

Positions	Models	▲ G (kcal/mol)
	Wildtype	3.9000
1	F1L	3.9000
	F1S	3.9000
	F1P	3.9000
2	P2S	3.9000
	P2F	3.9000
	P2L	3.9000
3	N3D	3.9000
	N3G	3.9000
	N3S	3.9000
4	I4A	3.9000
	I4T	3.9000
	I4V	3.9000
5	T5A	3.9000
	T5I	3.9000
	T5M	3.9000
	T5V	3.9000
6	N6D	3.9000
	N6G	3.9000
	N6S	3.9000
7	L7P	3.9000
	L7S	3.9000
8	C8H	3.9000
	C8R	3.9000
	C8Y	4.0000
9	P9F	3.9000
	P9L	3.9000
	P9S	3.9000
10	F10L	NA
	F10P	
	F10S	

11	G11D	N/A
	G11N	
	G11S	
12	E12G	3.9000
	E12K	3.9000
	E12R	3.9000
13	V13A	3.9000
	V13I	3.9000
	V13T	3.9000
14	F14L	N/A
	F14P	
	F14S	
15	N15D	N/A
	N15G	
	N15S	
16	A16I	3.9000
	A16T	3.9000
	A16V	3.9000
17	T17A	3.9000
	T17I	3.9000
	T17V	3.9000
18	R18E	3.9000
	R18G	3.9000
	R18K	3.9000
19	F19L	3.9000
	F19P	3.9000
	F19S	3.9000
20	A20I	3.9000
	A20M	3.9000
	A20T	3.9000
	A20V	3.9000

21	S21F	3.9000
	S21L	3.9000
	S21P	3.9000
22	V22I	3.9000
	V22A	3.9000
	V22T	3.9000
23	Y23C	3.9000
	Y23H	3.9000
	Y23R	3.9000
24	A24I	3.9000
	A24T	3.9000
	A24V	3.9000
25	W25Q	3.9000
	W25R	3.9000
26	N26D	3.9000
	N26G	3.9000
	N26S	3.9000
27	R27E	3.9000
	R27G	3.9000
	R27K	3.9000
28	K28E	3.9000
	K28G	3.9000
	K28R	3.9000
29	R29E	3.9000
	R29G	3.9000
	R29K	3.9000
30	I30A	3.9000
	I30T	3.9000
	I30V	3.9000
31	S31D	3.9000
	S31G	3.9000

	S31N	3.9000
32	N32D	3.9000
	N32G	3.9000
	N32S	3.9000
33	C33H	3.9000
	C33R	3.9000
	C33Y	3.9000
34	V34A	3.9000
	V34I	3.9000
	V34T	3.9000
35	A35I	3.9000
	A35T	3.9000
	A35V	3.9000
36	D36G	3.9000
	D36N	3.9000
	D36S	3.9000
37	Y37C	3.9000
	Y37H	3.9000
	Y37R	3.9000
38	S38F	3.9000
	S38L	3.9000
	S38P	3.9000
39	V39A	N/A
	V39I	
	V39T	
40	L40P	N/A
	L40S	
41	Y41C	3.9000
	Y41H	3.9000
	Y41R	3.9000
	N42D	3.9000

42	N42G	3.9000
	N42S	3.9000
43	S43F	3.4000
	S43L	3.6000
	S43P	3.8000
44	A44D	3.9000
	A44I	3.9000
	A44T	3.9000
	A44V	3.9000
45	S45L	3.9000
	S45P	4.1000
46	F46L	3.9000
	F46P	3.8000
	F46S	3.9000
47	S47F	3.9000
	S47L	3.9000
	S47P	3.9000
48	T48A	3.9000
	T48I	3.9000
	T48V	3.9000
49	F49L	3.9000
	F49P	3.9000
	F49S	3.9000
50	K50E	3.9000
	K50G	3.9000
	K50R	3.9000
51	C51H	3.9000
	C51R	3.9000
	C51Y	3.9000
52	Y52C	3.9000
	Y52H	3.9000

	Y52R	3.9000
53	G53E	3.9000
	G53K	3.9000
	G53R	3.9000
54	V54I	3.9000
	V54T	3.9000
	V54A	3.9000
	V54M	3.9000
55	S55F	3.9000
	S55L	3.9000
	S55P	3.9000
56	P56F	3.9000
	P56L	3.9000
	P56S	3.9000
57	T57A	3.9000
	T57I	3.9000
	T57V	3.9000
58	K58E	3.9000
	K58G	3.9000
	K58R	3.9000
59	L59P	3.9000
	L59S	3.9000
60	N60D	3.9000
	N60G	3.9000
	N60S	3.9000
61	D61G	3.9000
	D61N	3.9000
	D61S	3.9000
62	L62F	3.9000
	L62P	3.9000
	L62S	3.9000

63	C63H	3.8000
	C63R	3.9000
	C63Y	3.9000
64	F64L	3.9000
	F64P	3.9000
	F64S	3.9000
65	T65A	3.9000
	T65I	3.9000
	T65V	3.9000
66	N66D	3.9000
	N66G	3.9000
	N66S	3.9000
67	V67A	3.9000
	V67T	3.9000
	V67I	3.9000
68	Y68C	3.9000
	Y68H	3.9000
	Y68R	3.9000
69	A69I	3.9000
	A69M	3.9000
	A69T	3.9000
	A69V	3.9000
70	D70G	3.9000
	D70N	3.9000
	D70S	3.9000
71	S71L	3.9000
	S71P	3.9000
72	F72L	3.9000
	F72P	3.9000
	F72S	3.9000
	V73A	3.9000

73	V73I	3.9000
	V73M	3.9000
	V73T	3.9000
74	I74A	3.9000
	I74T	3.9000
	I74V	3.9000
75	R75E	3.9000
	R75G	3.9000
	R75K	3.9000
76	G76D	3.9000
	G76N	3.9000
	G76S	3.9000
77	D77G	3.9000
	D77N	3.9000
	D77S	3.9000
78	E78G	3.9000
	E78K	3.9000
	E78R	3.9000
79	V79A	3.9000
	V79I	3.9000
	V79T	3.9000
80	R80E	3.9000
	R80G	3.9000
	R80K	3.9000
81	Q81R	3.9000
	Q81W	3.9000
82	I82A	3.9000
	I82T	3.9000
	I82V	3.9000
83	A83I	3.9000
	A83T	3.9000

	A83V	3.9000
84	P84L	3.9000
	P84S	3.9000
85	G85E	3.9000
	G85K	3.9000
	G85R	3.9000
86	Q86R	3.9000
	Q86W	3.9000
87	T87A	3.9000
	T87I	3.9000
	T87V	3.9000
88	G88E	3.9000
	G88K	3.9000
	G88R	3.9000
89	K89E	3.9000
	K89G	3.9000
	K89R	3.9000
90	I90A	3.9000
	I90T	3.9000
	I90V	3.9000
91	A91I	3.9000
	A91T	3.9000
	A91V	3.9000
92	D92G	3.9000
	D92N	3.9000
	D92S	3.9000
93	Y93C	3.9000
	Y93H	3.9000
	Y93R	3.9000
94	N94D	3.9000
	N94G	3.9000

	N94S	3.9000
95	Y95C	3.9000
	Y95H	3.9000
	Y95R	3.9000
96	K96E	3.9000
	K96G	3.9000
	K96R	3.9000
97	L97P	3.9000
	L97S	3.9000
98	P98L	3.9000
	P98S	3.9000
99	D99G	3.9000
	D99N	3.9000
	D99S	3.9000
100	D100G	3.9000
	D100N	3.9000
	D100S	3.9000
101	F101L	3.9000
	F101P	3.9000
	F101S	3.9000
102	T102A	3.9000
	T102I	3.9000
	T102V	3.9000
	T102M	3.9000
103	G103D	3.9000
	G103N	3.9000
	G103S	3.9000
104	C104H	3.9000
	C104R	3.9000
	C104Y	3.9000
	V105A	3.9000

105	V105I	3.9000
	V105T	3.9000
106	I106A	3.9000
	I106M	3.9000
	I106T	3.9000
	I106V	3.9000
107	A107I	3.9000
	A107T	3.9000
	A107V	3.9000
108	W108Q	3.9000
	W108R	3.9000
109	N109D	3.9000
	N109G	3.9000
	N109S	3.9000
110	S110F	N/A
	S110L	3.9000
	S110P	3.9000
111	N111D	3.9000
	N111G	3.9000
	N111S	3.9000
112	N112D	3.9000
	N112G	3.9000
	N112S	3.9000
113	L113F	3.9000
	L113P	3.9000
	L113S	3.9000
114	D114G	3.9000
	D114N	3.9000
	D114S	3.9000
115	S115F	3.9000
	S115L	3.9000

	S115P	3.9000
116	K116E	3.9000
	K116G	3.9000
	K116R	3.9000
117	V117A	3.9000
	V117I	3.9000
	V117T	3.9000
118	G118D	3.9000
	G118N	3.9000
	G118S	3.9000
119	G119D	3.9000
	G119N	3.9000
	G119S	3.9000
120	N120D	3.9000
	N120G	3.9000
	N120S	3.9000
121	Y121C	3.9000
	Y121H	3.9000
	Y121R	3.9000
122	N122D	3.9000
	N122G	3.9000
	N122S	3.9000
123	Y123C	3.9000
	Y123H	3.9000
	Y123R	3.9000
124	L124P	3.9000
	L124S	3.9000
125	Y125C	3.9000
	Y125H	3.9000
	Y125R	3.9000
	R126G	3.9000

126	R126E	3.9000
	R126K	3.9000
127	L127P	3.9000
	L127S	3.9000
128	F128L	3.9000
	F128P	3.9000
	F128S	3.9000
129	R129E	3.9000
	R129G	3.9000
	R129K	3.9000
130	K130E	3.9000
	K130G	3.9000
	K130R	3.9000
131	S131F	3.9000
	S131L	3.9000
	S131P	3.9000
132	N132D	3.9000
	N132G	3.9000
	N132S	3.9000
133	L133F	3.9000
	L133P	3.9000
	L133S	3.9000
134	K134E	3.9000
	K134G	3.9000
	K134R	3.9000
135	P135F	3.9000
	P135L	3.9000
	P135S	3.9000
136	F136L	3.9000
	F136P	3.9000
	F136S	3.9000

137	E137G	3.9000
	E137K	3.9000
	E137R	3.9000
138	R138E	3.9000
	R138G	3.9000
	R138K	3.9000
139	D139G	3.9000
	D139N	3.9000
	D139S	3.9000
140	I140A	3.9000
	I140T	3.9000
	I140V	3.9000
141	S141L	3.9000
	S141P	3.9000
142	T142A	3.9000
	T142I	3.9000
	T142V	3.9000
143	E143G	3.9000
	E143K	3.9000
	E143R	3.9000
144	I144A	3.9000
	I144T	3.9000
	I144V	3.9000
145	Y145C	3.9000
	Y145H	3.9000
	Y145R	3.9000
146	Q146R	3.9000
	Q146W	3.9000
147	A147I	3.9000
	A147T	3.9000
	A147V	3.9000

148	G148D	3.9000
	G148N	3.9000
	G148S	3.9000
149	S149D	3.9000
	S149G	3.9000
	S149N	3.9000
150	T150A	3.9000
	T150I	3.9000
	T150V	3.9000
	T150M	3.9000
151	P151F	3.9000
	P151L	3.9000
	P151S	3.9000
152	C152H	3.9000
	C152R	3.9000
	C152Y	3.9000
153	N153G	3.9000
	N153D	3.9000
	N153S	3.9000
154	G154D	3.9000
	G154N	3.9000
	G154S	3.9000
155	V155A	3.9000
	V155I	3.9000
	V155T	3.9000
156	E156G	3.9000
	E156K	3.9000
	E156R	3.9000
157	G157D	3.9000
	G157N	3.9000
	G157S	3.9000

158	F158L	3.9000
	F158P	3.9000
	F158S	3.9000
159	N159D	3.9000
	N159G	3.9000
	N159S	3.9000
160	C160H	3.9000
	C160R	3.9000
	C160Y	3.9000
161	Y161C	3.9000
	Y161H	3.9000
	Y161R	3.9000
162	F162L	3.9000
	F162P	3.9000
	F162S	3.9000
163	P163F	3.9000
	P163L	3.9000
	P163S	3.9000
164	L164P	3.9000
	L164S	3.9000
165	Q165R	3.9000
	Q165W	3.9000
166	S166L	3.9000
	S166P	3.9000
167	Y167C	3.9000
	Y167H	3.9000
	Y167R	3.9000
168	G168D	3.9000
	G168N	3.9000
	G168S	3.9000
	F169L	3.9000

169	F169P	3.9000
	F169S	3.9000
170	Q170R	3.9000
	Q170W	3.9000
171	P171F	3.9000
	P171L	3.9000
	P171S	3.9000
172	T172A	3.9000
	T172I	3.9000
	T172V	3.9000
173	N173D	3.9000
	N173G	3.9000
	N173S	3.9000
174	G174D	3.9000
	G174N	3.9000
	G174S	3.9000
175	V175A	3.9000
	V175I	3.9000
	V175T	3.9000
176	G176D	3.9000
	G176N	3.9000
	G176S	3.9000
177	Y177C	3.9000
	Y177H	3.9000
	Y177R	3.9000
178	Q178R	3.9000
	Q178W	3.9000
179	P179L	3.9000
	P179S	3.9000
180	Y180C	3.9000
	Y180H	3.9000

	Y180R	3.9000
181	R181E	3.9000
	R181G	3.9000
	R181K	3.9000
182	V182A	3.9000
	V182I	3.9000
	V182M	3.9000
	V182T	3.9000
183	V183A	3.9000
	V183I	3.9000
	V183M	3.9000
	V183T	3.9000
184	V184A	3.9000
	V184I	3.9000
	V184M	3.9000
	V184T	3.9000
185	L185F	3.9000
	L185P	3.9000
	L185S	3.9000
186	S186F	3.9000
	S186L	3.9000
	S186P	3.9000
187	F187L	3.9000
	F187P	3.9000
	F187S	3.9000
188	E188G	3.9000
	E188K	3.9000
	E188R	3.9000
189	L189F	3.9000
	L189P	3.9000
	L189S	3.9000

190	L190P	3.9000
	L190S	3.9000
191	H191C	3.9000
	H191R	3.9000
	H191Y	3.9000
192	A192I	3.9000
	A192T	3.9000
	A192V	3.9000
	A192M	3.9000
193	P193L	3.9000
	P193S	3.9000
194	A194I	3.9000
	A194M	3.9000
	A194T	3.9000
	A194V	3.9000
195	T195I	3.9000
	T195A	3.9000
	T195V	3.9000
196	V196A	3.9000
	V196I	3.9000
	V196T	3.9000
197	C197H	3.9000
	C197R	3.9000
	C197Y	3.8000
198	G198E	3.9000
	G198K	3.9000
	G198R	3.9000
199	P199F	3.9000
	P199L	3.9000
	P199S	3.9000
	K200E	3.9000

200	K200G	3.9000
	K200R	3.9000