Supplementary Materials for

Robust deep learning based protein sequence design using ProteinMPNN

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Tables S1 to S1

	HALC1_878 (PDB ID: 8CYK)
Data Collection	
Space group	I 1 2 1
Cell dimensions	
a, b, c (Å)	64.17, 55.45, 82.81
α, β, γ (°)	90.00, 94.00, 90.00
Resolution (Å)	48.98 - 1.65 (1.709 - 1.65)
Rmerge (%)	2.1 (19.4)
Rpim (%)	2.1 (19.4)
/σ(I)	15.91 (3.96)
CC 1/2	0.999 (0.942)
Completeness (%)	96.85 (95.70)
Redundancy	2.0 (2.0)
Refinement	
No. unique reflections	33946 (3322)
Rwork / Rfree (%)	18.5 (24.0) / 21.7 (28.1)
No. non-hydrogen atoms	2366
Macromolecules	2151
Water	215
Ramachandran favoured/allowed	98.83/1.17
R.m.s. deviations	
Bond lengths (Å)	0.011
Bond angles (°)	1.12
B-factors (Å2)	
Macromolecules	28.36
Solvent	39.25

Table S1. Crystallographic statistics for HALC1_878.