

JSCH-2005 data set: Results with infinite non-bonded cut-offs

	MM2*	MM2*+LP	MM3*	AMBER*	AMBER*+LP	AMBER+1012	OPLS	OPLS-AA	MMFF-94	MMFF-94s
H-bonding										
ME	-13.04	-13.04	-13.09	-4.84	-4.47	-4.90	-5.18	-4.80	-4.38	-4.55
MUE	12.74	12.74	13.13	5.04	4.68	5.22	5.21	4.68	4.26	4.43
RMSE	15.13	15.13	15.98	6.41	5.98	6.56	5.98	5.36	5.26	5.29
Interstrand										
ME	-0.60	-0.61	0.14	0.86	0.86	0.84	0.80	0.89	0.82	-0.06
MUE	1.37	1.37	1.43	0.87	0.87	0.86	0.77	0.85	0.97	0.41
RMSE	1.85	1.85	1.77	1.11	1.11	1.10	1.01	1.06	1.25	0.68
Stacking										
ME	-3.96	-3.96	-3.46	0.92	0.92	0.90	-0.33	-0.11	-1.08	-2.44
MUE	4.37	4.37	3.91	1.75	1.75	1.74	1.45	1.32	1.74	2.77
RMSE	5.14	5.14	4.75	2.17	2.17	2.16	1.77	1.65	2.11	2.97
Amino acids										
ME	-2.08	-2.41	-1.30	-3.21	-3.23	-3.15	-1.02	-0.94	-2.71	-2.73
MUE	2.18	2.42	2.70	3.21	3.23	3.15	1.72	1.39	2.77	2.78
RMSE	3.01	3.34	2.96	4.29	4.30	4.30	2.53	1.74	3.24	3.24
Total:										
MUE	4.76	4.80	4.36	2.41	2.31	2.43	2.10	1.87	2.13	2.47
RMSE	6.72	6.74	6.46	3.60	3.39	3.62	3.06	2.59	2.79	3.11

JSCH-2005 data set: Results with default (vdW 7 Å, electrostatic 12 Å) non-bonded cut-offs

	MM2*	MM2*+LP	MM3*	AMBER*	AMBER*+LP	AMBER+1012	OPLS	OPLS-AA	MMFF-94	MMFF-94s
H-bonding										
ME	-13.28	-13.28	-12.79	-4.74	-4.42	-4.80	-4.97	-4.17	-4.05	-4.21
MUE	12.97	12.97	12.87	4.96	4.66	5.13	5.00	4.06	3.97	4.10
RMSE	14.65	14.65	14.99	6.39	6.03	6.50	5.80	4.64	4.85	4.89
Interstrand										
ME	-0.47	-0.47	0.90	1.67	1.67	1.65	2.24	2.33	2.15	1.31
MUE	1.45	1.45	1.71	1.66	1.66	1.64	2.12	2.18	2.06	1.41
RMSE	1.92	1.92	2.02	1.85	1.85	1.84	2.51	2.52	2.47	1.81
Stacking										
ME	-3.96	-2.09	-3.44	0.95	0.95	0.93	-0.27	-0.06	-1.01	-2.36
MUE	4.37	3.49	3.95	1.74	1.74	1.73	1.50	1.38	1.78	2.83
RMSE	5.15	4.49	4.76	2.17	2.17	2.17	1.91	1.80	2.23	3.05
Amino acids										
ME	-2.26	-2.55	-1.46	-3.13	-3.13	-3.13	-1.12	-0.99	-2.71	-2.72
MUE	2.42	2.55	2.77	3.20	3.20	3.31	1.93	1.79	2.92	2.93
RMSE	3.30	3.42	3.11	4.42	4.42	4.49	2.87	2.46	3.52	3.52
Total:										
MUE	4.88	4.55	4.41	2.59	2.51	2.63	2.44	2.16	2.37	2.68
RMSE	6.83	6.66	6.42	3.78	3.62	3.81	3.34	2.82	3.03	3.24

JSCH-2005 data set: Results with default bond dipole cut-offs

	MM2*	MM2*+LP	MM3*	AMBER*	AMBER*+LP	AMBER+1012	OPLS	OPLS-AA	MMFF-94	MMFF-94s
H-bonding										
ME	-10.74	-10.74	-10.75	-4.43	-3.99	-4.43	-4.81	-4.33	-3.69	-3.93
MUE	10.45	10.45	10.45	4.66	4.23	4.79	4.85	4.20	3.58	3.81
RMSE	11.90	11.90	12.98	6.03	5.47	6.07	5.57	4.69	4.24	4.43
Interstrand										
ME	-0.68	-0.68	0.05	0.76	0.76	0.74	0.67	0.78	0.82	-0.06
MUE	1.38	1.38	1.41	0.80	0.80	0.80	0.68	0.77	0.97	0.42
RMSE	1.88	1.88	1.76	1.04	1.04	1.03	0.92	0.98	1.25	0.68
Stacking										
ME	-3.97	-3.97	-3.48	0.91	0.91	0.88	-0.35	-0.14	-1.08	-2.44
MUE	4.38	4.38	3.92	1.75	1.75	1.73	1.45	1.33	1.74	2.77
RMSE	5.16	5.16	4.76	2.16	2.16	2.16	1.77	1.65	2.11	2.97
Amino acids										
ME	-2.20	-2.54	-1.42	-3.32	-3.35	-3.26	-1.19	-1.08	-2.74	-2.75
MUE	2.29	2.54	2.78	3.32	3.35	3.26	1.82	1.48	2.79	2.80
RMSE	3.09	3.42	3.02	4.37	4.38	4.37	2.59	1.83	3.25	3.26
Total:										
MUE	4.81	4.84	4.40	2.43	2.33	2.44	2.12	1.89	2.13	2.47
RMSE	6.76	6.78	6.55	3.64	3.43	3.65	3.10	2.63	2.79	3.10