

Supplementary material: Table 1. Optimized direct pair potentials derived in the context of Rigid trap states.

ALA	ALA	-2.88	ALA	ARG	1.97	ALA	ASN	0.90	ALA	ASP	1.52
ALA	CYS	-2.67	ALA	GLN	1.25	ALA	GLU	1.99	ALA	GLY	0.09
ALA	HIS	-0.16	ALA	ILE	-3.33	ALA	LEU	-2.85	ALA	LYS	3.22
ALA	MET	-0.56	ALA	PHE	-1.30	ALA	PRO	1.17	ALA	SER	-0.86
ALA	THR	0.34	ALA	TRP	-1.34	ALA	TYR	-1.55	ALA	VAL	-3.15
ARG	ARG	2.31	ARG	ASN	1.63	ARG	ASP	1.80	ARG	CYS	0.75
ARG	GLN	2.14	ARG	GLU	1.66	ARG	GLY	0.77	ARG	HIS	0.41
ARG	ILE	1.45	ARG	LEU	1.96	ARG	LYS	3.48	ARG	MET	0.92
ARG	PHE	1.56	ARG	PRO	1.94	ARG	SER	1.70	ARG	THR	1.06
ARG	TRP	-2.32	ARG	TYR	0.97	ARG	VAL	1.43	ASN	ASN	-1.91
ASN	ASP	1.02	ASN	CYS	0.86	ASN	GLN	1.41	ASN	GLU	2.42
ASN	GLY	1.03	ASN	HIS	0.48	ASN	ILE	2.11	ASN	LEU	0.64
ASN	LYS	2.66	ASN	MET	1.69	ASN	PHE	-0.45	ASN	PRO	0.09
ASN	SER	0.70	ASN	THR	1.14	ASN	TRP	1.48	ASN	TYR	0.97
ASN	VAL	2.68	ASP	ASP	1.73	ASP	CYS	1.46	ASP	GLN	2.99
ASP	GLU	3.13	ASP	GLY	1.41	ASP	HIS	-0.35	ASP	ILE	1.77
ASP	LEU	2.67	ASP	LYS	2.49	ASP	MET	2.33	ASP	PHE	1.90
ASP	PRO	2.56	ASP	SER	0.63	ASP	THR	0.42	ASP	TRP	1.18
ASP	TYR	2.35	ASP	VAL	1.36	CYS	CYS	-5.23	CYS	GLN	1.77
CYS	GLU	-0.22	CYS	GLY	-9.49	CYS	HIS	-0.30	CYS	ILE	-0.32
CYS	LEU	-2.86	CYS	LYS	3.17	CYS	MET	-0.64	CYS	PHE	-2.10
CYS	PRO	-1.74	CYS	SER	-4.84	CYS	THR	0.42	CYS	TRP	-1.08
CYS	TYR	-2.07	CYS	VAL	-2.63	GLN	GLN	0.08	GLN	GLU	2.65
GLN	GLY	1.13	GLN	HIS	1.76	GLN	ILE	1.50	GLN	LEU	1.42
GLN	LYS	2.67	GLN	MET	-0.64	GLN	PHE	-0.31	GLN	PRO	0.53
GLN	SER	1.83	GLN	THR	2.26	GLN	TRP	1.80	GLN	TYR	2.41
GLN	VAL	0.61	GLU	GLU	2.55	GLU	GLY	2.74	GLU	HIS	3.21
GLU	ILE	2.25	GLU	LEU	2.19	GLU	LYS	2.50	GLU	MET	1.39
GLU	PHE	1.87	GLU	PRO	1.99	GLU	SER	0.80	GLU	THR	1.72
GLU	TRP	3.17	GLU	TYR	1.63	GLU	VAL	2.80	GLY	GLY	-3.77
GLY	HIS	0.95	GLY	ILE	-2.84	GLY	LEU	-0.42	GLY	LYS	2.37
GLY	MET	-1.76	GLY	PHE	0.15	GLY	PRO	0.81	GLY	SER	0.11
GLY	THR	-1.49	GLY	TRP	-0.61	GLY	TYR	-0.77	GLY	VAL	-0.35
HIS	HIS	-1.88	HIS	ILE	1.71	HIS	LEU	-1.67	HIS	LYS	3.30
HIS	MET	-1.06	HIS	PHE	0.65	HIS	PRO	-0.36	HIS	SER	1.16
HIS	THR	2.09	HIS	TRP	-0.44	HIS	TYR	-1.41	HIS	VAL	0.12
ILE	ILE	-8.67	ILE	LEU	-3.70	ILE	LYS	3.52	ILE	MET	-3.31
ILE	PHE	-5.97	ILE	PRO	-1.51	ILE	SER	1.05	ILE	THR	-1.92
ILE	TRP	-2.58	ILE	TYR	-5.09	ILE	VAL	-5.26	LEU	LEU	-8.34
LEU	LYS	2.77	LEU	MET	-1.92	LEU	PHE	-4.86	LEU	PRO	-0.31

LEU	SER	−0.38		LEU	THR	−0.24		LEU	TRP	−2.85		LEU	TYR	−0.27
LEU	VAL	−5.07		LYS	LYS	2.54		LYS	MET	2.30		LYS	PHE	2.54
LYS	PRO	2.42		LYS	SER	2.37		LYS	THR	2.78		LYS	TRP	2.74
LYS	TYR	2.01		LYS	VAL	2.03		MET	MET	−2.66		MET	PHE	−3.23
MET	PRO	0.19		MET	SER	−0.55		MET	THR	1.35		MET	TRP	−0.42
MET	TYR	−0.77		MET	VAL	−3.69		PHE	PHE	−5.09		PHE	PRO	−2.35
PHE	SER	1.96		PHE	THR	0.36		PHE	TRP	−1.96		PHE	TYR	−1.30
PHE	VAL	−4.74		PRO	PRO	1.49		PRO	SER	0.90		PRO	THR	0.91
PRO	TRP	−3.27		PRO	TYR	−2.29		PRO	VAL	0.02		SER	SER	−0.80
SER	THR	−0.17		SER	TRP	−0.23		SER	TYR	1.25		SER	VAL	0.68
THR	THR	−2.48		THR	TRP	−4.71		THR	TYR	0.31		THR	VAL	0.20
TRP	TRP	−0.61		TRP	TYR	−1.63		TRP	VAL	0.93		TYR	TYR	−3.47
TYR	VAL	−1.54		VAL	VAL	−13.07								

Supplementary material: Table 2. Optimized water-mediated pair potentials derived in the context of Rigid trap states.

ALA	ALA	-0.22	ALA	ARG	1.00	ALA	ASN	0.20	ALA	ASP	0.66
ALA	CYS	0.54	ALA	GLN	0.83	ALA	GLU	1.11	ALA	GLY	-2.03
ALA	HIS	1.59	ALA	ILE	0.45	ALA	LEU	0.32	ALA	LYS	0.02
ALA	MET	1.16	ALA	PHE	-0.80	ALA	PRO	-0.39	ALA	SER	-1.03
ALA	THR	-0.12	ALA	TRP	1.31	ALA	TYR	2.02	ALA	VAL	-0.46
ARG	ARG	-1.50	ARG	ASN	-0.17	ARG	ASP	-1.90	ARG	CYS	0.03
ARG	GLN	-0.75	ARG	GLU	-1.56	ARG	GLY	-0.63	ARG	HIS	-3.40
ARG	ILE	-0.83	ARG	LEU	0.63	ARG	LYS	0.72	ARG	MET	0.94
ARG	PHE	-0.73	ARG	PRO	-0.05	ARG	SER	-0.28	ARG	THR	0.21
ARG	TRP	-0.34	ARG	TYR	-2.54	ARG	VAL	1.16	ASN	ASN	-2.55
ASN	ASP	-1.14	ASN	CYS	1.15	ASN	GLN	0.90	ASN	GLU	0.73
ASN	GLY	0.04	ASN	HIS	1.42	ASN	ILE	2.50	ASN	LEU	0.31
ASN	LYS	1.75	ASN	MET	-0.68	ASN	PHE	0.33	ASN	PRO	-1.81
ASN	SER	0.52	ASN	THR	0.54	ASN	TRP	-1.01	ASN	TYR	0.02
ASN	VAL	0.60	ASP	ASP	-1.70	ASP	CYS	1.17	ASP	GLN	0.73
ASP	GLU	1.55	ASP	GLY	0.38	ASP	HIS	-2.20	ASP	ILE	2.97
ASP	LEU	0.67	ASP	LYS	-0.95	ASP	MET	1.06	ASP	PHE	2.31
ASP	PRO	-0.21	ASP	SER	-1.31	ASP	THR	-1.47	ASP	TRP	1.25
ASP	TYR	-1.37	ASP	VAL	-0.14	CYS	CYS	0.40	CYS	GLN	1.15
CYS	GLU	0.21	CYS	GLY	0.60	CYS	HIS	0.42	CYS	ILE	0.93
CYS	LEU	0.92	CYS	LYS	1.88	CYS	MET	0.31	CYS	PHE	0.49
CYS	PRO	0.14	CYS	SER	0.36	CYS	THR	1.62	CYS	TRP	0.22
CYS	TYR	0.46	CYS	VAL	0.79	GLN	GLN	0.09	GLN	GLU	0.50
GLN	GLY	-1.16	GLN	HIS	1.49	GLN	ILE	1.73	GLN	LEU	-0.30
GLN	LYS	0.41	GLN	MET	0.47	GLN	PHE	-1.08	GLN	PRO	0.01
GLN	SER	0.54	GLN	THR	0.50	GLN	TRP	-0.70	GLN	TYR	-0.85
GLN	VAL	-0.71	GLU	GLU	0.77	GLU	GLY	0.12	GLU	HIS	-2.05
GLU	ILE	1.65	GLU	LEU	1.72	GLU	LYS	-1.07	GLU	MET	0.92
GLU	PHE	1.91	GLU	PRO	0.72	GLU	SER	-0.06	GLU	THR	0.45
GLU	TRP	0.57	GLU	TYR	-0.29	GLU	VAL	0.67	GLY	GLY	-2.97
GLY	HIS	-0.10	GLY	ILE	0.77	GLY	LEU	1.02	GLY	LYS	0.30
GLY	MET	0.27	GLY	PHE	-2.72	GLY	PRO	-0.31	GLY	SER	0.40
GLY	THR	0.99	GLY	TRP	0.52	GLY	TYR	0.50	GLY	VAL	-1.17
HIS	HIS	-0.73	HIS	ILE	-1.10	HIS	LEU	0.10	HIS	LYS	1.52
HIS	MET	0.58	HIS	PHE	-0.94	HIS	PRO	-0.91	HIS	SER	0.95
HIS	THR	-2.13	HIS	TRP	-0.63	HIS	TYR	-0.51	HIS	VAL	0.13
ILE	ILE	-0.54	ILE	LEU	-0.17	ILE	LYS	1.51	ILE	MET	0.81
ILE	PHE	-1.72	ILE	PRO	-0.85	ILE	SER	0.45	ILE	THR	1.20
ILE	TRP	0.14	ILE	TYR	-1.37	ILE	VAL	0.18	LEU	LEU	0.49
LEU	LYS	0.73	LEU	MET	-0.35	LEU	PHE	-0.62	LEU	PRO	0.83

LEU	SER	0.48		LEU	THR	0.18		LEU	TRP	0.24		LEU	TYR	−0.44
LEU	VAL	0.80		LYS	LYS	1.26		LYS	MET	−0.69		LYS	PHE	0.22
LYS	PRO	0.37		LYS	SER	0.57		LYS	THR	0.30		LYS	TRP	−1.32
LYS	TYR	−0.85		LYS	VAL	1.58		MET	MET	−0.79		MET	PHE	0.30
MET	PRO	−0.26		MET	SER	1.67		MET	THR	−0.29		MET	TRP	0.40
MET	TYR	−1.35		MET	VAL	−1.81		PHE	PHE	−1.47		PHE	PRO	0.31
PHE	SER	0.79		PHE	THR	1.95		PHE	TRP	0.15		PHE	TYR	−0.58
PHE	VAL	−1.08		PRO	PRO	−0.36		PRO	SER	0.76		PRO	THR	−0.06
PRO	TRP	−2.20		PRO	TYR	−3.50		PRO	VAL	0.46		SER	SER	−1.19
SER	THR	−0.50		SER	TRP	0.60		SER	TYR	−2.29		SER	VAL	0.97
THR	THR	−3.10		THR	TRP	−1.64		THR	TYR	0.16		THR	VAL	0.67
TRP	TRP	−0.98		TRP	TYR	−1.62		TRP	VAL	0.82		TYR	TYR	−1.91
TYR	VAL	0.73		VAL	VAL	−0.58								

Supplementary material: Table 3. Optimized direct pair potentials derived in the context of Semi-Flexible trap states.

ALA	ALA	-3.18	ALA	ARG	2.24	ALA	ASN	0.98	ALA	ASP	1.68
ALA	CYS	-3.88	ALA	GLN	1.14	ALA	GLU	1.64	ALA	GLY	0.67
ALA	HIS	0.02	ALA	ILE	-3.11	ALA	LEU	-2.35	ALA	LYS	3.21
ALA	MET	-0.21	ALA	PHE	-0.87	ALA	PRO	1.23	ALA	SER	-0.86
ALA	THR	0.54	ALA	TRP	-0.72	ALA	TYR	-0.79	ALA	VAL	-3.09
ARG	ARG	2.06	ARG	ASN	1.45	ARG	ASP	1.58	ARG	CYS	1.10
ARG	GLN	2.07	ARG	GLU	1.09	ARG	GLY	1.00	ARG	HIS	0.49
ARG	ILE	1.84	ARG	LEU	2.32	ARG	LYS	3.65	ARG	MET	0.78
ARG	PHE	1.69	ARG	PRO	1.97	ARG	SER	1.91	ARG	THR	1.26
ARG	TRP	-3.05	ARG	TYR	1.34	ARG	VAL	1.81	ASN	ASN	-3.03
ASN	ASP	0.77	ASN	CYS	1.21	ASN	GLN	1.27	ASN	GLU	2.36
ASN	GLY	1.27	ASN	HIS	0.33	ASN	ILE	2.70	ASN	LEU	0.83
ASN	LYS	2.47	ASN	MET	2.01	ASN	PHE	-0.43	ASN	PRO	-0.22
ASN	SER	0.60	ASN	THR	1.12	ASN	TRP	2.55	ASN	TYR	1.46
ASN	VAL	3.35	ASP	ASP	1.40	ASP	CYS	2.28	ASP	GLN	3.04
ASP	GLU	3.07	ASP	GLY	1.73	ASP	HIS	-0.78	ASP	ILE	2.26
ASP	LEU	3.44	ASP	LYS	2.14	ASP	MET	2.76	ASP	PHE	2.36
ASP	PRO	2.79	ASP	SER	0.61	ASP	THR	0.46	ASP	TRP	2.20
ASP	TYR	2.70	ASP	VAL	1.80	CYS	CYS	-4.72	CYS	GLN	2.26
CYS	GLU	-0.51	CYS	GLY	-4.72	CYS	HIS	-0.21	CYS	ILE	-0.31
CYS	LEU	-3.24	CYS	LYS	3.73	CYS	MET	-1.03	CYS	PHE	-2.62
CYS	PRO	-2.72	CYS	SER	-4.72	CYS	THR	0.65	CYS	TRP	-1.40
CYS	TYR	-2.36	CYS	VAL	-3.09	GLN	GLN	-0.84	GLN	GLU	2.50
GLN	GLY	1.25	GLN	HIS	2.18	GLN	ILE	1.92	GLN	LEU	1.67
GLN	LYS	2.56	GLN	MET	-1.30	GLN	PHE	-0.83	GLN	PRO	0.14
GLN	SER	1.92	GLN	THR	2.46	GLN	TRP	2.72	GLN	TYR	2.82
GLN	VAL	0.72	GLU	GLU	2.08	GLU	GLY	2.86	GLU	HIS	3.46
GLU	ILE	2.34	GLU	LEU	2.30	GLU	LYS	2.05	GLU	MET	0.87
GLU	PHE	1.63	GLU	PRO	1.59	GLU	SER	0.52	GLU	THR	1.49
GLU	TRP	3.79	GLU	TYR	1.55	GLU	VAL	3.04	GLY	GLY	-3.70
GLY	HIS	1.47	GLY	ILE	-1.83	GLY	LEU	0.20	GLY	LYS	2.05
GLY	MET	-1.20	GLY	PHE	1.02	GLY	PRO	1.03	GLY	SER	0.32
GLY	THR	-1.04	GLY	TRP	-0.08	GLY	TYR	0.33	GLY	VAL	0.44
HIS	HIS	-2.85	HIS	ILE	3.06	HIS	LEU	-2.37	HIS	LYS	3.49
HIS	MET	-1.65	HIS	PHE	1.02	HIS	PRO	-0.82	HIS	SER	1.59
HIS	THR	2.51	HIS	TRP	-0.52	HIS	TYR	-1.37	HIS	VAL	0.20
ILE	ILE	-4.72	ILE	LEU	-3.28	ILE	LYS	3.72	ILE	MET	-3.75
ILE	PHE	-4.72	ILE	PRO	-1.78	ILE	SER	1.90	ILE	THR	-1.65
ILE	TRP	-2.85	ILE	TYR	-3.25	ILE	VAL	-4.72	LEU	LEU	-4.72
LEU	LYS	2.79	LEU	MET	-2.10	LEU	PHE	-4.72	LEU	PRO	-0.30

LEU	SER	0.10		LEU	THR	0.26		LEU	TRP	−3.23		LEU	TYR	0.80
LEU	VAL	−4.72		LYS	LYS	2.08		LYS	MET	2.00		LYS	PHE	2.47
LYS	PRO	2.24		LYS	SER	2.26		LYS	THR	2.70		LYS	TRP	2.87
LYS	TYR	1.84		LYS	VAL	1.96		MET	MET	−3.78		MET	PHE	−4.63
MET	PRO	−0.11		MET	SER	−0.80		MET	THR	1.81		MET	TRP	−0.36
MET	TYR	−0.29		MET	VAL	−4.72		PHE	PHE	−4.72		PHE	PRO	−3.24
PHE	SER	2.79		PHE	THR	0.59		PHE	TRP	−2.39		PHE	TYR	−0.13
PHE	VAL	−4.72		PRO	PRO	1.33		PRO	SER	0.95		PRO	THR	0.88
PRO	TRP	−4.32		PRO	TYR	−1.86		PRO	VAL	−0.02		SER	SER	−1.53
SER	THR	0.01		SER	TRP	0.57		SER	TYR	1.88		SER	VAL	1.15
THR	THR	−2.66		THR	TRP	−4.54		THR	TYR	1.14		THR	VAL	0.94
TRP	TRP	−0.75		TRP	TYR	−1.64		TRP	VAL	1.56		TYR	TYR	−3.68
TYR	VAL	−0.46		VAL	VAL	−4.72								

Supplementary material: Table 4. Optimized water-mediated pair potentials derived in the context of Semi-Flexible trap states.

ALA	ALA	0.53	ALA	ARG	1.19	ALA	ASN	0.12	ALA	ASP	0.75
ALA	CYS	0.90	ALA	GLN	0.71	ALA	GLU	0.78	ALA	GLY	-1.52
ALA	HIS	2.32	ALA	ILE	1.20	ALA	LEU	0.90	ALA	LYS	-1.02
ALA	MET	2.04	ALA	PHE	-0.31	ALA	PRO	-0.59	ALA	SER	-0.85
ALA	THR	0.14	ALA	TRP	2.37	ALA	TYR	2.85	ALA	VAL	0.21
ARG	ARG	-3.33	ARG	ASN	-0.83	ARG	ASP	-2.99	ARG	CYS	0.17
ARG	GLN	-1.80	ARG	GLU	-3.66	ARG	GLY	-0.63	ARG	HIS	-4.72
ARG	ILE	-0.93	ARG	LEU	0.87	ARG	LYS	-0.41	ARG	MET	1.00
ARG	PHE	-1.07	ARG	PRO	-0.60	ARG	SER	-0.39	ARG	THR	0.23
ARG	TRP	-0.37	ARG	TYR	-2.42	ARG	VAL	1.51	ASN	ASN	-3.84
ASN	ASP	-1.74	ASN	CYS	1.87	ASN	GLN	0.58	ASN	GLU	0.07
ASN	GLY	0.26	ASN	HIS	1.84	ASN	ILE	3.06	ASN	LEU	0.53
ASN	LYS	1.31	ASN	MET	-1.04	ASN	PHE	0.72	ASN	PRO	-2.92
ASN	SER	0.49	ASN	THR	0.47	ASN	TRP	-1.10	ASN	TYR	0.43
ASN	VAL	0.95	ASP	ASP	-3.00	ASP	CYS	1.85	ASP	GLN	0.25
ASP	GLU	0.99	ASP	GLY	0.61	ASP	HIS	-3.00	ASP	ILE	3.58
ASP	LEU	1.13	ASP	LYS	-2.66	ASP	MET	1.43	ASP	PHE	2.91
ASP	PRO	-0.75	ASP	SER	-1.62	ASP	THR	-1.49	ASP	TRP	2.09
ASP	TYR	-1.01	ASP	VAL	0.09	CYS	CYS	0.70	CYS	GLN	1.63
CYS	GLU	0.38	CYS	GLY	1.25	CYS	HIS	0.77	CYS	ILE	1.46
CYS	LEU	1.73	CYS	LYS	2.55	CYS	MET	0.47	CYS	PHE	0.91
CYS	PRO	0.32	CYS	SER	0.90	CYS	THR	2.52	CYS	TRP	0.43
CYS	TYR	1.01	CYS	VAL	1.67	GLN	GLN	-0.85	GLN	GLU	-0.25
GLN	GLY	-1.54	GLN	HIS	1.87	GLN	ILE	2.17	GLN	LEU	-0.37
GLN	LYS	-0.63	GLN	MET	0.43	GLN	PHE	-1.66	GLN	PRO	-0.61
GLN	SER	0.24	GLN	THR	0.48	GLN	TRP	-0.76	GLN	TYR	-0.79
GLN	VAL	-0.86	GLU	GLU	-0.86	GLU	GLY	-0.19	GLU	HIS	-3.94
GLU	ILE	1.89	GLU	LEU	1.83	GLU	LYS	-3.92	GLU	MET	0.38
GLU	PHE	1.99	GLU	PRO	-0.22	GLU	SER	-0.49	GLU	THR	-0.00
GLU	TRP	0.68	GLU	TYR	-0.38	GLU	VAL	0.57	GLY	GLY	-2.61
GLY	HIS	0.27	GLY	ILE	1.71	GLY	LEU	1.83	GLY	LYS	-0.32
GLY	MET	1.12	GLY	PHE	-2.22	GLY	PRO	-0.33	GLY	SER	0.77
GLY	THR	1.77	GLY	TRP	1.30	GLY	TYR	1.34	GLY	VAL	-0.30
HIS	HIS	-1.13	HIS	ILE	-1.16	HIS	LEU	0.12	HIS	LYS	1.12
HIS	MET	0.70	HIS	PHE	-1.27	HIS	PRO	-1.56	HIS	SER	1.39
HIS	THR	-2.80	HIS	TRP	-0.84	HIS	TYR	-0.35	HIS	VAL	0.38
ILE	ILE	-0.29	ILE	LEU	0.39	ILE	LYS	1.38	ILE	MET	1.43
ILE	PHE	-1.81	ILE	PRO	-0.77	ILE	SER	1.14	ILE	THR	1.86
ILE	TRP	0.50	ILE	TYR	-0.87	ILE	VAL	1.10	LEU	LEU	0.71
LEU	LYS	0.40	LEU	MET	-0.17	LEU	PHE	-0.37	LEU	PRO	1.13

LEU	SER	1.05		LEU	THR	0.59		LEU	TRP	0.71		LEU	TYR	0.17
LEU	VAL	1.62		LYS	LYS	-0.41		LYS	MET	-2.02		LYS	PHE	-0.30
LYS	PRO	-0.79		LYS	SER	-0.08		LYS	THR	-0.52		LYS	TRP	-2.13
LYS	TYR	-1.47		LYS	VAL	1.61		MET	MET	-1.10		MET	PHE	0.42
MET	PRO	-0.44		MET	SER	2.54		MET	THR	-0.30		MET	TRP	0.62
MET	TYR	-1.50		MET	VAL	-2.29		PHE	PHE	-1.96		PHE	PRO	0.59
PHE	SER	1.48		PHE	THR	2.73		PHE	TRP	0.40		PHE	TYR	-0.03
PHE	VAL	-0.74		PRO	PRO	-1.51		PRO	SER	0.82		PRO	THR	-0.18
PRO	TRP	-2.92		PRO	TYR	-3.29		PRO	VAL	0.80		SER	SER	-1.84
SER	THR	-0.12		SER	TRP	1.25		SER	TYR	-1.83		SER	VAL	1.59
THR	THR	-3.22		THR	TRP	-1.56		THR	TYR	0.90		THR	VAL	1.39
TRP	TRP	-1.30		TRP	TYR	-1.93		TRP	VAL	1.37		TYR	TYR	-2.02
TYR	VAL	1.91		VAL	VAL	-0.02								

Supplementary material: Table 5. Optimized direct pair potentials derived in the context of Flexible trap states.

ALA	ALA	-2.11	ALA	ARG	1.60	ALA	ASN	0.36	ALA	ASP	0.88
ALA	CYS	-0.89	ALA	GLN	0.12	ALA	GLU	0.60	ALA	GLY	0.73
ALA	HIS	-0.14	ALA	ILE	-0.41	ALA	LEU	-0.36	ALA	LYS	2.23
ALA	MET	0.72	ALA	PHE	0.43	ALA	PRO	0.89	ALA	SER	-0.95
ALA	THR	0.38	ALA	TRP	0.20	ALA	TYR	-0.19	ALA	VAL	-0.71
ARG	ARG	0.87	ARG	ASN	0.02	ARG	ASP	0.08	ARG	CYS	1.74
ARG	GLN	0.97	ARG	GLU	-1.01	ARG	GLY	-0.27	ARG	HIS	-1.90
ARG	ILE	1.20	ARG	LEU	1.62	ARG	LYS	4.14	ARG	MET	-0.39
ARG	PHE	1.09	ARG	PRO	0.49	ARG	SER	1.00	ARG	THR	-0.09
ARG	TRP	-3.69	ARG	TYR	0.29	ARG	VAL	1.20	ASN	ASN	-4.47
ASN	ASP	-0.94	ASN	CYS	1.83	ASN	GLN	-0.19	ASN	GLU	1.36
ASN	GLY	0.45	ASN	HIS	-1.10	ASN	ILE	2.21	ASN	LEU	0.64
ASN	LYS	1.64	ASN	MET	1.56	ASN	PHE	-0.66	ASN	PRO	-2.37
ASN	SER	-0.83	ASN	THR	0.09	ASN	TRP	2.13	ASN	TYR	0.67
ASN	VAL	2.71	ASP	ASP	-0.20	ASP	CYS	2.63	ASP	GLN	2.62
ASP	GLU	2.71	ASP	GLY	0.72	ASP	HIS	-3.07	ASP	ILE	1.56
ASP	LEU	2.61	ASP	LYS	1.20	ASP	MET	2.05	ASP	PHE	1.65
ASP	PRO	2.10	ASP	SER	-0.76	ASP	THR	-1.02	ASP	TRP	1.42
ASP	TYR	2.04	ASP	VAL	1.09	CYS	CYS	-4.47	CYS	GLN	2.73
CYS	GLU	0.09	CYS	GLY	-4.47	CYS	HIS	0.60	CYS	ILE	1.60
CYS	LEU	-0.35	CYS	LYS	2.92	CYS	MET	0.10	CYS	PHE	-0.87
CYS	PRO	-1.45	CYS	SER	-4.06	CYS	THR	1.49	CYS	TRP	-0.73
CYS	TYR	-0.99	CYS	VAL	-0.11	GLN	GLN	-3.44	GLN	GLU	1.75
GLN	GLY	0.28	GLN	HIS	1.02	GLN	ILE	1.29	GLN	LEU	1.10
GLN	LYS	2.04	GLN	MET	-2.23	GLN	PHE	-1.28	GLN	PRO	-1.79
GLN	SER	1.02	GLN	THR	1.78	GLN	TRP	2.43	GLN	TYR	2.30
GLN	VAL	0.20	GLU	GLU	0.92	GLU	GLY	2.02	GLU	HIS	2.79
GLU	ILE	1.48	GLU	LEU	1.46	GLU	LYS	1.11	GLU	MET	-0.14
GLU	PHE	0.77	GLU	PRO	-0.10	GLU	SER	-1.37	GLU	THR	0.14
GLU	TRP	3.17	GLU	TYR	0.34	GLU	VAL	2.07	GLY	GLY	-3.87
GLY	HIS	0.84	GLY	ILE	-0.43	GLY	LEU	0.90	GLY	LYS	0.71
GLY	MET	-0.84	GLY	PHE	1.41	GLY	PRO	0.29	GLY	SER	-0.33
GLY	THR	-1.83	GLY	TRP	0.08	GLY	TYR	0.11	GLY	VAL	1.08
HIS	HIS	-3.36	HIS	ILE	2.67	HIS	LEU	-1.56	HIS	LYS	2.93
HIS	MET	-1.65	HIS	PHE	1.39	HIS	PRO	-2.80	HIS	SER	0.95
HIS	THR	1.89	HIS	TRP	-0.39	HIS	TYR	-1.75	HIS	VAL	0.60
ILE	ILE	-3.90	ILE	LEU	-0.25	ILE	LYS	2.51	ILE	MET	-1.20
ILE	PHE	-1.82	ILE	PRO	-1.00	ILE	SER	1.89	ILE	THR	-0.69
ILE	TRP	-1.83	ILE	TYR	-1.27	ILE	VAL	-0.83	LEU	LEU	-4.38
LEU	LYS	1.68	LEU	MET	-0.24	LEU	PHE	-1.20	LEU	PRO	0.01

LEU	SER	0.52		LEU	THR	0.63		LEU	TRP	−0.97		LEU	TYR	1.44
LEU	VAL	−0.98		LYS	LYS	1.23		LYS	MET	0.85		LYS	PHE	1.26
LYS	PRO	0.92		LYS	SER	1.21		LYS	THR	2.03		LYS	TRP	1.85
LYS	TYR	0.42		LYS	VAL	0.68		MET	MET	−3.51		MET	PHE	−3.08
MET	PRO	−0.40		MET	SER	−0.36		MET	THR	1.66		MET	TRP	0.11
MET	TYR	0.30		MET	VAL	−1.49		PHE	PHE	−4.47		PHE	PRO	−2.79
PHE	SER	2.51		PHE	THR	0.74		PHE	TRP	−1.23		PHE	TYR	0.76
PHE	VAL	−1.33		PRO	PRO	−0.02		PRO	SER	−0.18		PRO	THR	−0.23
PRO	TRP	−4.15		PRO	TYR	−2.85		PRO	VAL	0.19		SER	SER	−3.49
SER	THR	−1.27		SER	TRP	0.58		SER	TYR	1.41		SER	VAL	1.33
THR	THR	−4.33		THR	TRP	−4.01		THR	TYR	0.60		THR	VAL	0.90
TRP	TRP	−0.49		TRP	TYR	−1.06		TRP	VAL	2.16		TYR	TYR	−3.58
TYR	VAL	0.26		VAL	VAL	−4.47								

Supplementary material: Table 6. Optimized water-mediated pair potentials derived in the context of Flexible trap states.

ALA	ALA	0.94	ALA	ARG	1.58	ALA	ASN	0.44	ALA	ASP	1.10
ALA	CYS	2.55	ALA	GLN	0.94	ALA	GLU	0.93	ALA	GLY	-0.40
ALA	HIS	2.78	ALA	ILE	1.97	ALA	LEU	1.74	ALA	LYS	-1.25
ALA	MET	2.89	ALA	PHE	1.17	ALA	PRO	0.04	ALA	SER	-0.20
ALA	THR	0.74	ALA	TRP	3.39	ALA	TYR	3.20	ALA	VAL	1.45
ARG	ARG	-4.47	ARG	ASN	-2.88	ARG	ASP	-4.47	ARG	CYS	1.15
ARG	GLN	-4.47	ARG	GLU	-4.47	ARG	GLY	-1.27	ARG	HIS	-4.47
ARG	ILE	0.17	ARG	LEU	1.54	ARG	LYS	-3.19	ARG	MET	0.85
ARG	PHE	-0.38	ARG	PRO	-2.67	ARG	SER	-1.54	ARG	THR	-0.38
ARG	TRP	-0.33	ARG	TYR	-3.36	ARG	VAL	2.24	ASN	ASN	-4.47
ASN	ASP	-3.95	ASN	CYS	2.76	ASN	GLN	-0.42	ASN	GLU	-1.35
ASN	GLY	0.07	ASN	HIS	0.95	ASN	ILE	3.39	ASN	LEU	1.20
ASN	LYS	0.52	ASN	MET	-0.69	ASN	PHE	1.28	ASN	PRO	-4.47
ASN	SER	-0.17	ASN	THR	0.05	ASN	TRP	-0.80	ASN	TYR	0.25
ASN	VAL	1.52	ASP	ASP	-4.47	ASP	CYS	2.93	ASP	GLN	-0.94
ASP	GLU	-0.17	ASP	GLY	0.51	ASP	HIS	-4.47	ASP	ILE	3.97
ASP	LEU	1.74	ASP	LYS	-4.47	ASP	MET	1.44	ASP	PHE	3.41
ASP	PRO	-2.44	ASP	SER	-3.03	ASP	THR	-2.66	ASP	TRP	2.25
ASP	TYR	-1.42	ASP	VAL	0.73	CYS	CYS	1.32	CYS	GLN	2.34
CYS	GLU	1.71	CYS	GLY	2.96	CYS	HIS	1.32	CYS	ILE	2.71
CYS	LEU	3.17	CYS	LYS	3.65	CYS	MET	1.12	CYS	PHE	1.96
CYS	PRO	1.49	CYS	SER	2.28	CYS	THR	3.86	CYS	TRP	0.86
CYS	TYR	1.98	CYS	VAL	3.15	GLN	GLN	-1.67	GLN	GLU	-2.21
GLN	GLY	-2.06	GLN	HIS	1.07	GLN	ILE	2.76	GLN	LEU	0.41
GLN	LYS	-2.99	GLN	MET	0.53	GLN	PHE	-1.14	GLN	PRO	-1.94
GLN	SER	-0.36	GLN	THR	0.14	GLN	TRP	-0.52	GLN	TYR	-0.85
GLN	VAL	-0.14	GLU	GLU	-3.85	GLU	GLY	-0.89	GLU	HIS	-4.47
GLU	ILE	2.44	GLU	LEU	2.36	GLU	LYS	-4.47	GLU	MET	0.44
GLU	PHE	2.50	GLU	PRO	-1.96	GLU	SER	-1.67	GLU	THR	-0.80
GLU	TRP	0.72	GLU	TYR	-1.01	GLU	VAL	1.02	GLY	GLY	-2.02
GLY	HIS	0.23	GLY	ILE	2.44	GLY	LEU	2.41	GLY	LYS	-1.32
GLY	MET	1.85	GLY	PHE	-0.34	GLY	PRO	-0.37	GLY	SER	0.95
GLY	THR	2.04	GLY	TRP	2.14	GLY	TYR	1.82	GLY	VAL	1.13
HIS	HIS	-1.36	HIS	ILE	-0.36	HIS	LEU	1.00	HIS	LYS	-0.17
HIS	MET	0.84	HIS	PHE	-0.67	HIS	PRO	-2.30	HIS	SER	1.07
HIS	THR	-3.23	HIS	TRP	-0.58	HIS	TYR	-0.40	HIS	VAL	1.14
ILE	ILE	0.79	ILE	LEU	1.38	ILE	LYS	2.08	ILE	MET	2.56
ILE	PHE	0.01	ILE	PRO	0.73	ILE	SER	2.10	ILE	THR	2.49
ILE	TRP	1.30	ILE	TYR	0.63	ILE	VAL	1.91	LEU	LEU	1.45
LEU	LYS	0.83	LEU	MET	1.15	LEU	PHE	1.42	LEU	PRO	2.01

LEU	SER	1.82		LEU	THR	1.47		LEU	TRP	1.93		LEU	TYR	1.51
LEU	VAL	2.11		LYS	LYS	-3.38		LYS	MET	-2.10		LYS	PHE	-0.04
LYS	PRO	-3.24		LYS	SER	-1.44		LYS	THR	-1.77		LYS	TRP	-2.11
LYS	TYR	-2.89		LYS	VAL	1.92		MET	MET	-0.82		MET	PHE	1.34
MET	PRO	-0.01		MET	SER	3.26		MET	THR	0.42		MET	TRP	0.96
MET	TYR	-0.78		MET	VAL	-0.72		PHE	PHE	-0.97		PHE	PRO	1.50
PHE	SER	2.17		PHE	THR	3.15		PHE	TRP	1.15		PHE	TYR	1.11
PHE	VAL	1.02		PRO	PRO	-2.71		PRO	SER	0.61		PRO	THR	-0.73
PRO	TRP	-2.42		PRO	TYR	-3.44		PRO	VAL	1.65		SER	SER	-3.19
SER	THR	-0.61		SER	TRP	1.79		SER	TYR	-1.94		SER	VAL	2.21
THR	THR	-3.96		THR	TRP	-0.90		THR	TYR	1.24		THR	VAL	1.99
TRP	TRP	-1.03		TRP	TYR	-1.29		TRP	VAL	2.44		TYR	TYR	-1.71
TYR	VAL	2.41		VAL	VAL	1.18								

Supplementary material: Table 7. PDB identifiers and chain names for the training set of protein complexes.

1AAR-A-B	1AKS-A-B	1AOR-A-B	1APY-A-C	1BBP-B-D	1BCM-A-B
1BHM-A-B	1BMF-C-D	1BND-A-B	1BSR-A-B	1CDC-A-B	1CHO-E-I
1CPC-A-B	1CYD-C-D	1DER-F-G	1DOK-A-B	1DVR-A-B	1ECM-A-B
1EPT-A-C	1FAG-A-C	1FC1-A-B	1FLE-E-I	1FUQ-A-B	1GFL-A-B
1GLU-A-B	1GRI-A-B	1GTP-B-I	1HCG-A-B	1HIW-A-R	1HLP-A-B
1HSB-A-B	1KNY-A-B	1LEH-A-B	1LTS-A-C	1LWI-A-B	1MAS-A-B
1MDY-A-B	1MHL-A-C	1MSA-A-D	1NAL-2-3	1NCI-A-B	1NOY-A-B
1OBP-A-B	1ONE-A-B	1ORT-B-F	1OTG-B-C	1OVO-A-B	1PIO-A-B
1PNK-A-B	1PRT-A-F	1PSA-A-B	1PVC-1-3	1PVU-A-B	1PYT-A-C
1QRD-A-B	1RCO-R-V	1RTH-A-B	1RVV-1-2	1SCU-D-E	1SFT-A-B
1SRI-A-B	1SVA-2-3	1TBR-K-S	1THE-A-B	1TII-E-F	1TME-1-3
1TRK-A-B	1TTA-A-B	1UCY-E-H	1VFB-A-B	1VRT-A-B	1WDC-A-C
1WTL-A-B	1XSO-A-B	1YPT-A-B	2BBK-H-L	2BTF-A-P	2CST-A-B
2GLS-B-H	2KAI-B-I	2LIG-A-B	2MEV-1-2	2PHL-B-C	2POL-A-B
2RSP-A-B	2ZTA-A-B	3PGA-2-4	4AAH-C-D	4HTC-H-I	4SGB-E-I
6GSV-A-B	8CAT-A-B	1ABR-A-B	1ADU-A-B	1APX-A-B	1ASY-A-B
1BBB-A-B	1BDM-A-B	1BIN-A-B	1BMV-1-2	1BPL-A-B	1BVP-2-3
1CGJ-E-I	1CHR-A-B	1CPC-A-K	1DAA-A-B	1DIF-A-B	1ECE-A-B
1EPT-B-C	1FAT-A-B	1FIE-A-B	1FVP-A-B	1GDT-A-B	1GIF-B-C
1GYL-A-B	1HJR-B-D	1HMP-A-B	1HTM-D-F	1HUC-A-B	1HYH-A-B
1IDS-A-C	1INH-A-B	1KPB-A-B	1LTS-D-E	1MCO-H-L	1MEC-1-4
1NHK-L-R	1ORD-A-B	1OSJ-A-B	1OVA-A-B	1PDG-A-B	1PP2-L-R
1PRT-H-J	1PSD-A-B	1PVC-3-4	1PXT-A-B	1RCP-A-B	1RTM-1-2
1SCE-B-D	1SGP-E-I	1STF-E-I	1TAB-E-I	1TCO-A-B	1THJ-B-C
1TLF-A-B	1TME-2-3	1TVX-B-D	1UDI-E-I	1VHI-A-B	1VSC-A-B
1WFB-A-B	1XIK-A-B	1YHA-A-B	1YRN-A-B	2ACH-A-B	2BBV-B-C
2CCY-A-B	2DLD-A-B	2KAU-A-C	2LTN-A-B	2MEV-2-3	2PKA-A-B
3MDE-A-B	3SIC-E-I	4CHA-A-B	4KBP-B-C	6PFK-C-D	9LDT-A-B
1AHS-B-C	1APY-A-B	1BBH-A-B	1BGL-A-D	1BNC-A-B	1CAX-C-F
1CLX-A-B	1DBQ-A-B	1DPR-A-B	1ECZ-A-B	1EXT-A-B	1FCD-B-D
1FOD-1-3	1FUG-A-B	1GES-A-B	1GPM-B-D	1HBH-C-D	1HLE-A-B
1HTR-B-P	1HYL-A-B	1KIF-B-F	1LMK-E-G	1LYL-A-C	1MEE-A-I
1MMO-C-H	1MYK-A-B	1NIP-A-B	1OTF-B-E	1PGE-A-B	1POX-A-B
1PRT-H-L	1PVD-A-B	1QOR-A-B	1RHG-A-C	1SCM-A-B	1SLU-A-B
1STM-B-C	1TCR-A-B	1TME-1-2	1TPH-1-2	1UBS-A-B	1VOK-A-B
1WHT-A-B	1YPP-A-B	2AFN-B-C	2CHT-D-E	2HNT-C-F	2LTN-A-C
2PEL-B-C	2RSL-A-B	2UTG-A-B	3MON-C-D	4CTS-A-B	6FAB-H-L

Supplementary material: Table 8. PDB identifiers and chain names for the test set of protein complexes.

1ACB-E-I	1ATN-A-D	1BBT-2-3	1BLB-A-B	1BRS-C-F	1CHM-A-B
1CSM-A-B	1DIR-A-B	1ECF-A-B	1EPT-A-B	1FIN-A-B	1FRT-A-C
1GAD-O-P	1GLQ-A-B	1GTO-B-C	1HGE-C-D	1HRD-B-C	1HUL-A-B
1IES-B-E	1KPT-A-B	1LUC-A-B	1MDA-H-L	1MLD-A-B	1MPM-B-C
1NSC-A-B	1ORO-A-B	1OVA-C-D	1PMA-C-D	1PPF-E-I	1PRE-A-B
1PVC-1-2	1PYI-A-B	1RBA-A-B	1RVA-A-B	1SET-A-B	1SPB-P-S
1TAF-A-B	1TII-A-C	1TMF-1-3	1TSR-A-B	1UNA-A-B	1VSG-A-B
1XIM-A-C	1YTF-B-D	2BPA-1-3	2EIP-A-B	2KAU-B-C	2NAC-A-B
2PLV-1-4	2SPC-A-B	3HHR-A-B	4AAH-A-C	4SBV-A-B	8ATC-A-B