1A2K	-9.066	2
1ACB	20.070	4
1AHW	-50.795	1
1AK4	3.901	5
1AKJ	-85.876	1
1AVX	-6.888	2
1AY7	-16.907	1
1AZS	20.233	4

1B6C	0.111	5
1BGX	-35.679	1
1BJ1	9.708	3
1BKD	-43.236	1
1BUH	-3.138	5
1BVK	-5.512	2
1BVN	7.710	3
1CGI	16.991	4
1D6R	-16.923	1
1DE4	-26.011	1
1DFJ	-69.825	1
1DQJ	-6.238	2
1E4K	-2.311	5
1E6J	3.103	5
1E96	-8.643	2
1EAW	-12.842	2
1EER	-92.275	1
1EFN	-9.494	2
1EWY	-47.833	1
1EZU	13.981	3
1F34	-4.804	5
1F51	-8.883	2
1FAK	-27.105	1
1FC2	19.583	4
1FQ1	-21.172	1
1FQJ	-49.094	1
1FSK	-8.490	2
1GCQ	3.761	5
1GHQ	-1.233	5
1GLA	-20.311	1
1GP2	-27.219	1
1GPW	-46.550	1
1GRN	-35.551	1
1H1V	-9.622	2
1HE1	-3.027	5
1HE8	-28.506	1
1HIA	-20.386	1
1I2M	-89.927	1
1I4D	12.958	3
1I9R	-39.700	1
1IB1	-45.044	1
1IBR	-120.679	1
1IJK	-50.571	1
1IQD	-18.517	1
1IRA	-30.730	1
1J2J	9.828	3

1JMO	-47.796	1
1JPS	-56.304	1
1K4C	-7.187	2
1K5D	-86.871	1
1K74	-56.574	1
1KAC	-15.765	1
1KKL	-8.540	2
1KLU	5.009	3
1KTZ	-7.361	2
1KXP	-30.281	1
1KXQ	1.795	5
1M10	-71.704	1
1MAH	-8.537	2
1ML0	-60.229	1
1MLC	-4.904	5
1N2C	-80.532	1
1N8O	12.546	3
1NCA	-26.102	1
1NSN	-1.914	5
1NW9	22.954	4
1OPH	-10.547	2
1PPE	0.608	5
1PXV	-6.611	2
1QA9	-54.607	1
1QFW	-12.085	2
1R0R	0.636	5
1R8S	0.225	5
1RLB	-10.353	2
1S1Q	-8.035	2
1SBB	5.952	3
1T6B	-26.688	1
1UDI	-42.577	1
1VFB	-10.293	2
1WEJ	-34.047	1
1WQ1	-51.092	1
1XD3	-26.823	1
1XQS	-90.208	1
1Y64	-45.176	1
1YVB	11.304	3
1Z0K	-13.341	2
1Z5Y	18.405	4
1ZHI	-20.348	1
2AJF	-8.159	2
2B42	-17.856	1
2C0L	-26.957	1
2CFH	-1.216	5

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2FD6             7.039           3
2H7V            -7.695           2
2HLE           -27.350           1
2HMI            13.747           3
2HQS           -26.093           1
2HRK             2.974           5
2I25           -22.604           1
2JEL           -11.133           2
2MTA             9.901           3
2NZ8            -7.852           2
2O8V             8.464           3
2OOB             9.610           3
2OT3            12.643           3
2PCC           -55.606           1
2QFW            15.627           4
2SIC             4.840           5
2SNI            -0.966           5
2UUY             3.727           5
2VIS             0.984           5
7CEI           -80.907           1

*************************
Group 14s -

REMARK Please use this file to submit your results for both designs and
REMARK the docking benchmark.
REMARK Change the file name from GroupXXX.txt to represent your group's
name (Group14s.txt, Fan Jiang).
REMARK Add raw and normalized scores in the table below.
REMARK Fill in the units in which the raw scores were computed below.

Raw scores are given in units of sigma for z-score
                    Raw score        normalized score

design_1 -1.08693 5
design_2 -1.35818 5
design_3 -3.06294 1
design_4 -1.23158 5
design_5 -0.842242 3
design_6 -1.07451 5
design_7 -1.56007 5
design_8 -1.97668 5
design_9 -1.13102 5
design_10 -1.7418 5
design_11 -1.24259 5
design_12 -1.92746 5
```

design_13 -1.76039 5
design_14 -1.46755 5
design_15 -2.37907 2
design_16 -2.01954 2
design_17 -1.06874 5
design_18 -1.77489 5
design_19 -2.74962 2
design_20 -3.78682 1
design_21 -1.5616 5
design_22 -2.15015 2
design_23 -2.25417 2
design_24 -1.60173 5
design_25 -1.5688 5
design_26 -1.4783 5
design_27 -1.72965 5
design_28 -1.57068 5
design_29 -1.69227 5
design_30 -2.67521 2
design_31 -1.22768 5
design_32 -1.15291 5
design_33 -2.91998 2
design_34 -2.42303 2
design_35 -2.6151 2
design_36 -1.53769 5
design_37 -2.12691 2
design_38 -2.13424 2
design_39 -1.43388 5
design_40 -1.39641 5
design_41 -1.60583 5
design_42 -2.39886 2
design_43 -1.52213 5
design_44 -2.39127 2
design_45 -1.92207 5
design_46 -1.33028 5
design_47 -1.80545 5
design_48 -2.40938 2
design_49 -2.19936 2
design_50 -1.42003 5
design_51 -2.03172 2
design_52 -2.11574 2
design_53 -2.10822 2
design_54 -1.96452 5
design_55 -1.65291 5
design_56 -1.82464 5
design_57 -2.04356 2
design_58 -1.65652 5

design_59 -1.91108 5
design_60 -1.83141 5
design_61 -1.93248 5
design_62 -2.70277 2
design_63 -1.92635 5
design_64 -1.1933 5
design_65 -1.49893 5
design_66 -1.4743 5
design_67 -1.0701 5
design_68 -1.62964 5
design_69 -2.15877 2
design_70 -1.807 5
design_71 -1.73998 5
design_72 -2.44903 2
design_73 -1.30951 5
design_74 -2.08992 2
design_75 -1.77386 5
design_76 -1.49479 5
design_77 -1.83341 5
design_78 -1.25023 5
design_79 -0.850169 3
design_80 -1.60543 5
design_81 -2.11844 2
design_82 -2.18513 2
design_83 -3.55153 1
design_84 -1.8779 5
design_85 -1.943 5
design_86 -1.49382 5
design_87 -2.15792 2
1A2K -2.78674 2
1ACB -2.86472 2
1AHW -1.35257 5
1AK4 -2.36668 2
1AKJ -1.98801 5
1AVX -3.19702 1
1AY7 -2.84233 2
1AZS -3.34508 1
1B6C -1.98758 5
1BGX -8.45875 1
1BJ1 -4.00269 1
1BKD -4.14363 1
1BUH -1.61304 5
1BVK -1.72327 5
1BVN -3.27283 1
1CGI -4.60108 1
1D6R -2.57204 2

1DE4 -2.80802 2
1DFJ -3.23371 1
1DQJ -1.65302 5
1E4K -1.09153 5
1E6J -1.99995 5
1E96 -1.61624 5
1EAW -3.78369 1
1EER -5.16181 1
1EFN -2.17831 2
1EWY -1.3379 5
1EZU -5.6465 1
1F34 -5.27284 1
1F51 -2.1125 2
1FAK -3.00209 1
1FC2 -1.70571 5
1FQ1 -1.68519 5
1FQJ -2.60303 2
1FSK -4.23723 1
1GCQ -1.92281 5
1GHQ -1.04601 5
1GLA -2.014 2
1GP2 -2.6143 2
1GPW -3.07566 1
1GRN -2.30799 2
1H1V -2.46166 2
1HE1 -3.48787 1
1HE8 -1.06702 5
1HIA -3.21836 1
1I2M -4.48648 1
1I4D -1.71891 5
1I9R -2.26922 2
1IB1 -3.85149 1
1IBR -4.55961 1
1IJK -1.89163 5
1IQD -3.37454 1
1IRA -3.53553 1
1J2J -1.38083 5
1JMO -6.95177 1
1JPS -2.37978 2
1K4C -3.92671 1
1K5D -5.1897 1
1K74 -2.49634 2
1KAC -1.56719 5
1KKL -1.63771 5
1KLU -2.00472 2
1KTZ -1.63229 5

1KXP -3.0578 1
1KXQ -4.22967 1
1M10 -2.91073 2
1MAH -3.42041 1
1ML0 -4.22161 1
1MLC -2.66435 2
1N2C -8.3291 1
1N8O -3.5563 1
1NCA -2.3463 2
1NSN -1.01797 5
1NW9 -4.64067 1
1OPH -2.68631 2
1PPE -3.58191 1
1PXV -4.42404 1
1QA9 -2.71108 2
1QFW -1.49758 5
1R0R -3.53876 1
1R8S -3.9972 1
1RLB -1.25755 5
1S1Q -1.74319 5
1SBB -1.59586 5
1T6B -1.39347 5
1UDI -1.25385 5
1VFB -2.56165 2
1WEJ -2.13313 2
1WQ1 -3.99341 1
1XD3 -3.82592 1
1XQS -3.0143 1
1Y64 -1.21679 5
1YVB -2.31595 2
1Z0K -1.66084 5
1Z5Y -2.55802 2
1ZHI -2.20038 2
2AJF -2.05521 2
2B42 -4.68982 1
2C0L -2.4401 2
2CFH -3.40305 1
2FD6 -2.57422 2
2H7V -1.55653 5
2HLE -3.3068 1
2HMI -1.55506 5
2HQS -3.2061 1
2HRK -1.21433 5
2I25 -2.69766 2
2JEL -1.91034 5
2MTA -1.9606 5

2NZ8 -3.06954 1
2O8V -3.70833 1
2OOB -0.919975 3
2OT3 -4.67878 1
2PCC -0.279167 4
2QFW -2.07956 2
2SIC -4.53697 1
2SNI -3.38707 1
2UUY -2.46463 2
2VIS -2.34114 2
7CEI -1.63299 5

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Group 16s-

	Raw score	normalized score
design_1	-15.76	3
design_2	-15.08	3
design_3	-18.6	5
design_4	-11.44	4
design_5	-11.72	4
design_6	-12.12	4
design_7	-14.88	3
design_8	-10.48	4
design_9	-10.56	4
design_10	-13.92	3
design_11	-10.48	4
design_12	-13.08	4
design_13	-14.6	3
design_14	-12.68	4
design_15	-13.36	4
design_16	-15	3
design_17	-14.04	3
design_18	-12.8	4
design_19	-14.92	3
design_20	-21.88	1
design_21	-11.96	4
design_22	-12.4	4
design_23	-12.88	4
design_24	-14.64	3
design_25	-10.28	4
design_26	-12.48	4
design_27	-14.32	3
design_28	-10.68	4
design_29	-13.08	4
design_30	-20.48	1

design_31	-12.12	4
design_32	-9.12	4
design_33	-15.4	3
design_34	-18.24	5
design_35	-18.64	5
design_36	-13.56	4
design_37	-12.92	4
design_38	-17.4	5
design_39	-11.52	4
design_40	-12.2	4
design_41	-12.4	4
design_42	-16.24	3
design_43	-14.12	3
design_44	-21.12	1
design_45	-16.44	3
design_46	-13.28	4
design_47	-14.88	3
design_48	-14.04	3
design_49	-10.68	4
design_50	-12.48	4
design_51	-12.2	4
design_52	-20.08	2
design_53	-15.76	3
design_54	-13.28	4
design_55	-10.68	4
design_56	-13.28	4
design_57	-17.4	5
design_58	-18.64	5
design_59	-17	5
design_60	-12.48	4
design_61	-15.56	3
design_62	-13.48	4
design_63	-14.6	3
design_64	-8.96	4
design_65	-14.04	3
design_66	-16.04	3
design_67	-14.92	3
design_68	-9.92	4
design_69	-13.92	3
design_70	-12.2	4
design_71	-13.84	3
design_72	-19.12	5
design_73	-9.04	4
design_74	-10.68	4
design_75	-8.76	4
design_76	-19.6	5

design_77	-17.76	5
design_78	-11.52	4
design_79	-13.64	4
design_80	-12.96	4
design_81	-15.48	3
design_82	-13.2	4
design_83	-16.36	3
design_84	-13.68	4
design_85	-15.28	3
design_86	-12.68	4
design_87	-14.32	3
1A2K	-20.4	2
1ACB	-24.48	1
1AHW	-24.88	1
1AK4	-12.66	4
1AKJ	-21.6	1
1AVX	-24.48	1
1AY7	-14.24	3
1B6C	-22	1
1BGX	-75.64	1
1BJ1	-27.84	1
1BUH	-17.76	5
1BVK	-15.84	3
1BVN	-27.76	1
1CGI	-33.52	1
1D6R	-19.32	5
1DE4	-22.08	1
1DFJ	-23.72	1
1DQJ	-24.48	1
1E6J	-15.28	3
1E96	-14.24	3
1EAW	-26.36	1
1EER	-41.52	1
1EWY	-11.84	4
1EZU	-36.52	1
1F34	-42.28	1
1F51	-22.68	1
1FAK	-27.84	1
1FC2	-13.92	3
1FQ1	-16.8	5
1FQJ	-20.08	2
1FSK	-22.68	1
1GCQ	-17.15	5
1GHQ	-7.68	4
1GP2	-26.24	1
1GRN	-24.92	1

1H1V	-19.23	5
1HE1	-23.79	1
1HE8	-13.92	3
1HIA	-24.96	1
1I2M	-33.52	1
1I4D	-18.6	5
1I9R	-19.52	5
1IB1	-30.08	1
1IBR	-41.28	1
1IJK	-15.84	3
1IQD	-30.44	1
1JPS	-25.2	1
1K4C	-20.68	2
1K5D	-36.07	1
1KAC	-18.84	5
1KKL	-21.16	1
1KLU	-13.12	4
1KTZ	-11.04	4
1KXP	-40.24	1
1KXQ	-24.12	1
1M10	-23.96	1
1MAH	-23.24	1
1ML0	-30.28	1
1MLC	-22.56	1
1N2C	-20.36	2
1NCA	-24.32	1
1NSN	-15.68	3
1PPE	-24.68	1
1QA9	-12.96	4
1QFW	-20.76	2
1RLB	-12.96	4
1SBB	-10.88	4
1UDI	-21.3	1
1VFB	-18.72	5
1WEJ	-16.04	3
1WQ1	-29.32	1
2HNI	-14.4	3
2JEL	-19.4	5
2MTA	-13.48	4
2PCC	-9.35	4
2QFW	-19.68	5
2SIC	-25.64	1
2SNI	-22.76	1
2VIS	-17.4	5
7CEI	-21.04	2
1AZS	-21.6	1

1BKD	-36.24	1
1E4K	-14.04	3
1EFN	-13.16	4
1GLA	-14.4	3
1GPW	-24.6	1
1IRA	-34	1
1J2J	-11.92	4
1JMO	0	
1K74	-21.96	1
1N8O	-30.11	1
1NW9	-30.12	1
1OPH	-21.08	1
1PXV	-32.12	1
1R0R	-21.08	1
1R8S	-36.52	1
1S1Q	-11.76	4
1T6B	-22.32	1
1XD3	-31.92	1
1XQS	-27.88	1
1Y64	-16.92	5
1YVB	-19.52	5
1Z0K	-24.96	1
1Z5Y	-17.8	5
1ZHI	-13.6	4
2AJF	-16.32	3
2B42	-35.72	1
2C0L	-21.58	1
2CFH	-27.92	1
2FD6	-18.24	5
2H7V	-17.4	5
2HLE	-31.52	1
2HQS	-30.92	1
2HRK	-15.36	3
2I25	-23.08	1
2NZ8	-27.4	1
2O8V	-22.48	1
2OOB	-8.68	4
2OT3	-30.18	1
2UUY	-22.8	1

We found that using rpscore alone can achieve better results than our combinatorial scoring function for this issue.
The raw scores above are rpscores, the normalized scores are determined by raw scores.
****

Group 17s-
% result files with explanations in email from Charles Rober

(robert@ibpc.fr)
****
Group 20s-
design_1.pdb -152.033 5
design_2.pdb -273.597 3
design_3.pdb -157.047 5
design_4.pdb -237.936 3
design_5.pdb -156.308 5
design_6.pdb -122.828 5
design_7.pdb -234.427 3
design_8.pdb -287.733 3
design_9.pdb -258.069 3
design_10.pdb -345.66 2
design_11.pdb -158.197 5
design_12.pdb -361.55 2
design_13.pdb -242.971 3
design_14.pdb -143.996 5
design_15.pdb -164.076 5
design_16.pdb -257.84 3
design_17.pdb -250.72 3
design_18.pdb -254.208 3
design_19.pdb -109.389 5
design_20.pdb -320.652 2
design_21.pdb -294.817 3
design_22.pdb -126.708 5
design_23.pdb -114.739 5
design_24.pdb -95.7908 4
design_25.pdb -204.503 3
design_26.pdb -185.622 5
design_27.pdb -189.851 5
design_28.pdb -84.5884 4
design_29.pdb -89.284 4
design_30.pdb -164.311 5
design_31.pdb -147.865 5
design_32.pdb -231.319 3
design_33.pdb -256.135 3
design_34.pdb -232.38 3
design_35.pdb -293.433 3
design_36.pdb -320.842 2
design_37.pdb -248.711 3
design_38.pdb -130.828 5
design_39.pdb -185.137 5
design_40.pdb -225.944 3
design_41.pdb -204.625 3
design_42.pdb -206.632 3
design_43.pdb -256.143 3

design_44.pdb -288.19 3
design_45.pdb -348.732 2
design_46.pdb -175.431 5
design_47.pdb -134.367 5
design_48.pdb -260.064 3
design_49.pdb -101.043 5
design_50.pdb -185.067 5
design_51.pdb -126.811 5
design_52.pdb -308.295 2
design_53.pdb -252.179 3
design_54.pdb -127.3 5
design_55.pdb -328.584 2
design_56.pdb -173.654 5
design_57.pdb -96.0207 4
design_58.pdb -126.128 5
design_59.pdb -146.607 5
design_60.pdb -206.318 3
design_61.pdb -329.308 2
design_62.pdb -162.817 5
design_63.pdb -133.447 5
design_64.pdb -265.829 3
design_65.pdb -171.924 5
design_66.pdb -288.694 3
design_67.pdb -145.077 5
design_68.pdb -152.497 5
design_69.pdb -249.792 3
design_70.pdb -158.451 5
design_71.pdb -102.163 5
design_72.pdb -285.102 3
design_73.pdb -179.176 5
design_74.pdb -189.111 5
design_75.pdb -211.597 3
design_76.pdb -286.164 3
design_77.pdb -236.676 3
design_78.pdb -182.811 5
design_79.pdb -79.9939 4
design_80.pdb -209.237 3
design_81.pdb -127.469 5
design_82.pdb -316.599 2
design_83.pdb -360.262 2
design_84.pdb -225.875 3
design_85.pdb -272.298 3
design_86.pdb -159.549 5
design_87.pdb -169.339 5
1A2K.pdb -212.858 3
1ACB.pdb -295.49 3

1AHW.pdb -316.106 2
1AK4.pdb -143.433 5
1AKJ.pdb -27.0674 4
1AVX.pdb -353.548 2
1AY7.pdb -192.135 5
1AZS.pdb -203.629 3
1B6C.pdb -368.857 2
1BGX.pdb -680.46 1
1BJ1.pdb -291.849 3
1BKD.pdb -410.239 1
1BUH.pdb -136.266 5
1BVK.pdb -213.917 3
1BVN.pdb -443.535 1
1CGI.pdb -433.596 1
1D6R.pdb -181.635 5
1DE4.pdb -344.569 2
1DFJ.pdb -188.285 5
1DQJ.pdb -262.143 3
1E4K.pdb -97.2931 4
1E6J.pdb -190.087 5
1E96.pdb -173.945 5
1EAW.pdb -526.362 1
1EER.pdb -99.7758 4
1EFN.pdb -98.4382 4
1EWY.pdb -84.8175 4
1EZU.pdb -381.278 2
1F34.pdb -346.43 2
1F51.pdb -246.524 3
1FAK.pdb -221.007 3
1FC2.pdb -152.516 5
1FQ1.pdb -170.358 5
1FQJ.pdb -106.434 5
1FSK.pdb -356.89 2
1GCQ.pdb -137.863 5
1GHQ.pdb -22.4147 4
1GLA.pdb -120.582 5
1GP2.pdb -178.874 5
1GPW.pdb -234.614 3
1GRN.pdb -270.135 3
1H1V.pdb -343.143 2
1HE1.pdb -344.653 2
1HE8.pdb -100.669 5
1HIA.pdb -272.141 3
1I2M.pdb -160.036 5
1I4D.pdb -188.885 5
1I9R.pdb -183.982 5

1IB1.pdb -206.912 3
1IBR.pdb -273.309 3
1IJK.pdb -232.686 3
1IQD.pdb -234.026 3
1IRA.pdb -202.86 3
1J2J.pdb -214.06 3
1JMO.pdb -343.453 2
1JPS.pdb -253.278 3
1K4C.pdb -207.609 3
1K5D.pdb -211.76 3
1K74.pdb -452.897 1
1KAC.pdb -100.437 5
1KKL.pdb -325.869 2
1KLU.pdb -124.391 5
1KTZ.pdb -48.7399 4
1KXP.pdb -516.192 1
1KXQ.pdb -309.133 2
1M10.pdb -109.776 5
1MAH.pdb -202.605 3
1ML0.pdb -149.925 5
1MLC.pdb -249.877 3
1N2C.pdb -755.82 1
1N8O.pdb -384.953 2
1NCA.pdb -228.226 3
1NSN.pdb -171.256 5
1NW9.pdb -263.128 3
1OPH.pdb -125.578 5
1PPE.pdb -352.1 2
1PXV.pdb -339.407 2
1QA9.pdb -47.721 4
1QFW.pdb -183.678 5
1R0R.pdb -374.238 2
1R8S.pdb -494.181 1
1RLB.pdb -110.069 5
1S1Q.pdb -114.674 5
1SBB.pdb -135.491 5
1T6B.pdb -156.518 5
1UDI.pdb -311.854 2
1VFB.pdb -227.228 3
1WEJ.pdb -175.364 5
1WQ1.pdb -237.277 3
1XD3.pdb -275.048 3
1XQS.pdb -167.711 5
1Y64.pdb -98.4158 4
1YVB.pdb -277.378 3
1Z0K.pdb -330.2 2

1Z5Y.pdb -194.627 5
1ZHI.pdb -137.667 5
2AJF.pdb -211.92 3
2B42.pdb -401.066 1
2C0L.pdb -246.865 3
2CFH.pdb -784.149 1
2FD6.pdb -195.907 5
2H7V.pdb -222.925 3
2HLE.pdb -231.588 3
2HMI.pdb -87.5356 4
2HQS.pdb -186.229 5
2HRK.pdb -196.893 5
2I25.pdb -180.515 5
2JEL.pdb -281.384 3
2MTA.pdb -147.316 5
2NZ8.pdb -275.324 3
2O8V.pdb -197.512 5
2OOB.pdb -41.5053 4
2OT3.pdb -385.037 2
2PCC.pdb -81.9344 4
2QFW.pdb -208.647 3
2SIC.pdb -352.935 2
2SNI.pdb -320.712 2
2UUY.pdb -370.853 2
2VIS.pdb -244.655 3
7CEI.pdb -99.2515 4
****
Group 21s-
CAPRI T45 predictions - Furman Group, The Hebrew University, Jerusalem, Israel.
Raw scores are the delta in polar solvent accessible surface area between the monomers apart and the complex
and are given in units of Angstrem^2.
#
#Complex	Raw score	normalized score
design_1	-402.2	4
design_2	-425.2	3
design_3	-471.6	3
design_4	-378.6	4
design_5	-321.3	5
design_6	-293.6	5
design_7	-495.6	2
design_8	-268.1	5
design_9	-281.4	5
design_10	-303.9	5
design_11	-405.8	4

design_12	-430.3	3
design_13	-465.3	3
design_14	-263	5
design_15	-289.8	5
design_16	-388.1	4
design_17	-328.5	5
design_18	-398.5	4
design_19	-333.1	5
design_20	-466.1	3
design_21	-272.2	5
design_22	-259.7	5
design_23	-342.6	4
design_24	-378.4	4
design_25	-336.2	4
design_26	-446.8	3
design_27	-332.5	5
design_28	-278.6	5
design_29	-353	4
design_30	-498.6	2
design_31	-363.9	4
design_32	-185	5
design_33	-351.9	4
design_34	-468.2	3
design_35	-461.6	3
design_36	-406.2	4
design_37	-334.4	5
design_38	-332.5	5
design_39	-405.5	4
design_40	-380.1	4
design_41	-349	4
design_42	-417.9	3
design_43	-355.2	4
design_44	-461.6	3
design_45	-408	4
design_46	-340.9	4
design_47	-400.5	4
design_48	-294.9	5
design_49	-247.6	5
design_50	-325.5	5
design_51	-352.7	4
design_52	-610.3	2
design_53	-481.5	3
design_54	-361.9	4
design_55	-259.8	5
design_56	-321.7	5
design_57	-390.8	4

design_58	-417.5	3
design_59	-373.5	4
design_60	-399.4	4
design_61	-478.9	3
design_62	-354.3	4
design_63	-422.3	3
design_64	-283.4	5
design_65	-498	2
design_66	-291.5	5
design_67	-446.3	3
design_68	-312.9	5
design_69	-321.7	5
design_70	-308.7	5
design_71	-298.7	5
design_72	-528	2
design_73	-358.2	4
design_74	-260.3	5
design_75	-314.5	5
design_76	-530.8	2
design_77	-449	3
design_78	-330.3	5
design_79	-434.9	3
design_80	-306.1	5
design_81	-474.8	3
design_82	-267.9	5
design_83	-321.7	5
design_84	-352.7	4
design_85	-324.6	5
design_86	-292.5	5
design_87	-344.2	4
1A2K	-433.3	3
1ACB	-347.2	4
1AHW	-904.4	1
1AK4	-216.7	5
1AKJ	-961.8	1
1AVX	-623.4	2
1AY7	-478.8	3
1AZS	-536.3	2
1B6C	-491.1	3
1BGX	-2287.7	1
1BJ1	-630.2	2
1BKD	-1150.7	1
1BUH	-436.1	3
1BVK	-468.7	3
1BVN	-751.5	1
1CGI	-547	2

1D6R	-470.4	3
1DE4	-753.7	1
1DFJ	-990.8	1
1DQJ	-714.9	1
1E4K	-339.2	4
1E6J	-334.5	4
1E96	-376.8	4
1EAW	-580.2	2
1EER	-1219.9	1
1EFN	-411.5	3
1EWY	-617.1	2
1EZU	-798.9	1
1F34	-1006	1
1F51	-676.8	1
1FAK	-1123.3	1
1FC2	-311.4	5
1FQ1	-565.9	2
1FQJ	-640.2	2
1FSK	-626.8	2
1GCQ	-410.4	3
1GHQ	-222	5
1GLA	-480	3
1GP2	-719.6	1
1GPW	-776.5	1
1GRN	-747	1
1H1V	-657.4	1
1HE1	-575.1	2
1HE8	-499.5	2
1HIA	-532.3	2
1I2M	-1276.7	1
1I4D	-466.1	3
1I9R	-654.2	2
1IB1	-1020.5	1
1IBR	-1315	1
1IJK	-563.2	2
1IQD	-665.7	1
1IRA	-1103.4	1
1J2J	-207.2	5
1JMO	-1268.4	1
1JPS	-810.1	1
1K4C	-507.5	2
1K5D	-866.9	1
1K74	-708.7	1
1KAC	-383.8	4
1KKL	-499.6	2
1KLU	-384	4

1KTZ	-253.1	5
1KXP	-1003	1
1KXQ	-667.8	1
1M10	-842.6	1
1MAH	-575.1	2
1ML0	-747.7	1
1MLC	-493.7	2
1N2C	-1314.2	1
1N8O	-456.2	3
1NCA	-701.6	1
1NSN	-635.4	2
1NW9	-514.8	2
1OPH	-378.4	4
1PPE	-494.9	2
1PXV	-684.4	1
1QA9	-566.4	2
1QFW	-596.4	2
1R0R	-348.9	4
1R8S	-761.5	1
1RLB	-488	3
1S1Q	-417.7	3
1SBB	-353.4	4
1T6B	-621.5	2
1UDI	-616.6	2
1VFB	-553.4	2
1WEJ	-530.2	2
1WQ1	-1040	1
1XD3	-649.5	2
1XQS	-1027.4	1
1Y64	-789.7	1
1YVB	-389.9	4
1Z0K	-600.4	2
1Z5Y	-412.9	3
1ZHI	-442.1	3
2AJF	-572.3	2
2B42	-983.5	1
2C0L	-470.2	3
2CFH	-543	2
2FD6	-415	3
2H7V	-473.1	3
2HLE	-673.5	1
2HMI	-351	4
2HQS	-788.1	1
2HRK	-310.3	5
2I25	-607.7	2
2JEL	-551.4	2

2MTA	-314.2	5
2NZ8	-754	1
2O8V	-416.5	3
2OOB	-116.2	5
2OT3	-595.3	2
2PCC	-402.4	4
2QFW	-478.8	3
2SIC	-455.8	3
2SNI	-486.3	3
2UUY	-396.6	4
2VIS	-447.1	3
7CEI	-607.1	2

****

Group 22s-

Raw scores are a product of SVM classification

	Raw score	normalized score
1a2k	1	1
1acb	1	1
1ahw	1	1
1ak4	0	4
1akj	0	4
1avx	1	1
1ay7	0	4
1azs	1	1
1b6c	1	1
1bgx	1	1
1bj1	0	4
1bkd	1	1
1buh	0	4
1bvk	0	4
1bvn	0	4
1cgi	0	4
1d6r	0	4
1de4	1	1
1dfj	1	1
1dqj	0	4
1e4k	0	4
1e6j	0	4
1e96	0	4
1eaw	1	1
1eer	1	1
1efn	0	4
1ewy	0	4
1ezu	1	1
1f34	1	1

```
1f51        1  1
1fak        1  1
1fc2        0  4
1fq1        1  1
1fqj        0  4
1fsk        0  4
1gcq        0  4
1ghq        0  4
1gla        0  4
1gp2        1  1
1gpw        1  1
1grn        1  1
1h1v        0  4
1he1        1  1
1he8        0  4
1hia        1  1
1i2m        1  1
1i4d        1  1
1i9r        0  4
1ib1        1  1
1ibr        1  1
1ijk        0  4
1iqd        1  1
1ira        1  1
1j2j        0  4
1jmo        1  1
1jps        1  1
1k4c        0  4
1k5d        1  1
1k74        1  1
1kac        0  4
1kkl        0  4
1klu        0  4
1ktz        0  4
1kxp        1  1
1kxq        0  4
1m10        1  1
1mah        1  1
1ml0        1  1
1mlc        0  4
1n2c        1  1
1n8o        1  1
1nca        0  4
1nsn        0  4
1nw9        1  1
1oph        0  4
```

```
1ppe         1  1
1pxv         0  4
1qa9         0  4
1qfw         0  4
1r0r         0  4
1r8s         1  1
1rlb         0  4
1s1q         0  4
1sbb         0  4
1t6b         1  1
1udi         1  1
1vfb         0  4
1wej         0  4
1wq1         1  1
1xd3         1  1
1xqs         1  1
1y64         0  4
1yvb         0  4
1z0k         1  1
1z5y         0  4
1zhi         0  4
2ajf         0  4
2b42         1  1
2c0l         1  1
2cfh         1  1
2fd6         0  4
2h7v         0  4
2hle         1  1
2hmi         0  4
2hqs         1  1
2hrk         0  4
2i25         0  4
2jel         0  4
2mta         0  4
2nz8         1  1
2o8v         0  4
2oob         0  4
2ot3         1  1
2pcc         0  4
2qfw         0  4
2sic         0  4
2sni         1  1
2uuy         0  4
2vis         0  4
7cei         1  1
design_1     0  4
```

design_2	0	4
design_3	0	4
design_4	0	4
design_5	0	4
design_6	0	4
design_7	0	4
design_8	0	4
design_9	0	4
design_10	0	4
design_11	0	4
design_12	0	4
design_13	0	4
design_14	0	4
design_15	0	4
design_16	0	4
design_17	0	4
design_18	0	4
design_19	0	4
design_20	1	1
design_21	0	4
design_22	0	4
design_23	0	4
design_24	0	4
design_25	0	4
design_26	0	4
design_27	0	4
design_28	0	4
design_29	0	4
design_30	1	1
design_31	0	4
design_32	0	4
design_33	0	4
design_34	0	4
design_35	0	4
design_36	0	4
design_37	0	4
design_38	1	1
design_39	0	4
design_40	0	4
design_41	0	4
design_42	0	4
design_43	0	4
design_44	0	4
design_45	0	4
design_46	0	4
design_47	0	4

```
design_48    0  4
design_49    0  4
design_50    0  4
design_51    0  4
design_52    0  4
design_53    0  4
design_54    0  4
design_55    0  4
design_56    0  4
design_57    0  4
design_58    0  4
design_59    0  4
design_60    0  4
design_61    0  4
design_62    0  4
design_63    0  4
design_64    0  4
design_65    0  4
design_66    0  4
design_67    0  4
design_68    0  4
design_69    0  4
design_70    0  4
design_71    1  1
design_72    0  4
design_73    0  4
design_74    0  4
design_75    0  4
design_76    0  4
design_77    0  4
design_78    0  4
design_79    0  4
design_80    0  4
design_81    0  4
design_82    0  4
design_83    0  4
design_84    0  4
design_85    0  4
design_86    0  4
design_87    0  4

************************
Group 23s-
*Models with "-" could not be calculated the scores.

### Normalized score ###
```

Score >=0.5	1(bind)
0<= Score <0.5	2(likely to bind)
-0.5<= Score <0	5(uncertain)
-1.0<= Score <-0.5	3(likely not to bind)
Score <-1.0	4(does not to bind)

Model	Raw score	Normazied score
design_1	-2.027	4
design_2	-2.570	4
design_3	-1.651	4
design_4	-0.550	3
design_5	-0.930	3
design_6	0.743	1
design_7	-0.872	3
design_8	-0.049	5
design_9	-1.507	4
design_10	-2.515	4
design_11	-1.534	4
design_12	-2.349	4
design_13	-0.316	5
design_14	-1.487	4
design_15	-1.042	4
design_16	-1.709	4
design_17	-1.804	4
design_18	-1.604	4
design_19	-0.433	5
design_20	0.070	2
design_21	-0.685	3
design_22	0.166	2
design_23	-1.127	4
design_24	-0.026	5
design_25	0.165	2
design_26	0.273	2
design_27	-0.155	5
design_28	-1.155	4
design_29	-0.044	5
design_30	-1.719	4
design_31	-	-
design_32	-1.570	4
design_33	-0.387	5
design_34	-1.055	4
design_35	-1.607	4
design_36	-1.709	4
design_37	0.155	2
design_38	0.347	2

design_39	-2.123	4
design_40	-0.099	5
design_41	-2.217	4
design_42	-0.902	3
design_43	-	-
design_44	-1.960	4
design_45	-2.476	4
design_46	-2.032	4
design_47	-1.427	4
design_48	-2.758	4
design_49	-2.213	4
design_50	-1.425	4
design_51	0.187	2
design_52	-1.421	4
design_53	-0.308	5
design_54	-2.393	4
design_55	-1.279	4
design_56	-2.406	4
design_57	-0.832	3
design_58	-2.342	4
design_59	-1.060	4
design_60	-2.726	4
design_61	0.651	1
design_62	-1.008	4
design_63	0.480	2
design_64	-1.642	4
design_65	-0.691	3
design_66	-0.590	3
design_67	-1.992	4
design_68	-0.924	3
design_69	0.262	2
design_70	0.199	2
design_71	-0.771	3
design_72	0.290	2
design_73	-0.380	5
design_74	-2.441	4
design_75	-0.398	5
design_76	-1.682	4
design_77	0.151	2
design_78	0.625	1
design_79	-2.099	4
design_80	-1.453	4
design_81	-1.052	4
design_82	-0.714	3
design_83	0.442	2
design_84	0.062	2

```
design_85       -0.353  5
design_86       -1.959  4
design_87       -0.520  3
1A2K    0.658   1
1ACB    -0.105  5
1AHW    0.719   1
1AK4    -0.610  3
1AKJ    0.311   2
1AVX    0.422   2
1AY7    -0.908  3
1AZS    0.364   2
1B6C    -0.207  5
1BGX    0.570   1
1BJ1    -0.499  5
1BKD    0.185   2
1BUH    -1.118  4
1BVK    -0.870  3
1BVN    -0.992  3
1CGI    -0.204  5
1D6R    -0.164  5
1DE4    -       -
1DFJ    0.058   2
1DQJ    -1.024  4
1E4K    0.320   2
1E6J    0.551   1
1E96    0.626   1
1EAW    0.593   1
1EER    1.764   1
1EFN    0.114   2
1EWY    -0.825  3
1EZU    -0.880  3
1F34    -0.282  5
1F51    -0.516  3
1FAK    -0.463  5
1FC2    -1.410  4
1FQ1    0.264   2
1FQJ    -0.087  5
1FSK    -0.756  3
1GCQ    -0.874  3
1GHQ    -1.729  4
1GLA    0.011   2
1GP2    0.203   2
1GPW    0.908   1
1GRN    0.721   1
1H1V    -1.842  4
1HE1    0.359   2
```

1HE8	-0.046	5
1HIA	0.211	2
1I2M	0.964	1
1I4D	-1.195	4
1I9R	-0.074	5
1IB1	-0.054	5
1IBR	1.106	1
1IJK	0.833	1
1IQD	-0.537	3
1IRA	0.800	1
1J2J	0.117	2
1JMO	-	-
1JPS	0.696	1
1K4C	0.275	2
1K5D	0.193	2
1K74	0.874	1
1KAC	0.165	2
1KKL	-0.360	5
1KLU	-0.633	3
1KTZ	0.007	2
1KXP	1.236	1
1KXQ	0.392	2
1M10	0.045	2
1MAH	1.153	1
1ML0	1.189	1
1MLC	-0.379	5
1N2C	-	-
1N8O	-1.292	4
1NCA	-0.401	5
1NSN	-0.321	5
1NW9	-0.297	5
1OPH	0.260	2
1PPE	0.398	2
1PXV	0.465	2
1QA9	-0.187	5
1QFW	0.271	2
1R0R	-0.878	3
1R8S	0.860	1
1RLB	-0.112	5
1S1Q	-0.878	3
1SBB	-0.843	3
1T6B	-1.107	4
1UDI	0.975	1
1VFB	-1.011	4
1WEJ	-0.192	5
1WQ1	1.010	1

```
1XD3    0.905   1
1XQS    0.967   1
1Y64    0.495   2
1YVB    -       -
1Z0K    -0.122  5
1Z5Y    -0.713  3
1ZHI    0.459   2
2AJF    -0.224  5
2B42    -0.024  5
2C0L    0.425   2
2CFH    0.948   1
2FD6    -       -
2H7V    -       -
2HLE    0.626   1
2HMI    -0.023  5
2HQS    -0.014  5
2HRK    0.075   2
2I25    -0.591  3
2JEL    -2.441  4
2MTA    0.104   2
2NZ8    0.131   2
2O8V    -0.199  5
2OOB    -0.384  5
2OT3    1.074   1
2PCC    0.758   1
2QFW    -1.011  4
2SIC    -1.010  4
2SNI    0.118   2
2UUY    0.030   2
2VIS    -0.568  3
7CEI    0.809   1


**********
Group 24s-
REMARK Submission from Group 24s
REMARK Oregon State University
REMARK Victor Hsu - hsuv AT onid.orst.edu
REMARK Camden Driggers - driggers AT science.oregonstate.edu
REMARK Robert Hall - hallro AT onid.orst.edu
REMARK Jessica Morgan - morganje AT onid.orst.edu

Raw scores are given in arbitrary units

design_1  8.46  3
design_2  7.97  2
```

design_3 6.83 1
design_4 5.71 1
design_5 7.85 2
design_6 7.33 2
design_7 5.54 1
design_8 10.38 4
design_9 6.48 1
design_10 9.84 4
design_11 5.19 1
design_12 7.70 2
design_13 11.63 4
design_14 11.94 4
design_15 6.81 1
design_16 6.70 1
design_17 8.27 3
design_18 7.02 2
design_19 6.79 1
design_20 8.30 3
design_21 8.81 3
design_22 10.12 4
design_23 9.94 4
design_24 6.69 1
design_25 7.90 2
design_26 7.14 2
design_27 8.25 3
design_28 6.78 1
design_29 6.40 1
design_30 7.80 2
design_31 7.55 2
design_32 7.56 2
design_33 8.48 3
design_34 12.84 4
design_35 11.09 4
design_36 6.90 1
design_37 8.01 3
design_38 9.56 4
design_39 7.13 2
design_40 6.52 1
design_41 8.06 3
design_42 8.80 3
design_43 6.30 1
design_44 10.10 4
design_45 14.11 4
design_46 9.43 4
design_47 9.92 4
design_48 17.18 4

design_49 23.82 4
design_50 6.66 1
design_51 9.45 4
design_52 4.59 1
design_53 6.69 1
design_54 8.71 3
design_55 9.17 4
design_56 16.10 4
design_57 5.25 1
design_58 6.34 1
design_59 5.65 1
design_60 7.34 2
design_61 7.00 2
design_62 8.32 3
design_63 6.80 1
design_64 6.22 1
design_65 4.93 1
design_66 10.04 4
design_67 5.76 1
design_68 6.82 1
design_69 5.96 1
design_70 8.39 3
design_71 9.29 4
design_72 5.73 1
design_73 5.68 1
design_74 8.55 3
design_75 9.55 4
design_76 6.56 1
design_77 7.43 2
design_78 16.14 4
design_79 7.26 2
design_80 7.30 2
design_81 5.95 1
design_82 9.68 4
design_83 11.38 4
design_84 8.86 3
design_85 9.30 4
design_86 7.48 2
design_87 7.55 2
1A2K 5.55 1
1ACB 12.58 4
1AHW 4.51 1
1AK4 8.11 3
1AKJ 3.48 1
1ATN 6.78 1
1AVX 7.08 2

1AY7 4.38 1
1AZS 8.74 3
1B6C 8.47 3
1BGX 8.38 3
1BJ1 9.39 4
1BKD 5.74 1
1BUH 5.98 1
1BVK 5.97 1
1BVN 8.64 3
1CGI 10.10 4
1D6R 4.85 1
1DE4 7.60 2
1DFJ 4.94 1
1DQJ 5.52 1
1E4K 5.92 1
1E6E 4.25 1
1E6J 7.01 2
1E96 5.10 1
1EAW 6.02 1
1EER 5.80 1
1EFN 5.37 1
1EWY 3.78 1
1EZU 7.94 2
1F34 6.76 1
1F51 5.58 1
1FAK 5.94 1
1FC2 12.94 4
1FQ1 4.93 1
1FQJ 4.34 1
1FSK 5.90 1
1GCQ 6.46 1
1GHQ 3.47 1
1GLA 5.06 1
1GP2 5.39 1
1GPW 5.16 1
1GRN 5.11 1
1H1V 5.43 1
1HE1 7.50 2
1HE8 3.59 1
1HIA 6.21 1
1I2M 4.91 1
1I4D 10.01 4
1I9R 4.49 1
1IB1 4.95 1
1IBR 5.25 1
1IJK 4.82 1

```
1IQD  6.30  1
1IRA  5.91  1
1J2J  8.12  3
1JMO  6.94  1
1JPS  4.54  1
1K4C  5.74  1
1K5D  5.92  1
1K74  4.33  1
1KAC  4.62  1
1KKL  4.88  1
1KLU  5.87  1
1KTZ  5.03  1
1KXP  6.39  1
1KXQ  8.63  3
1M10  4.88  1
1MAH  6.43  1
1ML0  7.01  2
1MLC  6.65  1
1N2C  5.94  1
1N8O  8.63  3
1NCA  5.27  1
1NSN  5.66  1
1NW9  11.09  4
1OPH  5.58  1
1PPE  6.86  1
1PXV  6.88  1
1QA9  2.86  1
1QFW  7.84  2
1QFW  5.09  1
1R0R  8.45  3
1R8S  6.94  1
1RLB  5.54  1
1S1Q  7.21  2
1SBB  9.25  4
1T6B  4.65  1
1TMQ  6.93  1
1UDI  5.52  1
1VFB  6.09  1
1WEJ  4.10  1
1WQ1  4.97  1
1XD3  5.35  1
1XQS  4.29  1
1Y64  4.85  1
1YVB  6.60  1
1Z0K  5.00  1
1Z5Y  12.10  4
```

1ZHI 4.88 1
2AJF 7.36 2
2B42 7.18 2
2BTF 5.02 1
2C0L 4.95 1
2CFH 7.16 2
2FD6 6.43 1
2H7V 5.54 1
2HLE 5.83 1
2HMI 8.77 3
2HQS 5.44 1
2HRK 8.13 3
2i25 4.58 1
2JEL 6.21 1
2MTA 6.75 1
2NZ8 6.52 1
2O8V 6.05 1
2OOB 8.25 3
2OT3 8.89 3
2PCC 3.69 1
2SIC 7.09 2
2SNI 7.02 2
2UUY 6.87 1
2VIS 6.41 1
7CEI 3.73 1
****

Group 26s-
The following table is our scoring results for CAPRI Round 21 (our participant code is 26s). Three columns were prepared according to the format requirements. Raw scores were normalized as:

1 binds
2 likely to bind
3 likely not to bind
4 does not bind

If there is something missed, please contact me as soon as possible.

Bests,
Jian

Model ID	Raw Score	Normalized Score
1A2K	-4.3033	2
1ACB	-4.0664	2
1AHW	-4.3285	1
1AK4	-2.6089	4
1AKJ	-2.9691	3

1AVX	-4.9187	1
1AY7	-2.6741	4
1AZS	-4.229	2
1B6C	-3.1844	4
1BGX	-9.868	1
1BJ1	-4.439	2
1BKD	-7.7723	1
1BUH	-2.8412	4
1BVK	-2.0767	4
1BVN	-4.9685	1
1CGI	-5.3519	2
1D6R	-3.3038	4
1DE4	-3.52	3
1DFJ	-4.4911	1
1DQJ	-4.3985	1
1E4K	-2.9954	4
1E6J	-3.4832	4
1E96	-2.6764	4
1EAW	-4.6466	2
1EER	-8.026	1
1EFN	-3.7208	4
1EWY	-1.8186	3
1EZU	-6.2556	1
1F34	-6.3977	2
1F51	-4.2641	2
1FAK	-5.4979	1
1FC2	-2.9652	4
1FQ1	-3.1673	4
1FQJ	-3.0386	3
1FSK	-4.6558	1
1GCQ	-3.1267	4
1GHQ	-1.2898	4
1GLA	-2.3857	4
1GP2	-5.196	1
1GPW	-4.85	1
1GRN	-5.5872	1
1H1V	-3.949	3
1HE1	-5.6012	2
1HE8	-3.6117	4
1HIA	-3.911	4
1I2M	-6.764	1
1I4D	-3.8979	4
1I9R	-3.151	3
1IB1	-4.6806	1
1IBR	-8.4036	1
1IJK	-4.4034	2

1IQD	-5.4772	2
1IRA	-6.2854	1
1J2J	-2.7905	4
1JMO	-8.523	1
1JPS	-3.886	3
1K4C	-4.9217	2
1K5D	-5.52	1
1K74	-4.946	1
1KAC	-3.3382	4
1KKL	-2.8362	4
1KLU	-2.591	3
1KTZ	-3.0264	4
1KXP	-6.593	1
1KXQ	-6.1849	1
1M10	-4.4808	1
1MAH	-5.0261	2
1ML0	-6.4384	2
1MLC	-4.0621	2
1N2C	-10.509	1
1N8O	-4.2532	2
1NCA	-4.594	1
1NSN	-2.7432	3
1NW9	-6.1887	2
1OPH	-2.7911	4
1PPE	-4.3636	2
1PXV	-5.6637	1
1QA9	-3.0818	3
1QFW	-3.5917	4
1R0R	-4.7221	2
1R8S	-8.3683	2
1RLB	-2.6078	4
1S1Q	-2.0272	4
1SBB	-1.8749	4
1T6B	-4.1407	1
1UDI	-3.9641	4
1VFB	-2.5329	4
1WEJ	-3.311	3
1WQ1	-6.5023	1
1XD3	-5.91	2
1XQS	-5.096	1
1Y64	-3.647	3
1YVB	-3.6384	4
1Z0K	-4.0704	2
1Z5Y	-4.4255	2
1ZHI	-2.6248	4
2AJF	-3.9928	3

2B42	-6.1402	1
2C0L	-4.0636	2
2CFH	-7.639	2
2FD6	-3.743	4
2H7V	-3.8826	4
2HLE	-4.2059	2
2HMI	-2.358	4
2HQS	-3.7274	3
2HRK	-3.0518	4
2I25	-4.1498	2
2JEL	-2.344	4
2MTA	-1.6688	4
2NZ8	-5.143	1
2O8V	-4.5027	2
2OOB	-1.5714	4
2OT3	-5.6468	2
2PCC	-1.9434	4
2QFW	-2.628	4
2SIC	-5.0128	2
2SNI	-4.9204	2
2UUY	-3.9187	4
2VIS	-3.395	4
7CEI	-4.7854	2
design_1	-2.5501	4
design_2	-2.6796	4
design_3	-4.2356	2
design_4	-2.3435	3
design_5	-2.5629	4
design_6	-1.9154	4
design_7	-3.3333	3
design_8	-2.2382	4
design_9	-2.2556	4
design_10	-3.4009	4
design_11	-2.7611	4
design_12	-4.5416	2
design_13	-2.6238	4
design_14	-2.5561	4
design_15	-1.4823	4
design_16	-2.8196	4
design_17	-2.7862	4
design_18	-3.0472	4
design_19	-2.1024	4
design_20	-3.7478	4
design_21	-3.5645	4
design_22	-2.4194	4
design_23	-3.1563	4

design_24	-2.2446	4
design_25	-2.544	4
design_26	-2.0714	3
design_27	-1.8728	4
design_28	-0.9618	4
design_29	-1.5205	4
design_30	-3.9114	4
design_31	-2.217	4
design_32	-1.9363	4
design_33	-3.166	4
design_34	-3.4434	3
design_35	-4.2443	2
design_36	-3.628	4
design_37	-2.9272	4
design_38	-3.0197	4
design_39	-2.493	3
design_40	-2.289	4
design_41	-3.1069	4
design_42	-3.0584	4
design_43	-3.4382	4
design_44	-3.8292	4
design_45	-4.2311	2
design_46	-2.8551	4
design_47	-2.7076	4
design_48	-3.4101	4
design_49	-3.0123	4
design_50	-2.568	4
design_51	-1.9426	4
design_52	-4.6407	2
design_53	-4.3904	2
design_54	-2.944	4
design_55	-2.6457	4
design_56	-2.8902	4
design_57	-3.6813	4
design_58	-3.7299	4
design_59	-3.5145	4
design_60	-2.2263	4
design_61	-3.567	4
design_62	-2.3705	4
design_63	-3.1996	4
design_64	-2.1455	4
design_65	-3.3877	3
design_66	-3.6497	4
design_67	-2.5025	4
design_68	-1.8158	4
design_69	-3.5581	4

```
design_70       -2.1632         4
design_71       -3.6069         4
design_72       -3.5224         4
design_73       -2.195          4
design_74       -2.7727         4
design_75       -2.1319         4
design_76       -3.5511         4
design_77       -2.9556         4
design_78       -2.2757         4
design_79       -2.397          4
design_80       -2.6819         4
design_81       -3.6407         4
design_82       -3.1818         4
design_83       -3.6133         4
design_84       -1.7588         4
design_85       -3.7949         4
design_86       -2.6104         4
design_87       -2.4788         4
********************
Group 28s -
# CAPRI T45 predictions - Bonvin group, Utrecht University, the Netherlands
# Raw scores are given after the calculating of the pKd for each complex
#
#Complex        Raw score       normalized score
design_1        4.8     4
design_2        4.0     4
design_3        6.4     3
design_4        2.3     5
design_5        2.9     5
design_6        5.0     3
design_7        4.2     4
design_8        4.8     4
design_9        3.3     4
design_10       1.7     5
design_11       1.4     5
design_12       3.6     4
design_13       4.2     4
design_14       3.6     4
design_15       4.7     4
design_16       4.7     4
design_17       5.1     3
design_18       2.2     5
design_19       5.9     3
design_20       7.1     2
design_21       4.9     4
design_22       6.0     3
```

design_23	4.0	4
design_24	5.6	3
design_25	3.4	4
design_26	4.9	4
design_27	4.9	4
design_28	2.2	5
design_29	4.1	4
design_30	7.0	2
design_31	4.1	4
design_32	2.6	5
design_33	4.9	4
design_34	5.3	3
design_35	5.4	3
design_36	4.9	4
design_37	5.0	3
design_38	6.7	3
design_39	1.1	5
design_40	4.3	4
design_41	3.2	4
design_42	3.4	4
design_43	3.5	4
design_44	5.2	3
design_45	4.5	4
design_46	2.6	5
design_47	3.8	4
design_48	2.7	5
design_49	2.7	5
design_50	3.9	4
design_51	5.3	3
design_52	4.3	4
design_53	5.7	3
design_54	5.6	3
design_55	2.3	5
design_56	3.6	4
design_57	8.8	2
design_58	3.4	4
design_59	4.6	4
design_60	3.8	4
design_61	5.3	3
design_62	4.7	4
design_63	6.4	3
design_64	1.6	5
design_65	1.9	5
design_66	2.5	5
design_67	5.2	3
design_68	4.1	4

design_69	3.1	4
design_70	2.5	5
design_71	4.0	4
design_72	4.4	4
design_73	2.7	5
design_74	2.5	5
design_75	3.7	4
design_76	5.3	3
design_77	4.1	4
design_78	0.4	5
design_79	3.8	4
design_80	3.3	4
design_81	4.8	4
design_82	5.5	3
design_83	6.1	3
design_84	6.0	3
design_85	3.7	4
design_86	3.4	4
design_87	5.0	3
1A2K	6.4	3
1ACB	8.1	2
1AHW	8.6	2
1AK4	3.7	4
1AKJ	3.2	4
1AVX	11.7	1
1AY7	7.9	2
1AZS	7.8	2
1B6C	5.8	3
1BGX	16.2	1
1BJ1	11.7	1
1BKD	8.8	2
1BUH	4.0	4
1BVK	4.2	4
1BVN	8.4	2
1CGI	10.8	1
1D6R	10.2	1
1DE4	7.8	2
1DFJ	8.1	2
1DQJ	6.8	3
1E4K	3.2	4
1E6J	4.4	4
1E96-	4.7	4
1EAW	10.8	1
1EER	15.6	1
1EFN	5.0	3
1EWY	3.8	4

1EZU	11.1	1
1F34	11.3	1
1F51	6.1	3
1FAK	5.7	3
1FC2	2.8	5
1FQ1	3.5	4
1FQJ	1.1	5
1FSK	11.5	1
1GCQ	5.0	3
1GHQ	1.7	5
1GLA	3.9	4
1GP2	8.1	2
1GPW	9.0	1
1GRN	6.4	3
1H1V	1.3	5
1HE1	4.9	4
1HE8	3.3	4
1HIA	9.9	1
1I2M	15.1	1
1I4D	5.9	3
1I9R	7.3	2
1IB1	3.4	4
1IBR	13.3	1
1IJK	9.5	1
1IQD	11.5	1
1IRA	7.1	2
1J2J	3.5	4
1JMO	15.3	1
1JPS	10.6	1
1K4C	10.8	1
1K5D	12.1	1
1K74	7.5	2
1KAC	3.5	4
1KKL	4.5	4
1KLU	5.7	3
1KTZ	2.7	5
1KXP	10.6	1
1KXQ	7.2	2
1M10	7.8	2
1MAH	8.1	2
1ML0	10.0	1
1MLC	7.7	2
1N2C	18.3	1
1N8O	7.1	2
1NCA	7.5	2
1NSN	4.4	4

1NW9	8.2	2
1OPH	12.5	1
1PPE	10.4	1
1PVX	9.3	1
1QA9	5.0	3
1QFW	4.2	4
1R0R	8.4	2
1R8S	9.2	1
1RLB	5.0	3
1S1Q	4.5	4
1SSB	2.2	5
1T6B	5.7	3
1UDI	5.0	3
1VFB	5.6	3
1WEJ	7.6	2
1WQ1	5.5	3
1XD3	9.9	1
1XQS	15.0	1
1Y64	4.1	4
1YVB	7.4	2
1Z0K	6.3	3
1Z5Y	5.8	3
1ZHI	5.1	3
2AJF	4.4	4
2B42	9.1	1
2C0L	6.8	3
2CFH	7.5	2
2FD6	5.9	3
2H7V	4.5	4
2HLE	11.1	1
2HMI	3.9	4
2HQS	5.1	3
2HRK	4.9	4
2I25	7.8	2
2JEL	5.4	3
2MTA	1.8	5
2NZ8	6.9	3
2O8V	7.0	2
2OOB	3.3	4
2OT3	9.9	1
2PCC	4.1	4
2QFW	5.2	3
2SIC	7.1	2
2SNI	7.6	2
2UUY	10.1	1
2VIS	5.8	3

7CEI 8.1 2
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Group 29s -
Has document file in email from weiyi.zhang2008@gmail.com
that explains method.

	Raw score	normalized score
design_1	-60.34	4
design_2	-43.15	4
design_3	-74.56	3
design_4	-51.43	4
design_5	-58.33	4
design_6	-71.32	3
design_7	-73.48	3
design_8	-74.66	3
design_9	-48.92	4
design_10	-59.72	4
design_11	-40.34	4
design_12	-71.44	3
design_13	-52.62	4
design_14	-58.11	4
design_15	-59.27	4
design_16	-84.48	2
design_17	-56.81	4
design_18	-63.14	4
design_19	-78.38	3
design_20	-101.57	1
design_21	-56.8	4
design_22	-64.75	4
design_23	-60.97	4
design_24	-76.73	3
design_25	-50.51	4
design_26	-62.75	4
design_27	-56.14	4
design_28	-61.99	4
design_29	-78.63	3
design_30	-74.24	3
design_31	-43.42	4
design_32	-47.27	4
design_33	-78.1	3
design_34	-83.95	2
design_35	-80.87	2
design_36	-61.95	4
design_37	-74	3
design_38	-91.85	1
design_39	-43.29	4

design_40	-69.67	3
design_41	-63.19	4
design_42	-61.78	4
design_43	-59.07	4
design_44	-77.91	3
design_45	-71.68	3
design_46	-50.36	4
design_47	-53.58	4
design_48	-57.85	4
design_49	-55.41	4
design_50	-50.04	4
design_51	-65.73	4
design_52	-71.85	3
design_53	-75.55	3
design_54	-52.47	4
design_55	-64.78	4
design_56	-50.13	4
design_57	-84.68	2
design_58	-75.73	3
design_59	-67.03	4
design_60	-39.89	4
design_61	-67.56	4
design_62	-77.99	3
design_63	-67.27	4
design_64	-43.95	4
design_65	-62.2	4
design_66	-72.58	3
design_67	-47.77	4
design_68	-60.28	4
design_69	-74.42	3
design_70	-54.99	4
design_71	-73.77	3
design_72	-73.68	3
design_73	-55.05	4
design_74	-37.22	4
design_75	-62.22	4
design_76	-84.95	2
design_77	-86.51	2
design_78	-47.34	4
design_79	-46.36	4
design_80	-47.17	4
design_81	-67.44	4
design_82	-81.16	2
design_83	-92.62	1
design_84	-75.13	3
design_85	-78.11	3

design_86	-40.81	4
design_87	-56.67	4
ZDock2_1A2K	-97.38	1
ZDock2_1ACB	-79.77	2
ZDock2_1AHW	-87.55	2
ZDock2_1AK4	-47.67	4
ZDock2_1AKJ	-91.23	1
ZDock2_1AVX	-96.55	1
ZDock2_1AY7	-68.8	4
ZDock2_1B6C	-92.36	1
ZDock2_1BGX	-218.2	1
ZDock2_1BJ1	-103.05	1
ZDock2_1BUH	-61.11	4
ZDock2_1BVK	-49.89	4
ZDock2_1BVN	-116.59	1
ZDock2_1CGI	-111.17	1
ZDock2_1D6R	-71.6	3
ZDock2_1DE4	-80.15	2
ZDock2_1DFJ	-110.79	1
ZDock2_1DQJ	-72.98	3
ZDock2_1E6J	-69.27	3
ZDock2_1E96	-69.73	3
ZDock2_1EAW	-105.89	1
ZDock2_1EER	-197.6	1
ZDock2_1EWY	-65.43	4
ZDock2_1EZU	-123.63	1
ZDock2_1F34	-149.97	1
ZDock2_1F51	-89.89	1
ZDock2_1FAK	-124.37	1
ZDock2_1FC2	-47.97	4
ZDock2_1FQ1	-67.55	4
ZDock2_1FQJ	-80.98	2
ZDock2_1FSK	-92	1
ZDock2_1GCQ	-63.79	4
ZDock2_1GHQ	-24.7	4
ZDock2_1GP2	-124.03	1
ZDock2_1GRN	-104.81	1
ZDock2_1H1V	-61.64	4
ZDock2_1HE1	-105.98	1
ZDock2_1HE8	-70.84	3
ZDock2_1HIA	-94.66	1
ZDock2_1I2M	-159.52	1
ZDock2_1I4D	-60.17	4
ZDock2_1I9R	-64.4	4
ZDock2_1IB1	-130.92	1

ZDock2_1IBR	-188.07	1
ZDock2_1IJK	-103.89	1
ZDock2_1IQD	-141.7	1
ZDock2_1JPS	-101.07	1
ZDock2_1K4C	-110.97	1
ZDock2_1K5D	-155.41	1
ZDock2_1KAC	-64.31	4
ZDock2_1KKL	-71.95	3
ZDock2_1KLU	-65.99	4
ZDock2_1KTZ	-62.82	4
ZDock2_1KXP	-171.56	1
ZDock2_1KXQ	-103.02	1
ZDock2_1M10	-108.51	1
ZDock2_1MAH	-106.77	1
ZDock2_1ML0	-133.66	1
ZDock2_1MLC	-69.22	3
ZDock2_1N2C	-193.23	1
ZDock2_1NCA	-93.69	1
ZDock2_1NSN	-52.97	4
ZDock2_1PPE	-103.97	1
ZDock2_1QA9	-65.98	4
ZDock2_1QFW	-73.08	3
ZDock2_1RLB	-58.07	4
ZDock2_1SBB	-44.95	4
ZDock2_1UDI	-100.6	1
ZDock2_1VFB	-57.22	4
ZDock2_1WEJ	-65	4
ZDock2_1WQ1	-124.4	1
ZDock2_2HMI	-30.36	4
ZDock2_2JEL	-73.51	3
ZDock2_2MTA	-59.69	4
ZDock2_2PCC	-58.75	4
ZDock2_2QFW	-54.11	4
ZDock2_2SIC	-79.94	2
ZDock2_2SNI	-93.93	1
ZDock2_2VIS	-60.6	4
ZDock2_7CEI	-112.73	1
ZDock3_1AZS	-95.61	1
ZDock3_1BKD	-139.26	1
ZDock3_1E4K	-66.74	4
ZDock3_1EFN	-74.43	3
ZDock3_1GLA	-76.82	3
ZDock3_1GPW	-112.97	1
ZDock3_1IRA	-134.35	1
ZDock3_1J2J	-61.23	4

ZDock3_1JMO	-186.68	1
ZDock3_1K74	-83.26	2
ZDock3_1N8O	-104.02	1
ZDock3_1NW9	-114.51	1
ZDock3_1OPH	-84.1	2
ZDock3_1PXV	-120.76	1
ZDock3_1R0R	-71.54	3
ZDock3_1R8S	-154.5	1
ZDock3_1S1Q	-46.92	4
ZDock3_1T6B	-63.06	4
ZDock3_1XD3	-129.72	1
ZDock3_1XQS	-152.32	1
ZDock3_1Y64	-84.08	2
ZDock3_1YVB	-65.99	4
ZDock3_1Z0K	-94.51	1
ZDock3_1Z5Y	-70.28	3
ZDock3_1ZHI	-68.53	4
ZDock3_2AJF	-72.52	3
ZDock3_2B42	-113.92	1
ZDock3_2C0L	-107.15	1
ZDock3_2CFH	-138.32	1
ZDock3_2FD6	-53.75	4
ZDock3_2H7V	-85.48	2
ZDock3_2HLE	-138.94	1
ZDock3_2HQS	-110.74	1
ZDock3_2HRK	-66.21	4
ZDock3_2I25	-89.76	1
ZDock3_2NZ8	-121.82	1
ZDock3_2O8V	-84.38	2
ZDock3_2OOB	-43.16	4
ZDock3_2OT3	-135.55	1
ZDock3_2UUY	-78.77	3

Raw scores are given in kcal/mole in this example.
****
Group 30s-
Raw scores are given in units of Angstrom^2 per residue
Index for normalized score : 1 - binds; 4 - does not bind; 5 - uncertain

Complex	Raw score	Normalized score
design_01	1.57	4
design_02	0.94	4
design_03	1.76	4
design_04	1.57	4
design_05	1.54	4
design_06	2.69	1

design_07	1.46	4
design_08	2.89	1
design_09	1.36	4
design_10	1.92	4
design_11	1.68	4
design_12	1.93	4
design_13	1.66	4
design_14	1.77	4
design_15	2.46	5
design_16	0.91	4
design_17	0.83	4
design_18	1.29	4
design_19	2.06	5
design_20	3.19	1
design_21	1.45	4
design_22	2.32	5
design_23	1.97	4
design_24	3.49	1
design_25	1.01	4
design_26	1.51	4
design_27	1.42	4
design_28	2.95	1
design_29	2.41	5
design_30	2.20	5
design_31	1.00	4
design_32	1.07	4
design_33	3.22	1
design_34	2.20	5
design_35	1.98	4
design_36	0.91	4
design_37	2.67	1
design_38	3.21	1
design_39	1.20	4
design_40	0.86	4
design_41	0.93	4
design_42	1.62	4
design_43	1.60	4
design_44	1.93	4
design_45	2.28	5
design_46	1.18	4
design_47	1.51	4
design_48	1.94	4
design_49	2.31	5
design_50	1.53	4
design_51	2.14	5
design_52	1.30	4

design_53	1.20	4
design_54	1.91	4
design_55	2.99	1
design_56	1.37	4
design_57	2.34	5
design_58	1.09	4
design_59	2.26	5
design_60	1.60	4
design_61	1.83	4
design_62	4.45	1
design_63	1.72	4
design_64	1.29	4
design_65	1.58	4
design_66	1.82	4
design_67	1.77	4
design_68	2.66	1
design_69	1.83	4
design_70	1.33	4
design_71	3.56	1
design_72	2.29	5
design_73	1.15	4
design_74	1.18	4
design_75	2.52	1
design_76	1.25	4
design_77	2.24	5
design_78	1.41	4
design_79	1.57	4
design_80	1.39	4
design_81	1.55	4
design_82	2.77	1
design_83	4.60	1
design_84	2.19	5
design_85	1.63	4
design_86	0.80	4
design_87	1.40	4
1ACB	2.58	1
1AK4	1.54	4
1AVX	2.15	5
1AY7	3.38	1
1B6C	2.09	5
1BKD	2.53	1
1BUH	1.89	4
1BVN	1.92	4
1CGI	3.44	1
1D6R	2.33	5
1DFJ	2.11	5

1E96	1.62	4
1EAW	3.06	1
1EFN	3.91	1
1EWY	1.81	4
1F34	3.27	1
1FC2	2.71	1
1FQ1	1.80	4
1FQJ	2.04	5
1GCQ	4.94	1
1GHQ	0.77	4
1GLA	1.04	4
1GPW	2.35	5
1GRN	2.89	1
1H1V	1.44	4
1HE1	3.28	1
1HE8	0.80	4
1I2M	2.56	1
1IBR	2.75	1
1IRA	3.48	1
1J2J	2.80	1
1KAC	2.28	5
1KKL	1.37	4
1KTZ	2.54	1
1KXP	2.15	5
1KXQ	1.67	4
1M10	2.18	5
1MAH	1.64	4
1N8O	2.48	5
1NW9	3.08	1
1OPH	1.08	4
1PPE	3.24	1
1PXV	3.98	1
1QA9	2.97	1
1R0R	2.11	5
1R8S	3.93	1
1RLB	1.07	4
1S1Q	2.94	1
1SBB	1.31	4
1T6B	1.12	4
1UDI	3.19	1
1WQ1	3.02	1
1XD3	3.61	1
1XQS	2.70	1
1Y64	1.48	4
1YVB	2.23	5
1Z0K	3.97	1

1Z5Y	2.55	1
1ZHI	1.91	4
2AJF	1.10	4
2B42	2.31	5
2C0L	2.23	5
2CFH	3.82	1
2H7V	1.67	4
2HLE	3.27	1
2HQS	2.16	5
2HRK	2.58	1
2I25	2.91	1
2NZ8	2.73	1
2O8V	2.32	5
2OOB	3.31	1
2OT3	2.76	1
2PCC	1.36	4
2SIC	2.08	5
2SNI	2.43	5
2UUY	2.44	5
7CEI	3.18	1

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Group 31s-

	Raw Score	normalized score
design_1	0.230	4
design_2	2.850	2
design_3	1.074	4
design_4	1.517	3
design_5	3.037	2
design_6	-0.822	4
design_7	1.695	3
design_8	1.177	4
design_9	0.628	4
design_10	3.168	2
design_11	0.509	4
design_12	0.021	4
design_13	1.339	4
design_14	1.139	4
design_15	1.755	3
design_16	0.951	4
design_17	0.126	4
design_18	-0.309	4
design_19	1.173	4
design_20	3.184	2
design_21	2.783	2
design_22	1.302	4

design_23	3.542	2
design_24	2.838	2
design_25	1.012	4
design_26	1.550	3
design_27	4.166	1
design_28	3.313	2
design_29	6.651	1
design_30	0.592	4
design_31	0.538	4
design_32	0.477	4
design_33	0.390	4
design_34	-0.272	4
design_35	6.703	1
design_36	-0.396	4
design_37	3.481	2
design_38	1.953	3
design_39	6.779	1
design_40	0.984	4
design_41	-0.593	4
design_42	-1.182	4
design_43	0.047	4
design_44	-1.259	4
design_45	1.413	4
design_46	1.538	3
design_47	0.225	4
design_48	2.105	3
design_49	0.925	4
design_50	-1.213	4
design_51	6.506	1
design_52	0.108	4
design_53	0.958	4
design_54	1.590	3
design_55	6.054	1
design_56	3.023	2
design_57	2.416	3
design_58	0.557	4
design_59	6.096	1
design_60	1.969	3
design_61	1.804	3
design_62	1.483	4
design_63	0.581	4
design_64	-0.614	4
design_65	6.112	1
design_66	2.921	2
design_67	2.045	3
design_68	1.876	3

design_69	-0.351	4
design_70	-0.716	4
design_71	1.505	3
design_72	1.844	3
design_73	3.584	2
design_74	-0.859	4
design_75	3.201	2
design_76	0.725	4
design_77	0.352	4
design_78	0.170	4
design_79	0.446	4
design_80	1.397	4
design_81	0.640	4
design_82	0.917	4
design_83	9.034	1
design_84	1.618	3
design_85	-0.159	4
design_86	-1.345	4
design_87	2.064	3
1A2K	1.464	4
1ACB	5.057	1
1AHW	4.171	1
1AK4	2.474	3
1AKJ	1.908	3
1AVX	1.962	3
1AY7	4.704	1
1AZS	4.450	1
1B6C	6.832	1
1BGX	14.433	1
1BJ1	1.098	4
1BKD	9.914	1
1BUH	1.445	4
1BVK	6.242	1
1BVN	7.157	1
1CGI	8.839	1
1D6R	2.568	2
1DE4	6.141	1
1DFJ	1.341	4
1DQJ	7.902	1
1E4K	2.221	3
1E6J	3.578	2
1E96	4.393	1
1EAW	7.492	1
1EER	9.040	1
1EFN	3.175	2
1EWY	-0.156	4

1EZU	8.157	1
1F34	9.752	1
1F51	7.557	1
1FAK	7.265	1
1FC2	6.068	1
1FQ1	2.595	2
1FQJ	-0.122	4
1FSK	3.359	2
1GCQ	5.891	1
1GHQ	3.527	2
1GLA	0.491	4
1GP2	4.191	1
1GPW	6.790	1
1GRN	6.180	1
1H1V	0.184	4
1HE1	7.189	1
1HE8	3.712	2
1HIA	6.705	1
1I2M	9.519	1
1I4D	2.430	3
1I9R	6.006	1
1IB1	4.444	1
1IBR	8.081	1
1IJK	1.871	3
1IQD	6.479	1
1IRA	10.078	1
1J2J	0.177	4
1JMO	11.478	1
1JPS	3.231	2
1K4C	4.925	1
1K5D	9.717	1
1K74	6.608	1
1KAC	6.621	1
1KKL	-0.689	4
1KLU	4.209	1
1KTZ	0.824	4
1KXP	9.238	1
1KXQ	4.134	1
1M10	7.108	1
1MAH	5.602	1
1ML0	6.907	1
1MLC	0.234	4
1N2C	9.521	1
1N8O	6.779	1
1NCA	5.878	1
1NSN	0.404	4

1NW9	7.540	1
1OPH	-0.271	4
1PPE	7.417	1
1PXV	8.093	1
1QA9	0.201	4
1QFW	1.362	4
1R0R	6.523	1
1R8S	10.229	1
1RLB	7.716	1
1S1Q	1.968	3
1SBB	1.356	4
1T6B	1.652	3
1UDI	6.299	1
1VFB	1.799	3
1WEJ	6.052	1
1WQ1	8.011	1
1XD3	9.721	1
1XQS	7.490	1
1Y64	7.582	1
1YVB	1.452	4
1Z0K	5.129	1
1Z5Y	2.383	3
1ZHI	0.390	4
2AJF	1.863	3
2B42	6.712	1
2C0L	7.290	1
2CFH	9.394	1
2FD6	-0.478	4
2H7V	7.288	1
2HLE	7.748	1
2HMI	-0.654	4
2HQS	0.770	4
2HRK	2.469	3
2I25	6.476	1
2JEL	0.483	4
2MTA	1.232	4
2NZ8	3.837	2
2O8V	5.683	1
2OOB	0.452	4
2OT3	9.097	1
2PCC	0.947	4
2QFW	2.185	3
2SIC	4.378	1
2SNI	4.838	1
2UUY	4.660	1
2VIS	3.572	2

7CEI 3.335 2

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Group 32s-
REMARK the docking benchmark.
REMARK Change the file name from GroupXXX.txt to represent your group's name.
REMARK Add raw and normalized scores in the table below.
REMARK Fill in the units in which the raw scores were computed below.
Raw scores are given in units of "occurences of frequent interaction patterns"

	Raw score	normalized score
design_1	7.54	3
design_2	7.74	3
design_3	9.66	2
design_4	8.01	3
design_5	7.37	3
design_6	9.61	2
design_7	7.81	3
design_8	8.70	3
design_9	8.88	3
design_10	6.63	4
design_11	7.30	3
design_12	8.00	3
design_13	8.09	3
design_14	6.55	4
design_15	6.67	4
design_16	8.55	3
design_17	9.56	2
design_18	8.09	3
design_19	9.84	2
design_20	9.74	2
design_21	7.79	3
design_22	9.65	2
design_23	7.19	3
design_24	9.92	2
design_25	6.73	4
design_26	5.92	4
design_27	8.30	3
design_28	6.07	4
design_29	8.00	3
design_30	8.38	3
design_31	7.39	3
design_32	6.69	4
design_33	8.55	3
design_34	7.29	3

design_35	6.42	4
design_36	8.92	3
design_37	9.43	3
design_38	9.76	2
design_39	4.70	4
design_40	7.89	3
design_41	8.14	3
design_42	8.06	3
design_43	8.13	3
design_44	9.00	3
design_45	8.79	3
design_46	8.60	3
design_47	6.51	4
design_48	6.99	4
design_49	5.64	4
design_50	5.57	4
design_51	6.23	4
design_52	8.24	3
design_53	9.53	2
design_54	7.09	3
design_55	8.79	3
design_56	7.75	3
design_57	9.30	3
design_58	9.19	3
design_59	8.93	3
design_60	8.40	3
design_61	6.81	4
design_62	9.53	2
design_63	7.52	3
design_64	8.03	3
design_65	6.77	4
design_66	9.13	3
design_67	8.08	3
design_68	9.53	2
design_69	6.73	4
design_70	4.44	4
design_71	9.80	2
design_72	9.45	3
design_73	6.75	4
design_74	6.26	4
design_75	7.90	3
design_76	8.74	3
design_77	7.45	3
design_78	6.95	4
design_79	8.78	3
design_80	7.51	3

design_81	8.59	3
design_82	10.05	2
design_83	9.23	3
design_84	9.56	2
design_85	7.18	3
design_86	7.59	3
design_87	7.36	3
1A2K	10.26	2
1ACB	14.57	2
1AHW	8.98	3
1AK4	12.49	2
1AKJ	9.34	3
1AVX	23.91	1
1AY7	11.67	2
1AZS	5.99	4
1B6C	8.60	3
1BGX	11.66	2
1BJ1	13.56	2
1BKD	14.15	2
1BUH	5.68	4
1BVK	12.78	2
1BVN	10.15	2
1CGI	13.48	2
1D6R	15.29	1
1DE4	8.99	3
1DFJ	7.98	3
1DQJ	13.28	2
1E4K	8.85	3
1E6J	10.35	2
1.00E+96	7.61	3
1EAW	15.91	1
1EER	10.45	2
1EFN	7.84	3
1EWY	9.48	3
1EZU	14.48	2
1F34	11.24	2
1F51	9.52	2
1FAK	7.64	3
1FC2	8.44	3
1FQ1	9.17	3
1FQJ	11.91	2
1FSK	10.44	2
1GCQ	8.21	3
1GHQ	8.47	3
1GLA	8.86	3
1GP2	9.74	2

1GPW	9.40	3
1GRN	14.53	2
1H1V	12.20	2
1HE1	13.52	2
1HE8	7.76	3
1HIA	16.11	1
1I2M	10.65	2
1I4D	9.44	3
1I9R	8.23	3
1IB1	9.55	2
1IBR	10.03	2
1IJK	9.13	3
1IQD	10.68	2
1IRA	9.98	2
1J2J	9.17	3
1JMO	13.23	2
1JPS	8.88	3
1K4C	13.85	2
1K5D	12.26	2
1K74	13.52	2
1KAC	9.43	3
1KKL	13.22	2
1KLU	9.78	2
1KTZ	6.56	4
1KXP	14.68	2
1KXQ	10.52	2
1M10	12.11	2
1MAH	12.09	2
1ML0	9.26	3
1MLC	11.86	2
1N2C	16.53	1
1N8O	14.58	2
1NCA	12.85	2
1NSN	9.40	3
1NW9	9.70	2
1OPH	25.54	1
1PPE	25.24	1
1PXV	15.48	1
1QA9	7.16	3
1QFW	9.86	2
1R0R	16.75	1
1R8S	11.02	2
1RLB	9.06	3
1S1Q	9.66	2
1SBB	9.00	3
1T6B	11.46	2

1UDI 11.75 2
1VFB 13.99 2
1WEJ 7.28 3
1WQ1 11.20 2
1XD3 11.41 2
1XQS 9.70 2
1Y64 8.66 3
1YVB 11.29 2
1Z0K 10.25 2
1Z5Y 9.73 2
1ZHI 10.96 2
2AJF 10.47 2
2B42 12.76 2
2C0L 10.21 2
2CFH 12.15 2
2FD6 6.04 4
2H7V 10.03 2
2HLE 10.83 2
2HMI 9.57 2
2HQS 8.79 3
2HRK 8.79 3
2I25 11.34 2
2JEL 8.23 3
2MTA 6.92 4
2NZ8 13.52 2
2O8V 9.38 3
2OOB 8.70 3
2OT3 9.94 2
2PCC 6.74 4
2QFW 7.09 3
2SIC 15.69 1
2SNI 14.46 2
2UUY 16.97 1
2VIS 15.79 1
7CEI 8.78 3

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Group 33s -
Raw scores are linear combinations of vdW, electrostatic potential,
solvation as well as a knowledge based terms

	Raw score	normalized score
design_1	-6149.89	5
design_2	-6056.9	5
design_3	-7068.63	5
design_4	-6812.61	5
design_5	-5562.09	3

design_6 -5375.61 3
design_7 -8099.27 2
design_8 -5069.54 3
design_9 -7049.64 5
design_10 -7193.2 5
design_11 -6843.25 5
design_12 -7365.21 5
design_13 -5922.59 3
design_14 -4692.49 3
design_15 -5216.05 3
design_16 -8049.22 2
design_17 -6739.93 5
design_18 -7504 2
design_19 -6131.61 5
design_20 -7935.78 2
design_21 -7619.84 2
design_22 -5795.06 3
design_23 -5579.71 3
design_24 -5652.95 3
design_25 -5802.69 3
design_26 -8322.78 2
design_27 -6526.95 5
design_28 -5096.19 3
design_29 -6135.18 5
design_30 -7320.04 5
design_31 -5865.2 3
design_32 -5679.57 3
design_33 -6950.94 5
design_34 -9252.39 2
design_35 -9085.81 2
design_36 -6521.74 5
design_37 -6338.99 5
design_38 -7151.85 5
design_39 -7216.29 5
design_40 -6794.72 5
design_41 -7061.05 5
design_42 -6270.39 5
design_43 -7003.14 5
design_44 -7342.44 5
design_45 -8123.37 2
design_46 -5538.8 3
design_47 -7254.36 5
design_48 -7046.99 5
design_49 -5188.31 3
design_50 -5922.71 3
design_51 -6167.84 5

design_52	-8088.45	2
design_53	-8668.82	2
design_54	-5635.14	3
design_55	-5111.67	3
design_56	-6155.46	5
design_57	-8004.78	2
design_58	-7393.19	5
design_59	-6484.32	5
design_60	-6385.02	5
design_61	-7390.72	5
design_62	-6673.9	5
design_63	-5797.31	3
design_64	-6219.41	5
design_65	-8121.46	2
design_66	-7653.03	2
design_67	-4503.54	3
design_68	-5476.3	3
design_69	-8405.98	2
design_70	-5610.76	3
design_71	-6563.23	5
design_72	-9184.3	2
design_73	-5307.61	3
design_74	-5863.4	3
design_75	-5278.38	3
design_76	-7289.84	5
design_77	-7909.3	2
design_78	-5255.46	3
design_79	-4445.84	3
design_80	-5579.95	3
design_81	-6342.2	5
design_82	-6127.26	5
design_83	-8127.99	2
design_84	-6019.38	5
design_85	-8380.39	2
design_86	-5875	3
design_87	-7346.99	5
1A2K	-16462.2	1
1ACB	-9090.35	2
1AHW	-23307.6	1
1AK4	-5683.02	3
1AKJ	-29101.5	1
1AVX	-10099.4	1
1AY7	-5797.01	3
1AZS	-21551.5	1
1B6C	-8548.57	2
1BGX	-31744.6	1

1BJ1	-34392.7	1
1BKD	-15948.3	1
1BUH	-6253.16	5
1BVK	-13279.7	1
1BVN	-12134.2	1
1CGI	-11684	1
1D6R	-7261.67	5
1DE4	-47252.7	1
1DFJ	-10449.8	1
1DQJ	-22158.9	1
1E4K	-18866.3	1
1E6J	-19608.6	1
1E96	-5590.24	3
1EAW	-9202.65	2
1EER	-16120.2	1
1EFN	-5369.71	3
1EWY	-7023.89	5
1EZU	-26115	1
1F34	-12743.2	1
1F51	-23624.1	1
1FAK	-20907.5	1
1FC2	-5372.28	3
1FQ1	-6733.55	5
1FQJ	-11322	1
1FSK	-25046.1	1
1GCQ	-5183.11	3
1GHQ	-3605.25	3
1GLA	-6906.43	5
1GP2	-31881.9	1
1GPW	-10255.2	1
1GRN	-8944.74	2
1H1V	-8829.6	2
1HE1	-9905.52	1
1HE8	-7092.59	5
1HIA	-34826.4	1
1I2M	-11183.3	1
1I4D	-22456.8	1
1I9R	-45643	1
1IB1	-22751.1	1
1IBR	-14720.4	1
1IJK	-27160.4	1
1IQD	-23429.2	1
1IRA	-13596.2	1
1J2J	-5800.09	3
1JMO	-31112	1
1JPS	-23862.8	1

1K4C	-22614.1	1
1K5D	-35267.6	1
1K74	-21259.5	1
1KAC	-6221.35	5
1KKL	-30623.6	1
1KLU	-27418.3	1
1KTZ	-3980.51	3
1KXP	-12474.6	1
1KXQ	-10066.3	1
1M10	-10560	1
1MAH	-9509.98	1
1ML0	-22721.2	1
1MLC	-21410.2	1
1N2C	-192251	1
1N8O	-37013.3	1
1NCA	-23564.3	1
1NSN	-20025.4	1
1NW9	-9884.29	1
1OPH	-6538.53	5
1PPE	-9453.91	2
1PXV	-10719.9	1
1QA9	-8934.37	2
1QFW	-21564.5	1
1R0R	-8100.49	2
1R8S	-12168.3	1
1RLB	-31765.1	1
1S1Q	-4658.88	3
1SBB	-4900.7	3
1T6B	-8342.11	2
1UDI	-7744.8	2
1VFB	-13119.7	1
1WEJ	-24860.9	1
1WQ1	-12399	1
1XD3	-10266.5	1
1XQS	-12011.3	1
1Y64	-9041.25	2
1YVB	-9032.23	2
1Z0K	-8401.79	2
1Z5Y	-7403.15	5
1ZHI	-5016.17	3
2AJF	-7102.21	5
2B42	-9746.03	1
2C0L	-9415.78	2
2CFH	-11306.7	1
2FD6	-21367.3	1
2H7V	-7013.89	5

2HLE -10336.4 1
2HMI -45606 1
2HQS -11138.4 1
2HRK -5953.38 3
2I25 -5643.07 3
2JEL -21932.1 1
2MTA -19783.9 1
2NZ8 -12770.7 1
2O8V -7675.77 2
2OOB -4266.58 3
2OT3 -12279.9 1
2PCC -6076.02 5
2QFW -20194.1 1
2SIC -8946.57 2
2SNI -9128.92 2
2UUY -8573.8 2
2VIS -21264.7 1
7CEI -6743.58 5
****

Group 35s-

To discriminate between the native protein-protein interfaces and the designed ones, we chose to use a set of four metrics that can be computed from the structures: predicted binding energy per interface area, number of unsatisfied hydrogen bonds per interface area, ratio of hydrogen bond energy to total binding energy and the RosettaHoles score. All designed and native structures used in this analysis were repacked and minimized using the Rosetta energy function.

The predicted binding energy was calculated by taking the difference in energy between the structure of the complex and the separated binding partners. The area of the interface was computed in the same manner. The first metric, dG/dSASA, was obtained by dividing the binding energy by the area of the interface. The second metric, Unsat/dSASA, is the number of buried-unsatisfied polar atoms located at the interface divided by the area of the interface. The third metric, HBond energy/dG, is the proportion of hydrogen bond energy to the total binding energy.

A normal distribution was fit to each of the described metrics for native structures with resolution better than or equal to 2.2 angstroms. The corresponding cumulative distribution function for each metric was used to represent a score for how well a structure compares to natives. For each metric a score of 1.0 represents an above average comparison to natives while a score of 0.0 represents no correspondence to natives.

The final metric is the RosettaHoles score. The RosettaHoles score represents the probability that a set of solvent inaccessible voids comes

from a high-resolution crystal structure. Voids are determined by finding the largest spherical hole adjacent to all buried atoms, pruning away solvent accessible regions, and then clustering the holes into contiguous cavities. The scores for this metric are similar to the previous three, with 1.0 being ideal and 0.0 being completely unlike native proteins.

The scores for each of the four metrics for all native and designed structures were summed to yield the final raw score. This score ranged between 0.0 and 4.0 with 0.0 being no correspondence to native interfaces (does not bind) and 4.0 being as good as or better than native interfaces (binds). The normalized scores are as follows where RS represents the raw score: 4 (does not bind) for RS <1.5; 3 (likely not to bind) for 1.5<RS<2.0; 2 (likely to bind) for 2.0<RS<2.5; 1 (binds) for RS>2.5.

Some native structures were not evaluated due to problems obtaining a suitable minimized structure.
REMARK KuhlmanGroup scores for CAPRI round 21
REMARK Method described in KuhlmanMethod.txt
Raw scores are the sum of three cumulative distribution functions and the RosettaHoles score.
The raw score ranges from 0.0-4.0 with a higher score being more likely to bind.

MODEL	Raw_score	Normalized_score
design_1	1.74	3
design_2	0.97	4
design_3	1.54	3
design_4	1.50	3
design_5	0.81	4
design_6	1.08	4
design_7	1.17	4
design_8	1.58	3
design_9	1.42	4
design_10	1.43	4
design_11	1.28	4
design_12	1.31	4
design_13	1.66	3
design_14	1.30	4
design_15	0.98	4
design_16	1.40	4
design_17	1.33	4
design_18	1.05	4
design_19	0.93	4
design_20	1.50	3
design_21	1.44	4
design_22	1.92	3

design_23	1.29	4
design_24	1.58	3
design_25	1.80	3
design_26	2.07	2
design_27	1.56	3
design_28	0.66	4
design_29	1.63	3
design_30	1.52	3
design_31	0.74	4
design_32	1.23	4
design_33	1.54	3
design_34	1.16	4
design_35	1.48	4
design_36	1.04	4
design_37	1.56	3
design_38	1.82	3
design_39	1.30	4
design_40	1.19	4
design_41	1.12	4
design_42	0.95	4
design_43	1.52	3
design_44	0.72	4
design_45	1.19	4
design_46	0.92	4
design_47	1.60	3
design_48	1.01	4
design_49	1.70	3
design_50	1.82	3
design_51	1.11	4
design_52	1.15	4
design_53	1.41	4
design_54	1.48	4
design_55	1.67	3
design_56	1.02	4
design_57	1.17	4
design_58	0.97	4
design_59	1.18	4
design_60	1.12	4
design_61	1.62	3
design_62	1.68	3
design_63	1.22	4
design_64	1.17	4
design_65	1.31	4
design_66	1.36	4
design_67	1.13	4
design_68	1.12	4

design_69	1.47	4
design_70	1.12	4
design_71	0.98	4
design_72	0.82	4
design_73	1.47	4
design_74	1.86	3
design_75	1.51	3
design_76	0.86	4
design_77	0.97	4
design_78	0.96	4
design_79	1.54	3
design_80	1.79	3
design_81	0.84	4
design_82	1.52	3
design_83	1.64	3
design_84	1.76	3
design_85	0.91	4
design_86	0.78	4
design_87	1.53	3
1A2K	1.95	3
1ACB	1.58	3
1AHW	2.40	2
1AK4	2.01	2
1AKJ	2.83	1
1AVX	1.59	3
1AY7	2.86	1
1AZS	1.26	4
1B6C	1.42	4
1BGX	0.71	4
1BJ1	2.54	1
1BKD	2.18	2
1BUH	1.43	4
1BVK	2.94	1
1BVN	2.10	2
1CGI	1.47	4
1D6R	2.42	2
1DE4	1.75	3
1DFJ	1.66	3
1DQJ	2.21	2
1E4K	0.88	4
1E6J	2.12	2
1E96	1.35	4
1EAW	2.58	1
1EER	2.79	1
1EFN	2.02	2
1EWY	nd	5

1EZU	2.08	2
1F34	1.22	4
1F51	1.44	4
1FAK	2.55	1
1FC2	1.09	4
1FQ1	1.85	3
1FQJ	2.79	1
1FSK	1.91	3
1GCQ	1.63	3
1GHQ	1.40	4
1GLA	1.50	3
1GP2	1.60	3
1GPW	1.53	3
1GRN	2.03	2
1H1V	2.08	2
1HE1	1.76	3
1HE8	2.45	2
1HIA	2.21	2
1I2M	2.70	1
1I4D	1.34	4
1I9R	1.47	4
1IB1	2.40	2
1IBR	2.10	2
1IJK	2.08	2
1IQD	2.78	1
1IRA	1.91	3
1J2J	1.20	4
1JMO	2.49	2
1JPS	3.33	1
1K4C	2.48	2
1K5D	1.08	4
1K74	1.79	3
1KAC	1.84	3
1KKL	1.61	3
1KLU	1.97	3
1KTZ	2.87	1
1KXP	1.83	3
1KXQ	1.68	3
1M10	2.16	2
1MAH	1.40	4
1ML0	2.12	2
1MLC	1.93	3
1N2C	1.55	3
1N8O	2.03	2
1NCA	2.01	2
1NSN	2.19	2

1NW9	2.22	2
1OPH	1.91	3
1PPE	2.22	2
1PXV	2.31	2
1QA9	2.89	1
1QFW	2.37	2
1R0R	2.84	1
1R8S	1.74	3
1RLB	1.04	4
1S1Q	2.19	2
1SBB	2.25	2
1T6B	1.80	3
1UDI	2.04	2
1VFB	3.14	1
1WEJ	2.46	2
1WQ1	0.84	4
1XD3	2.16	2
1XQS	1.83	3
1Y64	nd	5
1YVB	0.74	4
1Z0K	2.66	1
1Z5Y	2.11	2
1ZHI	2.15	2
2AJF	1.64	3
2B42	1.42	4
2C0L	1.90	3
2CFH	1.55	3
2FD6	2.98	1
2H7V	1.78	3
2HLE	2.54	1
2HQS	2.10	2
2HRK	0.75	4
2I25	2.36	2
2JEL	2.89	1
2MTA	0.96	4
2NZ8	1.82	3
2O8V	nd	5
2OOB	1.93	3
2OT3	nd	5
2PCC	2.31	2
2QFW	1.97	3
2SIC	1.54	3
2SNI	1.84	3
2UUY	2.32	2
2VIS	1.91	3
7CEI	2.34	2

****
Group 36s-
ITScore/PP [1] was used to evaluate the 87 designed complex models from the Baker lab and 120 native complexes of T45. ITScore/PP is an all-atomic distance-dependent knowledge-based scoring function derived by a new iterative method that circumvents the long-standing reference state problem in the knowledge-based/statistical approaches. The basic idea of the method is to improve a set of effective pair potentials by iteration until the derived potentials can reproduce the atomic pair distribution functions in experimentally determined complex structures [2,3]. In addition to circumventing the reference state problem by iteration, another major advantage of ITScore/PP is that it considers the binding energy landscape of the complexes by including both the native structures and decoys according to a Boltzmann probability, instead of considering only the energy minima (i.e., native structures) like what conventional knowledge-based scoring functions do [4]. ITScore/PP was derived on the basis of 20 heavy atom types and 851 biological protein-protein complex structures [1].

ITScore/PP has been extensively validated with diverse benchmarks [1] and the recent CAPRI experiments [5] for its ability in binding mode prediction. However, further improvements are still needed for ITScore/PP in future studies, particularly for the purpose of discriminating binders from non-binders (like the CAPRI experiments in round 20 and 21). First, current ITScore/PP consists of only the inter-molecular interaction potentials. In order to better evaluate computationally designed models, it will be necessary for ITScore/PP to include intra-molecular interaction energy terms such as the torsional energies from side-chains and backbones. Second, entropy is currently ignored in ITScore/PP and needs to be included [6].

[1] Huang S-Y, Zou X. An iterative knowledge-based scoring function for protein-protein recognition. Proteins 2008;72:557-579.

[2] Huang S-Y, Zou X. An iterative knowledge-based scoring function to predict protein-ligand interactions: I. Derivation of interaction potentials. J Comput Chem 2006;27:1865-1875.

[3] Huang S-Y, Zou X. An iterative knowledge-based scoring function to predict protein-ligand interactions: II. Validation of the scoring function. J Comput Chem 2006;27:1876-1882.

[4] Huang S-Y, Zou X. Mean-force scoring functions for protein-ligand binding. Annu Rep Comput Chem 2010;6:281-296.(in press)

[5] Huang S-Y, Zou X. MDockPP: A hierarchical approach for protein-protein docking and its application to CAPRI rounds 15-19. 2010, DOI: 10.1002/prot.22797.

[6] Huang S-Y, Zou X. Inclusion of solvation and entropy in the knowledge-based scoring function for protein-ligand interactions. J Chem Inf Model 2010;50:262-273.

Raw scores are given in units of knowledge-based potentials that are not scaled to the experimental affinity data.

	Raw score	normalized score
design_1	-145.302	4
design_2	-139.746	4
design_3	-226.956	1
design_4	-120.767	4
design_5	-137.660	4
design_6	-161.184	3
design_7	-174.954	3
design_8	-172.194	3
design_9	-131.343	4
design_10	-141.188	4
design_11	-129.587	4
design_12	-180.953	5
design_13	-153.922	3
design_14	-160.362	3
design_15	-182.927	5
design_16	-184.665	5
design_17	-155.229	3
design_18	-156.503	3
design_19	-191.344	5
design_20	-260.669	1
design_21	-154.823	3
design_22	-178.583	5
design_23	-173.932	3
design_24	-188.239	5
design_25	-131.907	4
design_26	-158.362	3
design_27	-154.079	3
design_28	-161.448	3
design_29	-183.792	5
design_30	-224.418	2
design_31	-131.271	4
design_32	-118.529	4
design_33	-214.338	2
design_34	-213.088	2
design_35	-215.810	2

design_36	-147.137	4
design_37	-182.173	5
design_38	-218.510	2
design_39	-137.108	4
design_40	-152.208	3
design_41	-160.137	3
design_42	-160.590	3
design_43	-180.443	5
design_44	-204.018	2
design_45	-191.022	5
design_46	-138.927	4
design_47	-161.761	3
design_48	-165.333	3
design_49	-163.911	3
design_50	-172.478	3
design_51	-203.662	2
design_52	-198.505	5
design_53	-172.758	3
design_54	-149.281	4
design_55	-161.674	3
design_56	-150.012	3
design_57	-207.741	2
design_58	-171.397	3
design_59	-172.007	3
design_60	-142.899	4
design_61	-193.489	5
design_62	-191.447	5
design_63	-187.762	5
design_64	-123.810	4
design_65	-151.448	3
design_66	-170.220	3
design_67	-157.723	3
design_68	-137.584	4
design_69	-170.724	3
design_70	-146.584	4
design_71	-203.157	2
design_72	-178.247	5
design_73	-137.232	4
design_74	-132.643	4
design_75	-148.768	4
design_76	-200.476	2
design_77	-183.426	5
design_78	-133.858	4
design_79	-129.782	4
design_80	-135.108	4
design_81	-195.870	5

design_82	-181.330	5
design_83	-260.885	1
design_84	-199.564	5
design_85	-191.827	5
design_86	-128.349	4
design_87	-179.371	5
1A2K	-222.155	2
1ACB	-220.671	2
1AHW	-235.828	1
1AK4	-139.462	4
1AKJ	-203.935	2
1AVX	-290.994	1
1AY7	-199.636	5
1AZS	-253.324	1
1B6C	-210.181	2
1BGX	-627.896	1
1BJ1	-328.285	1
1BKD	-387.047	1
1BUH	-171.780	3
1BVK	-163.737	3
1BVN	-299.563	1
1CGI	-303.881	1
1D6R	-163.184	3
1DE4	-279.442	1
1DFJ	-238.882	1
1DQJ	-239.573	1
1E4K	-135.847	4
1E6J	-151.741	3
1E96	-170.931	3
1EAW	-260.874	1
1EER	-478.606	1
1EFN	-192.374	5
1EWY	-114.048	4
1EZU	-356.185	1
1F34	-343.051	1
1F51	-217.358	2
1FAK	-336.361	1
1FC2	-166.494	3
1FQ1	-153.896	3
1FQJ	-213.775	2
1FSK	-262.823	1
1GCQ	-173.798	3
1GHQ	-65.460	4
1GLA	-149.922	4
1GP2	-282.372	1
1GPW	-247.649	1

1GRN	-255.811	1
1H1V	-179.161	5
1HE1	-269.257	1
1HE8	-154.571	3
1HIA	-248.208	1
1I2M	-423.682	1
1I4D	-177.368	5
1I9R	-156.891	3
1IB1	-297.654	1
1IBR	-436.202	1
1IJK	-218.550	2
1IQD	-337.312	1
1IRA	-334.964	1
1J2J	-140.879	4
1JMO	-497.300	1
1JPS	-270.273	1
1K4C	-291.518	1
1K5D	-308.468	1
1K74	-193.584	5
1KAC	-148.475	4
1KKL	-168.281	3
1KLU	-183.488	5
1KTZ	-147.794	4
1KXP	-366.884	1
1KXQ	-278.268	1
1M10	-230.067	1
1MAH	-240.411	1
1ML0	-285.507	1
1MLC	-218.818	2
1N2C	-487.419	1
1N8O	-260.992	1
1NCA	-228.299	1
1NSN	-166.140	3
1NW9	-289.895	1
1OPH	-228.973	1
1PPE	-286.507	1
1PXV	-326.183	1
1QA9	-155.771	3
1QFW	-184.418	5
1R0R	-220.131	2
1R8S	-374.606	1
1RLB	-118.714	4
1S1Q	-128.508	4
1SBB	-127.819	4
1T6B	-192.473	5
1UDI	-211.140	2

1VFB -185.018 5
1WEJ -224.914 2
1WQ1 -303.424 1
1XD3 -314.161 1
1XQS -322.157 1
1Y64 -141.019 4
1YVB -196.599 5
1Z0K -248.840 1
1Z5Y -196.354 5
1ZHI -159.094 3
2AJF -158.559 3
2B42 -331.869 1
2C0L -225.499 1
2CFH -344.390 1
2FD6 -172.843 3
2H7V -191.404 5
2HLE -270.510 1
2HMI -132.249 4
2HQS -272.134 1
2HRK -152.068 3
2I25 -253.316 1
2JEL -192.712 5
2MTA -110.883 4
2NZ8 -318.314 1
2O8V -218.270 2
2OOB -90.480 4
2OT3 -340.345 1
2PCC -92.675 4
2QFW -177.254 5
2SIC -223.171 2
2SNI -224.962 2
2UUY -235.849 1
2VIS -136.422 4
7CEI -222.426 2
****
::::::::::::::
The data used to produce Fig. 3
data/two_best_discriminators.txt
::::::::::::::
Ôø°
Group 06 -
"Here are all the raw scores used in for generating the final predicted delta G score.",,,,,,,,,,
"Normalised scores given previously correspond to converting these into z-scores for the complexes for which we found an empirical binding free energy, then finding the modulus of the normalised weighting.",,,,,,,,,,

,,,,,,,,,,,
"Name ","SD_top_ranked_under_5Armds? ","SD_biggest_cluster? ","NIP ","NSC
","fine_pair_potential ","coarse_pair_potential ","BS_association
","GBSW_solvation ","all_vdw ","ACE_self ","Weights for raw scores:"
"1A2K ",0,1,0,0,-4.44,-4.57,78.1,-28.33,-38.51,699.41,"- 0.494 *
SD_top_ranked_under_5Armds?"
"1ACB ",0,0,0,0,-4.46,7.44,16.3,-28.84,-30.66,571.2,"- 0.060 *
SD_biggest_cluster?"
"1AHW ",0,1,0,0,-13.29,-18.07,53.2,-31.9,-40.72,1222.25,"- 0.184 *
fine_pair_potential"
"1AK4 ",0,0,0,0,-0.02,-4.15,54.9,-18.03,-25.39,328.53,"- 0.036 *
coarse_pair_potential"
"1AKJ ",0,1,0,0,-10.54,-18.75,38.9,-24.2,-34.26,978.68,"- 0.032 * all_vdw"
"1AVX ",0,1,0,0,-5.78,-15.79,26.7,-32.4,-43.76,915.41,"- 0.002 *
BS_association"
"1AY7 ",0,1,0,0,-3.79,-3.95,47,-21.95,-38.04,699.07,"+ 4208.615 * NIP"
"1B6C ",1,1,0,0,-3.4,-3.14,93.4,-30.32,-41.64,703.25,"- 3196.587 * NSC"
"1BGX ",1,0,0,0,-21.97,-25.53,26.8,-91.53,-112.52,2542.48,"- 0.007 *
ACE_self"
"1BJ1 ",0,1,0,0,-2.73,-4.12,40.5,-36.77,-61.96,763.09,"- 0.018 *
GBSW_solvation"
"1BUH ",0,1,0,0,-4.87,-5.62,41.5,-21.32,-29.74,577.94,
"1BVK ",0,1,0,0,-4.28,-10.56,67.9,-18.01,-28.63,660.95,
"1BVN ",1,0,0,0,-3.6,5.66,14.4,-33.06,28.66,808.73,
"1CGI ",1,1,0,0,-3.54,-0.2,8.8,-41.35,-50.98,864.26,
"1D6R ",0,0,0,0,-3.63,-10.27,16.7,-22.27,-31.74,697.17,
"1DE4 ",0,1,0,0,-7.6,-13.24,119.2,-36.48,-38.34,829.9,
"1DFJ ",1,1,0,0,-15.48,-35.92,51.7,-26.66,-2.1,1161.94,
"1DQJ ",0,1,0,0,-4.15,-19.63,91.2,-29.77,-48.5,1005.1,
"1E4K ",0,0,0,0,-8.2,-6.28,79.5,-18.63,-15.69,506.78,
"1E6J ",0,1,0,0,-1.88,-2.98,40.4,-24.11,-26,517.73,
1.00E+096,0,0,0,0,-4.94,-1.36,66.6,-23.63,-28.74,587.41,
"1EAW ",0,1,0,0,-5.02,-3.02,31,-36.36,-38.91,964.42,
"1EER ",1,1,0,0,-22.5,-17.78,29.4,-57.08,-57.24,1772.36,
"1EFN ",0,0,0,0,-3.9,-12.45,36.8,-20.51,-28.44,561.02,
"1EWY ",0,0,0,0,-8.52,-11.2,52.3,-15.27,-20.56,696.31,
"1EZU ",1,0,0,0,-7.63,-8.79,15.5,-44.88,-63.79,1069.66,
"1F34 ",1,1,0,0,-7.69,-4.83,4.3,-47.53,-63.28,1283.46,
"1FC2 ",0,1,0,0,-5.35,-4.09,75.9,-21.04,-26.12,475.21,
"1GCQ ",1,1,0,0,-0.46,-1.2,9.8,-21.57,-31.42,480.33,
"1GHQ ",0,0,0,0,-1.91,-2.31,39.8,-11.04,-14.79,301.28,
"1GLA ",0,1,0,0,-5.02,4.79,144.5,-18.71,-21.81,466.2,
"1GPW ",1,1,0,0,-6.48,-11.83,55.9,-30.51,-44.99,1070.2,
"1GRN ",1,1,0,0,-10.44,-20.2,42.9,-36.39,-48.32,1052.36,
"1HE8 ",0,0,0,0,-9.2,-13.59,169.2,-20.81,-25.06,570.55,
"1HIA ",1,1,0,0,-3.18,-2.1,16.6,-31.1,-45.74,784.04,

"1I2M ",1,1,0,0,-15.49,-30.72,81.1,-42.45,-65.49,1674.68,
"1I4D ",0,1,0,0,-5.75,-4.11,25.8,-27.74,-31.83,616.15,
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"1IJK ",0,1,0,0,-10.84,-15.16,41.6,-25.62,-30.45,756.35,
"1IQD ",0,1,0,0,-8.39,-5.7,45.6,-37.98,-53.6,993.03,
"1IRA ",1,1,0,0,-6.23,-6.38,3.2,-43.47,-60.52,1314.86,
"1J2J ",0,1,0,0,-4.31,-1.06,17.9,-20.69,-22.84,322.13,
"1JPS ",0,1,0,0,-8.4,-17.22,45.2,-34.6,-48.1,1217.18,
"1K5D ",1,1,0,0,-13.39,-30.22,39.3,-45.55,-50.29,1426.55,
"1KAC ",0,1,0,0,-4.6,-13.96,39.9,-22.05,-25.43,699.96,
"1KKL ",0,1,0,0,-3.91,-1.18,97.3,-32.8,-27.46,788.52,
"1KLU ",0,0,0,0,-4.11,-9.45,138.7,-21.16,-30.41,604.17,
"1KTZ ",0,1,0,0,-3.07,-7.07,16.7,-17,-22.66,409.6,
"1KXP ",1,1,0,0,-14.74,-17.32,22,-52.45,-60.02,1463.78,
"1KXQ ",0,1,0,0,-6.51,-14.4,75.1,-34.67,-47.42,821.79,
"1M10 ",0,1,0,0,-16.9,-21.39,90.4,-28.51,-41.13,1158.72,
"1MAH ",1,1,0,0,-2.55,-1.44,70.2,-31.39,-40.74,695.75,
"1ML0 ",1,1,0,0,-9.2,-10.03,150,-36.04,-47.24,885.57,
"1MLC ",0,1,0,0,-4.86,-16.36,67.7,-23.3,11.5,741.36,
"1N8O ",1,1,0,0,-3.78,2.68,23.9,-36.03,-51.8,774.66,
"1NCA ",0,1,0,0,-7.23,-16.25,64.9,-29.63,-43.21,863.09,
"1OPH ",0,0,0,0,-1.41,2.93,64.3,-27.97,-27.67,639.98,
"1PPE ",1,1,0,0,-0.36,0.5,5.2,-33.53,-45.52,819.55,
"1PXV ",1,1,0,0,-9.48,-7.85,19.4,-44.3,-67.38,1163.03,
"1QA9 ",0,1,0,0,-17.83,-29.92,109.9,-15.57,-23.29,841.92,
"1QFW ",0,0,0,0,-4.02,-8.82,22.9,-21.59,-27.94,739.99,
"1R0R ",0,0,0,0,-2.01,-2.95,19.9,-29.04,-41.06,626.4,
"1R8S ",1,1,0,0,-9.91,-16.53,21.7,-51.29,-64.03,1043.63,
"1RLB ",0,0,0,0,-4.49,-1.19,69.3,-17.87,-22.34,484.09,
"1S1Q ",0,0,0,0,-3.86,4.33,25.9,-19.22,-28.15,478.36,
"1SBB ",0,0,0,0,-4.17,-10.74,59.3,-15.86,-22.45,470.85,
"1T6B ",1,1,0,0,-6.43,-11.61,110.1,-27.98,-36.4,862.33,
"1VFB ",0,1,0,0,-3.49,-9.49,41.2,-20.43,-36.41,770.36,
"1WEJ ",0,1,0,0,-8.09,-12.76,184.2,-23.58,-36.44,927.12,
"1WQ1 ",1,1,0,0,-7.9,-21.38,19.4,-42.35,-56.65,1443.34,
"1XD3 ",1,1,0,0,-8.27,-9.47,24.7,-43.66,-57.97,1031.61,
"1XQS ",1,1,0,0,-21.05,-25.84,48,-36.89,-55,1497.47,
"1Y64 ",0,1,0,0,-9.48,-17.28,2.4,-24.17,-22.36,763.17,
"1Z0K ",1,1,0,0,-3.79,1.43,17.4,-30.72,-39.46,865.46,
"1ZHI ",0,0,0,0,-6.66,-1.17,87.9,-18.9,-28.11,566.85,
"2AJF ",0,1,0,0,-8.45,-11.35,70.6,-19,-29.07,611.08,
"2B42 ",1,1,0,0,-4.57,-24.18,10,-38.73,-59.11,1220.68,
"2C0L ",0,0,0,0,-6.06,-3.44,69.3,-34.91,-42.02,826.88,
"2FD6 ",0,0,0,0,-1.06,-11.9,106.6,-18.04,-32.73,503.96,
"2HLE ",0,1,0,0,-7.72,-6.93,19.9,-36.29,-48.98,1126.75,
"2HQS ",1,1,0,0,-7.9,-9.12,12.4,-37.05,-50.15,1146.82,

"2HRK ",0,1,0,0,-2.26,1.44,18.7,-25.72,-29.15,504.04,
"2I25 ",0,0,0,0,-12.3,-5.38,26.9,-27.44,-45.74,867.76,
"2JEL ",0,0,0,0,-4.12,-13.41,75.9,-25.25,-34.72,807.92,
"2MTA ",0,1,0,0,-3.07,1.5,89.7,-17.79,-21.38,380.44,
"2O8V ",0,1,0,0,-1.92,-5.49,76,-28.6,-37.63,576.42,
"2OOB ",0,0,0,0,-0.83,5.05,5.2,-16.88,-20.46,241.1,
"2OT3 ",0,1,0,0,-3.07,1.76,16.3,-46.35,-53.89,992.21,
"2PCC ",0,0,0,0,-8.55,-11.57,140.7,-14.53,-14.93,532.09,
"2QFW ",0,0,0,0,-2.67,-7.38,27.3,-17.63,-25.28,567.69,
"2SIC ",0,0,0,0,-1.72,-5.43,29.4,-28.81,-35.19,619.38,
"2SNI ",0,0,0,0,-3.73,-0.09,30.9,-31.21,-43.55,691.24,
"2UUY ",0,0,0,0,-1.2,-3.39,16.8,-30.34,-44.68,839.23,
"2VIS ",0,0,0,0,-1.56,-3.97,35,-20.16,-24.15,473.94,
"7CEI ",1,1,0,0,-10.75,-18.8,128.8,-24.7,-36.51,971.61,
"1AZS ",0,1,0,0,-9.01,-4.2,41.7,-28.41,-42.24,592.87,
"1BKD ",1,1,0,0,-16.09,-25.57,26.5,-49.38,-64.04,1360.91,
"1F51 ",1,1,0,0,-10.23,-0.82,43.7,-35.39,-36.49,927.6,
"1FAK ",1,0,0,0,-20.89,-15.8,35.1,-41.86,-53.96,1451.39,
"1FQ1 ",0,1,0,0,-8.81,-18.07,74.7,-21.37,-27.27,666.75,
"1FQJ ",0,0,0,0,-13.15,-14,39.4,-30.57,-28.17,1121.79,
"1FSK ",0,1,0,0,-7.08,-11.93,96.2,-27.42,-48.73,913.17,
"1GP2 ",1,1,0,0,-13.56,-16.72,75.4,-34.25,-45.11,1012.08,
"1H1V ",0,1,0,0,-4.6,-10.28,103.6,-32.35,-37.03,739.1,
"1HE1 ",1,1,0,0,-4.6,-8.88,19.4,-36.72,-48.25,951.11,
"1I9R ",0,0,0,0,-5.52,-9.67,86.4,-21.95,-27.12,734.98,
"1IB1 ",0,0,0,0,-19.48,-3.13,17.7,-45.09,-54.2,1273.22,
"1JMO ",1,1,0,0,-10.56,-26.44,35.1,-60.55,-81.32,1494.69,
"1K4C ",0,0,0,0,-3.58,-7.42,35.5,-28,-46.91,763.61,
"1K74 ",1,1,0,0,-13.98,-16.92,85.1,-31.8,-18.57,1022.8,
"1N2C ",1,1,0,0,-24.12,-22.94,63.8,-60.48,24.46,1140.59,
"1NSN ",0,1,0,0,-9.85,-12.16,74.6,-24.74,-13.68,832.35,
"1NW9 ",1,1,0,0,-5.32,1.41,34,-37.5,-53.6,750.42,
"1UDI ",1,1,0,0,-6.07,-3.98,33.8,-31.34,-36.99,719.52,
"1YVB ",0,1,0,0,-2.73,5.56,23.2,-26.27,-31.55,556.82,
"1Z5Y ",0,1,0,0,-4.24,-9.55,24.6,-20.12,-18.28,535.31,
"2CFH ",1,1,0,0,-11.06,-7.38,61.9,-50.65,-50.13,1009.81,
"2H7V ",0,1,0,0,-4,-6.38,20.7,-24.89,-29.95,624.82,
"2HMI ",0,1,0,0,-0.86,-4.22,179.6,-16.03,-17.86,301.14,
"2NZ8 ",1,1,0,0,-5.4,-9.07,18.2,-43.46,-52.44,1129.48,
"1D01 ",0,0,0,0,-3.89,-1.7,8.4,-18.31,-26.17,441.35,
"1D02 ",0,0,0,0,-6.35,-5.57,44.6,-17.79,-20.93,450.95,
"1D03 ",0,0,0,0,-4.69,-8.75,29.2,-25.53,-41.84,687.06,
"1D04 ",0,1,0,0,-6.36,-2.67,18.6,-18.12,-19.88,500.02,
"1D05 ",0,0,0,0,-4.81,-2.73,11.2,-19.18,39.84,452.84,
"1D06 ",0,0,0,0,-6.76,-1.9,53.6,-20.71,-28.46,480.64,
"1D07 ",0,0,0,0,-11.37,-10.42,10.8,-21.19,-28.86,625.39,

"1D08 ",0,0,0,0,-2.04,0.81,15.5,-22.11,-24.6,460.38,
"1D09 ",0,0,0,0,-4.76,-2.1,14,-16.54,-22.77,351.5,
"1D10 ",0,1,0,0,-4.03,-2.73,16.3,-18.11,-23.58,345.23,
"1D11 ",0,0,0,0,-7.89,-1.87,13.5,-16.42,-23.6,462.01,
"1D12 ",0,1,0,0,-3.38,-5.33,40.4,-26.15,-32.01,509.82,
"1D13 ",0,0,0,0,-4.82,-7.61,24.6,-17.97,-27.82,541.67,
"1D14 ",0,0,0,0,-0.31,-0.81,14.4,-17.17,-20.52,302.22,
"1D15 ",0,1,0,0,-4.15,-0.07,21.8,-20.94,-25.94,558.59,
"1D16 ",0,0,0,0,-4.84,-5.13,39.6,-21.35,-31.54,533.69,
"1D17 ",0,0,0,0,-5.93,-5.26,39,-17.26,-28.2,428.32,
"1D18 ",0,0,0,0,-8.29,-0.3,35.1,-16.65,-25.89,483.61,
"1D19 ",0,0,0,0,-4,-2.74,55.4,-24.08,-24.37,558.37,
"1D20 ",0,1,0,0,-10.65,0.68,37,-33.04,-27.29,759.61,
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"1D22 ",0,0,0,0,-3.06,-2.46,24,-21.02,-23.05,441.62,
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"1D29 ",0,0,0,0,-7.18,-4.08,30.9,-21.72,-28.35,558.53,
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"1D33 ",0,1,0,0,-4.16,-1.87,35.7,-26.97,-36.36,560.67,
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"1D35 ",0,1,0,0,-5.93,-9.25,25,-23.36,-38.25,587.62,
"1D36 ",0,0,0,0,-3.12,-8.6,21.5,-21.26,-25.14,432.04,
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"1D38 ",1,0,0,0,-6.65,-1.6,49.4,-27.61,-30.96,538.58,
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"1D42 ",0,0,0,0,-7.46,-2.6,33.1,-21.63,-23.95,503.98,
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"1D45 ",0,1,0,0,-4.6,-0.52,13.5,-25.45,-34.14,517.22,
"1D46 ",0,0,0,0,-4.17,-1.55,18.3,-14.78,-26.49,409.62,
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"1D50 ",0,0,0,0,-5.42,-1.05,52.2,-21.17,-26.41,429.58,
"1D51 ",0,0,0,0,-1.62,0.89,110.4,-18.28,-28.64,434.61,
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"1D56 ",0,0,0,0,-3.03,-0.12,29.4,-20.13,-27.74,406.46,
"1D57 ",0,0,0,0,-5.98,-7.89,53.7,-22.8,-32.03,646.11,
"1D58 ",0,0,0,0,-5.13,-5.89,24.3,-25.21,-29.87,529.65,
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"1D60 ",0,0,0,0,-2.91,-3.55,17.8,-15.86,-23.88,377.5,
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"1D62 ",0,1,0,0,-4.33,1.15,20.2,-23.27,-32.63,512.87,
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"1D64 ",0,0,0,0,-4.64,1.26,21.8,-16.45,-21.26,373.06,
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"1D66 ",0,0,0,0,-5.2,3.13,22.7,-22.45,-25.02,367.63,
"1D67 ",0,0,0,0,-5.56,-6.09,16.7,-20.9,-28.66,512.54,
"1D68 ",0,1,0,0,-4.08,4.32,45.5,-21.13,-22.11,474.73,
"1D69 ",0,0,0,0,-9.65,-3.89,21.4,-21.26,-24.51,496.87,
"1D70 ",0,0,0,0,-2.47,-5.12,16,-19.2,-28.76,442.03,
"1D71 ",0,1,0,0,-3.69,-1.75,18.3,-25.49,-24.6,519.2,
"1D72 ",0,0,0,0,-9.8,-5.25,16,-24.67,-34.44,675.61,
"1D73 ",0,0,0,0,-3.66,-2.77,37.7,-14.9,-23.76,392.77,
"1D74 ",0,0,0,0,-2.84,-2.72,28.1,-14.12,-23.95,310.24,
"1D75 ",0,0,0,0,-1.11,2.59,21.9,-17.92,-22.98,405.59,
"1D76 ",0,0,0,0,-7.39,-5.96,32.1,-27.23,-32.6,623.33,
"1D77 ",0,0,0,0,-7.42,-1.62,7.2,-22.56,-29.54,574.91,
"1D78 ",0,0,0,0,-2.92,1.31,24.6,-16.44,-24.99,362.38,
"1D79 ",0,0,0,0,-6.41,-9.7,26.5,-15.8,-21.23,449.62,
"1D80 ",0,0,0,0,-3.48,-10.96,24.9,-16.6,-23.94,365.2,
"1D81 ",0,0,0,0,-7.58,-9.9,29.03,-23.47,-33.95,633.08,
"1D82 ",0,1,0,0,-3.16,2.56,29.03,-27,-30.79,503.43,
"1D83 ",0,1,0,0,-6.38,1.43,29.03,-31.77,-40.44,603.27,
"1D84 ",0,0,0,0,-5.77,-0.99,29.03,-24.27,-25.35,590.93,
"1D85 ",0,0,0,0,-6.07,-0.23,29.03,-21.49,-30.82,457.79,
"1D86 ",0,0,0,0,-3.27,-4.61,29.03,-16.82,-21.88,335.66,
"1D87 ",0,0,0,0,-4.27,-0.27,29.03,-21.16,-29.74,436.4,

REMARK Top two descriminators for group 6, Iain H. Moal, Xiaofan Li and Paul A. Bates.

Units for ACE_self: kcal/mol
Units for Rosetta_fine: REU

Ace_self	Rosetta_fine	
design_1	441.35221	-3.890000
design_2	450.95477	-6.351000
design_3	687.06172	-4.689000
design_4	500.02184	-6.364000

design_5	452.84427	-4.810000
design_6	480.63589	-6.762000
design_7	625.39191	-11.370000
design_8	460.37543	-2.035000
design_9	351.49874	-4.763000
design_10	345.23206	-4.033000
design_11	462.00974	-7.889000
design_12	509.81702	-3.377000
design_13	541.66852	-4.824000
design_14	302.21809	-0.306000
design_15	558.58957	-4.154000
design_16	533.68756	-4.838000
design_17	428.32468	-5.930000
design_18	483.6136	-8.293000
design_19	558.36724	-3.995000
design_20	759.61015	-10.646000
design_21	378.1947	-4.290000
design_22	441.61667	-3.061000
design_23	364.08877	-3.402000
design_24	580.22214	-5.148000
design_25	388.82013	-7.116000
design_26	476.16206	-9.753000
design_27	432.12012	-4.237000
design_28	456.86103	-3.551000
design_29	558.52622	-7.176000
design_30	572.58354	-6.403000
design_31	396.08788	-1.463000
design_32	274.01709	-1.739000
design_33	560.66567	-4.161000
design_34	555.81453	-3.830000
design_35	587.6179	-5.931000
design_36	432.04206	-3.120000
design_37	539.79162	-3.355000
design_38	538.57983	-6.649000
design_39	403.63856	-4.297000
design_40	473.19782	-3.690000
design_41	414.74018	-5.582000
design_42	503.97733	-7.457000
design_43	466.08804	-7.665000
design_44	535.05564	-3.159000
design_45	517.22237	-4.599000
design_46	409.62412	-4.173000
design_47	450.39902	-5.899000
design_48	408.77631	-3.116000
design_49	228.60946	-0.862000
design_50	429.58165	-5.416000

design_51	434.60648	-1.618000
design_52	653.43299	-10.778000
design_53	579.65271	-10.645000
design_54	419.79665	-3.759000
design_55	366.12935	-2.517000
design_56	406.46393	-3.030000
design_57	646.10996	-5.982000
design_58	529.647	-5.131000
design_59	523.44885	-5.606000
design_60	377.49847	-2.905000
design_61	585.53069	-6.444000
design_62	512.87029	-4.331000
design_63	514.02865	-4.672000
design_64	373.06198	-4.639000
design_65	565.40046	-13.003000
design_66	367.63007	-5.204000
design_67	512.53812	-5.563000
design_68	474.73063	-4.079000
design_69	496.86781	-9.654000
design_70	442.02704	-2.474000
design_71	519.19557	-3.694000
design_72	675.61356	-9.800000
design_73	392.77039	-3.661000
design_74	310.23785	-2.836000
design_75	405.58872	-1.113000
design_76	623.33211	-7.393000
design_77	574.90942	-7.422000
design_78	362.38031	-2.924000
design_79	449.61552	-6.409000
design_80	365.20313	-3.484000
design_81	633.08277	-7.576000
design_82	503.43224	-3.156000
design_83	603.26757	-6.375000
design_84	590.93379	-5.766000
design_85	457.78971	-6.068000
design_86	335.65669	-3.273000
design_87	436.39842	-4.273000
1A2K	699.40758	-4.442000
1ACB	571.19633	-4.459000
1AHW	1222.24834	-13.286000
1AK4	328.53187	-0.019000
1AKJ	978.6798	-10.538000
1AVX	915.41087	-5.783000
1AY7	699.06927	-3.789000
1AZS	592.87483	-9.010000
1B6C	703.24898	-3.403000

1BGX	2542.48221	-21.970000
1BJ1	763.09447	-2.727000
1BKD	1360.91439	-16.087000
1BUH	577.93506	-4.870000
1BVK	660.94561	-4.276000
1BVN	808.73265	-3.598000
1CGI	864.26354	-3.541000
1D6R	697.16586	-3.630000
1DE4	829.90182	-7.598000
1DFJ	1161.93587	-15.477000
1DQJ	1005.10199	-4.153000
1E4K	506.77611	-8.199000
1E6J	517.73289	-1.880000
1E96	587.40504	-4.942000
1EAW	964.42454	-5.023000
1EER	1772.35574	-22.498000
1EFN	561.02136	-3.898000
1EWY	696.30784	-8.521000
1EZU	1069.66445	-7.634000
1F34	1283.45678	-7.694000
1F51	927.60028	-10.225000
1FAK	1451.3894	-20.886000
1FC2	475.20581	-5.352000
1FQ1	666.7464	-8.812000
1FQJ	1121.79303	-13.149000
1FSK	913.16991	-7.083000
1GCQ	480.33133	-0.463000
1GHQ	301.27524	-1.913000
1GLA	466.19906	-5.015000
1GP2	1012.08262	-13.558000
1GPW	1070.19891	-6.475000
1GRN	1052.35851	-10.435000
1H1V	739.09834	-4.598000
1HE1	951.11292	-4.604000
1HE8	570.54844	-9.197000
1HIA	784.03553	-3.177000
1I2M	1674.67612	-15.485000
1I4D	616.14671	-5.753000
1I9R	734.9849	-5.519000
1IB1	1273.21739	-19.484000
1IBR	1631.06512	-21.671000
1IJK	756.35282	-10.836000
1IQD	993.03027	-8.389000
1IRA	1314.85765	-6.227000
1J2J	322.13265	-4.311000
1JMO	1494.69091	-10.559000

1JPS	1217.17984	-8.402000
1K4C	763.61243	-3.583000
1K5D	1426.54802	-13.387000
1K74	1022.80258	-13.979000
1KAC	699.96152	-4.601000
1KKL	788.51979	-3.914000
1KLU	604.16541	-4.107000
1KTZ	409.59829	-3.071000
1KXP	1463.78078	-14.738000
1KXQ	821.79181	-6.513000
1M10	1158.71871	-16.904000
1MAH	695.74727	-2.546000
1ML0	885.57276	-9.202000
1MLC	741.35715	-4.856000
1N2C	1140.58958	-24.121000
1N8O	774.65594	-3.783000
1NCA	863.09222	-7.231000
1NSN	832.34604	-9.851000
1NW9	750.42132	-5.320000
1OPH	639.98134	-1.406000
1PPE	819.55235	-0.361000
1PXV	1163.02675	-9.484000
1QA9	841.92318	-17.834000
1QFW	739.98754	-4.022000
1R0R	626.39716	-2.008000
1R8S	1043.62688	-9.912000
1RLB	484.08506	-4.490000
1S1Q	478.35655	-3.863000
1SBB	470.84781	-4.166000
1T6B	862.33194	-6.426000
1UDI	719.52091	-6.067000
1VFB	770.36234	-3.489000
1WEJ	927.11812	-8.094000
1WQ1	1443.33874	-7.900000
1XD3	1031.60787	-8.272000
1XQS	1497.46828	-21.049000
1Y64	763.16749	-9.481000
1YVB	556.82453	-2.731000
1Z0K	865.46251	-3.793000
1Z5Y	535.31189	-4.237000
1ZHI	566.84629	-6.664000
2AJF	611.07684	-8.445000
2B42	1220.67969	-4.570000
2C0L	826.88422	-6.060000
2CFH	1009.80655	-11.055000
2FD6	503.96202	-1.056000

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2H7V    624.82199       -3.997000
2HLE    1126.74661      -7.719000
2HMI    301.13977       -0.862000
2HQS    1146.81692      -7.901000
2HRK    504.04066       -2.255000
2I25    867.75525       -12.304000
2JEL    807.92144       -4.118000
2MTA    380.43792       -3.071000
2NZ8    1129.48204      -5.402000
2O8V    576.41564       -1.921000
2OOB    241.09823       -0.833000
2OT3    992.2117        -3.065000
2PCC    532.09434       -8.554000
2QFW    567.68557       -2.671000
2SIC    619.37596       -1.716000
2SNI    691.24416       -3.726000
2UUY    839.2346        -1.197000
2VIS    473.93992       -1.562000
7CEI    971.609 -10.751000
********************************************************************************
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Group 05

REMARK Please use this file to submit your results for both designs and
REMARK the ZDock benchmark.
REMARK Change the file name from GroupXXX.txt to represent your group's
number.
REMARK Change 'Column1' and 'Column2' below to the first- and second-most
REMARK imporant parameters in your score function

REMARK Specify the units for each column below:

Units for Column1:Z-score of Atom-atom contact potential
Units for Column2:Raw energy score of Atom-atom contact potential

Column1         Column2
1A2K    4.958   5.333
1ACB    5.213   4.558
1AHW    4.541   4.836
1AK4    4.081   2.978
1AKJ    3.431   3.171
1AVX    4.811   5.180
1AY7    3.356   2.964
1AZS    3.412   3.945
1B6C    4.625   5.799
1BGX    6.778   12.632
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1BJ1	3.900	3.716
1BKD	6.343	7.264
1BUH	2.962	3.177
1BVK	2.320	2.830
1BVN	5.423	5.498
1CGI	4.525	5.098
1D6R	1.100	1.788
1DE4		
1DFJ	3.702	3.465
1DQJ	4.910	4.870
1E4K	2.494	2.737
1E6J	4.655	4.384
1E96	2.290	2.784
1EAW	2.823	3.608
1EER	6.672	9.258
1EFN	3.538	3.668
1EWY	1.989	2.258
1EZU	5.288	4.852
1F34	5.466	5.930
1F51	4.728	4.337
1FAK	6.095	5.752
1FC2	3.840	3.043
1FQ1	3.308	3.229
1FQJ	1.595	2.121
1FSK	5.042	5.533
1GCQ	3.826	3.334
1GHQ	-0.279	1.530
1GLA	3.014	3.039
1GP2	4.036	3.852
1GPW	3.972	3.764
1GRN	5.748	6.587
1H1V	4.782	4.672
1HE1	5.359	6.015
1HE8	2.542	2.475
1HIA	3.153	2.796
1I2M	6.383	6.632
1I4D	3.261	4.237
1I9R	1.526	2.346
1IB1	5.013	5.310
1IBR	5.980	7.829
1IJK	4.880	4.441
1IQD	6.625	7.444
1IRA	6.263	6.032
1J2J	3.682	4.590
1JMO	6.118	8.404
1JPS	5.054	4.355

1K4C	3.985	4.426
1K5D	4.758	6.539
1K74	5.496	5.414
1KAC	4.126	3.294
1KKL	2.860	3.132
1KLU	2.860	2.845
1KTZ	0.971	1.970
1KXP	6.098	8.379
1KXQ	6.225	5.200
1M10	4.323	3.702
1MAH	4.412	4.568
1ML0	4.255	5.303
1MLC	4.703	4.020
1N2C	6.272	9.143
1N8O	3.478	3.365
1NCA	3.751	3.767
1NSN	3.516	3.043
1NW9	3.459	5.634
1OPH	3.423	3.575
1PPE	3.942	4.374
1PXV	5.159	6.279
1QA9	1.813	1.848
1QFW	3.231	4.083
1R0R	4.690	4.709
1R8S	5.895	7.698
1RLB	2.274	2.552
1S1Q	2.420	2.505
1SBB	1.540	2.204
1T6B	5.510	5.621
1UDI	4.711	4.970
1VFB	3.405	3.165
1WEJ	3.905	2.768
1WQ1	4.629	6.011
1XD3	6.122	7.440
1XQS	4.343	4.758
1Y64	2.086	2.779
1YVB	4.179	4.427
1Z0K	5.462	5.703
1Z5Y	4.093	4.148
1ZHI	2.495	2.661
2AJF	4.587	4.222
2B42	5.636	6.962
2C0L	6.465	5.297
2CFH	5.631	11.846
2FD6	2.472	2.731
2H7V	5.005	5.000

2HLE	4.029	4.442
2HMI		
2HQS	4.863	4.753
2HRK	3.805	4.882
2I25	4.328	3.871
2JEL	1.963	2.410
2MTA	1.817	2.278
2NZ8	4.697	5.640
2O8V	4.074	3.642
2OOB	1.112	1.832
2OT3	6.061	6.973
2PCC	1.679	1.821
2QFW	2.828	4.233
2SIC	2.217	2.804
2SNI	5.063	4.798
2UUY	2.609	3.190
2VIS	3.199	3.451
7CEI	6.004	3.672
design_1	1.789	2.855
design_10	2.418	3.134
design_11	1.649	2.443
design_12	3.078	3.691
design_13	1.482	2.471
design_14	0.502	1.773
design_15	2.937	3.323
design_16	1.593	2.416
design_17	0.527	2.037
design_18	1.782	2.197
design_19	3.362	4.166
design_2	1.914	2.324
design_20	4.460	5.807
design_21	2.845	3.238
design_22	5.558	4.882
design_23	0.843	1.632
design_24	5.216	4.404
design_25	1.010	2.135
design_26	0.119	1.460
design_27	1.635	2.628
design_28	2.254	2.607
design_29	2.353	3.686
design_3	2.367	2.427
design_30	2.650	2.797
design_31	0.492	1.909
design_32	-0.539	1.309
design_33	3.391	4.094
design_34	2.674	2.746

design_35	2.632	2.933
design_36	2.195	2.637
design_37	4.719	4.547
design_38	4.285	6.159
design_39	1.023	2.035
design_4	1.489	2.443
design_40	1.520	2.430
design_41	2.040	2.541
design_42	0.927	2.454
design_43	1.867	2.456
design_44	3.287	2.928
design_45	2.754	4.090
design_46	1.849	2.097
design_47	2.157	2.606
design_48	2.663	3.521
design_49	2.055	2.195
design_5	0.983	2.108
design_50	1.062	2.043
design_51	1.757	2.428
design_52	3.048	3.301
design_53	1.900	2.618
design_54	0.174	1.608
design_55	4.509	4.454
design_56	1.494	2.467
design_57	1.498	2.044
design_58	1.928	2.831
design_59	0.857	1.883
design_6	5.277	4.184
design_60	0.342	1.703
design_61	1.723	3.060
design_62	1.769	4.517
design_63	2.672	3.363
design_64	1.332	2.220
design_65	1.509	2.307
design_66	4.178	4.179
design_67	1.767	2.295
design_68	3.958	2.897
design_69	1.230	2.221
design_7	1.621	2.612
design_70	1.002	2.026
design_71	4.417	5.240
design_72	2.472	2.813
design_73	1.140	2.079
design_74	-0.789	2.001
design_75	4.101	3.593
design_76		

```
design_77       3.115   3.306
design_78       1.297   2.467
design_79       0.303   1.625
design_8        3.577   3.869
design_80       0.842   1.939
design_81       2.026   2.964
design_82       4.704   4.543
design_83       3.047   5.879
design_84       4.070   3.814
design_85       3.140   3.491
design_86       1.662   2.449
design_87       1.207   1.984
design_9        1.656   2.458
**********************************************
REMARK Group35_top_two_discriminators.txt
REMARK Specify the units for each column below:

Units for Column1: Raw score HbondEnergy/deltaGbinding ratio (Unitless
Energy/Energy cancles out)
Units for Column2: Raw score BurriedUnsatisfiedH-bonds/InterfaceBurriedSASA
(number/Angstrom^2)

struc           Column1 Column2
1A2K.pdb        0.404   0.0032
1ACB.pdb        0.235   0.0052
1AHW.pdb        0.560   0.0016
1AK4.pdb        0.289   0.0035
1AKJ.pdb        0.619   0.0005
1AVX.pdb        0.407   0.0035
1AY7.pdb        0.526   0.0008
1AZS.pdb        0.157   0.0041
1B6C.pdb        0.261   0.0016
1BGX.pdb        0.321   0.0044
1BJ1.pdb        0.281   0.0011
1BKD.pdb        0.488   0.0013
1BUH.pdb        0.213   0.0017
1BVK.pdb        0.522   0.0015
1BVN.pdb        0.352   0.0029
1CGI.pdb        0.240   0.0034
1D6R.pdb        0.506   0.0022
1DE4.pdb        0.336   0.0005
1DFJ.pdb        0.446   0.0021
1DQJ.pdb        0.547   0.0034
1E4K.pdb        0.248   0.0038
1E6J.pdb        0.283   0.0024
1E96.pdb        0.395   0.0028
```

1EAW.pdb	0.547	0.0011
1EER.pdb	0.463	0.0009
1EFN.pdb	0.311	0.0009
1EWY.pdb	0.388	0.0047
1EZU.pdb	0.252	0.0019
1F34.pdb	0.379	0.0038
1F51.pdb	0.335	0.0019
1FAK.pdb	0.496	0.001
1FC2.pdb	0.155	0.0026
1FQ1.pdb	0.449	0.0014
1FQJ.pdb	0.507	0.0006
1FSK.pdb	0.355	0.0057
1GCQ.pdb	0.335	0.0025
1GHQ.pdb	0.351	0.0026
1GLA.pdb	0.293	0.0024
1GP2.pdb	0.334	0.0021
1GPW.pdb	0.458	0.0031
1GRN.pdb	0.457	0.0017
1H1V.pdb	0.470	0.001
1HE1.pdb	0.318	0.001
1HE8.pdb	0.473	0.0011
1HIA.pdb	0.398	0.003
1I2M.pdb	0.709	0.0007
1I4D.pdb	0.107	0.0012
1I9R.pdb	0.286	0.0015
1IB1.pdb	0.517	0.001
1IBR.pdb	0.510	0.0015
1IJK.pdb	0.401	0.0013
1IQD.pdb	0.423	0.001
1IRA.pdb	0.448	0.0019
1J2J.pdb	0.155	0.0019
1JMO.pdb	0.425	0.0021
1JPS.pdb	0.564	0.0006
1K4C.pdb	0.418	0.0027
1K5D.pdb	0.344	0.0046
1K74.pdb	0.355	0.0004
1KAC.pdb	0.433	0.0015
1KKL.pdb	0.265	0.0006
1KLU.pdb	0.334	0.0019
1KTZ.pdb	0.527	0.0011
1KXP.pdb	0.356	0.0012
1KXQ.pdb	0.323	0.0021
1M10.pdb	0.425	0.0006
1MAH.pdb	0.288	0.0019
1ML0.pdb	0.306	0.0029
1MLC.pdb	0.324	0.0008

1N2C.pdb	0.291	0.0012
1N8O.pdb	0.242	0.0026
1NCA.pdb	0.422	0.0029
1NSN.pdb	0.674	0.0014
1NW9.pdb	0.311	0.001
1OPH.pdb	0.471	0.0054
1PPE.pdb	0.417	0.0024
1PXV.pdb	0.307	0.0018
1QA9.pdb	0.475	0
1QFW.pdb	0.490	0.0023
1R0R.pdb	0.278	0
1R8S.pdb	0.381	0.002
1RLB.pdb	0.334	0.003
1S1Q.pdb	0.431	0.0009
1SBB.pdb	0.409	0
1T6B.pdb	0.403	0.0022
1UDI.pdb	0.381	0.001
1VFB.pdb	0.554	0.0016
1WEJ.pdb	0.526	0.0045
1WQ1.pdb	0.333	0.0041
1XD3.pdb	0.455	0.0023
1XQS.pdb	0.586	0.0038
1YVB.pdb	0.258	0.0039
1Z0K.pdb	0.489	0.0012
1Z5Y.pdb	0.234	0.0016
1ZHI.pdb	0.405	0
2AJF.pdb	0.297	0.0006
2B42.pdb	0.412	0.0037
2C0L.pdb	0.446	0.0026
2CFH.pdb	0.278	0.002
2FD6.pdb	0.462	0.0018
2H7V.pdb	0.473	0.0027
2HLE.pdb	0.576	0.0014
2HQS.pdb	0.496	0.0023
2HRK.pdb	0.134	0.004
2I25.pdb	0.494	0.0036
2JEL.pdb	0.463	0
2MTA.pdb	0.187	0.0033
2NZ8.pdb	0.405	0.0015
2OOB.pdb	0.278	0
2PCC.pdb	0.537	0.0008
2QFW.pdb	0.333	0.0023
2SIC.pdb	0.359	0.0051
2SNI.pdb	0.347	0.0052
2UUY.pdb	0.544	0.004
2VIS.pdb	0.358	0.0008

7CEI.pdb	0.876	0.0015
design_1_mpm	0.38644222	0.0017
design_10_mpm	0.232179226	0.0024
design_11_mpm	0.221148126	0.0025
design_12_mpm	0.24177502	0.0013
design_13_mpm	0.406802613	0.0024
design_14_mpm	0.237636609	0.0039
design_15_mpm	0.401149125	0.0062
design_16_mpm	0.268679245	0.0034
design_17_mpm	0.252458854	0.0049
design_18_mpm	0.353486774	0.0046
design_19_mpm	0.412245527	0.0041
design_2_mpm	0.36316068	0.004
design_20_mpm	0.277714204	0.0011
design_21_mpm	0.221550252	0.0025
design_22_mpm	0.384964225	0.0009
design_23_mpm	0.247426285	0.0063
design_24_mpm	0.5321248	0.0008
design_25_mpm	0.332567559	0.0011
design_26_mpm	0.195685542	0.0019
design_27_mpm	0.301869907	0.0041
design_28_mpm	0.486297299	0.0058
design_29_mpm	0.335901801	0.0025
design_3_mpm	0.319663956	0.0021
design_30_mpm	0.232053422	0.0021
design_31_mpm	0.346559518	0.0055
design_32_mpm	0.242469319	0.0063
design_33_mpm	0.31830367	0.0015
design_34_mpm	0.185527502	0.0028
design_35_mpm	0.146615314	0.0033
design_36_mpm	0.366129505	0.0024
design_37_mpm	0.410373208	0
design_38_mpm	0.239289762	0.0014
design_39_mpm	0.211769017	0.0029
design_4_mpm	0.349438546	0.003
design_40_mpm	0.490196078	0.0034
design_41_mpm	0.272722322	0.0027
design_42_mpm	0.300838779	0.0032
design_43_mpm	0.309697361	0.0017
design_44_mpm	0.196493656	0.0064
design_45_mpm	0.224746841	0.0028
design_46_mpm	0.245262114	0.006
design_47_mpm	0.291365818	0.0026
design_48_mpm	0.125685904	0.003
design_49_mpm	0.069713484	0.002
design_5_mpm	0.34329988	0.0051

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design_50_mpm   0.358207462     0.0019
design_51_mpm   0.264592263     0.0038
design_52_mpm   0.422646671     0.0021
design_53_mpm   0.423233417     0.0031
design_54_mpm   0.25052101      0.0028
design_55_mpm   0.366002316     0
design_56_mpm   0.22731681      0.0037
design_57_mpm   0.419863935     0.0036
design_58_mpm   0.347446472     0.0036
design_59_mpm   0.31268475      0.0042
design_6_mpm    0.172630923     0.0025
design_60_mpm   0.217168881     0.0032
design_61_mpm   0.253796694     0.0013
design_62_mpm   0.203851079     0.0007
design_63_mpm   0.410011919     0.0026
design_64_mpm   0.301096951     0.0021
design_65_mpm   0.282047042     0.005
design_66_mpm   0.188052976     0.0018
design_67_mpm   0.599531929     0.0025
design_68_mpm   0.364227739     0.0028
design_69_mpm   0.158223456     0.0021
design_7_mpm    0.218252348     0.0036
design_70_mpm   0.18357608      0.0048
design_71_mpm   0.355073952     0.0029
design_72_mpm   0.252224971     0.0035
design_73_mpm   0.486963107     0.0032
design_74_mpm   0.22371184      0.0024
design_75_mpm   0.487403533     0.0009
design_76_mpm   0.341107753     0.004
design_77_mpm   0.307604833     0.0029
design_78_mpm   0.327183199     0.0062
design_79_mpm   0.493601774     0.0021
design_8_mpm    0.410100614     0
design_80_mpm   0.198755304     0.001
design_81_mpm   0.431535091     0.0042
design_82_mpm   0.271087775     0.0007
design_83_mpm   0.220336091     0
design_84_mpm   0.380659753     0.0016
design_85_mpm   0.181626343     0.0037
design_86_mpm   0.157102827     0.0048
design_87_mpm   0.2237447       0.0026
design_9_mpm    0.232508902     0.0041
******************************
Group 08
REMARK Please use this file to submit your results for both designs and
REMARK the ZDock benchmark.
```

REMARK Change the file name from GroupXXX.txt to represent your group's number.
REMARK Change 'Column1' and 'Column2' below to the first- and second-most
REMARK imporant parameters in your score function

REMARK Specify the units for each column below:

Units for Sequence-Conservation: arbitrary unit
Units for Hydrogen-bond: kcal/mol

	Sequence-Conservation	Hydrogen-bond
design_1	-8.1200	-0.4611
design_2	-7.6424	-0.2946
design_3	-0.9553	-0.5498
design_4	-6.2094	-0.2393
design_5	-5.2541	-0.0498
design_6	-5.2541	-0.0082
design_7	-5.2541	-0.1115
design_8	-10.0306	-0.2275
design_9	-8.1200	-0.1838
design_10	-6.2094	-0.1913
design_11	-10.0306	-0.1612
design_12	-10.5083	-0.2235
design_13	-7.6424	-0.5203
design_14	-3.3435	-0.2984
design_15	-10.9859	-0.4326
design_16	-4.7765	-0.1657
design_17	-5.7318	-0.3320
design_18	-5.2541	-0.2596
design_19	-9.0753	-0.2528
design_20	-10.9859	-0.3607
design_21	-9.0753	-0.2135
design_22	-10.9859	-0.1799
design_23	-2.3882	-0.1930
design_24	-6.6871	-0.2507
design_25	-4.7765	-0.2450
design_26	-3.3435	-0.2068
design_27	-5.7318	-0.2974
design_28	-5.2541	-0.3754
design_29	-5.7318	-0.3854
design_30	-9.0753	-0.3731
design_31	-7.1647	-0.1456
design_32	-4.2988	-0.2081
design_33	-9.0753	-0.3502
design_34	-12.4189	-0.2498
design_35	-7.1647	-0.1507

design_36	-6.2094	-0.4514
design_37	-13.3742	-0.3323
design_38	-14.3294	-0.2515
design_39	-3.3435	-0.0014
design_40	-5.2541	-0.4278
design_41	-5.2541	-0.3414
design_42	-1.9106	-0.3892
design_43	-13.3742	-0.2861
design_44	-5.2541	-0.2345
design_45	-10.5083	-0.2806
design_46	-5.7318	-0.1228
design_47	-5.7318	-0.2752
design_48	-6.6871	-0.1677
design_49	-4.7765	-0.0794
design_50	-6.6871	-0.4039
design_51	-5.2541	-0.2214
design_52	-6.6871	-0.3535
design_53	-8.5977	-0.4769
design_54	-2.3882	-0.3092
design_55	-8.5977	-0.1213
design_56	-7.1647	-0.2922
design_57	-0.9553	-0.5264
design_58	-10.5083	-0.2200
design_59	-1.9106	-0.5467
design_60	-8.5977	-0.2147
design_61	-5.7318	-0.1405
design_62	-10.5083	-0.2785
design_63	-5.7318	-0.3629
design_64	-5.7318	-0.1558
design_65	-10.0306	-0.4205
design_66	-7.1647	-0.3189
design_67	-5.2541	-0.6709
design_68	-9.5530	-0.2135
design_69	-7.6424	-0.1781
design_70	-7.6424	-0.0657
design_71	-7.1647	-0.2797
design_72	-10.5083	-0.2077
design_73	-10.5083	-0.6897
design_74	-3.3435	-0.1152
design_75	-10.0306	-0.3240
design_76	-10.0306	-0.3041
design_77	-9.5530	-0.3808
design_78	-5.7318	-0.2830
design_79	-4.2988	-0.6364
design_80	-5.7318	-0.2067
design_81	-7.6424	-0.3531

design_82	-6.2094	-0.0797
design_83	-8.1200	-0.2586
design_84	-5.7318	-0.3747
design_85	-9.0753	-0.2614
design_86	-3.8212	-0.1026
design_87	-3.3435	-0.2937
1A2K	-21.0165	-0.7804
1ACB	-30.5695	-0.5408
1AHW	-3.3435	-0.9235
1AK4	-33.4354	-0.4379
1AKJ	-8.5977	-0.6566
1AVX	-30.5695	-0.5456
1AY7	-11.9412	-0.6297
1AZS	-4.2988	-0.0694
1B6C	-21.9718	-0.1551
1BGX	0.0000	0.0000
1BJ1	-4.2988	-0.4431
1BKD	-25.7930	-1.0183
1BUH	-16.7177	-0.2980
1BVK	-4.7765	-0.4571
1BVN	-8.1200	-0.3806
1CGI	-35.3460	-0.6704
1D6R	-33.4354	-0.6624
1DE4	0.0000	0.0000
1DFJ	-16.7177	-0.3650
1DQJ	-6.2094	-0.7136
1E4K	-0.9553	-0.1037
1E6J	-10.5083	-0.4530
1E96	-6.6871	-0.6642
1EAW	-39.1672	-0.5637
1EER	-3.8212	-0.7750
1EFN	-18.1506	-0.2879
1EWY	-10.9859	-0.2702
1EZU	-42.9883	-0.6969
1F34	-14.8071	-0.9747
1F51	-27.7036	-0.4473
1FAK	-16.7177	-1.0487
1FC2	-2.3882	-0.0842
1FQ1	-18.1506	-0.1733
1FQJ	-9.0753	-0.7453
1FSK	-8.1200	-0.6723
1GCQ	-12.8965	-0.5177
1GHQ	-2.8659	-0.1732
1GLA	-9.0753	-0.1124
1GP2	-19.1059	-0.7585
1GPW	-41.0777	-0.6171

1GRN	-41.0777	-0.6142
1H1V	-13.8518	-0.5178
1HE1	-20.0612	-0.7766
1HE8	-11.4636	-0.3629
1HIA	-23.8824	-0.8605
1I2M	-21.0144	-1.5992
1I4D	-15.7624	-0.1400
1I9R	-2.3882	-0.2215
1IB1	-17.1953	-1.1654
1IBR	-17.6730	-0.6563
1IJK	-2.8659	-0.4362
1IQD	-0.4776	-1.0937
1IRA	-6.2094	-0.9910
1J2J	-11.4636	-0.0879
1JMO	-32.4801	-1.4287
1JPS	-3.3435	-0.9684
1K4C	-2.3882	-0.5813
1K5D	-25.3154	-0.6779
1K74	-15.7608	-0.2904
1KAC	-3.8212	-0.4010
1KKL	-17.1953	-0.3186
1KLU	0.0000	-0.2773
1KTZ	-7.1647	-0.5160
1KXP	-12.8952	-0.9468
1KXQ	-19.5836	-0.6461
1M10	-1.4328	-0.8364
1MAH	-3.3435	-0.5422
1ML0	-10.5083	-0.8744
1MLC	-5.2541	-0.3461
1N2C	0.0000	0.0000
1N8O	-32.0024	-0.6183
1NCA	-8.1200	-0.5403
1NSN	-3.3435	-0.1793
1NW9	-13.3742	-0.5268
1OPH	-29.6142	-0.6569
1PPE	-36.7789	-0.8165
1PXV	-5.2541	-0.6362
1QA9	-0.9553	-0.3484
1QFW	-8.1200	-0.4570
1R0R	-45.8542	-0.7529
1R8S	-20.5368	-0.6802
1RLB	-1.9106	-0.1560
1S1Q	-14.8071	-0.3032
1SBB	-2.3882	-0.2698
1T6B	-6.2094	-0.6164
1UDI	-16.2400	-0.6097

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1VFB                   -5.2541       -0.7765
1WEJ                   -3.8212       -0.7503
1WQ1                  -22.4495       -0.4254
1XD3                  -25.3154       -0.9119
1XQS                  -21.0165       -1.1821
1Y64                  -19.1059       -0.1390
1YVB                  -24.8377       -0.2236
1Z0K                  -26.7483       -0.9349
1Z5Y                  -12.4189       -0.2921
1ZHI                           -0.4776       -0.2781
2AJF                           -3.8212       -0.2339
2B42                  -15.2847       -0.3982
2C0L                   -8.5977       -0.6159
2CFH                  -21.9718       -0.7419
2FD6                   -3.3435       -0.5515
2H7V                  -17.6730       -0.4232
2HLE                   -8.5977       -0.9689
2HMI                    0.0000        0.0000
2HQS                   -6.2094       -0.7396
2HRK                  -10.5083       -0.0272
2I25                           0.0000        0.0000
2JEL                         -10.0306       -0.5498
2MTA                  -10.5083        0.0000
2NZ8                  -29.6142       -0.9307
2O8V                  -30.0918       -0.1562
2OOB                  -12.4189       -0.2023
2OT3                  -32.4801       -0.5291
2PCC                   -6.6871       -0.2195
2QFW                   -4.2988       -0.1162
2SIC                  -39.1672       -0.7933
2SNI                  -39.1672       -0.6488
2UUY                  -29.1365       -0.8890
2VIS                   -4.7765       -0.2537
7CEI                   -7.1647       -1.0035
****************************************
Group 23-
REMARK Please use this file to submit your results for both designs and
REMARK the ZDock benchmark.
REMARK Change the file name from GroupXXX.txt to represent your group's
number.
REMARK Change 'Column1' and 'Column2' below to the first- and second-most
REMARK imporant parameters in your score function

REMARK Specify the units for each column below:

Units for Column1: complementarity score of electrostatic potential (Ecmp)
```

Units for Column2: complementarity score of hydrophobicity (Hcmp)

Column1	Column2	
design_1	0.240	0.127
design_2	0.128	0.078
design_3	0.324	0.088
design_4	0.629	0.165
design_5	0.459	0.268
design_6	0.908	0.210
design_7	0.539	0.125
design_8	0.706	0.207
design_9	0.329	0.222
design_10	0.088	0.161
design_11	0.382	0.130
design_12	0.072	0.225
design_13	0.722	0.092
design_14	0.391	0.104
design_15	0.456	0.187
design_16	0.307	0.121
design_17	0.279	0.138
design_18	0.350	0.113
design_19	0.610	0.172
design_20	0.702	0.138
design_21	0.538	0.224
design_22	0.778	0.187
design_23	0.430	0.170
design_24	0.716	0.201
design_25	0.843	0.116
design_26	0.903	0.047
design_27	0.742	0.106
design_28	0.445	0.141
design_29	0.759	0.110
design_30	0.289	0.095
design_31	-	-
design_32	0.440	0.215
design_33	0.608	0.183
design_34	0.487	0.064
design_35	0.359	0.048
design_36	0.292	0.176
design_37	0.731	0.221
design_38	0.806	0.164
design_39	0.239	0.078
design_40	0.790	0.080
design_41	0.174	0.137
design_42	0.493	0.186

design_43	-	-
design_44	0.218	0.119
design_45	0.056	0.182
design_46	0.395	0.058
design_47	0.374	0.134
design_48	0.017	0.149
design_49	0.206	0.038
design_50	0.379	0.132
design_51	0.853	0.045
design_52	0.367	0.138
design_53	0.695	0.099
design_54	0.125	0.124
design_55	0.439	0.121
design_56	0.139	0.130
design_57	0.508	0.179
design_58	0.115	0.180
design_59	0.430	0.188
design_60	0.057	0.119
design_61	0.903	0.147
design_62	0.457	0.148
design_63	0.893	0.122
design_64	0.296	0.213
design_65	0.557	0.183
design_66	0.546	0.238
design_67	0.212	0.154
design_68	0.459	0.237
design_69	0.794	0.216
design_70	0.794	0.183
design_71	0.523	0.173
design_72	0.781	0.197
design_73	0.767	0.143
design_74	0.258	0.099
design_75	0.687	0.109
design_76	0.248	0.183
design_77	0.788	0.151
design_78	0.952	0.133
design_79	0.207	0.123
design_80	0.403	0.114
design_81	0.461	0.119
design_82	0.479	0.272
design_83	0.787	0.205
design_84	0.742	0.177
design_85	0.691	0.093
design_86	0.218	0.195
design_87	0.622	0.137
1A2K	0.875	0.163

1ACB	0.627	0.234
1AHW	0.880	0.075
1AK4	0.686	0.177
1AKJ	0.828	0.106
1AVX	0.827	0.072
1AY7	0.549	0.083
1AZS	0.794	0.116
1B6C	0.627	0.182
1BGX	0.529	0.110
1BJ1	0.545	0.038
1BKD	0.574	0.156
1BUH	0.507	0.098
1BVK	0.602	0.032
1BVN	0.399	0.085
1CGI	0.550	0.138
1D6R	0.710	0.123
1DE4	-	-
1DFJ	0.769	0.058
1DQJ	0.500	0.047
1E4K	0.857	0.135
1E6J	0.904	0.161
1E96	0.883	0.246
1EAW	0.844	0.123
1EER	0.944	0.161
1EFN	0.788	0.137
1EWY	0.559	0.136
1EZU	0.353	0.121
1F34	0.423	0.193
1F51	0.478	0.264
1FAK	0.483	0.124
1FC2	0.339	0.198
1FQ1	0.826	0.172
1FQJ	0.703	0.121
1FSK	0.556	0.032
1GCQ	0.530	0.127
1GHQ	0.407	0.184
1GLA	0.760	0.173
1GP2	0.722	0.177
1GPW	0.915	0.133
1GRN	0.823	0.219
1H1V	0.153	0.240
1HE1	0.694	0.223
1HE8	0.768	0.163
1HIA	0.757	0.147
1I2M	0.834	0.101
1I4D	0.389	0.191

1I9R	0.796	0.065
1IB1	0.592	0.207
1IBR	0.800	0.173
1IJK	0.961	0.170
1IQD	0.478	0.161
1IRA	0.745	0.169
1J2J	0.720	0.293
1JMO	-	-
1JPS	0.875	0.100
1K4C	0.797	0.090
1K5D	0.595	0.219
1K74	0.868	0.217
1KAC	0.765	0.248
1KKL	0.595	0.233
1KLU	0.646	0.070
1KTZ	0.921	0.134
1KXP	0.789	0.244
1KXQ	0.820	0.110
1M10	0.775	0.083
1MAH	0.990	0.169
1ML0	0.955	0.173
1MLC	0.696	0.073
1N2C	-	-
1N8O	0.321	0.139
1NCA	0.610	0.098
1NSN	0.727	0.083
1NW9	0.569	0.141
1OPH	0.758	0.201
1PPE	0.781	0.143
1PXV	0.675	0.184
1QA9	0.780	0.084
1QFW	0.878	0.074
1R0R	0.444	0.198
1R8S	0.729	0.193
1RLB	0.718	0.196
1S1Q	0.550	0.146
1SBB	0.577	0.134
1T6B	0.387	0.166
1UDI	0.923	0.231
1VFB	0.537	0.047
1WEJ	0.762	0.041
1WQ1	0.837	0.154
1XD3	0.811	0.241
1XQS	0.916	0.111
1Y64	0.831	0.207
1YVB	-	-

1Z0K	0.661	0.148
1Z5Y	0.636	0.042
1ZHI	0.890	0.132
2AJF	0.714	0.123
2B42	0.587	0.084
2C0L	0.710	0.294
2CFH	0.752	0.312
2FD6	-	-
2H7V	-	-
2HLE	0.820	0.164
2HMI	0.777	0.136
2HQS	0.602	0.177
2HRK	0.690	0.288
2I25	0.611	0.075
2JEL	0.115	0.087
2MTA	0.751	0.253
2NZ8	0.600	0.214
2O8V	0.671	0.171
2OOB	0.676	0.352
2OT3	0.808	0.207
2PCC	0.999	0.164
2QFW	0.524	0.053
2SIC	0.368	0.239
2SNI	0.697	0.195
2UUY	0.729	0.138
2VIS	0.671	0.058
7CEI	0.978	0.089

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Group 33-

REMARK Please use this file to submit your results for both designs and
REMARK the ZDock benchmark.
REMARK Change the file name from Group33.txt to represent your group's
number.
REMARK Change 'Column1' and 'Column2' below to the first- and second-most
REMARK imporant parameters in your score function

REMARK Specify the units for each column below:

Units for Column1: 12-6 Lennard-Jones Potential potential (CHARMM-based)
Units for Column2: Atom Contact Potential (see methods section)

vdw_attr	atom_contact_potential
design_1	-19.03942337 -1.789190923
design_2	-18.77413121 -0.502496294
design_3	-30.9419549 -2.03805566
design_4	-18.85804009 -0.709955479

design_5	-19.53897966	-0.900893462
design_6	-21.06502619	-0.137760721
design_7	-22.81517504	-1.329733913
design_8	-20.81640728	-2.002594486
design_9	-17.56596171	-2.307179379
design_10	-19.5046959	-3.488646828
design_11	-19.12619334	-0.44158851
design_12	-24.57296991	-2.46215051
design_13	-21.95147098	-0.870078876
design_14	-19.26520288	-4.067709271
design_15	-25.51195025	0.687776332
design_16	-23.89671662	-2.014751997
design_17	-22.88660365	0.385550095
design_18	-20.4319359	-0.860258804
design_19	-25.62545662	-0.591743314
design_20	-34.42483942	-0.733142447
design_21	-20.07252372	-3.654396345
design_22	-21.55767639	-2.093036747
design_23	-21.54332161	-3.903841022
design_24	-23.4800333	-0.357260367
design_25	-16.02797753	-0.887742275
design_26	-21.44106229	-0.936860315
design_27	-22.01712808	-1.630499693
design_28	-20.6971294	0.339257845
design_29	-23.69431912	-0.564581639
design_30	-28.72549761	-3.187088936
design_31	-18.85971729	-0.787296059
design_32	-15.73437044	-2.021265707
design_33	-28.51254368	-2.075656245
design_34	-28.04233824	-1.610021466
design_35	-29.15870619	-3.793086736
design_36	-19.74769128	-1.430551432
design_37	-24.50963128	-2.036591667
design_38	-28.03242308	-3.540813086
design_39	-17.53064204	-1.109615076
design_40	-19.74048923	0.079345968
design_41	-20.3151738	-1.721967456
design_42	-21.60305921	-1.619470235
design_43	-22.92236728	-1.68495742
design_44	-27.63744459	-3.479686057
design_45	-26.55289393	-3.288362626
design_46	-18.83707521	-0.741813249
design_47	-21.22855231	-2.312367008
design_48	-22.69594649	-2.451068009
design_49	-20.08426406	-3.167339169
design_50	-20.92764451	-0.638103106

design_51	-23.66610285	-2.051256355
design_52	-26.78508623	1.560362385
design_53	-24.18139513	-0.497375854
design_54	-20.8939527	-2.233017857
design_55	-19.44214654	-1.825613948
design_56	-19.93553668	-1.812614817
design_57	-24.92937301	-1.977604048
design_58	-23.93336817	-1.552801955
design_59	-23.4580325	-2.637900445
design_60	-18.60547485	-1.489454182
design_61	-25.79791132	-0.255264228
design_62	-25.05723416	-1.89085006
design_63	-22.81729619	-0.614106344
design_64	-16.96981896	-1.354908235
design_65	-20.77428019	-0.055215538
design_66	-21.05516036	-4.469847755
design_67	-21.49029278	1.544887904
design_68	-20.1848462	-1.543254172
design_69	-22.7936182	-2.588626811
design_70	-19.86691983	-1.560514442
design_71	-25.69496139	-2.986436967
design_72	-26.42700595	-0.795111096
design_73	-18.59284659	0.39408652
design_74	-17.26643512	-1.858903885
design_75	-18.99857884	-1.462865373
design_76	-26.78355703	1.283932844
design_77	-23.69959734	-0.891144115
design_78	-18.20595808	-1.222890683
design_79	-19.44382373	0.786656004
design_80	-19.49122904	-1.196772191
design_81	-25.31853066	1.087959289
design_82	-23.79485192	-2.424613577
design_83	-31.08308559	-2.87679659
design_84	-26.6562385	0.240597418
design_85	-24.48087239	-3.099712574
design_86	-17.71118673	-1.073259239
design_87	-22.63867535	-2.540315028
1A2K	-83.54828514	-0.988556257
1ACB	-29.92656371	-7.246201666
1AHW	-97.07236443	-3.642762194
1AK4	-18.79361623	-2.365056627
1AKJ	-107.650507	-2.425154618
1AVX	-36.81113696	-1.207904199
1AY7	-28.41275081	3.25513634
1AZS	-83.0929771	0.329659494
1B6C	-32.36963911	-1.919153933

1BGX	-154.7203803	0.843051577
1BJ1	-146.1898907	-22.02931732
1BKD	-51.47792597	2.332739149
1BUH	-26.40352527	0.923475737
1BVK	-59.31139472	-1.39067706
1BVN	-40.96144485	-3.743791885
1CGI	-43.00880182	-7.928196285
1D6R	-22.87358075	0.496028555
1DE4	-180.0153809	0.062843509
1DFJ	-33.52596368	5.147209931
1DQJ	-95.51553651	-4.93829029
1E4K	-67.10638673	0.203534338
1E6J	-82.9829731	-7.890500222
1E96	-24.1177112	0.779466877
1EAW	-36.63355203	-0.101826047
1EER	-59.92307616	1.706309092
1EFN	-22.98516328	-0.61583909
1EWY	-19.70482425	2.601240494
1EZU	-107.4226063	-12.23467086
1F34	-53.05596543	-5.755120825
1F51	-85.73800603	-10.92432602
1FAK	-82.81081438	-0.057589753
1FC2	-20.15075975	-1.05870771
1FQ1	-23.60843707	1.359827111
1FQJ	-32.84561606	4.015550085
1FSK	-100.4686763	-6.870867699
1GCQ	-22.7590878	-1.982993241
1GHQ	-11.8887687	-0.467823696
1GLA	-18.63339515	-1.280615873
1GP2	-108.2755073	-12.09357584
1GPW	-34.82016321	0.727381951
1GRN	-37.40969685	2.718879792
1H1V	-31.86460729	-0.274023146
1HE1	-36.45937081	-0.900387783
1HE8	-21.32203105	0.894492911
1HIA	-166.7196956	-35.60085464
1I2M	-50.78337157	7.311480213
1I4D	-89.19449945	-9.851155186
1I9R	-189.306526	-16.92945732
1IB1	-77.11675079	6.56081228
1IBR	-56.37877686	7.275693707
1IJK	-106.0576688	-12.19626755
1IQD	-95.93779402	-9.237904607
1IRA	-48.94556482	1.091799619
1J2J	-18.57232567	-3.033535828
1JMO	-143.2552996	-8.168234627

1JPS	-98.16500507	-3.5809845
1K4C	-100.8578833	-6.719659103
1K5D	-134.5541312	-3.98354733
1K74	-67.36931109	-1.790690278
1KAC	-21.75943261	0.696079367
1KKL	-116.1144023	-13.14397344
1KLU	-122.8137939	-9.003241313
1KTZ	-17.82962601	-2.454218777
1KXP	-50.71233759	2.56219006
1KXQ	-37.14420737	-1.855519726
1M10	-33.8045747	3.454327852
1MAH	-33.57297435	-4.197064053
1ML0	-83.47133167	-7.826600799
1MLC	-91.05963455	-4.221181046
1N2C	-724.7290477	-19.07434913
1N8O	-177.2322304	-41.6247986
1NCA	-97.10689484	-6.425445931
1NSN	-78.75349193	-5.019693982
1NW9	-41.37038349	-6.412220483
1OPH	-30.04520031	-2.438037053
1PPE	-35.78523867	-4.661687474
1PXV	-47.68841147	-2.741225141
1QA9	-18.78404637	4.597540515
1QFW	-129.4051547	-18.38220558
1R0R	-30.91151882	-5.194453777
1R8S	-50.25357651	-6.294747387
1RLB	-117.9558594	-23.36568871
1S1Q	-19.30185444	-1.169023504
1SBB	-18.28715386	0.483298178
1T6B	-33.26821888	1.072431764
1UDI	-31.29485563	-0.573202933
1VFB	-62.96471144	0.348637304
1WEJ	-104.8165474	-1.758390481
1WQ1	-45.1790377	5.333639239
1XD3	-41.74582764	-3.310605424
1XQS	-43.62625477	7.234461429
1Y64	-24.2190826	2.761010269
1YVB	-28.64731091	-5.436684574
1Z0K	-34.69920814	-1.654461093
1Z5Y	-25.50751062	-3.157504953
1ZHI	-21.16309253	0.554241743
2AJF	-23.45379019	0.332859062
2B42	-49.02360353	3.413997308
2C0L	-30.44703556	-0.04248516
2CFH	-44.60168935	-6.697274855
2FD6	-94.0223432	-9.270013448

2H7V	-25.88882494	-0.920257781
2HLE	-39.30492272	-0.621026719
2HMI	-173.5394503	-15.0163291
2HQS	-42.74311503	3.14923728
2HRK	-23.38892236	-2.168018671
2I25	-33.8624378	2.710827828
2JEL	-92.53457608	-5.697515866
2MTA	-81.5874515	-3.798532509
2NZ8	-43.7237785	0.953650269
2O8V	-30.18021419	-5.543867281
2OOB	-15.03014752	-1.742109743
2OT3	-48.56055082	-5.642633794
2PCC	-12.95319306	2.634516286
2QFW	-126.7921897	-16.6149109
2SIC	-30.81221924	-6.676411181
2SNI	-32.40890511	-4.890798909
2UUY	-31.38488132	-0.764681958
2VIS	-86.42269461	-10.03871608
7CEI	-29.84230953	5.223273938
****
Group 31 -
REMARK Please use this file to submit your results for both designs and
REMARK the ZDock benchmark.
REMARK Change the file name from GroupXXX.txt to represent your group's
number.
REMARK Change 'Column1' and 'Column2' below to the first- and second-most
REMARK imporant parameters in your score function

REMARK Specify the units for each column below:

Units for Column1: Z_1
Units for Column2: Z_k

REMARK Z_1 and Z_k are our used score for interaction prediction based on
MEGADOCK.

Column1(Z_1),	Column2(Z_k)
design_01,	0.230,	4.424
design_02,	1.074,	4.418
design_03,	3.037,	5.193
design_04,	1.695,	4.256
design_05,	0.628,	4.750
design_06,	0.509,	4.471
design_07,	1.339,	4.568
design_08,	1.755,	4.665
design_09,	0.126,	4.163

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design_10,      1.173,  5.209
design_11,      2.783,  4.753
design_12,      3.542,  4.935
design_13,      1.012,  4.640
design_14,      4.166,  4.696
design_15,      1.363,  6.651
design_16,      0.538,  5.366
design_17,      0.390,  5.202
design_18,      -0.513, 6.703
design_19,      3.481,  5.312
design_20,      4.718,  6.779
design_21,      -0.593, 4.544
design_22,      0.047,  5.111
design_23,      1.413,  4.932
design_24,      0.225,  5.049
design_25,      0.925,  4.636
design_26,      1.334,  6.506
design_27,      0.958,  4.356
design_28,      2.985,  6.054
design_29,      2.416,  5.955
design_30,      2.340,  6.096
design_31,      1.804,  5.552
design_32,      0.581,  4.781
design_33,      6.112,  6.112
design_34,      2.045,  4.528
design_35,      -0.351, 4.197
design_36,      1.505,  5.098
design_37,      3.584,  4.789
design_38,      3.201,  4.947
design_39,      0.352,  4.459
design_40,      0.446,  5.571
design_41,      0.640,  4.857
design_42,      1.962,  9.034
design_43,      -0.159, 4.367
design_44,      2.064,  4.478
design_45,      2.159,  7.982
design_46,      -0.791, 5.964
design_47,      0.972,  5.534
design_48,      -0.121, 4.520
design_49,      4.203,  5.567
design_50,      2.968,  6.413
design_51,      1.922,  4.631
design_52,      1.329,  4.302
design_53,      1.070,  5.821
design_54,      3.140,  4.799
design_55,      0.986,  4.544
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design_56,      2.015,  5.086
design_57,      2.907,  4.814
design_58,      -0.267, 5.860
design_59,      1.494,  4.925
design_60,      0.788,  4.604
design_61,      1.685,  4.388
design_62,      5.595,  5.595
design_63,      0.216,  5.158
design_64,      0.248,  4.388
design_65,      0.854,  5.502
design_66,      -0.762, 6.310
design_67,      0.652,  5.035
design_68,      3.763,  5.804
design_69,      0.354,  4.920
design_70,      2.332,  4.201
design_71,      1.892,  4.452
design_72,      0.219,  4.987
design_73,      1.381,  4.008
design_74,      3.631,  6.508
design_75,      1.091,  4.417
design_76,      2.806,  4.090
design_77,      1.929,  5.070
design_78,      2.818,  6.700
design_79,      0.336,  4.772
design_80,      -0.294, 4.758
design_81,      -0.721, 4.904
design_82,      5.337,  5.337
design_83,      4.863,  7.294
design_84,      1.074,  5.258
design_85,      2.042,  5.114
design_86,      0.134,  6.334
design_87,      -0.030, 4.734
1A2K,   1.464,  4.735
1ACB,   5.057,  5.057
1AHW,   4.171,  5.736
1AK4,   2.474,  4.892
1AKJ,   1.908,  5.010
1AVX,   1.962,  5.923
1AY7,   4.704,  5.568
1AZS,   4.450,  5.497
1B6C,   6.832,  6.832
1BGX,   14.433, 14.433
1BJ1,   1.098,  5.311
1BKD,   9.914,  9.914
1BUH,   1.445,  4.825
1BVK,   1.004,  6.242
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1BVN,   7.157,  7.157
1CGI,   8.839,  8.839
1D6R,   2.568,  5.806
1DE4,   -0.200, 6.141
1DFJ,   1.341,  4.820
1DQJ,   1.140,  7.902
1E4K,   2.221,  4.542
1E6J,   3.578,  5.753
1E96,   4.393,  5.018
1EAW,   6.565,  7.492
1EER,   8.452,  9.040
1EFN,   3.175,  4.376
1EWY,   -0.156, 5.236
1EZU,   6.932,  8.157
1F34,   9.752,  9.752
1F51,   5.831,  7.557
1FAK,   7.265,  7.265
1FC2,   1.708,  6.068
1FQ1,   2.595,  5.425
1FQJ,   -0.122, 5.209
1FSK,   3.359,  5.877
1GCQ,   5.891,  5.891
1GHQ,   3.527,  5.396
1GLA,   0.491,  5.386
1GP2,   4.191,  5.667
1GPW,   6.424,  6.790
1GRN,   5.598,  6.180
1H1V,   0.184,  4.911
1HE1,   5.631,  7.189
1HE8,   3.712,  5.124
1HIA,   1.199,  6.705
1I2M,   8.455,  9.519
1I4D,   2.430,  4.994
1I9R,   0.200,  6.006
1IB1,   4.444,  5.074
1IBR,   8.081,  8.081
1IJK,   1.871,  5.048
1IQD,   6.479,  6.479
1IRA,   10.078, 10.078
1J2J,   0.177,  5.351
1JMO,   10.518, 11.478
1JPS,   3.231,  4.865
1K4C,   4.925,  4.931
1K5D,   7.464,  9.717
1K74,   6.448,  6.608
1KAC,   1.179,  6.621
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1KKL, -0.689, 4.488
1KLU, 4.209, 4.302
1KTZ, 0.824, 4.251
1KXP, 9.238, 9.238
1KXQ, 4.134, 4.666
1M10, 7.108, 7.108
1MAH, 5.602, 5.883
1ML0, 5.545, 6.907
1MLC, 0.234, 5.327
1N2C, 7.851, 9.521
1N8O, 2.585, 6.779
1NCA, 5.878, 5.878
1NSN, 0.404, 5.159
1NW9, 7.540, 7.540
1OPH, -0.271, 5.334
1PPE, 7.417, 7.417
1PXV, 8.093, 8.093
1QA9, 0.201, 4.006
1QFW, 1.362, 5.350
1R0R, 0.730, 6.523
1R8S, 9.424, 10.229
1RLB, -1.162, 7.716
1S1Q, 1.968, 5.492
1SBB, 1.356, 5.708
1T6B, 1.652, 5.716
1UDI, 1.951, 6.299
1VFB, 1.799, 5.679
1WEJ, 1.270, 6.052
1WQ1, 7.426, 8.011
1XD3, 9.036, 9.721
1XQS, 6.380, 7.490
1Y64, 1.650, 7.582
1YVB, 1.452, 4.305
1Z0K, 5.129, 5.216
1Z5Y, 2.383, 4.487
1ZHI, 0.390, 4.683
2AJF, 1.863, 5.712
2B42, 6.405, 6.712
2C0L, 7.290, 7.290
2CFH, 6.546, 9.394
2FD6, -0.478, 4.985
2H7V, 1.659, 7.288
2HLE, 4.315, 7.748
2HMI, -0.654, 5.756
2HQS, 0.770, 5.882
2HRK, 2.469, 4.829

2I25,   6.476, 6.476
2JEL,   0.483, 5.909
2MTA,   1.232, 3.593
2NZ8,   3.837, 4.543
2O8V,   5.683, 5.683
2OOB,   0.452, 4.127
2OT3,   8.787, 9.097
2PCC,   0.947, 5.438
2QFW,   2.185, 5.156
2SIC,   4.378, 4.618
2SNI,   4.838, 4.838
2UUY,   4.660, 5.047
2VIS,   3.572, 5.216
7CEI,   3.335, 4.768
****
Group 11-
REMARK Please use this file to submit your results for both designs and
REMARK the ZDock benchmark.
REMARK Change the file name from GroupXXX.txt to represent your group's
number.
REMARK Change 'Column1' and 'Column2' below to the first- and second-most
REMARK imporant parameters in your score function

REMARK Specify the units for each column below:

Units for Column1: kcal/mol (these are the 'raw values', not yet multiplied
with the weight specified in Table 2)
Units for Column2: kcal/mol (these are the 'raw values', not yet multiplied
with the weight specified in Table 2)

vdW(attractive) Desolvation(ACE)
design_1   -59.211 -5.060
design_2   -56.604 -1.408
design_3   -90.800 -5.772
design_4   -58.342 -2.065
design_5   -60.512 -2.596
design_6   -64.586 -0.390
design_7   -71.300 -3.730
design_8   -61.544 -5.597
design_9   -52.135 -6.524
design_10   -60.785 -9.846
design_11   -57.970 -1.277
design_12   -74.782 -7.072
design_13   -66.480 -2.505
design_14   -57.645 -11.533
design_15   -74.065 2.023

design_16 -71.865 -5.685
design_17 -66.819 1.112
design_18 -63.008 -2.433
design_19 -74.548 -1.673
design_20 -103.010 -2.059
design_21 -60.396 -10.370
design_22 -63.594 -5.837
design_23 -66.785 -10.960
design_24 -70.290 -1.010
design_25 -49.424 -2.550
design_26 -66.516 -2.649
design_27 -65.795 -4.611
design_28 -59.110 0.959
design_29 -68.124 -1.597
design_30 -88.040 -9.013
design_31 -56.225 -2.226
design_32 -45.850 -5.716
design_33 -80.882 -5.915
design_34 -86.106 -4.554
design_35 -88.992 -10.821
design_36 -61.574 -4.090
design_37 -72.348 -5.759
design_38 -81.454 -10.013
design_39 -56.400 -3.166
design_40 -59.345 0.178
design_41 -61.144 -4.870
design_42 -66.668 -4.619
design_43 -66.594 -4.795
design_44 -83.359 -9.864
design_45 -78.610 -9.299
design_46 -59.006 -2.098
design_47 -63.968 -6.594
design_48 -69.579 -6.901
design_49 -59.021 -8.901
design_50 -64.798 -1.720
design_51 -68.176 -5.749
design_52 -81.641 4.354
design_53 -74.510 -1.504
design_54 -64.937 -6.404
design_55 -58.331 -5.163
design_56 -59.447 -5.104
design_57 -74.124 -5.795
design_58 -73.496 -4.355
design_59 -70.413 -7.515
design_60 -57.813 -4.300
design_61 -79.648 -0.722

design_62	-74.618	-5.347
design_63	-67.777	-1.737
design_64	-50.724	-3.860
design_65	-62.670	-0.156
design_66	-62.801	-12.640
design_67	-66.081	4.386
design_68	-60.169	-4.496
design_69	-69.636	-7.386
design_70	-60.055	-4.456
design_71	-74.971	-8.445
design_72	-81.564	-2.248
design_73	-51.074	1.114
design_74	-50.711	-5.319
design_75	-55.231	-4.137
design_76	-83.435	3.631
design_77	-72.862	-2.616
design_78	-55.220	-3.458
design_79	-60.058	2.254
design_80	-58.315	-3.441
design_81	-77.324	3.077
design_82	-71.819	-6.820
design_83	-93.150	-8.135
design_84	-77.284	0.680
design_85	-73.123	-8.766
design_86	-53.359	-3.035
design_87	-67.293	-7.184
1A2K	-87.348	-5.415
1ACB	-92.239	-20.575
1AHW	-110.399	13.443
1AK4	-53.350	-6.688
1AKJ	-90.952	12.565
1AVX	-115.029	-3.416
1AY7	-83.044	9.145
1AZS	-98.373	-8.108
1B6C	-97.748	-5.443
1BGX	-331.511	22.395
1BJ1	-131.143	-7.178
1BKD	-156.196	6.588
1BUH	-79.766	2.631
1BVK	-73.410	7.215
1BVN	-125.282	-10.624
1CGI	-129.611	-22.420
1D6R	-72.814	1.384
1DE4	-111.444	7.764
1DFJ	-108.041	14.611
1DQJ	-102.260	9.318

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1E4K    -64.499 -2.672
1E6J    -74.843 -6.445
1E96    -71.076 2.206
1EAW    -115.413        -0.288
1EER    -181.832        3.838
1EFN    -72.109 -1.761
1EWY    -60.272 7.274
1EZU    -147.063        -17.776
1F34    -161.957        -16.213
1F51    -102.772        0.355
1FAK    -141.154        10.976
1FC2    -64.540 -2.972
1FQ1    -73.902 3.717
1FQJ    -96.992 11.356
1FSK    -118.122        -0.069
1GCQ    -67.671 -5.674
1GHQ    -35.472 -1.323
1GLA    -57.608 -3.591
1GP2    -111.312        1.382
1GPW    -110.355        2.057
1GRN    -113.559        7.689
1H1V    -97.035 -0.775
1HE1    -109.627        -2.546
1HE8    -65.197 2.530
1HIA    -105.017        -8.187
1I2M    -147.846        20.676
1I4D    -83.289 -0.043
1I9R    -78.824 5.841
1IB1    -133.574        15.286
1IBR    -177.170        20.179
1IJK    -76.349 4.946
1IQD    -126.301        -5.014
1IRA    -154.764        3.028
1J2J    -54.694 -8.578
1JMO    -207.283        -15.387
1JPS    -114.687        15.502
1K4C    -99.144 -2.609
1K5D    -145.965        12.589
1K74    -100.013        9.727
1KAC    -67.092 1.968
1KKL    -85.229 0.012
1KLU    -67.302 0.098
1KTZ    -52.892 -6.940
1KXP    -157.666        7.246
1KXQ    -113.013        -5.267
1M10    -104.880        9.711
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1MAH    -103.722        -11.874
1ML0    -122.958        -9.033
1MLC    -87.222 2.712
1N2C    -203.385        -2.531
1N8O    -106.058        -19.525
1NCA    -109.869        6.190
1NSN    -75.190 8.640
1NW9    -125.360        -18.411
1OPH    -89.242 -6.894
1PPE    -108.268        -13.608
1PXV    -142.986        -7.806
1QA9    -56.817 13.001
1QFW    -80.756 4.463
1R0R    -91.890 -14.689
1R8S    -149.111        -17.765
1RLB    -55.621 -1.851
1S1Q    -59.223 -3.248
1SBB    -55.095 1.386
1T6B    -100.892        3.033
1UDI    -95.447 -1.605
1VFB    -79.931 9.549
1WEJ    -84.120 15.623
1WQ1    -141.802        15.083
1XD3    -122.628        -11.004
1XQS    -133.180        20.458
1Y64    -80.931 7.718
1YVB    -88.242 -15.403
1Z0K    -102.206        -4.745
1Z5Y    -76.601 -8.929
1ZHI    -65.549 1.567
2AJF    -74.064 0.941
2B42    -151.548        9.596
2C0L    -93.457 -1.583
2CFH    -131.061        -19.005
2FD6    -74.863 -2.010
2H7V    -78.216 -2.602
2HLE    -118.014        -1.756
2HMI    -61.616 -6.269
2HQS    -125.283        8.942
2HRK    -70.978 -6.242
2I25    -100.796        7.666
2JEL    -84.438 4.702
2MTA    -57.673 -3.345
2NZ8    -128.527        2.681
2O8V    -92.166 -15.677
2OOB    -42.484 -4.926
```

2OT3   -142.081   -15.957
2PCC   -41.453 7.250
2QFW   -80.150 -1.168
2SIC   -93.009 -18.916
2SNI   -97.905 -14.070
2UUY   -95.930 -2.162
2VIS   -68.584 -2.827
7CEI   -87.152 14.771
****
Group 7 -
REMARK Please use this file to submit your results for both designs and
REMARK the ZDock benchmark.
REMARK Change the file name from GroupXXX.txt to represent your group's
number.
REMARK Change 'Column1' and 'Column2' below to the first- and second-most
REMARK important parameters in your score function

REMARK Specify the units for each column below:

Units for Column1: in units of RT
Units for Column2: no units; it is the logarithm of the Rank of the docking
solution

ATTRACT-Score after re-minimization   Logarithm of the Rank of
the docking   solution closest to
the provided complex
after a systematic docking search

design_1 -16.644   3.497
design_2 -14.679   4.920
design_3 -18.373   0.693
design_4 -13.671   5.541
design_5 -16.405   3.258
design_6 -17.422   1.099
design_7 -19.515   1.386
design_8 -17.867   0.693
design_9   -9.871   7.958
design_10 -16.906   3.332
design_11 -14.069   5.517
design_12   -7.862   8.160
design_13 -14.283   5.513
design_14 -15.778   4.718
design_15 -15.339   2.639
design_16 -21.667   0.000
design_17 -13.071   5.313
design_18 -15.396   3.761

design_19	-13.826	3.401
design_20	-24.610	0.000
design_21	-22.813	1.386
design_22	-12.965	5.004
design_23	-14.035	5.268
design_24	-16.301	2.890
design_25	-9.276	7.640
design_26	-10.853	7.809
design_27	-13.170	6.087
design_28	-13.558	4.564
design_29	-17.639	0.000
design_30	-22.989	0.000
design_31	-15.037	3.611
design_32	-11.572	7.288
design_33	-21.587	0.693
design_34	-23.192	0.000
design_35	-23.096	0.000
design_36	-19.520	2.639
design_37	-22.080	0.693
design_38	-14.043	3.045
design_39	-17.866	2.079
design_40	-15.769	5.209
design_41	-14.878	5.434
design_42	-12.192	5.956
design_43	-11.207	7.604
design_44	-21.438	1.609
design_45	-16.757	3.434
design_46	-14.514	4.369
design_47	-9.683	8.543
design_48	-13.283	5.666
design_49	-14.129	5.011
design_50	-17.068	1.099
design_51	-17.126	2.303
design_52	-19.405	1.099
design_53	-20.689	2.996
design_54	-13.519	5.412
design_55	-14.356	5.347
design_56	-9.645	8.339
design_57	-19.523	1.609
design_58	-15.294	4.511
design_59	-12.465	5.455
design_60	-15.338	4.682
design_61	-23.168	0.693
design_62	-14.888	3.807
design_63	-15.806	5.037
design_64	-13.182	5.638

design_65	-14.691	3.829
design_66	-16.136	3.497
design_67	-15.665	4.394
design_68	-11.068	6.576
design_69	-12.113	6.538
design_70	-14.251	5.707
design_71	-16.027	3.178
design_72	-13.028	5.956
design_73	-11.408	7.339
design_74	-13.150	6.347
design_75	-14.066	5.333
design_76	-11.357	7.274
design_77	-27.318	0.000
design_78	-11.425	7.430
design_79	-11.950	6.304
design_80	-16.292	3.367
design_81	-22.026	0.000
design_82	-17.344	1.609
design_83	-17.319	4.263
design_84	-16.923	3.367
design_85	-18.457	1.609
design_86	-12.172	6.205
design_87	-15.243	5.288
1A2K	-21.196	0.000
1ACB	-23.441	0.000
1AHW	-18.820	2.079
1AK4	-19.938	1.099
1AKJ	-18.428	0.693
1AVX	-27.226	0.000
1AY7	-20.298	0.000
1B6C	-27.424	0.000
1BGX	-5.782	9.185
1BJ1	-28.518	0.000
1BUH	-20.029	0.000
1BVK	-18.058	2.079
1BVN	-31.345	0.000
1CGI	-30.790	0.000
1D6R	-20.888	0.000
1DFJ	-29.619	0.000
1DQJ	-15.870	3.689
1E6J	-22.270	0.000
1E96	-17.651	0.693
1EAW	-27.000	0.000
1EER	-31.699	0.000
1EWY	-15.768	3.850
1EZU	-28.307	0.000

1F34	-32.465	0.693
1F51	-25.894	0.000
1FAK	-30.314	0.000
1FC2	-22.534	0.000
1FQ1	-23.561	0.000
1FQJ	-20.311	0.000
1FSK	-30.278	0.000
1GCQ	-19.403	1.099
1GHQ	-5.870	9.527
1GP2	-6.608	8.515
1GRN	-18.455	1.386
1H1V	-23.177	0.000
1HE1	-23.992	0.000
1HE8	-16.981	2.197
1HIA	-25.430	0.000
1I2M	-36.317	0.000
1I4D	-18.496	1.609
1I9R	-18.056	0.000
1IB1	-21.416	0.000
1IBR	-27.969	0.000
1IJK	-25.971	0.000
1IQD	-27.911	0.000
1JPS	-22.721	0.000
1K4C	-29.713	0.000
1K5D	-29.208	0.000
1KAC	-17.231	2.565
1KKL	-18.439	3.296
1KLU	-21.236	0.000
1KTZ	-13.716	4.796
1KXP	-32.477	0.000
1KXQ	-27.394	0.000
1M10	-22.822	0.000
1MAH	-18.722	1.386
1ML0	-26.423	0.693
1MLC	-22.416	0.000
1NCA	-21.519	0.693
1NSN	-21.242	0.000
1PPE	-24.538	0.000
1QA9	-17.660	1.609
1QFW	-21.309	0.000
1RLB	-17.971	0.000
1SBB	-21.381	0.000
1UDI	-24.829	0.000
1VFB	-19.408	0.000
1WEJ	-20.421	0.000
1WQ1	-26.479	0.000

2HMI	-15.128	4.489
2JEL	-16.492	2.833
2MTA	-18.357	2.197
2PCC	-15.929	2.197
2QFW	-18.038	1.792
2SIC	-22.684	0.000
2SNI	-22.158	0.000
2VIS	-21.912	1.099
7CEI	-23.151	0.000
1J2J	-21.213	0.000
1IRA	-23.087	0.000
1GPW	-26.651	0.000
1GLA	-19.289	1.386
1EFN	-21.268	1.386
1E4K	-27.875	1.099
1BKD	-38.822	0.000
1AZS	-20.472	0.693
1Y64	-18.682	2.485
1XQS	-30.959	0.000
1XD3	-29.763	0.000
1T6B	-27.147	0.000
1S1Q	-15.847	1.099
1R8S	-34.505	0.693
1R0R	-25.159	0.000
1PXV	-28.588	0.000
1OPH	-26.582	0.000
1NW9	-25.493	0.000
1N8O	-25.978	0.000
1K74	-29.452	1.609
1JMO	-36.874	0.000
2CFH	-37.068	0.693
2C0L	-23.069	0.000
2B42	-31.694	0.000
2AJF	-21.583	1.099
1ZHI	-19.302	1.946
1Z5Y	-21.417	0.693
1Z0K	-23.677	0.000
1YVB	-19.780	1.386
2UUY	-20.116	0.000
2OT3	-20.509	0.000
2OOB	-16.177	2.079
2O8V	-23.684	0.000
2NZ8	-28.925	0.000
2I25	-23.232	1.099
2HRK	-19.743	0.000
2HQS	-27.587	0.000

```
2HLE  -16.555    1.792
2H7V  -18.759    0.000
2FD6  -22.064    0.693

**************************

::::::::::::
From this point on scripts for producing and analyzing the data
::::::::::::

::::::::::::::
scripts/ddg_sasa1.xml
::::::::::::::
Report the binding energy and buried surface area. Suggested commandline:

rosetta_scripts -s <PDB> -parser:protocol ddg_sasa1.xml -database ~/
minirosetta_database -ex1 -ex2 -use_input_sc
<dock_design>
        <SCOREFXNS>
        </SCOREFXNS>
        <FILTERS>
                <Sasa name=sasa confidence=0/> buried surface area
                <Ddg name=ddg confidence=0 repeats=3/> binding energy;
repeats: takes the average of several computations to reduce numerical
error
        </FILTERS>
        <MOVERS>
                <AtomTree name=docking_tree docking_ft=1/> forms a docking-
compatible fold tree
        </MOVERS>
        <APPLY_TO_POSE>
        </APPLY_TO_POSE>
        <PROTOCOLS>
                <Add mover_name=docking_tree filter_name=ddg/>
                <Add filter_name=sasa/>
        </PROTOCOLS>
</dock_design>
::::::::::::::
scripts/ddg_sasa2.xml
::::::::::::::
Used to compute binding energies across the interface formed between chains
1/2 and 3. See ddg_sasa1.xml for details

<dock_design>
        <SCOREFXNS>
        </SCOREFXNS>
```

```
        <FILTERS>
                <Sasa name=sasa confidence=0 jump=2/>
                <Ddg name=ddg confidence=0 repeats=3 jump=2/>
        </FILTERS>
        <MOVERS>
                <AtomTree name=docking_tree docking_ft=1/>
        </MOVERS>
        <APPLY_TO_POSE>
        </APPLY_TO_POSE>
        <PROTOCOLS>
                <Add mover_name=docking_tree filter_name=ddg/>
                <Add filter_name=sasa/>
        </PROTOCOLS>
</dock_design>
::::::::::::::
scripts/degree.xml
::::::::::::::
Used to compute the average degree of residues at the interface. See Figure
S2 for examples

Suggested commandline:

rosetta_scripts -s <PDB> -parser:protocol degree.xml -database ~/
minirosetta_database

<dock_design>
        <TASKOPERATIONS>
          <ProteinInterfaceDesign name=pido repack_chain1=0
design_chain1=0/> for computations spanning both chains, use
repack_chain1=1 design_chain1=1
        </TASKOPERATIONS>
        <SCOREFXNS>
        </SCOREFXNS>
        <FILTERS>
                <AverageDegree name=degree distance_threshold=8
threshold=8.5 task_operations=pido confidence=0/> distance_threshold: what
radius sphere to use around each residue; threshold: how many residue
neighbours to require within sphere; confidence: change to 1 to effect an
actual filter; with 0, only reports values
        </FILTERS>
        <MOVERS>
                <AtomTree name=docking_tree docking_ft=1/>
        </MOVERS>
        <APPLY_TO_POSE>
        </APPLY_TO_POSE>
        <PROTOCOLS>
```

```
                <Add mover=docking_tree filter=degree/>
        </PROTOCOLS>
</dock_design>
::::::::::::::
scripts/dock1.xml
::::::::::::::
Docking refinement of a complex using high-resolution RosettaDock (Gray et
al. 2003, JMB 331, 281). Also reports binding energy, buried surface area
and RMSD from starting structure.

Suggested commandline:
rosetta_scripts -s <PDB> -parser:protocol dock1.xml -database ~/
minirosetta_database -ex1 -ex2 -use_input_sc -nstruct 100

<dock_design>
        <SCOREFXNS>
        </SCOREFXNS>
        <FILTERS>
                <Sasa name=sasa confidence=0/> buried surface area
                <Ddg name=ddg confidence=0/> binding energy
                <Rmsd name=rmsd confidence=0/>
        </FILTERS>
        <MOVERS>
                <Docking name=dock1 fullatom=1 local_refine=1
score_high=score12/> To do more exansive docking use local_refine=0
        </MOVERS>
        <APPLY_TO_POSE>
        </APPLY_TO_POSE>
        <PROTOCOLS>
                <Add mover_name=dock1/>
                <Add filter_name=sasa/>
                <Add filter_name=ddg/>
                <Add filter_name=rmsd/>
        </PROTOCOLS>
</dock_design>
::::::::::::::
scripts/dock2.xml
::::::::::::::
Docking across the interface between chains 1/2 and 3. See dock1.xml for
details.
<dock_design>
        <SCOREFXNS>
        </SCOREFXNS>
        <FILTERS>
                <Sasa name=sasa confidence=0/>
                <Ddg name=ddg confidence=0/>
```

```
                <Rmsd name=rmsd confidence=0/>
        </FILTERS>
        <MOVERS>
                <Docking name=dock1 fullatom=1 local_refine=1
movable_jumps=2 score_high=score12/>
        </MOVERS>
        <APPLY_TO_POSE>
        </APPLY_TO_POSE>
        <PROTOCOLS>
                <Add mover_name=dock1/>
                <Add filter_name=sasa/>
                <Add filter_name=ddg/>
                <Add filter_name=rmsd/>
        </PROTOCOLS>
</dock_design>
::::::::::::::
scripts/ppk0.xml
::::::::::::::
Prepack a protein structure without separating the chains. Carries out
sidechain minimization, repacking and minimization.

Suggested commandline:

rosetta_scripts -s <PDB> -parser:protocol ppk0.xml -database ~/
minirosetta_database -ex1 -ex2 -use_input_sc

<dock_design>
        <SCOREFXNS>
        </SCOREFXNS>
        <FILTERS>
        </FILTERS>
        <MOVERS>
                <Prepack name=ppk jump_number=0 scorefxn=score12/>
        </MOVERS>
        <APPLY_TO_POSE>
        </APPLY_TO_POSE>
        <PROTOCOLS>
                <Add mover_name=ppk/>
        </PROTOCOLS>
</dock_design>
::::::::::::::
scripts/ppk1.xml
::::::::::::::
Prepack a structure by first separating the chains. See ppk0.xml for
details.
```

```
<dock_design>
        <SCOREFXNS>
        </SCOREFXNS>
        <FILTERS>
        </FILTERS>
        <MOVERS>
                <Prepack name=ppk jump_number=1 scorefxn=score12/>
        </MOVERS>
        <APPLY_TO_POSE>
        </APPLY_TO_POSE>
        <PROTOCOLS>
                <Add mover_name=ppk/>
        </PROTOCOLS>
</dock_design>
::::::::::::::
scripts/ppk2.xml
::::::::::::::
Prepack a structure by separating chains 1/2 from 3. See ppk0.xml for
details.
<dock_design>
        <SCOREFXNS>
        </SCOREFXNS>
        <FILTERS>
        </FILTERS>
        <MOVERS>
                <Prepack name=ppk jump_number=2 scorefxn=score12/>
        </MOVERS>
        <APPLY_TO_POSE>
        </APPLY_TO_POSE>
        <PROTOCOLS>
                <Add mover_name=ppk/>
        </PROTOCOLS>
</dock_design>
::::::::::::::
scripts/generic_ROC.gnu
::::::::::::::
#A script to generate a histogram with gnuplot. Switch XXX with the name of
the histogram and YYY with the data file. Use on the output from
ROC_coords.sh
#Sarel Fleishman 2011
set style fill solid 1.0 border -1
set style line 10 linetype 1
set xtics border nomirror
set ytics border nomirror
set xrange [0:1]
set yrange [0:1]
```

```
set xlabel 'Designs'
set ylabel 'Natives'
set title 'XXX'
set nokey
plot 'YYY' u 1:2 w lines, x
set terminal postscript enhanced color
set output 'XXX.eps'
replot
::::::::::::::
scripts/hist_generic.gnu
::::::::::::::
#Generates a histogram with gnuplot. Histograms are only supported from
gnuplot v4.4 onwards.
#Change XXX to the data file name
#Sarel Fleishman 2011

set style data histogram
set style histogram cluster gap 1
set boxwidth 0.9
set style fill solid 1.0 border -1
set style line 10 linetype 1
set xtics border nomirror
set ytics border nomirror
set xlabel 'Binding categories'
set ylabel 'Counts'
set xtic rotate by -45 scale 0
set terminal postscript enhanced color
set output 'XXX.eps'
plot 'XXX' using 4 ti 'designs', '' u 3:xticlabels(1) ti 'natives'
replot
```