Table S1. Interacting chains used as prediction targets.

1a2xAB[1]	1ds6AB	1go4BF	1kgyAE	1ofhAG	1sq0AB	1wmhAB	2assBC
1a9nAB	1dtdAB	1gpqAD	1ki1BA	1ofuAX	1sq2LN	1wmiCD	2atqAB
1acbEI	1dx5MI	1gpwAB	1klfBA	1ohzAB	1stfEI	1wpxAB	2auhAB
1agrAE	1e0fDI	1gvnBA	1kpsAB	1oiuAB	1sv0AC	1wq1RG	2aw2AB
1aisBA	1e44BA	1gxdAC	1kshAB	1ol5AB	1svxBA	1wr6AE	2ayoAB
1aroPL	1e96AB	1gzsAB	1ktkEA	1oo0AB	1syxAB	1wrdAB	2b3tBA
1avaAC	1eaiBD	1h2sAB	1ktzBA	1ophAB	1t0fAC	1wywAB	2b4sAB
1avgHI	1ebdBC	1h4lAD	1ku6AB	1oqdAK	1t6bXY	1x3wAB	2b59AB
1avwAB	1eerBA	1h59AB	1kxqAH	1oqeAK	1t6gAC	1x86AB	2b5iBA
1axiBA	1eerCA	1h6kAX	1kz7AB	1or7AC	1t9gDS	1xb2AB	2b5iCA
1ay7AB	1efnAB	1h9dAB	1kzyCA	1oryAB	1ta3BA	1xd3AB	2bcjAQ
1b0nAB	1efuCD	1h9hEI	1l4dAB	1otsAC	1tafAB	1xdkBA	2bfxAD
1b34AB	1ewyAC	1he1AC	1l6xAB	1oxbAB	1tbrKS	1xdtTR	2bh1AX
1b6cAB	1f02IT	1he8AB	1l7vAC	1oyvBI	1tdqAB	1xg2AB	2bkhAB
1bh9BA	1f34AB	1hl6BA	1ldjAB	1oyvAI	1te1AB	1xk4BD	2bkkAB
1blxAB	1f3vBA	1hx1AB	1lfdBA	1p5vAB	1th1AC	1xl3AC	2bkrAB
1bmlCA	1f5qAB	1i1rAB	1lpbBA	1p8vAC	1th8AB	1xouBA	2bo9AB
1bndAB	1f60AB	1i2mBA	1ltxAR	1p9mCB	1tk5AB	1xqsAC	2bseFC
1brsAD	1f6fBA	1i7wCD	1m1eAB	1p9MAB	1tmqAB	1xtgAB	2btfAP
1buhAB	1f6fCA	1i8lAC	1m27AC	1pk1AB	1tnrAR	1xu1AR	2c1mAB
1buiAC	1f6mAC	1iarBA	1m2vBA	1ppfEI	1tocBR	1y4hAC	2c2vHT
1bvnPT	1f93BE	1ib1AE	1m9fAD	1pq1AB	1tt5AB	1y64AB	2c5dAC
1bzqAL	1fbvAC	1ibrBA	1ma9AB	1pqzAB	1tueAB	1y8xAB	2c5dAD
1c1yAB	1fccBD	1iilEA	1mbxAC	1pufAB	1tx4AB	1ycsAB	2ckhAB
1c4zAD	1ffgAB	1im3AD	1moxAC	1pvhAB	1tx6AI	1yvbAI	2ey4AE
1c9pAB	1fleEI	1iraYX	1mq8AB	1pxvAC	1txqAB	1z0jAB	2ey4AC
1cd9BA	1fm9AD	1itbBA	1mr1AD	1qa9AB	1tygAB	1z2cBA	2f9dAP
1cf7BA	1foeAB	1ixsBA	1mvfAE	1qavBA	1u0sYA	1z3eAB	2fi4EI
1ci6AB	1fqjAB	1iyjBA	1mzwAB	1qbkBC	1u7fAB	1z3gHA	2g45AB
1clvAI	1fqJCA	1j2jAB	1n0wAB	1qo3AC	1uadAC	1z5yED	2gooAC
1cseEI	1fr2BA	1jatAB	1nbfAD	1r0rEI	1ueaAB	1z92AB	2gy7AB
1cxzAB	1fs1BA	1jchAB	1nexBA	1r1kAD	1ughEI	1zbdAB	2hppHP
1d2zBA	1fyhAB	1jdhAB	1nf3AC	1r4aAE	1ujwAB	1zbxAB	2mtaCA
1d3bAB	1g3nAC	1jiwPI	1nkpAB	1r8sAE	1ukvGY	1zc3AD	2sniEI
1d4xAG	1g3nAB	1jk9BA	1nmuAB	1rp3AB	1ul1XA	1zlhAB	2trcBP
1d6rAI	1g4uSR	1jmaAB	1npeAB	1rzrCT	1us7AB	1zm2AB	3fapAB
1devAB	1g6vAK	1jowBA	1nqlAB	1s1qAB	1usuAB	2a01AD	3hhrCA
1df9BC	1g73AC	1jtdAB	1nt2BA	1s3sFG	1uuzAD	2a19BA	3proAC
1df9AC	1gc1GC	1jtgAB	1nu9AC	1s4yBA	1uw4BA	2a41AC	3sicEI
1dfjEI	1gcqAC	1jtpAL	1nunBA	1s6vAB	1uzxAB	2a42AB	3ygsCP
1dhkAB	1gcqBC	1jw9BD	1nvuSR	1sbbAD	1v5iAB	2a5dBA	4cpaAI
1dkfBA	1gh6BA	1k5dAB	1nvuSQ	1sgfGB	1v74AB	2a5tAB	4htcHI
1dkgDA	1ghqAB	1k8rAB	1nw9BA	1sgpEI	1vetAB	2a5yBA	4sgbEI
1dmlAB	1gl0EI	1k90AD	1o6sAB	1shwAB	1vg0AB	2a78BA	
1dn1AB	1gl1AI	1k93AD	1o94AC	1shyBA	1w1iAF	2ajfAE	
1dowAB	1gl4AB	1kacAB	1oc0AB	1shzAC	1w1wCG	2apoAB	
1dp5AB	1glbFG	1kg0BC	1oeyJA	1sppAB	1w98AB	2assBA	

[1] First four symbols are the PDB code, followed by the chain IDs of receptor and ligand.
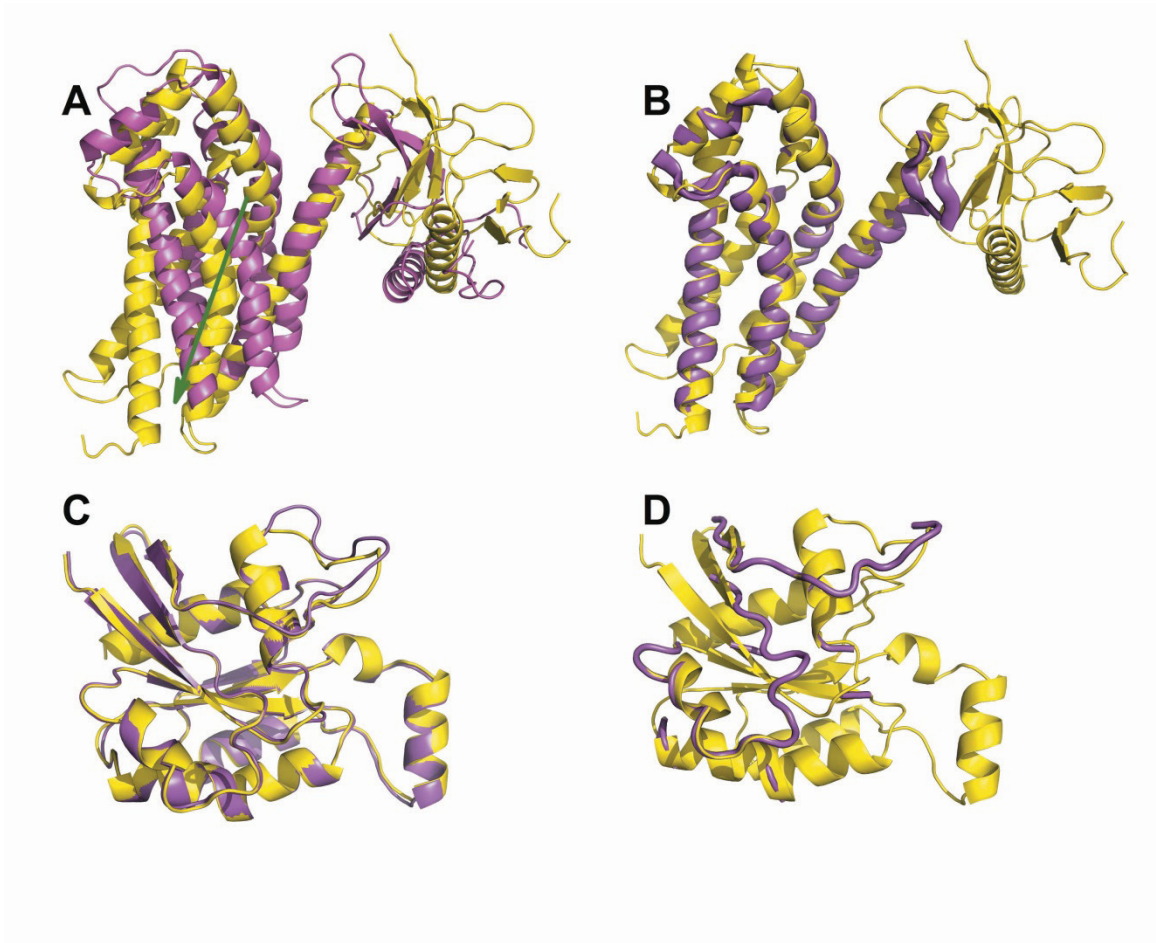
Figure S1. *Structural similarity in hetero-complexes with domain structure.* (A) Alignments of the receptors (chains B of the target 1ki1 and template 2nz8) by FSA and (B) PSA. (C) Alignments of the ligands (chains A) by FSA and (D) PSA.
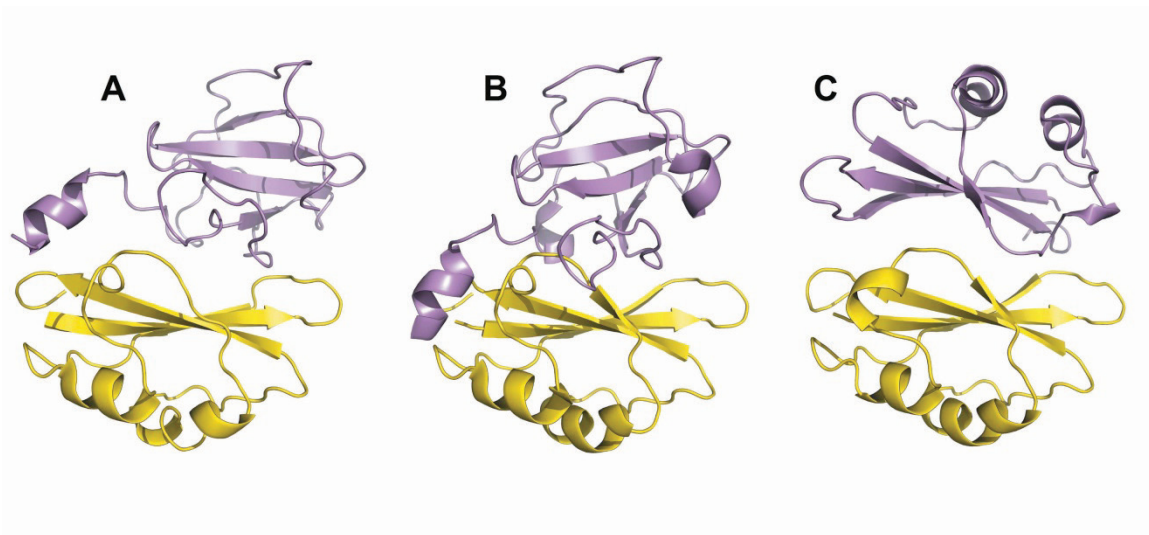
Figure S2. *Structural similarity of biological and crystal packing interfaces.* (A) PSA model and (B) X-ray structure of the biologically functional complex (1e44, chains A and B). (C) X-ray structure of the crystal-packing complex (3eip, chains A and B).
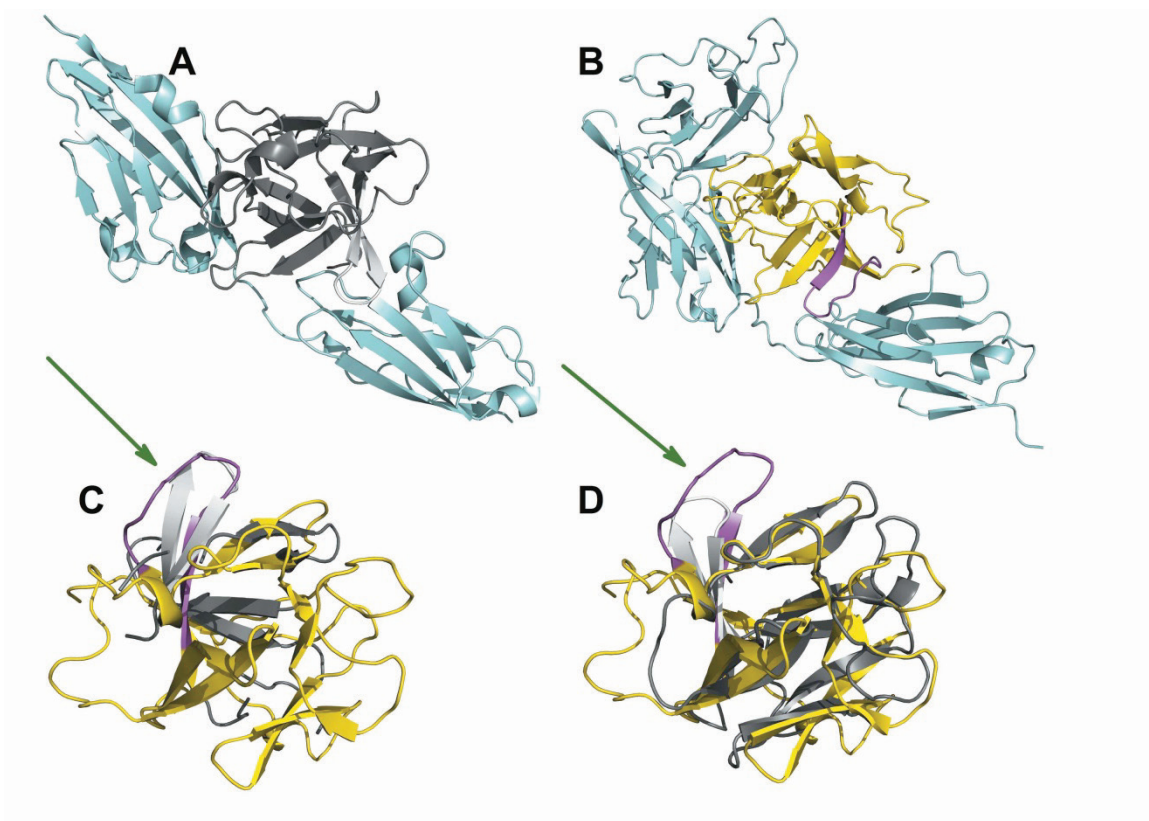
Figure S3. *Dissimilar interface loops.* (A) X-ray structures of the template (chains A and C from 1cvs) and (B) the target (chains A and B from 1itb). (C) PSA and (D) FSA alignments of the target and the template ligands. The receptors are in cyan, target ligands are in gray and template ligands in yellow. Parts of ligand β-strands essential for the model building are in magenta for the target and white for the template, and marked by arrows in C and D.
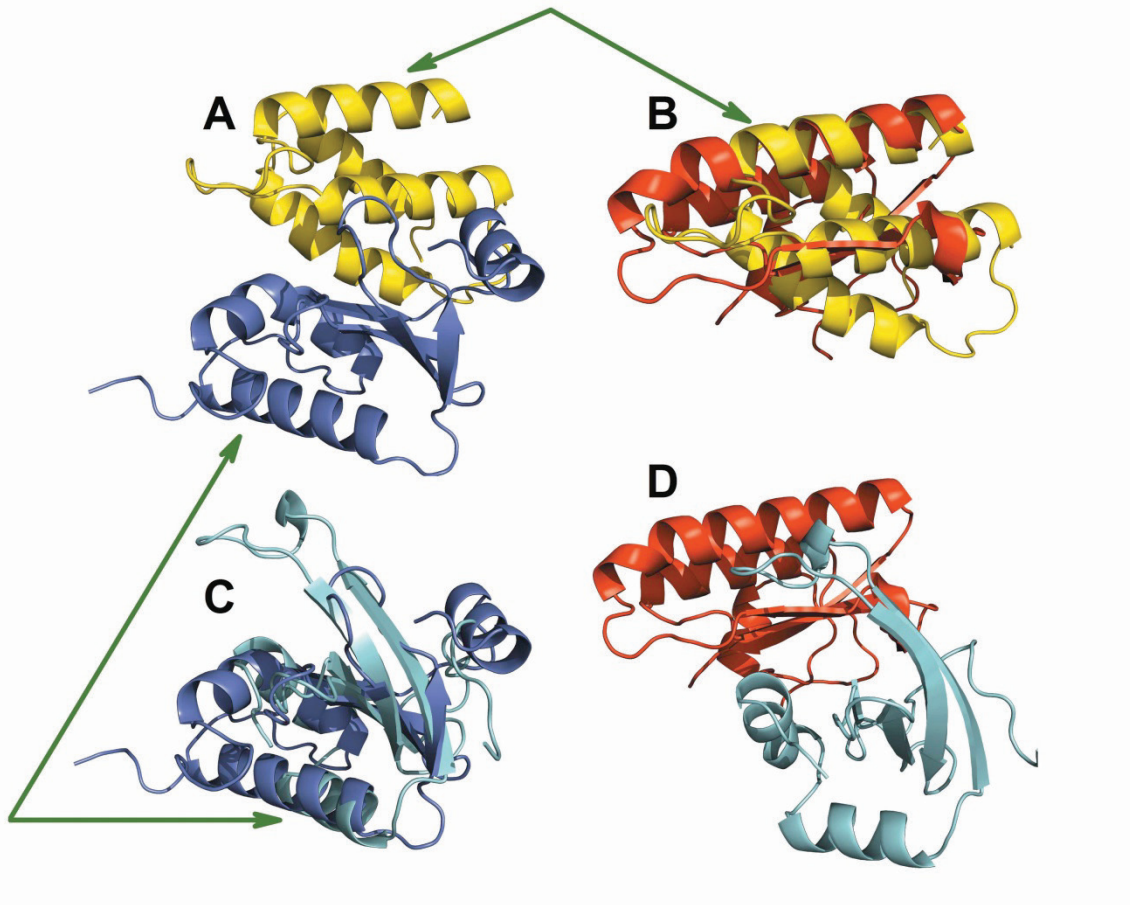
Figure S4. *Local structural similarity away from the interface*. (A) X-ray structures of the target (chains A and B of 1v74) and (D) template 2fhz (chains A and B of 2fhz). (B) FSA alignments of the ligands and (C) receptors.