

Dynamic Allostery based molecular workings of Kinase:Peptide complexes

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Fig S2: Comparison of the RMSF (snapshots over simulation time) with the B-factors obtained from the crystal structures of the IP20 and Phospholamban bound structures of PKA. Simulations provide the phospholamban peptide the desired conformational flexibility as is already reported in its crystal structure.

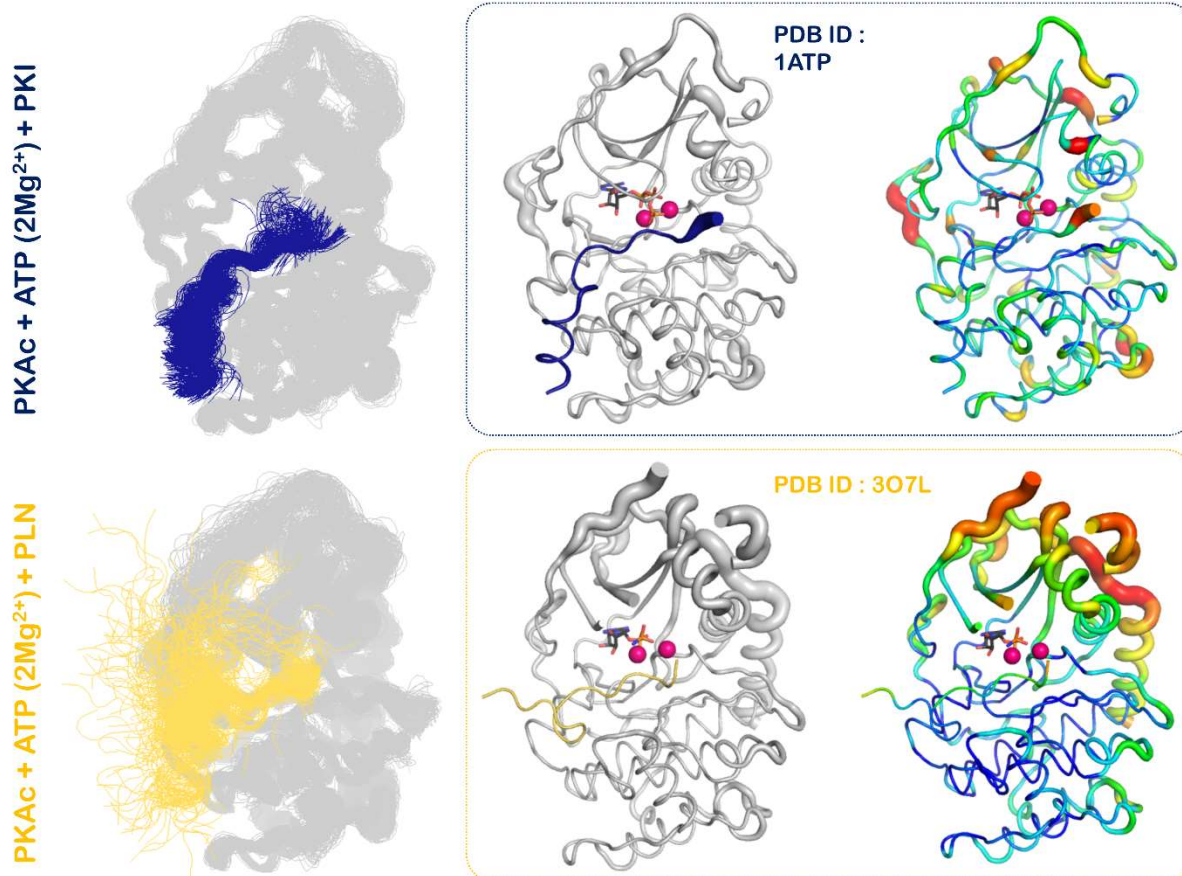


Fig S3: Contact Maps for the seven Kinase:Peptide complexes obtained over the 5.4 μ sec simulation time

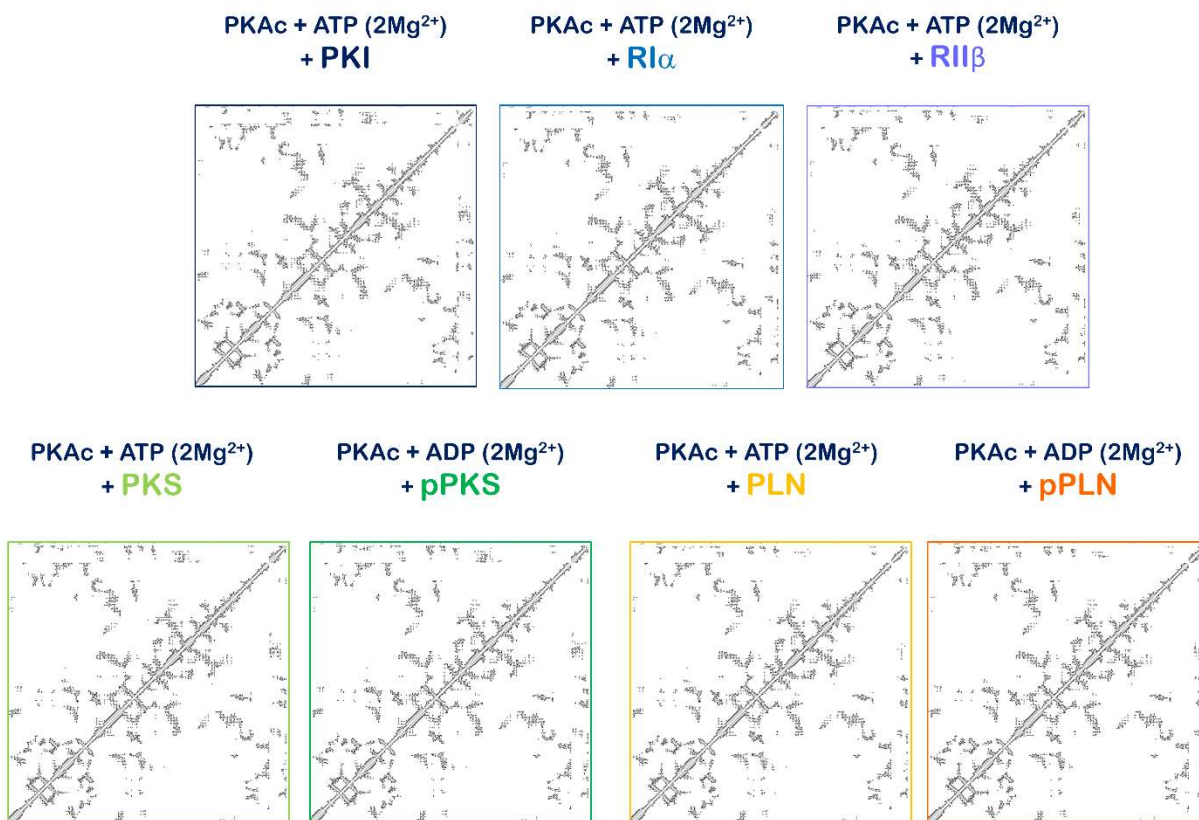


Fig S4: Mutual Information Matrices for the seven Kinase:Peptide complexes obtained over the 5.4 μ sec simulation time

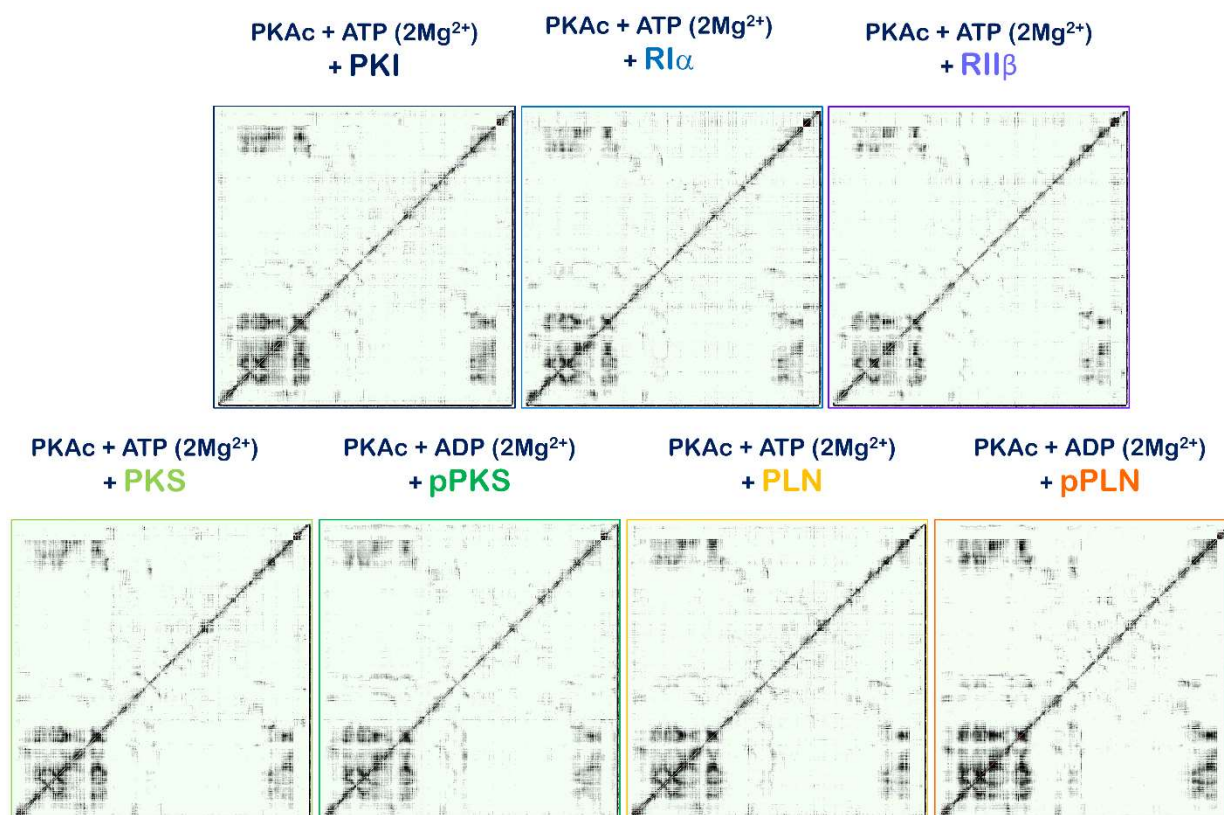


Fig S5: The community network at the hydrophobic core varies in the seven Kinase:Peptide complexes in accordance with the signatures of their molecular recognition.

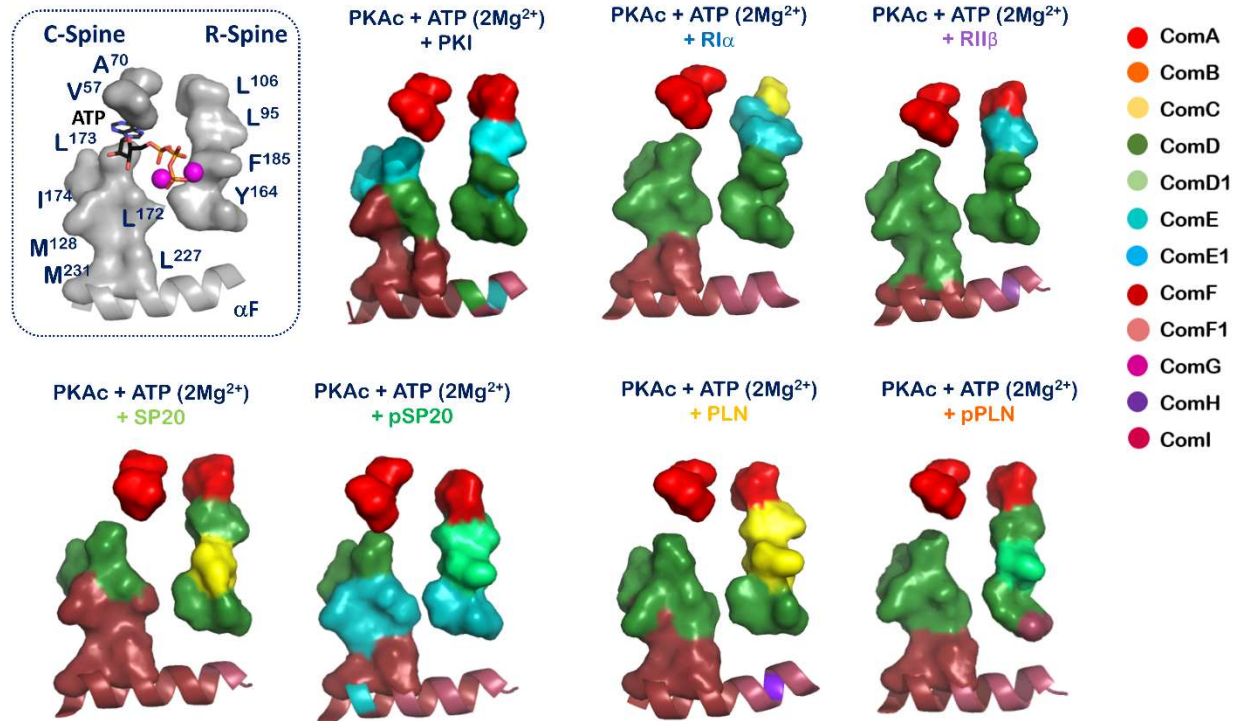


Fig S6: Community Maps of the three Kinase:inhibitor complexes showing the community dynamic behavior of R133 and D328 residues.

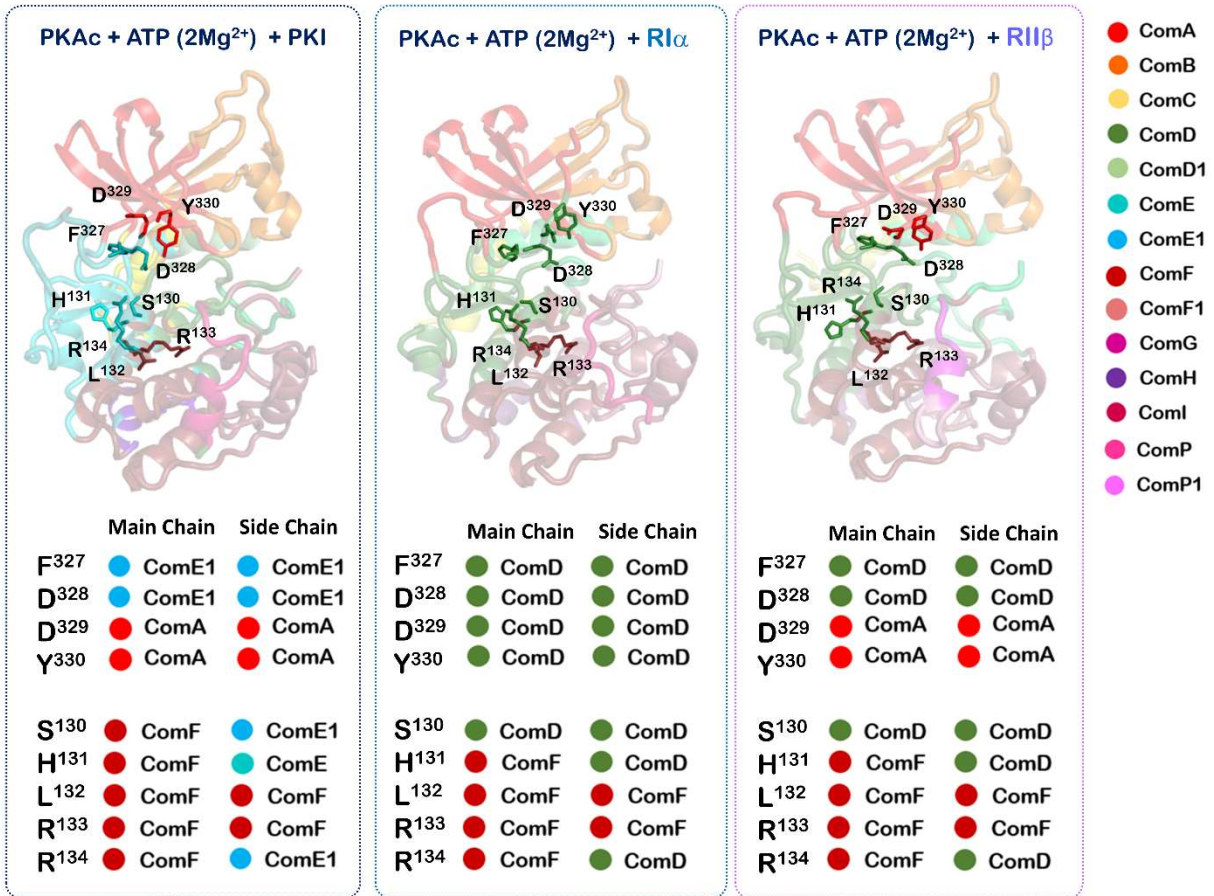


Fig S7: Free energy landscape of the MD simulations of the seven Kinase:Peptide complexes. Dynamics is measured for the peptide in the complex. Dynamics measured between P-site (Ser/Ala etc)- Calpha of the peptide and D166- Calpha of the YRD motif alongside between R-Calpha and E170-Calpha of the activation segment.

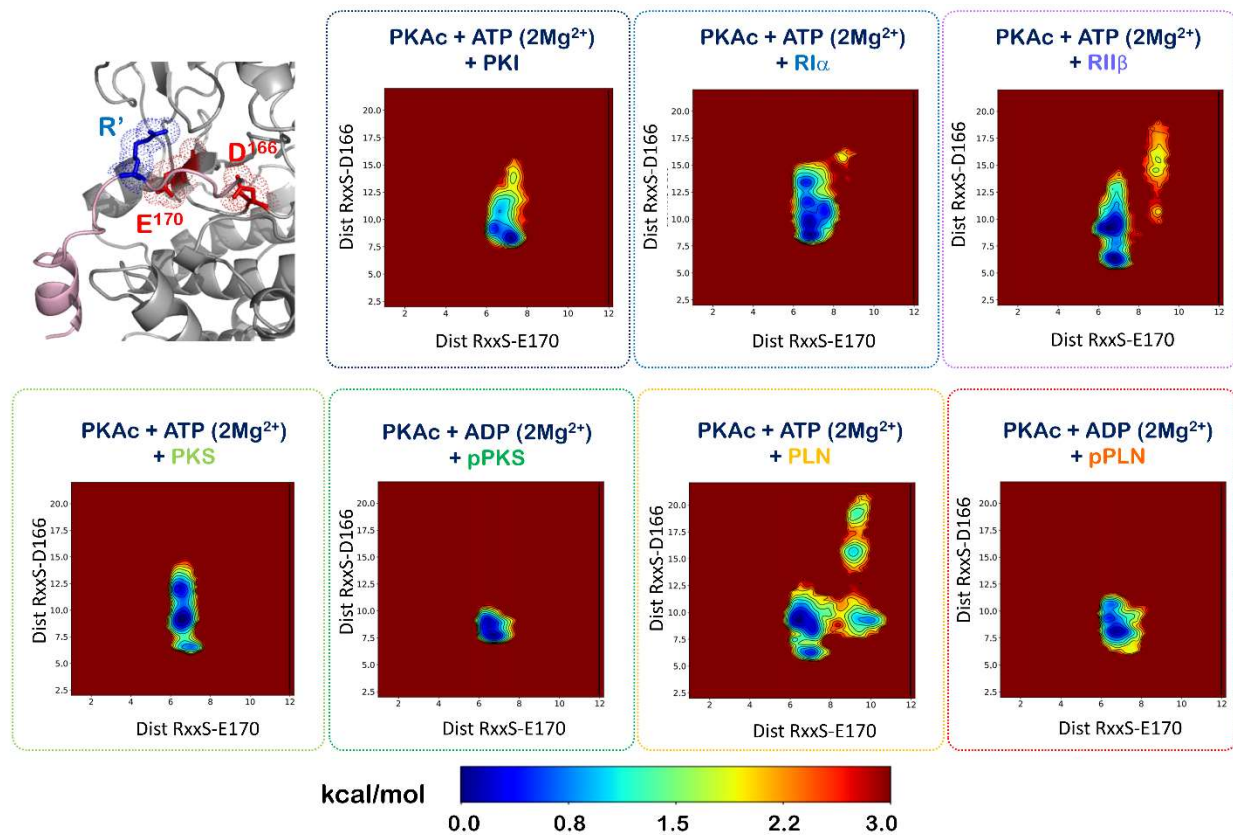


Table S1: Bridging residues for community maps of PKAc: PKI complex

Number	Residue	Main Chain	Side Chain
1	SER 34	COM A	COM C
2	SER 35	COM A	COM C
3	LYS 72	COM A	COM B
4	GLU 86	COM B	COM D2
5	LYS 92	COM B	COM A
6	ARG 93	COM C	COM E
7	LEU 95	COM C	COM E
8	GLN 96	COM C	COM B
9	PHE 100	COM C	COM E
10	MET 118	COM A	COM B
11	ALA 124	COM E	COM E1
12	SER 130	COM F	COM E1
13	HIS 131	COM F	COM E
14	ARG 134	COM F	COM E1
15	PHE 154	COM E	COM D
16	LEU 157	COM D1	COM D
17	HIS 158	COM D	COM H
18	ILE 163	COM D	COM D1
19	ARG 165	COM D	COM D1
20	LYS 168	COM F	COM D
21	VAL 182	COM E	COM D
22	THR 183	COM E	COM D
23	PHE 185	COM D	COM E
24	ARG 190	COM D1	COM C
25	ARG 194	COM D1	COM F1
26	T2P 197	COM F1	COM D1
27	THR 201	COM F1	COM D
28	TYR 204	COM F1	COM F
29	ASN 216	COM D1	COM F1
30	LYS 217	COM D	COM F1
31	ASP 220	COM F	COM F1
32	TRP 221	COM F	COM E
33	TRP 222	COM F	COM F1
34	ALA 223	COM F	COM D
35	ASN 271	COM F	COM H
36	LEU 273	COM F1	COM F
37	LYS 292	COM H	COM E
38	HIS 294	COM F	COM H
39	THR 299	COM E	COM F
40	TYR 306	COM E	COM C
41	PRO 313	COM F	COM E
42	THR 324	COM E1	COM A

43	GLU 334	COM B	COM A
44	ILE 335	COM B	COM A
45	THR 354	COM D	COM A
46	ILE 360 (PKI)	COM P	COM F
47	ARG 368 (PKI)	COM D	COM E1
48	ASN 360 (PKI)	COM F1	COM F
49	ILE 371 (PKI)	COM D	COM F1

RES 34



RES 35



RES 72



RES 86



RES 92



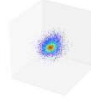
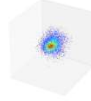
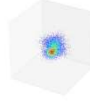
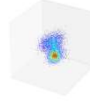
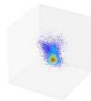
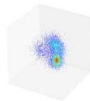
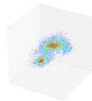
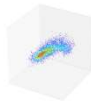
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RES 95



RES 96



RES 100



RES 118



RES 124



RES 130



RES 131



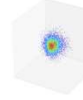
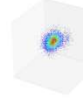
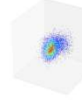
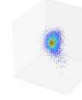
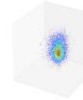
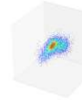
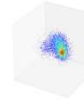
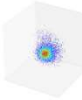
RES 134



RES 154



RES 157



RES 158



RES 163



RES 165



RES 168



RES 182



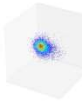
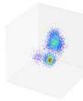
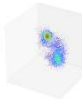
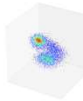
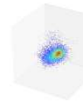
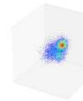
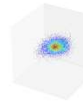
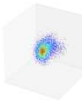
RES 183



RES 185



RES 190



RES 194



RES 197



RES 201



RES 204



RES 216



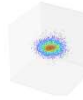
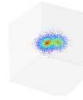
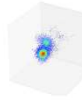
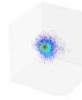
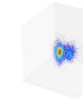
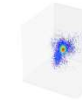
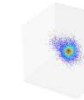
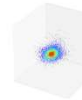
RES 217



RES 220



RES 221



RES 222



RES 223



RES 271



RES 273



RES 292



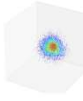
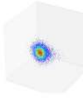
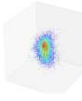
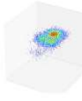
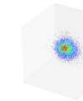
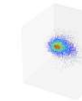
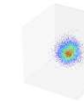
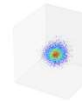
RES 294



RES 299



RES 306



RES 313



RES 324



RES 334



RES 335



RES 354



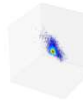
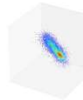
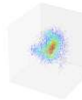
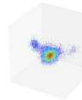
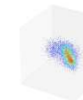
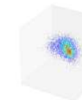
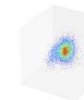
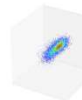
RES 360



RES 368



RES 370



RES 371

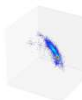


Table S2: Bridging residues for community maps of PKAc : RI α complex

Number	Residue	Main Chain	Side Chain
1	TRP 30	COM C	COM E
2	SER 34	COM A	COM C
3	GLY 55	COM B	COM A
4	ILE 73	COM B	COM A
5	THR 88	COM E	COM B
6	LYS 92	COM E	COM B
7	ILE 94	COM C	COM E
8	GLN 96	COM C	COM E
9	LEU 103	COM D	COM C
10	VAL 104	COM E	COM D
11	LYS 105	COM E	COM C
12	TYR 117	COM A	COM B
13	MET 128	COM A	COM B
14	HIS 131	COM F	COM D
15	ARG 134	COM F	COM D
16	ALA 147	COM D	COM F
17	PHE 154	COM H	COM F1
18	LEU 157	COM C	COM D
19	HIS 158	COM C	COM H
20	PRO 169	COM F	COM D
21	GLU 170	COM D	COM F
22	PHE 187	COM E	COM F1
23	ARG 190	COM E	COM C
24	T2P 197	COM F1	COM E
25	GLY 200	COM F1	COM E
26	THR 201	COM F1	COM F
27	GLU 203	COM F1	COM F
28	LEU 224	COM F	COM D
29	ASN 271	COM H	COM F
30	LEU 273	COM F1	COM F
31	LYS 285	COM H	COM F1
32	ALA 298	COM H	COM F
33	THR 300	COM D	COM F
34	TRP 302	COM D	COM H
35	PRO 313	COM F	COM D
36	LYS 317	COM D	COM A
37	ASP 329	COM A	COM D
38	TYR 330	COM A	COM D
39	ILE 335	COM B	COM A
40	ARG 364 (R1a)	COM F	COM D
41	GLY 366 (R1a)	COM F	COM P1

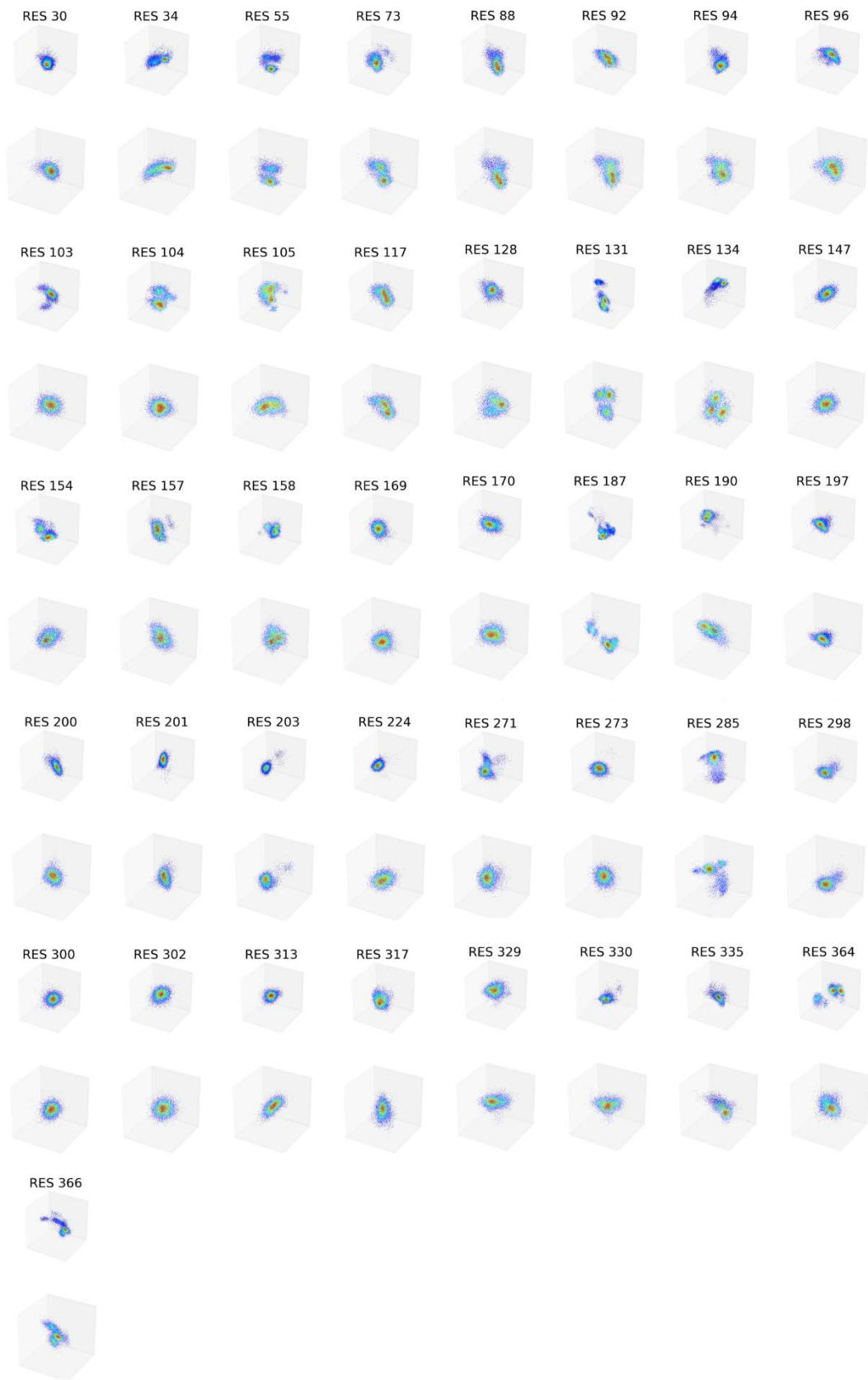
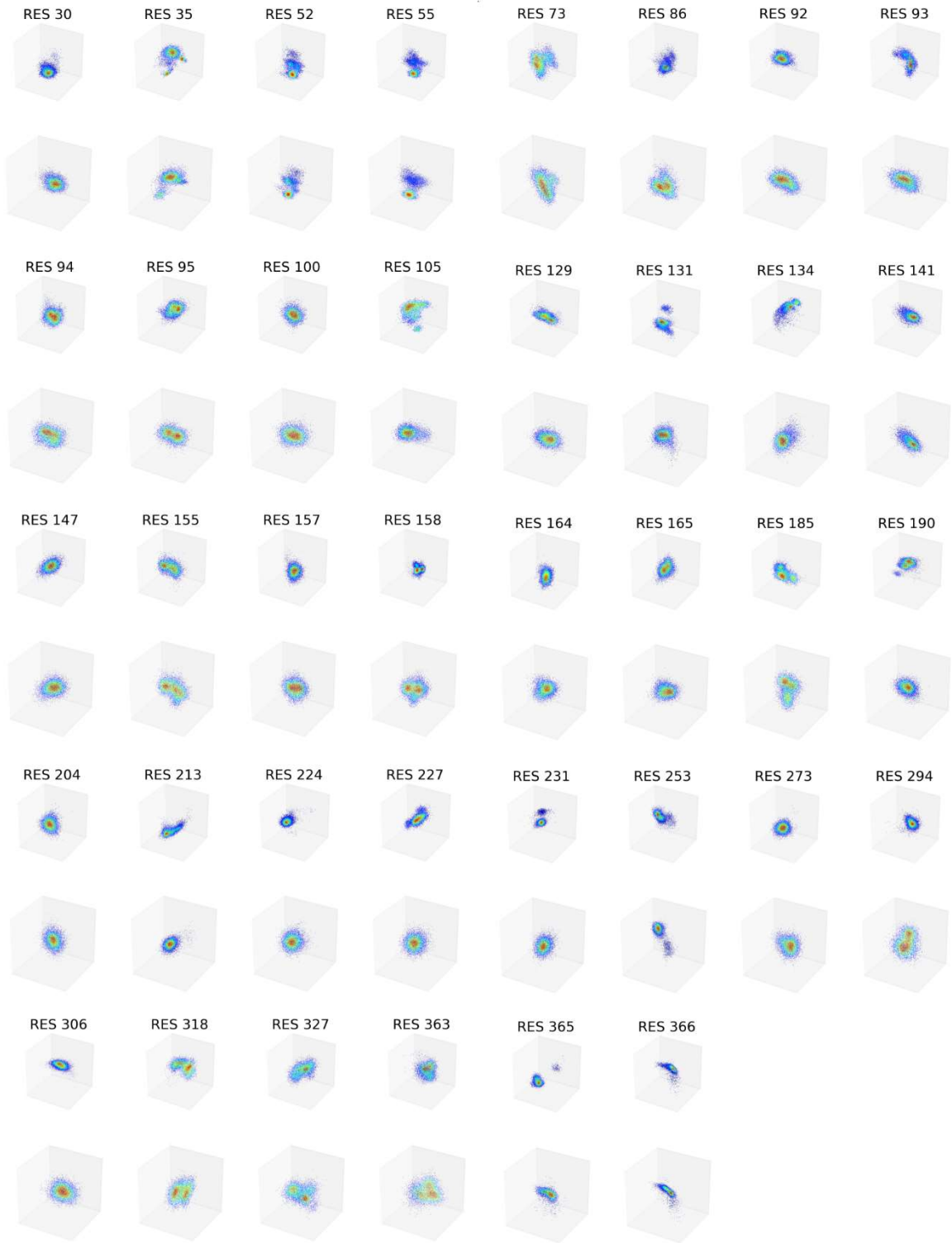


Table S3: Bridging residues for community maps of PKAc : RII β complex

Number	Residue	Main Chain	Side Chain
1	TRP 30	COM C	COM D1
2	GLN 35	COM A	COM C
3	GLY 52	COM A	COM B
4	GLY 55	COM B	COM A
5	ILE 73	COM A	COM B
6	GLU 86	COM D1	COM B
7	LYS 92	COM D1	COM B
8	ARG 93	COM C	COM D1
9	ILE 94	COM C	COM D1
10	LEU 95	COM C	COM D1
11	PHE 100	COM C	COM D
12	LYS 105	COM D	COM A
13	PHE 129	COM D	COM F
14	HIS 131	COM F	COM D
15	ARG 134	COM F	COM D
16	PRO 141	COM F	COM D
17	ALA 147	COM D	COM F
18	GLU 155	COM H	COM D
19	LEU 157	COM C	COM D1
20	HIS 158	COM C	COM H
21	TYR 164	COM D1	COM D
22	ARG 165	COM F1	COM D1
23	PHE 185	COM D1	COM D
24	ARG 180	COM D1	COM C
25	TYR 204	COM F1	COM F
26	LYS 213	COM D1	COM F1
27	LEU 224	COM F	COM D
28	LEU 227	COM F	COM D
29	MET 231	COM F	COM D
30	GLY 253	COM F1	COM F
31	LEU 273	COM F1	COM F
32	HIS 294	COM H	COM F
33	TYR 306	COM D	COM C
34	PHE 318	COM D	COM A
35	PHE 327	COM A	COM D
36	THR 363 (RIIb)	COM F	COM P
37	ARG 365 (RIIb)	COM D	COM F
38	ALA 366 (RIIb)	COM D1	COM D



Video S1: Community Map of PKA:ATP:IP20 mapped on the Kinase domain

Video S2: Community Map of PKA:ATP:RI α mapped on the Kinase domain

Video S3: Community Map of PKA:ATP:RII β mapped on the Kinase domain

Video S4: Community Map of PKA:ATP:SP20 mapped on the Kinase domain

Video S5: Community Map of PKA:ATP:pSP20 mapped on the Kinase domain

Video S6: Community Map of PKA:ATP:PLN mapped on the Kinase domain

Video S7: Community Map of PKA:ATP:pPLN mapped on the Kinase domain