PDB ID	Score of lowest scoring model		RMSD of lowest scoring model	
	TransRot/MCM	Transform/MCM	TransRot/MCM	Transform/MCM
2q89	-17.1	-16.1	1.0	0.8
3bgz	-15.8	-15.5	6.7	4.5
1ukb	-9.8	-10.4	4.3	1.2
1vot	-13.6	-13.6	4.0	2.8
2p7g	-16.5	-15.8	1.6	0.8
2rca	-14.8	-14.0	1.1	1.1
2vuk	-15.2	-14.2	2.2	1.3
2nta	-13.6	-15.6	1.0	1.1
2are	-11.7	-9.4	2.2	1.4
2z4b	-14.2	-13.2	2.3	1.3
2jj3	-18.9	-17.3	1.7	3.8
2b3f	-14.8	-13.3	2.7	2.7
2bbf	-17.0	-17.4	1.6	1.9
2pwg	-11.5	-12.9	2.4	3.7
2otz	-9.9	-11.0	1.0	1.0
2ou0	-9.2	-9.4	2.1	0.9
2pzv	-8.6	-7.6	3.1	5.0
2q88	-16.8	-16.7	1.4	1.3
1ui0	-8.8	-9.6	2.1	2.2
1uz1	-12.9	-9.8	3.3	1.3
1uz4	-11.4	-10.3	3.2	1.8
1v0l	-11.3	-11.1	2.6	1.5
1ws4	-9.6	-10.2	3.6	3.7
1y20	-14.7	-14.3	0.5	0.4
2fai	-14.9	-14.5	2.1	1.8
2fqw	-17.1	-15.2	2.2	1.4
2j78	-13.6	-12.7	3.9	3.3
1bky	-8.5	-9.4	4.4	4.3
1q4w	-14.6	-13.5	1.6	1.2
1fcx	-23.7	-22.2	1.4	1.3
1fh8	-11.0	-9.3	2.7	1.9
1y93	-6.9	-7.2	3.1	1.7
1lhw	-16.9	-15.1	3.3	1.1
1fh9	-12.9	-11.1	6.0	5.9
1s9t	-11.2	-10.5	4.9	5.0
1fhd	-13.0	-11.3	5.6	3.5
1lnm	-18.0	-17.3	5.2	1.1
1nli	-15.5	-13.9	1.0	0.7
1ow4	-16.2	-14.8	2.9	1.3
1r5y	-14.2	-14.3	1.2	1.2
1s38	-15.3	-15.0	1.3	0.8
1s39	-12.2	-11.9	1.4	1.8
1sw1	-13.5	-13.4	2.2	1.9

S 3 Table: PDB IDs, RMSDs and Scores for lowest scoring models generated by the Transform/MCM and the TransRot/MCM protocols docking ligands into the set of 43 relaxed protein models.