## SUPPLEMENTARY MATERAL

## Analysis of the *a*CP1-KH3-poly(C)RNA model

Following are tables describing the oligonucleotide stereochemistry and hydrogen bonding interactions that occur during the molecular dynamics simulation of the  $\alpha$ CP1-KH3/8-nt poly(C)-RNA model as described in the manuscript.

## Sterochemistry of modelled RNA

The backbone dihedral angles of the poly(C)-RNA in the  $\alpha$ CP1-KH3-RNA model were calculated at every picosecond timestep in the 1 ns molecular dynamics simulation. The mean and std deviation (second and third value in each cell) of these angles are listed and allow the degree of movement over the simulation as well as any departure from the original model (first value - in bold) to be noted. The six dihedral angles which describe the oligonucleotide backbone are defined (as per standard nomenclature) by the following atoms:

alpha:	-03'	Р	O5'	C5'
beta:	Р	O5'	C5'	C4'
gamma:	O5'	C5'	C4'	C3'
delta:	C5'	C4'	C3'	O3'
epsilon:	C4'	C3'	O3'	+P
zeta:	C3'	O3'	+P	+05'

Base*	alpha	beta	gamma	delta	epsilon	zeta
9	N/A	173.7	43.0	85.8	66.6	-57.2
		23.8	60.10	75.8	-65.4	94.7
		149.5	13.02	6.4	142.0	94.7
10	-127.5	170.7	93.0	105.5	-127.8	-60.9
	-31.5	100.9	51.5	141.7	-112.6	-77.4
	61.0	99.3	19.0	7.9	16.7	17.3
11	124.9	137.9	42.8	118.6	-76.2	165.4
	109.2	92.7	57.2	139.5	-116.9	-110.5
	30.8	130.8	14.9	7.4	31.3	15.0
12	-102.4	160.9	40.11	92.9	79.4	<b>98.8</b>
	-72.9	130.0	38.1	74.9	39.7	8.8
	18.7	34.8	15.1	5.9	8.7	169.2
13	111.3	-110.8	133.3	112.7	-112.4	132.7
	-62.2	146.2	30.2	146.5	-103.0	123.2
	27.0	51.4	25.0	6.6	18.4	19.3
14	-76.9	143.5	37.7	78.5	-135.7	-60.0
	-105.0	145.1	53.8	78.1	105.9	25.5
	22.2	27.6	11.0	5.7	127.0	16.3
15	-63.8	179.5	<b>48.7</b>	82.1	-132.9	-63.9
	-131.5	74.3	64.0	79.7	-86.1	-33.2
	14.1	155.6	9.6	5.2	102.6	31.0
16	-65.2	172.5	51.0	N/A	N/A	N/A
	-82.6	99.5	59.8			
	29.7	133.2	10.7			

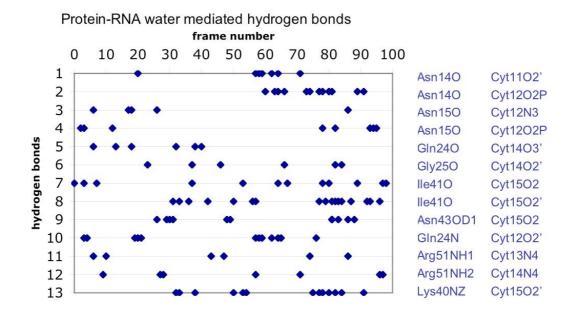
\* the numbering system is based on the oligonucleotide numbering within the Nova2-KH3-RNA structure (accession code: 1EC6) with bases **12-15** corresponding to the binding tetrad.

## Hydrogen bonding

The lifetime of potentially important hydrogen bond interactions occurring between the protein and oligonucleotide assessed by determining their existence at each picosecond of the 1 ns molecular dynamics simulation (shown as a dot at each timepoint). Their presence was defined by the hydrogen bond acceptor and donor occurring within 3.8 Å of one another and within an X-H-X angle of  $30^{\circ}$  degrees where X = the heavy atom. Water mediated hydrogen bonds occurring between the protein and oligonucleotide were defined as simultaneous hydrogen bonds occurring between the protein and the oligonucleotide to the same water oxygen.

					frame								
	0	10	20	30	40	50	60	70	80	90	100		
1		•	•	••	• •	•	••	• •	-	•		Gly18CA	Cyt12O2
2		• • •	• ••		••	• •	• • •	•	• •	• •		lle21CG2	Cyt13O4'
3		٠	* *		•		٠		•			lle21CD	Cyt13O4'
<b>"</b> 4						• •	• • •	• ••	•		•	Arg23CA	Cyt13OP1
ipuc						••		•	•		•	GIn24N	Cyt13OP1
q 6	; +=	•	• •	٠								Gly25CA	Cyt13O2'
hydrogen bonds	•	• •	٠		• •			٠	•	•	•	lle28CG2	Cyt14O2
grd	; +			•				•••			••	Arg32NH1	Cyt14O2
۲ p	••	• •	٠		• ••	• •		••		• •	•	Arg32NH1	Cyt14C2'
10	)			•	**	٠	•	••	**			Arg32NH1	Cyt14O2'
11	. 🖂	• • •		4		••		٠	•			Arg32NH2	Cyt14C2
12		• •••						• •		• •	•	Arg32NH2	Cyt14 O2
13	: +			-	٠	• •	••		***			Lys40CD	Cyt15O2'
14	-	****		•	•							Lys40NZ	Cyt15O2'
15	;					•	•					Lys40NZ	Cyt16O1P
16								• •		•		lle41CB	Cyt14N3
17	·			٠			٠	٠				lle41CB	Cyt14N4
18	; +	• •	•	•	•	• •	•		**		•••	lle41CD	Cyt14N3
19	-			• ••••		•	-	• • •		•		Arg51NH1	Cyt13C2
20	)	•	-	• • •	•							Arg51NH1	Cyt13O2
21	. 🗰			• •						•	5	Arg51NH1	Cyt13N3
22	•			++	•	• • • • • • •	* *		• •			Arg51NH1	Cyt13C4
23			-	• •••						•		Arg51NH2	Cyt13O2
24	. –	**	•	***	•••			• •	••	•		Gly18O	Cyt12C2'
25			**			٠		•				Gly22O	Cyt13C5'
26	; +	•		••		•		• •				Gln24O	Cyt14C4'
27	' +	٠			• •				٠	•	•	lle28CG2	Cyt14C1'
28	; +					•	-	٠		-		lle41CB	Cyt14N4
29	) +					•	-			••	•	lle41CG2	Cyt14N4
30	•	•	•	•		****		٠	• •			lle41C	Cyt14N4
31		• •						•••				lle410	Cyt14N4

Protein-RNA hydrogen bonds



\* the numbering system is based on the oligonucleotide numbering within the Nova2-KH3-RNA structure (accession code: 1EC6) with bases 12-15 corresponding to the binding tetrad.