Supplement to "Relationship between Hot Spot Residues and Ligand Binding Hot Spots in Protein-Protein Interfaces"

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Table S1: End group atom from the standard PDB used to represent each of the 18 amino acids (not including alanine and glycine).

Residue	**End group atom**
Arg	CZ
Asn	ND2
Asp	OD1
Cys	SG
Gln	CD
Glu	CD
His	CG
Ile	CD1
Leu	CG
Lys	NZ
Met	CE
Phe	CG
Pro	CG
Ser	OG
Thr	OG1
Trp	CH2
Tyr	OH
Val	CG1

Table S2: Identity, change in Gibbs free energy of the complex or energy class, and density correlation for all hot spot residues within the data set.

PDB(chain)	Residue	Energy ($\frac{kcal}{mol}$ or class)	Density Correlation
1a4y(A)	Tyr434	3.3	19899
1a4y(A)	Asp435	3.5	10886
1brs(D)	Tyr29	3.4	14233
1brs(D)	Asp35	4.5	17075
1brs(D)	Asp39	7.7	6733
1bxl(B)	Val574	S	9164
1bxl(B)	Leu578	S	19704
1bxl(B)	Ile581	S	18430
1bxl(B)	Ile585	S	11126
1cbw(D)	Lys15	2.0	9323
1cdl(E)	Trp800	S	14951
1cdl(E)	Ile810	S	5214
1cdl(E)	Leu813	S	3951
1dfj(I)	Trp259	2.2	0
1dfj(I)	Tyr430	5.9	8798
1dfj(I)	Asp431	3.6	10590
1dfj(I)	Tyr433	2.6	613
1dva(X)	Leu2	S	26103
1dva(X)	Trp11	S	8656
1dva(X)	Tyr12	S	9656
1dva(X)	Phe15	S	5016
1ebp(C)	Trp13	S	1805
1f47(A)	Ile8	2.5	28637
1f47(A)	Phe11	2.5	3859
1f47(A)	Leu12	2.3	976
1nfi(F)	Tyr181	S	3646
1osg(G)	Asp26	S	65
1osg(G)	Leu28	S	29450
1osg(G)	Val29	S	6012
1osg(G)	Arg30	S	11395
1osg(G)	Val33	S	0
1ycr(B)	Phe19	S	23625
1ycr(B)	Trp23	S	33083
1ycr(B)	Leu26	2.39	13361
2ptc(I)	Lys15	10	7051
3brv(A,C)	Trp739	S	1468
3brv(A,C)	Trp741	S	6658

Table S3: Identity, change in Gibbs free energy of the complex or energy class, and density correlation for all hot spot residues within the data set.

PDB(chain)	Residue	Energy ($\frac{kcal}{mol}$ or class)	Density Correlation
1a4y(A)	Trp261	0.10	0
1a4y(A)	Trp263	1.20	0
1a4y(A)	Ser289	0.00	0
1a4y(A)	Trp318	1.50	0
1a4y(A)	Lys320	-0.30	0
1a4y(A)	Glu344	0.20	0
1a4y(A)	Trp375	1.00	0
1a4y(A)	Glu401	0.90	0
1a4y(A)	Tyr437	0.80	2108
1a4y(A)	Ile459	0.70	43
1brs(D)	Thr42	1.80	78
1brs(D)	Glu76	1.30	0
1bxl(B)	Arg576	N	0
1bxl(B)	Ile580	N	0
1bxl(B)	Asp584	N	0
1cbw(D)	Thr11	0.20	0
1cbw(D)	Arg17	0.50	442
1cbw(D)	Arg39	0.20	0
1cdl(E)	Lys799	N	0
1cdl(E)	Lys802	N	0
1cdl(E)	Arg808	N	0
1dfj(I)	Glu202	1.0	0
1dfj(I)	Trp257	1.3	0
1dfj(I)	Glu283	1.3	0
1dfj(I)	Ser285	0.8	0
1dfj(I)	Trp314	1.0	0
1dfj(I)	Lys316	1.3	0
1dfj(I)	Glu397	1.3	0
1dfj(I)	Arg453	0.8	0
1dfj(I)	Ile455	0.3	3
1dva(X)	Arg7	N	7
1dva(X)	Val8	N	299
1dva(X)	Asp9	N	75
1ebp(C)	Leu11	N	316
1ebp(C)	Thr12	N	0
1f47(A)	Asp4	0.7	0
1f47(A)	Tyr5	0.9	0
1f47(A)	Leu6	0.9	12730
1f47(A)	Gln15	0.0	0
1lqb(D)	Met561	N	0
1lqb(D)	Leu562	N	1896
1nfi(F)	Cys215	N	3832
1osg(G)	Leu27	N	3
1osg(G)	His31	N	1
1ycr(B)	Glu17	0.14	0
1ycr(B)	Thr18	0.58	0
1ycr(B)	Ser20	-0.43	0
1ycr(B)	Leu22	0.37	0
1ycr(B)	Leu25	0.30	0
1ycr(B)	Pro27	-1.26	548
1ycr(B)	Glu28	-0.36	0
3brv(A,C)	Leu737	N	89
3brv(A,C)	Leu742	N	441.5