Supplementary Information for:

ProPOSE: Direct exhaustive protein docking with side chain flexibility

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Antibody dataset selection. The SAbDab Antibody database (http://opig.stats.ox.ac.uk/webapps/abdb/web_front/Welcome.php) (Sept. 28, 2014) was queried

using the following criteria.

- Method=Xray
- Resolution<3.2A
- Complex=True
- Antigen=Protein

This resulted in a list of 517 Ab:Ag. From this list a hand-curated subset with the following selection criteria was extracted.

- Complete Fab region of the Ab (no breaks in the Ab)
- No small molecule at the interface
- Selection of Ab based on sequence/conformational diversity for a specific target. For example, if a single mutation results in the same loop conformation these cases are typically removed.
- Selection of Ab based on unique epitope for a specific target.

Only systems that went through the preparation steps and that executed to completion without error by all 6 docking programs in all 4 scenarios (BB, RB, BR and RR) are reported. The final Antibody dataset is comprised of 241 Ab:Ag complexes (Table S1).

1ahw1bj11bq11bvk1dqj1e6j1egj1e81fbi1fbi1fe81fj11fns1fsk1h0d1i9r1iqd1jhl1jps1jrh1k4c1kb51lk31mlc1nca1nfd1nsn1oaz1ors1osp1ots1p2c1pkq1r0a1rj11sy61t031tpx1tqb1tzh1tzi1v7m1vfb1w721wej1xiw1yjd1ynt1yqv1yy91ztx2adf2aep2aeq2arj2b2x2bdn2cmr2dd82fd62fjg2fjh2h8p2h9g2hmi2i912f882je12nr62ny12ny72oz42q8b2qqk2qqn2r012r562uzi2vxq2vxs2vxt2we2wuc2x712xqy2xra2xtj2xwt3d853d9a3ebb3eoa3g043gbn3g133jgd3grw3hfz3hfn3hi13hi63hmx3i503idx3iu33jwd3k2u3hk13ks03ks03ifs31953id83i1z3lzf3ma93my3my3mg3my3ng3hi63hmx3id93up3up3up3ks03ks03ks03ks03ifs3id83iz3iz73e93ksj3ss03so33so33so33ks03up3up3up3up3up3up <t< th=""><th></th><th></th><th></th><th></th><th></th><th></th><th></th><th></th><th></th><th></th></t<>										
1kbs11k31mlc1nca1nfd1nsn1oaz1ors1osp1ots1p2c1pkq1r0a1rj11sy61t031tpx1tqb1tzh1tzi1v7m1vfb1w721wej1xiw1yjd1ynt1yqv1yy91ztx2adf2aep2aeq2arj2b2x2bdn2cmr2dd82fd62fjg2fjh2h8p2h9g2hmi2i912j882je12nr62ny12ny72oz42q8b2qqk2qqn2r012r562uzi2vxq2vxs2vxt2w9e2wuc2x712xqy2xra2xtj2xwt2yc12ypv2yss2zch3ab03b2u3b9k3bdy3bgf3bn93cvh3d853d9a3ehb3eoa3g043gbn3gi33jgjf3grw3h423hfm3hi13hi63hmx3i503idx3iu33jwd3k2u3klh3kr33ks0315x31953ld83liz3lzf3ma93mj93mxw3nfp3nh73nps3o2d3p0y3pgf3pnw3qls3q3g3qwo3rlg3raj3rkd3ru83ru74aei4ag44al84am04bz14bz24cmh4cni4d9q4d9r4dkf4dn44dvr4ene4faf4ffv4ffy4fp84fqi4fqj4g3y4g6j4g6m4g7v<	1ahw	1bj1	1bql	1bvk	1dqj	1e6j	1egj	1eo8	1fbi	1fe8
1p2c1pkq1r@a1rjl1sy61t@31tpx1tqb1tzh1tzi1v7m1vfb1w721wej1xiw1yjd1ynt1yqv1yy91ztx2adf2aep2aeq2arj2b2x2bdn2cmr2dd82fd62fjg2fjh2h8p2h9g2hmi2i9l2j882jel2nr62ny12ny72oz42q8b2qqk2qqn2r0l2r562uzi2vxq2vxs2vxt2w9e2wuc2x712xqy2xra2xtj2ypv2yss2yss2zch3ab03b2u3b9k3bdy3bgf3bn93cvh3d853d9a3ehb3eoa3g043gbn3gi93gjf3grw3h423hfm3hi13hi63hmx3i503idx3iu33jwd3k2u3klh3kr33ks0315x319531d83liz3lzf3ma93mj93mxw3nfp3nh73nps3o2d3p0y3pgf3pnw3q1s3q3g3qwo3r1g3raj3rkd3ru83rvv3s353s373se93skj3sm53so33sob3sqo3typ3u303u9p3ubx3uc03v6o3vg93w2d3w9e3wd53zkm3ztn4aei4ag44al84am04bz14bz24cmh4cni4d9q4d9r4dkf4dn44dvr4ene4f3f<	1fj1	1fns	1fsk	1h0d	1i9r	1iqd	1jhl	1jps	1jrh	1k4c
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2adf2aep2aeq2arj2b2x2bdn2cmr2dd82fd62fjg2fjh2h8p2h9g2hmi2i9l2j882jel2nr62ny12ny72oz42q8b2qqk2qqn2r0l2r562uzi2vxq2vxs2vxt2w9e2wuc2x712xqy2xra2xtj2xwt2yc12ypv2yss2zch3ab03b2u3b9k3bdy3bgf3bn93cvh3d853d9a3ehb3eoa3g043gbn3gi93gjf3grw3h423hfm3hi13hi63hmx3i503idx3iu33jwd3k2u3klh3kr33ks03l5x3l953ld83liz3lzf3ma93mj93mxw3nfp3nh73nps3o2d3p0y3pgf3pnw3qls3q3g3qwo3rlg3raj3rkd3ru83rvv3s353s373se93skj3sm53so33sob3sqo3t3p3u303u9p3ubx3uc03v6o3vg93w2d3w9e3wd53zkm3ztn4aei4ag44al84am04bz14bz24cmh4ffy4fp84fqi4fqj4g3y4g6j4g6m4g7v4gms4h884h8w4hc14hcr4hf54hfu4hj04h1z4ht14hwb4i2x4i3r4i774i9w4ij34irz4j6r4jan </td <td>1p2c</td> <td>1pkq</td> <td>1r0a</td> <td>1rjl</td> <td>1sy6</td> <td>1t03</td> <td>1tpx</td> <td>1tqb</td> <td>1tzh</td> <td>1tzi</td>	1p2c	1pkq	1r0a	1rjl	1sy6	1t03	1tpx	1tqb	1tzh	1tzi
2fjh2h8p2h9g2hmi2i9l2j882jel2nr62ny12ny72oz42q8b2qqk2qqn2r0l2r562uzi2vxq2vxs2vxt2w9e2wuc2x712xqy2xra2xtj2xwt2yc12ypv2yss2zch3ab03b2u3b9k3bdy3bgf3bn93cvh3d853d9a3ehb3eoa3g043gbn3gi93gjf3grw3h423hfm3hi13hi63hmx3i503idx3iu33jwd3k2u3klh3kr33ks0315x319531d831iz31zf3ma93mj93mxw3nfp3nh73nps3o2d3p0y3pgf3pnw3q1s3q3g3qwo3r1g3raj3rkd3ru83rvv3s353s373se93skj3sm53so33sob3sqo3t3p3u303u9p3ubx3uc03v6o3vg93w2d3w9e3wd53zkm3ztn4aei4ag44al84am04bz14bz24cmh4cni4d9q4d9r4dkf4dn44dvr4ene4f3f4ffv4ffy4fp84fqi4fqj4g3y4g6j4g6m4g7v4gms4h884h8w4hc14hcr4hf54hfu4hj04h1z4ht14hwb4i2x4i3r4i774i9w4ij34irz4j6r4jan4j1r </td <td>1v7m</td> <td>1vfb</td> <td>1w72</td> <td>1wej</td> <td>1xiw</td> <td>1yjd</td> <td>1ynt</td> <td>1yqv</td> <td>1yy9</td> <td>1ztx</td>	1v7m	1vfb	1w72	1wej	1xiw	1yjd	1ynt	1yqv	1yy9	1ztx
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2w9e2wuc2x712xqy2xra2xtj2xwt2yc12ypv2yss2zch3ab03b2u3b9k3bdy3bgf3bn93cvh3d853d9a3ehb3eoa3g043gbn3gi93gjf3grw3h423hfm3hi13hi63hmx3i503idx3iu33jwd3k2u3klh3kr33ks0315x31953ld83liz3lzf3ma93mj93mxw3nfp3nh73nps3o2d3p0y3pgf3pnw3q1s3q3g3qwo3r1g3raj3rkd3ru83rvv3s353s373se93skj3sm53so33sob3sqo3t3p3u303u9p3ubx3uc03v6o3vg93w2d3w9e3wd53zkm3ztn4aei4ag44al84am04bz14bz24cmh4cni4d9q4d9r4dkf4dn44dvr4ene4f3f4ffv4ffy4fp84fqi4fqj4g3y4g6j4g6m4g7v4gms4h884h8w4hc14hcr4hf54hfu4hj04h1z4ht14hwb4i2x4i3r4i774i9w4ij34irz4j6r4jan4j1r4jpk4jpw4k3j4k944k9e4kht4ki54kuc4kxz415f4mwf4np44o584ogy4oii4okv4olz4ot14py84u0r </td <td>2fjh</td> <td>2h8p</td> <td>2h9g</td> <td>2hmi</td> <td>2i9l</td> <td>2j88</td> <td>2jel</td> <td>2nr6</td> <td>2ny1</td> <td>2ny7</td>	2fjh	2h8p	2h9g	2hmi	2i9l	2j88	2jel	2nr6	2ny1	2ny7
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3hi6 3hmx 3i50 3idx 3iu3 3jwd 3k2u 3klh 3kr3 3ks0 315x 3195 31d8 31iz 31zf 3ma9 3mj9 3mxw 3nfp 3nh7 3nps 3o2d 3p0y 3pgf 3pnw 3q1s 3q3g 3qwo 3r1g 3raj 3rkd 3ru8 3rvv 3s35 3s37 3se9 3skj 3sm5 3so3 3sob 3sqo 3t3p 3u30 3u9p 3ubx 3uc0 3v6o 3vg9 3w2d 3w9e 3wd5 3zkm 3ztn 4aei 4ag4 4al8 4am0 4bz1 4bz2 4cmh 4cni 4d9q 4d9r 4dkf 4dn4 4dvr 4ene 4f2m 4f3f 4ffv 4ffy 4fp8 4fqi 4fqj 4g3y 4g6j 4g6m 4g7v 4gms 4h88 4h8w 4hc1 4hcr 4hf5 4hfu 4hj0 4h1z 4ht1 4hwb 4i2x 4i3r 4i77 4i9w	2zch	3ab0	3b2u	3b9k	3bdy	3bgf	3bn9	3cvh	3d85	3d9a
315x 3195 31d8 31iz 31zf 3ma9 3mj9 3mxw 3nfp 3nh7 3nps 3o2d 3p0y 3pgf 3pnw 3q1s 3q3g 3qwo 3r1g 3raj 3rkd 3ru8 3rvv 3s35 3s37 3se9 3skj 3sm5 3so3 3sob 3sqo 3t3p 3u30 3u9p 3ubx 3uc0 3v6o 3vg9 3w2d 3w9e 3wd5 3zkm 3ztn 4aei 4ag4 4al8 4am0 4bz1 4bz2 4cmh 4cni 4d9q 4d9r 4dkf 4dn4 4dvr 4ene 4f2m 4f3f 4ffv 4ffy 4fp8 4fqi 4fqj 4g3y 4g6j 4g6m 4g7v 4gms 4h88 4h8w 4hc1 4hcr 4hf5 4hfu 4hj0 4h1z 4ht1 4hwb 4i2x 4i3r 4i77 4i9w 4ij3 4irz 4j6r 4jan 4j1r 4jpk 4jpw 4k3j 4k94 4k9e	3ehb	3eoa	3g04	3gbn	3gi9	3gjf	3grw	3h42	3hfm	3hi1
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3wd5 3zkm 3ztn 4aei 4ag4 4al8 4am0 4bz1 4bz2 4cmh 4cni 4d9q 4d9r 4dkf 4dn4 4dvr 4ene 4f2m 4f3f 4ffv 4ffy 4fp8 4fqi 4fqj 4g3y 4g6j 4g6m 4g7v 4gms 4h88 4h8w 4hc1 4hcr 4hf5 4hfu 4hj0 4hlz 4ht1 4hwb 4i2x 4i3r 4i77 4i9w 4ij3 4irz 4j6r 4jan 4jlr 4jpk 4jpw 4k3j 4k94 4k9e 4kht 4ki5 4kuc 4kxz 4l5f 4leo 4lf3 4liq 4lmq 4lst 4lsu 4lvh 4lvn 4m48 4m5z 4mwf 4np4 4o58 4ogy 4oii 4okv 4olz 4ot1 4pg8 4u0r 4u1g 4u6h	3rkd	3ru8	3rvv	3s35	3s37	3se9	3skj	3sm5	3so3	3sob
4cni 4d9q 4d9r 4dkf 4dn4 4dvr 4ene 4f2m 4f3f 4ffv 4ffy 4fp8 4fqi 4fqj 4g3y 4g6j 4g6m 4g7v 4gms 4h88 4h8w 4hc1 4hcr 4hf5 4hfu 4hj0 4hlz 4ht1 4hwb 4i2x 4i3r 4i77 4i9w 4ij3 4irz 4j6r 4jan 4jlr 4jpk 4jpw 4k3j 4k94 4k9e 4kht 4ki5 4kuc 4kxz 415f 4leo 41f3 4liq 4lmq 4lst 4lsu 4lvh 4lvn 4m88 4m5z 4mwf 4np4 4o58 4ogy 4oii 4okv 4olz 4ot1 4py8 4u0r 4u1g 4u6h	3sqo	3t3p	3u30	3u9p	3ubx	3uc0	3v6o	3vg9	3w2d	3w9e
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4h8w4hc14hcr4hf54hfu4hj04hlz4ht14hwb4i2x4i3r4i774i9w4ij34irz4j6r4jan4jlr4jpk4jpw4k3j4k944k9e4kht4ki54kuc4kxz4l5f4leo4lf34liq4lmq4lst4lsu4lvh4lvn4m484m5z4mwf4np44o584ogy4oii4okv4olz4ot14py84u0r4u1g4u6h	4cni	4d9q	4d9r	4dkf	4dn4	4dvr	4ene	4f2m	4f3f	4ffv
4i3r4i774i9w4ij34irz4j6r4jan4jlr4jpk4jpw4k3j4k944k9e4kht4ki54kuc4kxz4l5f4leo4lf34liq4lmq4lst4lsu4lvh4lvn4m484m5z4mwf4np44o584ogy4oii4okv4olz4ot14py84u0r4u1g4u6h	4ffy	4fp8	4fqi	4fqj	4g3y	4g6j	4g6m	4g7v	4gms	4h88
4k3j 4k94 4k9e 4kht 4ki5 4kuc 4kxz 415f 4leo 41f3 4liq 4lmq 4lst 4lsu 4lvh 4lvn 4m48 4m5z 4mwf 4np4 4o58 4ogy 4oii 4okv 4olz 4ot1 4py8 4u0r 4u1g 4u6h	4h8w	4hc1	4hcr	4hf5	4hfu	4hj0	4hlz	4ht1	4hwb	4i2x
4liq 4lmq 4lst 4lsu 4lvh 4lvn 4m48 4m5z 4mwf 4np4 4o58 4ogy 4oii 4okv 4olz 4ot1 4py8 4u0r 4u1g 4u6h	4i3r	4i77	4i9w	4ij3	4irz	4j6r	4jan	4jlr	4jpk	4jpw
405840gy40ii40kv40lz40t14py84u0r4u1g4u6h	4k3j	4k94	4k9e	4kht	4ki5	4kuc	4kxz	415f	4leo	41f3
	4liq	41mq	4lst	4lsu	4lvh	4lvn	4m48	4m5z	4mwf	4np4
4u6v	4058	4ogy	4oii	4okv	4olz	4ot1	4py8	4u0r	4u1g	4u6h
	4u6v									

 Table S1. PDB codes of the selected Antibody complexes

Benchmark dataset selection. Quality criteria similar to that of the Antibody dataset was applied to the Protein Benchmark 5.0 complexed and unbound structures in addition to the requirement that all interface residues be present in the bound and unbound forms of the proteins. All antibody systems were removed from the set.

Only systems that went through the preparation steps and that executed to completion without error by all 6 docking programs in all 7 scenarios (BB, RB, BR, RR, UB, BU, UU) are reported. The final Benchmark dataset contained 150 complexes (Table S2).

1acb	1ak4	1akj	1atn	1avx	1ay7	1b6c	1bkd	1buh	1bvn
1cgi	1clv	1d6r	1e6e	1eaw	1eer	1efn	1ewy	1ezu	1f34
1f51	1fc2	1fcc	1ffw	1fle	1fq1	1fqj	1gcq	1ghq	1gl1
1gla	1gpw	1grn	1gxd	1h1v	1h9d	1he1	1hia	1i2m	1i4d
1ibr	1ijk	1j2j	1jiw	1jtd	1jtg	1jwh	1jzd	1k74	1kac
1kkl	1ktz	1kxp	1lfd	1m10	1m27	1mah	1ml0	1mq8	1oc0
1ofu	1oph	1oyv	1ppe	1pxv	1qa9	1r0r	1r6q	1r8s	1rke
1rlb	1rv6	1s1q	1sbb	1syx	1t6b	1tmq	1udi	1us7	1xqs
1xu1	1y64	1yvb	1z5y	1zhh	1zhi	2a1a	2a5t	2a9k	2abz
2ajf	2ayo	2b42	2b4j	2btf	2c01	2cfh	2g77	2gaf	2gtp
2h7v	2hle	2hqs	2hrk	2i9b	2ido	2j0t	2j7p	2nz8	2o3b
2oob	2ot3	2oul	2pcc	2sic	2sni	2uuy	2vdb	2x9a	2z0e
3a4s	3aaa	3aad	3biw	3bp8	3bx7	3cph	3d5s	3daw	3f1p
3fn1	3h11	3h2v	3k75	3189	3p57	3pc8	3r9a	3s9d	3sgq
3szk	3vlb	4сра	4fza	4h03	4hx3	4iz7	41w4	4m76	7cei

Table S2. PDB codes of the selected Protein benchmark dataset 5.0 complexes.

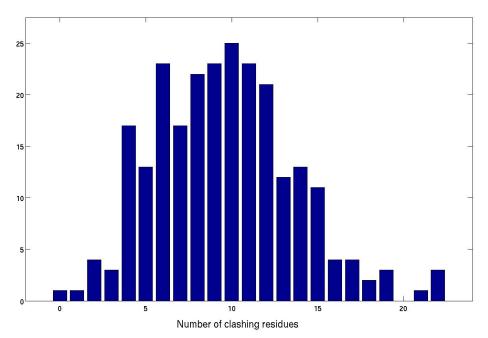
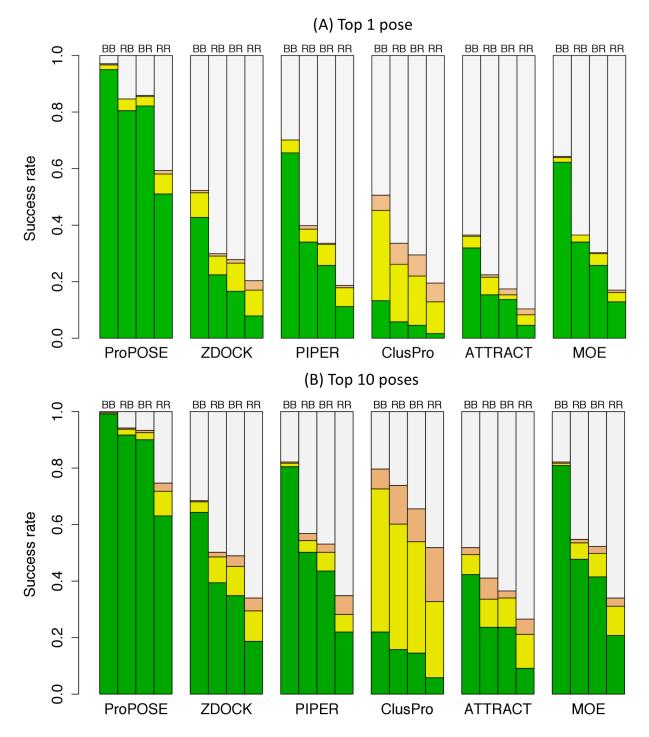
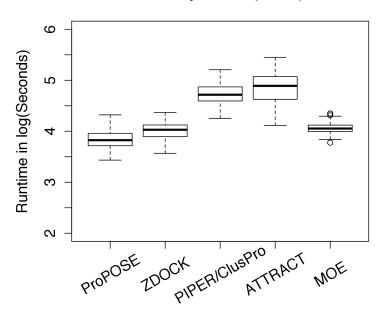


Fig. S1. Distribution of the number of interfering sidechains when both repacked proteins in the Antibody dataset are overlaid to the bound position. A sidechain is considered clashing when its AMBER van der Waals interaction energy > 5 kcal/mol.



Antibody dataset (N=241)

Figure S2. Absolute docking success rate using the Top 1 and Top 10 pose predictions under four scenarios: (BB) Bound ligand with bound receptor; (UB) Unbound ligand with bound receptor; (UU) Bound ligand with unbound receptor; (UB) Unbound ligand with bound receptor; (UU) Unbound ligand with unbound receptor; Colors indicate the quality of the predictions according to the CAPRI metric as High (green), Medium (yellow) or Acceptable (coral).



Antibody dataset (N=241)

Benchmark dataset (N=150)

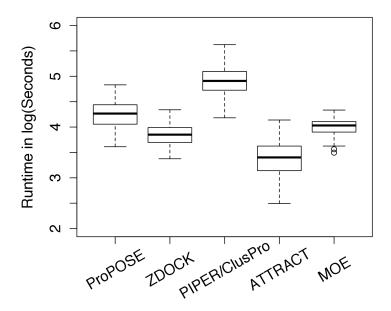


Figure S3. Runtime of the 6 programs tested on the Antibody and Benchmark dataset.

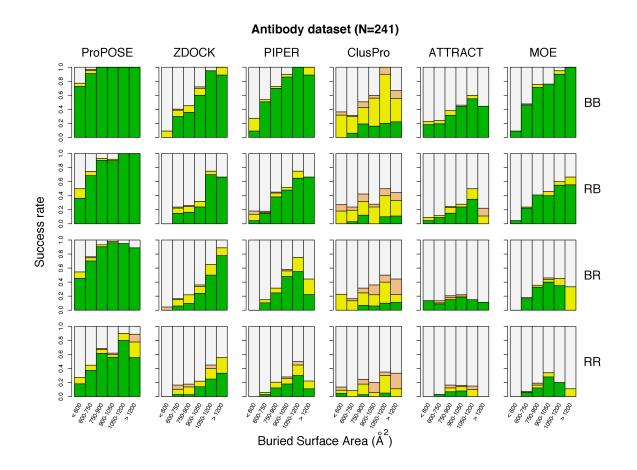


Figure S4. Absolute docking success rate for the top-pose prediction dependence on the buried surface area on the Antibody dataset under four sidechain perturbation scenarios: (RR) Repacked ligand with repacked receptor; (BR) Bound ligand with repacked receptor; (RB) Repacked ligand with bound receptor; (BB) Bound ligand with bound receptor. Colors indicate the quality of the predictions according to the CAPRI metric as High (green), Medium (yellow) or Acceptable (coral). From left to right the BSA bins contain 22, 67, 73, 50, 20 and 9 systems, respectively.

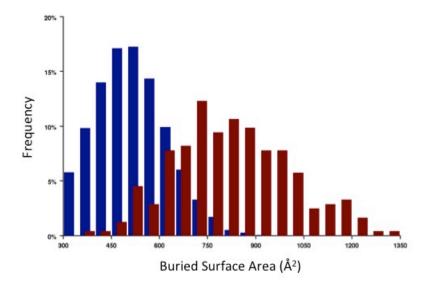
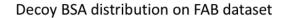


Figure S5. BSA distribution for the Antibody complexes (red) compared to the best decoys (blue). Decoys are defined as best 5000 poses of each Antibody that are more than 10 Å RMSD away from their native state



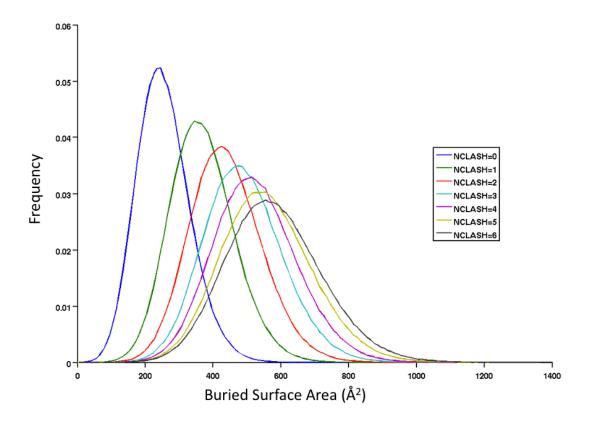
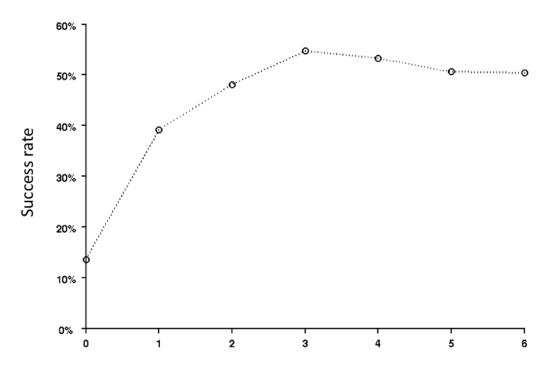


Figure S6. BSA distribution of best decoy poses with different number of tolerated sidechain conflicts on the Fab dataset. NCLASH=0 means that no sidechain clash was tolerated. NCLASH=N means that at most N clashing sidechains are tolerated on the ligand and N are tolerated on the receptor.



Number of tolerated sidechain conflicts

Figure S7. Success rate on the repacked-repacked (RR) Antibody dataset for various number of sidechain conflicts tolerated on each protein in the initial docking stage (Stage1).