

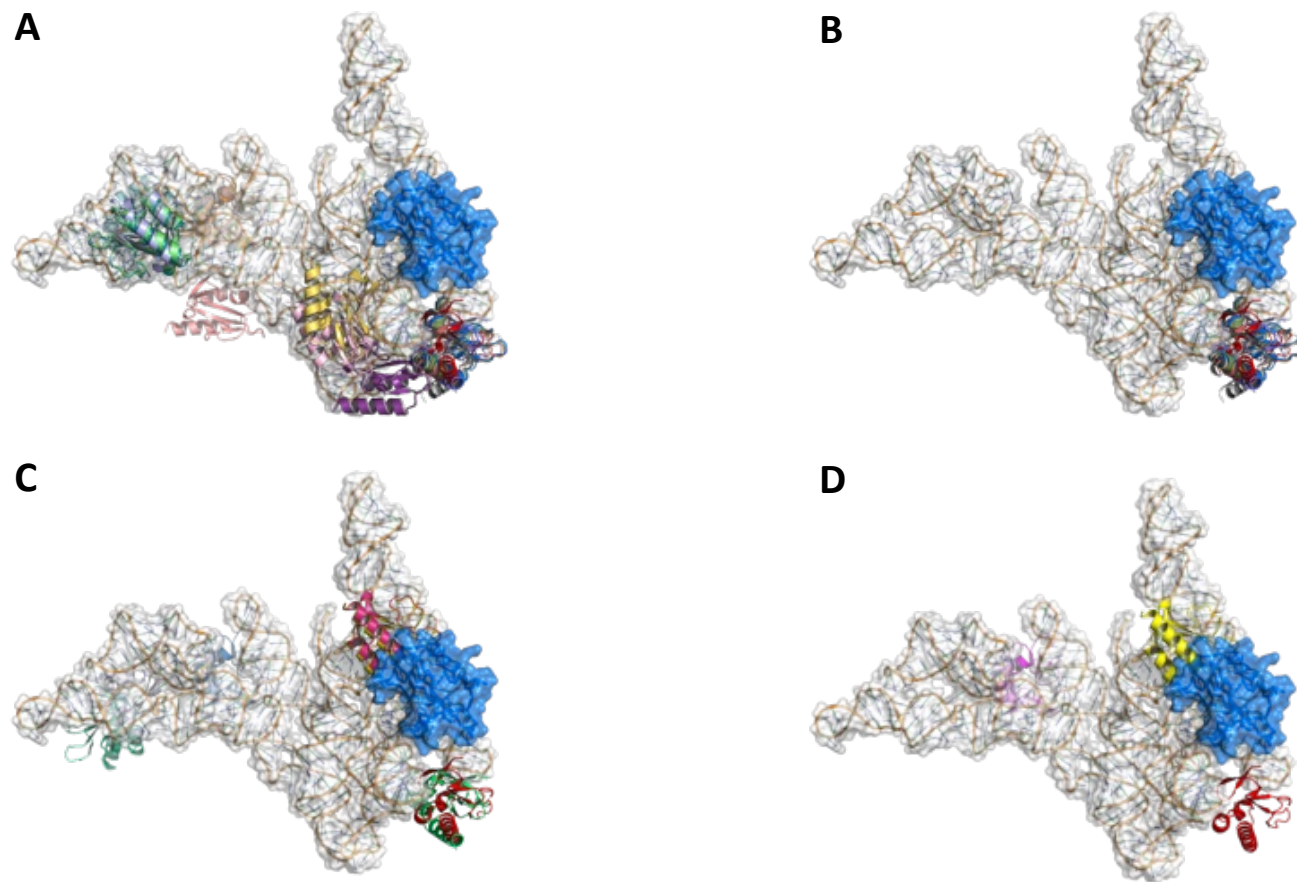


Fig S1. Decoys obtained from blind docking using RnpM-P RNA cross-linking data sets. P RNA and P protein are depicted in transparent white and marine, respectively, and the decoys each in a different color. The decoys obtained from *in silico* blind docking were checked for compatibility with cross-linking data sets with the localization scores (LS) 1.0 (A), 1.0 top populated cluster (B), 1.5 (C) and 2.0 (D).

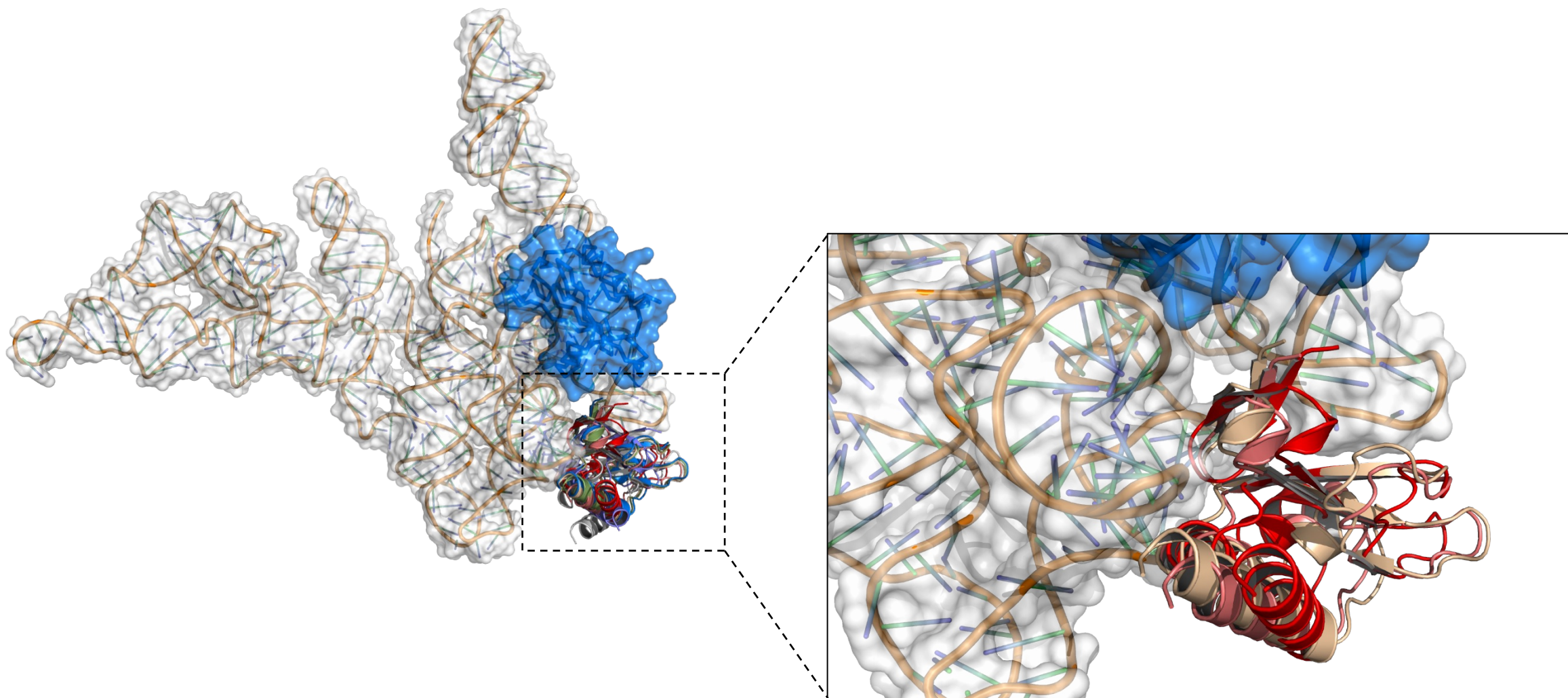


Fig S2. Accumulation of RnpM hits in the predicted P RNA binding site. Multiple RnpM decoys (cartoon representation) were predicted to bind in close proximity to the RnpA protein (transparent surface, marine).

Table S1. Cross-links identified for RnpM and P RNA

RnpM peptide sequence	RNA-adduct	Crosslinked nucleotide	Localization score	#q-value	Crosslinker
Localization score (LS) 1.0					
CVVTGEM(Oxidation)K PK	G+C4H6O2	G	2,641	0	DEB
CVVTGEM(Oxidation)K PK	U+C4H6O2	U	1,422	1,15E-06	DEB
CVVTGEM(Oxidation)K PK	A+C4H6O2	A	3,699	1,00E-06	DEB
CVVTGEMKPK	A+C4H6O2	A	3,315	2,35E-06	DEB
CVVTGEM(Oxidation)K PK	U+C4H6O2	U	1,181	1,93E-06	DEB
SKEGEISVDPTGK	U+C4H6O2	U	1,902	3,30E-06	DEB
SKEGEISVDPTGK	U+C4H6O2	U	1,826	2,39E-06	DEB
SKEGEISVDPTGK	U+C4H6O2	U	1,096	8,78E-07	DEB
KCVVTGEM(Oxidation)KPK	CG+C5H9N1	C	1,196	3,65E-06	NM
CVVTGEM(Oxidation)K PK	A+C5H9N1	A	3,116	2,25E-06	NM
CVVTGEM(Oxidation)K PK	U+C5H9N1	U	2,811	3,61E-06	NM
CVVTGEM(Oxidation)K PK	A+C5H9N1	A	2,908	2,97E-06	NM
CVVTGEM(Oxidation)K PK	G+C5H9N1	G	1,132	2,96E-06	NM
CVVTGEMKPK	C+C5H9N1	C	1,608	2,10E-06	NM
KCVVTGEMKPK	A+C5H9N1	A	1,454	3,87E-06	NM
ECILAAK	G+C5H9N1	G	1,029	4,38E-06	NM
SKEGEISVDPTGKK	G+C5H9N1	G	1,638	4,42E-06	NM
SKEGEISVDPTGKK	G+C5H9N1	G	1,787	4,52E-06	NM
ECILAAK	A+C5H9N1	A	1,647	4,53E-06	NM
EGEISVDPTGK	G+C5H9N1	G	1,208	3,90E-06	NM
CVVTGEM(Oxidation)K PK	AA+C5H9N1	A	1,094	4,30E-06	NM
EGEISVDPTGKK	G+C5H9N1	G	2,106	4,09E-06	NM
GAYLTLDKECILAAK	CC+C5H9N1-H3O4P1	C	1,166	8,91E-03	NM
CVVTGEMKPK	U+C5H9N1	U	1,147	3,98E-06	NM
ECILAAK	A+C5H9N1	A	1,000	4,82E-06	NM
GAYLTLDKECILAAK	CC+C5H9N1-H3O4P1	C	2,010	9,55E-04	NM

GAYLTLDKECILAAK	GU+C5H9N1-H1O3P1	G	1,229	1,86E-03	NM
GAYLTLDKECILAAK	AU+C5H9N1-H1O3P1	A	1,583	4,97E-06	NM
GAYLTLDKECILAAK	AU+C5H9N1-H1O3P1	A	1,040	2,76E-03	NM
GAYLTLDKECILAAK	CC+C5H9N1-H3O4P1	C	1,435	5,36E-06	NM
GAYLTLDKECILAAK	G+C5H9N1	G	1,187	4,93E-06	NM
GAYLTLDKECILAAK	U+C5H9N1	U	1,883	4,48E-06	NM
GAYLTLDKECILAAK	A+C5H9N1	A	1,848	2,76E-03	NM
GAYLTLDKECILAAK	G+C5H9N1-H2O1	G	1,270	4,13E-06	NM
GAYLTLDKECILAAK	U+C5H9N1	U	1,218	8,91E-03	NM
LS 1.5					
CVVTGEM(Oxidation)K PK	G+C4H6O2	G	2,641	0	DEB
CVVTGEM(Oxidation)K PK	A+C4H6O2	A	3,699	1,00E-06	DEB
CVVTGEMKPK	A+C4H6O2	A	3,315	2,35E-06	DEB
CVVTGEM(Oxidation)K PK	U+C4H6O2	U	1,591	2,15E-06	DEB
SKEGEISVDPTGK	U+C4H6O2	U	1,902	3,30E-06	DEB
SKEGEISVDPTGK	U+C4H6O2	U	1,826	2,39E-06	DEB
CVVTGEM(Oxidation)K PK	A+C5H9N1	A	3,116	2,25E-06	NM
CVVTGEM(Oxidation)K PK	U+C5H9N1	U	2,811	3,61E-06	NM
CVVTGEM(Oxidation)K PK	A+C5H9N1	A	2,908	2,97E-06	NM
CVVTGEMKPK	C+C5H9N1	C	1,608	2,10E-06	NM
SKEGEISVDPTGKK	G+C5H9N1	G	1,638	4,42E-06	NM
SKEGEISVDPTGKK	G+C5H9N1	G	1,787	4,52E-06	NM
ECILAAK	A+C5H9N1	A	1,647	4,53E-06	NM
EGEISVDPTGKK	G+C5H9N1	G	2,106	4,09E-06	NM
GAYLTLDKECILAAK	CC+C5H9N1-H3O4P1	C	2,010	9,55E-04	NM
GAYLTLDKECILAAK	AU+C5H9N1-H1O3P1	A	1,583	4,97E-06	NM

GAYLTLDKECILAAK	A+C5H9N1	A	2,929	3,66E-06	NM
GAYLTLDKECILAAK	U+C5H9N1	U	1,883	4,48E-06	NM
GAYLTLDKECILAAK	A+C5H9N1	A	1,848	2,76E-03	NM
LS 2.0					
CVVTGEM(Oxidation)K PK	G+C4H6O2	G	2,641	0	DEB
CVVTGEM(Oxidation)K PK	A+C4H6O2	A	3,699	1,00E-06	DEB
CVVTGEMKPK	A+C4H6O2	A	3,315	2,35E-06	DEB
SKEGEISVDPTGK	U+C4H6O2	U	2,042	2,33E-06	DEB
EGEISVDPTGK	U+C4H6O2	U	5,763	3,09E-06	DEB
CVVTGEM(Oxidation)K PK	A+C5H9N1	A	3,116	2,25E-06	NM
CVVTGEM(Oxidation)K PK	U+C5H9N1	U	2,811	3,61E-06	NM
CVVTGEM(Oxidation)K PK	A+C5H9N1	A	2,908	2,97E-06	NM
SKEGEISVDPTGKK	G+C5H9N1	G	3,365	4,93E-06	NM
EGEISVDPTGKK	G+C5H9N1	G	2,106	4,09E-06	NM
GAYLTLDKECILAAK	CC+C5H9N1- H3O4P1	C	2,010	9,55E-04	NM
GAYLTLDKECILAAK	A+C5H9N1	A	2,929	3,66E-06	NM
GAYLTLDKECILAAK	A+C5H9N1	A	2,474	3,68E-06	NM
GAYLTLDKECILAAK	U+C5H9N1	U	2,336	4,73E-06	NM

Table S2. Cross-links identified for RnpA and P RNA

RnpA peptide sequence	RNA-adduct	Crosslinked nucleotide	Localization score	#q-value	Crosslinker
Localization score (LS) 1.0					
IGNAVM(Oxidation)R	U+C4H6O2	U	1,132	3,57E-06	DEB
PASQLTYEETKK	U+C4H6O2	U	1,185	1,64E-06	DEB
KPASQLTYEETK	G+C5H9N1	G	1,253	1,24E-06	NM
KPASQLTYEETK	AU+C5H9N1	A	2,006	1,26E-06	NM
KPASQLTYEETK	C+C5H9N1	C	1,056	2,43E-06	NM
KPASQLTYEETK	G+C5H9N1	G	1,069	3,12E-06	NM
HGTSVANR	G+C5H9N1	G	1,227	3,26E-06	NM
HGTSVANR	A+C5H9N1	A	1,523	3,37E-06	NM
VFKHGTSVANR	G+C5H9N1	G	1,112	3,62E-06	NM
IGNAVMR	G+C5H9N1	G	1,598	3,69E-06	NM
SLQHLLFR	G+C5H9N1	G	1,614	4,00E-06	NM
KIGNAVM(Oxidation)R	G+C5H9N1	G	1,219	4,31E-06	NM
VGLSVSKK	G+C5H9N1	G	1,416	4,33E-06	NM
KPASQLTYEETKK	A+C5H9N1	A	1,148	4,52E-06	NM
NEDFQK	A+C5H9N1	A	1,775	4,53E-06	NM
LS 1.5					
IGNAVM(Oxidation)R	U+C4H6O2	U	1,669	2,54E-06	DEB
KPASQLTYEETK	AU+C5H9N1	A	2,006	1,26E-06	NM
HGTSVANR	A+C5H9N1	A	1,523	3,37E-06	NM
IGNAVMR	G+C5H9N1	G	1,598	3,69E-06	NM
SLQHLLFR	G+C5H9N1	G	1,614	4,00E-06	NM
NEDFQK	A+C5H9N1	A	1,775	4,53E-06	NM
KPASQLTYEETK	AU+C5H9N1	A	2,006	1,26E-06	NM
HGTSVANR	A+C5H9N1	A	2,931	4,03E-06	NM

Table S3. RnpM decoys predicted and classified according to the localization score of cross-linking data

Model abbreviation	Buried surface area	Number of hydrogen bonds	d0	d0-ALL	d2	d2-ALL	d3	d3-ALL	d5	d5-All	Number of interactions	Number of short range contacts
Localization score (LS) 1.0												
model_3216	814,94	14	31	54	35	91	36	114	37	176	43	2
model_4971	932,448	27	28	57	34	93	35	118	36	160	50	4
model_6561	703,288	18	31	55	35	100	36	118	37	173	29	3
model_1228	947,319	40	34	61	35	95	35	119	37	163	97	10
model_742	860,192	24	31	57	35	96	37	119	37	164	45	1
model_1268	886,657	24	33	55	35	100	37	120	37	185	30	3
model_2804	906,434	24	32	56	35	99	37	121	37	186	31	4
model_156	775,197	34	33	70	36	108	36	123	37	163	55	2
model_3530	628,927	22	33	56	33	93	35	124	37	173	41	2
model_8396	754,519	32	31	60	33	90	35	124	35	165	40	3
model_2463	801,658	37	31	63	33	91	35	125	35	172	46	6
model_345	967,083	32	32	55	35	100	36	125	37	174	53	4

model_3219	885,739	24	30	57	35	107	35	127	37	176	52	6
model_214	905,135	29	32	54	36	99	36	128	37	175	48	2
model_4338	844,206	28	30	55	34	108	36	131	37	182	47	7
model_636	1064,82	25	31	65	36	114	37	132	37	191	56	5
model_30	1002,58	35	33	59	36	107	36	137	37	190	67	2
model_85	876,26	32	34	63	36	112	36	138	37	192	68	1
model_4911	678,253	23	31	63	35	108	35	139	37	181	42	2
model_3350	774,026	27	29	56	35	113	36	140	37	193	41	3

LS 1.5

model_1228	947,319	40	19	33	20	54	20	64	20	78	97	10
model_742	860,192	24	17	35	19	55	20	67	20	81	45	1
model_167	1093,14	49	17	34	19	60	20	69	20	99	62	6
model_695	1145,62	52	17	37	19	58	20	70	20	106	72	9
model_156	775,197	34	19	39	20	60	20	71	20	86	55	2
model_1950	851,603	37	17	33	19	75	20	86	20	110	67	8
model_926	780,727	24	17	37	19	76	19	96	20	133	53	1
model_1228	947,319	40	19	33	20	54	20	64	20	78	97	10

LS 2.0												
model_742	860,192	24	13	27	14	42	15	51	15	59	45	1
model_695	1145,62	52	13	30	14	44	15	53	15	79	72	9
model_156	775,197	34	14	30	15	46	15	54	15	66	55	2

Table S4. Best scoring decoys for the RnpM-P RNA complex

Model abbreviation	Buried surface area	Number of hydrogen bonds	d0	d0-ALL	d2	d2-ALL	d3	d3-ALL	d5	d5-All	Number of interactions	Number of short range contacts
model_6561	703,288	18	31	55	35	100	36	118	37	173	29	3
model_1228	947,319	40	34	61	35	95	35	119	37	163	97	10
model_156	775,197	34	33	70	36	108	36	123	37	163	55	2
model_345	967,083	32	32	55	35	100	36	125	37	174	53	4
model_214	905,135	29	32	54	36	99	36	128	37	175	48	2
model_30	1002,58	35	33	59	36	107	36	137	37	190	67	2
model_85	876,26	32	34	63	36	112	36	138	37	192	68	1