

Additional file 2 —

		Nter	R1	Fulcrum	Catalytic	R2	Elbow	Flaps	Cantilever	R3	Wall	R4	Helix	Cter
Asymmetry in the three 3EBZ _{mini} wild-type structures														
51 common symmetric positions	3, 6-11, 13, 14, 16, 17, 20, 24-26, 28-31, 34-36, 38, 39, 43, 45, 48, 49, 52-55, 57, 61-63, 65, 66, 68, 69, 71, 73, 76, 78, 81, 82, 84, 87, 94-96	1	4	7	6	4	2	9	9	2	2	1	3	1
27 common asymmetric positions	4, 5, 12, 18, 19, 21, 33, 40-42, 50, 51, 58-60, 64, 74, 75, 77, 83, 88, 89, 91-93, 97, 98	2	0	4	0	1	3	3	5	2	0	0	5	2
Asymmetry in the 150 mutant structures														
25 common symmetric positions	7, 9, 10, 13, 16, 17, 20, 28, 30, 35, 45, 52, 53, 55, 61, 66, 68, 69, 71, 73, 81, 82, 87, 94, 95	0	2	5	2	1	0	4	6	0	2	0	3	0
36 Or _{asym} positions	4, 5, 12, 15, 18, 19, 21, 23, 32, 33, 37, 42, 44, 47, 50, 51, 58-60, 64, 67, 74, 75, 77, 79, 80, 83, 86, 88-93, 97, 98	2	0	6	0	2	2	5	6	2	2	1	6	2
Comparison of the asymmetry in the three 3EBZ _{mini} and the 150 mutant structures														
25 positions are OR _{asym} in the mutant set and asymmetric in the three 3EBZ _{mini} structures	4, 5, 12, 18, 19, 21, 33, 42, 50, 51, 58-60, 64, 74, 75, 77, 83, 88, 89, 91-93, 97, 98	2	0	4	0	1	1	3	5	1	1	0	5	2
11 are Or _{asym} positions in the mutant set and are not asymmetric in the three 3EBZ _{mini} structures	15, 23, 32, 37, 44, 47, 67, 79, 80, 86, 90	0	0	2	0	1	1	2	1	1	1	1	1	0
2 are asymmetric in the three 3EBZ _{mini} structures and not over-represented in the mutant set	40 and 41	0	0	0	0	0	2	0	0	0	0	0	0	0

Figure S2: Summary of structural asymmetry in the three wild-type structures 3EBZ_{mini} and the 150 mutant structures. OR_{asym}: over-represented asymmetric positions.