Ligand conformation \rightarrow







	Ligand poses	Side chain rotamers	crystal structure / predicted structure	RMS error
ABP-arabinose			d and i	0.677 Å
RBP-ribose				0.148 Å



Crystal structure / Predicted structure







Seq. #	Best sequence	Protein-ligand hydrogen bonds	Shape complementarity	Dissociation energy	Unfolding enerav	
	•	5 6 7 8 9 10 11 12	0.78 0.88	-35 -10 15	-5 0 5 10	
2709	Q <mark>F</mark> LM <mark>R</mark> QFNAQ					
2764	RAL <mark>D</mark> L <mark>RFN</mark> SQ					
4384	RYE <mark>DRRFN</mark> AV					
4640	RYL <mark>D</mark> A <mark>RFN</mark> AQ					
4663	mil <mark>drrfn</mark> s <mark>Q</mark>					
5030	MYL <mark>DRRFN</mark> S <mark>Q</mark>					
5474	l <mark>f</mark> l <mark>drrfn</mark> SQ					
5727	QY <mark>FDRRFN</mark> S <mark>Q</mark>					
5916	MYM <mark>DRR</mark> Y <mark>N</mark> SQ					
5928	QY <mark>FDRR</mark> Y <mark>N</mark> S <mark>Q</mark>					
6461	Q <mark>FFDRRFN</mark> S <mark>Q</mark>					
6496	SY <mark>FDRR</mark> Y <mark>N</mark> SQ					
6559	NY <mark>FDRR</mark> Y <mark>N</mark> SQ					
7071	S <mark>F</mark> M <mark>DRRFNDQ</mark>					
7199	L <mark>FFDRR</mark> Y <mark>N</mark> SQ					
8618	S <mark>FFDRRFNDQ</mark>					
8782	<mark>nffdrrfn</mark> S <mark>Q</mark>					
8871	<mark>NFFDRRF</mark> SS <mark>Q</mark>					
8888	L <mark>FFDRRFNDQ</mark>					
native (8964)	<mark>NFFDRRFNDQ</mark>					

Design calc.	Rotamers per position	Local minimization	Solvent treatment		Rank	# of residues identical to native	K _d (experime	ental)	Sequence (10 primary contacts)
(a)	2800	yes	Lee	ſ	1	3	210 ± 80	mM*	<mark>N</mark> IMLMM <mark>FN</mark> AN
					2	4	$\textbf{8.8}\pm\textbf{0.4}$	mM*	<mark>NF</mark> MLNM <mark>FN</mark> AN
				l	3	4	83 ± 32	mM*	<mark>NF</mark> MLMM <mark>FN</mark> AN
(b)	5449	no	Lee	ſ	1	8	12 ± 0.9	mM*	<mark>NFFDRRF</mark> SS <mark>Q</mark>
				ł	2	9	48 ± 13	mM*	<mark>NFFDRRFN</mark> S <mark>Q</mark>
					3	8	84 ± 10	mM*	NMFDRRFN <mark>S</mark> Q
(c)	5449	yes	Qiu	ſ	1	6	99 ± 2	mM*	NYY <mark>DRR</mark> Y <mark>N</mark> AQ
				ł	2	6	84 ± 2	mM*	<mark>N</mark> YM <mark>DRR</mark> Y <mark>N</mark> SQ
					3	7	13 ± 1	mM*	NY <mark>FDRR</mark> Y <mark>N</mark> AQ
(d)	5449	yes	Lee	{	1	9	19 ± 8	μM^{\dagger}	L <mark>FFDRRFNDQ</mark>
					2	10	0.30 ± 0.07	μM^{\dagger}	<mark>NFFDRRFNDQ</mark>
				l	3	9	80 ± 2	μM^{\dagger}	N <mark>TFDRRFNDQ</mark>
Native						10	0.30 ± 0.07	μM^{\dagger}	NFFDRRFNDQ

Table 1