

Supporting Information

Engineering the Biomimetic Cofactors of NMNH for Cytochrome P450 BM3 Based on Binding Conformation Refinement

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19 Table S1 Primer sequence for site-directed mutagenesis^a

Primer	Sequence(5'-3')
G1001R-F	<u>CGT</u> GACGGAAGCCAAATGGC
G1001R-R	GCAAATATAGAAGTGCGCTCCTTGATCAAG
D943R-F	<u>CGT</u> TATCTGTATCAAGAAGAGCTTGAAAACG
D943R-R	TTCATGAGGTGAACGGCAGCC
G1001Q-F	<u>CAG</u> GACGGAAGCCAAATGGC
G1001Q-R	GCAAATATAGAAGTGCGCTCCTTGATCAAG
G907P-F	<u>CCG</u> GTCGCGCCGTTTAGAG
G907P-R	TGTTCCCGGTCCGACCATG
S848R-F	<u>CGT</u> GTTGTCTCAGGAGAAGCGTGG
S848R-R	GACCGTGATGCTTGCTTGTTTTTCATCG
S866R-F	<u>CGT</u> AACTATCTTGCCGAGCTGC
S866R-R	CGCAATTCCTTTATATTCTCCATATCCGC
D943M-F	<u>ATG</u> TATCTGTATCAAGAAGAGCTTGAAAACG
D943M-R	TTCATGAGGTGAACGGCAGCC
G907T-F	<u>ACG</u> GTCGCGCCGTTTAGAG
G907T-R	TGTTCCCGGTCCGACCATG
G905T-F	<u>ACC</u> ACAGGCGTCGCG
G905T-R	CGGTCCGACCATGATAAGCG
D1002N-F	<u>AAT</u> GGAAGCCAAATGGCACC
D1002N-R	TCCGCAAATATAGAAGTGCGCTCC

20 ^aThe underline represents the mutated residue.

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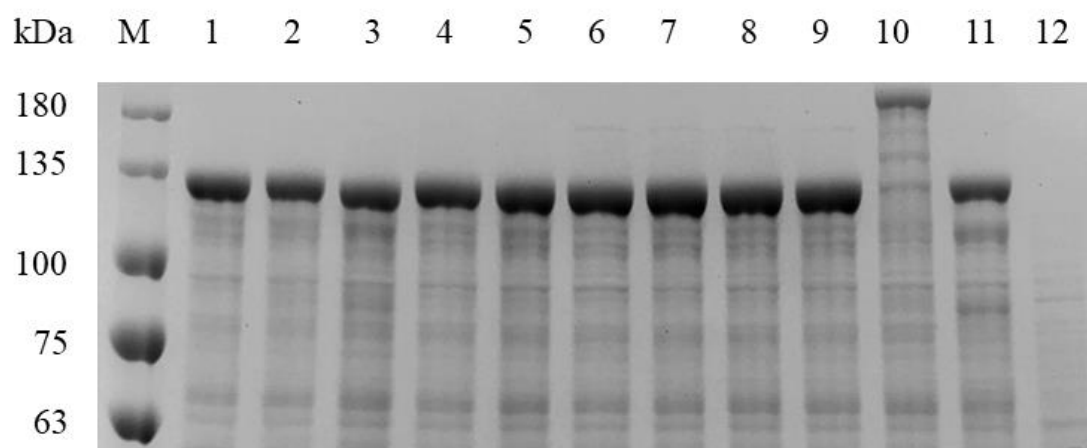


Fig. S1 SDS-PAGE analysis of expressed WT P450 BM3 and mutants. Lane M, protein marker; lane 1, wild-type; lane 2, G1001R; lane 3, D943R; lane 4, G1001Q; lane 5, G907P; lane 6, S848R; lane 7, S866R; lane 8, G907T; lane 9, G905T; lane 10, D943M; lane 11, D1002N; lane 12, empty vector control.

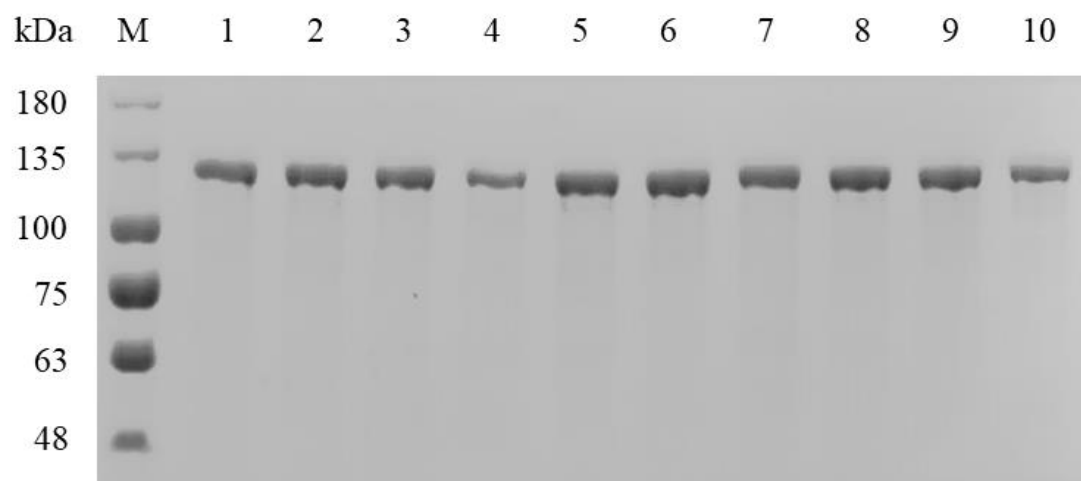


Fig. S2 SDS-PAGE analysis of purified WT P450 BM3 and mutants. Lane M, protein marker; lane 1, wild-type; lane 2, G1001R; lane 3, D943R; lane 4, G1001Q; lane 5, G907P; lane 6, S848R; lane 7, S866R; lane 8, G907T; lane 9, G905T; lane 10, D1002N.

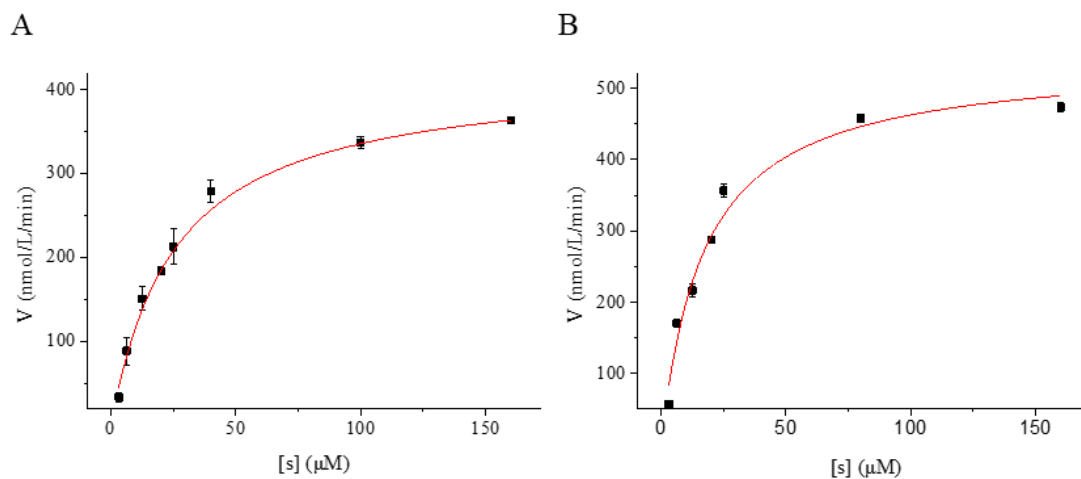
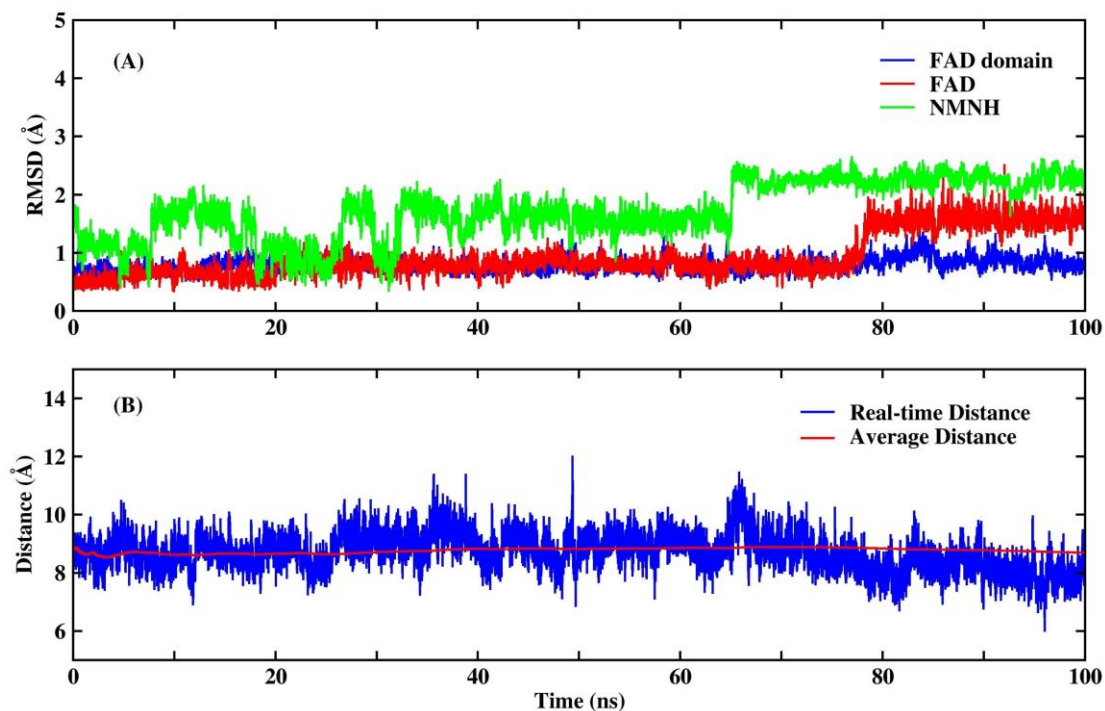
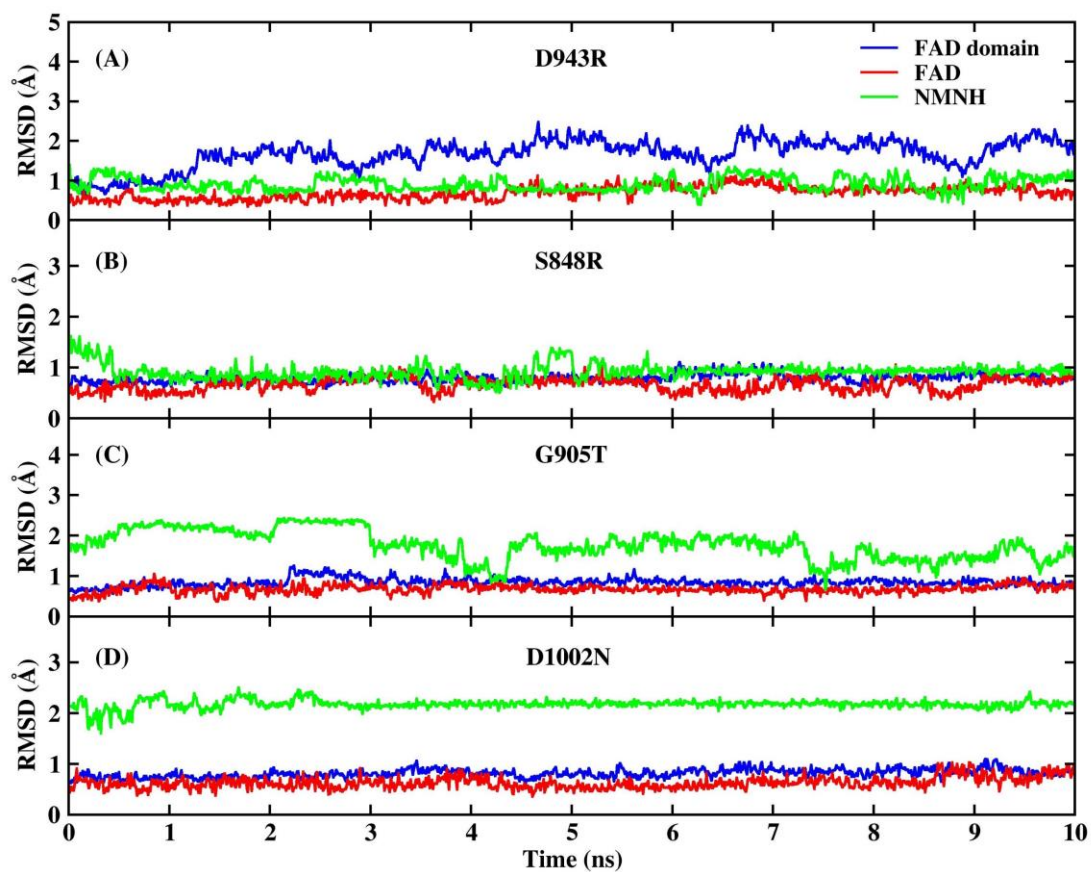


Fig. S3 The kinetic investigations of cytochrome *c* reduction with NMNH based on the Michaelis-Menten. A. The Michaelis-Menten plots of WT BM3. B. The Michaelis-Menten plots of mutant S848R.



39 Fig. S4 The longer time (100 ns) simulation on FAD domain-NMNH complex. (A) The
 40 RMSD of FAD domain-NMNH simulations. (B) The real-time and average distance between
 41 the N-5 and C-4 atoms of 100-ns simulation.

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Fig. S5 The RMSD of protein binding pocket backbone atoms, FAD and NMNH in the four mutant simulations. (A) D943R mutant. (B) S848R mutant. (C) G905T mutant. (D) D1002N mutant.

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48 Table S2 Mutants Screened and corresponding binding free energy(ΔG_{bind}).

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
1	1001	GLY	ARG	-46.18	-4.643
2	943	ASP	ARG	-44.997	-3.46
3	905	GLY	LYS	-44.654	-3.117
4	1001	GLY	LYS	-44.474	-2.937
5	1001	GLY	GLN	-44.119	-2.582
6	907	GLY	PRO	-43.832	-2.295
7	1001	GLY	HIE	-43.79	-2.253
8	1001	GLY	ASN	-43.638	-2.101
9	1001	GLY	ILE	-43.571	-2.034
10	848	SER	ARG	-43.35	-1.813
11	866	SER	ARG	-43.221	-1.684
12	907	GLY	THR	-43.213	-1.676
13	1001	GLY	LEU	-43.191	-1.654
14	909	ALA	ARG	-43.13	-1.593
15	943	ASP	LYS	-43.113	-1.576
16	1001	GLY	VAL	-43.108	-1.571
17	848	SER	LYS	-42.93	-1.393
18	1002	ASP	TRP	-42.762	-1.225
19	1047	TRP	THR	-42.707	-1.17
20	904	PRO	TRP	-42.655	-1.118
21	828	ARG	LEU	-42.64	-1.103
22	828	ARG	GLN	-42.604	-1.067
23	845	ILE	ARG	-42.582	-1.045
24	909	ALA	VAL	-42.572	-1.035
25	935	PHE	TRP	-42.49	-0.953
26	905	GLY	THR	-42.489	-0.952
27	907	GLY	VAL	-42.48	-0.943
28	847	VAL	TRP	-42.471	-0.934
29	909	ALA	LYS	-42.446	-0.909
30	1046	VAL	ARG	-42.446	-0.909
31	943	ASP	MET	-42.438	-0.901
32	845	ILE	LYS	-42.393	-0.856
33	909	ALA	ILE	-42.39	-0.853
34	943	ASP	TRP	-42.389	-0.852
35	1004	SER	PRO	-42.389	-0.852
36	907	GLY	ILE	-42.328	-0.791
37	1003	GLY	ILE	-42.309	-0.772
38	830	TYR	ARG	-42.307	-0.77
39	1001	GLY	TYR	-42.283	-0.746
40	1048	ALA	TRP	-42.282	-0.745
41	863	GLY	LYS	-42.239	-0.702
42	830	TYR	LYS	-42.21	-0.673

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
43	907	GLY	ARG	-42.21	-0.673
44	866	SER	LYS	-42.201	-0.664
45	905	GLY	PHE	-42.189	-0.652
46	943	ASP	PHE	-42.188	-0.651
47	1003	GLY	VAL	-42.168	-0.631
48	700	HIE	TRP	-42.167	-0.63
49	863	GLY	LEU	-42.166	-0.629
50	943	ASP	GLN	-42.159	-0.622
51	828	ARG	ILE	-42.137	-0.6
52	833	SER	TRP	-42.135	-0.598
53	943	ASP	HIE	-42.128	-0.591
54	903	GLY	LYS	-42.125	-0.588
55	903	GLY	THR	-42.112	-0.575
56	903	GLY	ARG	-42.094	-0.557
57	1002	ASP	TYR	-42.071	-0.534
58	845	ILE	MET	-42.068	-0.531
59	905	GLY	GLN	-42.068	-0.531
60	1001	GLY	MET	-42.066	-0.529
61	1002	ASP	ASN	-42.053	-0.516
62	828	ARG	MET	-42.05	-0.513
63	943	ASP	ILE	-42.046	-0.509
64	908	VAL	LYS	-42.042	-0.505
65	943	ASP	TYR	-42.032	-0.495
66	907	GLY	LYS	-42.031	-0.494
67	1046	VAL	MET	-42.028	-0.491
68	845	ILE	HIE	-42.019	-0.482
69	1048	ALA	GLN	-42.014	-0.477
70	828	ARG	LYS	-42.011	-0.474
71	908	VAL	ARG	-42.009	-0.472
72	907	GLY	ASN	-42.006	-0.469
73	903	GLY	LEU	-41.999	-0.462
74	943	ASP	VAL	-41.996	-0.459
75	905	GLY	HIE	-41.993	-0.456
76	866	SER	TRP	-41.979	-0.442
77	943	ASP	LEU	-41.973	-0.436
78	904	PRO	LYS	-41.956	-0.419
79	943	ASP	CYS	-41.955	-0.418
80	847	VAL	ARG	-41.953	-0.416
81	907	GLY	GLN	-41.951	-0.414
82	943	ASP	ALA	-41.949	-0.412
83	1002	ASP	PHE	-41.944	-0.407
84	943	ASP	GLY	-41.94	-0.403
85	943	ASP	ASN	-41.919	-0.382

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
86	829	TYR	VAL	-41.917	-0.38
87	937	CYS	ARG	-41.911	-0.374
88	907	GLY	PHE	-41.907	-0.37
89	863	GLY	MET	-41.906	-0.369
90	966	SER	ARG	-41.901	-0.364
91	863	GLY	GLN	-41.888	-0.351
92	943	ASP	SER	-41.887	-0.35
93	845	ILE	GLN	-41.885	-0.348
94	847	VAL	LEU	-41.879	-0.342
95	830	TYR	PRO	-41.876	-0.339
96	936	GLY	LYS	-41.874	-0.337
97	1048	ALA	PHE	-41.873	-0.336
98	829	TYR	THR	-41.869	-0.332
99	829	TYR	ILE	-41.867	-0.33
100	907	GLY	SER	-41.866	-0.329
101	907	GLY	CYS	-41.864	-0.327
102	1004	SER	ARG	-41.849	-0.312
103	903	GLY	PRO	-41.846	-0.309
104	1046	VAL	LYS	-41.845	-0.308
105	830	TYR	GLN	-41.842	-0.305
106	1004	SER	LYS	-41.839	-0.302
107	847	VAL	LYS	-41.825	-0.288
108	700	HIE	ARG	-41.822	-0.285
109	1046	VAL	GLN	-41.817	-0.28
110	863	GLY	PRO	-41.815	-0.278
111	936	GLY	ARG	-41.813	-0.276
112	1046	VAL	PRO	-41.813	-0.276
113	943	ASP	THR	-41.811	-0.274
114	966	SER	MET	-41.811	-0.274
115	904	PRO	ARG	-41.809	-0.272
116	1001	GLY	CYS	-41.808	-0.271
117	966	SER	LYS	-41.801	-0.264
118	1004	SER	THR	-41.8	-0.263
119	828	ARG	VAL	-41.797	-0.26
120	828	ARG	ASN	-41.796	-0.259
121	832	ILE	LYS	-41.795	-0.258
122	937	CYS	LYS	-41.795	-0.258
123	678	SER	LYS	-41.787	-0.25
124	945	LEU	LYS	-41.785	-0.248
125	943	ASP	PRO	-41.783	-0.246
126	845	ILE	TYR	-41.781	-0.244
127	907	GLY	MET	-41.78	-0.243
128	903	GLY	VAL	-41.777	-0.24

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
129	1048	ALA	LEU	-41.777	-0.24
130	1047	TRP	ASP	-41.768	-0.231
131	680	ARG	LYS	-41.767	-0.23
132	851	SER	ARG	-41.767	-0.23
133	674	GLN	ARG	-41.766	-0.229
134	851	SER	LYS	-41.764	-0.227
135	1002	ASP	LYS	-41.761	-0.224
136	1048	ALA	TYR	-41.761	-0.224
137	832	ILE	ARG	-41.759	-0.222
138	678	SER	ARG	-41.754	-0.217
139	935	PHE	LYS	-41.75	-0.213
140	1001	GLY	PRO	-41.75	-0.213
141	1002	ASP	ILE	-41.75	-0.213
142	849	VAL	ARG	-41.749	-0.212
143	847	VAL	TYR	-41.746	-0.209
144	1048	ALA	HIE	-41.744	-0.207
145	830	TYR	VAL	-41.742	-0.205
146	845	ILE	PHE	-41.736	-0.199
147	849	VAL	LYS	-41.736	-0.199
148	903	GLY	ILE	-41.733	-0.196
149	847	VAL	ILE	-41.731	-0.194
150	1048	ALA	MET	-41.73	-0.193
151	1048	ALA	ARG	-41.727	-0.19
152	847	VAL	GLN	-41.725	-0.188
153	1048	ALA	PRO	-41.725	-0.188
154	828	ARG	CYS	-41.717	-0.18
155	866	SER	TYR	-41.717	-0.18
156	903	GLY	SER	-41.715	-0.178
157	850	VAL	LYS	-41.714	-0.177
158	863	GLY	ALA	-41.714	-0.177
159	946	TYR	ARG	-41.71	-0.173
160	935	PHE	TYR	-41.708	-0.171
161	1002	ASP	PRO	-41.707	-0.17
162	1048	ALA	THR	-41.706	-0.169
163	903	GLY	ALA	-41.704	-0.167
164	866	SER	THR	-41.703	-0.166
165	1005	GLN	ARG	-41.703	-0.166
166	1003	GLY	MET	-41.696	-0.159
167	936	GLY	PHE	-41.693	-0.156
168	1003	GLY	GLN	-41.693	-0.156
169	855	TRP	LYS	-41.691	-0.154
170	908	VAL	ILE	-41.69	-0.153
171	845	ILE	LEU	-41.685	-0.148

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
172	845	ILE	VAL	-41.684	-0.147
173	1048	ALA	LYS	-41.682	-0.145
174	828	ARG	HIE	-41.676	-0.139
175	863	GLY	VAL	-41.674	-0.137
176	1003	GLY	HIE	-41.674	-0.137
177	1003	GLY	ARG	-41.673	-0.136
178	682	THR	PRO	-41.672	-0.135
179	936	GLY	PRO	-41.668	-0.131
180	909	ALA	ASN	-41.667	-0.13
181	1003	GLY	LEU	-41.666	-0.129
182	828	ARG	GLU	-41.665	-0.128
183	847	VAL	ASN	-41.665	-0.128
184	855	TRP	ARG	-41.664	-0.127
185	673	LEU	LYS	-41.659	-0.122
186	674	GLN	LYS	-41.652	-0.115
187	863	GLY	ASN	-41.652	-0.115
188	1003	GLY	LYS	-41.651	-0.114
189	966	SER	VAL	-41.648	-0.111
190	966	SER	ALA	-41.646	-0.109
191	847	VAL	MET	-41.645	-0.108
192	966	SER	GLY	-41.645	-0.108
193	845	ILE	CYS	-41.644	-0.107
194	830	TYR	ILE	-41.641	-0.104
195	1048	ALA	ILE	-41.634	-0.097
196	863	GLY	SER	-41.627	-0.09
197	847	VAL	GLY	-41.626	-0.089
198	681	SER	ARG	-41.624	-0.087
199	909	ALA	SER	-41.624	-0.087
200	847	VAL	PHE	-41.62	-0.083
201	1003	GLY	ALA	-41.62	-0.083
202	1004	SER	LEU	-41.617	-0.08
203	903	GLY	MET	-41.616	-0.079
204	846	THR	ASN	-41.614	-0.077
205	674	GLN	ILE	-41.613	-0.076
206	1003	GLY	GLU	-41.613	-0.076
207	847	VAL	CYS	-41.612	-0.075
208	847	VAL	SER	-41.612	-0.075
209	936	GLY	ILE	-41.611	-0.074
210	935	PHE	ARG	-41.609	-0.072
211	829	TYR	CYS	-41.607	-0.07
212	943	ASP	GLU	-41.607	-0.07
213	681	SER	TRP	-41.606	-0.069
214	1004	SER	MET	-41.602	-0.065

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
215	1006	MET	LYS	-41.601	-0.064
216	904	PRO	ILE	-41.599	-0.062
217	833	SER	TYR	-41.598	-0.061
218	966	SER	GLN	-41.597	-0.06
219	907	GLY	ALA	-41.595	-0.058
220	936	GLY	VAL	-41.595	-0.058
221	946	TYR	LYS	-41.592	-0.055
222	1001	GLY	THR	-41.592	-0.055
223	937	CYS	VAL	-41.591	-0.054
224	1004	SER	GLN	-41.591	-0.054
225	863	GLY	THR	-41.59	-0.053
226	1004	SER	PHE	-41.59	-0.053
227	851	SER	PHE	-41.587	-0.05
228	866	SER	MET	-41.584	-0.047
229	829	TYR	ALA	-41.583	-0.046
230	850	VAL	ARG	-41.583	-0.046
231	861	TYR	TRP	-41.583	-0.046
232	861	TYR	ARG	-41.582	-0.045
233	936	GLY	ASN	-41.581	-0.044
234	673	LEU	VAL	-41.58	-0.043
235	678	SER	THR	-41.58	-0.043
236	681	SER	LYS	-41.58	-0.043
237	850	VAL	THR	-41.58	-0.043
238	1003	GLY	ASP	-41.58	-0.043
239	1003	GLY	TRP	-41.579	-0.042
240	833	SER	ALA	-41.578	-0.041
241	909	ALA	CYS	-41.578	-0.041
242	681	SER	THR	-41.577	-0.04
243	855	TRP	ASN	-41.577	-0.04
244	936	GLY	THR	-41.575	-0.038
245	966	SER	ILE	-41.575	-0.038
246	1004	SER	ALA	-41.575	-0.038
247	847	VAL	ALA	-41.574	-0.037
248	845	ILE	THR	-41.573	-0.036
249	678	SER	ILE	-41.572	-0.035
250	830	TYR	THR	-41.572	-0.035
251	910	PRO	ARG	-41.569	-0.032
252	1003	GLY	THR	-41.569	-0.032
253	1006	MET	PRO	-41.569	-0.032
254	1003	GLY	CYS	-41.568	-0.031
255	1004	SER	HIE	-41.568	-0.031
256	855	TRP	MET	-41.566	-0.029
257	966	SER	PRO	-41.566	-0.029

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
258	681	SER	CYS	-41.564	-0.027
259	673	LEU	THR	-41.563	-0.026
260	674	GLN	THR	-41.563	-0.026
261	830	TYR	HIE	-41.563	-0.026
262	833	SER	THR	-41.563	-0.026
263	1004	SER	VAL	-41.562	-0.025
264	904	PRO	SER	-41.561	-0.024
265	674	GLN	PRO	-41.558	-0.021
266	833	SER	LYS	-41.556	-0.019
267	855	TRP	PHE	-41.556	-0.019
268	678	SER	CYS	-41.555	-0.018
269	909	ALA	LEU	-41.554	-0.017
270	1003	GLY	ASN	-41.554	-0.017
271	1048	ALA	CYS	-41.554	-0.017
272	861	TYR	ASN	-41.552	-0.015
273	935	PHE	PRO	-41.552	-0.015
274	1004	SER	ILE	-41.551	-0.014
275	1004	SER	CYS	-41.551	-0.014
276	681	SER	MET	-41.55	-0.013
277	830	TYR	MET	-41.55	-0.013
278	833	SER	CYS	-41.55	-0.013
279	845	ILE	PRO	-41.55	-0.013
280	851	SER	ASN	-41.55	-0.013
281	910	PRO	LYS	-41.55	-0.013
282	1004	SER	ASN	-41.55	-0.013
283	905	GLY	TYR	-41.549	-0.012
284	1005	GLN	LYS	-41.548	-0.011
285	829	TYR	SER	-41.547	-0.01
286	851	SER	ILE	-41.547	-0.01
287	678	SER	ALA	-41.546	-0.009
288	682	THR	SER	-41.546	-0.009
289	845	ILE	ALA	-41.546	-0.009
290	861	TYR	PRO	-41.546	-0.009
291	967	ARG	LYS	-41.546	-0.009
292	1005	GLN	MET	-41.546	-0.009
293	674	GLN	ALA	-41.545	-0.008
294	847	VAL	PRO	-41.545	-0.008
295	861	TYR	VAL	-41.545	-0.008
296	935	PHE	GLN	-41.545	-0.008
297	674	GLN	CYS	-41.544	-0.007
298	851	SER	CYS	-41.544	-0.007
299	851	SER	THR	-41.544	-0.007
300	851	SER	ALA	-41.543	-0.006

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
301	674	GLN	GLY	-41.541	-0.004
302	678	SER	GLY	-41.541	-0.004
303	851	SER	VAL	-41.541	-0.004
304	908	VAL	GLN	-41.541	-0.004
305	673	LEU	ASN	-41.538	-0.001
306	908	VAL	LEU	-41.538	-0.001
307	937	CYS	HIE	-41.538	-0.001
308	833	SER	GLY	-41.537	0
309	845	ILE	GLY	-41.537	0
310	861	TYR	HIE	-41.537	0
311	674	GLN	SER	-41.536	0.001
312	851	SER	GLY	-41.536	0.001
313	855	TRP	VAL	-41.536	0.001
314	904	PRO	LEU	-41.535	0.002
315	851	SER	MET	-41.534	0.003
316	681	SER	ALA	-41.533	0.004
317	849	VAL	LEU	-41.533	0.004
318	851	SER	GLN	-41.533	0.004
319	935	PHE	LEU	-41.532	0.005
320	935	PHE	MET	-41.532	0.005
321	851	SER	TRP	-41.531	0.006
322	861	TYR	ALA	-41.531	0.006
323	866	SER	ALA	-41.531	0.006
324	673	LEU	CYS	-41.53	0.007
325	847	VAL	GLU	-41.53	0.007
326	1002	ASP	MET	-41.53	0.007
327	855	TRP	SER	-41.529	0.008
328	861	TYR	SER	-41.529	0.008
329	861	TYR	GLN	-41.529	0.008
330	829	TYR	ASN	-41.528	0.009
331	847	VAL	THR	-41.528	0.009
332	855	TRP	THR	-41.528	0.009
333	861	TYR	CYS	-41.527	0.01
334	1004	SER	TRP	-41.527	0.01
335	861	TYR	ILE	-41.525	0.012
336	908	VAL	PHE	-41.525	0.012
337	1003	GLY	PHE	-41.525	0.012
338	682	THR	ALA	-41.524	0.013
339	851	SER	HIE	-41.524	0.013
340	855	TRP	CYS	-41.524	0.013
341	855	TRP	GLY	-41.524	0.013
342	937	CYS	ALA	-41.524	0.013
343	855	TRP	TYR	-41.523	0.014

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
344	861	TYR	GLY	-41.523	0.014
345	1003	GLY	SER	-41.523	0.014
346	845	ILE	SER	-41.522	0.015
347	855	TRP	ALA	-41.522	0.015
348	1047	TRP	ALA	-41.522	0.015
349	861	TYR	THR	-41.519	0.018
350	1005	GLN	HIE	-41.519	0.018
351	681	SER	GLY	-41.517	0.02
352	935	PHE	GLY	-41.517	0.02
353	1004	SER	GLY	-41.517	0.02
354	861	TYR	LEU	-41.516	0.021
355	1005	GLN	PHE	-41.516	0.021
356	673	LEU	SER	-41.515	0.022
357	674	GLN	ASN	-41.515	0.022
358	1004	SER	TYR	-41.514	0.023
359	678	SER	PRO	-41.513	0.024
360	673	LEU	ALA	-41.512	0.025
361	846	THR	SER	-41.511	0.026
362	935	PHE	THR	-41.511	0.026
363	945	LEU	ILE	-41.511	0.026
364	846	THR	CYS	-41.51	0.027
365	849	VAL	TRP	-41.51	0.027
366	910	PRO	THR	-41.51	0.027
367	935	PHE	ILE	-41.51	0.027
368	936	GLY	TYR	-41.51	0.027
369	1005	GLN	LEU	-41.51	0.027
370	682	THR	VAL	-41.508	0.029
371	673	LEU	GLY	-41.507	0.03
372	681	SER	ASN	-41.507	0.03
373	935	PHE	ALA	-41.505	0.032
374	935	PHE	CYS	-41.505	0.032
375	904	PRO	GLN	-41.503	0.034
376	681	SER	VAL	-41.502	0.035
377	832	ILE	MET	-41.502	0.035
378	678	SER	TYR	-41.501	0.036
379	966	SER	ASN	-41.501	0.036
380	1006	MET	CYS	-41.5	0.037
381	681	SER	HIE	-41.499	0.038
382	937	CYS	GLY	-41.499	0.038
383	908	VAL	THR	-41.497	0.04
384	937	CYS	ASN	-41.496	0.041
385	1002	ASP	HIE	-41.496	0.041
386	830	TYR	CYS	-41.495	0.042

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
387	904	PRO	ALA	-41.495	0.042
388	850	VAL	LEU	-41.494	0.043
389	935	PHE	SER	-41.494	0.043
390	830	TYR	ALA	-41.493	0.044
391	833	SER	PRO	-41.492	0.045
392	861	TYR	LYS	-41.492	0.045
393	678	SER	LEU	-41.49	0.047
394	678	SER	ASN	-41.489	0.048
395	846	THR	ALA	-41.489	0.048
396	909	ALA	GLN	-41.489	0.048
397	936	GLY	SER	-41.489	0.048
398	1006	MET	SER	-41.489	0.048
399	1048	ALA	ASN	-41.489	0.048
400	673	LEU	ARG	-41.487	0.05
401	966	SER	THR	-41.487	0.05
402	936	GLY	CYS	-41.485	0.052
403	966	SER	LEU	-41.485	0.052
404	832	ILE	SER	-41.484	0.053
405	903	GLY	CYS	-41.484	0.053
406	832	ILE	ASN	-41.48	0.057
407	850	VAL	CYS	-41.48	0.057
408	674	GLN	MET	-41.479	0.058
409	832	ILE	CYS	-41.479	0.058
410	1005	GLN	THR	-41.479	0.058
411	851	SER	PRO	-41.478	0.059
412	855	TRP	LEU	-41.477	0.06
413	674	GLN	VAL	-41.476	0.061
414	850	VAL	ILE	-41.475	0.062
415	849	VAL	ASN	-41.474	0.063
416	946	TYR	GLY	-41.474	0.063
417	845	ILE	GLU	-41.473	0.064
418	936	GLY	LEU	-41.473	0.064
419	681	SER	LEU	-41.472	0.065
420	833	SER	VAL	-41.471	0.066
421	946	TYR	CYS	-41.469	0.068
422	678	SER	GLN	-41.468	0.069
423	833	SER	PHE	-41.468	0.069
424	850	VAL	ALA	-41.468	0.069
425	946	TYR	SER	-41.468	0.069
426	850	VAL	MET	-41.467	0.07
427	946	TYR	ALA	-41.466	0.071
428	674	GLN	LEU	-41.465	0.072
429	832	ILE	ALA	-41.463	0.074

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
430	946	TYR	THR	-41.463	0.074
431	832	ILE	THR	-41.46	0.077
432	850	VAL	SER	-41.46	0.077
433	904	PRO	VAL	-41.458	0.079
434	1003	GLY	TYR	-41.458	0.079
435	678	SER	VAL	-41.457	0.08
436	861	TYR	MET	-41.457	0.08
437	673	LEU	ILE	-41.456	0.081
438	850	VAL	ASN	-41.456	0.081
439	936	GLY	TRP	-41.456	0.081
440	937	CYS	ILE	-41.456	0.081
441	946	TYR	PRO	-41.456	0.081
442	866	SER	CYS	-41.455	0.082
443	682	THR	GLY	-41.454	0.083
444	680	ARG	PHE	-41.453	0.084
445	1006	MET	ALA	-41.452	0.085
446	966	SER	CYS	-41.451	0.086
447	850	VAL	HIE	-41.45	0.087
448	866	SER	GLY	-41.448	0.089
449	1005	GLN	ALA	-41.448	0.089
450	1006	MET	ASN	-41.448	0.089
451	1005	GLN	VAL	-41.447	0.09
452	935	PHE	VAL	-41.446	0.091
453	829	TYR	LEU	-41.445	0.092
454	1002	ASP	ARG	-41.443	0.094
455	908	VAL	CYS	-41.441	0.096
456	936	GLY	ALA	-41.441	0.096
457	866	SER	VAL	-41.44	0.097
458	908	VAL	TYR	-41.44	0.097
459	829	TYR	GLY	-41.436	0.101
460	851	SER	LEU	-41.436	0.101
461	833	SER	LEU	-41.434	0.103
462	850	VAL	PRO	-41.434	0.103
463	908	VAL	ALA	-41.434	0.103
464	904	PRO	GLY	-41.433	0.104
465	849	VAL	THR	-41.432	0.105
466	904	PRO	CYS	-41.431	0.106
467	935	PHE	HIE	-41.431	0.106
468	937	CYS	MET	-41.43	0.107
469	830	TYR	GLY	-41.429	0.108
470	904	PRO	TYR	-41.429	0.108
471	908	VAL	ASN	-41.429	0.108
472	1046	VAL	THR	-41.428	0.109

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
473	850	VAL	GLY	-41.426	0.111
474	910	PRO	SER	-41.425	0.112
475	1006	MET	THR	-41.421	0.116
476	673	LEU	TRP	-41.42	0.117
477	682	THR	ASN	-41.42	0.117
478	828	ARG	SER	-41.42	0.117
479	849	VAL	CYS	-41.42	0.117
480	855	TRP	ILE	-41.42	0.117
481	866	SER	ASN	-41.42	0.117
482	681	SER	ILE	-41.419	0.118
483	678	SER	HIE	-41.416	0.121
484	855	TRP	HIE	-41.416	0.121
485	908	VAL	TRP	-41.416	0.121
486	1006	MET	GLY	-41.416	0.121
487	908	VAL	SER	-41.415	0.122
488	904	PRO	MET	-41.413	0.124
489	936	GLY	HIE	-41.413	0.124
490	833	SER	ASN	-41.412	0.125
491	866	SER	PRO	-41.412	0.125
492	861	TYR	PHE	-41.411	0.126
493	937	CYS	THR	-41.411	0.126
494	829	TYR	HIE	-41.41	0.127
495	850	VAL	GLN	-41.41	0.127
496	850	VAL	TRP	-41.409	0.128
497	946	TYR	ASN	-41.409	0.128
498	910	PRO	CYS	-41.408	0.129
499	681	SER	PRO	-41.406	0.131
500	946	TYR	LEU	-41.406	0.131
501	833	SER	HIE	-41.405	0.132
502	936	GLY	MET	-41.404	0.133
503	946	TYR	MET	-41.404	0.133
504	1005	GLN	CYS	-41.404	0.133
505	1048	ALA	GLU	-41.403	0.134
506	908	VAL	GLY	-41.401	0.136
507	849	VAL	GLN	-41.4	0.137
508	910	PRO	ALA	-41.399	0.138
509	937	CYS	SER	-41.397	0.14
510	681	SER	GLN	-41.396	0.141
511	700	HIE	PHE	-41.396	0.141
512	849	VAL	HIE	-41.396	0.141
513	910	PRO	VAL	-41.396	0.141
514	849	VAL	MET	-41.395	0.142
515	966	SER	HIE	-41.394	0.143

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
516	847	VAL	HIE	-41.393	0.144
517	908	VAL	MET	-41.393	0.144
518	829	TYR	GLN	-41.392	0.145
519	1006	MET	LEU	-41.391	0.146
520	680	ARG	HIE	-41.389	0.148
521	1005	GLN	SER	-41.389	0.148
522	910	PRO	ASN	-41.387	0.15
523	829	TYR	LYS	-41.386	0.151
524	851	SER	TYR	-41.386	0.151
525	966	SER	TYR	-41.386	0.151
526	855	TRP	GLN	-41.385	0.152
527	945	LEU	ASN	-41.385	0.152
528	966	SER	PHE	-41.384	0.153
529	832	ILE	TYR	-41.382	0.155
530	680	ARG	MET	-41.38	0.157
531	830	TYR	ASN	-41.379	0.158
532	937	CYS	GLN	-41.379	0.158
533	846	THR	GLY	-41.377	0.16
534	678	SER	PHE	-41.376	0.161
535	832	ILE	PRO	-41.374	0.163
536	910	PRO	GLY	-41.374	0.163
537	673	LEU	TYR	-41.372	0.165
538	946	TYR	GLN	-41.372	0.165
539	832	ILE	GLY	-41.37	0.167
540	904	PRO	THR	-41.369	0.168
541	905	GLY	SER	-41.368	0.169
542	681	SER	TYR	-41.366	0.171
543	678	SER	MET	-41.364	0.173
544	674	GLN	TRP	-41.361	0.176
545	903	GLY	GLU	-41.361	0.176
546	945	LEU	THR	-41.361	0.176
547	830	TYR	SER	-41.358	0.179
548	673	LEU	PRO	-41.357	0.18
549	935	PHE	ASN	-41.357	0.18
550	946	TYR	ILE	-41.356	0.181
551	937	CYS	LEU	-41.355	0.182
552	673	LEU	GLN	-41.353	0.184
553	832	ILE	LEU	-41.352	0.185
554	849	VAL	SER	-41.352	0.185
555	1048	ALA	SER	-41.352	0.185
556	673	LEU	MET	-41.348	0.189
557	681	SER	PHE	-41.348	0.189
558	936	GLY	GLN	-41.347	0.19

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
559	945	LEU	CYS	-41.347	0.19
560	1005	GLN	ILE	-41.346	0.191
561	1006	MET	ARG	-41.344	0.193
562	832	ILE	PHE	-41.342	0.195
563	863	GLY	CYS	-41.342	0.195
564	909	ALA	GLY	-41.342	0.195
565	674	GLN	PHE	-41.34	0.197
566	682	THR	CYS	-41.34	0.197
567	855	TRP	PRO	-41.34	0.197
568	863	GLY	ILE	-41.34	0.197
569	673	LEU	PHE	-41.338	0.199
570	946	TYR	TRP	-41.338	0.199
571	674	GLN	TYR	-41.337	0.2
572	849	VAL	ALA	-41.337	0.2
573	847	VAL	ASP	-41.335	0.202
574	946	TYR	VAL	-41.334	0.203
575	849	VAL	GLY	-41.333	0.204
576	945	LEU	SER	-41.333	0.204
577	946	TYR	HIE	-41.332	0.205
578	680	ARG	ASN	-41.33	0.207
579	846	THR	PRO	-41.33	0.207
580	845	ILE	ASN	-41.327	0.21
581	908	VAL	HIE	-41.327	0.21
582	673	LEU	HIE	-41.326	0.211
583	945	LEU	ALA	-41.326	0.211
584	850	VAL	PHE	-41.322	0.215
585	866	SER	PHE	-41.322	0.215
586	937	CYS	PRO	-41.322	0.215
587	861	TYR	ASP	-41.319	0.218
588	904	PRO	PHE	-41.319	0.218
589	967	ARG	THR	-41.318	0.219
590	945	LEU	VAL	-41.317	0.22
591	849	VAL	ILE	-41.316	0.221
592	855	TRP	GLU	-41.316	0.221
593	849	VAL	PHE	-41.315	0.222
594	1005	GLN	ASN	-41.315	0.222
595	828	ARG	TYR	-41.314	0.223
596	850	VAL	TYR	-41.312	0.225
597	945	LEU	GLY	-41.312	0.225
598	910	PRO	LEU	-41.311	0.226
599	966	SER	TRP	-41.311	0.226
600	832	ILE	HIE	-41.31	0.227
601	849	VAL	TYR	-41.31	0.227

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
602	680	ARG	GLN	-41.307	0.23
603	680	ARG	PRO	-41.305	0.232
604	829	TYR	PRO	-41.304	0.233
605	903	GLY	GLN	-41.303	0.234
606	829	TYR	MET	-41.301	0.236
607	1006	MET	VAL	-41.301	0.236
608	967	ARG	GLY	-41.3	0.237
609	678	SER	TRP	-41.296	0.241
610	1005	GLN	PRO	-41.294	0.243
611	680	ARG	LEU	-41.293	0.244
612	907	GLY	HIE	-41.293	0.244
613	828	ARG	ASP	-41.283	0.254
614	680	ARG	GLY	-41.279	0.258
615	908	VAL	PRO	-41.278	0.259
616	828	ARG	GLY	-41.272	0.265
617	851	SER	GLU	-41.27	0.267
618	1001	GLY	GLU	-41.27	0.267
619	945	LEU	ARG	-41.269	0.268
620	1048	ALA	VAL	-41.268	0.269
621	680	ARG	THR	-41.267	0.27
622	946	TYR	PHE	-41.267	0.27
623	967	ARG	ILE	-41.267	0.27
624	829	TYR	TRP	-41.264	0.273
625	680	ARG	ALA	-41.263	0.274
626	832	ILE	VAL	-41.262	0.275
627	851	SER	ASP	-41.262	0.275
628	681	SER	ASP	-41.259	0.278
629	967	ARG	CYS	-41.259	0.278
630	680	ARG	CYS	-41.258	0.279
631	846	THR	LEU	-41.258	0.279
632	967	ARG	SER	-41.258	0.279
633	700	HIE	ILE	-41.256	0.281
634	828	ARG	ALA	-41.256	0.281
635	967	ARG	ALA	-41.256	0.281
636	832	ILE	GLN	-41.254	0.283
637	966	SER	GLU	-41.251	0.286
638	967	ARG	PHE	-41.251	0.286
639	830	TYR	LEU	-41.25	0.287
640	833	SER	ILE	-41.249	0.288
641	967	ARG	MET	-41.248	0.289
642	967	ARG	ASN	-41.247	0.29
643	680	ARG	SER	-41.246	0.291
644	829	TYR	PHE	-41.244	0.293

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
645	828	ARG	THR	-41.243	0.294
646	967	ARG	GLN	-41.243	0.294
647	1004	SER	GLU	-41.243	0.294
648	855	TRP	ASP	-41.239	0.298
649	967	ARG	LEU	-41.237	0.3
650	674	GLN	GLU	-41.236	0.301
651	1005	GLN	ASP	-41.234	0.303
652	861	TYR	GLU	-41.233	0.304
653	1002	ASP	GLN	-41.233	0.304
654	833	SER	GLN	-41.232	0.305
655	946	TYR	ASP	-41.231	0.306
656	967	ARG	HIE	-41.23	0.307
657	674	GLN	HIE	-41.229	0.308
658	829	TYR	ASP	-41.225	0.312
659	832	ILE	TRP	-41.225	0.312
660	1004	SER	ASP	-41.224	0.313
661	1005	GLN	GLU	-41.221	0.316
662	1047	TRP	SER	-41.219	0.318
663	945	LEU	GLN	-41.217	0.32
664	904	PRO	HIE	-41.216	0.321
665	700	HIE	THR	-41.215	0.322
666	904	PRO	ASN	-41.213	0.324
667	967	ARG	TRP	-41.21	0.327
668	967	ARG	PRO	-41.21	0.327
669	1046	VAL	ALA	-41.207	0.33
670	1005	GLN	TRP	-41.205	0.332
671	1048	ALA	GLY	-41.205	0.332
672	673	LEU	ASP	-41.204	0.333
673	909	ALA	THR	-41.202	0.335
674	1006	MET	TRP	-41.202	0.335
675	866	SER	GLN	-41.198	0.339
676	1005	GLN	TYR	-41.198	0.339
677	1047	TRP	CYS	-41.198	0.339
678	680	ARG	VAL	-41.196	0.341
679	848	SER	GLU	-41.194	0.343
680	905	GLY	MET	-41.187	0.35
681	1006	MET	TYR	-41.185	0.352
682	905	GLY	ILE	-41.183	0.354
683	1048	ALA	ASP	-41.183	0.354
684	910	PRO	HIE	-41.178	0.359
685	832	ILE	GLU	-41.174	0.363
686	907	GLY	GLU	-41.174	0.363
687	846	THR	ILE	-41.172	0.365

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
688	866	SER	LEU	-41.172	0.365
689	905	GLY	ASN	-41.17	0.367
690	1047	TRP	HIE	-41.17	0.367
691	680	ARG	ILE	-41.167	0.37
692	1046	VAL	SER	-41.167	0.37
693	674	GLN	ASP	-41.166	0.371
694	910	PRO	ILE	-41.165	0.372
695	967	ARG	VAL	-41.164	0.373
696	673	LEU	GLU	-41.159	0.378
697	849	VAL	PRO	-41.158	0.379
698	936	GLY	ASP	-41.158	0.379
699	700	HIE	TYR	-41.157	0.38
700	700	HIE	PRO	-41.155	0.382
701	1002	ASP	VAL	-41.155	0.382
702	828	ARG	PHE	-41.153	0.384
703	866	SER	ASP	-41.149	0.388
704	833	SER	MET	-41.148	0.389
705	966	SER	ASP	-41.148	0.389
706	908	VAL	GLU	-41.146	0.391
707	828	ARG	PRO	-41.145	0.392
708	910	PRO	MET	-41.144	0.393
709	945	LEU	MET	-41.143	0.394
710	678	SER	ASP	-41.142	0.395
711	935	PHE	GLU	-41.141	0.396
712	866	SER	GLU	-41.14	0.397
713	945	LEU	PRO	-41.14	0.397
714	681	SER	GLU	-41.139	0.398
715	967	ARG	TYR	-41.139	0.398
716	910	PRO	TYR	-41.137	0.4
717	910	PRO	TRP	-41.135	0.402
718	863	GLY	GLU	-41.13	0.407
719	903	GLY	ASP	-41.13	0.407
720	910	PRO	PHE	-41.129	0.408
721	1002	ASP	GLU	-41.128	0.409
722	1003	GLY	PRO	-41.127	0.41
723	680	ARG	TRP	-41.118	0.419
724	832	ILE	ASP	-41.115	0.422
725	909	ALA	MET	-41.112	0.425
726	945	LEU	TRP	-41.112	0.425
727	945	LEU	PHE	-41.111	0.426
728	700	HIE	CYS	-41.11	0.427
729	1006	MET	ASP	-41.102	0.435
730	937	CYS	ASP	-41.093	0.444

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
731	945	LEU	HIE	-41.092	0.445
732	700	HIE	LYS	-41.091	0.446
733	846	THR	TRP	-41.084	0.453
734	830	TYR	GLU	-41.081	0.456
735	935	PHE	ASP	-41.081	0.456
736	1006	MET	ILE	-41.08	0.457
737	678	SER	GLU	-41.078	0.459
738	700	HIE	ALA	-41.076	0.461
739	845	ILE	ASP	-41.071	0.466
740	1006	MET	PHE	-41.065	0.472
741	1047	TRP	TYR	-41.058	0.479
742	866	SER	ILE	-41.057	0.48
743	680	ARG	TYR	-41.047	0.49
744	700	HIE	ASN	-41.045	0.492
745	936	GLY	GLU	-41.044	0.493
746	1046	VAL	ILE	-41.042	0.495
747	938	ARG	LYS	-41.04	0.497
748	700	HIE	GLY	-41.039	0.498
749	905	GLY	VAL	-41.039	0.498
750	700	HIE	SER	-41.034	0.503
751	833	SER	ASP	-41.025	0.512
752	849	VAL	GLU	-41.023	0.514
753	863	GLY	ASP	-41.022	0.515
754	1006	MET	HIE	-41.021	0.516
755	700	HIE	LEU	-41.016	0.521
756	850	VAL	ASP	-41.016	0.521
757	1001	GLY	ALA	-41.008	0.529
758	849	VAL	ASP	-41	0.537
759	903	GLY	ASN	-40.996	0.541
760	1001	GLY	SER	-40.996	0.541
761	863	GLY	ARG	-40.994	0.543
762	908	VAL	ASP	-40.993	0.544
763	850	VAL	GLU	-40.992	0.545
764	846	THR	GLU	-40.991	0.546
765	1046	VAL	GLY	-40.987	0.55
766	938	ARG	GLY	-40.986	0.551
767	833	SER	GLU	-40.985	0.552
768	846	THR	VAL	-40.985	0.552
769	938	ARG	SER	-40.985	0.552
770	1047	TRP	ARG	-40.984	0.553
771	938	ARG	ALA	-40.981	0.556
772	909	ALA	ASP	-40.98	0.557
773	967	ARG	ASP	-40.974	0.563

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
774	937	CYS	GLU	-40.972	0.565
775	967	ARG	GLU	-40.972	0.565
776	700	HIE	MET	-40.971	0.566
777	829	TYR	GLU	-40.97	0.567
778	700	HIE	GLU	-40.962	0.575
779	938	ARG	CYS	-40.961	0.576
780	1047	TRP	MET	-40.953	0.584
781	1006	MET	GLN	-40.95	0.587
782	910	PRO	ASP	-40.947	0.59
783	945	LEU	TYR	-40.944	0.593
784	700	HIE	GLN	-40.943	0.594
785	846	THR	ASP	-40.941	0.596
786	904	PRO	GLU	-40.94	0.597
787	910	PRO	GLN	-40.939	0.598
788	910	PRO	GLU	-40.939	0.598
789	946	TYR	GLU	-40.929	0.608
790	1005	GLN	GLY	-40.919	0.618
791	938	ARG	MET	-40.917	0.62
792	938	ARG	PRO	-40.915	0.622
793	1002	ASP	THR	-40.915	0.622
794	1046	VAL	CYS	-40.912	0.625
795	909	ALA	GLU	-40.911	0.626
796	1001	GLY	PHE	-40.901	0.636
797	1047	TRP	LYS	-40.901	0.636
798	907	GLY	LEU	-40.9	0.637
799	700	HIE	VAL	-40.897	0.64
800	700	HIE	ASP	-40.885	0.652
801	680	ARG	GLU	-40.879	0.658
802	938	ARG	ILE	-40.86	0.677
803	905	GLY	LEU	-40.85	0.687
804	945	LEU	ASP	-40.843	0.694
805	938	ARG	VAL	-40.829	0.708
806	938	ARG	THR	-40.819	0.718
807	905	GLY	PRO	-40.807	0.73
808	846	THR	HIE	-40.803	0.734
809	938	ARG	HIE	-40.803	0.734
810	1047	TRP	ASN	-40.801	0.736
811	830	TYR	ASP	-40.8	0.737
812	938	ARG	GLN	-40.784	0.753
813	1047	TRP	GLY	-40.784	0.753
814	1046	VAL	ASN	-40.779	0.758
815	938	ARG	TYR	-40.77	0.767
816	938	ARG	LEU	-40.769	0.768

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
817	938	ARG	TRP	-40.765	0.772
818	1047	TRP	LEU	-40.765	0.772
819	938	ARG	ASN	-40.753	0.784
820	680	ARG	ASP	-40.743	0.794
821	1002	ASP	SER	-40.74	0.797
822	1047	TRP	GLU	-40.739	0.798
823	1047	TRP	PHE	-40.73	0.807
824	848	SER	CYS	-40.72	0.817
825	1046	VAL	ASP	-40.714	0.823
826	938	ARG	PHE	-40.692	0.845
827	905	GLY	ALA	-40.689	0.848
828	848	SER	LEU	-40.688	0.849
829	938	ARG	GLU	-40.687	0.85
830	1046	VAL	GLU	-40.656	0.881
831	945	LEU	GLU	-40.655	0.882
832	848	SER	ASN	-40.645	0.892
833	1002	ASP	CYS	-40.642	0.895
834	904	PRO	ASP	-40.629	0.908
835	907	GLY	TRP	-40.594	0.943
836	682	THR	ASP	-40.581	0.956
837	938	ARG	ASP	-40.578	0.959
838	848	SER	GLN	-40.574	0.963
839	1006	MET	GLU	-40.568	0.969
840	682	THR	ILE	-40.565	0.972
841	846	THR	PHE	-40.556	0.981
842	907	GLY	ASP	-40.539	0.998
843	909	ALA	TRP	-40.532	1.005
844	905	GLY	TRP	-40.526	1.011
845	863	GLY	TYR	-40.515	1.022
846	1047	TRP	VAL	-40.501	1.036
847	1047	TRP	ILE	-40.492	1.045
848	863	GLY	PHE	-40.477	1.06
849	905	GLY	CYS	-40.476	1.061
850	845	ILE	TRP	-40.46	1.077
851	1047	TRP	GLN	-40.454	1.083
852	905	GLY	ARG	-40.442	1.095
853	866	SER	HIE	-40.428	1.109
854	1002	ASP	ALA	-40.402	1.135
855	1046	VAL	HIE	-40.396	1.141
856	846	THR	GLN	-40.395	1.142
857	906	THR	SER	-40.387	1.15
858	909	ALA	HIE	-40.356	1.181
859	846	THR	TYR	-40.353	1.184

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
860	828	ARG	TRP	-40.326	1.211
861	863	GLY	HIE	-40.306	1.231
862	682	THR	LEU	-40.274	1.263
863	833	SER	ARG	-40.21	1.327
864	863	GLY	TRP	-40.199	1.338
865	848	SER	PRO	-40.188	1.349
866	1002	ASP	LEU	-40.177	1.36
867	682	THR	LYS	-40.162	1.375
868	829	TYR	ARG	-40.16	1.377
869	848	SER	TYR	-40.135	1.402
870	906	THR	CYS	-40.132	1.405
871	848	SER	ASP	-40.117	1.42
872	906	THR	ASN	-40.114	1.423
873	907	GLY	TYR	-40.08	1.457
874	848	SER	ILE	-40.023	1.514
875	848	SER	VAL	-40.014	1.523
876	909	ALA	TYR	-40.014	1.523
877	909	ALA	PHE	-39.999	1.538
878	848	SER	PHE	-39.969	1.568
879	682	THR	GLU	-39.926	1.611
880	848	SER	ALA	-39.914	1.623
881	937	CYS	TYR	-39.819	1.718
882	937	CYS	TRP	-39.815	1.722
883	848	SER	HIE	-39.814	1.723
884	848	SER	TRP	-39.797	1.74
885	848	SER	THR	-39.782	1.755
886	682	THR	TRP	-39.773	1.764
887	682	THR	GLN	-39.766	1.771
888	937	CYS	PHE	-39.753	1.784
889	906	THR	ALA	-39.744	1.793
890	906	THR	ARG	-39.725	1.812
891	906	THR	GLN	-39.68	1.857
892	1046	VAL	TYR	-39.674	1.863
893	906	THR	LYS	-39.666	1.871
894	905	GLY	GLU	-39.641	1.896
895	846	THR	LYS	-39.604	1.933
896	1002	ASP	GLY	-39.593	1.944
897	848	SER	MET	-39.578	1.959
898	846	THR	ARG	-39.509	2.028
899	846	THR	MET	-39.339	2.198
900	1046	VAL	LEU	-39.312	2.225
901	1001	GLY	ASP	-39.287	2.25
902	848	SER	GLY	-39.233	2.304

number	ID	wild	mutant	ΔG_{bind}	$\Delta\Delta G_{bind}^a$
903	905	GLY	ASP	-39.149	2.388
904	906	THR	MET	-39.144	2.393
905	906	THR	ASP	-39.095	2.442
906	906	THR	PHE	-39.036	2.501
907	830	TYR	PHE	-38.945	2.592
908	830	TYR	TRP	-38.911	2.626
909	909	ALA	PRO	-38.885	2.652
910	1046	VAL	PHE	-38.857	2.68
911	906	THR	HIE	-38.846	2.691
912	906	THR	TRP	-38.841	2.696
913	906	THR	TYR	-38.776	2.761
914	906	THR	LEU	-38.528	3.009
915	906	THR	GLY	-38.443	3.094
916	682	THR	ARG	-38.072	3.465
917	906	THR	PRO	-38.066	3.471
918	682	THR	MET	-37.863	3.674
919	1047	TRP	PRO	-37.776	3.761
920	682	THR	HIE	-37.655	3.882
921	903	GLY	TYR	-37.421	4.116
922	903	GLY	TRP	-37.319	4.218
923	906	THR	VAL	-37.299	4.238
924	906	THR	GLU	-37.06	4.477
925	682	THR	PHE	-36.656	4.881
926	682	THR	TYR	-36.425	5.112
927	903	GLY	PHE	-36.107	5.43
928	906	THR	ILE	-35.573	5.964
929	1046	VAL	TRP	-35.127	6.41
930	903	GLY	HIE	-34.124	7.413
931	1001	GLY	TRP	-34.049	7.488

^a $\Delta\Delta G_{bind} = \Delta G_{bind}(\text{mut}) - \Delta G_{bind}(\text{WT})$

All energies are in kcal/mol.