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Supplementary information

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De novo design of buttressed loops for sculpting protein functions

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Supplementary Table 1. Crystallographic data collection and refinement statistics.

	RBL4	RBL7_C2_3
Wavelength (Å)	1.033	0.9795
Resolution range (Å)	59.84 - 1.8 (1.864 - 1.8)	45.3 - 2.986 (3.092 - 2.986)
Space group	P 21 21 2	P 21 21 21
Unit cell (Å, °)	62.287 215.442 28.008 90 90 90	111.961 117.644 142.056 90 90 90
Total reflections	258923 (25447)	258197 (25212)
Unique reflections	35977 (3521)	38693 (3751)
Multiplicity	7.2 (7.2)	6.7 (6.7)
Completeness (%)	98.67 (96.09)	99.02 (92.46)
Mean I/sigma(I)	5.70 (0.36)	5.34 (0.64)
Wilson B-factor	40.77	67.39

R-sym	0.1381 (3.305)	0.3314 (3.08)
R-meas	0.1498 (3.557)	0.3597 (3.336)
R-pim	0.05685 (1.298)	0.1385 (1.269)
CC1/2	0.989 (0.335)	0.996 (0.395)
Reflections used in refinement	35803 (3439)	38424 (3544)
Reflections used for R-free	1974 (193)	1988 (179)
R-work	0.2329 (0.6169)	0.2097 (0.3431)
R-free	0.2835 (0.6811)	0.2593 (0.3912)
Number of non-hydrogen atoms	3216	12376
macromolecules	3066	12331
ligands	28	7
solvent	122	38

Protein residues	410	1648
RMS(bonds) (Å)	0.011	0.004
RMS(angles) (°)	1.07	0.70
Ramachandran favored (%)	99.51	98.35
Ramachandran allowed (%)	0.49	1.65
Ramachandran outliers (%)	0.00	0.00
Rotamer outliers (%)	0.96	3.80
Clashscore	2.22	7.38
Average B-factor (Å^2)	52.05	77.82
macromolecules	52.07	77.86
ligands	51.18	121.17
solvent	51.77	55.70

Number of TLS groups	4	8

Statistics for the highest-resolution shell are shown in parentheses.