

Supplementary Information

FlexAID: Revisiting docking on non native-complex structures

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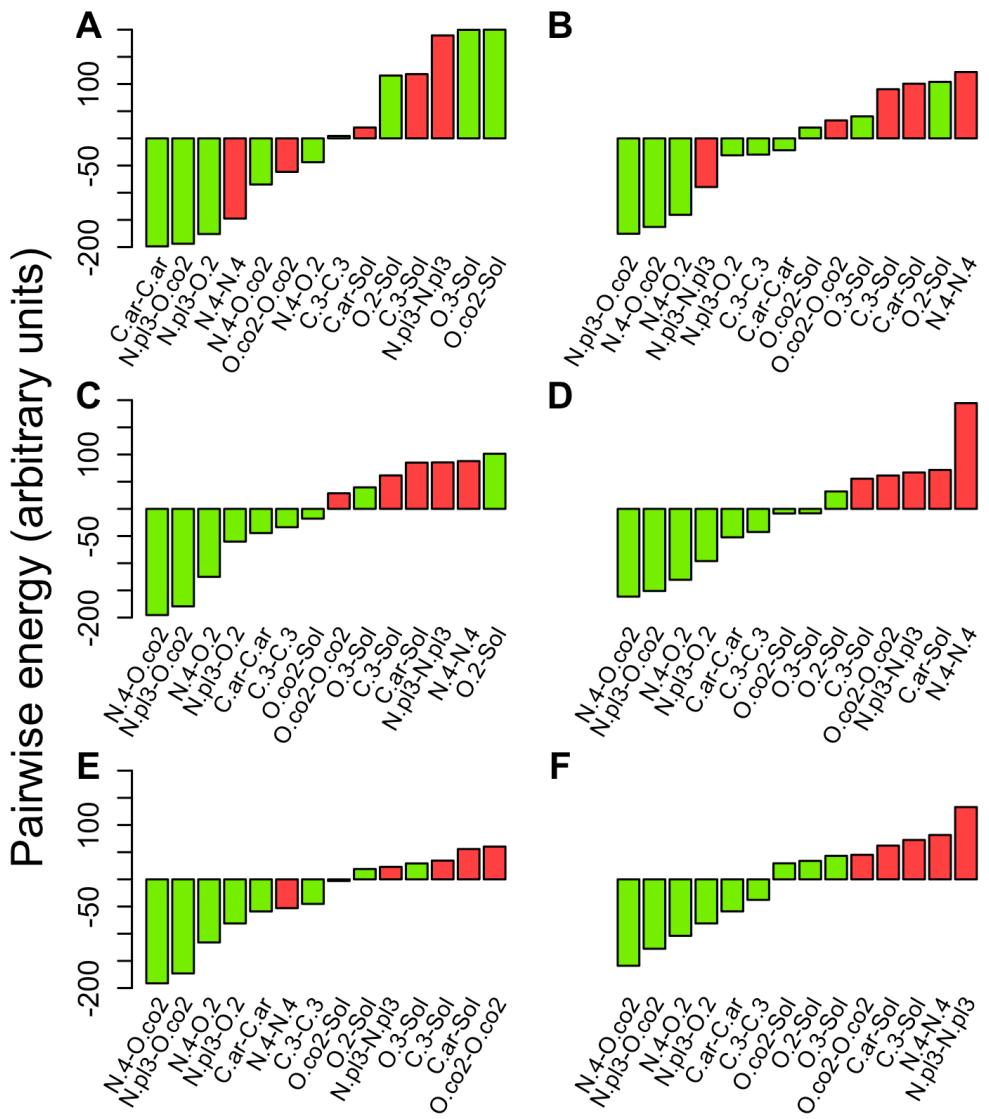


Figure S1. Pairwise interaction parameters for selected interactions for the potentials derived in consecutive MC iterations. Normalized values of the initial potentials (A) and potentials at iterations 1 (B), 2 (C), 3 (D), 4 (E) and 5 (F) are displayed. For the colour coding and atom types nomenclature, refer to the legend of Figure 2.

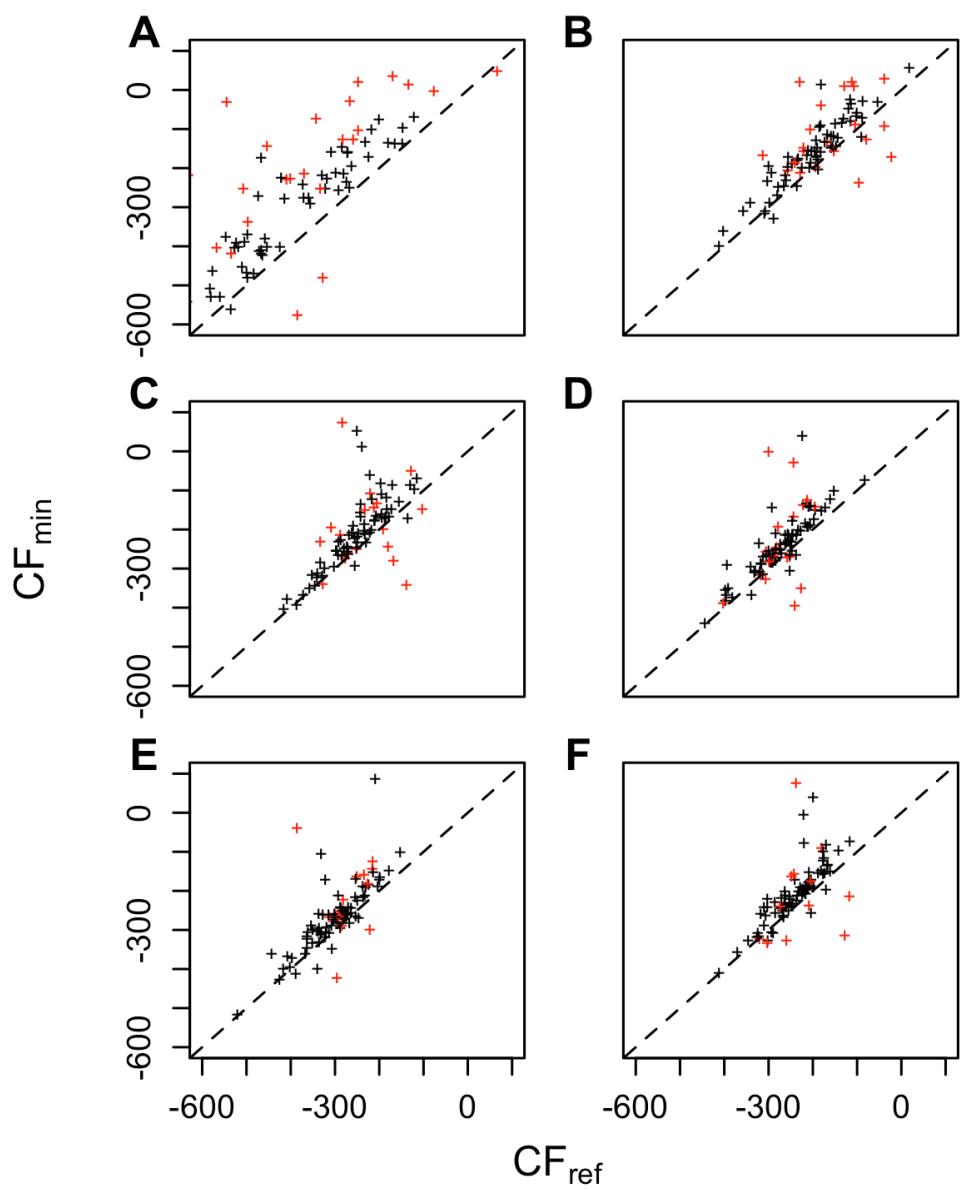


Figure S2. Best CF (CF_{min}) predicted as a function of the reference CF (CF_{ref}). Values for the initial potentials (A) and potentials at iterations 1 (B), 2 (C), 3 (D), 4 (E) and 5 (F) are displayed. Each point represents a unique protein-ligand complex in the Astex diverse set. Points above the dashed line are cases that were optimized relative to the reference CF. Points marked in red are complexes for which no success was observed.

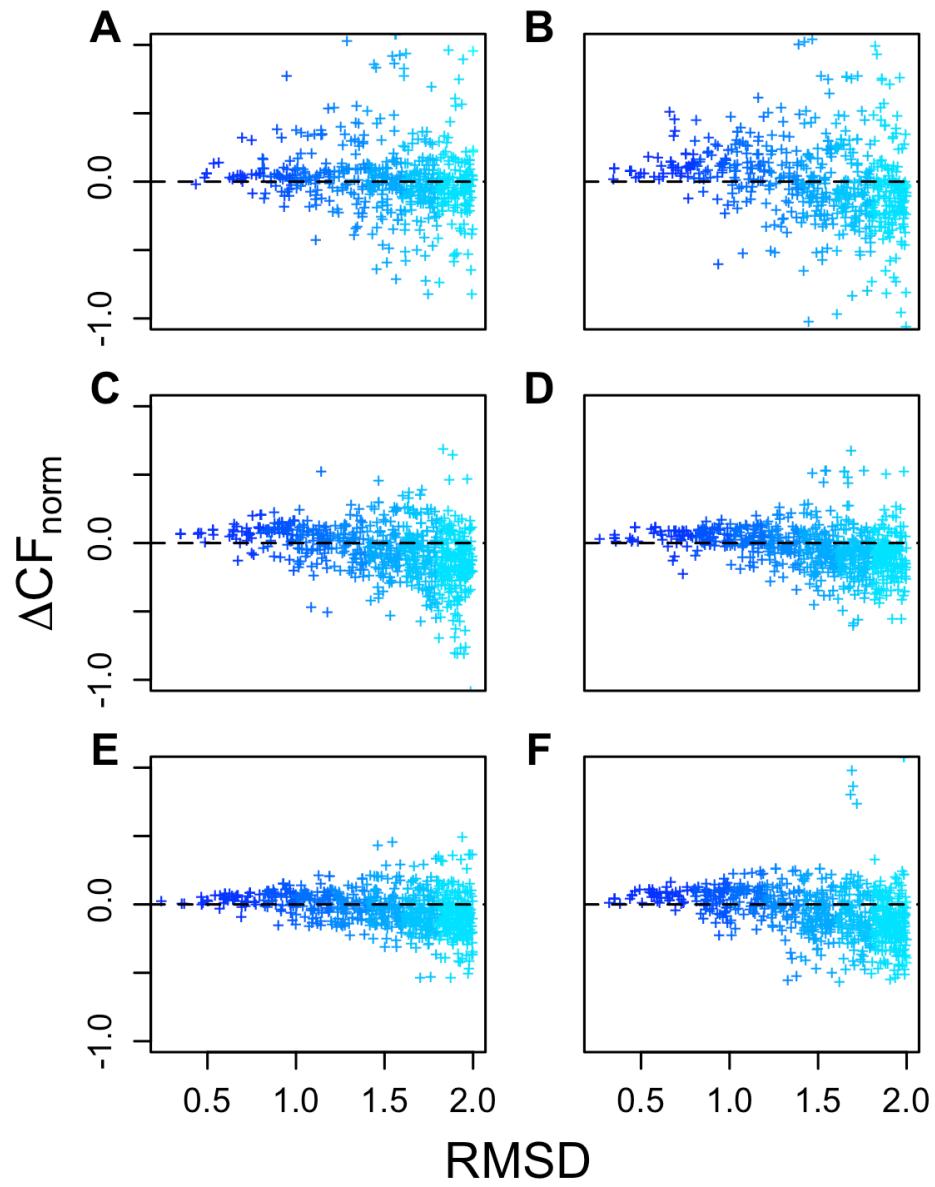


Figure S3. Smoothness of the scoring function for each iteration. Differences in CF between successful poses relative to the reference pose for the initial potentials (A) and potentials at iterations 1 (B), 2 (C), 3 (D), 4 (E) and 5 (F) are displayed. Each point represents a successful prediction in the Astex diverse set. For the colour coding and further detail refer to the legend of Figure 3.

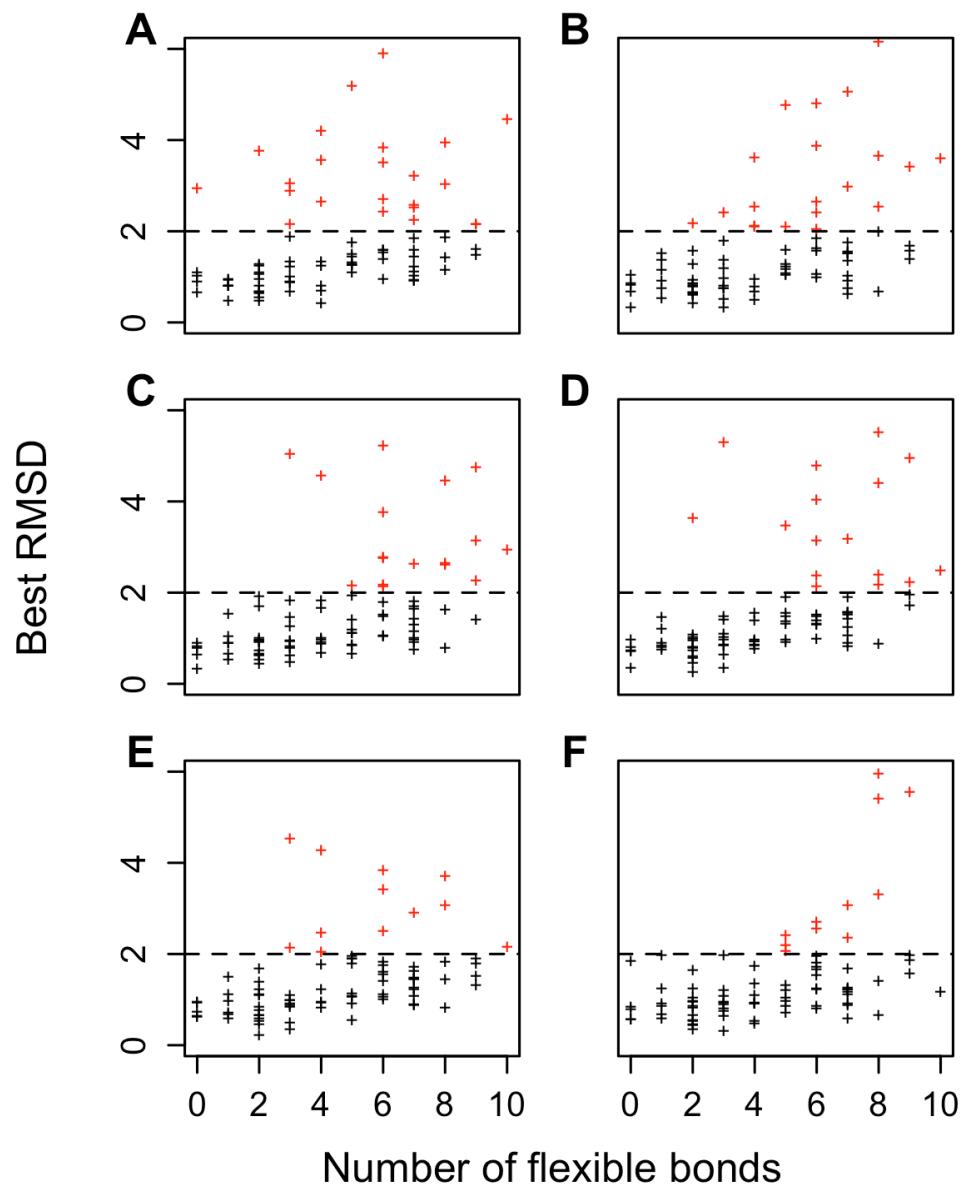


Figure S4. Best RMSD as a function of the number of flexible bonds of the ligand. Values for the initial potentials (A) and potentials at iterations 1 (B), 2 (C), 3 (D), 4 (E) and 5 (F) are displayed. Each point represents the best-predicted pose in terms of RMSD for each complex in the Astex diverse set. A RMSD of 2.0 \AA is used as cut-off for successful predictions. Points marked in red are failures.

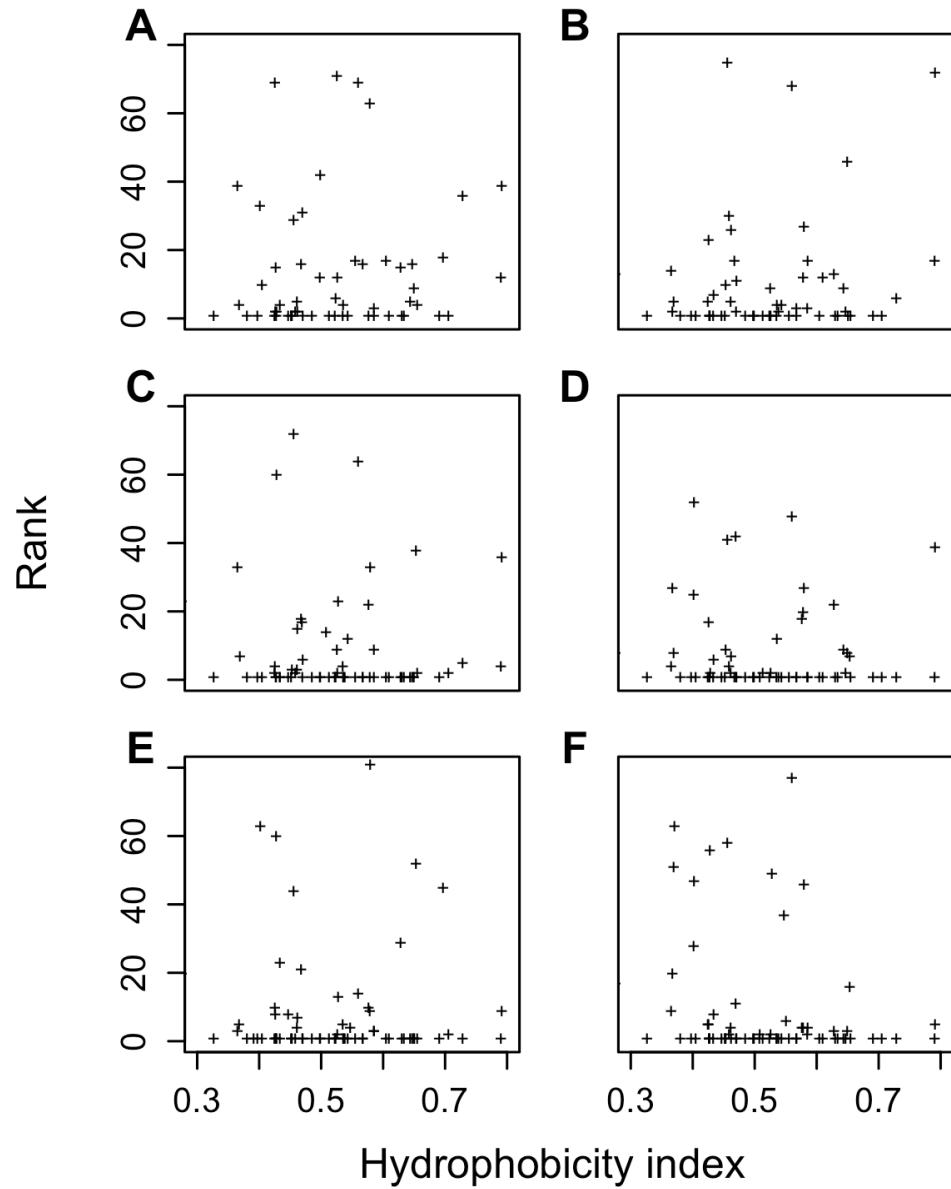
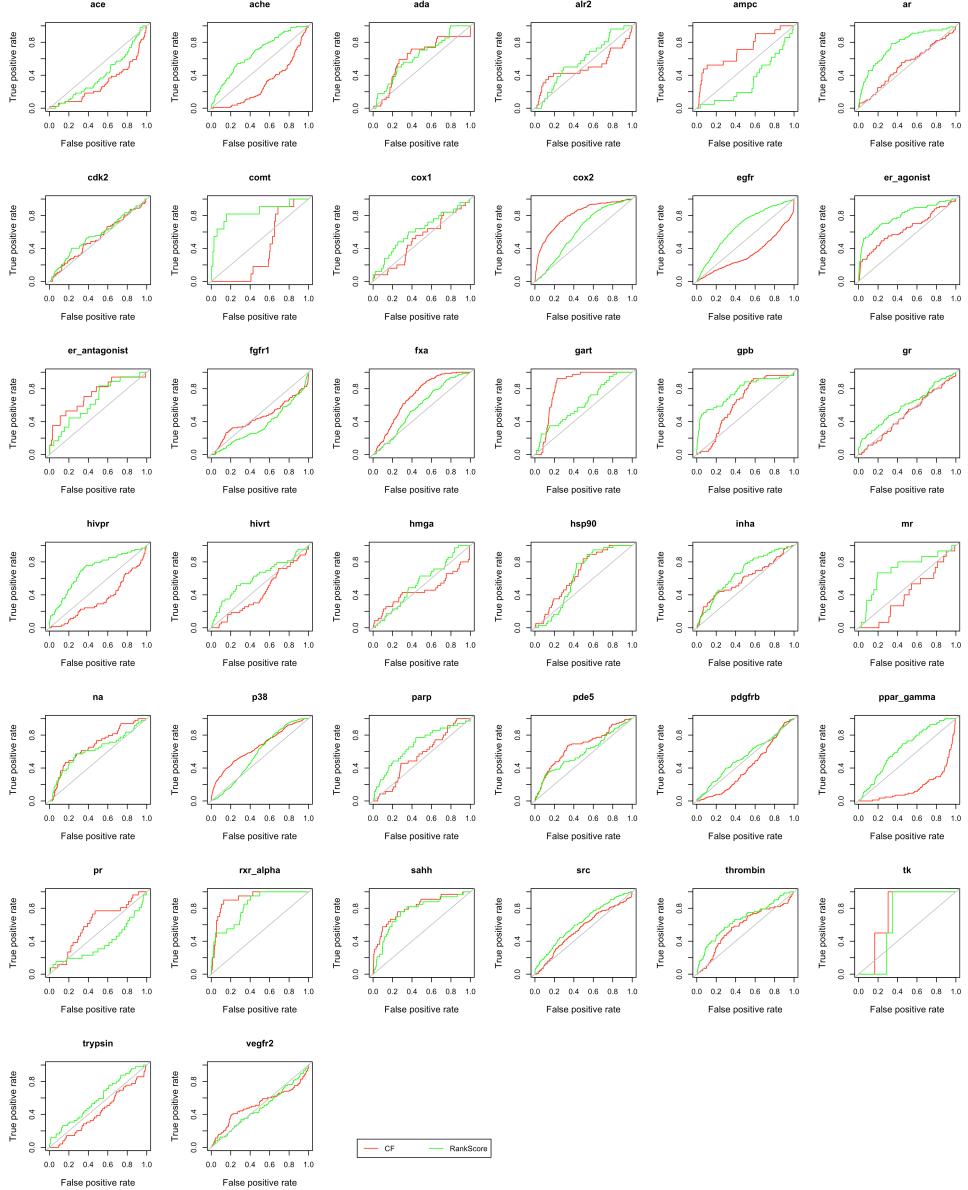


Figure S5. Rank as a function of the hydrophobicity index of the binding-site. Values for the initial potentials (A) and potentials at iterations 1 (B), 2 (C), 3 (D), 4 (E) and 5 (F) are displayed. The hydrophobicity index of a binding-site is defined as the hydrophobic SAS over the total SAS. Each point represents a unique protein-ligand complex in the Astex diverse set.

A

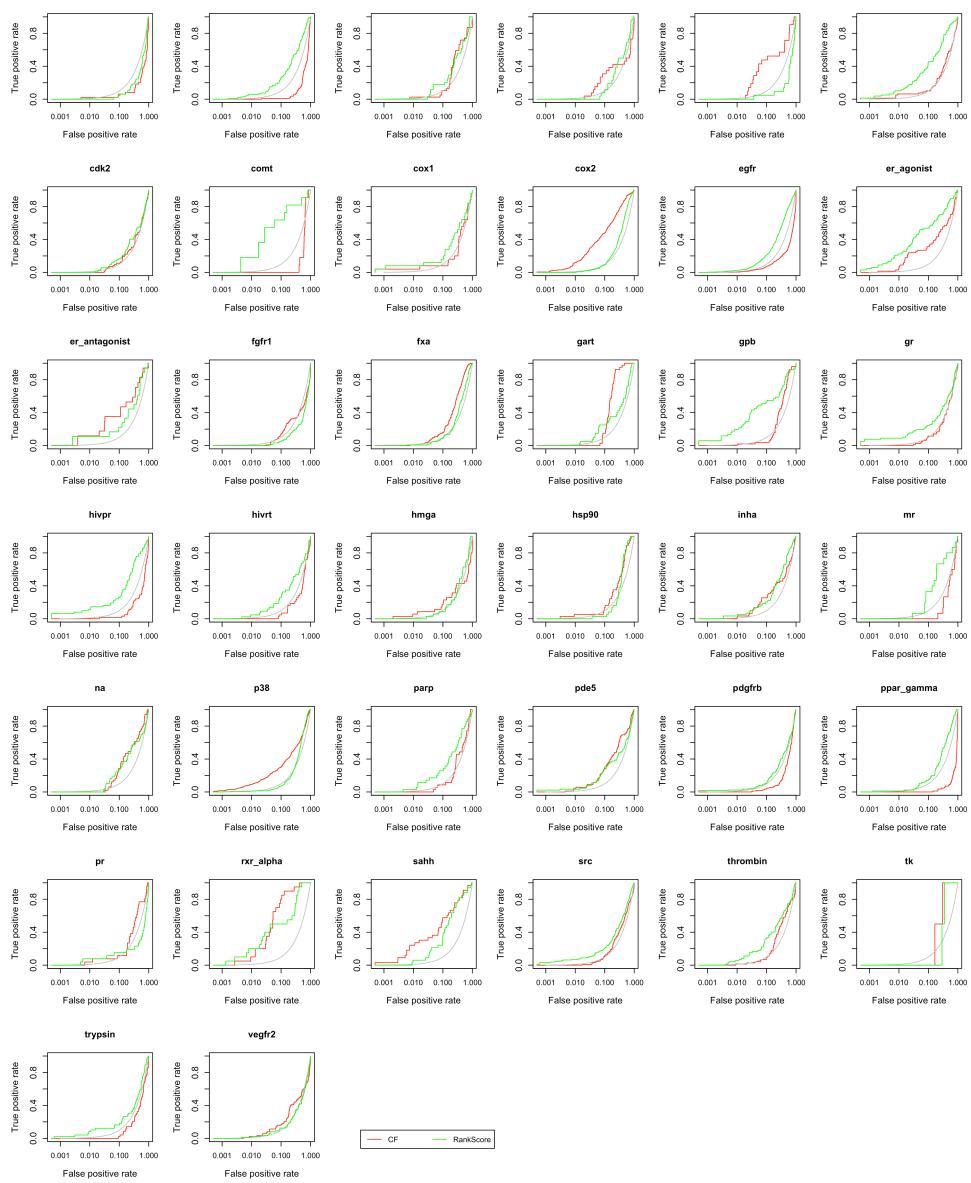
B

Figure S6. ROC curves of targets in the DUD dataset. The ROC (A) and semi-logarithmic ROC (B) curves of 38 targets in the DUD dataset are displayed. We use the CF (red) and RankScore (green) as scoring functions to discriminate true from false positives. We use RankScore only to re-score the best predicted pose for each unique molecule according to the CF. The grey bars indicate random predictions.

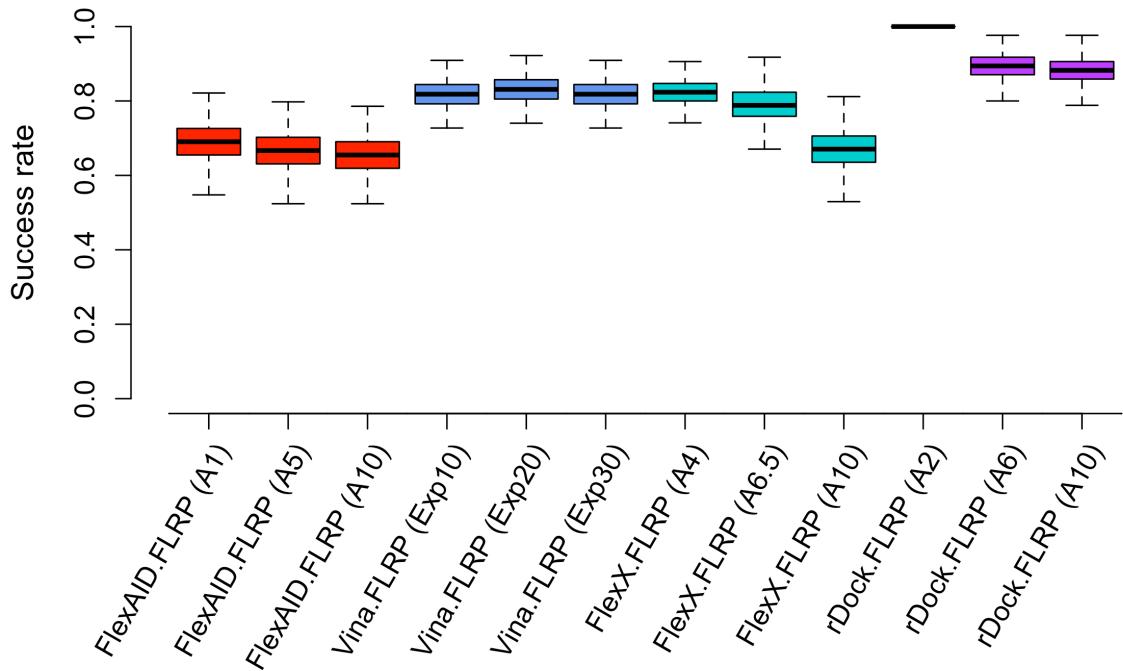
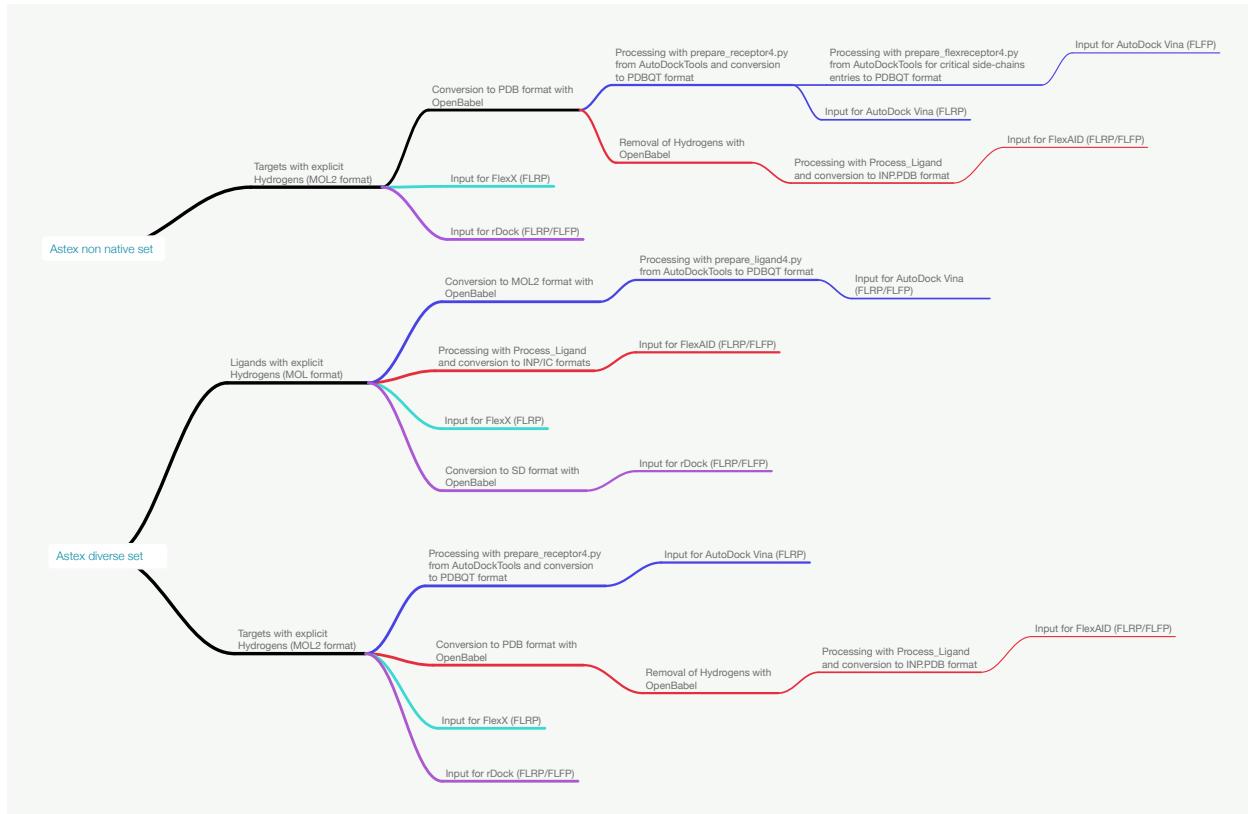


Figure S7. Performance of FlexAID, AutoDock Vina, FlexX and rDock as a function of an increasing definition of the binding-site. The performance of FlexAID (red), AutoDock Vina (blue), FlexX (cyan) and rDock (purple) were evaluated on the Astex diverse set in the presence of ligand flexibility. FlexAID: We retained grid vertexes within 1, 5 and 10Å of the reference ligand (denoted as A1, A5 and A10). AutoDock Vina: The size of the box was expanded by 10, 20 and 30Å in each dimension (denoted as Exp10, Exp20 and Exp30). FlexX: The set of protein atoms was restricted to those within 4.0, 6.5 and 10.0Å of the reference ligand (denoted as A4, A6.5 and A10). rDock: We used spheres of radii 2, 6 and 10Å that overlap the reference ligand (denoted as A2, A6 and A10).

A

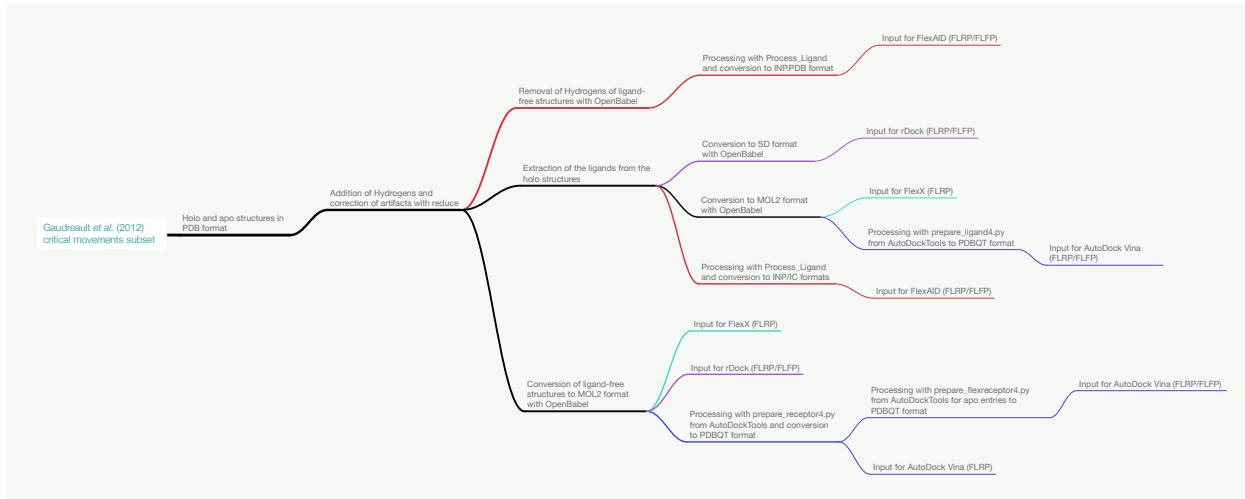
B

Figure S8. Detailed pipeline of the preparation and processing of the molecules of the Astex diverse and non-native sets (A) and of the HAP2 dataset (B). Specific steps for a given method are color-coded according to Figure 3. Black lines represent common steps for methods. For higher resolution images, please refer to: <http://bcb.med.usherbrooke.ca/FlexAID-SI>

Table S1. Atom types and their frequency in the training and test sets

SYBYL Atom type	C.1	C.2	C.3	C.ar	C.cat	N.1	N.2	N.3	N.4	N.ar
PDBbind	56	10,933	44,032	28,904	875	23	674	0	1,478	3,096
Astex	4	604	2,767	1,877	36	2	14	18	60	225
	N.am	N.pl3	O.2	O.3	O.co2	O.ar	S.2	S.3	S.o	S.o2
PDBbind	10,288	3,616	11,411	7,308	6,562	0	17	1,208	266	0
Astex	569	193	736	330	285	0	6	96	11	1
	S.ar	P.3	F	Cl	Br	I	Se	Mg	Sr	Cu
PDBbind	0	367	322	185	63	13	1	67	1	4
Astex	0	6	25	17	1	0	0	3	0	0
	Mn	Hg	Cd	Ni	Zn	Ca	Fe	Co.oh	Du	
PDBbind	18	2	1	2	210	30	0	3	0	
Astex	2	0	0	0	14	1	3	0	0	

Table S2. Values of pairwise interactions

C.1	C.1	0.000	C.1	C.2	-119.400	C.1	C.3	-162.900
C.1	C.AR	-179.100	C.1	C.CAT	0.000	C.1	N.1	0.000
C.1	N.2	0.000	C.1	N.3	0.000	C.1	N.4	0.000
C.1	N.AR	157.100	C.1	N.AM	60.540	C.1	N.PL3	-78.630
C.1	O.2	-198.300	C.1	O.3	-180.800	C.1	O.CO2	93.260
C.1	O.AR	0.000	C.1	S.2	0.000	C.1	S.3	0.000
C.1	S.O	0.000	C.1	S.O2	0.000	C.1	S.AR	0.000
C.1	P.3	0.000	C.1	F	0.000	C.1	CL	0.000
C.1	BR	0.000	C.1	I	0.000	C.1	SE	0.000
C.1	MG	0.000	C.1	SR	0.000	C.1	CU	0.000
C.1	MN	0.000	C.1	HG	0.000	C.1	CD	0.000
C.1	NI	0.000	C.1	ZN	0.000	C.1	CA	0.000
C.1	FE	0.000	C.1	CO.OH	0.000	C.1	DU	0.000
C.1	SOL	159.100	C.2	C.2	-198.900	C.2	C.3	-69.110
C.2	C.AR	-149.400	C.2	C.CAT	194.100	C.2	N.1	165.400
C.2	N.2	-88.780	C.2	N.3	0.000	C.2	N.4	36.970
C.2	N.AR	15.810	C.2	N.AM	-21.590	C.2	N.PL3	-61.990
C.2	O.2	-10.060	C.2	O.3	61.290	C.2	O.CO2	14.760
C.2	O.AR	0.000	C.2	S.2	-115.000	C.2	S.3	-123.100
C.2	S.O	81.350	C.2	S.O2	0.000	C.2	S.AR	0.000
C.2	P.3	76.920	C.2	F	-186.100	C.2	CL	-193.700
C.2	BR	0.000	C.2	I	13.040	C.2	SE	0.000
C.2	MG	152.500	C.2	SR	0.000	C.2	CU	0.000
C.2	MN	119.800	C.2	HG	0.000	C.2	CD	121.200
C.2	NI	0.000	C.2	ZN	-40.540	C.2	CA	0.000
C.2	FE	0.000	C.2	CO.OH	0.000	C.2	DU	0.000
C.2	SOL	61.750	C.3	C.3	-37.750	C.3	C.AR	-53.320
C.3	C.CAT	-191.900	C.3	N.1	-71.640	C.3	N.2	-68.710
C.3	N.3	0.000	C.3	N.4	87.280	C.3	N.AR	-63.970
C.3	N.AM	26.900	C.3	N.PL3	-0.949	C.3	O.2	-50.230
C.3	O.3	-44.360	C.3	O.CO2	-30.770	C.3	O.AR	0.000
C.3	S.2	0.000	C.3	S.3	-48.670	C.3	S.O	-121.800
C.3	S.O2	0.000	C.3	S.AR	0.000	C.3	P.3	-8.391
C.3	F	-74.040	C.3	CL	-93.410	C.3	BR	0.000
C.3	I	-157.600	C.3	SE	0.000	C.3	MG	131.200
C.3	SR	0.000	C.3	CU	-180.800	C.3	MN	0.000
C.3	HG	0.000	C.3	CD	0.000	C.3	NI	0.000
C.3	ZN	95.360	C.3	CA	0.000	C.3	FE	0.000
C.3	CO.OH	0.000	C.3	DU	0.000	C.3	SOL	72.500
C.AR	C.AR	-58.920	C.AR	C.CAT	-183.900	C.AR	N.1	0.000
C.AR	N.2	-124.200	C.AR	N.3	0.000	C.AR	N.4	36.650
C.AR	N.AR	-18.300	C.AR	N.AM	23.980	C.AR	N.PL3	-16.940
C.AR	O.2	-5.605	C.AR	O.3	-21.650	C.AR	O.CO2	25.600
C.AR	O.AR	0.000	C.AR	S.2	-135.600	C.AR	S.3	-51.640
C.AR	S.O	100.300	C.AR	S.O2	0.000	C.AR	S.AR	0.000
C.AR	P.3	-58.990	C.AR	F	-57.060	C.AR	CL	-25.050
C.AR	BR	-12.720	C.AR	I	0.000	C.AR	SE	0.000
C.AR	MG	0.000	C.AR	SR	0.000	C.AR	CU	0.000
C.AR	MN	0.000	C.AR	HG	0.000	C.AR	CD	0.000
C.AR	NI	0.000	C.AR	ZN	160.800	C.AR	CA	0.000
C.AR	FE	0.000	C.AR	CO.OH	0.000	C.AR	DU	0.000
C.AR	SOL	62.170	C.CAT	C.CAT	0.000	C.CAT	N.1	0.000
C.CAT	N.2	-161.800	C.CAT	N.3	0.000	C.CAT	N.4	174.800
C.CAT	N.AR	-118.300	C.CAT	N.AM	180.900	C.CAT	N.PL3	-83.100
C.CAT	O.2	195.900	C.CAT	O.3	67.990	C.CAT	O.CO2	-54.190
C.CAT	O.AR	0.000	C.CAT	S.2	0.000	C.CAT	S.3	-167.900
C.CAT	S.O	0.000	C.CAT	S.O2	0.000	C.CAT	S.AR	0.000
C.CAT	P.3	167.700	C.CAT	F	-28.170	C.CAT	CL	0.000
C.CAT	BR	-190.100	C.CAT	I	0.000	C.CAT	SE	0.000
C.CAT	MG	0.000	C.CAT	SR	0.000	C.CAT	CU	0.000

C.CAT	MN	0.000	C.CAT	HG	0.000	C.CAT	CD	0.000
C.CAT	NI	0.000	C.CAT	ZN	0.000	C.CAT	CA	0.000
C.CAT	FE	0.000	C.CAT	CO.OH	0.000	C.CAT	DU	0.000
C.CAT	SOL	120.300	N.1	N.1	0.000	N.1	N.2	0.000
N.1	N.3	0.000	N.1	N.4	0.000	N.1	N.AR	0.000
N.1	N.AM	-168.900	N.1	N.PL3	0.000	N.1	O.2	0.000
N.1	O.3	-71.740	N.1	O.CO2	0.000	N.1	O.AR	0.000
N.1	S.2	0.000	N.1	S.3	0.000	N.1	S.O	0.000
N.1	S.O2	0.000	N.1	S.AR	0.000	N.1	P.3	0.000
N.1	F	0.000	N.1	CL	0.000	N.1	BR	0.000
N.1	I	0.000	N.1	SE	0.000	N.1	MG	0.000
N.1	SR	0.000	N.1	CU	0.000	N.1	MN	0.000
N.1	HG	0.000	N.1	CD	0.000	N.1	NI	0.000
N.1	ZN	0.000	N.1	CA	0.000	N.1	FE	0.000
N.1	CO.OH	0.000	N.1	DU	0.000	N.1	SOL	167.200
N.2	N.2	0.000	N.2	N.3	0.000	N.2	N.4	84.570
N.2	N.AR	-55.800	N.2	N.AM	-195.700	N.2	N.PL3	-122.300
N.2	O.2	-87.380	N.2	O.3	-144.800	N.2	O.CO2	-197.600
N.2	O.AR	0.000	N.2	S.2	0.000	N.2	S.3	28.130
N.2	S.O	0.000	N.2	S.O2	0.000	N.2	S.AR	0.000
N.2	P.3	0.000	N.2	F	0.000	N.2	CL	0.000
N.2	BR	0.000	N.2	I	0.000	N.2	SE	0.000
N.2	MG	0.000	N.2	SR	0.000	N.2	CU	0.000
N.2	MN	0.000	N.2	HG	0.000	N.2	CD	0.000
N.2	NI	0.000	N.2	ZN	0.000	N.2	CA	0.000
N.2	FE	0.000	N.2	CO.OH	0.000	N.2	DU	0.000
N.2	SOL	136.400	N.3	N.3	0.000	N.3	N.4	0.000
N.3	N.AR	0.000	N.3	N.AM	0.000	N.3	N.PL3	0.000
N.3	O.2	0.000	N.3	O.3	0.000	N.3	O.CO2	0.000
N.3	O.AR	0.000	N.3	S.2	0.000	N.3	S.3	0.000
N.3	S.O	0.000	N.3	S.O2	0.000	N.3	S.AR	0.000
N.3	P.3	0.000	N.3	F	0.000	N.3	CL	0.000
N.3	BR	0.000	N.3	I	0.000	N.3	SE	0.000
N.3	MG	0.000	N.3	SR	0.000	N.3	CU	0.000
N.3	MN	0.000	N.3	HG	0.000	N.3	CD	0.000
N.3	NI	0.000	N.3	ZN	0.000	N.3	CA	0.000
N.3	FE	0.000	N.3	CO.OH	0.000	N.3	DU	0.000
N.3	SOL	0.000	N.4	N.4	81.660	N.4	N.AR	-16.350
N.4	N.AM	160.200	N.4	N.PL3	160.400	N.4	O.2	-103.900
N.4	O.3	-101.800	N.4	O.CO2	-159.000	N.4	O.AR	0.000
N.4	S.2	0.000	N.4	S.3	-66.400	N.4	S.O	0.000
N.4	S.O2	0.000	N.4	S.AR	0.000	N.4	P.3	143.000
N.4	F	0.000	N.4	CL	45.570	N.4	BR	50.170
N.4	I	0.000	N.4	SE	0.000	N.4	MG	0.000
N.4	SR	0.000	N.4	CU	0.000	N.4	MN	0.000
N.4	HG	0.000	N.4	CD	0.000	N.4	NI	0.000
N.4	ZN	158.900	N.4	CA	0.000	N.4	FE	0.000
N.4	CO.OH	0.000	N.4	DU	0.000	N.4	SOL	147.100
N.AR	N.AR	156.700	N.AR	N.AM	-157.300	N.AR	N.PL3	-26.350
N.AR	O.2	-86.640	N.AR	O.3	-189.600	N.AR	O.CO2	-125.300
N.AR	O.AR	0.000	N.AR	S.2	0.000	N.AR	S.3	-190.100
N.AR	S.O	-169.000	N.AR	S.O2	0.000	N.AR	S.AR	0.000
N.AR	P.3	-148.800	N.AR	F	7.695	N.AR	CL	88.720
N.AR	BR	137.300	N.AR	I	0.000	N.AR	SE	0.000
N.AR	MG	0.000	N.AR	SR	0.000	N.AR	CU	0.000
N.AR	MN	0.000	N.AR	HG	0.000	N.AR	CD	0.000
N.AR	NI	0.000	N.AR	ZN	0.000	N.AR	CA	0.000
N.AR	FE	0.000	N.AR	CO.OH	0.000	N.AR	DU	0.000
N.AR	SOL	198.300	N.AM	N.AM	72.280	N.AM	N.PL3	86.550
N.AM	O.2	-141.100	N.AM	O.3	-70.050	N.AM	O.CO2	-140.100
N.AM	O.AR	0.000	N.AM	S.2	0.000	N.AM	S.3	46.220
N.AM	S.O	73.660	N.AM	S.O2	0.000	N.AM	S.AR	0.000
N.AM	P.3	-117.900	N.AM	F	-46.590	N.AM	CL	36.680

N.AM	BR	0.000	N.AM	I	0.000	N.AM	SE	0.000
N.AM	MG	-61.630	N.AM	SR	0.000	N.AM	CU	0.000
N.AM	MN	0.000	N.AM	HG	0.000	N.AM	CD	0.000
N.AM	NI	0.000	N.AM	ZN	-185.800	N.AM	CA	0.000
N.AM	FE	0.000	N.AM	CO.OH	0.000	N.AM	DU	0.000
N.AM	SOL	190.500	N.PL3	N.PL3	133.000	N.PL3	O.2	-81.100
N.PL3	O.3	-49.120	N.PL3	O.CO2	-127.700	N.PL3	O.AR	0.000
N.PL3	S.2	0.000	N.PL3	S.3	-50.590	N.PL3	S.O	159.900
N.PL3	S.O2	0.000	N.PL3	S.AR	0.000	N.PL3	P.3	44.250
N.PL3	F	-28.990	N.PL3	CL	0.000	N.PL3	BR	-1.934
N.PL3	I	0.000	N.PL3	SE	0.000	N.PL3	MG	92.970
N.PL3	SR	0.000	N.PL3	CU	0.000	N.PL3	MN	37.170
N.PL3	HG	0.000	N.PL3	CD	0.000	N.PL3	NI	0.000
N.PL3	ZN	0.000	N.PL3	CA	0.000	N.PL3	FE	0.000
N.PL3	CO.OH	0.000	N.PL3	DU	0.000	N.PL3	SOL	162.800
O.2	O.2	56.580	O.2	O.3	-33.000	O.2	O.CO2	52.000
O.2	O.AR	0.000	O.2	S.2	0.000	O.2	S.3	27.660
O.2	S.O	170.400	O.2	S.O2	0.000	O.2	S.AR	0.000
O.2	P.3	61.460	O.2	F	51.700	O.2	CL	19.200
O.2	BR	0.000	O.2	I	9.606	O.2	SE	0.000
O.2	MG	-61.550	O.2	SR	0.000	O.2	CU	0.000
O.2	MN	0.000	O.2	HG	0.000	O.2	CD	0.000
O.2	NI	0.000	O.2	ZN	-182.100	O.2	CA	0.000
O.2	FE	0.000	O.2	CO.OH	0.000	O.2	DU	0.000
O.2	SOL	33.990	O.3	O.3	-77.280	O.3	O.CO2	-95.080
O.3	O.AR	0.000	O.3	S.2	0.000	O.3	S.3	-79.640
O.3	S.O	170.800	O.3	S.O2	0.000	O.3	S.AR	0.000
O.3	P.3	-163.400	O.3	F	-149.500	O.3	CL	0.000
O.3	BR	0.000	O.3	I	0.000	O.3	SE	0.000
O.3	MG	67.590	O.3	SR	71.700	O.3	CU	0.000
O.3	MN	0.000	O.3	HG	0.000	O.3	CD	0.000
O.3	NI	0.000	O.3	ZN	-186.700	O.3	CA	-197.800
O.3	FE	0.000	O.3	CO.OH	0.000	O.3	DU	0.000
O.3	SOL	43.240	O.CO2	O.CO2	45.170	O.CO2	O.AR	0.000
O.CO2	S.2	0.000	O.CO2	S.3	32.660	O.CO2	S.O	-77.560
O.CO2	S.O2	0.000	O.CO2	S.AR	0.000	O.CO2	P.3	101.400
O.CO2	F	187.500	O.CO2	CL	-69.110	O.CO2	BR	0.000
O.CO2	I	0.000	O.CO2	SE	0.000	O.CO2	MG	-194.700
O.CO2	SR	0.000	O.CO2	CU	0.000	O.CO2	MN	0.000
O.CO2	HG	0.000	O.CO2	CD	0.000	O.CO2	NI	0.000
O.CO2	ZN	-173.400	O.CO2	CA	-68.340	O.CO2	FE	0.000
O.CO2	CO.OH	0.000	O.CO2	DU	0.000	O.CO2	SOL	29.560
O.AR	O.AR	0.000	O.AR	S.2	0.000	O.AR	S.3	0.000
O.AR	S.O	0.000	O.AR	S.O2	0.000	O.AR	S.AR	0.000
O.AR	P.3	0.000	O.AR	F	0.000	O.AR	CL	0.000
O.AR	BR	0.000	O.AR	I	0.000	O.AR	SE	0.000
O.AR	MG	0.000	O.AR	SR	0.000	O.AR	CU	0.000
O.AR	MN	0.000	O.AR	HG	0.000	O.AR	CD	0.000
O.AR	NI	0.000	O.AR	ZN	0.000	O.AR	CA	0.000
O.AR	FE	0.000	O.AR	CO.OH	0.000	O.AR	DU	0.000
O.AR	SOL	0.000	S.2	S.2	0.000	S.2	S.3	0.000
S.2	S.O	0.000	S.2	S.O2	0.000	S.2	S.AR	0.000
S.2	P.3	0.000	S.2	F	0.000	S.2	CL	0.000
S.2	BR	0.000	S.2	I	0.000	S.2	SE	0.000
S.2	MG	0.000	S.2	SR	0.000	S.2	CU	0.000
S.2	MN	0.000	S.2	HG	0.000	S.2	CD	0.000
S.2	NI	0.000	S.2	ZN	0.000	S.2	CA	0.000
S.2	FE	0.000	S.2	CO.OH	0.000	S.2	DU	0.000
S.2	SOL	0.000	S.3	S.3	-145.500	S.3	S.O	103.900
S.3	S.O2	0.000	S.3	S.AR	0.000	S.3	P.3	-41.280
S.3	F	5.702	S.3	CL	-167.500	S.3	BR	-119.700
S.3	I	0.000	S.3	SE	0.000	S.3	MG	0.000
S.3	SR	0.000	S.3	CU	0.000	S.3	MN	0.000

S.3	HG	0.000	S.3	CD	0.000	S.3	NI	0.000
S.3	ZN	-153.700	S.3	CA	0.000	S.3	FE	0.000
S.3	CO.OH	0.000	S.3	DU	0.000	S.3	SOL	94.930
S.O	S.O	0.000	S.O	S.O2	0.000	S.O	S.AR	0.000
S.O	P.3	0.000	S.O	F	0.000	S.O	CL	0.000
S.O	BR	0.000	S.O	I	0.000	S.O	SE	0.000
S.O	MG	0.000	S.O	SR	0.000	S.O	CU	0.000
S.O	MN	0.000	S.O	HG	0.000	S.O	CD	0.000
S.O	NI	0.000	S.O	ZN	-134.400	S.O	CA	0.000
S.O	FE	0.000	S.O	CO.OH	0.000	S.O	DU	0.000
S.O	SOL	-176.200	S.O2	S.O2	0.000	S.O2	S.AR	0.000
S.O2	P.3	0.000	S.O2	F	0.000	S.O2	CL	0.000
S.O2	BR	0.000	S.O2	I	0.000	S.O2	SE	0.000
S.O2	MG	0.000	S.O2	SR	0.000	S.O2	CU	0.000
S.O2	MN	0.000	S.O2	HG	0.000	S.O2	CD	0.000
S.O2	NI	0.000	S.O2	ZN	0.000	S.O2	CA	0.000
S.O2	FE	0.000	S.O2	CO.OH	0.000	S.O2	DU	0.000
S.O2	SOL	0.000	S.AR	S.AR	0.000	S.AR	P.3	0.000
S.AR	F	0.000	S.AR	CL	0.000	S.AR	BR	0.000
S.AR	I	0.000	S.AR	SE	0.000	S.AR	MG	0.000
S.AR	SR	0.000	S.AR	CU	0.000	S.AR	MN	0.000
S.AR	HG	0.000	S.AR	CD	0.000	S.AR	NI	0.000
S.AR	ZN	0.000	S.AR	CA	0.000	S.AR	FE	0.000
S.AR	CO.OH	0.000	S.AR	DU	0.000	S.AR	SOL	0.000
P.3	P.3	0.000	P.3	F	0.000	P.3	CL	0.000
P.3	BR	0.000	P.3	I	0.000	P.3	SE	0.000
P.3	MG	-163.000	P.3	SR	0.000	P.3	CU	0.000
P.3	MN	0.000	P.3	HG	0.000	P.3	CD	0.000
P.3	NI	0.000	P.3	ZN	89.370	P.3	CA	0.000
P.3	FE	0.000	P.3	CO.OH	0.000	P.3	DU	0.000
P.3	SOL	134.700	F	F	0.000	F	CL	0.000
F	BR	0.000	F	I	0.000	F	SE	0.000
F	MG	0.000	F	SR	0.000	F	CU	0.000
F	MN	0.000	F	HG	0.000	F	CD	0.000
F	NI	0.000	F	ZN	-118.700	F	CA	0.000
F	FE	0.000	F	CO.OH	0.000	F	DU	0.000
F	SOL	3.117	CL	CL	0.000	CL	BR	0.000
CL	I	0.000	CL	SE	0.000	CL	MG	0.000
CL	SR	0.000	CL	CU	0.000	CL	MN	0.000
CL	HG	0.000	CL	CD	0.000	CL	NI	0.000
CL	ZN	0.000	CL	CA	0.000	CL	FE	0.000
CL	CO.OH	0.000	CL	DU	0.000	CL	SOL	198.800
BR	BR	0.000	BR	I	0.000	BR	SE	0.000
BR	MG	0.000	BR	SR	0.000	BR	CU	0.000
BR	MN	0.000	BR	HG	0.000	BR	CD	0.000
BR	NI	0.000	BR	ZN	0.000	BR	CA	0.000
BR	FE	0.000	BR	CO.OH	0.000	BR	DU	0.000
BR	SOL	138.400	I	I	0.000	I	SE	0.000
I	MG	0.000	I	SR	0.000	I	CU	0.000
I	MN	0.000	I	HG	0.000	I	CD	0.000
I	NI	0.000	I	ZN	0.000	I	CA	0.000
I	FE	0.000	I	CO.OH	0.000	I	DU	0.000
I	SOL	0.000	SE	SE	0.000	SE	MG	0.000
SE	SR	0.000	SE	CU	0.000	SE	MN	0.000
SE	HG	0.000	SE	CD	0.000	SE	NI	0.000
SE	ZN	0.000	SE	CA	0.000	SE	FE	0.000
SE	CO.OH	0.000	SE	DU	0.000	SE	SOL	0.000
MG	MG	0.000	MG	SR	0.000	MG	CU	0.000
MG	MN	0.000	MG	HG	0.000	MG	CD	0.000
MG	NI	0.000	MG	ZN	0.000	MG	CA	0.000
MG	FE	0.000	MG	CO.OH	0.000	MG	DU	0.000
MG	SOL	0.000	SR	SR	0.000	SR	CU	0.000
SR	MN	0.000	SR	HG	0.000	SR	CD	0.000

SR	NI	0.000	SR	ZN	0.000	SR	CA	0.000
SR	FE	0.000	SR	CO.OH	0.000	SR	DU	0.000
SR	SOL	0.000	CU	CU	0.000	CU	MN	0.000
CU	HG	0.000	CU	CD	0.000	CU	NI	0.000
CU	ZN	0.000	CU	CA	0.000	CU	FE	0.000
CU	CO.OH	0.000	CU	DU	0.000	CU	SOL	0.000
MN	MN	0.000	MN	HG	0.000	MN	CD	0.000
MN	NI	0.000	MN	ZN	0.000	MN	CA	0.000
MN	FE	0.000	MN	CO.OH	0.000	MN	DU	0.000
MN	SOL	0.000	HG	HG	0.000	HG	CD	0.000
HG	NI	0.000	HG	ZN	0.000	HG	CA	0.000
HG	FE	0.000	HG	CO.OH	0.000	HG	DU	0.000
HG	SOL	0.000	CD	CD	0.000	CD	NI	0.000
CD	ZN	0.000	CD	CA	0.000	CD	FE	0.000
CD	CO.OH	0.000	CD	DU	0.000	CD	SOL	0.000
NI	NI	0.000	NI	ZN	0.000	NI	CA	0.000
NI	FE	0.000	NI	CO.OH	0.000	NI	DU	0.000
NI	SOL	0.000	ZN	ZN	0.000	ZN	CA	0.000
ZN	FE	0.000	ZN	CO.OH	0.000	ZN	DU	0.000
ZN	SOL	0.000	CA	CA	0.000	CA	FE	0.000
CA	CO.OH	0.000	CA	DU	0.000	CA	SOL	0.000
FE	FE	0.000	FE	CO.OH	0.000	FE	DU	0.000
FE	SOL	0.000	CO.OH	CO.OH	0.000	CO.OH	DU	0.000
CO.OH	SOL	0.000	DU	DU	0.000	DU	SOL	0.000
SOL	SOL	0.000						

Table S3. Internal probabilities of rotamer changes for protein side-chains

Residue ^a	Probability
ARG	0.381
ASN	0.279
ASP	0.220
CYS	0.048
GLN	0.347
GLU	0.188
HIS	0.168
ILE	0.172
LEU	0.136
LYS	0.532
MET	0.342
PHE	0.203
SER	0.195
THR	0.058
TRP	0.090
TYR	0.190
VAL	0.070

^aGly and Ala are excluded as their side-chain has no flexible bond as well as Pro as movements in the side-chain inevitably accompanies backbone movements.

Table S4. List of PDB entries used in each of the scenario

		<p>*1h8i(1oyt) 1hag(1oyt) *1hah(1oyt) *1hai(1oyt) *1hgt(1oyt) *1hxe(1oyt) *1hx(1oyt) *1k21(1oyt) 1k22(1oyt) 1kts(1oyt) 1ktt(1oyt) *1lhc(1oyt) 1hd(1oyt) *1lhe(1oyt) *1lhf(1oyt) *1lhg(1oyt) *1mu6(1oyt) *1mu8(1oyt) *1muc(1oyt) *1nm6(1oyt) *1no9(1oyt) *1nrr(1oyt) *1nt1(1oyt) 1nzq(1oyt) *1o0d(1oyt) *1o2g(1oyt) *1o5g(1oyt) *1qbv(1oyt) *1sb1(1oyt) 1sfq(1oyt) 1sg8(1oyt) *1sgii(1oyt) 1shh(1oyt) *1s13(1oyt) *1t4u(1oyt) *1t4v(1oyt) *1ta6(1oyt) *1thr(1oyt) *1ths(1oyt) *1tmb(1oyt) *1tmu(1oyt) *1tom(1oyt) *1uma(1oyt) 1vr1(1oyt) *1vzq(1oyt) *1w7g(1oyt) *1way(1oyt) 1xml(1oyt) *1xmn(1oyt) *1ype(1oyt) *1ypg(1oyt) *1ypj(1oyt) *1ypk(1oyt) *1ypl(1oyt) *1ypm(1oyt) *1z71(1oyt) *1zgi(1oyt) *1zgv(1oyt) 1zrb(1oyt) *2a2x(1oyt) *2ank(1oyt) *2ann(1oyt) *2bvr(1oyt) *2bsv(1oyt) 2bx(1oyt) *2c8w(1oyt) *2c8x(1oyt) 2c8y(1oyt) *2c8z(1oyt) 2c90(1oyt) *2c93(1oyt) *2cf8(1oyt) *2cf9(1oyt) *2cn0(1oyt) *2feq(1oyt) *2fes(1oyt) *2gde(1oyt) 2gp9(1oyt) 2od3(1oyt) *4thn(1oyt) *5gd5(1oyt) *7kme(1oyt) 8kme(1oyt) 1akd(1oyt) 1cp4(1p2y) 1d24(1p2y) 1dz6(1p2y) 1dz8(1p2y) 1dz9(1p2y) 1gek(1p2y) 1gem(1p2y) 1gjm(1p2y) 1iwi(1p2y) 1iwj(1p2y) *1iwk(1p2y) 1lw1(1p2y) 1noo(1p2y) 1e76(1p2y) *1pha(1p2y) 1phb(1p2y) 1phd(1p2y) 1phe(1p2y) 1phf(1p2y) *1phg(1p2y) 1re9(1p2y) 185(1p2y) 186(1p2y) 187(1p2y) 188(1p2y) 1uyu(1p2y) 1yre(1p2y) 1rd(1p2y) 2a1m(1p2y) 2cpp(1p2y) 2h7(1p2y) 3cp4(1p2y) 4cp4(1p2y) 5cp4(1p2y) 5cp5(1p2y) 6cpp(1p2y) *7cpp(1p2y) 8cpp(1p2y) *1p5z(1p62) *1p60(1p62) *2no9(1p62) *2noa(1p62) *2noa(1p62) 1s9(1t1) *1s3d(1t1) *1u1d(1u1c) *1u1e(1u1c) *1u1f(1u1c) 2j0f(1luu) 1ob3(1v0p) 1vb6(1v0p) 1v0o(1v0p) *1a4g(1vcj) *1a4q(1vcj) 1b9s(1vcj) *1b9(1vcj) 1b9v(1vcj) *1inf(1vcj) 1inv(1vcj) *1ivb(1vcj) *1nsb(1vcj) 1nscl(1vcj) *1nsd(1vcj) 1e15(1wl1p) 1efr(1wl1p) 1gpf(1wl1p) 1hg(1wl1p) 1h0i(1wl1p) 1o6i(1wl1p) 1ur8(1wl1p) 1wt(1wl1p) *1w1v(1wl1p) 1w1y(1wl1p) *1g3u(1w2g) *1gsi(1w2g) *1mm(1w2g) *1mrs(1w2g) *1n5i(1w2g) *1n5k(1w2g) *1n5l(1w2g) *1n5t(1w2g) *1w2h(1w2g) *1w9s(1xoz) 1tbfl(1xoz) 1xp0(1xoz) 2chm(1xoz) 1fmv(1yv3) 1fmw(1yv3) 1jwy(1yv3) 1jx2(1yv3) 1mma(1yv3) 1mmg(1yv3) 1mmn(1yv3) 1nb4(1yv) 2ax8(1z95) 1byq(2bsm) *1osf(2bsm) 1uy6(2bsm) 1uy7(2bsm) 1uy8(2bsm) 1uy9(2bsm) *1yc(2bsm) 1uyd(2bsm) 1uye(2bsm) *1yc1(2bsm) *1yc2(2bsm) 1yc3(2bsm) 1yc4(2bsm) *1yer(2bsm) *1yes(2bsm) *1yet(2bsm) 2byh(2bsm) *2byi(2bsm) 2bz5(2bsm) 2cs(2bsm) 2ct(2bsm) *2cdd(2bsm) 2fwy(2bsm) *2fwz(2bsm) 2h55(2bsm) 2uwd(2bsm) </p>	<p>6cpp(1p2y) *7cpp(1p2y) 8cpp(1p2y) *1p5z(1p62) *1p60(1p62) *1p61(1p62) *2no9(1p62) *2noa(1p62) 1s9(1t1) *1s3d(1t1) *1u1d(1u1c) *1u1e(1u1c) *1u1f(1u1c) 2j0f(1luu) 1ob3(1v0p) 1vb6(1v0p) 1v0o(1v0p) *1a4g(1vcj) *1a4q(1vcj) 1b9s(1vcj) *1b9(1vcj) 1b9v(1vcj) *1inf(1vcj) 1inv(1vcj) *1ivb(1vcj) *1nsb(1vcj) 1nscl(1vcj) *1nsd(1vcj) 1e15(1wl1p) 1efr(1wl1p) 1gpf(1wl1p) 1hg(1wl1p) 1h0i(1wl1p) 1o6i(1wl1p) 1ur8(1wl1p) 1wt(1wl1p) *1w1v(1wl1p) 1w1y(1wl1p) *1g3u(1w2g) *1gsi(1w2g) *1mm(1w2g) *1mrs(1w2g) *1n5i(1w2g) *1n5k(1w2g) *1n5l(1w2g) *1n5t(1w2g) *1w2h(1w2g) *1w9s(1xoz) 1tbfl(1xoz) 1xp0(1xoz) 2chm(1xoz) 1fmv(1yv3) 1fmw(1yv3) 1jwy(1yv3) 1jx2(1yv3) 1mma(1yv3) 1mmg(1yv3) 1mmn(1yv3) 1nb4(1yv) 2ax8(1z95) 1byq(2bsm) *1osf(2bsm) 1uy6(2bsm) 1uy7(2bsm) 1uy8(2bsm) 1uy9(2bsm) *1yc(2bsm) 1uyd(2bsm) 1uye(2bsm) *1yc1(2bsm) *1yc2(2bsm) 1yc3(2bsm) 1yc4(2bsm) *1yer(2bsm) *1yes(2bsm) *1yet(2bsm) 2byh(2bsm) *2byi(2bsm) 2bz5(2bsm) 2cs(2bsm) 2ct(2bsm) *2cdd(2bsm) 2fwy(2bsm) *2fwz(2bsm) 2h55(2bsm) 2uwd(2bsm) </p>
rDock		<p>1a0u(1g9v) *1a0z(1g9v) 1a3n(1g9v) 1a3o(1g9v) 1b86(1g9v) 1bij(1g9v) 1b20(1g9v) 1bbz(1g9v) 1cls(1g9v) 1dx1(1g9v) 1dxu(1g9v) 1dxv(1g9v) 1fn3(1g9v) 1gbu(1g9v) 1gbv(1g9v) 1gx2(1g9v) 1hab(1g9v) 1hbh(1g9v) 1hdb(1g9v) *1j7s(1g9v) *1j7w(1g9v) *1j7y(1g9v) *1k0y(1g9v) 1kd2(1g9v) 1m9(1g9v) 1nej(1g9v) 1nej(1g9v) 1qsi(1g9v) 1qsh(1g9v) 1qsi(1g9v) 1rps(1g9v) 1rq3(1g9v) *1r4q(1g9v) 1sdc(1g9v) 1sdl(1g9v) 1xt(1g9v) 1xy0(1g9v) *1xye(1g9v) *1xz2(1g9v) *1xz4(1g9v) 1xz5(1g9v) *1xz7(1g9v) 1y09(1g9v) 1y0t(1g9v) 1y0w(1g9v) 1y2z(1g9v) 1y2z(1g9v) 1y5k(1g9v) 1y4q(1g9v) 1y4r(1g9v) 1y4v(1g9v) 1y5f(1g9v) 1y5f(1g9v) 1y5k(1g9v) 1y7c(1g9v) 1y7d(1g9v) 1y7g(1g9v) 1y83(1g9v) 1y85(1g9v) 1y86(1g9v) 1y9h(1g9v) 1yhe(1g9v) 1yhe(1g9v) *2d5z(1g9v) 2d60(1g9v) 2dn2(1g9v) 2hhd(1g9v) 2hhe(1g9v) 6bw6(1g9v) 1fxh(1gm8) 1fxv(1gm8) 1gkf(1gm8) 1gn7(1gm8) 1dx6(1gpk) 1e66(1gpk) *1eve(1gpk) *1gpn(1gpk) 1h22(1gpk) 1h23(1gpk) *1jbj(1gpk) *1ode(1gpk) 1qid(1gpk) 1qie(1gpk) 1qif(1gpk) 1qig(1gpk) 1qih(1gpk) 1qit(1gpk) *1ut6(1gpk) 1vot(1gpk) *1vxr(1gpk) 1w4l(1gpk) 1w6r(1gpk) 1w6r(1gpk) 1w75(1gpk) 1zbg(1gpk) 1zcg(1gpk) 2ack(1gpk) *2c5g(1gpk) *2ck(1gpk) 1w6r(1gpk) 1w75(1gpk) 1zbg(1gpk) *2cmf(1gpk) *1yv3(1hnn) *2an3(1hnn) *2an3(1hnn) *2an4(1hnn) *2g71(1hnn) *2g8m(1hnn) *2f1(1hp0) *1q0n(1hq2) *1hyt(1hww) *1hxx(1hww) *1ps3(1hww) *1r33(1hww) *1r33(1hww) *1r34(1hww) 1tqs(1hww) *1tqt(1hww) 1tqu(1hww) *1tqv(1hww) *1tqv(1hww) *1tqv(1hww) *2alw(1hww) 2f18(1hww) 2f1a(1hww) *2f1b(1hww) *2f1b(1hww) 2f18(1hww) 2f17(1hww) 2f18(1hww) 2f1a(1hww) *2f1b(1hww) *2f1b(1hww) 2f17(1hww) 2f17(1hww) 2f17(1hww) *2f1v(1hww) *1ai9(1ia1) *1aoe(1ia1) *1ia1(1ia1) *1m78(1ia1) *1m7a(1ia1) *2f17(1ig3) *1dd6(1ije) *1ijt(1ije) 1jkh(1ila) *1a50(1k3u) *1c29(1k3u) *1c8v(1k3u) *1c9d(1k3u) *1c9d(1k3u) *1c9e(1k3u) *1fuy(1k3u) *1qop(1k3u) *1tip(1k3u) *1tip(1k3u) *1tip(1k3u) *1ps3(1hww) *1r33(1hww) *1r34(1hww) 1tqs(1hww) *1tqv(1hww) 1tqu(1hww) *1tqv(1hww) *1tqv(1hww) *2alw(1hww) 2f18(1hww) 2f1a(1hww) *2f1b(1hww) *2f17(1hww) *2f17(1hww) 2f17(1hww) 2f17(1hww) 2f17(1hww) *2f1v(1hww) *1ai9(1ia1) *1aoe(1ia1) *1ia1(1ia1) *1m78(1ia1) *1m7a(1ia1) *2f17(1ig3) *1dd6(1ije) *1ijt(1ije) 1jkh(1ila) *1a50(1k3u) *1c29(1k3u) *1c8v(1k3u) *1c9d(1k3u) *1c9d(1k3u) *1c9e(1k3u) *1fuy(1k3u) *1qop(1k3u) *1tip(1k3u) *1tip(1k3u) *1tip(1k3u) *1ao1(1ke5) 1b38(1ke5) *1b39(1ke5) *1ckp(1ke5) *1d8(1ke5) 1e1v(1ke5) 1e1x(1ke5) 1e9h(1ke5) *1fin(1ke5) *1fvt(1ke5) 1g28(1ke5) *1h00(1ke5) *1h01(1ke5) *1h08(1ke5) *1h08(1ke5) 1h0v(1ke5) 1h0w(1ke5) 1h1p(1ke5) *1h1p(1ke5) *1h1q(1ke5) *1h1r(1ke5) *1h1s(1ke5) *1h24(1ke5) *1h25(1ke5) *1h26(1ke5) *1h27(1ke5) 1hck(1ke5) *1h27(1ke5) *1jsw(1ke5) *1ke8(1ke5) *1ke8(1ke5) *1ke8(1ke5) *1ke9(1ke5) 1tsy(1ke5) *1o1q(1ke5) *1o1q(1ke5) *1o1t(1ke5) *1o1u(1ke5) *1oiy(1ke5) *1okv(1ke5) *1okw(1ke5) *1okw(1ke5) *1p2a(1ke5) *1p5e(1ke5) *1pkd(1ke5) *1v0x(1ke5) 1w4l(1ke5) 1w6r(1ke5) 1w6r(1ke5) *1p7(1ke5) 1w75(1ke5) *1w8(1ke5) 1w8(1ke5) *1w98(1ke5) 1wcc(1ke5) 1y8y(1ke5) *1y91(1ke5) *1h1s(1ke5) *1h24(1ke5) *1h25(1ke5) *1h26(1ke5) 1hck(1ke5) 1hcl(1ke5) 1jsv(1ke5) *1ke6(1ke5) *1ke8(1ke5) *1ke9(1ke5) *1o19(1ke5) *1o1q(1ke5) *1o1t(1ke5) *1o1u(1ke5) *1o1y(1ke5) *1okv(1ke5) *1okw(1ke5) *1p2a(1ke5) *1p5e(1ke5) *1pkd(1ke5) 1pw2(1ke5) 1pxi(1ke5) 1pxj(1ke5) *1pxl(1ke5) *1qmz(1ke5) *1urw(1ke5) *1v1k(1ke5) *1vyz(1ke5) *1w0x(1ke5) 1w8c(1ke5) *1w98(1ke5) 1wcc(1ke5) 1y8y(1ke5) *1y91(1ke5) *1ykr(1ke5) *2a0c(1ke5) 2a4l(1ke5) *2b52(1ke5) *2b53(1ke5) *2b54(1ke5) *2btr(1ke5) *2c5n(1ke5) *2c5o(1ke5) *2c5p(1ke5) *2c5y(1ke5) 2c68(1ke5) 2c69(1ke5) 2c6i(1ke5) 2c6k(1ke5) 2c6m(1ke5) *2c6o(1ke5) *2cch(1ke5) *2ch(1ke5) *2cjm(1ke5) *2clx(1ke5) *2duv(1ke5) 2exm(1ke5) *2fdv(1ke5) *2g9x(1ke5) *2uee(1ke5) *1a8g(1kzk) *1a8k(1kzk) *1a94(1kzk) </p>	

		<p>*1fxh(1gm8) *1fxv(1gm8) 1gkf(1gm8) 1gm7(1gm8) *1dx6(1gpk) *1e66(1gpk) *1ea5(1gpk) *1evf(1gpk) *1gp(1gpk) *1h22(1gpk) *1h23(1gpk) *1jib(1gpk) *1odc(1gpk) *1qid(1gpk) *1jic(1gpk) *1qif(1gpk) *1qig(1gpk) *1qih(1gpk) *1qit(1gpk) *1ut6(1gpk) *1vot(1gpk) *1vxr(1gpk) *1w4l(1gpk) *1w6r(1gpk) *1w75(1gpk) *1zgb(1gpk) *1zge(1gpk) *2ack(1gpk) *2c5g(1gpk) *2cek(1gpk) *2cmk(1gpk) *2cmf(1gpk) *1y2z(1hn) *2an3(1hn) *2an4(1hn) *2an5(1hn) *2g71(1hn) *2g8n(1hn) *2ff1(1hp0) *10n(1hq2) *1hyt(1hw) *1hxk(1hw) 1ps1(1hww) *1r33(1hww) *1r34(1hww) *1r35(1hww) *1r36(1hww) *1tq1(1hww) *1tq2(1hww) *1tq3(1hww) *1tq4(1hww) *1tq5(1hww) *2f1a(1hww) *2f1b(1hww) *2f1c(1hww) *2f1d(1hww) *2f1e(1hww) *2f1f(1hww) *2f1g(1hww) *2f1h(1hww) *2f1i(1hww) *2f1j(1hww) *1m7a(1ial) *2fl7(1ig3) 1dd6(1je) *1ji(1ije) 1jkh(1jla) *1a50(1k3u) *1c29(1k3u) 1c8v(1k3u) *1c9d(1k3u) *1cw2(1k3u) 1cx9(1k3u) *1fuy(1k3u) *1pok(1k3u) *1jp1(1k3u) *1wb1(1k3u) *2trs(1k3u) 2tzy(1k3u) *1aq1(1ke5) *1b38(1ke5) *1b39(1ke5) *1ckp(1ke5) *1di8(1ke5) 1e1v(1ke5) *1e1x(1ke5) *1e9h(1ke5) *1f1n(1ke5) *1f1t(1ke5) 1gz2(1ke5) *1h0n(1ke5) *1h0s(1ke5) *1e9h(1ke5) *1f1n(1ke5) *1f1t(1ke5) 1gz2(1ke5) *1h0n(1ke5) *1h0s(1ke5) 1h0v(1ke5) *1h0w(1ke5) *1h1p(1ke5) *1h1q(1ke5) *1h1r(1ke5) *1h1s(1ke5) *1h24(1ke5) *1h25(1ke5) *1h26(1ke5) *1h27(1ke5) 1hek(1ke5) 1hcl(1ke5) *1jsv(1ke5) *1ke6(1ke5) *1ke7(1ke5) *1ke8(1ke5) *1ke9(1ke5) *1o19(1ke5) *1oiq(1ke5) *1oit(1ke5) *1oiu(1ke5) *1oiy(1ke5) 1okv(1ke5) 1okw(1ke5) *1p2a(1ke5) *1p5e(1ke5) *1pkd(1ke5) 1pw2(1ke5) *1pxi(1ke5) *1pxj(1ke5) *1pxl(1ke5) 1qmz(1ke5) *1urw(1ke5) *1vk(1ke5) *1vyt(1ke5) *1w8c(1ke5) *1w8e(1ke5) *1w98(1ke5) *1wec(1ke5) *1y8y(1ke5) *1y91(1ke5) *1ykr(1ke5) *2a0c(1ke5) *2a4l(1ke5) *2b52(1ke5) *2b53(1ke5) 2b54(1ke5) *2btr(1ke5) 2c5n(1ke5) *2c5p(1ke5) *2c5v(1ke5) 2c68(1ke5) 2c69(1ke5) *2c6i(1ke5) *2c6k(1ke5) *2c6l(1ke5) *2c6m(1ke5) *2c6o(1ke5) 2cch(1ke5) *2cjm(1ke5) *2clx(1ke5) *2duv(1ke5)</p>
FLFP	FlexAID	<p>*1dx6(1gpk) *1e66(1gpk) *1ea5(1gpk) *1eve(1gpk) *1gp(1gpk) *1h22(1gpk) *1h23(1gpk) *1jib(1gpk) *1odc(1gpk) *1qid(1gpk) *1qie(1gpk) *1qif(1gpk) *1qif(1gpk) *1qig(1gpk) *1qih(1gpk) *1ut6(1gpk) *1vot(1gpk) *1vxr(1gpk) *1w4l(1gpk) *1w6r(1gpk) *1w75(1gpk) *1zgb(1gpk) *1zge(1gpk) *2ack(1gpk) *2c5g(1gpk) *2cek(1gpk) *2cmk(1gpk) *2cmf(1gpk) *1y2z(1hn) *2an3(1hn) *2an4(1hn) *2an5(1hn) *2g71(1hn) *2g8n(1hn) *2ff1(1hp0) *1qon(1h2g) *1hyt(1hw) *1hxk(1hw) 1ps3(1hww) *1r33(1hww) *1r34(1hww) *1tq1(1hww) *1tq2(1hww) *1tq3(1hww) *1tq4(1hww) *1tq5(1hww) *2adw(1hww) 2f18(1hww) *2f1a(1hww) *2f1b(1hww) *2f1d(1hww) *2f1f(1hww) *2f1g(1hww) *2f1h(1hww) *2f1i(1hww) *2f1j(1hww) *1jih(1jla) *1a50(1k3u) *1c29(1k3u) 1c8v(1k3u) *1c9d(1k3u) *1cw2(1k3u) 1cx9(1k3u) *1fuy(1k3u) *1qop(1k3u) *1tjp(1k3u) *1wbi(1k3u) *1wbr(1k3u) *1wbs(1k3u) *1wbt(1k3u) 1cyt(1k3u) *1wbu(1k3u) *1wby(1k3u) *1wca(1k3u) *1wcb(1k3u) *1wcc(1k3u) *1wcd(1k3u) *1wce(1k3u) *1wcf(1k3u) *1wch(1k3u) *1wci(1k3u) *1wck(1k3u) *1wcl(1k3u) 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			1wbn(1ywr) *1wbo(1ywr) 1wbs(1ywr) 1wbt(1ywr) 1wbu(1ywr) 1wbw(1ywr) *1wfc(1ywr) *1yqf(1ywr) 1zz2(1ywr) 1zzl(1ywr) *2bak(1ywr) *2bal(1ywr) 2gfs(1ywr) 2ghf(1ywr) *2ghm(1ywr) *2gtn(1ywr) 2ihf(1ywr) *2axs(1z95) *2fpz(2bm2) *1ia8(2br1) *1nvq(2br1) *1nvr(2br1) *1nvs(2br1) *1zlt(2br1) *1ys(2br1) *2brb(2br1) *2brg(2br1) *2brh(2br1) *2brm(2br1) *2bro(2br1) *2c3l(2br1) 2cgu(2br1) *2cgw(2br1) 2gx(2br1) *2hog(2br1) *ibyg(2bsm) *1osf(2bsm) *1uy6(2bsm) *1uy7(2bsm) *1uy8(2bsm) *1uy9(2bsm) *1uyd(2bsm) *1uyd(2bsm) *1uye(2bsm) *1uyf(2bsm) *1uyg(2bsm) *1uyh(2bsm) *1uyi(2bsm) *1uyk(2bsm) *1uyl(2bsm) *1yc1(2bsm) *1yc3(2bsm) *1yc4(2bsm) *1yer(2bsm) *1yes(2bsm) *1yet(2bsm) *2bt0(2bsm) *2byh(2bsm) *2byi(2bsm) *2bz5(2bsm) *2ccs(2bsm) *2cct(2bsm) *2dd(2bsm) *2fwy(2bsm) *2fwz(2bsm) *2h55(2bsm) *2uwd(2bsm)	
NATIVE FLRP	FlexAID	FlexAID	1b8v 1bq4 *1br5 *1bzs *1e8z *1eqc 1hon 1ikg *1it8 *1j1s *1js0 1lee 1if *1lm *1lo0 1nx3 1ra1 *1s5o *1tqm 1uak *1v2g 1v8l *1wk9 1wpr 1x6n 1xcw *1y2w 1yon 1yxt 1z3w 1zg3 *2bf6 *2bu7 2c05 2d5a 2e15 2ejt 2oxd 2uyq *2x0u 2x1t 2z1s 2zlz *2y1 3aar *3acd 3adp 3baz 3cj7 3csj 3cuf *3d5i 3eha 3erk 3go6 3jyn *3sl1 4a3h *7jdw	1b8v 1bq4 *1br5 *1bzs *1e8z *1eqc 1hon 1ikg *1it8 *1j1s *1js0 1lee 1if *1lm *1lo0 1nx3 1ra1 *1s5o *1tqm 1uak *1v2g 1v8l *1wk9 1wpr 1x6n 1xcw *1y2w 1yon 1yxt 1z3w 1zg3 *2bu7 2d5a 2e15 2ejt 2oxd 2x1t 2z1s 2zlz *2y1 3aar *3acd 3adp 3baz 3cj7 3csj 3cuf *3d5i 3eha 3erk 3go6 3jyn *3sl1 4a3h *7jdw
		Vina	*1b8v 1bq4 *1br5 *1bzs *1e8z *1eqc 1hon *1ikg *1it8 *1j1s *1js0 *1lee *1lm *1lo0 *1nx3 *1ra1 *1s5o 1tqm *1uak *1v2g 1v8l *1wk9 1wpr *1xcw *1y2w *1yon *1yxt 1z3w 1zg3 *2bf6 *2c05 *2d5a 2e15 *2ejt 2oxd 2uyq *2x0u *2x1t 2z1s 2zlz 2zy1 3aar *3acd *3adp *3baz 3cj7 3csj *3cuf *3d5i *3eha 3erk *3go6 *3jyn *3sl1 *4a3h *7jdw	*1b8v 1bq4 *1br5 *1bzs *1e8z *1eqc 1hon *1ikg *1it8 *1j1s 1js0 *1lee *1lm *1lo0 *1nx3 *1ra1 *1s5o *1tqm *1uak *1v2g 1v8l *1wk9 *1wpr *1xcw *1y2w *1yon *1yxt 1z3w 1zg3 *2bu7 2d5a 2e15 *2ejt 2oxd *2ejt 2oxd *2x1t 2z1s 2zlz 2zy1 3aar *3acd *3adp *3baz 3cj7 3csj *3cuf *3d5i *3eha *3erk *3go6 *3jyn *3sl1 *4a3h *7jdw
		FlexX	1b8v 1bq4 1br5 *1bzs 1e8z *1eqc 1hon 1ile *1ikg *1it8 *1j1s 1js0 *1lee *1lm *1lo0 *1nx3 *1ra1 *1rbp *1s5o *1tqm *1uak *1v2g 1v8l 1wk9 *1wpr 1x6n 1xcw 1y2w 1yon 1yxt 1z3w 1zg3 *2bf6 2bu7 2d5a 2e15 *2ejt 2oxd *2x1t 2z1s 2zlz *2y1 3aar *3acd *3adp *3baz 3cj7 3csj *3cuf *3d5i *3sl1 4a3h *7jdw	1b8v 1bq4 1br5 *1bzs 1e8z *1eqc 1hon *1ikg *1it8 *1j1s 1js0 *1lee *1lm *1lo0 *1nx3 *1ra1 *1s5o *1tqm *1uak *1v2g 1v8l 1wk9 *1wpr 1x6n 1xcw 1y2w 1yon 1yxt 1z3w 1zg3 *2bu7 2d5a 2e15 *2ejt 2oxd *2x1t 2z1s 2zlz 2zy1 3aar *3acd *3adp *3baz 3cj7 3csj *3cuf *3d5i *3eha 3erk 3go6 3jyn *3sl1 4a3h *7jdw
		rDock	1b8v 1bq4 *1br5 1bzs *1e8z *1eqc *1hon *1ile *1ikg *1it8 *1j1s *1js0 *1lee *1if 1lm *1lo0 1nx3 *1ra1 *1rbp *1s5o *1tqm *1uak *1v2g 1v8l 1wk9 1wpr *1x6n *1xcw *1y2w 1yon *1yxt *1z3w *1zg3 *2bu7 2d5a 2e15 2ejt 2oxd *2x1t 2z1s *2zlz 2zy1 3aar *3acd *3adp *3baz 3cj7 3csj *3cuf *3d5i *3eha 3erk 3go6 *3jyn *3sl1 *4a3h *7jdw	1b8v 1bq4 *1br5 1bzs *1e8z *1eqc *1hon *1ikg *1it8 *1j1s 1js0 *1lee *1if 1lm *1lo0 1nx3 *1ra1 *1s5o *1tqm *1uak *1v2g 1v8l 1wk9 1wpr *1x6n *1xcw *1y2w *1yon *1yxt *1z3w *1zg3 *2bu7 2d5a 2e15 *2ejt 2oxd *2x1t 2z1s *2zlz 2zy1 3aar *3acd *3adp *3baz 3cj7 3csj *3cuf *3d5i *3eha 3erk 3go6 *3jyn *3sl1 *4a3h *7jdw
HAPPY FLRP	FlexAID	FlexAID	1czl(1eqc) 1e8y(1e8z) 1erk(3erk) 1gpi(1z3w) *1i76(1bzs) *1iq8(1it8) *1j1q(1j1s) 1j4b(1loo) 1jam(2oxd) *1jrl(1v2g) *1jsm(1js0) *1kxo(1lnm) *1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1py3(3d5i) 1rte(1br5) *1sll(3sli) 1tqi(1tqm) *1wka(1wk9) 1xqz(1yx1) 1y2v(1y2w) 1zhf(1zg3) 2btz(2bu7) 2dul(2ejt) 2ebg(2ei5) 2j1x(2x0u) 2jdw(7jdw) *2uyo(2uyq) *2vk5(2bf6) 2zco(2zy1) 3acb(3acd) 3pte(1ikg) 3wrp(1wpr) 4pgm(1bq4)	1czl(1eqc) 1erk(3erk) *1i76(1bzs) *1j1q(1j1s) *1jrl(1v2g) 1kxo(1lnm) *1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1rte(1br5) *1sll(3sli) 1tqi(1tqm) 2dul(2ejt) 2jdw(7jdw) *2zco(2zy1) 3acb(3acd) 3pte(1ikg) 3wrp(1wpr)
		Vina	16gs(3csj) *1a3h(4a3h) 1adi(1hon) 1b8p(1b8v) *1bsi(1xcw) 1czl(1eqc) 1e8y(1e8z) 1erk(3erk) 1gpi(1z3w) 1i76(1bzs) *1iq8(1it8) *1j1q(1j1s) 1j4b(1loo) 1jam(2oxd) *1jrl(1v2g) *1jsm(1js0) *1kxo(1lnm) *1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1py3(3d5i) 1rte(1br5) *1sll(3sli) 1kxo(1lnm) 1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1py3(3d5i) 1rte(1br5) 1tqi(1tqm) *1wka(1wk9) 1xqz(1yx1) 1y2v(1y2w) 1zhf(1zg3) 2btz(2bu7) 2dul(2ejt) 2exo(3uaf) 2jdw(7jdw) *2x16(2x1t) 2zco(2zy1) *3acb(3acd) 3acb(3acd) 3ado(3adp) *3ba1(3baz) 3cj1(3cj7) 3pq(1lee) 3go7(3go6) 3jyl(3jyn) *3pte(1ikg) 3wrp(1wpr) 4pgm(1bq4) 5df(1ra1)	1czl(1eqc) 1erk(3erk) 1i76(1bzs) 1j1q(1j1s) *1jrl(1v2g) 1kxo(1lnm) 1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1rte(1br5) *1sll(3sli) 1tqi(1tqm) 2dul(2ejt) 2jdw(7jdw) *2zco(2zy1) 3acb(3acd) *3pte(1ikg) 3wrp(1wpr)
		FlexX	1brp(1rbp) 1czl(1eqc) 1erk(3erk) 1gpi(1z3w) *1i76(1bzs) *1iq8(1it8) *1j1q(1j1s) 1j4b(1loo) 1jam(2oxd) *1jrl(1v2g) *1jsm(1js0) *1kxo(1lnm) *1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1py3(3d5i) 1rte(1br5) *1sll(3sli) 1tqi(1tqm) *1wka(1wk9) 1xqz(1yx1) 1y2v(1y2w) 1zhf(1zg3) 2btz(2bu7) 2dul(2ejt) 2exo(3uaf) 2jdw(7jdw) *2x16(2x1t) 2zco(2zy1) *3acb(3acd) 3ba1(3baz) 3jyl(3jyn) 3pte(1ikg) 3wrp(1wpr) 5df(1ra1)	1czl(1eqc) 1erk(3erk) 1i76(1bzs) *1j1q(1j1s) *1jrl(1v2g) 1kxo(1lnm) *1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1rte(1br5) *1sll(3sli) 1tqi(1tqm) *2dul(2ejt) 2jdw(7jdw) *2zco(2zy1) 3acb(3acd) *3pte(1ikg) 3wrp(1wpr)
		rDock	*16gs(3csj) *1a3h(4a3h) 1adi(1hon) 1alb(1if) 1brq(1rbp) *1bsi(1xcw) 1czl(1eqc) 1e8y(1e8z) 1erk(3erk) 1gpi(1z3w) 1i76(1bzs) *1iq8(1it8) *1j1q(1j1s) 1j4b(1loo) 1jam(2oxd) *1jrl(1v2g) *1jsm(1js0) *1kxo(1lnm) *1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) *1py3(3d5i) 1rte(1br5) *1sll(3sli) 1nx2(1nx3) 1njz(2zlz) 1py3(3d5i) 1rte(1br5) 1s0d(1i1e) *1sll(3sli) 1tqi(1tqm) *1wka(1wk9) 1xqz(1yx1) 1y2v(1y2w) 1zhf(1zg3) 2btz(2bu7) 2dul(2ejt) 2exo(3uaf) 2jdw(7jdw) *2x16(2x1t) 2zco(2zy1) *3acb(3acd) 3ba1(3baz) 3zco(2zy1) 3acb(3acd) 3cj1(3cj7) 3pq(1lee) 3go7(3go6) 3jyl(3jyn) *3pte(1ikg) 3wrp(1wpr) 4pgm(1bq4) *5df(1ra1)	1czl(1eqc) 1erk(3erk) 1i76(1bzs) *1j1q(1j1s) *1jrl(1v2g) 1kxo(1lnm) 1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1rte(1br5) *1sll(3sli) 1tqi(1tqm) 2dul(2ejt) 2jdw(7jdw) *2zco(2zy1) 3acb(3acd) 3pte(1ikg) 3wrp(1wpr)
FLFP	FlexAID	FlexAID	*1czl(1eqc) *1e8y(1e8z) 1erk(3erk) 1gpi(1z3w) 1i76(1bzs) *1iq8(1it8) *1j1q(1j1s) 1j4b(1loo) 1jam(2oxd) *1jrl(1v2g) *1jsm(1js0) *1kxo(1lnm) *1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1py3(3d5i) 1rte(1br5) *1sll(3sli) 1tqi(1tqm) *1wka(1wk9) 1xqz(1yx1) 1y2v(1y2w) 1zhf(1zg3) 2btz(2bu7) 2dul(2ejt) 2exo(3uaf) 2jdw(7jdw) *2x16(2x1t) 2zco(2zy1) *3acb(3acd) 3acb(3acd) 3ado(3adp) *3ba1(3baz) 3cj1(3cj7) 3pq(1lee) 3jyl(3jyn) 3pte(1ikg) 3wrp(1wpr) 4pgm(1bq4)	*1czl(1eqc) 1erk(3erk) 1i76(1bzs) *1j1q(1j1s) *1jrl(1v2g) *1kxo(1lnm) *1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1rte(1br5) *1sll(3sli) 1tqi(1tqm) 2dul(2ejt) *2jdw(7jdw) *2zco(2zy1) 3acb(3acd) 3pte(1ikg) 3wrp(1wpr)
		Vina	*1a3h(4a3h) *1b8p(1b8v) *1bsi(1xcw) *1czl(1eqc) 1e8y(1e8z) 1erk(3erk) 1gpi(1z3w) 1gqv(2c05) 1i76(1bzs) *1j1q(1j1s) 1j4b(1loo) 1jks(3eha) *1jrl(1v2g) *1jsm(1js0) 1ks9(1yon) *1kxo(1lnm) 1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1rte(1br5) 1sll(3sli) 1tqi(1tqm) 1ua1(1uak) *1wka(1wk9) 1x6l(1x6n) 1xqz(1yx1) 1zhf(1zg3) 2btz(2bu7) 2d59(2d5a) *2dul(2ejt) 2exo(3uaf) *2jdw(7jdw) 2uyo(2uyq) *2vk5(2bf6) *2zco(2zy1) 3acb(3acd) *3ado(3adp) *3ba1(3baz) 3cj1(3cj7) 3pq(1lee) 3jyl(3jyn) 3pte(1ikg) 3wrp(1wpr) 5df(1ra1)	*1czl(1eqc) 1erk(3erk) 1i76(1bzs) *1j1q(1j1s) *1jrl(1v2g) *1kxo(1lnm) 1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1rte(1br5) *1sll(3sli) 1tqi(1tqm) *2dul(2ejt) *2jdw(7jdw) *2zco(2zy1) 3acb(3acd) 3pte(1ikg) 3wrp(1wpr)
	rDock	rDock	16gs(3csj) *1a3h(4a3h) 1adi(1hon) 1alb(1if) 1brq(1rbp) *1bsi(1xcw) 1czl(1eqc) 1e8y(1e8z) 1erk(3erk) 1gpi(1z3w) 1i76(1bzs) *1iq8(1it8) *1j1q(1j1s) 1jks(3eha) *1jrl(1v2g) *1jsm(1js0) 1kxo(1lnm) 1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1py3(3d5i) 1rte(1br5) 1s0d(1i1e) *1sll(3sli) 1tqi(1tqm) *1wka(1wk9) 1xqz(1yx1) 1y2v(1y2w) 1zhf(1zg3) 2btz(2bu7) 2dul(2ejt) 2exo(3uaf) 2jdw(7jdw) *2x16(2x1t) 2zco(2zy1) *3acb(3acd) 3ba1(3baz) 3zco(2zy1) 3acb(3acd) 3cj1(3cj7) 3pq(1lee) 3jyl(3jyn) 3pte(1ikg) 3wrp(1wpr) 4pgm(1bq4) 5df(1ra1)	1czl(1eqc) 1erk(3erk) 1i76(1bzs) *1j1q(1j1s) *1jrl(1v2g) 1kxo(1lnm) 1nm8(1s5o) 1nx2(1nx3) 1njz(2zlz) 1rte(1br5) *1sll(3sli) 1tqi(1tqm) 2dul(2ejt) 2jdw(7jdw) *2zco(2zy1) 3acb(3acd) 3pte(1ikg) 3wrp(1wpr)

			1tqi(1tqm) *1uaj(1uak) 1v8i(1v8l) 1x6l(1x6n) 1xqz(1yxt) *1y2v(1y2w) 1zhf(1zg3) 2btz(2bu7) 2dul(2ejt) 2ebg(2ei5) *2exo(3cu) 2jdw(7jdw) 2x16(2x1) 2zco(2zy1) *3acb(3acd) 3ba1(3baz) 3cj1(3cj7) 3f9q(1lee) 3go7(3go6) 3jyl(3jyn) 3pte(1ikg) 3wrp(1wrp) 4pgm(1bq4) 5dfrr(1ra1)	
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^aEntries that are marked with an asterisk represent successes according to Figures 4 and 6.

^bThe PDB code in parenthesis represents the native protein structure associated to the non-native structure used for the simulation.