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Supplemental information

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Dynamics of the SARS-CoV-2 nucleoprotein N-terminal domain triggers RNA duplex destabilization

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SUPPLEMENTARY MATERIAL

Modeling the dsRNA melting activity

We used the software Kinetiscope (http://hinsberg.net/kinetiscope/), which is based on a stochastic algorithm developed by Bunker (1) and Gillespie (2). We used the elementary rate constants for individual chemical steps to produce an absolute time base (Figure 6A). The starting condition mimics exactly the experimental condition, varying the concentration of N-NTD over 50 nM dsRNA (dsTRS). The predictions were validated by direct comparison to the experimental data (3).

To simulate the melting curve, we had to constrain the kinetic space, which is large because each model is composed by 6 reactions and 12 individual rate constants, assuming the following boundaries: (B1) the kinetic model must be complete, complying all possible reactions for a given mechanism; (B2) the presence of N-NTD must lead to catalysis, with the melting of dsRNA being faster than the annealing reaction; (B3) the equilibrium of the annealing is shifted toward the dsRNA; and (B4) the equilibrium for the melting activity must be reached in less than 133 seconds, as described by Grossoehme et al. (3).

The criterion for choosing the rate constants for the annealing reaction (R1, Figure 6) was that it must be significantly slower than the melting activity (catalysis). As to our knowledge there is no experimental kinetic rate constant available for the annealing of dsTRS, we fixed a $k_{off} = 8\times10^{-4}\cdot s^{-1}$ for the simulations, which is the experimental value of the dissociation rate constant observed for the almost inactive Y127A N-NTD+SR mutant (3). This mutant has a melting activity of hours, 30 fold slower than the wild-type (3), while our simulation showed melting activities of tens of seconds (Figure 6B). To yield an equilibrium shifted toward the dsRNA, we used $k_{on} = 4\times10^{-1}\ M^{-}1\cdot s^{-1}$, which is true below

the melting temperature of the dsRNA. Any values of k_{off} < 1 s^{-1}, with an association constant K_a, gives the same molar fraction of dsRNA.

We constrained the binding reactions R2 and R3 of N-NTD to the sense (TRS) and antisense (cTRS) single-stranded RNA (ssRNA) (Figure 6A) based on the published experimental values for these association constants (3, 4). Since these values were very similar, to simplify the simulation, we used the same K_a for both reactions ($K_a = 4\times10^7$ M^{-1}). Note that $k_{on} < 10^6$ $M^{-1}\cdot s^{-1}$ makes the reaction too slow to reach equilibrium, violating the boundary B4 (Figures S14A and S16B).

For dsRNA (dsTRS) binding, there was no experimental data to constrain the simulation. However, simulations unambiguously showed that K_a for reaction R4 must be of the same order of that for ssRNAs, leading to the allowed ranges depicted in Figure 6A. We also determined k_{on} based on the simulations, taking boundaries B2 and B4 into consideration, which were also considered for reactions from R1 to R3 (Figure S16B, S17A and S18B). All the constraints applied to reactions from R1 to R4 are valid for both kinetic models (models 1 and 2). Conversely, reactions R5 and R6 are specific for each kinetic model, being essential to comply with boundary B1.

For model 1, there is no experimental data available to constrain reactions R5 and R6, but the simulations showed that they are tightly related to reactions R2 and R3, being both K_a and k_{off} of the same order of magnitude for reactions R2 and R3 (Figure S16C). Note that there is an intricate relationship between the formation of ssRNA-bound states (C2 and C3) and the decrease of free or bound dsRNA (dsTRS and C4). To illustrate this relationship, Figure 6B shows the kinetics at three concentrations of N-NTD. The simulated melting curves for model 1 resembled the near exponential decay observed experimentally (Figure 6C, left). Interestingly, when k_{off} of reactions R5 and R6 were bigger than k_{off} for

reactions R2 and R3, we observed a plateau in the exponential decay of the dsRNA melting curve (Figure 6C). Remarkably, melting curves that either decayed to zero or reached a plateau was observed experimentally, as mentioned before (3). It is worth mentioning that the kinetic model 1 is fully compatible with the experimental data by Grossoehme et al. (2009) (3), as well as with the triggering event suggested by the MD simulations, in which one N-NTD can initiate dsRNA melting, destabilizing the WC base-pairing.

We also evaluated the kinetic model 2, in which a sandwich of 2 N-NTD and 1 dsRNA is necessary for the melting reaction. This stoichiometry for N-NTD melting activity should be considered, since the full-length N protein is a biologically functional dimer and the recognition of the TRS duplex by the two N-NTD subunits for the melting activity is possible. In this model, a sandwich of two N-NTDs and one dsRNA is formed, and the final products are each N-NTD bound to TRS and cTRS ssRNA.

To build a kinetic model that would exclusively produce ssRNA from the sandwiched dsRNA, we had to replace reactions R5 and R6 of kinetic model 1. In this new model, reaction R5 forms the sandwiched dsRNA (C5, Figure 6A) and reaction R6 is the dissociation of C5 into the ssRNA-bound N-NTDs (C2 and C3, Figure 6A). To simulate N-NTD melting activity considering model 2, we used the same boundaries described earlier (B1, B2, B3 and B4), with reactions from R1 to R4 having almost the same constraints described for the model 1.

Reaction R5 and R6 of the model 2 has no parallel to any other reaction. We scanned all the kinetic space that led to the catalysis of melting activity and observed two contrasting situations. The first is when reaction R6 equilibrium is between 10^{-6} and 10^{7} M^{-1}, always having the dissociated forms C2 and C3 available and making the melting curve very stiff (model 2a). The second is the opposite situation, where equilibrium is skewed

toward the sandwich state (C5) with $K_a > 10^7$ M^{-1} (model 2b). Figure 6C illustrates the melting curves obtained for the two situations.

Model 2a is characterized for the high efficiency in the dissociation of the dsRNA, k_{on} and k_{off} can assume any value (*n* and *m*, Figure 6A) as long as K_a is between 10^{-6} to 10^7 M^{-1}. Particularly for model 2a, the kinetic of dsRNA melting is also independent of k_{on} for reactions R2 and R3, at fixed concentrations of N-NTD. For R5, the equilibrium should be shifted toward C5, to keep up with boundaries B2 and B4 ($K_a > 1$, Figure S17B). All simulated conditions led to the curve in red (Figure 6C), in which, the minimal amount of N-NTD (10 nM) led to complete dissociation of the dsRNA (molar fraction of zero). Figure S17 illustrates all the simulated boundaries. Note that for the model 2a there is never an accumulation of C5 (Figure S17C).

Model 2b corresponds to when the equilibrium of reaction R6 is shifted toward C5 ($K_a > 10^7$ M^{-1}). For R5, we determined that k_{on} has to be $> 10^7$ s^{-1} to keep up with boundaries B2 and B4. For the melting activity to take place, the equilibrium of reaction R5 was skilled toward C5 ($K_a > 10^7$ M^{-1}, Figure S18C). Figure S18 illustrates the reaction boundaries. In this situation, we were able to observe a melting curve (Figure 6C, blue) with a near exponential decay at a low concentration of N-NTD and a near exponential rise at higher concentrations of N-NTD. This behavior is explained by the accumulation of C5 and N-NTD concentration-dependent mutual compensation of C5 and dsRNA. Note how K_a modulates the accumulation of C5, transitioning between models 2a and 2b (Figure S18D). The increase in the concentration of N-NTD led to a decrease in dsRNA forming C2, C3 and free ssRNA. Further increase in N-NTD led to a decrease in dsRNA and a compensating increase in C5. None of the situations simulated for model 2 are parallel to the experimental observation.

TRS-L	**UUCUC-UAAACGAAC**
TRS-B S	ACAAC-UAAACGAAC
TRS-B ORF3a	UACACAUAAACGAAC
TRS-B E	UUGUA-AGCACAAGC
TRS-B M	UGGUC-UAAACGAAC
TRS-B ORF6	UACAG-UAAGUGACA
TRS-B ORF7a	UUGAU-UAAACGAAC
TRS-B ORF7b	CACUC-AAAAGAAAG
TRS-B ORF8	ACGCC-UAAACGAAC
TRS-B N	UCAUC-UAAACGAAC
TRS-B ORF9b	CAAAC-UAAAAUGUC
TRS-B ORF14	UACAC-CAAAAGAUC
TRS-B ORF10	AGGCC-UAAACUCAU

Figure S1. Pairwise alignment of the TRS-B sequences of each SARS-CoV-2 ORF (NCBI reference: NC_045512.3) with that of TRS-L performed by ClustalW2 (5). The bold sequence denotes the sequence used in this work.

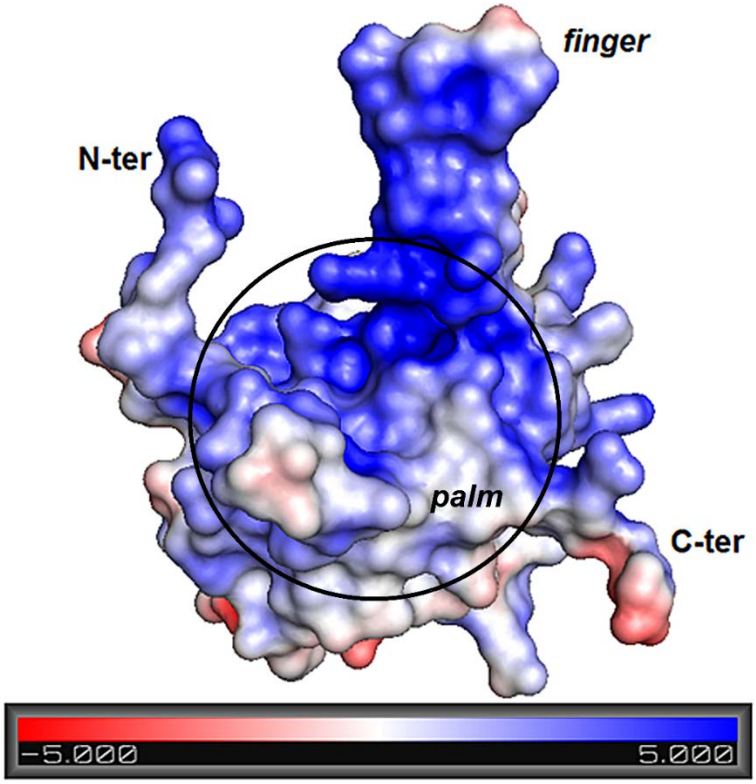

Figure S2. Electrostatic potential surface of SARS-CoV-2 N-NTD calculated from APBS software (6) using charge values and protonation states determined by PDB2PQR server (7) along with PROPKA program (pH 7.0, 50 mM NaCl, 25 °C) (8). The bar denotes the electrostatic potential range from –5 (red) to +5 kTe^{-1} (blue). The electrostatic potential surface of N-NTD was displayed using PyMOL (9).

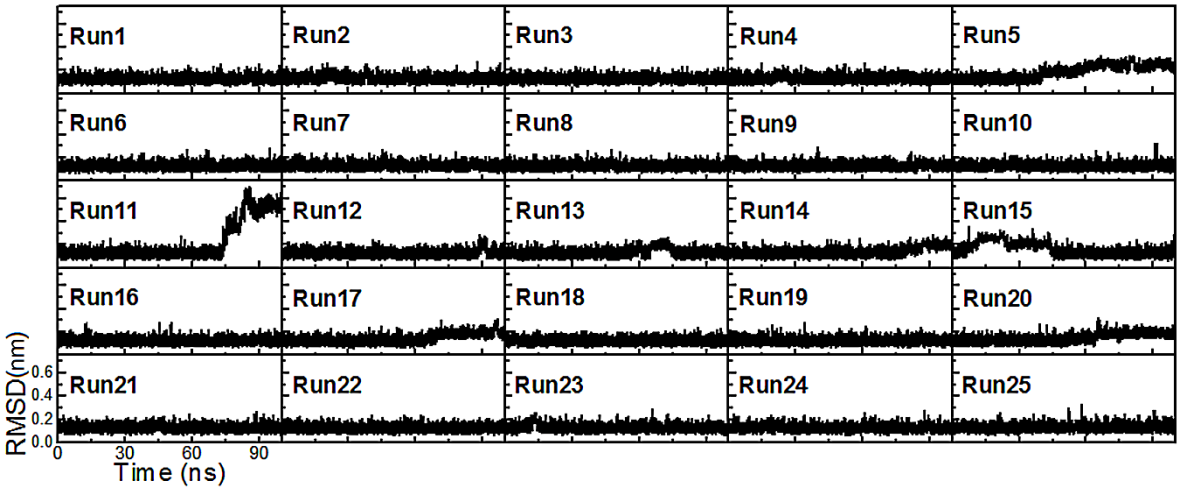

Figure S3. RMSD values of the backbone atoms of free dsTRS for the 25 replicas of 100 ns MD simulations.

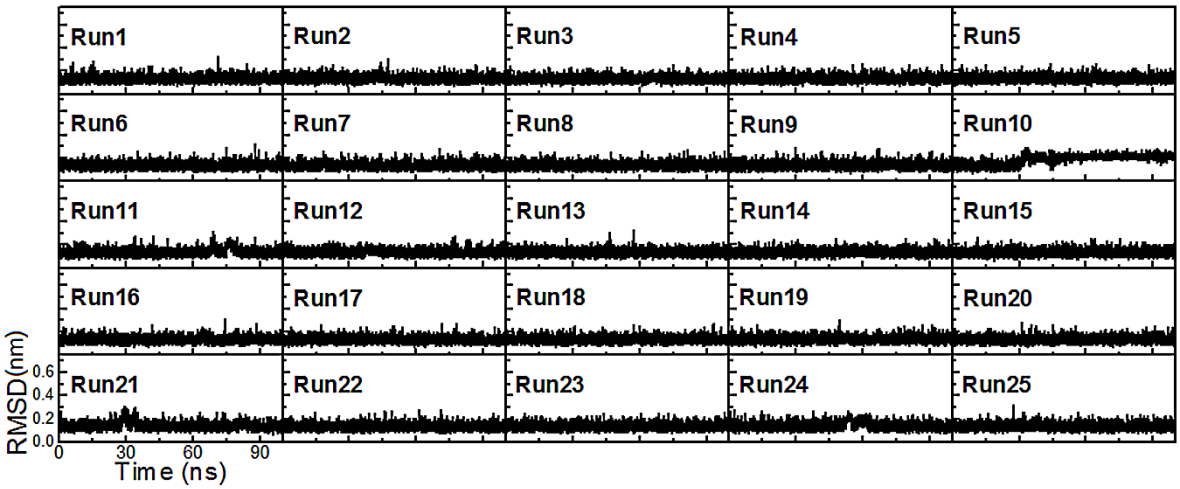

Figure S4. RMSD values of the backbone atoms of free dsNS for the 25 replicas of 100 ns MD simulations.

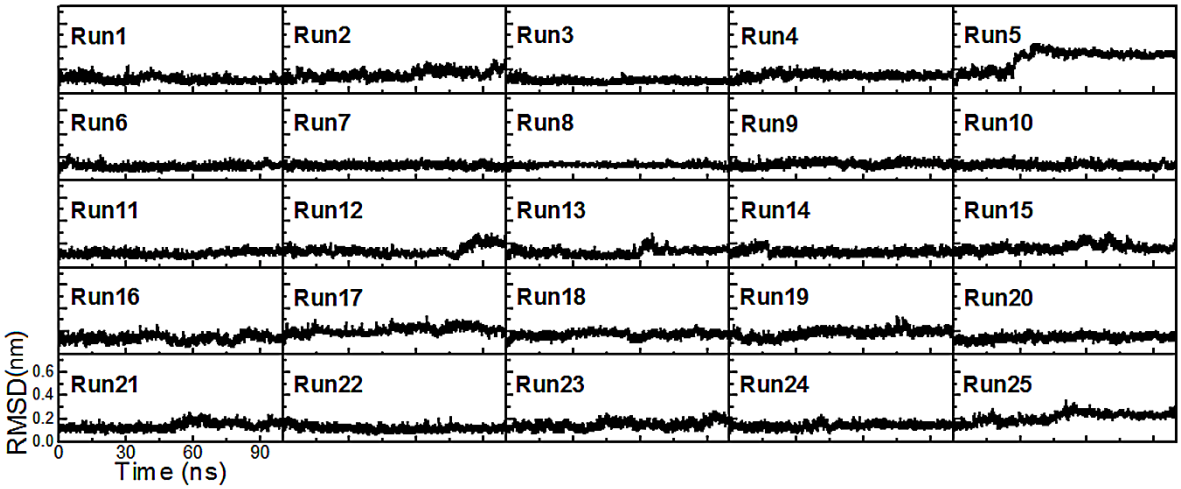

Figure S5. RMSD values of the backbone atoms of N-NTD-bound dsTRS for the 25 replicas of 100 ns MD simulations.

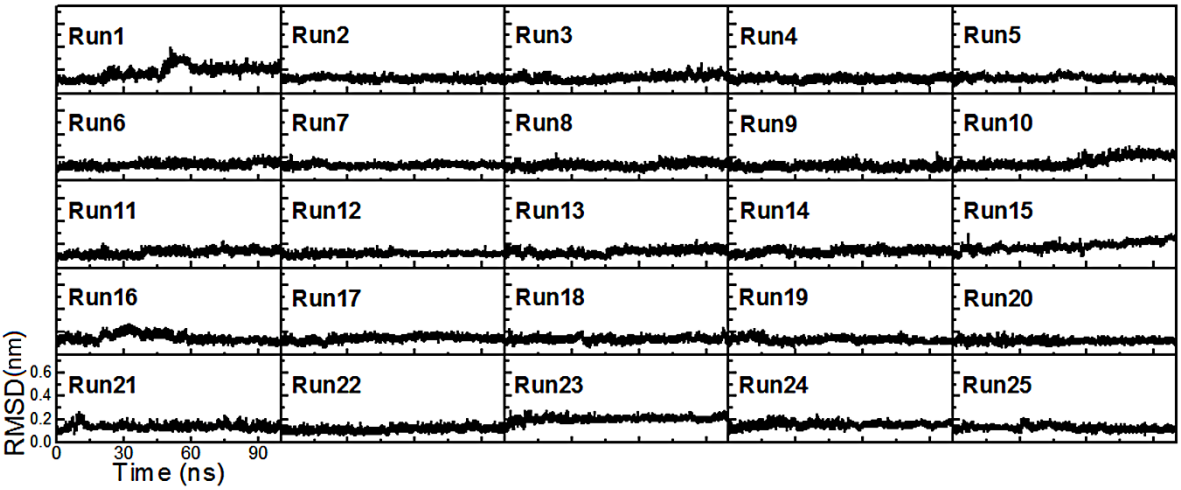

Figure S6. RMSD values of the backbone atoms of N-NTD-bound dsNS for the 25 replicas of 100 ns MD simulations.

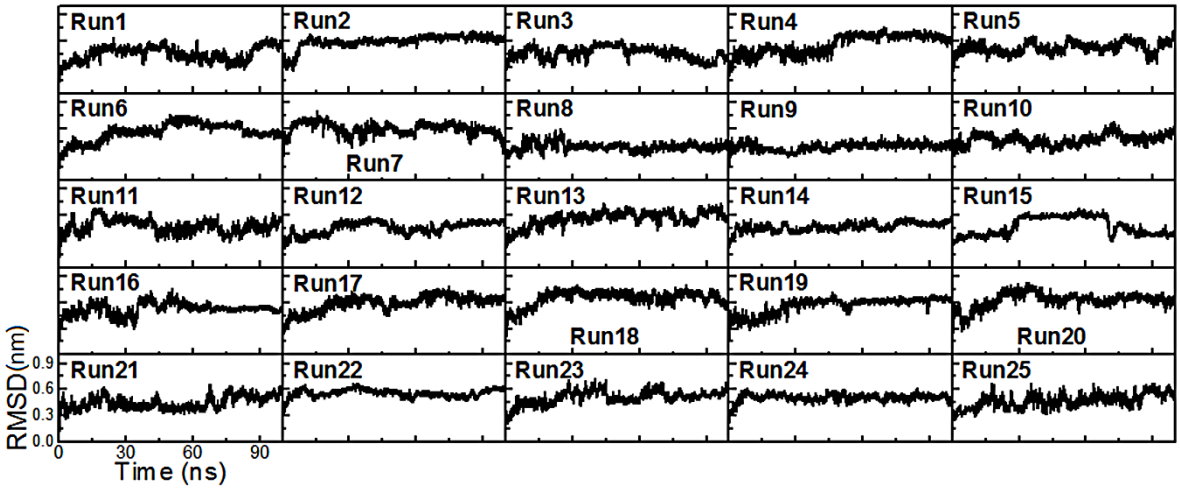

Figure S7. RMSD values of the backbone atoms of free N-NTD for the 25 replicas of 100 ns MD simulations.

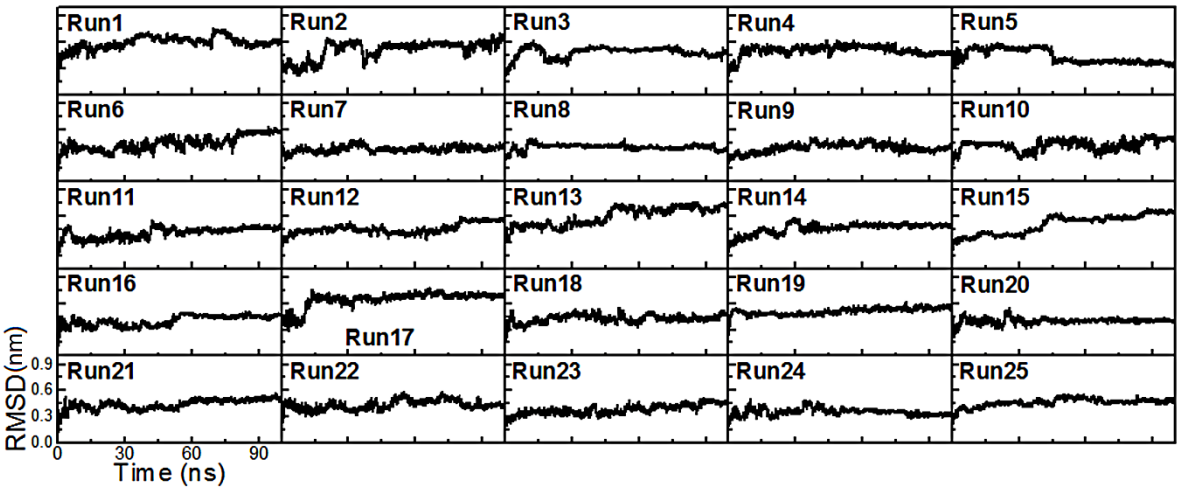

Figure S8. RMSD values of the backbone atoms of dsTRS-bound N-NTD for the 25 replicas of 100 ns MD simulations.

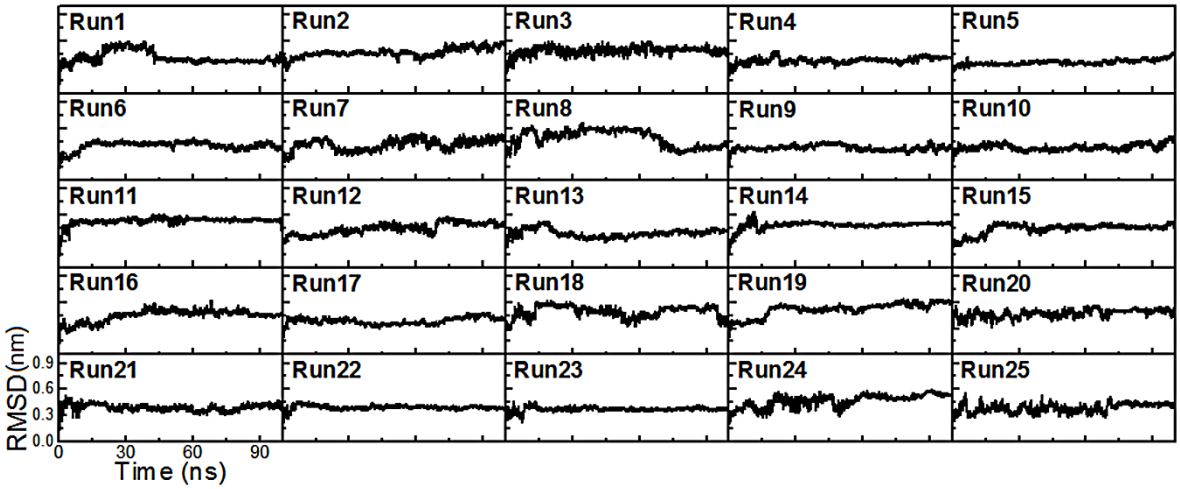

Figure S9. RMSD values of the backbone atoms of dsNS-bound N-NTD for the 25 replicas of 100 ns MD simulations.

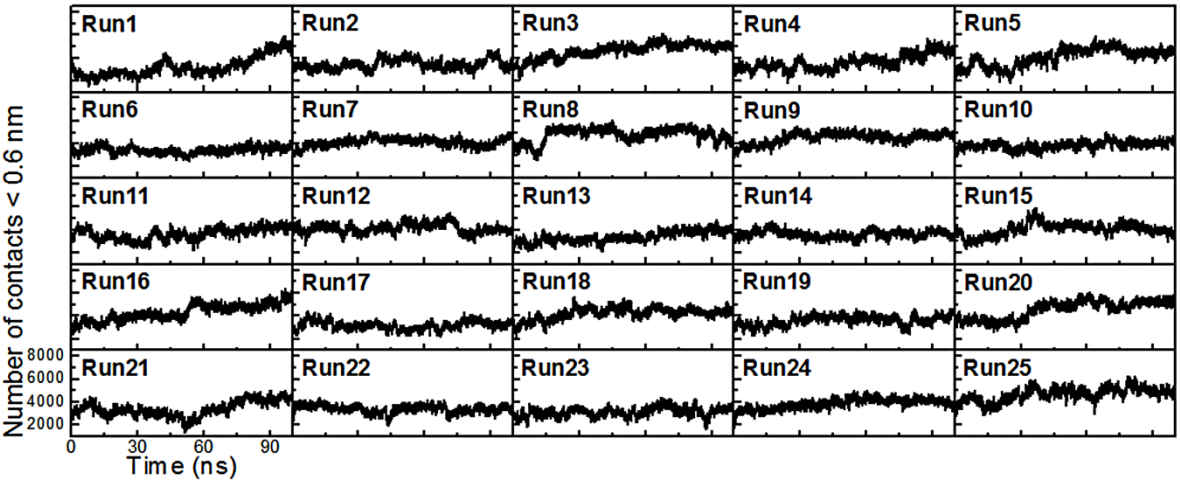

Figure S10. Number of contacts < 0.6 nm between the N-NTD and dsTRS atoms for the 25 replicas of 100 ns MD simulations.

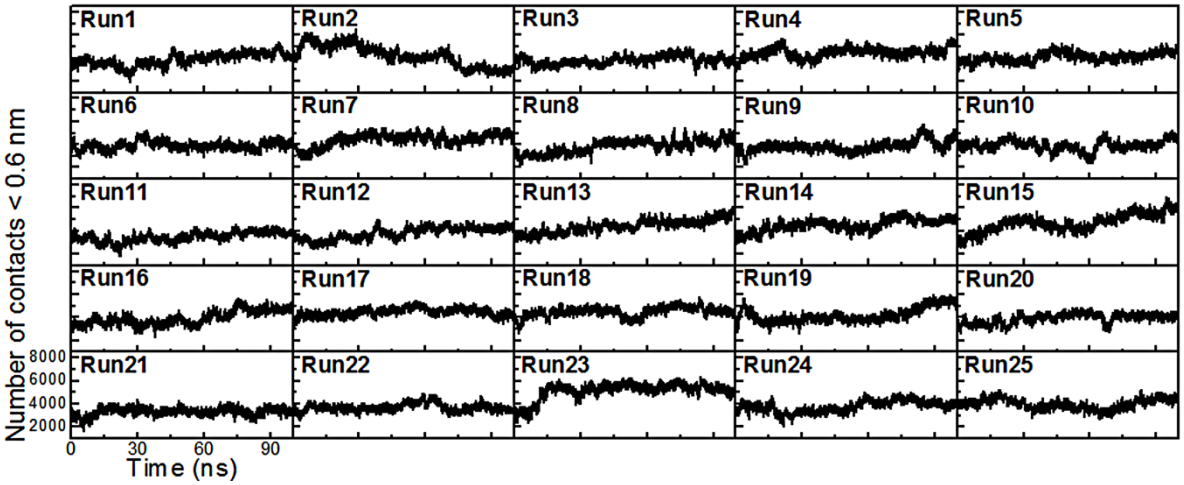

Figure S11. Number of contacts < 0.6 nm between the N-NTD and dsNS atoms for the 25 replicas of 100 ns MD simulations.

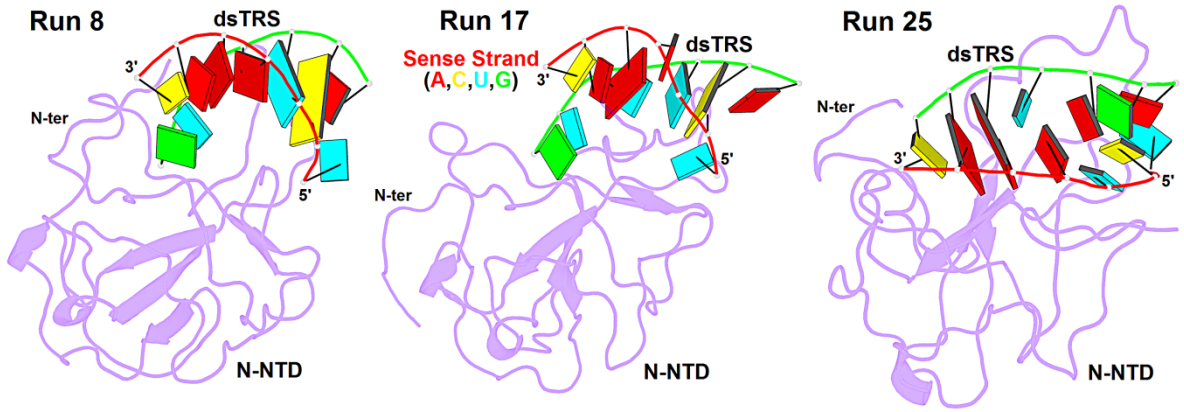

Figure S12. Structural model of the N-NTD:dsTRS complex representative of the MD simulation for runs 8, 17, and 25. The protein is shown as purple cartoon and dsTRS is denoted as ribbon model with nitrogenous bases and base-pairing as colored squares and rectangles, respectively. The color of the squares corresponds to the type of nitrogenous base, being A: red, C: yellow, U: cyan, and G: green. The color of the rectangles refers to the color of the nitrogenous base of the sense RNA strand.

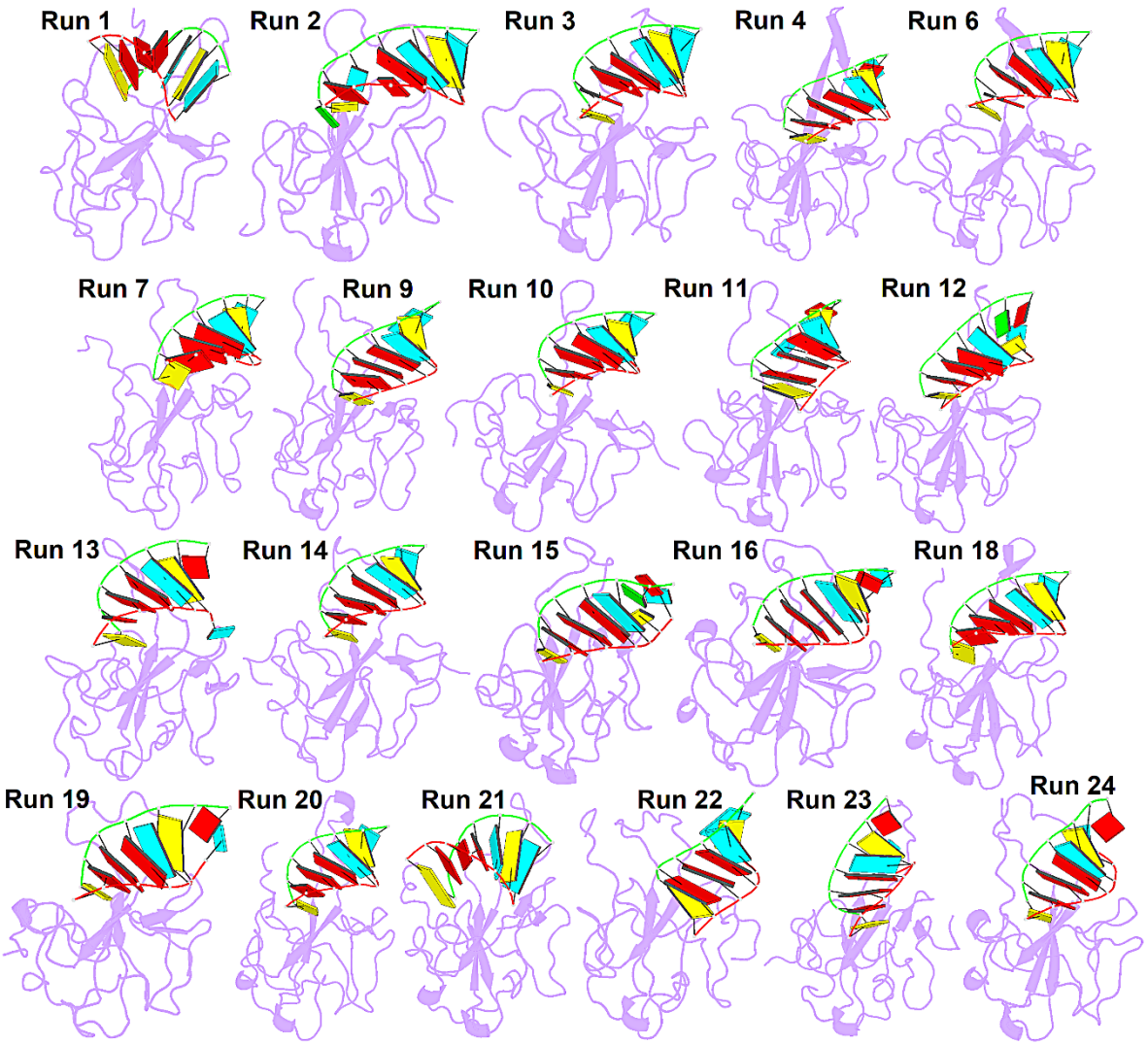

Figure S13. Structural model of the N-NTD:dsTRS complex of the MD simulations (last frames) for the runs that had no significant break of protein-nitrogenous base hydrogen bonds. The protein is shown as purple cartoon and dsTRS is denoted as ribbon model with nitrogenous bases and base-pairing as colored squares and rectangles, respectively. The color of the squares corresponds to the type of nitrogenous base, being A: red, C: yellow, U: cyan, and G: green. The color of the rectangles refers to the color of the nitrogenous base of the sense RNA strand. The protein structure representation is equally oriented in all runs, placing the N- and C-termini to the left and right, respectively, and the finger at the top.

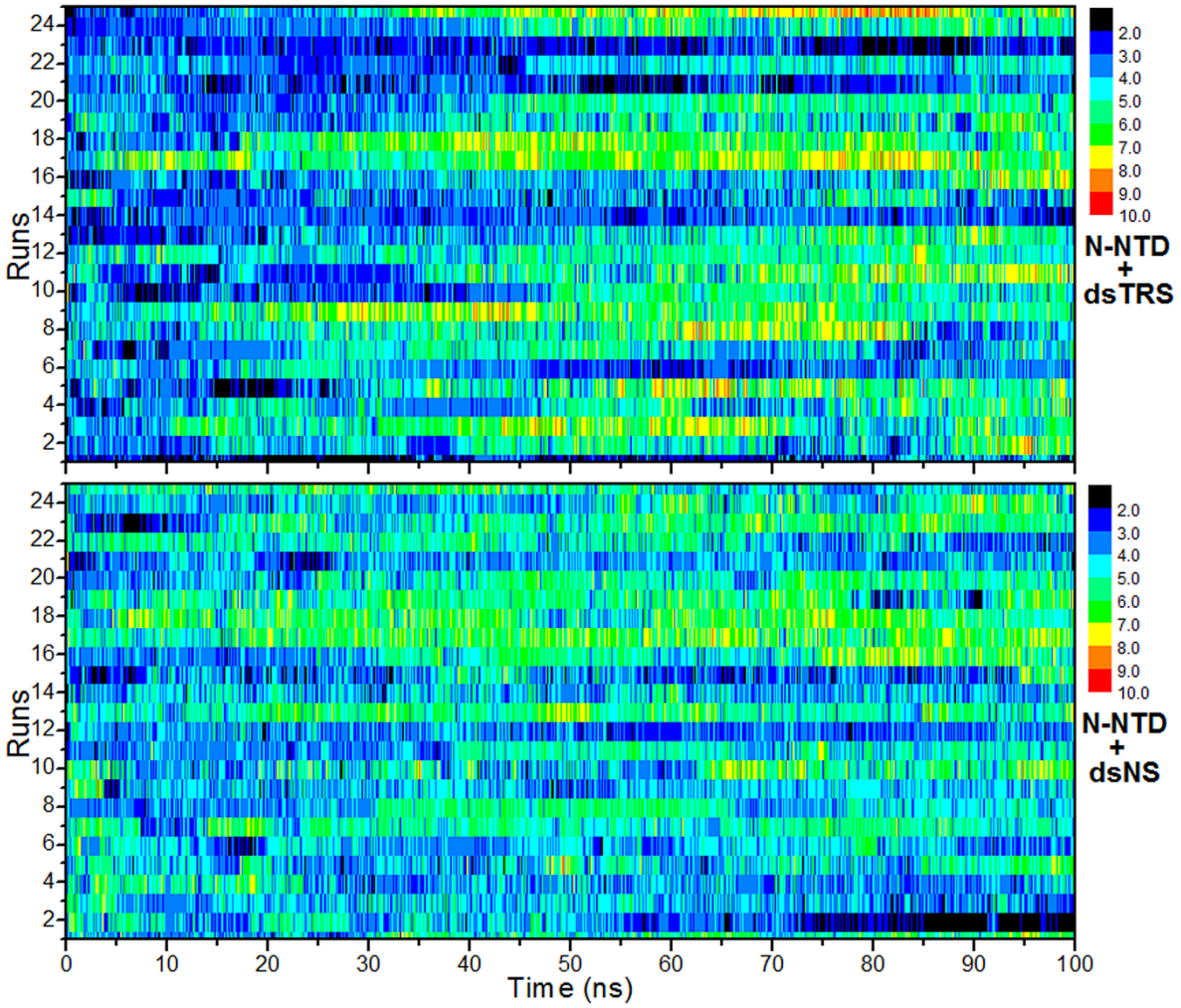

Figure S14. Number of intermolecular hydrogen bonds formed between the nitrogenous bases of the dsRNAs (dsTRS in top and dsNS in bottom) and N-NTD over the 100 ns simulations for the 25 MD replicas. The color bar denotes the correspondence between the color code and the number of intermolecular hydrogen bonds.

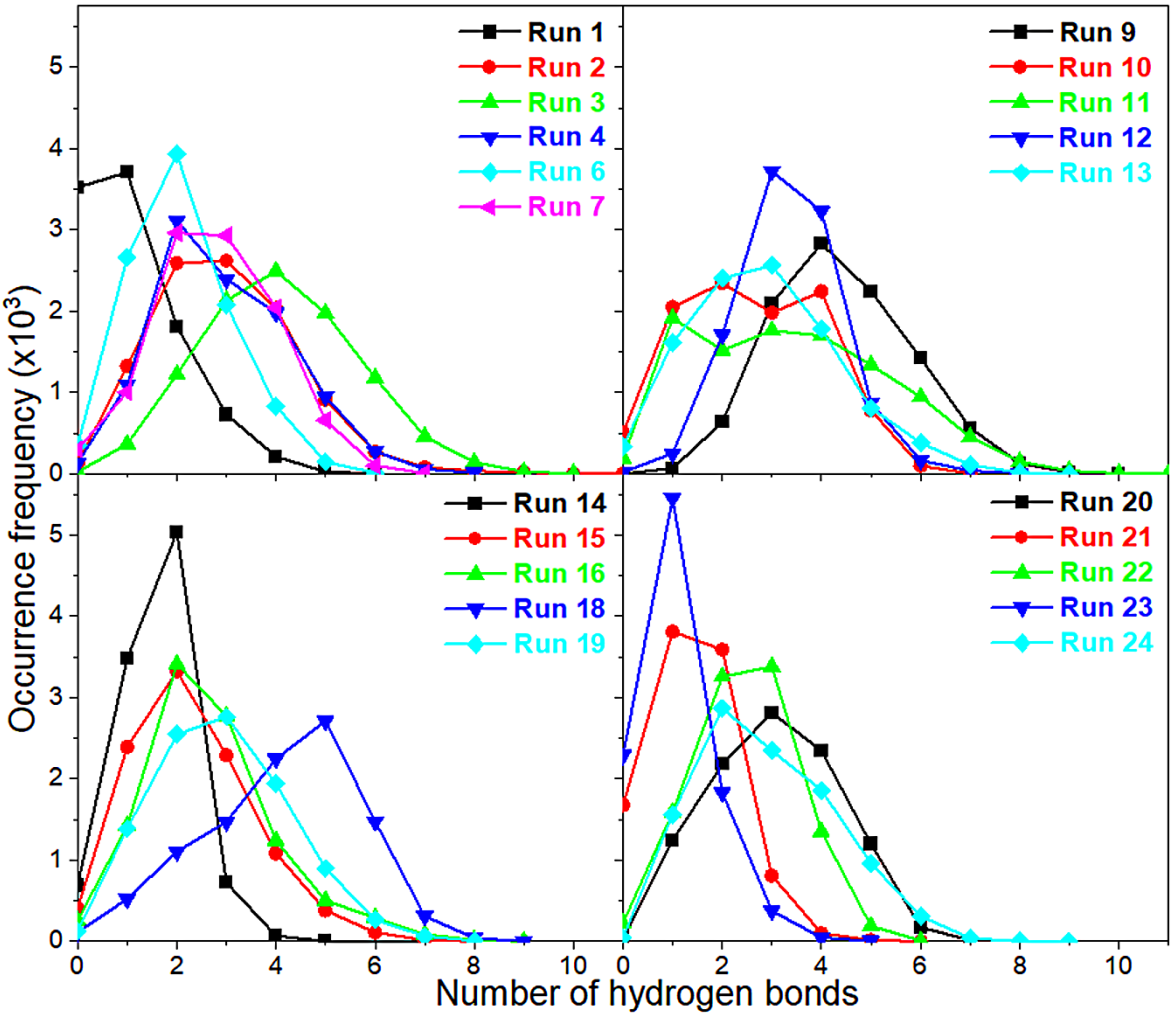

Figure S15. Distribution of the occurrence frequency of the number of hydrogen bonds between the nitrogenous bases of dsTRS and N-NTD along the 100 ns MD simulations.

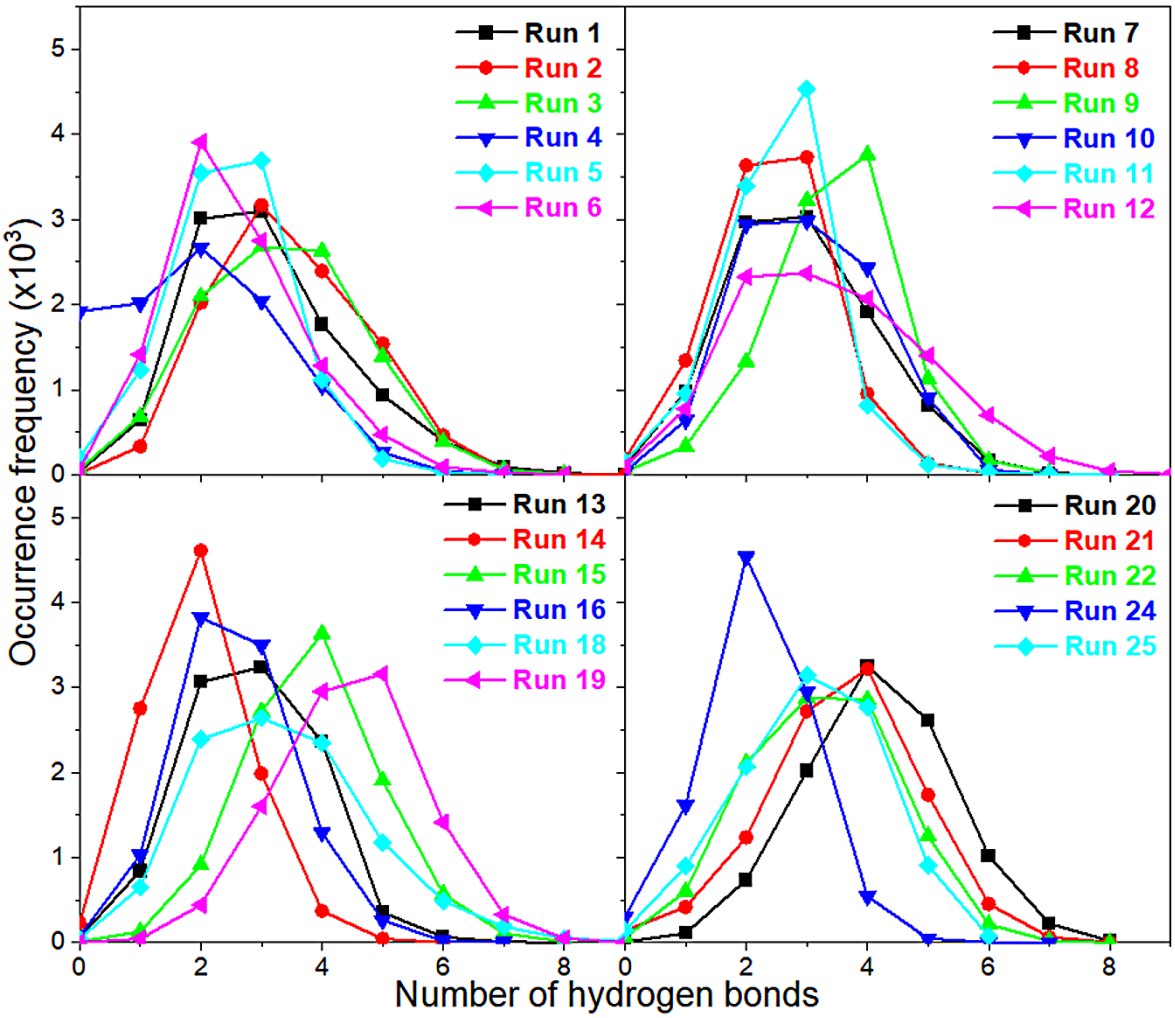

Figure S16. Distribution of the occurrence frequency of the number of hydrogen bonds between the nitrogenous bases of dsNS and N-NTD along the 100 ns MD simulations.

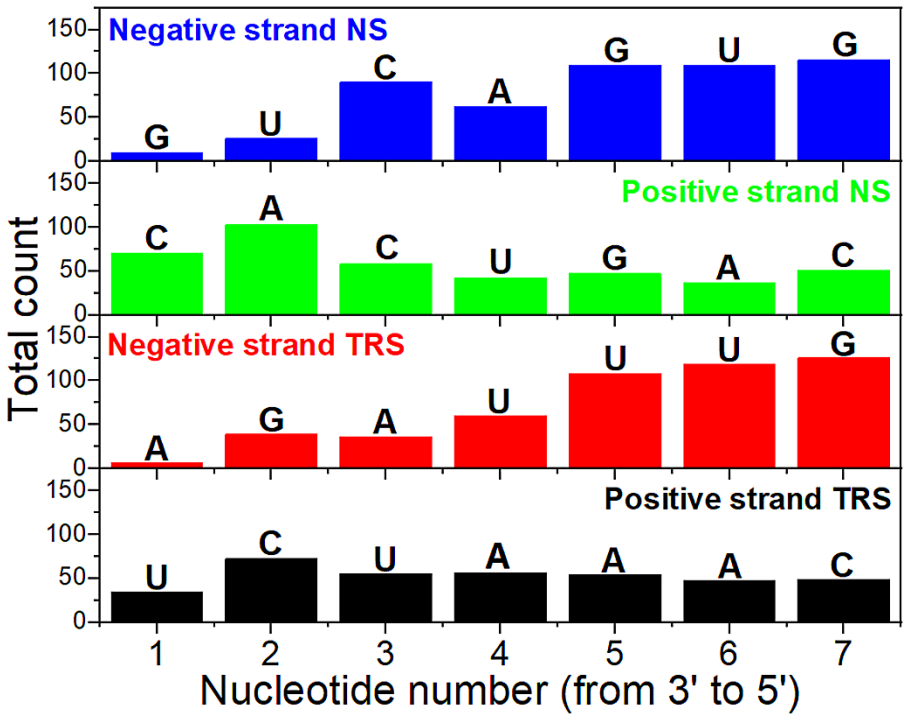

Figure S17. Total count of protein-RNA hydrogen bonds with persistency higher than 10% as a function of the residue number for 25 replicas along the 100 ns MD simulations.

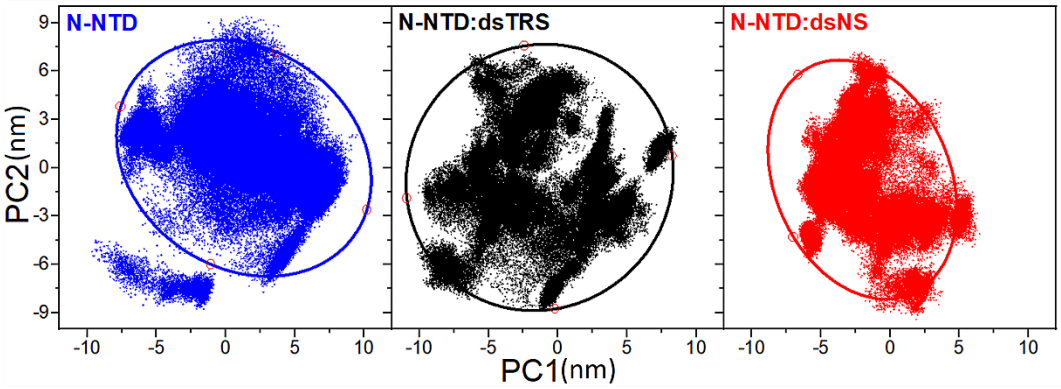

Figure S18. PCA scatter plots PC1 and PC2 for free N-NTD (blue dots – *left*) and for N-NTD complexed with either TRS (black dots – *middle*) or NS (red dots – *right*) dsRNAs, using the trajectories of all 25 replicas of free N-NTD concatenated with its bound states. The extent of the conformational space for each scatter plot was measured by fitting an elliptical shell (solid lines) that contains 95% of the density.

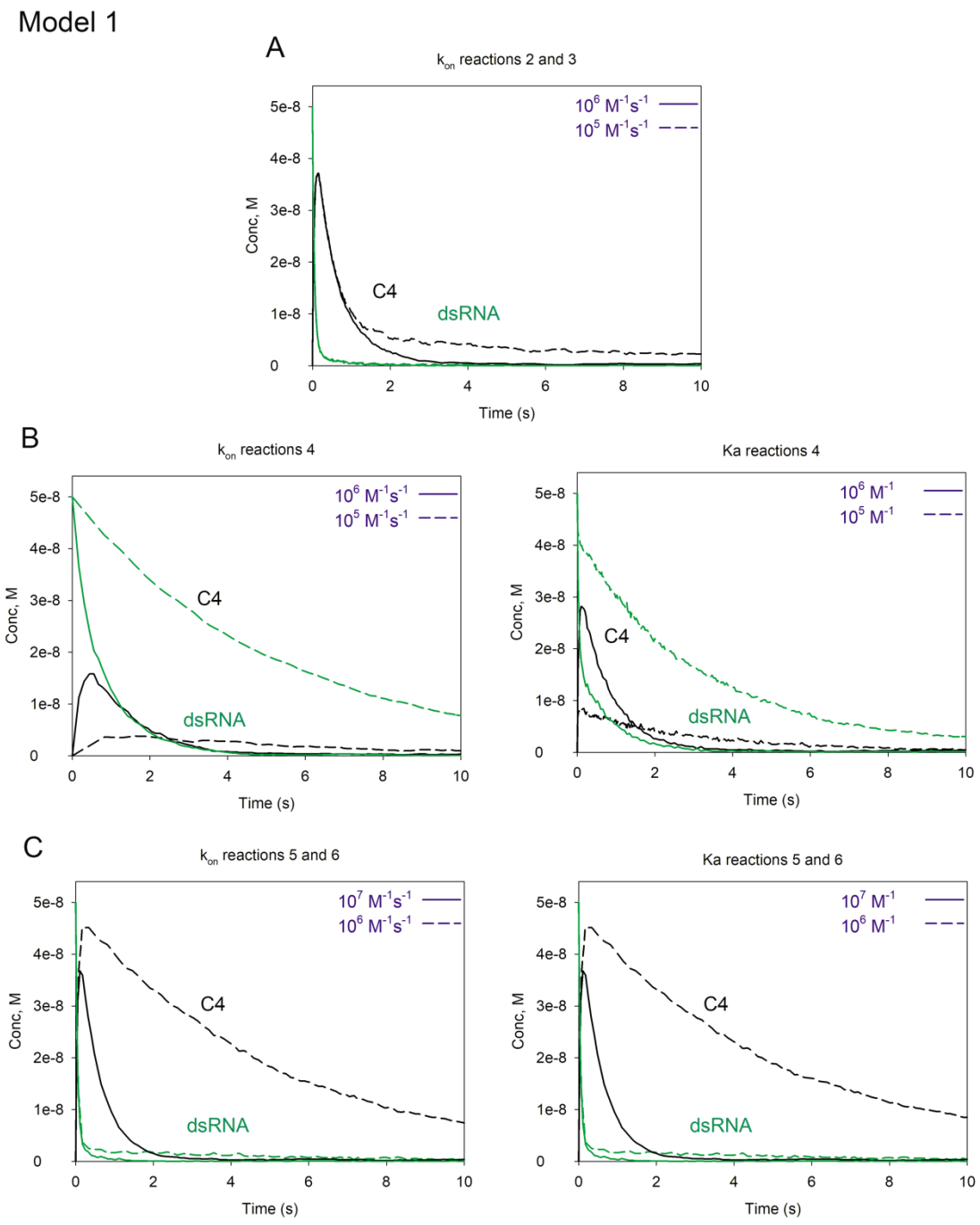

Figure S19. Simulations of the reactions progression for the validation of the ranges described in Figure 6A for model 1. A) Effect of the variation of k_{on} in reaction R2 and R3. Note that $k_{on} < 10^6$ $M^{-1}s^{-1}$ makes the reaction too slow to reach equilibrium, violating boundary B4. B) Effect of the variation of k_{on} (left) and K_a (right) in reaction R4. Note that $k_{on} < 10^6$ $M^{-1}s^{-1}$ or $K_a < 10^6$ M^{-1} make the reaction too slow to reach equilibrium, violating boundary B4. C) Effect of the variation of k_{on} (left) and K_a (right) in reactions R5 and R6. Note that $k_{on} < 10^6$ $M^{-1}s^{-1}$ or $K_a < 10^6$ M^{-1} make the reaction too slow to reach equilibrium, violating boundary B4. For model 1 simulations, we used the following reaction rates:

(R1) $k_{on} = 4\times10^{-1}$ $M^{-1}s^{-1}$ and $k_{off} = 8\times10^{-4}$ s^{-1}; (R2, R3) $k_{on} = 4\times10^{7}$ $M^{-1}s^{-1}$ and $k_{off} = 1$ s^{-1}; (R4) $k_{on} = 1\times10^{7}$ $M^{-1}s^{-1}$ and $k_{off} = 1$ s^{-1}; (R5, R6) $k_{on} = 4\times10^{7}$ $M^{-1}s^{-1}$ and $k_{off} = 1$ s^{-1} (red).

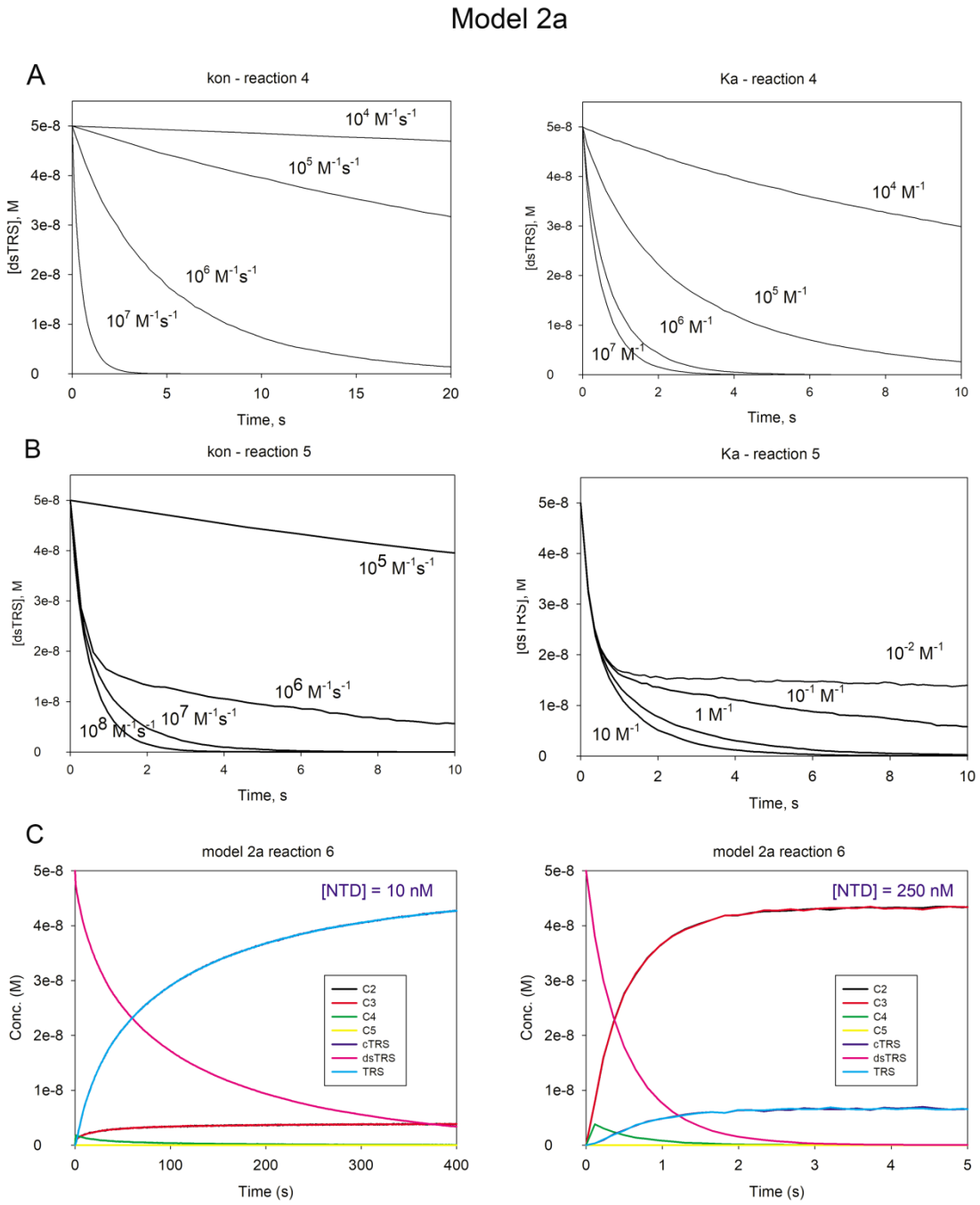

Figure S20. Simulations of the reactions progression for the validation of the ranges described in Figure 6A for model 2a. A) Effect of the variation of k_{on} (left) and K_a (right) in reaction R4. Note that $k_{on} < 10^6$ $M^{-1}s^{-1}$ or $K_a < 10^5$ M^{-1} make the reaction too slow to reach equilibrium, violating boundary B4. B) Effect of the variation of k_{on} (left) and K_a (right) in reaction R5. Note that $k_{on} < 10^7$ $M^{-1}s^{-1}$ or $K_a < 1$ M^{-1} make the reaction too slow to reach

equilibrium, violating boundary B4. C) Time course of the reaction R6 for each of the components. For model 2a, for $10^{7} > K_a > 10^{-6}$ M^{-1}, there is never accumulation of C5, resulting in a kinetic of dsRNA melting independent of k_{on} and k_{off} at fixed concentrations of N-NTD. The kinetics changes considerably with the [N-NTD] as showed in the figure. For values of $K_a > 10^{7}$ M^{-1} we observed the transition to model 2b with accumulation of C5. Note that for reactions R2 and R3, K_a was determined experimentally (4×10^{7} M^{-1}). Particularly for model 2a, the kinetic of dsRNA melting is independent of k_{on} and k_{off} of reactions R2 and R3, at fixed concentrations of N-NTD. For model 2a simulations, we used the following reaction rates: (R1) $k_{on} = 4\times10^{-1}$ $M^{-1}s^{-1}$ and $k_{off} = 8\times10^{-4}$ s^{-1}; (R2, R3) $k_{on} = 4\times10^{7}$ $M^{-1}s^{-1}$ and $k_{off} = 1$ s^{-1}; (R4) $k_{on} = 1\times10^{7}$ $M^{-1}s^{-1}$ and $k_{off} = 1$ s^{-1}; (R5) $k_{on} = 1\times10^{8}$ $M^{-1}s^{-1}$ and $k_{off} = 1$ s^{-1} and (R6) $k_{on} = 1\times10^{8}$ $M^{-1}s^{-1}$ and $k_{off} = 1\times10^{-1}$ s^{-1}.

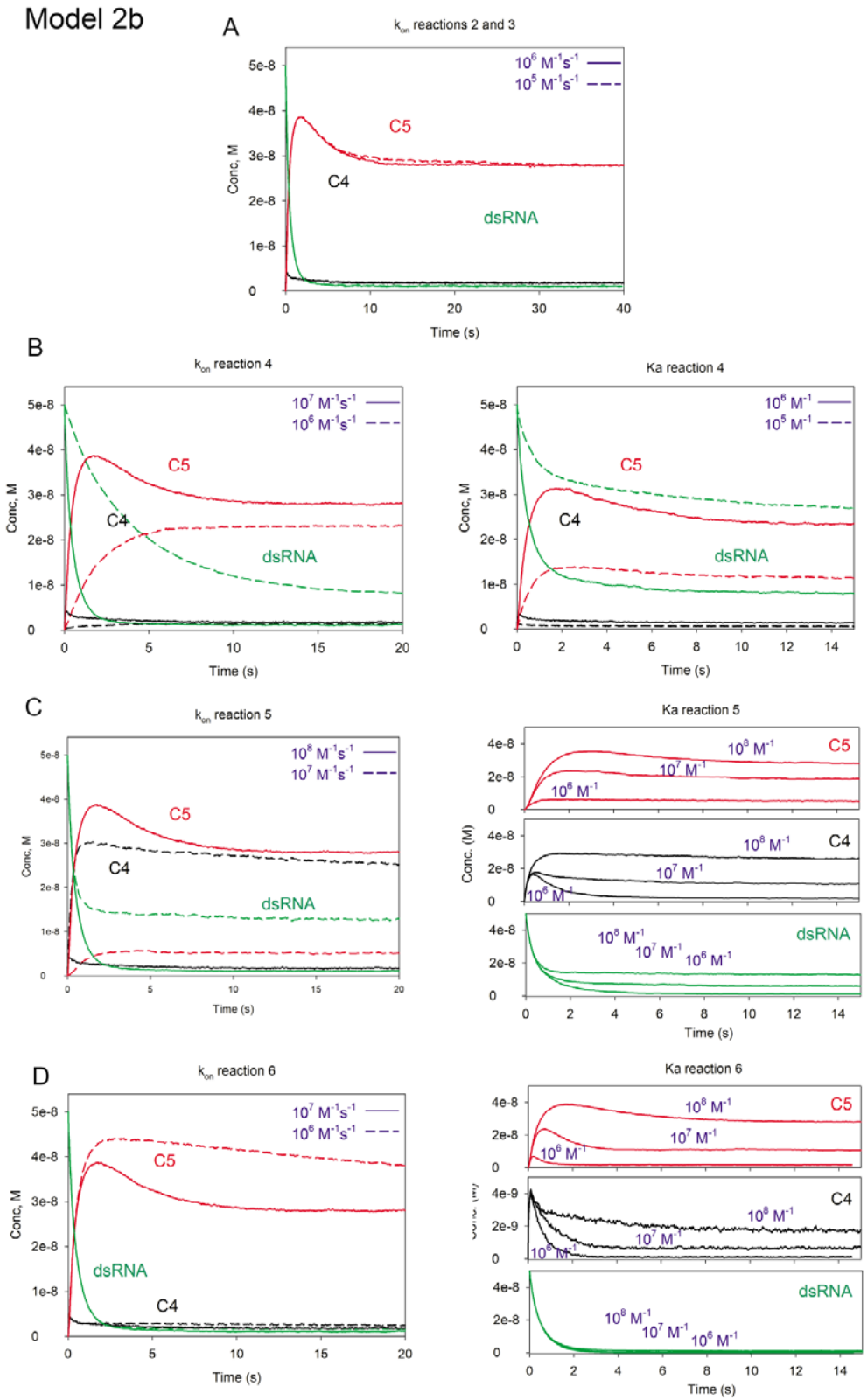

Figure S21. Simulations of the reactions progression for the validation of the ranges described in Figure 6A for model 2b. A) Effect of the variation of k_{on} in reactions R2 and

R3. Note that $k_{on} < 10^6$ $M^{-1}s^{-1}$ makes the reaction too slow to reach equilibrium, violating boundary B4. B) Effect of the variation of k_{on} (left) and K_a (right) in reaction R4. Note that $k_{on} < 10^7$ $M^{-1}s^{-1}$ or $K_a < 10^6$ M^{-1} make the reaction too slow to reach equilibrium, violating boundary B4. C) Effect of the variation of k_{on} (left) and K_a (right) in reaction R5. Note that $k_{on} < 10^7$ $M^{-1}s^{-1}$ or $K_a < 10^7$ M^{-1} make the reaction too slow to reach equilibrium, violating boundary B4. D) Effect of the variation of k_{on} (left) and K_a (right) in reaction R6. Note that $k_{on} < 10^6$ $M^{-1}s^{-1}$ or $K_a < 10^7$ M^{-1} make the reaction too slow to reach equilibrium, violating boundary B4. For model 2b simulations, we used the following reaction rates: (R1) $k_{on} = 4\times10^{-1}$ $M^{-1}s^{-1}$ and $k_{off} = 8\times10^{-4}$ s^{-1}; (R2, R3) $k_{on} = 4\times10^7$ $M^{-1}s^{-1}$ and $k_{off} = 1$ s^{-1}; (R4) $k_{on} = 1\times10^7$ $M^{-1}s^{-1}$ and $k_{off} = 1$ s^{-1}; (R5) $k_{on} = 1\times10^8$ $M^{-1}s^{-1}$ and $k_{off} = 1$ s^{-1} and (R6) $k_{on} = 1\times10^8$ $M^{-1}s^{-1}$ and $k_{off} = 1\times10^{-1}$ s^{-1}.

Table S1. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 1 of the N-NTD:dsTRS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
TYR69	OH	U9	O1P	89.971
ARG67	NH1	U10	O2P	86.851
ARG67	NH1	U9	O1P	86.201
ARG55	NE	U11	O1P	76.722
ARG67	NH2	U10	O2P	71.003
ARG55	NH2	U11	O1P	69.833
ARG52	NH2	U10	O1P	59.824
GLY59	N	A12	O1P	55.144
ARG52	NH1	U10	O1P	51.005
ARG137	NH2	A5	O2P	48.495
SER11	N	G8	O5'	41.626
GLY57	N	U11	O2P	39.596
ARG137	NH2	A4	O2P	38.366
ARG109	NH2	G8	N7	26.437
ASP58	N	U11	O3'	26.107
G8	O5'	PHE13	O	25.667
LYS60	NZ	G13	O2P	23.258
ARG55	NH2	U10	O3'	23.198
ARG137	NH2	A6	O2P	22.958
ARG137	NH1	A6	O2P	18.528
ARG137	NH1	A5	O2P	18.168
SER136	N	C2	O2P	17.718
ASP58	N	A12	O1P	17.248
U1	O5'	ALA133	O	17.078
GLY57	N	U11	O1P	17.008
ASP58	N	A12	O2P	16.048
ARG137	NH2	U3	O2P	12.999
ARG52	NH1	U9	O3'	12.499
U1	O5'	PHE131	O	11.629
LEU5	N	U9	O2'	11.319
G8	N2	PRO6	O	11.269

LYS60	NZ	A12	O2P	10.889
ARG137	NH2	C2	O1P	10.809
ARG137	NH1	A4	O2P	10.649

Table S2. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 2 of the N-NTD:dsTRS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG137	NH2	A4	O2P	86.341
TYR69	OH	U9	O2P	66.413
TYR132	OH	U3	O2P	65.723
TYR71	OH	G8	O5'	58.024
ARG137	NH2	U3	O1P	57.834
ARG52	NH2	U10	O1P	51.605
ARG52	NE	U10	O2P	49.785
ARG67	NH2	U10	O4	46.965
GLY20	N	C2	O1P	46.155
LYS62	NZ	G13	O6	45.335
SER65	OG	C2	O2P	43.236
ARG67	NH1	U10	O4	38.716
SER11	N	G8	O5'	37.536
ARG137	NH1	U3	O1P	35.976
ARG52	NH1	U9	O1P	35.806
A5	N6	GLU134	OE2	33.877
ARG137	NE	A4	O2P	32.117
SER11	N	G8	O4'	29.037
ARG52	NH2	U10	O2P	25.507
ARG137	NH2	U3	O5'	23.388
LYS60	NZ	G13	O2P	23.138
A5	N6	GLU134	OE1	22.968
ARG52	NH2	U9	O2P	19.138
GLY57	N	U11	O2P	17.598
ARG52	NH1	U9	O2P	16.108
ARG137	NE	A4	O1P	15.588
ARG137	NH2	U3	O2P	15.048
ARG137	NH1	U3	O2P	14.099
ALA15	N	G8	O6	14.009
GLY57	N	U11	O1P	13.279
LYS62	NZ	G13	N7	13.209
SER65	OG	U1	O5'	11.659
ARG52	NH2	U9	O1P	10.929
SER11	N	G8	N7	10.819
ARG52	NH2	U9	O5'	10.499
A6	N6	GLU134	OE2	10.199

Table S3. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 3 of the N-NTD:dsTRS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG137	NH2	A4	O2P	91.731
G8	N2	PRO111	O	88.321
ARG67	NH2	C2	O2P	84.022
U1	O5'	SER65	O	76.312
ARG52	NH1	U10	O2P	75.722
ARG52	NH1	U9	O1P	69.693
ARG137	NH2	U3	O1P	63.674
SER11	N	G8	O4'	62.444
ARG109	NH1	G8	N3	60.694
ARG52	NH2	U10	O2P	60.364
ARG137	NH1	U3	O1P	57.674
ARG67	NE	C2	O2P	56.654
ARG109	NH2	G8	N2	51.885
TYR132	OH	U3	O2P	49.315
GLY57	N	G13	N7	48.295
ARG55	NH2	U9	O2P	39.746
GLY57	N	G13	O6	35.236
ARG55	NH2	U10	O2P	30.607
ARG55	NH1	U10	O2P	28.607
ASN114	N	C7	O2'	25.517
ARG137	NE	A4	O2P	25.027
ARG55	NH1	U9	O2P	24.278
ALA116	N	G8	O6	23.448
C7	O2'	ALA112	O	22.748
LYS62	NZ	U1	O4	19.228
ARG137	NH2	U3	O5'	18.558
C2	N4	ARG55	O	18.248
ARG67	NH2	C2	O5'	16.658
ASN8	ND2	U9	O1P	14.839
TYR71	OH	G8	O5'	14.509
A12	N6	ARG55	O	14.279
ARG137	NH2	U3	O2P	12.839
SER11	N	G8	O5'	12.339
SER140	OG	A5	O1P	11.689
ARG52	NH2	U9	O1P	10.969
ARG52	NH1	U9	O2P	10.769

Table S4. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 4 of the N-NTD:dsTRS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
TYR69	OH	U9	O2P	73.193
GLY20	N	C2	O1P	54.375

SER11	N	G8	O5'	52.735
ARG137	NH2	A5	O2P	51.935
A6	N6	GLU134	OE1	51.705
ARG52	NH2	U11	O2P	41.666
ARG137	NH2	A4	O2P	38.346
TYR71	OH	G8	O5'	36.966
ARG137	NE	A5	O2P	36.126
HIS19	NE2	U3	O2P	32.097
ARG67	NH2	U9	O2P	32.037
SER11	N	G8	O4'	31.597
SER65	OG	C2	O2P	30.627
A6	N6	GLU134	OE2	30.107
LYS62	NZ	A14	N7	29.667
U1	O5'	ASP63	O	27.647
A14	N6	ASP63	O	27.547
C7	N4	GLU134	OE2	26.977
GLY20	N	C2	O2P	25.517
HIS19	NE2	U3	O1P	25.117
C7	N4	GLU134	OE1	23.288
SER140	N	A6	O1P	21.028
GLY139	N	A5	O1P	21.008
ARG52	NE	U10	O2P	19.868
ARG67	NE	U9	O2P	19.368
G8	N2	MET3	O	18.938
ARG52	NH1	U11	O2P	18.268
SER140	OG	A6	O1P	18.168
ARG137	NH1	A4	O2P	16.888
ARG52	NH2	U10	O2P	16.198
GLY57	N	G13	O2P	15.368
U9	O2'	ALA2	O	13.789
ARG52	NH1	U10	O2P	13.439
ARG137	NH2	A4	O1P	13.109
ARG67	NH2	U9	O1P	12.069
GLY139	N	A6	O1P	11.709
ARG52	NH2	U10	O1P	10.989
SER140	OG	A5	O1P	10.679
SER140	N	A5	O1P	10.539

Table S5. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 5 of the N-NTD:dsTRS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
A12	N6	ARG53	O	49.125
ARG55	NH2	A12	O2P	45.235
ARG53	NH1	U10	O2P	43.846
GLY138	N	C2	O2P	33.467
ASN8	ND2	G8	O2'	32.547
C2	N4	GLU134	OE2	26.847

ARG55	NH1	U11	O2P	26.437
ARG53	NH2	U11	O2P	26.187
GLY1	N	C7	O2	25.087
ARG53	NH2	U9	O2P	23.678
TYR69	OH	U9	O4	21.638
ARG55	NH2	U11	O5'	21.528
ARG55	NH2	A12	O1P	19.128
C2	N4	GLU134	OE1	19.128
ARG137	NH2	U3	O2P	18.888
ARG137	NH1	U3	O2P	18.668
ARG53	NH1	U9	O5'	18.318
GLY135	N	U3	O4	17.818
ASN8	N	G8	N2	17.578
U3	N3	GLU134	OE1	17.448
U1	O5'	ALA133	O	16.808
ARG55	NH2	U11	O2P	16.268
G8	N2	ASN7	OD1	15.448
ARG53	NH1	U9	O2P	15.418
A4	N6	GLU134	OE1	14.829
U1	O5'	SER136	O	13.989
ARG137	NE	C2	O2P	13.969
ARG137	NH1	C2	O2P	13.769
SER11	N	G8	O4'	13.479
ARG55	NH2	U11	O1P	13.169
SER140	OG	C2	O1P	12.949
ARG53	NH2	U10	O2P	12.749
TYR69	OH	U9	O2P	12.669
U3	N3	GLU134	OE2	12.539
ARG53	NH2	U9	O1P	11.959
GLY1	N	U9	O2'	11.909
ARG55	NH1	A12	O2P	11.419
ASN7	ND2	G8	O2'	10.639
ARG137	NH2	C2	O2P	10.619
ARG67	NH2	A4	N1	10.469
LEU5	N	C7	O2	10.379

Table S6. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 6 of the N-NTD:dsTRS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
G8	N2	PRO111	O	86.671
ARG67	NH2	C2	O2P	69.403
ARG52	NH1	U9	O2P	67.093
ASN8	ND2	U9	O1P	61.044
SER11	N	G8	O4'	58.784
ARG137	NH2	U3	O2P	56.054
ARG137	NH1	U3	O1P	54.095
ARG52	NH2	U9	O2P	53.275

G8	O2'	ASN8	OD1	53.085
SER65	N	U1	O5'	48.425
ARG67	NH1	C2	O2P	48.105
LYS62	NZ	G13	O6	44.366
ARG137	NH2	A4	O2P	25.317
C7	O2'	ALA112	O	24.528
ARG109	NH2	G8	N3	23.758
ARG137	NH2	U3	O1P	20.458
TYR69	OH	G8	O5'	17.708
GLY57	N	A12	O2P	16.808
ALA116	N	G8	O6	14.799
ARG137	NH1	C2	O1P	14.039
TYR132	OH	C2	O1P	13.669
LYS60	NZ	A12	O2P	13.179
ARG137	NE	A4	O1P	12.799
U1	O5'	ASP63	O	11.019
LYS60	NZ	U11	O1P	10.039

Table S7. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 7 of the N-NTD:dsTRS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG137	NH2	A4	O2P	97.16
ARG67	NH2	C2	O2P	89.071
ARG67	NH1	C2	O2P	80.562
SER11	N	G8	O4'	79.992
LYS62	NZ	G13	O6	76.422
ARG52	NH2	U10	O1P	75.512
SER65	N	U1	O5'	75.422
ARG52	NH1	U9	O1P	61.304
ASN8	ND2	U9	O1P	58.334
ARG52	NE	U10	O2P	53.455
ARG137	NE	A4	O1P	49.365
ARG137	NH2	U3	O2P	49.315
LYS60	NZ	A12	O2P	44.816
G8	O2'	ASN8	OD1	42.886
ARG137	NE	A4	O2P	41.996
SER140	N	A6	O2P	39.916
SER140	OG	A6	O1P	37.576
A5	N6	GLU134	OE1	37.456
A5	N6	GLU134	OE2	35.466
ARG109	NH1	G8	N3	33.557
ARG137	NH2	U3	O1P	32.707
ARG137	NH1	U3	O1P	31.147
GLY139	N	A5	O1P	23.978
ASN113	ND2	U9	O2'	23.348
ASP58	N	U11	O1P	20.628
ARG109	NH2	G8	N3	18.708

ALA116	N	C7	N4	17.628
ARG52	NE	U10	O1P	17.258
G8	N2	ASN113	OD1	16.218
ASN113	ND2	C7	O2	15.648
LYS60	NZ	U11	O1P	15.118
ASN8	ND2	G8	O3'	11.479
LYS60	NZ	A12	O1P	10.109

Table S8. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 8 of the N-NTD:dsTRS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG137	NH2	A4	O2P	82.132
G8	N2	PRO111	O	80.852
ARG137	NH1	U3	O2P	76.952
ARG52	NH2	U10	O2P	64.894
ARG52	NH1	U10	O2P	62.964
GLY57	N	A12	O2P	61.324
A14	N6	LYS62	O	56.154
GLY135	N	C2	O1P	54.405
ARG137	NH2	U3	O2P	53.525
MET3	N	U9	O2'	51.275
SER65	N	U1	O4'	50.005
GLY135	N	C2	O2P	43.826
TYR71	OH	G8	O5'	41.916
ARG52	NH1	U9	O1P	41.696
LYS62	NZ	G13	N7	38.956
LYS62	NZ	G13	O6	37.396
C7	O3'	ALA112	O	35.906
ARG109	NH2	G8	N3	35.036
SER11	N	G8	O5'	27.037
SER11	N	G8	O4'	24.868
HIS19	NE2	U1	O2'	23.508
ARG137	NH2	U3	O5'	22.778
HIS19	NE2	C2	O1P	20.788
ARG109	NH2	G8	N2	20.388
ARG52	NH2	U9	O1P	20.178
ARG109	NH1	G8	N2	16.878
U9	O2'	MET3	O	16.308
ARG52	NH2	U10	O1P	16.038
ARG67	NH1	U9	O4	15.498
C7	O2'	ALA112	O	15.158
C7	O2'	ASN114	O	15.128
ARG109	NH1	G8	N3	14.399
ASN8	ND2	G8	O2'	13.289
ASN8	ND2	G8	O3'	11.999
LYS60	NZ	G13	O2P	11.669
SER65	N	U1	O2	11.479

ARG52	NH1	U9	O2P	11.309
ARG52	NE	U9	O2P	10.269

Table S9. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 9 of the N-NTD:dsTRS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
G8	N2	PRO111	O	99.08
ASN8	ND2	U9	O1P	86.611
ARG109	NH1	G8	N3	85.681
SER11	N	G8	O4'	79.372
ARG67	NH2	C2	O2P	77.212
ARG52	NH2	U11	O2P	76.132
ARG52	NE	U10	O2P	71.663
C7	O2'	ALA112	O	61.164
ARG109	NH2	G8	N2	59.704
G8	O2'	ASN8	OD1	58.664
ARG137	NH1	A5	O2P	54.065
LYS62	NZ	G13	O6	48.295
ARG52	NH2	U10	O2P	45.505
ARG55	NH2	U11	O1P	42.186
ARG137	NH2	A4	O1P	42.006
ARG55	NH1	U11	O2P	35.626
ARG52	NH2	U10	O5'	35.026
ARG137	NH1	A4	O5'	33.207
A6	N6	SER136	OG	32.387
TYR132	OH	U3	O2P	31.307
ARG137	NH2	A4	O2P	28.827
ARG137	NH1	A4	O1P	25.097
ARG55	NH1	U10	O1P	24.578
ARG53	N	U9	O1P	23.738
C7	N4	GLY138	O	22.288
SER136	OG	A6	N7	22.028
ARG67	NH1	C2	O2P	20.618
ARG53	NH2	U10	O1P	19.758
LYS60	NZ	A12	O2P	18.438
ARG55	NH2	U11	O2P	17.558
ARG137	N	A5	O1P	16.428
SER136	OG	A6	O2P	16.028
LYS62	NZ	U1	O4	14.489
ARG53	NE	U10	O1P	14.299
ARG52	NH1	U10	O2P	14.199
ARG137	NH1	A4	O2P	14.149
ARG55	NH2	A12	O2P	13.959
ARG55	NH1	U11	O1P	12.549
ARG52	NH1	U11	O2P	11.389

Table S10. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 10 of the N-NTD:dsTRS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ASN8	ND2	U9	O1P	95.73
SER11	N	G8	O4'	85.051
G8	O2'	ASN8	OD1	81.052
ARG52	NH1	U9	O2P	68.343
ARG52	NH1	U10	O2P	67.613
ARG52	NH2	U10	O2P	61.284
G8	N2	ALA112	O	50.995
LYS62	NZ	G13	O6	43.876
ASN113	ND2	U9	O2	39.476
GLY139	N	A4	O1P	34.637
ARG67	NH2	C2	O2P	34.177
SER65	OG	C2	O2P	33.887
SER140	N	A5	O1P	32.147
THR14	OG1	G8	O6	31.217
G8	N2	PRO111	O	28.877
SER140	OG	A5	O1P	27.357
ARG53	NE	U9	O1P	27.327
ARG53	NH2	U9	O1P	22.408
ASN113	ND2	U10	O4'	22.008
ARG52	NH1	U9	O1P	21.678
ARG137	NH2	A4	O2P	19.688
ASN114	N	G8	N2	17.608
ARG67	NH1	C2	O2P	17.388
ARG53	NH2	G8	O3'	17.348
ARG55	NH1	U11	O2P	16.328
ARG55	NH2	A12	O2P	14.249
C7	O2'	ALA112	O	13.959
ASN114	N	C7	O2	13.819
SER140	OG	A4	O3'	13.199
U1	O5'	ASP63	O	12.209
ARG137	NH1	A4	O2P	11.969
SER65	OG	U1	O5'	11.059
C7	O3'	ASN113	O	10.749
GLY139	N	A5	O1P	10.439

Table S11. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 11 of the N-NTD:dsTRS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG137	NH1	A5	O2P	74.893
C7	O2'	ALA116	O	44.726
ARG137	NH2	A4	O2P	43.476
ARG67	NH2	C2	O2P	42.776

ARG137	NH2	A4	O1P	42.736
ARG109	NH2	G8	N3	41.366
SER65	OG	C2	O2P	38.096
A6	N6	GLU134	OE2	38.036
TYR69	OH	G8	N7	32.767
ARG137	NH1	A4	O5'	31.467
C2	N4	ASP63	O	31.467
LYS62	NZ	G13	O6	30.467
ARG137	NH1	A4	O1P	29.627
A6	N6	GLU134	OE1	28.987
ARG52	NH1	U9	O1P	28.437
ALA116	N	C7	O2	23.388
ARG137	NH1	A4	O2P	23.288
ARG52	NH2	U10	O1P	23.018
SER11	N	G8	O4'	21.028
ARG52	NH2	U10	O2P	19.338
ARG53	N	U9	O2P	17.758
ARG52	NE	U10	O2P	16.358
ARG67	NH1	C2	O2P	16.128
LYS62	NZ	G13	N7	14.779
G8	O5'	THR51	O	14.299
ASN8	ND2	U9	O1P	14.059
A5	N6	GLU134	OE2	13.409
GLY139	N	C7	O2P	12.949
LYS60	NZ	A12	O2P	12.929
A5	N6	GLU134	OE1	12.629
ARG52	NE	U9	O2P	12.349
ARG53	NH1	U9	O1P	11.029
ARG137	NH2	A5	O2P	11.019
LYS60	NZ	U11	O1P	10.119

Table S12. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 12 of the N-NTD:dsTRS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
SER11	N	G8	O4'	91.081
ALA15	N	G8	O6	88.661
ASN8	ND2	U9	O1P	64.134
ARG52	NH1	U9	O2P	62.854
ARG52	NH2	U10	O2P	58.784
SER65	OG	C2	O2P	52.505
LYS62	NZ	G13	O6	47.575
SER136	OG	C7	O2P	45.715
C7	N4	GLU134	O	43.316
ARG52	NH1	U10	O2P	42.966
C7	O2'	ALA116	O	42.726
G8	O2'	ASN8	OD1	28.927
A5	N6	GLU134	OE1	24.328

U1	O5'	ASP63	O	17.968
ARG137	NH2	A5	O2P	15.468
TYR69	OH	U9	O4	15.458
ARG52	NH2	U9	O2P	14.889
A5	N6	GLU134	OE2	13.379
A5	N6	GLU134	O	12.609
ARG137	NH1	A5	O2P	12.079
ARG109	NH2	G8	O2'	11.109
ARG137	NH2	A4	O2P	10.899
ARG137	NH2	A6	O1P	10.629
GLY1	N	U10	O1P	10.449
ARG52	NH2	U10	O5'	10.449
U1	O5'	LYS62	O	10.239

Table S13. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 13 of the N-NTD:dsTRS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG52	NH2	U10	O2P	65.473
ARG52	NH1	U10	O2P	56.324
ARG48	NH2	U9	O1P	49.485
THR9	OG1	G8	N2	46.625
LYS62	NZ	U11	O4	45.025
SER65	OG	C2	O2P	42.236
ARG52	NH1	U9	O1P	41.726
LYS62	NZ	U10	O4	35.426
THR9	OG1	G8	N3	35.096
LYS60	NZ	A12	O2P	34.437
ASN110	ND2	C7	O3'	30.657
C2	N4	LYS62	O	30.057
G8	N2	ASN8	O	29.557
ARG67	NH2	C2	O2P	27.337
TYR71	OH	G8	O5'	25.507
LYS60	NZ	G13	O2P	24.828
U1	O5'	ASP63	OD1	23.708
THR9	OG1	G8	O2'	21.988
ARG137	NH2	A4	O2P	20.918
ARG52	NH2	U10	O1P	18.808
ARG67	NH2	C2	O1P	16.548
C7	O2'	ASN110	OD1	15.298
SER140	OG	A4	O2P	14.269
ARG52	NH1	U9	O2P	14.109
ARG48	NH1	U9	O1P	12.929
C7	O2'	ASN8	OD1	12.719
ARG52	NE	U10	O2P	12.429
ARG52	NH2	U9	O2P	12.109
ARG52	NE	U9	O2P	11.909
ARG137	NH2	U3	O2P	11.179

ARG137	NH1	U3	O2P	10.049

Table S14. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 14 of the N-NTD:dsTRS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ASN8	ND2	U9	O1P	88.451
SER11	N	G8	O4'	79.162
ARG67	NH2	C2	O2P	77.662
G8	N2	PRO111	O	75.962
G8	O2'	ASN8	OD1	73.253
ARG137	NH2	A4	O2P	60.934
ARG52	NH1	U9	O1P	52.525
ARG52	NH2	U10	O1P	45.295
LYS60	NZ	A12	O2P	44.456
ARG52	NE	U10	O2P	43.366
ARG137	NH2	U3	O1P	33.547
ARG137	NH2	A5	O2P	33.437
LYS62	NZ	G13	O6	30.797
ARG137	NH1	U3	O1P	25.287
ARG67	NH1	C2	O2P	24.208
ARG137	NH1	A4	O1P	23.128
ARG137	NH1	A4	O2P	17.528
LYS60	NZ	U11	O1P	16.218
ARG137	NH2	A4	O1P	15.778
C7	O2'	ALA112	O	14.879
LYS62	NZ	U11	O4	14.739
LYS62	NZ	U10	O4	14.309
ARG52	NH2	U11	O2P	12.049
ARG137	NE	A5	O2P	11.019
ARG53	N	U9	O1P	10.179
ARG137	NE	A4	O1P	10.179

Table S15. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 15 of the N-NTD:dsTRS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG52	NH2	U10	O1P	90.731
SER11	N	G8	O4'	87.771
ARG52	NE	U10	O2P	81.122
ASN8	ND2	G8	O5'	70.823
SER65	OG	C2	O2P	63.744
ARG52	NH1	U9	O1P	56.774
ASP58	N	U11	O1P	51.925
ARG137	NH2	A6	O1P	47.055

LYS62	NZ	U11	O2P	46.425
A6	N6	GLU134	OE1	46.375
ASN7	N	U9	O1P	45.345
ALA15	N	G8	O6	44.186
A6	N6	GLU134	OE2	40.856
LYS60	NZ	A12	O2P	36.106
GLY4	N	U9	O2'	35.266
ARG137	NH2	C7	O2P	31.617
A5	N6	GLU134	OE2	31.057
ARG137	NE	A6	O2P	30.077
A5	N6	GLU134	OE1	29.237
ASN8	N	U9	O1P	23.178
GLY138	N	A5	O2P	22.298
ARG137	NE	A6	O1P	21.658
GLY57	N	U10	O3'	21.088
U1	O5'	ASP63	O	17.488
GLY57	N	U10	O1P	15.608
ARG137	NH1	C7	O2P	15.258
GLY57	N	U11	O1P	15.168
GLY20	N	U3	O1P	14.579
ARG137	NH2	A6	O2P	13.939
ARG109	NH2	G8	N3	12.389
ASN8	ND2	U9	O1P	11.059
GLY138	N	A5	O1P	11.039

Table S16. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 16 of the N-NTD:dsTRS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG52	NH2	U10	O1P	90.731
SER11	N	G8	O4'	87.771
ARG52	NE	U10	O2P	81.122
ASN8	ND2	G8	O5'	70.823
SER65	OG	C2	O2P	63.744
ARG52	NH1	U9	O1P	56.774
ASP58	N	U11	O1P	51.925
ARG137	NH2	A6	O1P	47.055
LYS62	NZ	U11	O2P	46.425
A6	N6	GLU134	OE1	46.375
ASN7	N	U9	O1P	45.345
ALA15	N	G8	O6	44.186
A6	N6	GLU134	OE2	40.856
LYS60	NZ	A12	O2P	36.106
GLY4	N	U9	O2'	35.266
ARG137	NH2	C7	O2P	31.617
A5	N6	GLU134	OE2	31.057
ARG137	NE	A6	O2P	30.077
A5	N6	GLU134	OE1	29.237

ASN8	N	U9	O1P	23.178
GLY138	N	A5	O2P	22.298
ARG137	NE	A6	O1P	21.658
GLY57	N	U10	O3'	21.088
U1	O5'	ASP63	O	17.488
GLY57	N	U10	O1P	15.608
ARG137	NH1	C7	O2P	15.258
GLY57	N	U11	O1P	15.168
GLY20	N	U3	O1P	14.579
ARG137	NH2	A6	O2P	13.939
ARG109	NH2	G8	N3	12.389
ASN8	ND2	U9	O1P	11.059
GLY138	N	A5	O1P	11.039

Table S17. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 17 of the N-NTD:dsTRS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
TYR69	OH	U9	O2P	85.441
ALA15	N	G8	O6	82.052
ARG52	NH1	U11	O2P	71.533
ARG137	NE	U3	O2P	67.643
ARG67	NH1	U9	O4	62.614
ARG52	NH2	U11	O2P	60.224
A6	N6	SER140	OC1	42.976
ARG52	NH1	U10	O2P	41.026
A6	N6	GLU134	OE2	36.776
A6	N6	GLU134	OE1	36.396
ARG52	NH1	U10	O1P	31.967
C7	N4	SER140	OC2	30.957
ARG137	NH1	A4	O2P	27.637
ARG55	NH1	U11	O1P	25.507
ARG137	NH2	U3	O2P	24.318
ARG55	NH2	A12	O1P	21.748
THR51	OG1	U9	O1P	20.888
C7	N4	SER140	OC1	18.278
THR51	N	U9	O2P	17.678
A6	N6	SER140	OC2	17.328
ARG52	NH2	U10	O1P	16.808
ARG55	NH1	A12	O2P	16.218
ARG55	NH2	A12	O2P	15.908
LYS60	NZ	G13	N7	13.709
SER11	N	G8	O4'	12.919
MET61	N	G13	O2P	12.719
ARG55	NH2	U11	O1P	12.459
ARG52	NE	U10	O2P	12.159
TYR71	OH	G8	O5'	11.879
LYS60	NZ	G13	O2P	11.549

LYS60	NZ	G13	O6	10.849
ARG109	NH1	C7	O2	10.399

Table S18. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 18 of the N-NTD:dsTRS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
SER65	OG	C2	O2P	92.471
SER65	OG	U1	O5'	86.661
GLY20	N	C2	O1P	78.272
LYS62	NZ	G13	O6	72.413
A6	N6	GLU134	OE1	67.753
SER11	N	G8	O4'	61.564
ARG67	NH2	U10	O4	55.734
ARG52	NH2	U11	O2P	50.715
A5	N6	GLU134	OE2	45.525
ARG52	NH2	U10	O2P	44.046
ARG52	NE	U10	O2P	41.696
ASN8	ND2	U9	O1P	41.566
ARG67	NH1	U9	O4	35.296
SER136	OG	C7	O2P	33.277
ARG137	NE	A6	O1P	32.447
ARG137	N	A6	O2P	30.087
SER11	N	G8	O5'	29.657
TYR69	OH	U9	O2P	28.207
ARG67	NH1	U10	O4	25.857
C7	N4	GLY135	O	24.758
TYR71	OH	G8	O5'	22.798
ARG52	NH2	U9	O1P	21.968
C7	N4	GLU134	OE1	21.908
ARG137	NH2	A6	O1P	21.708
TYR132	OH	A5	O2P	20.948
ARG137	NH2	A5	O1P	20.238
ARG137	NE	A6	O2P	19.918
LYS21	NZ	U1	O5'	19.888
HIS19	NE2	U3	O1P	19.878
HIS19	NE2	U3	O2P	17.838
ARG137	NH2	A6	O2P	17.218
ARG52	NH1	U10	O2P	15.668
ARG137	NH2	A5	O2P	15.108
ARG52	NH2	U10	O1P	14.939
C7	O2'	SER140	OC1	14.319
ARG55	NH1	U11	O1P	13.819
A6	N6	GLU134	OE2	13.519
ARG52	NH1	U9	O2P	13.379
ARG52	NH2	U10	O5'	13.139
LYS62	NZ	G13	N7	12.699
ARG52	NH1	U9	O1P	11.539

ARG55	NH2	A12	O1P	11.409
ARG55	NH2	U11	O1P	11.279
C7	O3'	SER140	OC1	10.769
GLY20	N	C2	O2P	10.349
ARG55	NE	A12	O1P	10.059

Table S19. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 19 of the N-NTD:dsTRS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
TYR69	OH	U9	O2P	59.374
ARG137	NH2	A6	O2P	56.354
TYR71	OH	G8	O5'	56.334
SER11	N	G8	O4'	53.535
A6	N6	GLU134	OE1	43.586
LYS62	NZ	G13	O6	43.226
ARG137	NE	A6	O2P	42.416
ARG52	NH2	U11	O2P	41.616
SER11	N	G8	O5'	40.796
ARG52	NH2	U10	O1P	40.716
ARG52	NE	U10	O2P	40.426
HIS19	NE2	U3	O1P	36.456
A5	N6	GLU134	OE2	36.376
HIS19	NE2	U3	O2P	29.877
GLY20	N	C2	O1P	27.647
TYR132	OH	U3	O2P	27.377
GLY20	N	C2	O2P	26.717
A5	N6	GLU134	OE1	25.167
ARG53	NE	U9	O1P	25.097
ARG67	NH1	U10	O4	24.988
ARG67	NH2	U10	O4	24.598
ARG52	NH1	U11	O2P	23.338
ARG53	NH2	G8	O3'	22.058
LYS62	NZ	G13	N7	16.408
A6	N6	GLU134	OE2	15.398
ARG137	NH1	A5	O2P	15.048
LYS60	NZ	A12	O2P	14.909
TYR132	OH	C2	O2P	14.329
SER65	OG	C2	O2P	13.099
LYS60	NZ	A12	O1P	12.779
ARG137	NH2	A4	O2P	12.659
ARG52	NE	U10	O1P	11.229
SER65	OG	U1	O5'	11.089
ARG52	NH1	U10	O1P	11.069
LYS60	NZ	G13	O2P	10.569

Table S20. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 20 of the N-NTD:dsTRS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
G8	N2	PRO111	O	98.31
ARG137	NH1	A4	O2P	94.911
SER11	N	G8	O4'	84.882
ARG137	NH2	U3	O1P	78.582
ARG55	NH1	U11	O2P	66.813
ARG55	NH2	U10	O1P	65.853
ARG53	NH1	U10	O2P	60.174
C7	O2'	ALA112	O	54.205
ARG109	NH1	G8	N3	53.995
ARG109	NH2	G8	N2	53.295
ARG137	NH1	U3	O1P	52.145
ARG55	NH1	U10	O1P	50.505
ARG137	NH1	U3	O5'	49.945
ARG53	NH1	U9	O1P	39.996
ARG55	NH1	U10	O5'	37.486
ARG53	NH2	U9	O1P	33.637
GLY4	N	U9	O2'	31.537
ARG52	NH1	C2	O2P	31.067
LYS60	NZ	G13	N7	30.737
LYS60	NZ	A12	N7	27.197
SER65	N	U1	O5'	24.268
GLY4	N	U9	O3'	23.618
ARG67	NH2	C2	O1P	23.098
ARG53	NH1	U9	O2P	20.328
ARG55	NH2	U11	O2P	15.928
ARG52	NH2	C2	O2P	15.418
SER65	N	C2	O2P	15.338
ARG109	NH2	G8	N3	15.168
ARG53	NH1	U9	O5'	14.229
ARG55	NH1	U10	O2P	12.899
ARG137	NH1	U3	O2P	11.879
GLY1	N	U10	O2'	10.909
ARG55	NH2	U10	O2P	10.119
C7	O3'	ASN113	O	10.009

Table S21. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 21 of the N-NTD:dsTRS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG52	NH1	U10	O2P	49.675

GLY138	N	C2	O1P	41.006
TYR69	OH	U9	O2P	38.796
ASN8	ND2	U9	O1P	36.816
ARG52	NH2	U10	O2P	34.217
ARG52	NH2	U9	O1P	33.167
G8	O2'	ASN8	OD1	32.797
ARG137	NH1	C2	O1P	31.787
ARG55	NH1	U11	O2P	31.477
GLY57	N	G13	O2P	30.967
THR51	OG1	U9	O1P	29.627
SER11	N	G8	O5'	27.787
U1	O5'	GLU134	OE1	26.817
TYR132	OH	C2	O1P	26.797
ARG137	NH2	U3	O2P	26.057
G8	N2	ASN7	OD1	25.907
THR51	N	U9	O1P	21.248
ARG52	NH1	U10	O1P	19.548
G8	N2	MET3	O	17.318
U1	O2'	SER136	O	17.008
ARG55	NH2	A12	O2P	16.418
ARG137	NH2	C2	O1P	15.888
ASP58	N	A12	O1P	15.038
LYS62	NZ	U1	O4	14.049
LEU5	N	C7	O2	13.909
TYR132	OH	C2	O2P	13.239
TYR71	OH	G8	O5'	12.999
G8	O2'	ASN7	O	12.699
ARG52	NH1	U9	O1P	12.669
LYS62	NZ	G13	O6	11.849
ARG137	NH2	U3	O1P	10.969
U1	O5'	SER65	O	10.599
ARG137	NH1	U3	O1P	10.179

Table S22. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 22 of the N-NTD:dsTRS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
LYS62	NZ	G13	O6	50.245
C7	O2'	ALA116	O	47.445
SER65	OG	C2	O2P	44.936
SER11	N	G8	O4'	42.196
ALA116	N	C7	O2	40.356
ARG52	NH1	U9	O1P	40.036
G8	N2	PRO111	O	32.907
ASN8	ND2	U9	O1P	32.897
ARG67	NH2	C2	O1P	31.247
LYS60	NZ	U10	O2P	30.787
ARG137	NH2	A4	O2P	28.767

G8	O2'	ASN8	OD1	26.877
G8	N2	ASN114	O	25.787
G8	N2	ASN114	OD1	25.467
ARG67	NH2	C2	O2P	23.338
ARG137	NE	A4	O2P	22.998
ARG52	NH2	U9	O1P	20.988
ARG52	NH1	U9	O2P	19.938
ASN114	ND2	G8	O2'	18.718
C7	O2'	ALA112	O	18.438
ASN114	N	U9	O2'	17.608
ARG137	NH2	U3	O2P	17.498
ARG52	NH2	U10	O1P	17.478
LYS60	NZ	U11	O2P	15.528
LYS60	NZ	U10	O1P	15.468
ALA116	N	G8	N2	14.709
ASN114	ND2	G8	N3	14.419
ARG52	NE	U10	O2P	14.129
U1	O5'	ASP63	O	14.029
TYR69	OH	G8	N7	13.439
G8	O2'	PRO111	O	12.699
ARG137	NH1	A5	O2P	12.589
SER65	N	C2	O2P	12.099
ARG137	NH2	A4	O1P	11.649
ARG52	NH1	U10	O2P	10.929
ARG52	NH2	U10	O2P	10.619
LYS60	NZ	U9	O1P	10.159

Table S23. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 23 of the N-NTD:dsTRS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
SER11	N	G8	O4'	54.355
LYS62	NZ	G13	O6	48.635
ASN114	ND2	C7	O2P	33.217
ARG52	NH2	C2	O2P	31.087
ARG137	NH1	U3	O1P	29.857
C7	O2'	PRO111	O	28.787
SER65	N	U1	O5'	23.648
ARG137	NH2	U3	O2P	21.728
SER11	N	G8	O2'	21.238
ARG137	NH2	U3	O1P	20.988
ASN8	ND2	U9	O1P	18.028
G8	O2'	ASN8	OD1	17.018
LYS60	NZ	G13	O2P	16.008
C7	O3'	ALA112	O	14.299
GLY57	N	A12	O2P	13.759
C7	O3'	PRO111	O	12.569
TYR71	OH	G8	O5'	12.389

GLY57	N	U11	O1P	11.369
GLY57	N	U11	O2P	10.819

Table S24. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 24 of the N-NTD:dsTRS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG52	NH2	U10	O1P	91.581
SER11	N	G8	O4'	90.611
ARG52	NE	U10	O2P	82.912
ARG55	NH1	U11	O2P	69.443
ARG137	NH1	A5	O2P	69.293
ARG137	NH2	A4	O1P	63.614
SER65	OG	C2	O2P	57.664
A6	N6	GLU134	OE1	54.195
LYS62	NZ	G13	O6	44.756
LYS60	NZ	A12	O2P	42.686
ARG55	NH2	U11	O2P	39.826
ASN8	ND2	U9	O2P	39.646
LYS60	NZ	U11	O1P	39.366
ARG137	NH1	A4	O5'	38.486
A6	N6	GLU134	OE2	38.146
ARG137	NH1	A4	O1P	36.986
ARG55	NH2	U11	O1P	27.577
ARG67	NH2	U9	O4	25.517
ARG52	NH1	U9	O1P	25.327
ARG137	NH2	A5	O2P	22.408
ASN8	ND2	U9	O1P	21.488
C2	N4	LYS62	O	20.548
LYS62	NZ	G13	N7	18.388
ARG55	NH1	U10	O1P	18.348
ARG137	NH2	A4	O2P	16.678
U1	O5'	ASP63	O	16.028
A14	N6	MET61	O	15.338
ARG137	NE	A5	O2P	14.089
SER65	N	C2	O2P	13.929
GLY139	N	A6	O1P	13.419
ARG109	NH2	G8	N3	12.049
C2	N4	ASP63	O	12.019
ARG52	NE	U10	O1P	11.889
LYS62	NZ	A12	N7	11.069
ARG67	NH2	C2	O2P	10.939
ARG137	NH1	A4	O2P	10.769
TYR132	OH	U3	O2P	10.509

Table S25. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 25 of the N-NTD:dsTRS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
TYR132	OH	A4	O2P	67.043
SER11	N	G8	O4'	41.796
A5	N6	GLU134	OE1	39.956
ARG67	NH1	U10	O4	32.547
TYR69	OH	U9	O2P	31.887
A5	N6	GLU134	OE2	30.637
A4	N6	GLU134	OE1	30.497
ARG67	NH2	U11	O4	29.777
ARG137	NH2	A5	O2P	29.407
ARG67	NH2	U10	O4	27.757
G8	N2	MET3	O	26.987
ARG52	NH2	U10	O1P	26.267
ARG55	NH2	U10	O1P	25.857
ARG52	NH1	U10	O2P	23.388
LYS60	NZ	A14	O2P	23.098
A4	N6	GLU134	OE2	23.058
ARG55	NH1	U10	O1P	22.818
TYR71	OH	G8	O5'	22.448
ARG52	NH2	U9	O1P	22.358
ARG52	NE	U9	O1P	21.988
ARG52	NH1	U9	O1P	21.898
ARG137	NH1	A5	O2P	21.748
ARG137	NH2	A5	O1P	21.608
LYS60	NZ	G13	O2P	21.158
ARG55	NH2	U11	O2P	20.478
ARG55	NH1	U11	O2P	20.018
G8	N2	ALA2	O	17.898
ARG137	NH1	A4	O1P	17.678
ARG52	NH1	U10	O1P	17.248
SER11	N	G8	N7	17.088
A6	N6	GLU134	OE2	16.428
ARG55	NH2	U11	O1P	15.848
LYS62	NZ	G13	O6	15.848
ARG55	NE	U11	O1P	15.178
LYS60	NZ	G13	O1P	14.659
ARG55	NH1	U10	O2P	14.359
THR51	N	U9	O1P	14.309
THR51	OG1	U9	O1P	13.749
ARG137	NH2	A4	O2P	13.599
ARG55	NE	U11	O2P	13.359
ARG52	NE	U10	O2P	13.199
ARG67	NH1	U9	O4	13.139
GLY20	N	U1	O4	12.489
LYS60	NZ	A12	O1P	12.019
LYS62	NZ	A14	N7	11.619

ARG137	NH1	U3	O1P	11.459
ARG55	NH2	U10	O2P	11.429
ARG137	NE	A5	O1P	11.269
ASN8	ND2	G8	N3	10.629
ARG55	NH1	U10	O5'	10.579
TYR132	OH	C2	O2P	10.129
ARG52	NH2	U10	O2P	10.019

Table S26. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 1 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
SER11	N	G8	O4'	80.052
ARG52	NH1	C10	O2P	66.783
ALA15	N	G8	O6	65.313
C7	N4	GLU134	O	63.594
ARG52	NH1	U9	O2P	58.534
ARG52	NH2	C10	O2P	53.675
LYS62	NZ	G12	O6	44.126
C7	O2'	ALA116	O	39.106
GLY57	N	G12	O2P	35.286
ARG137	NH2	A6	O1P	29.577
ARG52	NH2	C10	O1P	29.367
ASN8	ND2	U9	O1P	28.597
ARG137	NE	A6	O1P	27.877
LYS62	NZ	G12	N7	26.697
C1	N4	ASP63	O	24.568
ARG137	N	A6	O2P	24.008
G8	O2'	ASN8	OD1	22.768
C1	N4	LYS62	O	22.198
GLY138	N	G5	O2P	20.618
HIS19	NE2	C3	O2P	20.468
ARG52	NE	C10	O2P	20.368
GLY138	N	G5	O1P	20.228
ARG137	NH2	G5	O1P	20.098
A2	N6	ASP63	O	19.428
SER65	OG	A2	O2P	17.948
GLY1	N	C10	O1P	15.998
ARG67	NH2	A2	O2P	14.829
ARG137	NH1	A6	O2P	13.939
ARG137	NH2	A6	O2P	13.249
HIS19	NE2	A2	O1P	11.719

Table S27. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 2 of the N-NTD:dsNS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG52	NH2	C10	O1P	97.35
SER65	OG	A2	O2P	92.141
ARG52	NE	C10	O2P	90.011
THR17	OG1	A2	O1P	75.832
ARG67	NE	A2	O2P	65.743
C1	N4	ASP63	O	57.924
ARG67	NH2	A2	O1P	57.474
GLY57	N	A11	O1P	53.715
ARG67	NH2	C3	O2P	44.626
ARG137	NH1	U4	O2P	42.476
LYS62	NZ	A11	O2P	40.876
G8	N2	ASN8	OD1	34.557
LYS62	NZ	G12	O2P	33.557
ARG137	NH2	C3	O2P	30.877
ARG67	NH2	A2	O5'	28.617
GLY4	N	U9	O2'	27.887
ARG137	NH2	U4	O2P	26.877
LYS60	NZ	U13	O2P	20.118
ARG67	NE	A2	O1P	19.818
ARG137	NH1	G5	O2P	18.848
ARG137	NH1	C3	O5'	17.648
GLN18	N	A2	O1P	16.838
LYS62	NZ	G12	O6	15.048
ARG52	NE	C10	O1P	14.859
LYS62	NZ	G12	N7	14.419
C7	O3'	GLY139	O	13.549
C10	O2'	GLY1	O	10.639
LYS60	NZ	G12	O1P	10.189

Table S28. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 3 of the N-NTD:dsNS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
C1	N4	LYS62	O	75.152
C7	O2'	ASN8	OD1	52.695
ALA112	N	C7	O2'	50.375
LYS60	NZ	U13	O2P	48.035
LYS62	NZ	G12	O6	44.036
LYS62	NZ	G12	N7	42.216
ARG48	NH1	G8	O5'	41.666
G8	N2	ASN8	O	37.676
ARG52	NH2	C10	O2P	35.856

ASN8	ND2	C7	O3'	32.877
ARG55	NH2	C10	O1P	32.407
ARG52	NH2	C10	O1P	31.027
SER140	OG	U4	O1P	29.037
ARG67	NH2	A2	O2P	28.627
LYS60	N	G12	O2P	27.587
ARG67	NH1	A2	O2P	26.297
GLY59	N	A11	O1P	25.217
SER140	N	U4	O1P	24.618
ARG52	NH1	U9	O1P	23.948
LYS60	NZ	G12	O1P	23.848
GLY139	N	C3	O1P	23.708
ARG52	NH1	C10	O2P	20.408
HIS19	NE2	A2	O1P	20.158
ARG48	NH1	U9	O1P	18.688
ARG55	NH1	C10	O1P	17.008
THR51	OG1	U9	O1P	15.308
ARG52	NH2	U9	O1P	15.248
ARG67	NH2	A2	O1P	14.889
TYR132	OH	A2	O2P	13.599
ASN8	ND2	C7	O2'	13.289
TYR132	OH	A2	O1P	12.439
ALA2	N	C7	O1P	12.159
ARG52	NE	C10	O2P	11.749
SER65	OG	A2	O2P	11.579
GLY59	N	A11	O2P	10.569
SER65	OG	C1	O5'	10.529
GLY139	N	C3	O2P	10.169

Table S29. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 4 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
SER65	OG	A2	O2P	87.161
ARG52	NH2	C10	O1P	85.651
SER11	N	G8	O4'	85.191
C1	N4	LYS62	O	84.532
ARG52	NE	C10	O2P	77.712
SER65	OG	C1	O5'	64.964
ARG137	NE	G5	O2P	61.854
ASN8	N	U9	O1P	61.204
ARG137	NH2	G5	O2P	55.274
GLY59	N	A11	O1P	46.975
LYS60	N	G12	O2P	43.696
LYS62	NZ	G12	O6	39.706
G8	O2'	ASN8	O	36.476
ARG52	NH1	U9	O1P	34.137
ASN8	ND2	G8	O5'	32.617

SER140	OG	G5	O1P	32.057
SER140	N	G5	O1P	30.537
ARG137	NH1	U4	O2P	26.187
LYS62	NZ	G12	N7	25.167
G8	N2	PRO111	O	23.588
ASN8	ND2	U9	O2P	21.268
ARG109	NH2	G8	N3	19.318
GLY139	N	U4	O1P	17.508
TYR132	OH	C3	O2P	13.129
C7	O2'	ALA112	O	12.299
LYS60	NZ	U13	O2P	12.229
LYS62	NZ	A11	N7	12.219
GLY138	N	U4	O1P	10.289

Table S30. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 5 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
SER65	OG	A2	O2P	90.501
SER11	N	G8	O4'	85.341
ARG52	NH1	C10	O2P	83.422
ARG52	NH2	C10	O2P	80.322
GLY20	N	A2	O1P	76.402
C1	N4	ASP63	O	71.983
ARG52	NH1	U9	O2P	55.694
SER65	OG	C1	O5'	49.405
ARG137	NH2	A6	O1P	42.396
A6	N6	GLU134	OE1	37.476
ARG137	NH2	C7	O2P	36.096
A6	N6	GLU134	OE2	35.756
ARG137	NE	A6	O2P	35.056
ASN7	ND2	U9	O1P	25.607
GLY138	N	G5	O2P	22.628
ALA116	N	G8	N2	19.938
ARG137	NH2	A6	O2P	17.718
ARG137	NE	A6	O1P	17.378
ASN7	ND2	G8	O3'	16.648
ARG52	NH2	C10	O5'	16.338
ARG53	NH2	U9	O1P	16.178
G8	N2	ASN114	O	15.098
ARG137	NH2	A6	O5'	14.009
LYS62	NZ	G14	N7	13.939
C7	O2'	ALA116	O	12.509
ALA2	N	C10	O1P	12.079
G8	O2'	PRO111	O	11.719
ALA116	N	C7	O2	11.639
GLY1	N	A11	O2P	11.489
ASN7	N	U9	O1P	11.129

GLY1	N	A11	O1P	11.049
G8	O5'	SER11	OG	11.039
C1	N4	LYS62	O	11.009
ARG137	NH1	G5	O1P	10.269

Table S31. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 6 of the N-NTD:dsNS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
C1	N4	LYS62	O	81.532
ASN8	ND2	G8	N3	77.432
GLY4	N	C7	O2'	74.993
ARG67	NH1	A2	O2P	69.213
ARG67	NH2	A2	O2P	53.765
ARG52	NH1	C10	O2P	50.635
ARG52	NH2	C10	O2P	46.675
GLY57	N	G12	O2P	37.316
ARG67	NH2	A2	O1P	37.126
ARG137	NH2	U4	O2P	33.547
LYS62	NZ	G12	O6	27.497
ARG52	NH2	C10	O1P	23.258
ARG137	NH1	U4	O2P	22.898
ARG52	NE	U9	O2P	20.518
LYS62	NZ	G12	N7	18.668
ARG52	NE	C10	O2P	17.618
ARG137	NH1	C3	O2P	16.658
ARG52	NH2	A11	O2P	15.928
ARG52	NH1	A11	O2P	15.648
ARG52	NH2	U9	O2P	14.789
GLY1	N	C10	O2'	12.559
GLY57	N	A11	O1P	12.439
ARG137	NH1	C3	O1P	11.769
ALA2	N	U9	O2'	11.669
TYR132	OH	C3	O1P	11.439
HIS19	NE2	A2	O1P	10.949
THR17	OG1	A2	O1P	10.909
ARG137	NH2	C3	O1P	10.169
ARG55	NH2	A11	O1P	10.059

Table S32. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 7 of the N-NTD:dsNS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
SER11	N	G8	O4'	94.851
SER65	OG	A2	O2P	89.031

ALA15	N	G8	O6	85.081
C1	N4	ASP63	O	65.333
ARG52	NE	C10	O2P	58.954
ARG52	NH2	C10	O2P	55.604
SER136	OG	A6	O1P	54.115
ARG52	NH2	A11	O2P	42.076
GLY57	N	A11	O1P	38.496
GLY20	N	A2	O2P	36.296
A6	N6	GLU134	OE2	33.337
LYS21	N	A2	O1P	32.847
SER136	N	C7	O2P	31.717
A6	N6	GLU134	OE1	26.887
SER65	OG	C1	O5'	26.517
HIS19	NE2	C3	O1P	26.407
LYS60	NZ	U13	O2P	23.858
C1	N4	LYS62	O	22.278
C7	O2'	ALA116	O	22.188
LYS60	NZ	G12	O1P	21.778
LYS62	NZ	G12	N7	18.798
LYS21	NZ	A2	O1P	18.258
ARG137	N	A6	O1P	15.528
TYR69	OH	U9	O4	15.248
ASN8	ND2	U9	O1P	15.058
LYS62	NZ	G14	N7	15.018
ARG67	NH1	A2	O2P	13.569
HIS19	NE2	C3	O2P	13.299
LYS62	NZ	G12	O6	12.959
ARG109	NH2	G8	O2'	12.859
GLY20	N	A2	O1P	12.519
ARG137	NH2	G5	O2P	11.169
LYS62	NZ	G12	O2P	11.059
ARG137	NH2	U4	O2P	10.319
TYR132	OH	C3	O2P	10.009

Table S33. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 8 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
C1	N4	LYS62	O	94.421
ARG67	NH2	A2	O2P	84.162
ARG52	NH2	C10	O2P	64.974
LYS62	NZ	G12	O6	49.995
ARG52	NH1	U9	O2P	47.625
ARG52	NH2	U9	O2P	39.396
LYS62	NZ	G12	N7	39.256
LYS60	NZ	U13	O2P	35.936
ARG137	NH2	G5	O6	32.387
GLY138	N	C3	O1P	32.077

TYR132	OH	A2	O1P	30.667
GLY57	N	A11	O1P	29.957
ARG137	NE	U4	O2P	29.657
ARG52	NE	C10	O2P	28.397
ARG52	NH2	U9	O5'	28.317
ARG137	NH1	G5	N7	28.047
LYS60	NZ	G12	O1P	25.647
TYR71	OH	G8	O5'	23.838
ASN8	ND2	C7	O2'	23.358
ARG137	NH1	C3	O2P	22.248
SER65	OG	C1	O5'	21.838
ARG137	NH2	U4	O2P	21.828
ARG137	NH2	G5	O2P	20.568
ARG137	NH2	A2	O1P	19.948
G8	N2	ASN7	O	18.928
LYS60	NZ	G12	O2P	18.888
ARG137	NH1	A2	O5'	16.138
ARG52	NH2	U9	O1P	15.088
LYS62	NZ	U13	O4	14.099
ARG52	NH2	C10	O1P	13.889
ARG137	NH2	U4	O5'	11.729

Table S34. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 9 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
C1	N4	LYS62	O	77.592
G8	N2	ASN8	O	67.913
TYR132	OH	A2	O1P	65.993
GLY57	N	G12	O2P	53.935
ARG52	NH2	C10	O2P	53.765
LYS62	NZ	G12	O6	49.075
ARG52	NH1	U9	O1P	43.576
ARG52	NH2	U9	O5'	40.466
SER65	N	C1	O5'	38.166
ARG67	NH2	A2	O2P	37.606
G8	O2'	ASN8	OD1	32.927
SER65	OG	A2	O2P	32.407
ARG67	NH1	A2	O2P	31.167
LYS62	NZ	G12	N7	30.567
ARG48	NH2	U9	O1P	30.207
ARG137	NH2	C3	O1P	28.887
ARG52	NE	C10	O1P	24.328
LYS60	NZ	U13	O2P	22.848
ARG137	NH1	C3	O1P	22.838
ARG52	NH2	C10	O1P	20.548
THR51	N	U9	O2P	19.478
SER65	OG	C1	O5'	16.548

ARG137	NH2	C3	O2P	15.628
ARG137	NH2	A2	O1P	12.159
ARG52	NH2	U9	O1P	11.999
ARG52	N	U9	O1P	11.639
ARG137	NH1	A2	O1P	11.369
ARG137	NH1	C3	O2P	11.009
LYS60	NZ	G12	O1P	10.539

Table S35. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 10 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG52	NE	C10	O2P	59.434
C1	N4	LYS62	O	51.655
ARG52	NH2	A11	O2P	51.415
LYS62	NZ	G12	O6	44.436
ARG137	NH2	A6	O2P	40.586
ARG137	NH1	G5	O2P	34.097
ARG67	NH2	A2	O2P	32.607
ARG137	NE	A6	O2P	32.007
ALA15	N	G8	O6	30.957
LYS62	NZ	G12	N7	30.847
ARG52	NH2	C10	O1P	30.037
C7	N4	GLU134	O	29.597
TYR69	OH	U9	O2P	28.787
TYR71	OH	G8	O5'	28.197
SER11	N	G8	O4'	27.007
ARG52	NH2	C10	O2P	25.327
LYS60	NZ	G12	O2P	24.708
C1	N4	MET61	O	23.698
ARG67	NH1	A2	O2P	22.938
C7	O2'	PRO111	O	21.648
SER11	N	G8	O5'	21.168
GLY57	N	A11	O1P	20.968
SER11	N	G8	O2'	20.908
TYR69	OH	U9	O4	18.098
ARG137	NH2	G5	O2P	17.918
C7	O3'	ALA112	O	17.388
SER65	OG	A2	O2P	17.278
ARG137	NE	G5	O2P	17.138
LYS62	NZ	U13	O4	14.229
HIS19	NE2	U4	O2P	13.739
A2	N6	LYS62	O	13.639
ASP58	N	A11	O1P	13.509
ARG109	NH1	G8	N2	12.599
ARG52	NH1	A11	O2P	11.409
C1	O5'	ASP63	OD2	10.829
ARG109	NH2	G8	N3	10.779

Table S36. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 11 of the N-NTD:dsNS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
SER11	N	G8	O4'	84.352
ARG137	NH1	G5	O2P	59.954
GLY57	N	G12	O2P	57.064
ARG137	NH1	U4	O2P	55.964
SER65	OG	A2	O2P	55.254
ARG52	NH1	C10	O2P	53.945
C1	N4	LYS62	O	51.805
ARG52	NH2	C10	O2P	47.335
ARG52	NH1	U9	O1P	47.105
LYS62	NZ	G12	O6	45.005
A6	N6	GLU134	OE2	44.966
ARG137	NH2	U4	O2P	41.006
ARG67	NH2	U9	O4	37.746
C1	N4	ASP63	O	37.196
GLY20	N	A2	O1P	33.237
ARG52	NH2	C10	O1P	30.407
SER65	OG	C1	O5'	25.917
ARG137	NH1	U4	O5'	24.278
LYS62	NZ	G12	N7	23.878
ARG137	NH2	C3	O1P	22.468
LYS60	NZ	U13	O2P	19.898
A6	N6	GLU134	OE1	19.738
ARG137	NH1	C3	O1P	19.578
ARG52	NE	U9	O1P	18.948
ARG137	NH1	C3	O5'	18.388
HIS19	NE2	A2	O1P	17.738
ARG137	NH2	U4	O1P	17.058
ARG52	NH2	U9	O1P	15.328
LYS60	NZ	G12	O1P	15.128
C7	O3'	ASN114	OD1	11.779
ARG52	NH1	U9	O2P	11.379
SER11	OG	G8	O5'	11.029
ARG137	NH2	C3	O2P	10.489
SER65	N	C1	O5'	10.339

Table S37. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 12 of the N-NTD:dsNS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
SER11	N	G8	O4'	90.121

SER65	OG	A2	O2P	86.841
ARG67	NE	A2	O2P	72.663
C1	N4	ASP63	O	69.323
ARG67	NH2	C3	O2P	65.713
ARG67	NH2	A2	O5'	62.534
GLY138	N	G5	O2P	60.444
ARG137	NH2	C7	O2P	60.184
ARG137	NH1	A6	O2P	59.494
ARG137	NH1	C7	O2P	53.185
THR17	OG1	A2	O1P	50.225
GLN18	N	A2	O1P	44.686
ARG52	NH2	U9	O1P	43.566
LYS60	NZ	G12	O2P	36.716
LYS60	NZ	A11	O1P	35.616
ARG52	NH2	C10	O2P	33.627
LYS62	NZ	G12	O6	33.317
LYS62	NZ	G12	N7	32.647
GLY57	N	A11	O1P	28.327
ARG52	NH1	U9	O1P	27.307
ARG67	NH2	A2	O2P	25.587
ARG52	NH2	C10	O1P	23.158
C1	N4	LYS62	O	20.938
ARG52	NE	U9	O1P	20.088
ARG52	NH1	C10	O2P	18.368
GLY139	N	G5	O1P	16.468
ALA116	N	G8	N2	15.638
ARG52	NH1	C10	O1P	15.428
GLY139	N	U4	O1P	13.639
SER65	OG	C1	O5'	13.279
ARG52	NE	C10	O2P	12.309
LYS60	NZ	U13	O2P	11.779
ARG52	NE	U9	O2P	10.259
ARG137	NH2	A6	O2P	10.029

Table S38. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 13 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
SER11	N	G8	O4'	94.141
SER65	OG	A2	O2P	90.081
C1	N4	LYS62	O	79.142
ARG52	NH2	C10	O2P	78.582
ASN8	ND2	U9	O1P	77.602
ARG55	NH2	U9	O1P	68.813
ALA15	N	G8	O6	59.944
ARG137	NH2	U4	O2P	45.035
ARG52	NH2	A11	O2P	42.596
ASN8	N	U9	O1P	39.386

A6	N6	GLU134	OE1	39.266
ARG52	NE	C10	O2P	38.106
ARG55	NE	C10	O1P	37.796
SER65	OG	C1	O5'	35.796
GLY138	N	G5	O1P	35.566
G8	O2'	ASN7	OD1	34.527
C7	N4	GLU134	OE2	33.887
ARG137	NE	G5	O2P	33.797
ARG137	NH2	C3	O1P	32.777
LYS62	NZ	G12	O6	30.677
ARG137	N	G5	O1P	30.557
ARG67	NH2	U4	O4	29.047
ARG137	NE	U4	O2P	24.238
LYS60	NZ	G12	O1P	23.598
ARG52	NE	U9	O2P	23.488
ARG137	NH2	G5	O2P	21.958
LYS62	NZ	U13	O4	20.248
LYS62	NZ	G12	N7	20.148
ARG52	NH2	U9	O5'	17.938
ARG52	NH1	A11	O2P	17.488
ARG137	NH1	C3	O1P	16.348
ASN8	N	G8	O3'	16.258
LYS60	NZ	G12	O2P	15.518
TYR132	OH	C3	O2P	15.328
HIS19	NE2	C3	O1P	15.208
ARG137	NH1	U4	O2P	14.689
C1	N4	ASP63	O	14.029
SER136	OG	G5	O1P	13.599
G8	O5'	ASN8	O	13.299
LYS60	NZ	U13	O2P	13.269
ARG52	NH2	C10	O1P	13.039
LYS62	NZ	G12	O2P	13.009
ARG137	N	G5	O2P	12.949
ARG52	NH2	U9	O2P	12.559
A6	N6	GLU134	OE2	12.129
SER136	OG	G5	O2P	10.989
GLY20	N	A2	O1P	10.769
ARG55	NH1	U9	O1P	10.259

Table S39. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 14 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
C1	N4	LYS62	O	85.271
THR51	OG1	U9	O1P	65.843
TYR132	OH	A2	O1P	61.974
ARG67	NH2	A2	O2P	61.804
GLY57	N	G12	O2P	56.314

ARG137	NH1	G5	O2P	46.915
ARG137	NH2	G5	O2P	46.875
LYS62	NZ	U13	O4	44.666
ARG48	NH1	G8	O5'	34.477
THR51	N	U9	O2P	33.817
ARG137	NH1	U4	O2P	32.597
ARG55	NH2	C10	O1P	31.437
ARG48	NH1	U9	O1P	31.087
THR51	N	U9	O1P	30.937
ARG55	NH1	C10	O2P	29.287
ARG52	NH2	A11	O2P	27.697
ARG52	NE	C10	O2P	27.427
ASN8	ND2	C7	O2'	26.007
ARG52	NH2	C10	O1P	25.537
ARG137	NH2	U4	O2P	23.198
ARG52	NH2	C10	O2P	22.958
LYS62	NZ	G12	O6	22.758
ARG52	NE	C10	O1P	22.028
ARG52	NH1	C10	O1P	21.588
ARG48	NH2	U9	O1P	20.328
LYS62	NZ	G12	N7	17.198
HIS19	NE2	A2	O1P	16.858
ARG52	NH2	C10	O5'	16.528
G8	N2	ASN8	O	16.348
C7	O2'	ASN8	OD1	14.249
GLY1	N	A6	N3	13.079
GLY139	N	A6	O2P	13.069
C7	O3'	ALA2	O	12.889

Table S40. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 15 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid Residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG52	NH1	U9	O2P	91.581
ARG52	NH1	U9	O2P	91.581
C7	O2'	ALA116	O	91.461
C7	O2'	ALA116	O	91.461
ARG52	NH2	C10	O2P	89.651
ARG52	NH2	C10	O2P	89.651
ASN8	ND2	U9	O1P	88.301
ASN8	ND2	U9	O1P	88.301
ARG53	N	U9	O2P	82.602
ARG53	N	U9	O2P	82.602
ARG52	NH1	C10	O2P	80.812
ARG52	NH1	C10	O2P	80.812
G8	O2'	ASN8	OD1	60.344
G8	O2'	ASN8	OD1	60.344
ALA116	N	C7	O2	54.385

ALA116	N	C7	O2	54.385
ARG137	NH2	A6	O2P	50.195
ARG137	NH2	A6	O2P	50.195
GLY56	N	C10	O1P	45.425
GLY56	N	C10	O1P	45.425
ARG55	NH2	G12	O2P	43.026
ARG55	NH2	G12	O2P	43.026
ARG55	NE	A11	O2P	39.736
ARG55	NE	A11	O2P	39.736
ARG53	NH1	U9	O1P	37.546
ARG53	NH1	U9	O1P	37.546
C1	O5'	GLN18	O	34.197
C1	O5'	GLN18	O	34.197
ARG53	NE	U9	O1P	33.367
ARG53	NE	U9	O1P	33.367
ARG55	NH2	A11	O2P	30.387
ARG55	NH2	A11	O2P	30.387
ARG109	NH2	G8	N3	29.577
ARG109	NH2	G8	N3	29.577
SER65	OG	A2	O1P	27.427
SER65	OG	A2	O1P	27.427
ARG137	NE	A6	O2P	26.677
ARG137	NE	A6	O2P	26.677
GLY57	N	C10	O1P	26.017
GLY57	N	C10	O1P	26.017
ARG137	NH2	G5	O1P	24.388
ARG137	NH2	G5	O1P	24.388
GLY4	N	U9	O2'	22.428
GLY4	N	U9	O2'	22.428
ARG67	NH2	C3	O2P	18.848
ARG67	NH2	C3	O2P	18.848
ARG55	NH1	A11	O2P	18.828
ARG55	NH1	A11	O2P	18.828
GLY20	N	C1	O4'	18.308
GLY20	N	C1	O4'	18.308
ARG137	NH1	A6	O2P	18.048
ARG137	NH1	A6	O2P	18.048
ARG55	NH1	G12	O2P	17.798
ARG55	NH1	G12	O2P	17.798
ARG53	NH2	U9	O1P	17.678
ARG53	NH2	U9	O1P	17.678
ARG67	NH2	A2	O2P	16.618
ARG67	NH2	A2	O2P	16.618
ALA116	N	G8	N2	16.078
ALA116	N	G8	N2	16.078
ARG55	NH2	A11	O1P	15.898
ARG55	NH2	A11	O1P	15.898
SER65	OG	A2	O2P	15.688
SER65	OG	A2	O2P	15.688
ARG53	NH2	G8	O3'	15.648
ARG53	NH2	G8	O3'	15.648

ARG67	NE	A2	O2P	14.859
ARG67	NE	A2	O2P	14.859
G8	O5'	THR51	O	13.269
G8	O5'	THR51	O	13.269
SER65	N	C1	O4'	13.249
SER65	N	C1	O4'	13.249
ARG137	NH1	G5	O2P	12.739
ARG137	NH1	G5	O2P	12.739
MET3	N	U9	O2'	11.389
MET3	N	U9	O2'	11.389
LYS62	NZ	G14	O6	11.079
LYS62	NZ	G14	O6	11.079
ARG55	NH2	A11	O5'	10.919
ARG55	NH2	A11	O5'	10.919
SER65	N	A2	O2P	10.809
SER65	N	A2	O2P	10.809
LYS21	NZ	C1	N3	10.759
LYS21	NZ	C1	N3	10.759
GLY1	N	A11	O1P	10.669
GLY1	N	A11	O1P	10.669

Table S41. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 16 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
SER11	N	G8	O4'	81.732
ARG53	NH2	C10	O2P	54.775
ARG137	NH1	U4	O2P	53.725
ARG53	NH2	U9	O1P	49.395
SER65	N	C1	O5'	47.995
ARG137	NH2	C3	O1P	40.626
C7	N4	SER140	OC1	36.076
ARG137	NH1	C3	O5'	33.497
ARG137	NH2	C3	O2P	32.997
ARG55	NH2	G12	O2P	29.737
ASP58	N	G14	N7	28.777
ARG137	NH2	U4	O2P	28.397
C1	N4	LYS62	O	26.667
ARG137	NH1	C3	O1P	26.637
SER11	OG	G8	O5'	26.347
SER140	OG	C7	N4	25.727
A6	N6	SER140	OC2	24.278
ARG52	NH1	G12	O6	23.868
ARG55	NH2	U13	O2P	22.728
ARG52	NH2	G12	N7	22.538
GLY57	N	U13	O4	22.468
LYS60	NZ	U13	O2P	22.428
ARG53	NH1	C10	O2P	21.958

ARG52	NH2	C10	O2P	21.528
ARG137	NH1	C3	O2P	21.158
ARG109	NH1	G8	N3	20.918
ARG55	NE	G12	O2P	20.818
LYS60	NZ	G12	O1P	19.168
ARG137	NE	U4	O2P	17.498
ARG53	NH1	U9	O1P	15.188
GLY57	N	A11	O1P	15.018
MET3	N	C10	O1P	14.939
SER65	OG	A2	O2P	13.849
C7	O3'	ASN113	O	13.759
ARG53	NE	C10	O2P	13.439
ARG55	NH2	G12	O5'	12.899
LYS62	NZ	G12	N7	11.509
LYS62	NZ	G12	O6	10.489
ARG52	NH1	C10	O2P	10.319
G14	O2'	ASP58	OD2	10.129

Table S42. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 17 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
G8	N2	PRO111	O	97.34
SER65	OG	A2	O2P	82.622
ARG137	NH1	U4	O2P	79.712
ARG109	NH1	G8	N3	78.762
ARG52	NH2	C10	O2P	77.772
SER11	N	G8	O4'	65.673
ASN8	ND2	U9	O1P	65.143
SER65	OG	C1	O5'	63.294
C1	N4	LYS62	O	60.894
GLY57	N	G12	O2P	60.054
ARG52	NH1	C10	O2P	55.254
ARG109	NH2	G8	N2	54.205
LYS62	NZ	G12	O6	51.615
ARG137	NH2	C3	O1P	46.275
ARG52	NH2	U9	O1P	46.015
ARG137	NH1	C3	O5'	45.555
C7	O2'	ALA112	O	44.966
ARG137	NH2	C3	O2P	40.306
G8	O2'	ASN8	OD1	36.596
HIS19	NE2	C3	O2P	30.307
ARG137	NH1	C3	O2P	29.527
ARG137	NH1	C3	O1P	28.217
ARG52	NH2	U9	O2P	26.247
C1	N4	ASP63	O	25.577
ARG109	NH2	G8	N3	25.277
ARG55	NH1	A11	O2P	22.828

ARG55	NH2	C10	O1P	22.258
TYR71	OH	G8	O5'	21.258
LYS62	NZ	G12	N7	19.948
ARG52	NE	U9	O1P	18.228
ARG55	NH1	C10	O1P	15.788
SER11	N	G8	O5'	14.829
TYR69	OH	U9	O2P	14.709
ARG55	NH1	C10	O5'	14.509
SER140	N	G5	O1P	13.659
ARG52	NH1	U9	O2P	12.209
HIS19	NE2	A2	O3'	11.559
SER140	OG	G5	O1P	10.809
LYS62	NZ	U13	O4	10.629

Table S43. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 18 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG52	NE	C10	O2P	78.612
ARG52	NH2	A11	O2P	76.252
SER65	OG	A2	O2P	76.152
TYR132	OH	C3	O2P	73.163
SER11	N	G8	O4'	66.063
ARG109	NH2	G8	N3	55.014
G8	N2	PRO111	O	53.575
ARG52	NH2	C10	O2P	44.926
G8	N2	ALA112	O	41.006
C1	N4	LYS62	O	38.826
ARG137	NE	A6	O2P	38.556
ARG67	NH1	A2	O2P	35.286
ARG137	NH1	G5	O2P	31.697
C1	N4	ASP63	O	31.647
ASN113	ND2	U9	O2	30.457
A6	N6	GLU134	OE1	28.527
C7	O2'	ALA112	O	24.938
ARG67	NH2	A2	O2P	23.898
ARG137	NH2	A6	O2P	21.548
LYS62	NZ	G12	O6	21.368
GLY57	N	A11	O1P	20.888
HIS19	NE2	C3	O2P	19.948
LYS62	NZ	G12	N7	18.438
ARG52	NH1	A11	O2P	17.968
LYS60	NZ	G12	O2P	17.888
ARG109	NH1	G8	N2	16.308
LYS62	NZ	U13	O4	16.128
SER65	OG	C1	O5'	15.988
ARG52	NH2	C10	O5'	15.678
SER140	OG	C3	O1P	15.318

C7	O2'	ASN113	O	14.229
C7	O3'	ASN113	O	13.809
A6	N6	GLU134	OE2	13.059
ARG53	N	U9	O1P	11.899
TYR71	OH	G8	O5'	11.769
ARG137	NH2	G5	O2P	11.299
ARG137	NH1	G5	O1P	10.919
ARG53	NE	U9	O1P	10.879
SER11	OG	G8	O5'	10.859
GLY138	N	G5	O1P	10.359

Table S44. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 19 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
TYR132	OH	A2	O1P	76.752
C1	O5'	GLU134	OE2	72.473
ARG52	NH1	C10	O2P	53.155
ARG52	NH2	A11	O2P	51.675
TYR69	OH	U9	O2P	50.255
ARG137	NH1	G5	O6	48.125
GLY4	N	C7	O2'	44.836
ARG137	NH2	G5	N7	39.486
ARG52	NH1	A11	O2P	38.716
GLY135	N	A2	O1P	35.696
THR51	N	U9	O1P	32.567
SER11	N	G8	O5'	30.147
LYS62	NZ	G14	O6	28.587
THR51	OG1	U9	O1P	27.747
ARG137	NH2	G5	O6	26.887
G8	N2	GLY1	O	25.927
ARG52	NH2	C10	O2P	20.238
TYR69	OH	U9	O1P	19.758
G8	N2	MET3	O	19.108
ARG52	N	U9	O1P	17.948
LYS60	NZ	G12	O2P	17.948
ARG52	NH2	C10	O1P	17.498
TYR71	OH	G8	O5'	17.138
ARG52	NE	C10	O2P	16.828
ARG52	NH1	U9	O1P	15.878
ARG55	NH1	G12	O2P	15.438
ARG109	NH2	G8	N7	14.989
G8	N2	ALA2	O	14.899
ARG67	NH1	U9	O2P	14.739
ARG137	NE	G5	O2P	13.109
C1	N4	LYS62	O	12.789
ASN8	ND2	G8	N3	12.689
TYR132	OH	A2	O2P	12.689

GLY4	N	C7	O2	12.619
MET3	N	U9	O2'	12.009
SER11	N	G8	O4'	11.649
ARG137	NH2	U9	O4	11.589
ARG52	NH2	C10	O5'	10.949
ARG52	NH1	C10	O1P	10.919
LYS60	NZ	G12	O1P	10.479
ARG137	NH1	U4	O4	10.409
ARG55	NH2	G12	O2P	10.379
ALA2	N	U9	O2'	10.339
ARG55	NH2	U13	O2P	10.089

Table S45. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 20 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG52	NH2	C10	O1P	88.831
SER65	OG	A2	O2P	81.802
ARG52	NE	C10	O2P	78.032
ARG55	NH1	A11	O2P	66.743
G8	N2	ALA112	O	63.204
ARG55	NH1	C10	O1P	57.404
ASN113	ND2	C10	O4'	55.464
C1	N4	ASP63	O	55.424
ASN113	ND2	U9	O2	54.895
ASN8	ND2	U9	O1P	54.775
ARG55	NH2	A11	O1P	54.015
ALA115	N	C7	O2'	50.875
ARG67	NE	A2	O2P	49.375
SER11	N	G8	O4'	47.975
ARG67	NH2	C3	O2P	46.015
ARG67	NH2	A2	O5'	36.316
ARG67	NH2	A2	O2P	35.066
LYS60	NZ	G12	O2P	33.277
LYS62	NZ	G12	O6	32.757
C1	N4	LYS62	O	31.927
ARG55	NH2	A11	O2P	31.167
LYS62	NZ	G12	N7	31.117
C7	O3'	ASN113	O	29.147
ARG52	NH1	U9	O1P	26.737
SER65	OG	C1	O5'	25.917
SER11	N	G8	O5'	24.298
G8	O2'	ASN8	OD1	21.378
ARG55	NH2	C10	O1P	17.498
ARG109	NH2	G8	N3	16.208
THR17	OG1	A2	O1P	15.918
LYS60	NZ	G12	O1P	15.218
ARG55	NH1	A11	O1P	12.719

LYS60	NZ	U13	O2P	11.939
ASN114	N	G8	N2	11.179
U9	O2'	ASN113	OD1	10.729
TYR71	OH	G8	O5'	10.349

Table S46. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 21 of the N-NTD:dsNS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
GLY4	N	U9	O2'	64.064
C1	O5'	GLU134	OE1	55.134
ARG52	NH2	G12	N7	54.915
ARG52	NH1	G12	O6	54.275
ARG109	NH2	G8	O2'	39.316
ARG109	NH1	G8	O2'	38.976
ARG53	NH2	A11	O2P	34.387
ARG53	NH2	C10	O1P	33.097
ARG109	NH2	G8	O3'	32.647
C1	O5'	GLU134	OE2	32.137
ARG137	NH1	A2	O1P	31.657
C10	O2'	GLY1	O	29.727
ARG137	NH1	C3	O2P	29.297
LYS62	NZ	G14	N7	28.667
ASN8	ND2	C10	O1P	28.547
ARG109	NH2	U9	O1P	28.547
ARG67	NH2	C1	O5'	25.867
ARG55	NH2	G12	O1P	21.828
ALA116	N	G8	O5'	21.818
ARG55	NH1	U13	O2P	20.368
ARG109	NH1	G8	O3'	19.888
ARG137	NH2	C3	O2P	19.288
ARG67	NH2	C1	O4'	19.028
G8	O2'	PRO111	O	18.628
ARG55	NH1	G12	O5'	15.438
GLY1	N	A11	O1P	14.509
ARG53	NH1	C10	O1P	13.299
ARG137	NH2	C3	O1P	12.809
ALA116	N	G8	O4'	12.619
ASN8	ND2	U9	O3'	12.349
ARG53	NE	A11	O1P	11.749
ARG52	NH2	G12	O6	11.469
ARG55	NH1	G12	O1P	11.319

Table S47. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 22 of the N-NTD:dsNS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
SER11	N	G8	O4'	95.21
ARG137	NH1	C3	O2P	89.761
G8	N2	PRO111	O	72.873
ARG52	NH1	C10	O2P	69.073
C1	N4	LYS62	O	68.413
ARG52	NH2	C10	O2P	65.023
ASN8	ND2	U9	O1P	62.944
ALA116	N	G8	O6	55.934
ARG137	NH2	A2	O1P	48.615
ARG137	NH1	A2	O1P	44.976
ARG52	NH2	U9	O1P	41.226
LYS60	NZ	A11	O1P	33.247
ARG67	NH2	A2	O2P	31.587
ARG137	NH1	A2	O5'	30.007
G8	O2'	PRO111	O	29.657
ARG137	NH2	A2	O2P	28.747
LYS62	NZ	G12	O6	27.487
LYS60	NZ	A11	O2P	24.818
LYS62	NZ	U13	O4	23.478
GLY139	N	G5	O2P	23.418
C1	O5'	ASP63	O	22.408
SER65	N	C1	O5'	19.758
LYS62	NZ	G12	N7	17.238
ALA115	N	C7	O2'	15.408
C7	O3'	ASN113	O	15.118
ASN114	N	G8	N2	14.609
C7	O2'	ASN113	O	14.409
ASN8	ND2	G8	O3'	13.799
GLY1	N	C10	O1P	11.769
GLY139	N	U4	O1P	11.409
ASN8	ND2	G8	O5'	11.079
ARG137	NH1	A2	O2P	10.899
GLY138	N	U4	O2P	10.219

Table S48. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 23 of the N-NTD:dsNS complex.

Donor		Acceptor		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
G8	N2	ASN8	OD1	75.812
C10	N4	TYR69	OH	75.362
TYR69	OH	U9	O2P	71.933
ARG52	NH2	A11	O1P	71.273

GLY4	N	U9	O2	67.373
ARG137	NH2	G5	O2P	59.624
TYR71	OH	G8	O5'	53.325
GLY138	N	C3	O2P	51.675
SER11	N	G8	N7	47.645
ARG48	NH1	G8	O5'	47.445
ARG137	NE	U4	O2P	45.095
LYS60	NZ	G12	O2P	42.006
U9	O2'	ALA2	O	39.826
ARG137	NE	G5	O2P	38.326
C7	O2'	GLY4	O	35.136
C1	O5'	GLY130	O	26.087
ARG55	NH2	C10	O1P	23.328
ARG52	NH1	C10	O1P	22.938
ARG137	NH2	U4	O2P	22.538
ARG52	NE	A11	O1P	20.118
GLY139	N	A2	O1P	19.608
ARG109	NH2	G8	O6	19.448
GLY138	N	U4	O2P	19.388
ARG52	NE	A11	O2P	19.048
ARG53	N	C10	O2P	18.818
LYS60	NZ	A11	O1P	17.508
ARG52	NH1	A11	O2P	17.038
ARG109	NH2	C7	N4	16.718
ARG53	NE	C10	O1P	15.108
GLY138	N	U4	O1P	13.869
ARG55	NH1	C10	O1P	13.409
LYS60	NZ	G12	O1P	12.189
C1	O5'	PHE131	O	11.189
SER140	OG	A2	O1P	10.789
SER140	N	A2	O1P	10.669
ARG53	NE	U9	O1P	10.569
ARG53	NH2	U9	O1P	10.129

Table S49. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 24 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
C1	N4	LYS62	O	92.081
ARG67	NH2	A2	O2P	85.931
ARG48	NH1	U9	O2P	80.262
TYR71	OH	G8	O5'	70.093
ARG67	NH1	A2	O2P	63.084
SER65	N	C1	O5'	62.294
ARG52	NH2	A11	O2P	58.334
LYS62	NZ	G12	N7	44.626
ARG52	NH1	A11	O2P	42.696
LYS62	NZ	G12	O6	40.986

LYS60	NZ	G12	O1P	40.606
ARG52	NH1	C10	O2P	27.947
C7	O3'	LEU5	O	26.477
LYS60	NZ	U13	O2P	25.807
LEU5	N	C7	O1P	24.118
ARG52	NH1	C10	O1P	23.208
LYS62	NZ	U13	O4	22.538
ARG48	NH2	U9	O1P	21.428
ARG137	NH1	C3	O1P	21.408
SER11	N	G8	N7	20.958
TYR69	OH	U9	O4	19.518
ARG137	NH1	U4	O2P	19.388
ARG137	NH2	C3	O1P	18.128
ARG52	NH2	A11	N7	17.498
ARG137	NH2	U4	O2P	15.308
ASN8	ND2	G8	O2'	15.058
LYS60	NZ	G12	O2P	14.219
ARG52	NH2	A11	O1P	12.489
ARG137	NE	C3	O1P	11.559
ARG137	NH2	C3	O2P	10.329
LEU5	N	C7	O3'	10.239

Table S50. Protein-RNA hydrogen bonds with percentage of persistence higher than 10% for run 25 of the N-NTD:dsNS complex.

Donor		**Acceptor**		
Amino acid residue	**Atom**	**Nucleotide residue**	**Atom**	**%Persistence**
ARG137	NH2	C3	O1P	62.784
G8	N2	PRO111	O	56.434
ARG137	NH2	U4	O2P	55.394
ARG109	NH2	G8	N3	47.505
ASN8	ND2	U9	O1P	46.525
ARG137	NH1	C3	O1P	46.165
SER65	OG	A2	O2P	45.435
ARG52	NH1	U9	O2P	45.155
ARG67	NH2	A2	O2P	34.107
C1	N4	MET61	O	33.597
ARG52	NH1	C10	O2P	33.027
ARG137	NH1	U4	O2P	30.437
C7	O2'	ALA112	O	30.327
LYS62	NZ	G12	O6	25.967
ARG52	NH2	C10	O2P	25.237
ARG109	NH1	G8	N2	24.838
C1	N4	LYS62	O	24.578
ARG52	NH1	U9	O1P	24.388
TYR69	OH	G8	O6	24.098
ARG137	NE	U4	O1P	23.738
ARG52	NH2	C10	O1P	23.168
SER65	OG	A2	O1P	22.858

SER65	N	A2	O2P	21.338
LYS60	NZ	G12	O2P	20.268
C7	O2'	PRO111	O	19.308
C1	N4	ASP63	O	19.068
U9	O2'	GLY1	O	18.958
ARG67	NH1	A2	O2P	18.708
ARG52	NE	C10	O2P	18.658
LYS62	NZ	G12	N7	18.168
ARG137	NE	U4	O2P	18.018
C1	O5'	ASP63	O	17.768
SER11	N	G8	O4'	16.948
GLY1	N	C10	O1P	16.118
G8	O2'	ASN8	OD1	15.058
GLY57	N	A11	O2P	14.589
ARG67	NH2	A2	O1P	14.099
SER140	N	G5	O1P	13.819
LYS60	NZ	U13	O2P	13.209
SER65	OG	C1	O5'	12.529
LYS60	NZ	G14	N7	12.159
ARG137	NH1	C3	O5'	11.939
TYR69	OH	G8	N7	10.979
ARG67	NE	A2	O2P	10.179

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