

**Table 3.** Contact energies in RT units;  $e_{ij}$  for upper half and diagonal and  $e'_{ij}$  for lower half

Cys	Met	Phe	Ile	Leu	Val	Trp	Tyr	Ala	Gly	Thr	Ser	Asn	Gln	Asp	Glu	His	Arg	Lys	Pro	
Cys	-5.44	-4.99	-5.80	-5.50	-5.83	-4.96	-4.95	-4.16	-3.57	-3.16	-3.11	-2.86	-2.59	-2.85	-2.41	-2.27	-3.60	-2.57	-1.95	-3.07
Met	0.46	-5.46	-6.56	-6.02	-6.41	-5.32	-5.55	-4.91	-3.94	-3.39	-3.51	-3.03	-2.95	-3.30	-2.57	-2.89	-3.98	-3.12	-2.48	-3.45
Phe	0.54	-0.20	-7.26	-6.84	-7.28	-6.29	-6.16	-5.66	-4.81	-4.13	-4.28	-4.02	-3.75	-4.10	-3.48	-3.56	-4.77	-3.98	-3.36	-4.25
Ile	0.49	-0.01	0.06	-6.54	-7.04	-6.05	-5.78	-5.25	-4.58	-3.78	-4.03	-3.52	-3.24	-3.67	-3.17	-3.27	-4.14	-3.63	-3.01	-3.76
Leu	0.57	0.01	0.03	-0.08	-7.37	-6.48	-6.14	-5.67	-4.91	-4.16	-4.34	-3.92	-3.74	-4.04	-3.40	-3.59	-4.54	-4.03	-3.37	-4.20
Val	0.52	0.18	0.10	-0.01	-0.04	-5.52	-5.18	-4.62	-4.04	-3.38	-3.46	-3.05	-2.83	-3.07	-2.48	-2.67	-3.58	-3.07	-2.49	-3.32
Trp	0.30	-0.29	0.00	0.02	0.08	0.11	-5.06	-4.66	-3.82	-3.42	-3.22	-2.99	-3.07	-3.11	-2.84	-2.99	-3.98	-3.41	-2.69	-3.73
Tyr	0.64	-0.10	0.05	0.11	0.10	0.23	-0.04	-4.17	-3.36	-3.01	-3.01	-2.78	-2.76	-2.97	-2.76	-2.79	-3.52	-3.16	-2.60	-3.19
Ala	0.51	0.15	0.17	0.05	0.13	0.08	0.07	0.09	-2.72	-2.31	-2.32	-2.01	-1.84	-1.89	-1.70	-1.51	-2.41	-1.83	-1.31	-2.03
Gly	0.68	0.46	0.62	0.62	0.65	0.51	0.24	0.20	0.18	-2.24	-2.08	-1.82	-1.74	-1.66	-1.59	-1.22	-2.15	-1.72	-1.15	-1.87
Thr	0.67	0.28	0.41	0.30	0.40	0.36	0.37	0.13	0.10	0.10	-2.12	-1.96	-1.88	-1.90	-1.80	-1.74	-2.42	-1.90	-1.31	-1.90
Ser	0.69	0.53	0.44	0.59	0.60	0.55	0.38	0.14	0.18	0.14	-0.06	-1.67	-1.58	-1.49	-1.63	-1.48	-2.11	-1.62	-1.05	-1.57
Asn	0.97	0.62	0.72	0.87	0.79	0.77	0.30	0.17	0.36	0.22	0.02	0.10	-1.68	-1.71	-1.68	-1.51	-2.08	-1.64	-1.21	-1.53
Gln	0.64	0.20	0.30	0.37	0.42	0.46	0.19	-0.12	0.24	0.24	-0.08	0.11	-0.10	-1.54	-1.46	-1.42	-1.98	-1.80	-1.29	-1.73
Asp	0.91	0.77	0.75	0.71	0.89	0.89	0.30	-0.07	0.26	0.13	-0.14	-0.19	-0.24	-0.09	-1.21	-1.02	-2.32	-2.29	-1.68	-1.33
Glu	0.91	0.30	0.52	0.46	0.55	0.55	0.00	-0.25	0.30	0.36	-0.22	-0.19	-0.21	-0.19	0.05	-0.91	-2.15	-2.27	-1.80	-1.26
His	0.65	0.28	0.39	0.66	0.67	0.70	0.08	0.09	0.47	0.50	0.16	0.26	0.29	0.31	-0.19	-0.16	-3.05	-2.16	-1.35	-2.25
Arg	0.93	0.38	0.42	0.41	0.43	0.47	-0.11	-0.30	0.30	0.18	-0.07	-0.01	-0.02	-0.26	-0.91	-1.04	0.14	-1.55	-0.59	-1.70
Lys	0.83	0.31	0.33	0.32	0.37	0.33	-0.10	-0.46	0.11	0.03	-0.19	-0.15	-0.30	-0.46	-1.01	-1.28	0.23	0.24	-0.12	-0.97
Pro	0.53	0.16	0.25	0.39	0.35	0.31	-0.33	-0.23	0.20	0.13	0.04	0.14	0.18	-0.08	0.14	0.07	0.15	-0.05	-0.04	-1.75

$e_{rr}$  - 2.55  $e_{rr}$  -3.57 -3.92 -4.76 -4.42 -4.81 -3.89 -3.81 -3.41 -2.57 -2.19 -2.29 -1.98 -1.92 -2.00 -1.84 -1.79 -2.56 -2.11 -1.52 -2.09  
 $e_r$  - 3.60  $e_i$  -4.29 -4.73 -5.57 -5.29 -5.71 -4.72 -4.41 -3.87 -3.17 -2.53 -2.63 -2.27 -2.14 -2.35 -2.02 -2.07 -2.94 -2.43 -1.82 -2.53  
 $f_r$  - 3.60  $f_i$  -5.58 -6.14 -7.39 -7.09 -7.88 -6.15 -5.34 -4.60 -3.24 -2.22 -2.48 -1.92 -1.74 -1.93 -1.54 -1.49 -2.91 -2.07 -1.17 -1.97  
 $N_{ii}/N_i$  2.096 2.723 2.722 2.780 2.811 2.893 2.728 2.537 2.493 2.143 1.840 1.973 1.771 1.699 1.720 1.598 1.508 2.075 1.787 1.343 1.629  
 $q_i$  7.162 6.281 6.646 6.137 5.870 6.042 6.087 6.155 5.793 6.037 6.334 6.284 6.486 6.582 6.574 6.469 6.487 6.235 6.241 6.318 6.569 5.858