Figure S1: Pairwise distributions of each pair of LHOC metrics across the 1,040 structures in the Rosetta antibody database. A best-fit line (red) is drawn through each pairwise distribution, with its corresponding r^2 value labeled.
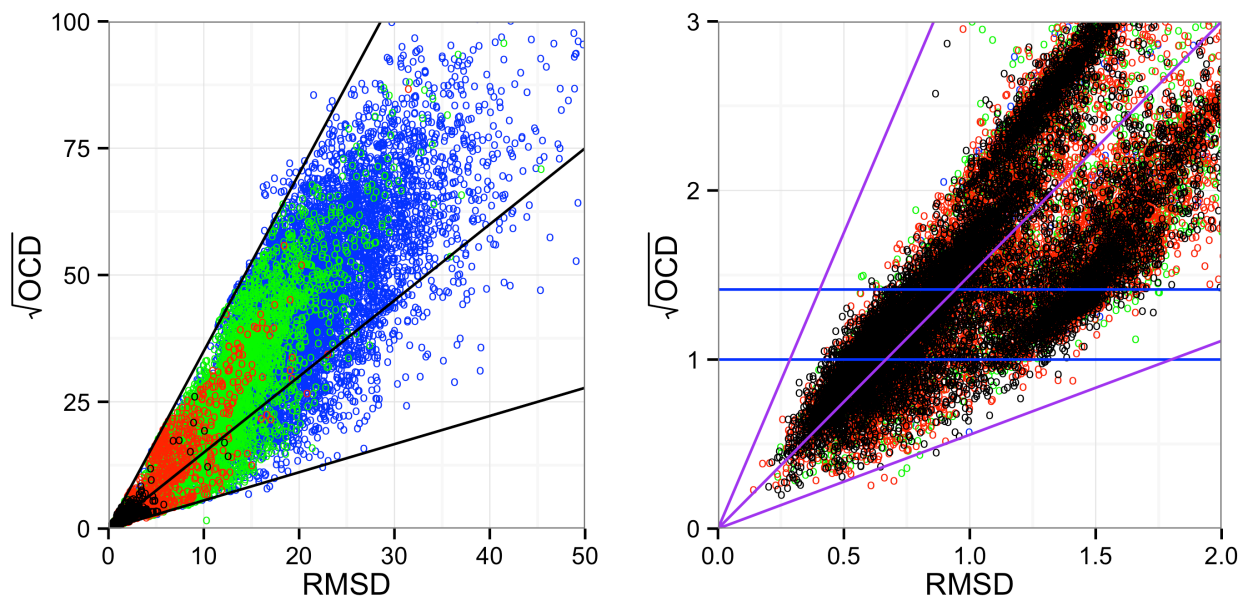
Figure S2: Correlation of OCD and RMSD in 40,000 candidate structures from rigid-body $V_L–V_H$ docking of a 1DLF homology model. To linearize the correlation, the square root of OCD is plotted against RMSD. The different colors represent the scale of perturbations in the docking simulations (blue > green > red > black, corresponding to size of rotations and translations). Zero-intercept lines highlight the center and the bounds of the correlation, and their slopes are noted. Horizontal lines corresponding to OCD values of 1.0 and 2.0 are also shown. The data are plotted over the RMSD ranges 0 Å-50 Å (left) and 0 Å-2 Å (right).

Table S3: Summary of the performance of the full ST, MT, bMT, and rMT RosettaAntibody protocols for each of the 46 benchmark antibodies. Target totals represent the number of targets in the benchmark set for which a given protocol achieved a given threshold of success. The four success thresholds are: (1) a single sub-2.0 OCD grafted structure, (2) a single sub-1.0 OCD candidate structure, (3) at least 100 sub-2.0 OCD candidate structures, and (4) at least 10 sub-1.0 OCD candidate structures. The grafted models for the MT and rMT protocols are identical, so the rMT column was omitted from this portion of the table.

Target	OCD, grafted model		Lowest OCD candidate structure				Sub-2.0 OCD candidate structures				Sub-1.0 OCD candidate structures			
	ST	MT (best)	ST	MT	bMT	rMT	ST	MT	bMT	rMT	ST	MT	bMT	rMT
1dlf	15.60	8.21	1.09	0.42	0.46	0.42	5	73	22	26	0	15	5	4
1fns	3.14	1.91	0.22	0.08	0.08	0.08	302	999	354	348	47	341	132	119
1gig	2.97	1.05	0.53	0.10	0.10	0.10	103	285	120	107	18	72	39	34
1jfq	2.52	0.64	0.45	0.22	0.24	0.24	93	451	172	163	5	72	26	28
1jpt	5.76	0.17	0.08	0.06	0.06	0.06	809	1593	598	568	472	665	261	252
1mfa	6.25	4.89	0.59	0.52	0.51	0.52	28	78	43	38	5	8	4	6
1mlb	4.48	1.07	0.50	0.10	0.10	0.22	179	620	290	231	23	142	71	65
1mqk	2.84	1.32	0.07	0.04	0.13	0.04	340	841	392	294	94	280	140	101
1nlb	7.02	0.97	0.32	0.12	0.31	0.12	69	201	60	70	14	50	14	23
1oaq	4.78	1.20	0.31	0.10	0.10	0.18	84	314	76	102	23	73	13	24
1seq	0.60	0.60	0.30	0.06	0.06	0.24	304	717	236	262	33	151	58	70
2adf	2.38	1.03	0.29	0.15	0.22	0.15	153	323	96	107	36	73	20	24
2d7t	20.47	15.18	2.93	1.55	2.93	2.29	0	1	0	0	0	0	0	0
2e27	6.70	1.52	1.11	0.68	0.98	1.13	18	41	15	15	0	3	1	0
2fb4	7.56	1.12	1.04	0.11	0.19	0.11	7	152	67	55	0	24	11	11
2fbj	9.96	0.85	1.12	0.10	0.10	0.36	7	258	60	84	0	77	16	27
2r8s	0.99	0.33	0.07	0.07	0.10	0.15	550	773	245	255	228	304	94	99
2v17	10.83	3.12	0.22	0.16	0.16	0.34	83	396	192	145	26	90	46	30
2vxv	0.45	0.45	0.12	0.12	0.12	0.12	775	1193	480	405	360	425	169	144
2xwt	0.85	0.85	0.04	0.04	0.04	0.10	467	880	381	341	137	261	101	96
2ypv	8.09	3.33	0.41	0.41	0.82	0.41	22	90	27	45	7	10	2	5
3e8u	4.02	1.30	0.03	0.03	0.03	0.03	432	1220	446	433	150	504	180	173
3eo9	4.45	2.55	0.03	0.03	0.29	0.13	243	620	231	239	43	102	30	48
3g5y	2.57	1.52	0.38	0.10	0.10	0.13	403	805	266	288	38	170	46	62
3giz	5.36	0.91	0.96	0.36	0.36	0.36	2	60	10	25	1	11	1	4
3gnm	2.55	0.53	0.07	0.04	0.04	0.11	220	1127	447	396	69	367	149	129
3go1	2.22	0.26	0.10	0.06	0.06	0.06	169	326	162	103	45	97	49	31
3hc4	10.99	2.13	1.61	0.13	0.47	0.13	2	57	22	14	0	7	5	3
3hnt	4.56	1.46	0.43	0.14	0.14	0.20	90	665	280	246	15	220	100	77
3i9g	0.29	0.29	0.05	0.05	0.05	0.05	569	710	417	243	367	390	235	136
3liz	8.47	1.18	0.38	0.18	0.29	0.18	24	424	187	144	3	89	38	28
3lmj	2.54	0.78	0.63	0.17	0.46	0.37	159	304	101	118	14	42	14	20
3m8o	31.92	15.63	9.06	7.00	10.02	7.00	0	0	0	0	0	0	0	0
3mlr	130.15	130.15	49.42	49.42	50.09	52.15	0	0	0	0	0	0	0	0
3mxw	1.47	1.20	0.06	0.06	0.07	0.07	547	1008	507	350	239	342	205	115
3nps	7.36	4.37	4.09	2.06	20.6	2.70	0	0	0	0	0	0	0	0
3oz9	2.54	2.54	0.65	0.39	0.86	0.60	86	214	90	88	5	19	2	7
3p0y	0.13	0.13	0.08	0.08	0.22	0.14	274	385	138	126	61	82	25	22
3t65	0.71	0.69	0.08	0.01	0.01	0.08	628	1704	639	610	233	745	280	252
3umt	1.10	1.10	0.25	0.10	0.10	0.29	184	334	109	117	48	79	26	30
3v0w	3.24	3.24	0.16	0.16	0.22	0.16	224	314	121	103	41	62	26	21
4f57	10.49	5.49	0.05	0.05	0.05	0.18	149	237	80	91	48	63	20	22
4h0h	4.69	1.30	0.62	0.20	0.21	0.20	118	471	124	165	7	73	12	30
4h20	0.32	0.32	0.16	0.10	0.13	0.10	465	1046	468	372	155	280	131	101
4hpy	0.54	0.54	0.32	0.17	0.17	0.30	247	450	251	160	18	58	31	17
4nzu	1.11	1.11	0.03	0.03	0.09	0.03	544	1154	444	408	171	378	142	134
Target Totals	Best Graft ≤ 2.0 OCD		Best Structure ≤ 1.0 OCD				≥ 100 Sub-2.0 OCD Models				≥ 10 Sub-1.0 OCD Models			
	12	33	37	42	42	41	27	36	29	31	30	39	35	35