

**Table 8. The highest-ranking designed sequences for the SH3 domain, using two different solvation terms**

Designer energy	Rank	Min. energy sequences by designer	ACE energy	ACE rank	Min. energy sequences reranked with ACE
-269.21	1	DKRVWARYWFWGRRRQQLPFQQGQEELEIQYEPDRYWKKAKDRRGREGQIPDPVQHQ	-233.1	892	DRKVQAQYWFWGRQRQMLPFRQGEELERRRDPDYYFQAQNRDGRQGIIPRPQVREG
-268.26	5	DKKVQARYWFWGRQYQQLPFRQGEELERQRPDYYWKAQVRRGQTGLIPQPQVYWK	-221.0	464	DRKCOMQYWFWGRWRQALPARQGEVEIQQHPDYYQKAKVRRGQYGLIPRPQVREK
-268.13	6	DKKVQMRREFRGRRRQQLPGYQGEELERQYEPDRYWKAQCRDRGTGQIPDPVYHK	-220.3	422	DRRCRIRYWFWGRQDRMLPVRQGEVEVRQRPDYYLKAQVRRGQGGILPRPQCEEQ
-267.61	8	DRRVQARHRFQGRRRQQLPFDQGEELERQHPDYYWQAQVRRGQTGLIPRPVQEK	-218.1	310	DRRVKARDDFWGRRRQQLPFRKGEELERRHPRSDQQAQDRRGWQGIIPRPVVEEA
-267.61	9	RDKVQARYWFWGRRRQQLPFRQGEELERQYEPDRYWLKAKVRRGDEGQAPRPVQSK	-216.0	114	DRKVKARDDFWGRRRQQLPFRKGEELERQYQDDRWFKAQVRYGREGQIPKPRVESA
-267.43	11	DKRVQARYWFWGRQYQQLPFWQGAELERQEPDYYKKGQDRRGWQGILPDPVYHK	-211.5	1065	DKKLECRDDFWGRQYQMLPARKGEELERQYHPDYYQKAKVRRGQTGKIPDRCKHK
-267.11	13	SYKVKARYWFWGRQYQQLPFRQGEELERIQQPDYYFKAKVRRGQYGIIPRPVQEA	-210.9	508	DKRVEVRYWFWGRQRQMLPFRQGEELERRRHPDYYIQVQVRRGQGGILPKPVKSK
-266.98	14	DRKVQARHRFQGRRRQQLPFDQGEELERQYQPDYWIKAQVRRGQEGQAPRPVQSK	-206.1	723	DRRVARREFRGRQRQMLPFRQGEELERQYQYQYFQARVRRGWQGLIPRPVVEEA
-266.81	18	DKRVWARYWFWGRRRQQLPFWQGALELRNEPDRYWKAQVQRGQGLIPDPVQHY	-205.8	804	DRRVKARYWFWGRQRMLPFWQGALELRQHPDYYQGGKVRGRTGILPRPVQEA
-266.79	19	DRRVKARYWFWGRDRRQLPFRQGEELERQPDYYKKGQVRYGRQLLPDPVVEHA	-193.4	301	DRRVEVRYFQGRQRQMLPADQGEELERQHPYQYQKAQDRRGQGLIPRPVKEK
-222.70	WT	AEYVRALFDFNGNDEEDLPFKKGDILRIDKPEEQWNAEDSEGKRGMI PVPYVEKY	-72.4	WT	AEYVRALFDFNGNDEEDLPFKKGDILRIDKPEEQWNAEDSEGKRGMI PVPYVEKY

One solvation term is the standard surface area-dependent solvation term of DESIGNER, and the other is the ACE solvation term by Schaefer *et al.* [Schaefer, M., Bartels, C. & Karplus, M. (1998) *J. Mol. Biol.* **284**, 835–848]. The sequences are listed in order of increasing energies, and their rank order is given in column 1. The rank order and energies of the native sequences in each ranking is given in the last row of each table.