Supplementary Information

Monobodies as enabling tools for structural and mechanistic biology

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Supplementary Figure 1. Observed packing modes of monobodies.

Supplementary Figure 2. Observed interactions between monobody symmetry mates.

Supplementary Table 1. Monobody-target structures available in the Protein Data Bank at the time of this article. (separate Excel file)



b

Mode	Interaction	# Observed	Structures (PDB codes)
А	diversified-loops to wt-loops	14	6bqo, 6bqo, 6byn, 5mtj, 5dc0, 5dc0, 5dc9, 5dc9, 4huk, 4je4, 4je4, 3rzw, 3qht, 3k2m
В	wt-loops to wt-loops	12	6bx4, 6byn, 5mtj, 5oc7, 5oc7, 5oc7, 5dc0, 5dc9, 5nkq (5a41), 4je4, 4je4, 3uyo
С	wt-loops to wt-face	10	6bqo, 6bqo, 6byn, 5oc7, 5oc7, 5ecj, 4huk, 4jeg, 4jeg, 3k2m
D	wt-face to wt-face	10	6bqo, 6bqo, 6bx5, 6byn, 5mtj, 5a40, 5ecj, 4huk, 3k2m
Е	diversified-loops to wt-face	7	6byn, 5dc0, 5nkq (5a41), 5nkq (5a41), 4jeg, 4jeg, 3t04
F	diversified-face to wt-loops	5	6bx4, 6bx4, 6bx5, 6b24, 6b24
G	edge to edge (anti-parallel)	3	5a40, 5a40, 3k2m
н	diversified-face to wt-face	2	6bx4, 5dc0
I	diversified-loops to diversified-loops	1	3t04
J	edge to edge (parallel)	0	
к	diversified-loops to diversified-face	0	
L	diversified-face to diversified-face	0	

Supplementary Fig. 1. Observed packing modes of monobodies

(a) Cartoon representations of modes of two-body interactions between monobody molecules, classified according to regions of monobody that are involved in crystal contacts.

(**b**) Summary table of observed monobody-monobody crystal packing interactions, using the criteria as described for Supplementary Table 1.



Supplementary Fig. 2. Observed interactions between monobody symmetry mates

(**a-c**) Representative crystal structures containing crystal contacts involving more than two monobody molecules. All structures as shown as cartoons.

(d) Hydrogen bonding observed between edge strands of monobodies. All structures are shown both as cartoons and as backbone models with hydrogen-bonds depicted as dotted lines.