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*** DrugScore-PPI 1.0 ***
Knowledge-based Scoring Function to
Predict Protein-Protein Interactions
D. M. Krüger, H. Gohlke
2009
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In silico alanine scanning on chain A for PDB-ID cluster2\_1.  
(file uploaded by user)

Date: 2018-05-08 15:38:12

Residue	ddGcalc [kcal/mol]	Degree Of Buriedness	Possible Saltbridges
TYR6A	0.44	4.88	-
TRP7A	0.24	2.83	-
LEU12A	0.67	1.83	-
MET34A	0.19	6.44	-
ASP39A	3.51	7.57	-
TYR40A	0.16	4.74	-
ASP41A	0.93	6.21	-
ARG42A	-0.05	3.03	-
SER43A	0.09	3.11	-
TRP45A	0.49	2.75	-
LEU46A	1.45	6.34	-
ASN47A	0.07	2.37	-
GLU48A	0.07	5.18	-
LYS49A	1.16	6.69	-
PHE50A	1.36	5.87	-
LYS51A	0.42	4.14	-
ASP55A	1.07	3.78	-
PHE56A	1.12	4.19	-
ASN58A	0.35	5.89	-
LEU59A	0.40	3.67	-
HIS67A	0.08	2.86	-
LYS68A	0.10	3.32	-
ILE69A	0.46	4.56	-
THR70A	0.25	6.08	-
GLN71A	0.28	7.07	-
SER72A	0.07	1.60	-
ASN73A	0.02	5.49	-
ILE75A	0.16	5.50	-
ARG77A	0.94	6.89	X
ARG81A	0.09	6.19	X
THR89A	0.15	4.96	-
GLU90A	0.38	4.23	-
LYS93A	0.94	8.32	-
ILE94A	0.76	4.56	-
ARG95A	0.18	6.10	-
VAL96A	0.23	5.38	-
ASP97A	2.55	8.71	-
ILE98A	0.05	1.83	-
GLU100A	0.58	7.33	-
ASN101A	0.59	5.89	-
VAL103A	0.12	4.27	-
MET104A	0.47	6.34	-
ASP105A	0.11	3.71	-
HIS107A	-0.06	3.80	-
MET108A	0.43	2.72	-
VAL111A	0.47	3.22	-
ARG112A	-0.06	5.01	-
TYR115A	0.27	6.45	-
ASP116A	1.61	8.71	-
ASP118A	0.39	2.50	-
LEU122A	0.05	1.83	-
PHE154A	0.15	2.50	-
SER211A	0.17	4.62	-

