A.  SUPPLEMENTARY MATERIALS

complexes with independent ligand and binding site information in SC-PDB:

1bdi 1boo 1cgp 1cy1 1cy7 1ea6 1efa 1fjx 1g38 1g6n 1g50 1gwq 1gwr 1h7u 1ih7 1iqr 1i5z 1i6x 1in5 1j7k 1knu 1ng9 1qp0 1qqb 1qtm 1r5k 1sxj\_1\_5 1uhl\_1\_2 1uom 1vpw 1w5t\_2\_3 1wbb 1wet 1xms 1xp8 1xv9 2bj4 2dt5 2hvc 2ijg 2j0v 2j4a 2j4d\_1\_3 2j7y 2j14 2jfa 2pub 2qpy 2rcw 2rfi 2uxh 2uxi 2uxo 2uxu 2vkv 2vuu 2x9d 2xrl 2y7p 2zl9 2zla 2zlc 2zno 2zoz 2zr9 3a78 3b6c 3bej 3bqd 3br2 3c1y 3c23 3cbp 3cs8 3d6y 3d57 3d70 3dr1 3fal 3frq 3g1l 3g1o 3g6x 3gbk 3gjw 3gn7 3h0a\_1\_2 3hgg 3hq5 3i59\_1\_2 3iid 3ipq 3ipu 3ix4 3ix8 3jpu 3k0f 3kcc 3kyt 3l3l 3l3m 3lmp 3o8g 3p7n 3q23 3qp6 3qqa 3sfi 3vkx 3wgw 4bjx 4bqy 4oay 4y17 4y29 5f54 5f56