Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for:
Consequences of Mg^{2+} binding on the geometry and stability of RNA base pairs

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S1 Number of possible base pairing geometries with Mg^{2+} bound nucleobases

- Each Mg^{2+} bound nucleobase has 2 free edges (WC and Sugar). Since we have considered Mg^{2+} binding at the Hoogsteen edge of only 3 bases (guanine, adenine and uracil), total number of interactive edges of the first base will be ($3 \times 2 = 6$).
- The Mg^{2+} bound base can interact with any of the 3 edges of the second base (any of the four nucleobases). Hence, there are total ($4 \times 3 = 12$) interactive edges for the second base.
- Therefore, if we consider only *cis* type base pairs, there could be total ($6 \times 12 = 72$) possible base pairing geometries. Out of which, base pairs like A:G W:W Cis and G:A W:W Cis basically correspond to the same base pairing geometry. Hence after removing 3 W:W, 3 S:S, 3 S:W and 3 W:S type geometries corresponding to A:G, A:U and G:U pairs and 3 S:W (or W:S) geometries corresponding to A:A, G:G and U:U pairs (total 15 base pairing geometries), there remain total (72 - 15 = 57) unique base pairing geometries.
- Therefore, if we consider both the *cis* and *trans* type base pairs, there will be total ($57 \times 2 = 114$) unique base pairing geometries.

S2 Root Mean Square Deviation (RMSD)

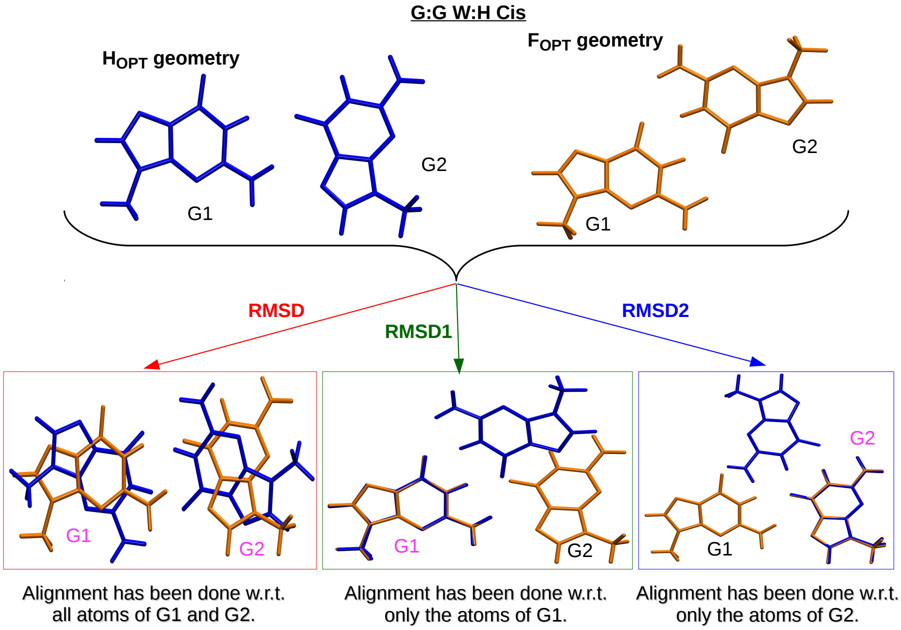
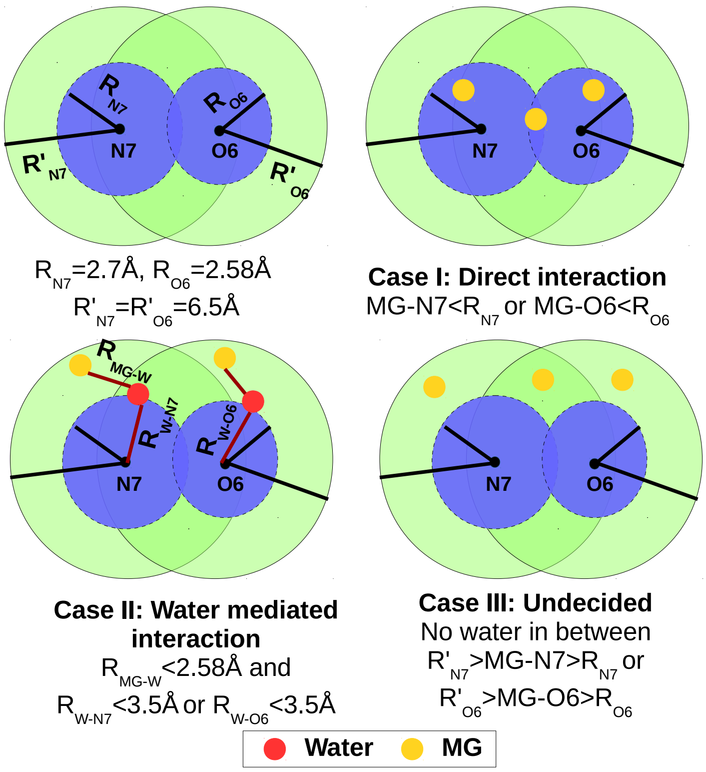


Figure S1: Pictorial description of different ways of calculating RMSD values between the H_{OPT} and F_{OPT} geometries.

S3 Algorithm to detect Mg^{2+}–nucleobase interactions



R_{N7}=2.7Å, R_{O6}=2.58Å
R'_{N7}=R'_{O6}=6.5Å

Case I: Direct interaction
MG-N7<R_{N7} or MG-O6<R_{O6}

Case II: Water mediated interaction
R_{MG-W}<2.58Å and
R_{W-N7}<3.5Å or R_{W-O6}<3.5Å

Case III: Undecided
No water in between
R'_{N7}>MG-N7>R_{N7} or
R'_{O6}>MG-O6>R_{O6}

Figure S2: Two dimensional schematic representation of detection criterion of Mg^{2+}–nucleobase interactions. This figure is specific to guanine which has two polar atoms, O6 and N7, at its hoogsteen edge. We have considered all those Mg^{2+} (yellow dot) which occur within the green circles (spheres). Mg^{2+} ions present within the blue circle (sphere) are counted as directly interacting cases (Case I). If the Mg^{2+} is located outside the blue circle but there is a water molecule (red dot) between the Mg^{2+} and N7/O6 in such a way that, it is directly bounded to Mg^{2+} and N7/O6 is within 3.5 Å of it, then they are counted as water mediated interactions (Case II). All other cases where the Mg^{2+} is outside the blue circle but there is no water molecule present between the Mg^{2+} and N7/O6, are counted as undecided (Case III).

For a given RNA crystal structure, first all those guanine residues are shortlisted for which one or more Mg^{2+} ions are found within 6.5 Å of their respective Hoogsteen edge carbonyl oxygen (O6) and/or imino nitrogen (N7) atoms. Depending on the mode of interaction between Mg^{2+} and nucleobase atoms (O6/N7), these short listed Mg^{2+}—nucleobase pairs may further be categorized into two classes — (i) direct interaction, and (ii) water mediated interaction. The ideal bond lengths of Mg–O and Mg–N bonds are taken as 2.08 Å and 2.20 Å, respectively. These are the mean distances observed in the Cambridge Structural Database[1] and also considered in earlier literature.[2] With a buffer length of 0.5 Å, if the Mg–O6 distance is found to be $\leq$ 2.70 Å and/or the Mg–N7 distance is found to be $\leq$ 2.58 Å, we have considered the corresponding Mg^{2+}—nucleobase interaction as a **direct interaction**. On the other hand, we have considered it as a water mediated interaction, if a water molecule (O_W) is found between the Mg^{2+} and the nucleobase atom in such a way that (i) it is directly bound to Mg^{2+} (i.e., Mg^{2+}–O_W distance $\leq$ 2.70 Å) and (ii) there is a possibility of hydrogen bonding interaction between the water molecule and nucleobase atom i.e., O_W–O6/N7 distance $\leq$ 3.5 Å, a reasonable cut-off for hydrogen bond donor-acceptor distance for biological systems.[3,4]

In a similar fashion Mg^{2+}-adenine and Mg^{2+}-uracil interactions can be identified. Note that adenine has N6 instead of O6. Hence, the cut-off distances must be taken accordingly. In case of uracil, there is only one Mg^{2+} binding site (i.e., O4) at the Hoogsteen edge.

S4 Optimized geometries

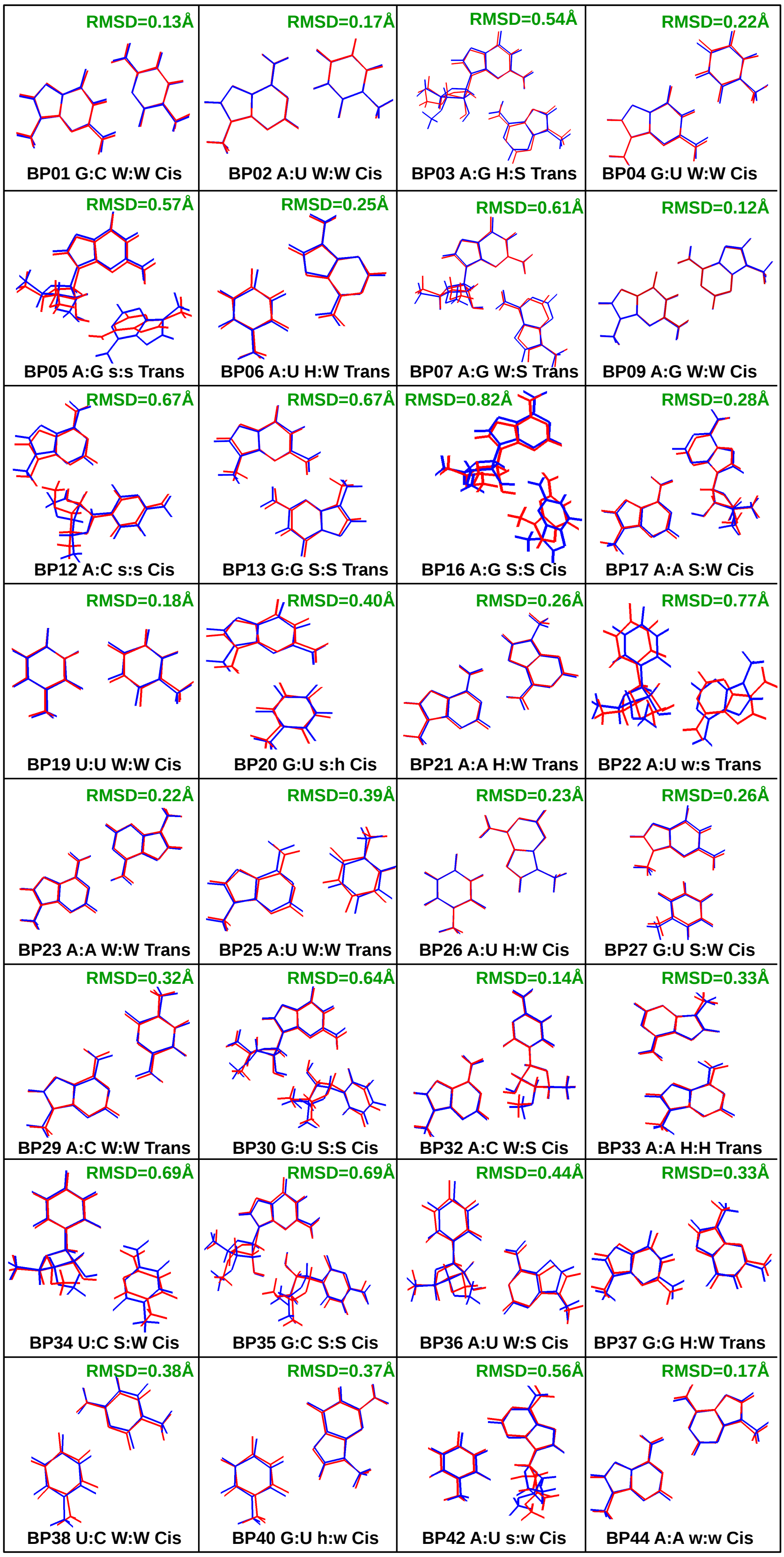


Figure S3: Structural alignment of H_{OPT} (blue) and F_{OPT} geometries (red) of all the base pairs which show smaller deviation (RMSD < 1Å) from their native geometries on gas phase geometry optimization.

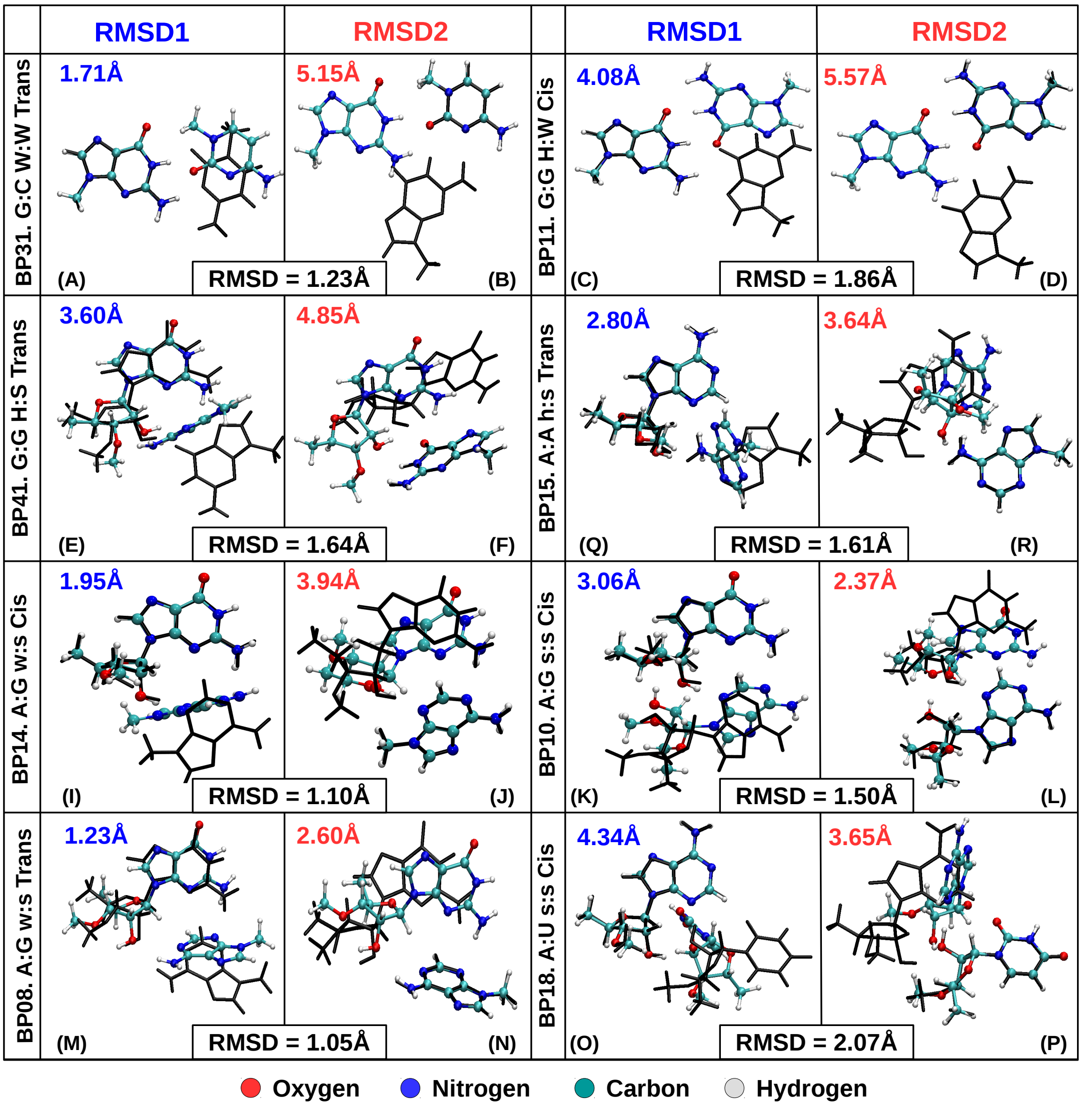


Figure S4: Structural superposition of H_{OPT} and F_{OPT} geometries and corresponding Root Mean Square Deviation values are reported. The H_{OPT} geometries are shown as *stick* model in black color and the F_{OPT} geometries are shown as *ball and stick* model in CPK color scheme. RMSD values are calculated after structural superposition with respect to all atoms. RMSD1 and RMSD2 values are calculated after structural alignments with respect to (a) the Mg^{2+} bound base and (b) the second base, respectively.

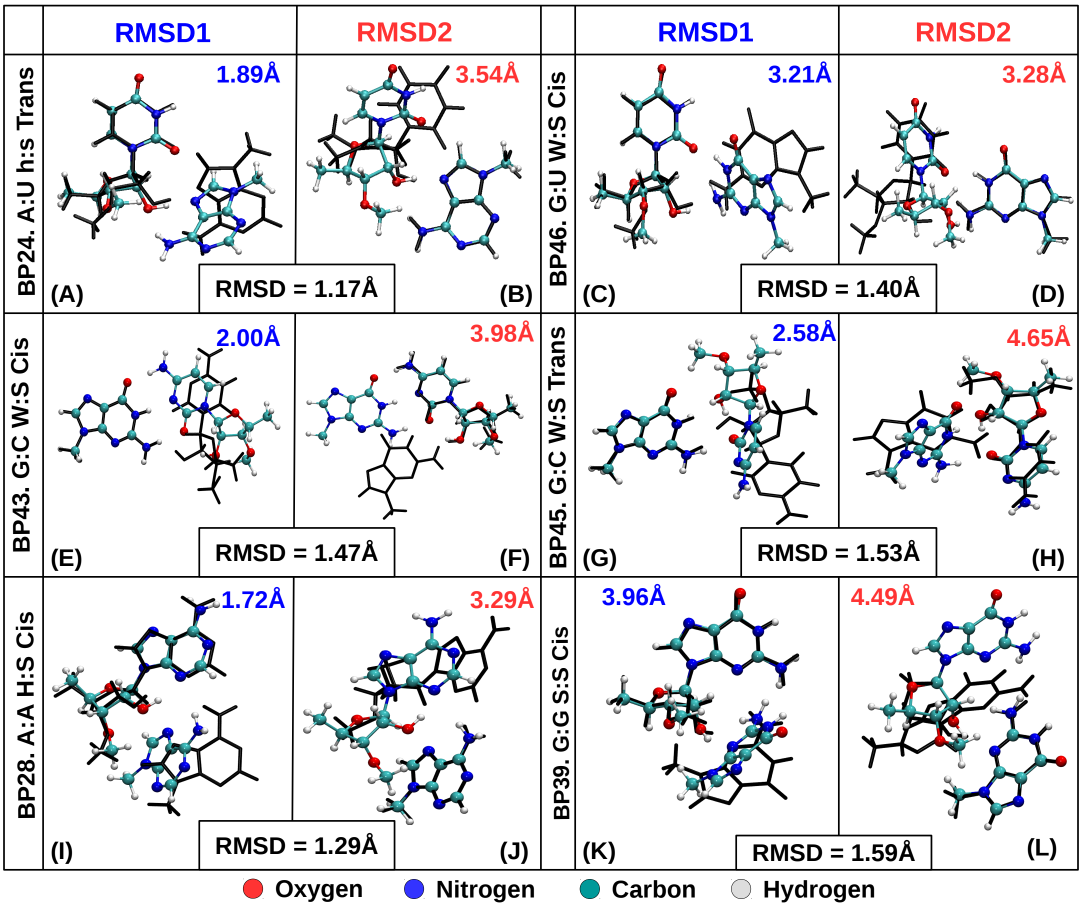


Figure S5: Structural superposition of H_{OPT} and F_{OPT} geometries and corresponding Root Mean Square Deviation values are reported. Other annotations are same as the Figure S4.

S5 Characterization of the optimized geometries on the basis of six geometrical parameters obtained using NUPARM

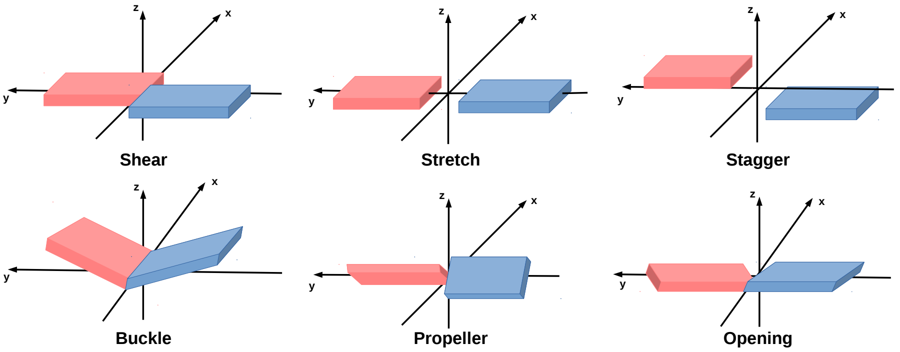


Figure S6: Illustration of 3 rotational (Buckle, Open, Propeller Twist) and 3 translational parameters (Stagger, Shear and Stretch) that characterize the geometry of a base pairing interaction.

Table S1: Three rotational (Buckle, Open and Propeller Twist) and three translational parameters (Stagger, Shear and Stretch) that characterize the optimized geometries of the Mg^{2+} bound base pairs.

Base Pair	Mg^{2+} bindng mode	Buckle	Open	Propel	Stagger	Shear	Stretch
BP11 G:G W:H Cis	Direct binding at N7	1.7	-5.5	1.1	0.0	2.9	2.9
	Direct binding at O6	-23.6	-0.1	-50.5	-0.3	0.6	2.8
	Water mediated binding	2.7	-4.3	-4.5	-0.0	2.9	2.9
BP41 G:G H:S Trans	Direct binding at N7	-2.3	-8.5	-22.2	0.2	2.1	3.5
	Direct binding at O6	-0.9	-10.6	-27.0	0.4	2.1	3.5
	Water mediated binding	-0.7	-10.5	-25.2	0.3	2.1	3.5
BP14 A:G w:s Cis	Direct binding at N7	-33.0	54.2	-36.6	-1.4	-1.9	2.5
	Direct binding at O6	-33.2	54.5	-35.7	-1.4	-1.9	2.4
	Water mediated binding	-34.6	54.8	-35.6	-1.4	-1.9	2.5
BP08 G:A s:w Trans	Direct binding at N7	-58.9	-41.0	12.8	2.7	-2.1	1.4
	Direct binding at O6	-56.8	-45.3	-33.0	1.5	-1.9	2.0
	Water mediated binding	-55.6	-45.9	-35.6	1.5	-1.9	2.0
BP10 A:G s:s Cis	Direct binding at N7	-58.6	-31.2	6.5	-1.7	2.2	2.3
	Direct binding at O6	-54.6	-31.8	13.0	-1.6	2.0	2.4
	Water mediated binding	-53.7	-31.5	11.8	-1.6	2.1	2.4
BP18 A:U s:s Cis	Direct binding at N7	-2.7	-51.2	-28.0	-0.4	1.8	4.3
	Water mediated binding	-2.0	-50.0	-29.6	-0.4	1.8	4.3
BP15 A:A s:h Trans	Direct binding at N7	-37.6	-31.3	74.0	-2.5	1.0	2.0
	Water mediated binding	-16.0	-2.1	38.5	-0.5	1.7	3.0

Table S2: Values of 3 rotational (Buckle, Open, Propeller Twist) and 3 translational parameters (Stagger, Shear and Stretch) that characterize the geometry of the optimized base pairs. Values are reported for H_{OPT} and F_{OPT} geometries of 14 base pairs, which show large deviation on full optimization, in the absence of Mg^{2+} binding.

Sl.	Base Pair	Geometry	Buckle	Open	Propel	Stagger	Shear	Stretch
1	BP11 G:G W:H Cis	H_{OPT}	-2.5	2.9	-17.5	-0.3	3.7	2.9
		F_{OPT}	14.8	-94.9	-7.0	-0.3	4.3	4.0
2	BP15 A:A s:h Trans	H_{OPT}	-15.1	-8.8	1.2	-0.2	2.4	2.7
		F_{OPT}	-23.4	-35.4	76.3	-2.7	1.3	1.7
3	BP18 A:U s:s Cis	H_{OPT}	25.8	-33.5	-36.6	-1.1	0.4	3.7
		F_{OPT}	-57.2	-91.6	-89.6	2.6	1.8	2.4
4	BP28 A:A S:H Cis	H_{OPT}	-5.2	-19.9	-2.9	1.0	2.5	3.2
		F_{OPT}	6.9	22.0	24.4	2.4	2.7	2.2
5	BP31 G:C W:W Trans	H_{OPT}	8.8	7.9	-7.6	0.1	-2.0	3.0
		F_{OPT}	-5.4	76.5	-4.5	0.2	-4.1	3.1
6	BP41 G:G S:H Trans	H_{OPT}	-23.2	-2.4	-4.9	-0.5	1.6	3.8
		F_{OPT}	-98.5	-16.3	31.0	-0.1	3.3	3.2
7	BP43 G:C W:S Cis	H_{OPT}	-1.1	-34.6	-19.3	0.0	3.8	3.2
		F_{OPT}	2.6	-88.7	-2.7	-0.2	5.5	2.7
8	BP08 G:A s:w Trans	H_{OPT}	-33.8	-46.4	-54.8	0.7	-2.0	2.7
		F_{OPT}	-81.1	-40.6	-46.1	2.0	-1.5	2.0
9	BP10 A:G s:s Cis	H_{OPT}	-13.1	-24.7	-24.6	-0.5	3.0	3.0
		F_{OPT}	-56.4	-27.3	23.1	-1.6	1.9	2.5
10	BP14 A:G w:s Cis	H_{OPT}	-9.3	60.8	-21.0	-0.7	-2.5	2.7
		F_{OPT}	-80.3	51.7	-46.5	-2.0	-0.8	2.1
11	BP24 A:U h:s Trans	H_{OPT}	-156.5	-17.3	-30.1	0.6	1.2	2.1
		F_{OPT}	129.8	-20.4	-39.0	3.3	1.0	-0.9
12	BP39 G:G S:S Cis	H_{OPT}	-81.0	-22.7	-0.1	-0.9	-2.8	4.2
		F_{OPT}	69.3	-86.7	-20.3	-4.2	-0.4	-1.4
13	BP45 G:C W:S Trans	H_{OPT}	-39.9	-61.8	-43.4	0.7	0.0	4.8
		F_{OPT}	-107.6	-25.9	-8.3	-0.9	1.9	3.7
14	BP46 G:U W:S Cis	H_{OPT}	-3.0	-37.4	-13.5	-0.2	4.1	3.2
		F_{OPT}	-24.9	-32.3	55.6	0.2	3.3	3.2

Table S3: Values of 3 rotational (Buckle, Open, Propeller Twist) and 3 translational parameters (Stagger, Shear and Stretch) that characterize the geometry of the optimized base pairs. Values are reported for H_{OPT} and F_{OPT} geometries of those 32 base pairs, which show small deviation (RMSD < 1Å) on full optimization, in the absence of Mg^{2+} binding.

Sl.	Base Pair	Geometry	Buckle	Open	Propel	Stagger	Shear	Stretch
1	(BP01) G:C W:W Cis	H_{OPT}	-4.5	2.9	-5.9	-0.3	-0.1	2.9
		F_{OPT}	-0.1	-3.9	0.1	0.0	-0.2	3.0
2	(BP02) A:U W:W Cis	H_{OPT}	-2.1	1.6	-14.1	-0.2	0.2	2.8
		F_{OPT}	0.1	3.0	-0.1	0.0	0.1	2.8
3	(BP03) A:G H:S Trans	H_{OPT}	-8.2	-14.2	-8.7	0.0	2.6	3.3
		F_{OPT}	4.6	-11.2	-25.7	-0.3	2.2	3.4
4	(BP04) G:U W:W Cis	H_{OPT}	-7.9	-0.6	-9.7	0.1	-2.0	2.9
		F_{OPT}	0.3	0.7	3.2	0.1	-2.4	2.9
5	(BP05) A:G s:s Trans	H_{OPT}	74.3	-100.7	136.1	-3.5	-2.5	1.2
		F_{OPT}	68.7	102.0	-88.1	-2.9	1.6	0.1
6	(BP06) A:U H:W Trans	H_{OPT}	-8.6	5.6	11.7	0.4	0.7	2.9
		F_{OPT}	0.2	4.1	0.1	0.0	0.1	2.8
7	(BP07) A:G W:S Trans	H_{OPT}	-33.8	46.4	-54.8	-0.7	-2.0	2.7
		F_{OPT}	-81.1	40.6	-46.1	-2.0	-1.5	2.0
8	(BP09) A:G W:W Cis	H_{OPT}	-13.6	8.5	-11.2	-0.7	0.2	2.8
		F_{OPT}	9.7	-2.8	-26.2	-0.3	-0.1	2.9
9	(BP12) A:C s:s Cis	H_{OPT}	141.0	17.8	-144.1	-4.2	3.9	-0.5
		F_{OPT}	119.6	0.0	-39.0	-4.3	2.3	-0.5
10	(BP13) G:G S:S Trans	H_{OPT}	7.7	1.7	8.5	0.0	-3.6	0.0
		F_{OPT}	42.3	0.0	-19.1	0.0	-3.7	0.0
11	(BP16) A:G S:S Cis	H_{OPT}	-93.2	38.3	108.7	-1.7	-1.8	2.8
		F_{OPT}	36.8	66.0	-52.1	0.1	-1.1	4.0
12	(BP17) A:A S:W Cis	H_{OPT}	4.1	-17.2	-20.7	-0.8	-2.5	3.3
		F_{OPT}	15.2	-23.0	-35.7	0.0	-2.6	3.4
13	(BP19) U:U W:W Cis	H_{OPT}	7.2	4.3	-6.6	0.0	2.5	2.9
		F_{OPT}	0.0	-0.7	0.0	0.0	2.7	2.9
14	(BP20) G:U s:h Cis	H_{OPT}	4.3	71.6	-13.9	-0.9	2.9	2.1
		F_{OPT}	-12.2	75.5	-5.8	-0.1	2.6	2.4
15	(BP21) A:A H:W Trans	H_{OPT}	5.7	6.3	19.7	0.7	2.3	2.8
		F_{OPT}	-1.4	1.5	9.2	0.0	2.5	3.0
16	(BP22) A:U w:s Trans	H_{OPT}	-31.4	78.1	-17.0	-1.5	0.3	4.0
		F_{OPT}	-35.3	41.1	-24.0	0.7	0.7	4.2
17	(BP23) A:A W:W Trans	H_{OPT}	4.0	-0.4	18.7	0.2	2.2	2.8
		F_{OPT}	-0.8	0.0	3.6	0.0	2.3	3.1
18	(BP25) A:U W:W Trans	H_{OPT}	-10.5	-3.3	18.1	0.2	-1.1	3.0
		F_{OPT}	-0.1	-4.7	0.0	0.0	-0.1	2.8
19	(BP26) A:U H:W Cis	H_{OPT}	15.2	2.4	-11.9	0.0	0.2	2.8
		F_{OPT}	0.1	1.7	0.0	0.0	0.1	2.8
20	(BP27) G:U S:W Cis	H_{OPT}	-4.1	61.8	29.3	0.7	1.9	2.6
		F_{OPT}	-11.2	59.6	43.8	0.7	1.7	2.5
21	(BP29) A:C W:W Trans	H_{OPT}	6.9	-0.3	-20.0	-0.1	2.6	3.0
		F_{OPT}	0.1	0.9	0.1	0.0	2.1	3.0
22	(BP30) G:U S:S Cis	H_{OPT}	12.0	-20.3	-18.8	-1.1	1.4	4.5
		F_{OPT}	-6.7	-22.2	-54.1	-1.0	0.6	4.3
23	(BP32) A:C W:S Cis	H_{OPT}	-28.3	-38.2	-10.7	-1.0	0.7	4.4
		F_{OPT}	-35.9	-35.1	-12.8	-1.1	0.9	4.2
24	(BP33) A:A H:H Trans	H_{OPT}	156.8	17.3	10.5	4.2	2.9	0.2
		F_{OPT}	-145.8	32.0	-0.2	-2.1	2.6	0.0
25	(BP34) U:C S:W Cis	H_{OPT}	34.0	-37.8	-3.7	0.2	-0.7	4.5
		F_{OPT}	31.3	-28.0	-51.1	-1.8	-0.4	4.1
26	(BP35) G:C S:S Cis	H_{OPT}	32.8	-16.9	-28.9	-1.2	0.4	4.0
		F_{OPT}	-6.2	-24.8	-53.1	-0.9	0.7	4.3
27	(BP36) A:U W:S Cis	H_{OPT}	46.4	-38.1	13.6	-0.2	-1.0	4.3
		F_{OPT}	35.6	-31.9	-17.2	-1.2	-0.7	4.3
28	(BP37) G:G H:W Trans	H_{OPT}	10.3	-4.7	-10.4	-0.2	0.0	3.0
		F_{OPT}	7.2	11.1	2.2	0.0	0.2	2.9
29	(BP38) U:C W:W Cis	H_{OPT}	8.4	-17.1	-15.8	0.4	-0.5	3.2
		F_{OPT}	-7.5	-3.0	-31.2	-0.5	-0.2	2.9
30	(BP40) G:U h:w Cis	H_{OPT}	-6.3	16.6	-17.5	0.1	-0.5	3.2
		F_{OPT}	-3.6	24.1	6.0	-0.1	0.0	3.0
31	(BP42) A:U s:w Cis	H_{OPT}	24.1	-5.9	-2.0	-0.1	-0.2	2.8
		F_{OPT}	-2.1	-4.9	-9.8	-0.1	-0.2	3.0
32	(BP44) A:A w:w Cis	H_{OPT}	15.8	13.1	-22.8	-0.5	-2.7	2.7
		F_{OPT}	14.0	18.6	-13.4	-0.1	-2.7	2.7

S6 Mg^{2+} binding induced charge redistribution of the monomers

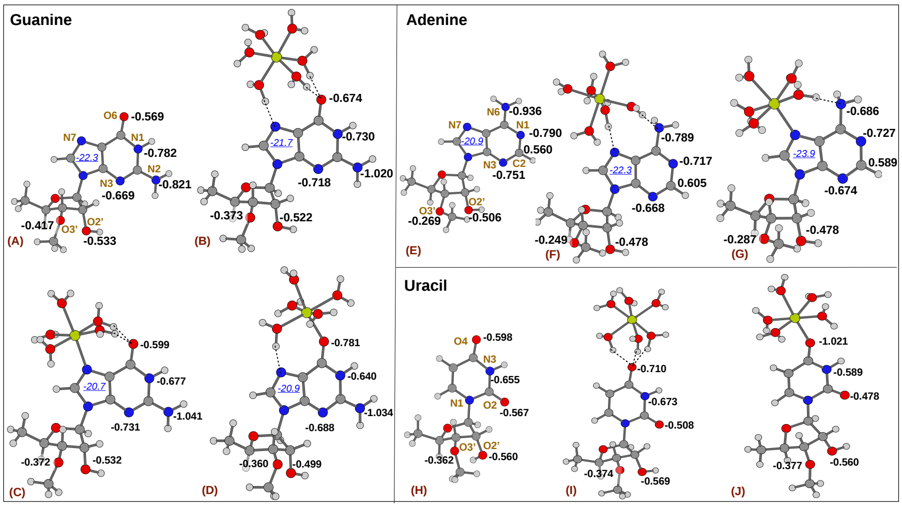


Figure S7: Partial charges at different sites of the three nucleobases in their isolated and Mg^{2+} bound forms are given as a fraction of the elementary charge (e). Partial charges obtained Molecular Electrostatic Potential (MESP) calculation are reported here. Hydrogen bonding interactions between the inner shell water molecules and the nucleobase atoms are shown in broken lines. NICS$(1)_{zz}$ values (in ppm unit) for the 5-member rings are reported in blue text (also underlined).

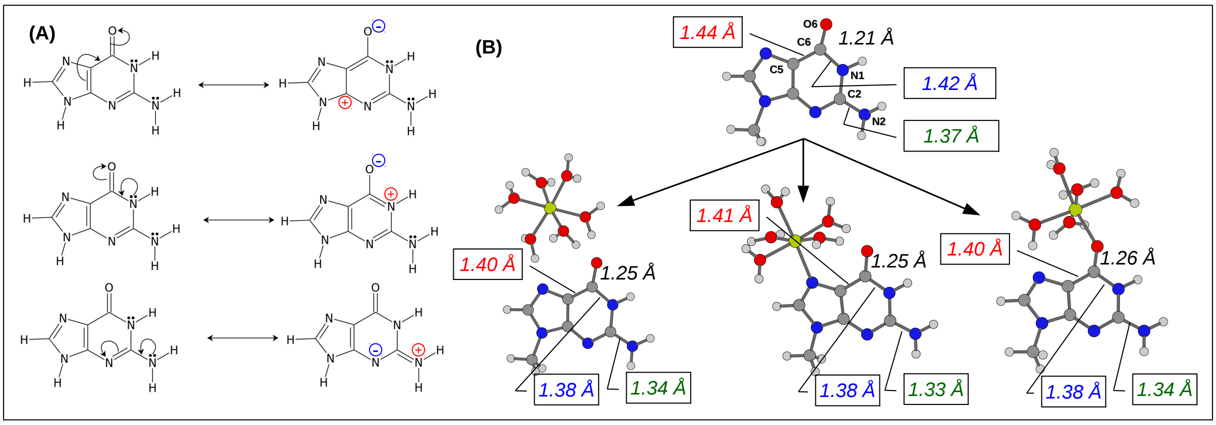


Figure S8: (A) Resonance canonical structures (valance bond structures) of guanine. (B) Optimized geometries of isolated guanine and guanine with different modes of Mg^{2+} binding. C6-O6, N1-C6, C5-C6 and C2-N2 bond lengths are reported in **black**, **blue**, **red** and **green** colored text, respectively.

In comparison to the optimized geometry of isolated guanine, optimized geometries of Mg^{2+} bound guanine (Figure S8B) display an elongated C6-O6 bond and shortened C5-C6, N1-C6 and N2-C2 bonds. This suggests that in the presence of Mg^{2+} binding, the major contributing resonance canonical structures or valance bond structures of guanine are the ones which are illustrated in Figure S8A. The distribution of formal charges in these resonance canonical structures clearly suggest that, on Mg^{2+} binding the electronic charge density increases at O6 and reduces at N1 and N2. Similar justification is also valid for other nucleobases.

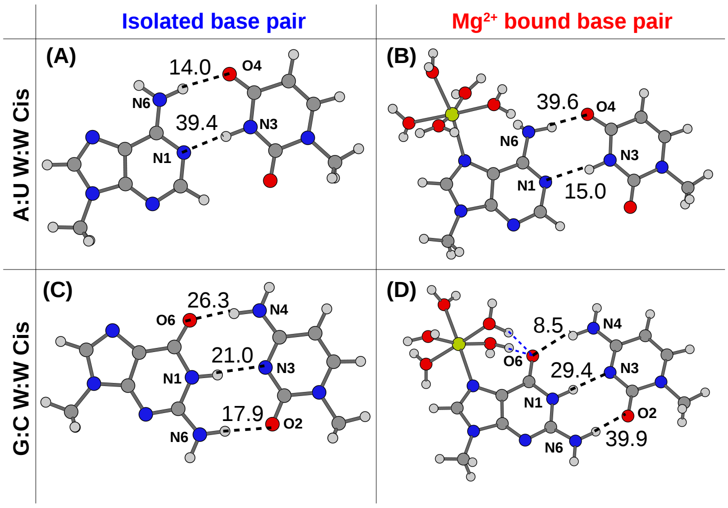


Figure S9: Optimized geometries of (A)isolated and (B) Mg^{2+} bound A:U W:W Cis pair. The inter-base hydrogen bonds are shown in black broken line. For each of the hydrogen bonds we have reported the values of the stabilization energy (E(2), in kcal mol^{-1}) obtained from NBO analysis. The same values are also reported for (C) isolated and (D) Mg^{2+} bound G:C W:W Cis pairs. Hydrogen bonds between Mg^{2+} coordiated water and O6 of guanine is represented in blue broken lines.

Within the Natural Bond Orbital framework, each hydrogen bond is treated as a $n\rightarrow\sigma^*$ type charge transfer interaction from the lone pair orbital of the acceptor to the anti-bonding orbital of the donor-hydrogen bond. Strength of individual inter-base hydrogen bonds can be measured using the stabilization energy (E(2)) due to charge delocalization between donor and acceptor natural bond orbitals. Larger value of E(2) represents a stronger hydrogen bond. As shown in the above Figure S9, in A:U W:W Cis pair Mg^{2+} binding increases the strength of the A(N6-H)$\cdots$O4(U) bond and reduces the strength of the U(N3-H)$\cdots$N1(A) bond. Analysis of the charge redistribution due to Mg^{2+} binding also suggested that on Mg^{2+} binding, N6 of adenine will become a better hydrogen bond donor, while hydrogen bonding potential of N1 will be reduced. In the same line, the partial charge distribution analysis suggested that hydrogen bonding potential of all the three polar atoms of the WC edge of guanine will be improved on Mg^{2+} binding. Interestingly, in G:C W:W Cis pair, the C(N4-H)$\cdots$O6(G) bond displays an exception. Unlike the other two bonds, it gets weaker on Mg^{2+} binding. However, it must be noted that in this case the O6 is involved in three hydrogen bond formation (two with water molecules and one with cytosine) and therefore should be treated separately. Therefore the final interaction energies of different Mg^{2+} bound base pairs are strongly influenced by the mode of Mg^{2+} binding.

Table S4: NBO (obtained from natural population analysis) and ESP charges (obtained from molecular electrostatic potential calculation) at the hydrogen atoms of isolated and Mg^{2+} bound nucleobases. Values are given as a fraction of the elementary charge (e). In guanine, the hydrogen atoms that are attached to the N2 atom are denoted by N2-H(W) (which belong to the Watson-Crick edge) and N-H(S) (which belong to the Sugar edge). Similarly in adenine, the hydrogen atoms that are attached to the N6 atom are denoted by N6-H(H) (which belong to the Hoogsteen edge) and N-H(W) (which belong to the Watson-Crick edge).

				Mode of Mg^{2+} binding		
Guanine	Atoms		isolated	Water mediated	Direct (N7)	Direct (O6)
	N1-H	NBO	0.453	0.468	0.473	0.461
		ESP	0.427	0.427	0.421	0.435
	N2-H(W)	NBO	0.422	0.446	0.449	0.445
		ESP	0.356	0.469	0.482	0.462
	N2-H(S)	NBO	0.437	0.466	0.466	0.468
		ESP	0.373	0.489	0.502	0.504
	O2′-H	NBO	0.514	0.522	0.525	0.522
		ESP	0.377	0.414	0.419	0.407
Adenine	Atoms		isolated	Water mediated	Direct (N7)	
	N6-H(H)	NBO	0.441	0.435	0.433	
		ESP	0.413	0.348	0.299	
	N6-H(W)	NBO	0.437	0.457	0.461	
		ESP	0.427	0.383	0.36	
	C2-H	NBO	0.22	0.252	0.255	
		ESP	0.063	0.094	0.108	
	O2′-H	NBO	0.513	0.522	0.524	
		ESP	0.389	0.42	0.439	
Uracil	Atoms		isolated	Water mediated	Direct (O4)	
	N3-H	NBO	0.47	0.472	0.478	
		ESP	0.388	0.404	0.409	
	O2′-H	NBO	0.501	0.526	0.527	
		ESP	0.372	0.427	0.432	

S7 Occurrence frequency of Mg^{2+} bound base pairs in HDRNAS database

S7.1 Base pairs having Mg^{2+} bound to O6 or N7 of guanine

	via N7		via O6		via both			No. of occurrences **in HDRNAS**
Base pairing geometry	Direct	Water mediated	Direct	Water mediated	Direct	Water mediated	Total	
G:A pairs								
G:A S:H Trans	23	9	32	29	1	27	121	1299
G:A s:s Trans	1	7	3	8	0	20	39	587
G:A s:w Trans	0	2	6	2	0	7	17	357
G:A W:W Cis	0	1	1	3	0	8	13	344
G:A S:W Trans	0	2	0	3	0	4	9	206
G:A s:s Cis	1	1	1	4	0	8	15	147
G:A S:S Cis	0	0	1	1	0	3	5	131
G:A s:w Cis	0	2	3	2	0	2	9	104
G:A w:w Trans	0	0	1	0	0	0	1	6
G:C pairs								
G:C W:W Cis	18	129	22	166	1	249	585	14090
G:C W:W Trans	0	1	0	2	0	1	4	116
G:C S:S Cis	0	0	0	2	0	1	3	83
G:C W:S Trans	1	0	0	0	0	0	1	40
G:C W:S Cis	0	0	1	1	0	0	2	14
G:C h:h Cis	0	0	1	0	0	0	1	2
G:G pairs								
G:G S:S Trans	1	1	7	1	0	2	12	150
G:G H:W Cis	0	0	2	2	0	0	4	123
G:G W:H Cis	2	0	9	1	0	2	14	123
G:G W:H Trans	0	1	1	0	0	0	2	65
G:G S:S Cis	0	2	0	2	0	0	4	54
G:G S:H Trans	0	0	1	0	0	1	2	11
G:G S:W Cis	0	0	0	0	0	0	0	6
G:U pairs								
G:U W:W Cis	0	11	21	20	0	40	92	2009
G:U s:h Cis	0	0	2	3	0	0	5	116
G:U S:W Cis	6	1	0	0	0	1	8	33
G:U w:h Trans	0	0	3	0	0	0	3	21
G:U W:W Trans	0	0	0	0	0	1	1	8

S7.2 Base pairs having Mg^{2+} bound to N6 or N7 of adenine

	via N6		via N7		via both			
Base pairing geometry	Direct	Water mediated	Direct	Water mediated	Direct	Water mediated	Total	No. of occurrences **in HDRNAS**
A:A pairs								
A:A H:H Trans	0	4	0	0	0	0	4	418
A:A W:W Trans	0	0	0	6	0	0	6	278
A:A H:W Trans	0	1	0	0	0	0	1	194
A:A W:H Trans	0	0	0	3	0	4	7	194
A:A S:W Cis	0	0	0	3	0	2	5	146
A:A W:S Cis	0	1	0	2	0	1	4	146
A:A h:s Trans	0	1	0	0	0	0	1	94
A:A s:h Trans	0	4	4	2	0	1	11	94
A:A w:w Cis	0	2	0	0	0	0	2	80
A:A S:H Cis	0	1	0	2	0	1	4	50
A:A s:s Trans	0	1	0	0	0	0	1	10
A:A h:h Cis	0	1	0	0	0	0	1	4
A:C pairs								
A:C s:s Cis	0	2	5	4	0	2	13	462
A:C W:S Cis	0	1	0	0	0	1	2	172
A:C S:W Cis	0	1	0	0	0	0	1	47
A:C W:W Trans	0	0	0	4	0	0	4	25
A:C s:h Cis	0	0	0	1	0	0	1	8
A:G pairs								
A:G H:S Trans	0	2	0	0	0	0	2	1299
A:G s:s Trans	0	3	0	9	0	2	14	584
A:G w:s Trans	0	0	0	0	0	1	1	360
A:G W:W Cis	0	4	0	0	0	1	5	344
A:G W:S Trans	0	0	0	3	0	0	3	206
A:G s:s Cis	0	0	2	3	0	0	5	147
A:G S:S Cis	0	0	4	2	0	0	6	131
A:G w:s Cis	0	0	0	1	0	0	1	104
A:G +:H Trans	0	0	0	0	0	2	2	9
A:G z:h Cis	0	0	0	1	0	0	1	3
A:U pairs								
A:U W:W Cis	0	21	4	30	0	18	73	3714
A:U H:W Cis	0	2	0	0	0	0	2	187
A:U s:s Cis	0	0	0	3	0	2	5	176
A:U W:W Trans	0	0	0	0	0	2	2	148
A:U w:s Trans	0	0	0	1	0	0	1	148

S7.3 Base pairs having Mg^{2+} bound to O4 of uracil

Base pairing geometry	Direct	Water mediated	Total	No. of occurrences in **HDRNAS**
U:A pairs				
U:A W:W Cis	10	62	72	3714
U:A W:H Trans	15	18	33	903
U:A W:H Cis	0	5	5	187
U:A s:s Cis	0	2	2	176
U:A s:w Trans	0	5	5	148
U:A W:W Trans	0	5	5	148
U:A S:W Cis	0	2	2	53
U:A s:h Trans	1	4	5	37
U:A w:s Cis	0	2	2	37
U:A w:s Trans	0	1	1	24
U:A h:h Trans	0	1	1	13
U:C pairs				
U:C W:W Cis	0	2	2	52
U:C S:W Cis	3	1	4	28
U:G pairs				
U:G W:W Cis	17	57	74	2009
U:G S:S Cis	0	4	4	54
U:G w:h Cis	0	1	1	19
U:G S:W Cis	1	0	1	14
U:G S:S Trans	0	1	1	8
U:G W:W Trans	0	1	1	8
U:U pairs				
U:U W:W Cis	1	5	6	452
U:U S:W Cis	0	1	1	6

S8 Occurrence frequency of Mg^{2+} bound base pairs in NDB database

S8.1 Base pairs having Mg^{2+} bound to O6 or N7 of guanine

	via N7		via O6		via both			
Base pairing geometry	Direct	Water mediated	Direct	Water mediated	Direct	Water mediated	Total	No. of occurrences **in NDB**
G:A pairs								
G:A S:H Trans	13	10	25	22	0	28	98	951
G:A s:s Trans	1	5	1	9	0	18	34	427
G:A W:W Cis	0	0	1	3	0	8	12	303
G:A s:w Trans	0	4	1	6	0	3	14	201
G:A S:W Trans	0	2	5	7	0	7	21	200
G:A s:s Cis	0	0	2	2	0	3	7	105
G:A S:S Cis	0	0	0	1	0	3	4	95
G:A s:w Cis	0	3	0	1	0	7	11	72
G:A w:w Trans	0	0	0	0	0	1	1	4
G:A h:z Cis	0	1	0	0	0	0	1	1
G:C pairs								
G:C W:W Cis	29	118	24	166	1	275	613	13182
G:C W:W Trans	0	0	1	2	0	0	3	86
G:C S:S Cis	0	0	1	0	0	1	2	49
G:C W:S Trans	2	0	0	0	0	0	2	30
G:C h:h Trans	0	0	0	1	0	0	1	12
G:C S:W Trans	1	0	0	0	0	0	1	27
G:C W:S Cis	0	0	1	0	0	0	1	4
G:C h:h Cis	0	0	0	1	0	0	1	3
G:G pairs								
G:G H:W Cis	0	0	4	2	0	0	6	222
G:G W:H Cis	0	0	7	1	0	1	9	222
G:G S:S Trans	0	0	7	3	0	1	11	120
G:G W:H Trans	0	2	1	0	0	0	3	72
G:G S:S Cis	0	0	0	1	0	2	3	44
G:G S:H Trans	0	0	0	0	0	1	1	4
G:U pairs								
G:U W:W Cis	3	13	9	21	0	24	70	1622
G:U s:h Cis	0	2	4	3	0	0	9	98
G:U S:S Cis	0	0	1	0	0	0	1	34
G:U h:w Cis	0	0	0	2	0	0	2	21
G:U S:W Cis	1	0	0	0	0	0	1	16
G:U S:W Trans	0	1	0	1	0	0	2	14
G:U W:W Trans	0	0	0	0	0	1	1	13

S8.2 Base pairs having Mg^{2+} bound to N6 or N7 of adenine

	via N6		via N7		via both			
Base pairing geometry	Direct	Water mediated	Direct	Water mediated	Direct	Water mediated	Total	No. of occurrences **in NDB**
A:A pairs								
A:A H:H Trans	0	2	0	0	0	0	2	412
A:A W:W Trans	0	0	0	4	0	2	6	214
A:A S:W Cis	0	0	0	4	0	1	5	137
A:A W:S Cis	0	0	0	1	0	1	2	137
A:A H:W Trans	0	0	0	1	0	0	1	127
A:A W:H Trans	0	2	0	4	0	0	6	127
A:A w:w Cis	0	2	0	0	0	1	3	106
A:A h:s Trans	0	2	0	0	0	0	2	103
A:A s:h Trans	0	1	2	3	0	0	6	103
A:A S:H Cis	0	3	0	2	0	0	5	43
A:A s:s Trans	0	1	0	0	0	0	1	32
A:A s:w Trans	0	2	0	0	0	0	2	19
A:A w:s Trans	0	0	0	1	0	0	1	19
A:C pairs								
A:C s:s Cis	0	4	2	3	0	0	9	303
A:C W:S Cis	0	0	0	1	0	4	5	136
A:C +:W Cis	0	0	0	1	0	0	1	101
A:C S:W Cis	0	1	0	0	0	0	1	31
A:C W:W Trans	0	1	0	3	0	0	4	21
A:G pairs								
A:G H:S Trans	1	1	0	0	0	0	2	951
A:G s:s Trans	0	1	0	8	0	3	12	427
A:G W:W Cis	0	2	0	1	0	1	4	303
A:G w:s Trans	0	0	2	0	0	1	3	201
A:G W:S Trans	0	1	0	2	0	0	3	200
A:G s:s Cis	0	0	1	0	0	0	1	105
A:G S:S Cis	0	0	2	1	0	1	4	95
A:G +:H Trans	0	0	0	0	0	2	2	10
A:G z:h Cis	0	0	0	1	0	0	1	1
A:U pairs								
A:U W:W Cis	0	31	2	33	0	34	100	6013
A:U H:W Trans	0	2	0	0	0	0	2	703
A:U H:W Cis	0	2	0	0	0	0	2	201
A:U s:s Cis	0	1	0	2	0	0	3	170
A:U w:s Trans	0	1	0	0	0	0	1	127
A:U W:W Trans	0	0	0	0	0	1	1	110
A:U h:s Trans	0	0	0	1	0	0	1	53
A:U s:w Cis	0	1	0	0	0	0	1	38
A:U s:h Trans	0	1	0	0	0	0	1	8
A:U S:S Trans	0	0	0	1	0	0	1	4

S8.3 Base pairs having Mg^{2+} bound to O4 of uracil

Base pairing geometry	Direct	Water mediated	Total	No. of occurrences in **NDB**
U:A pairs				
U:A W:W Cis	20	80	100	6013
U:A W:H Trans	16	20	36	703
U:A W:H Cis	0	5	5	201
U:A s:s Cis	0	6	6	170
U:A s:w Trans	0	7	7	127
U:A W:W Trans	0	2	2	110
U:A S:W Cis	0	3	3	65
U:A s:h Trans	4	1	5	53
U:A w:s Trans	0	1	1	21
U:C pairs				
U:C W:W Cis	0	2	2	62
U:C S:W Cis	1	0	1	32
U:C W:W Trans	1	0	1	7
U:G pairs				
U:G W:W Cis	9	42	51	1622
U:G S:S Cis	0	3	3	34
U:G w:h Cis	0	3	3	21
U:G S:W Cis	2	0	2	13
U:G W:W Trans	0	1	1	13
U:U pairs				
U:U W:W Cis	1	7	8	618

S9 PDB Ids of the RNA crystal structures studied in this work

S9.1 HD-RNAS (167 files)

URL: http://www.saha.ac.in/biop/www/HD-RNAS.html

2du6 ,2zue ,1f7u ,3kfu ,1b23 ,2fmt ,1yfg ,4arc ,3vjr ,2bte ,2azx ,3eph ,1o0c ,3knl ,3akz ,1euy ,1zjw ,3amt ,1ffy ,1qu2 ,2zni ,3foz ,1evv ,2zm5 ,3tup ,1ehz ,3a3a ,3hl2 ,3add ,2fk6 ,1qf6 ,2dr2 ,2y10 ,2xqd ,3am1 ,1c0a ,1il2 ,2der ,1gtr ,1n78 ,1qtq ,1wz2 ,3tvf ,3uye ,4as1 ,2ct8 ,3knh ,4dh9 ,2csx ,2du5 ,1h4s ,3rg5 ,1ser ,4gaq ,3uz6 ,1j1u ,3uz8 ,1j2b ,1gax ,1i6u ,2vqe ,3r8n ,3u5b ,2zjr ,3r8s ,1mms ,1vqo ,3v2d ,3u5d ,1un6 ,2xg0 ,1u8d ,1xok ,2vpl ,1zho ,2nz4 ,1hr2 ,1gid ,1c9s ,1sj3 ,3nkb ,3g78 ,2z75 ,2r8s ,2gcv ,1m5o ,3cul ,3d2v ,3f2q ,4enc ,2xnz ,3npq ,3irw ,3v7e ,4fe5 ,1y26 ,3q3z ,3gx5 ,3suh ,3dio ,2pxv ,1l9a ,1lng ,3ktw ,1hq1 ,2pxb ,2a64 ,1u9s ,1p6v ,3r9w ,3r9x ,2b57 ,3npb ,1gtn ,1gtf ,3snp ,3pu0 ,3pu1 ,2xd0 ,2zzn ,2zzm ,2ozb ,2gje ,3ptx ,3pu4 ,1fir ,3moj ,3hhz ,357d ,3knn ,1s03 ,3siv ,2xdb ,2xdd ,2il9 ,3nmu ,1kxk ,1vfg ,3pyu ,3kiq ,3kir ,3kit ,3pyn ,3u4m ,3ciy ,1jbr ,3nvk ,3hax ,3ovb ,3ovs ,3p22 ,1kh6 ,3pla ,1ddy ,3r4f ,3rw6 ,2zh1 ,3icq ,2gtt ,2nue ,2hvy ,1u6b ,2hw8 ,2jea ,3lwv ,1xjr ,3ds7

S9.2 NDB (838 files)

URL: http://rna.bgsu.edu/rna3dhub/nrlist/

1urn ,3iab ,1ooa ,3r4f ,3zp8 ,3snp ,4a3e ,4pqv ,1kxk ,4bxx ,3siu ,3la5 ,4tzx ,1cvj ,2bh2 ,4a3d ,4a3k ,3b5f ,4lx6 ,4q5s ,1p6v ,3egz ,364d ,1t0d ,1yfg ,3nvk ,1hys ,4boc ,3hk2 ,1i9v ,1mji ,2tra ,1y26 ,4n0t ,2du3 ,3moj ,2du6 ,1jbr ,2d2l ,3cw5 ,1h4s ,1qc0 ,4ngf ,3nkb ,1f7v ,1fir ,4c4w ,1vfg ,4jf2 ,3vjr ,4ol8 ,2ake ,4a93 ,2dlc ,1vby ,3tup ,1u0b ,total 3ouy ,2ozb ,3e2e ,1qu2 ,2g3s ,4kr2 ,2p7d ,2hoj ,1j1u ,1i6u ,3wqy ,3po2 ,1qf6 ,1q96 ,1b23 ,2rfk ,1VY9 ,3amu ,2zuf ,4k4w ,4p5j ,3umy ,2hvy ,1eiy ,1qrs ,4mcf ,1VY8 ,4qi2 ,2zzm ,3cz3 ,4lvz ,4db2 ,4kr6 ,2gjw ,3hjw ,3gtl ,4kr7 ,4k4u ,1qbp ,3am1 ,3hax ,3m3y ,1h3e ,3qsy ,4aob ,2i82 ,4b5r ,1feu ,3dh3 ,3al0 ,3bnq ,2nok ,1s03 ,2pn4 ,3gx5 ,4kzd ,4ts2 ,3fu2 ,1d4r ,4l81 ,1tfy ,4wkj ,1tfw ,4o26 ,4q0b ,3sux ,1nuv ,3p59 ,3zla ,1lng ,3htx ,3ciy ,1yyw ,2vpl ,4w92 ,1u63 ,3hou ,4pqu ,1ykv ,3w3s ,3ucz ,4wfl ,1duq ,4qlm ,4H6F ,1egk ,3a6p ,4jrc ,4qyz ,3f4g ,4qk9 ,4kqy ,1qa6 ,4g7o ,1zx7 ,4csf ,4mgm ,1fjg ,4qk8 ,3j7y ,2AW7 ,4un5 ,4un3 ,1un6 ,4v19 ,4ilm ,3rw6 ,1mfq ,3ivn ,3icq ,2o5i ,2oiu ,3slq ,3j7a ,3siv ,1hmh ,4uyk ,4u7u ,3eph ,2quw ,2zzn ,2ho7 ,4W23 ,1h38 ,3U5F ,2der ,2zni ,2zm5 ,3pla ,2azx ,1efw ,1il2 ,2qbz ,2wj8 ,3wfs ,2qux ,1u9s ,1j2b ,2y9h ,2csx ,3d2v ,3q3z ,2qwy ,2d6f ,4k4y ,2cv1 ,1gax ,3d0u ,3ol8 ,2bte ,4aq7 ,2gdi ,3ol7 ,4gxy ,4frg ,4rge ,3ol9 ,3rg5 ,3dir ,3owz ,1et4 ,1wz2 ,1g1x ,3add ,3adc ,4p9r ,3cun ,3iwn ,3ktw ,4k50 ,3p22 ,4frn ,2gtt ,4FY3 ,2xd0 ,4plx ,4uyj ,1m5o ,1u6b ,1VW3 ,4eya ,4oo8 ,2czj ,4ioa ,4m6d ,3v7e ,1s72 ,4QCN ,2il9 ,3ivk ,2QBG ,3rkf ,1nbs ,3r1c ,4qjd ,2a64 ,3U5H ,3kfu ,1kog ,1VX6 ,1gid ,4mgn ,3hga ,3ok4 ,1rmv ,4ejt ,3j06 ,4lck ,4W21 ,1rxa ,4ang ,3ahu ,3pdm ,1vtm ,2x1a ,1mdg ,1laj ,1osu ,2c4z ,2c50 ,1p79 ,2fz2 ,4afy

,4alp ,2xnr ,4lq3 ,4jiy ,4n2s ,333d ,3u2e ,2x1f ,1h2c ,4ohy ,4n2q ,3qjp ,2r7u ,2r7v ,4qu6 ,4lmz ,4faw ,2r7s ,3o8c ,3mj0 ,2tmv ,4r3i ,3hsb ,4ms9 ,4ohz ,2r7t ,283d ,3pf4 ,3qsu ,3gpq ,3rtj ,2vop ,1g2j ,3b0u ,3nj6 ,4dwa ,3q0q ,3q0r ,3q0s ,2a1r ,4jzv ,4jvh ,3k5q ,3k5y ,3k5z ,3k61 ,3k62 ,3k64 ,4tu0 ,3pf5 ,3rc8 ,3t3o ,1b2m ,2voo ,4i67 ,2xs7 ,4rkv ,3qgc ,1l3z ,1kq2 ,4hot ,4hos ,3avt ,4nku ,4lj0 ,2asb ,4j7m ,4qu7 ,3nna ,2g91 ,1n1h ,413d ,3o8r ,3v71 ,3v6y ,2xs2 ,3bsb ,4j7l ,4oau ,1nb7 ,4hor ,1fxl ,2bbv ,1si3 ,4nl3 ,3nma ,1i5l ,1pgl ,3mij ,3nmr ,4jab ,255d ,2q66 ,2r7w ,4oav ,3t5n ,3v74 ,3l26 ,1uvk ,4rcj ,1g2e ,4kre ,3nnc ,4d25 ,1uvi ,3ice ,3gib ,2c0b ,2po1 ,4ola ,3pey ,2q1r ,3g9y ,2vnu ,4am3 ,3mdg ,3mdi ,4e59 ,4u35 ,2v7r ,4u34 ,259d ,402d ,4cs1 ,3iev ,1wpu ,3sqw ,1uvj ,2jea ,3czw ,4fts ,4kxt ,1cwp ,4e78 ,2xs5 ,4c8y ,4g9z ,3r1e ,4al7 ,3nd3 ,3q0o ,3i5x ,3i5y ,1wmq ,1av6 ,2a8v ,4qm6 ,4ii9 ,4mdx ,2xgj ,4krf ,4c8z ,2vuq ,2a0p ,3p4c ,3p4d ,4c40 ,4f1n ,2xzo ,2b2d ,3jxr ,3oin ,2xli ,1kd5 ,438d ,1kfo ,3ie1 ,1uvm ,3q0p ,2bx2 ,1ddl ,3o7v ,2jlu ,2jlw ,2vrt ,4g0a ,3bx3 ,2g4b ,3aev ,3er9 ,2von ,1n38 ,4gv9 ,3kmq ,2f8k ,3knc ,4o8j ,3rer ,1uvl ,1pvo ,4ba2 ,4jvy ,4fsj ,2vod ,1zse ,1zdj ,4e58 ,2gxb ,3gvn ,421d ,479d ,4msr ,3bnt ,1bmv ,4ht9 ,4n48 ,3bx2 ,4dzs ,4b3g ,4ftb ,3kms ,3nl0 ,422d ,472d ,1dqh ,4jrd ,377d ,3ibk ,1m8y ,4ngd ,3qrr ,3bsx ,4nha ,4f3t ,3uld ,3vnu ,1wne ,165d ,2y8y ,439d ,4l8h ,3eqt ,2r22 ,2jlz ,1xpo ,1xpr ,1xpu ,1knz ,3fht ,2izn ,2y8w ,3avu ,2v6w ,4fvu ,3l25 ,4j39 ,3pkm ,4jk0 ,4w5n ,3qjj ,3qjl ,1zh5 ,3qrp ,1i9x ,1j6s ,4j5v ,2jlx ,3d2s ,2atw ,1n35 ,1uvn ,1ytu ,3vnv ,4nlf ,3fs0 ,1lnt ,157d ,3cjz ,4jrt ,4knq ,2ix1 ,354d ,3avv ,4e6b ,2pjp ,2r20 ,433d ,4pei ,4f02 ,3bso ,1fuf ,3boy ,2py9 ,3m85 ,3q2t ,3bsn ,3cgp ,3cgr ,3cgs ,3ssf ,1rna ,4kyy ,2gje ,3dd2 ,3m7n ,3nnh ,2ann ,2e9r ,4c9d ,4w5r ,3adi ,1l2x ,4h5p ,1b7f ,2e9z ,387d ,4tv0 ,3hxm ,3r2d ,4ay2 ,353d ,1csl ,2a43 ,466d ,435d ,405d ,3q50 ,2nz4 ,4pmw ,1f8v ,2izm ,1k8w ,3avw ,1mhk ,397d ,4gha ,2val ,1m8w ,4peh ,3r2c ,4bw0 ,1zbi ,1zbl ,4oq8 ,3avx ,2bgg ,3ncu ,3lrr ,3k49 ,3avy ,2j0s ,7msf ,3ho1 ,3tmi ,2xsl ,4pcj ,2w89 ,420d ,3og8 ,1jid ,1jzv ,4w5t ,2iz9 ,4ato ,4kji ,3hm9 ,3sn2 ,4h8k ,406d ,398d ,1f1t ,1j9h ,3p6y ,4bwm ,2zy6 ,1zev ,2jlt ,4m59 ,4w5q ,2bu1 ,3glp ,2oe5 ,4m7d ,4w5o ,1u1y ,2e9t ,3hjf ,1f27 ,3lrn ,3tzr ,3sj2 ,1o9m ,2ao5 ,3r9w ,2db3 ,4oo1 ,4m7a ,4ill ,1t0k ,4qil ,2ec0 ,1e7k ,1sa9 ,2hw8 ,1saq ,4pdb ,4e5c ,4ijs ,1UTF ,3mqk ,3szx ,1t0e ,4fxd ,4ghl ,2bq5 ,5msf ,4jah ,2dr8 ,361d ,3syw ,1mwl ,3bnl ,4qqb ,6msf ,3ova ,2fqn ,2az2 ,3td0 ,4k31 ,2grb ,4jng ,3bt7 ,1zbh ,1xok ,2o3x ,3td1 ,4ktg ,3mei ,2qek ,4bhh ,4u8t ,1br3 ,1ec6 ,1ntb ,4hkq ,4oog ,2o3v ,4kq0 ,409d ,1duh ,1sds ,3rzo ,1yzd ,1q2r ,4gg4 ,4nfo ,4qik ,2zi0 ,1nlc ,2awe ,2gic ,3ptx ,3pu0 ,4iqs ,3s1m ,3s1n ,2f8s ,3bnp ,2zko ,1xpe ,280d ,4j1g ,1gtn ,1gtf ,4o41 ,4mce ,1rpu ,2qk9 ,4erd ,3erc ,4lgt ,3npn ,3loa ,1yz9 ,3ks8 ,1xjr ,2nue ,3p4b ,3pu1 ,3zc0 ,1qcu ,3agv ,4wsb ,3r9x ,4wsa ,4wrt ,3b31 ,4py5 ,3ftm ,1kh6 ,1utd ,3s1r ,3ts0 ,1dfu ,429d ,4ig8 ,1r9f ,2q1o ,4k27 ,3s2d ,1rlg ,4enb ,3wbm ,4oji ,2f8t ,3ts2 ,2i91 ,3s14 ,2ply ,1sdr ,2xb2 ,1VW4 ,3s49 ,3s15 ,3ftf ,2nug ,2pxv ,3s16 ,1i6h ,3r1d ,3s17 ,3e5c ,2b3j ,1qln ,488d ,3nvi ,3nj7 ,3po3 ,4k4v ,1mzp ,4m30 ,3t5q ,4a3g ,4gcw ,1jbs ,4m4o ,1m8v ,2w2h ,1s77 ,1yvp ,2ez6 ,4kz2 ,3fo4 ,1msw ,4e48 ,3f73 ,1r3e ,1f7y ,4c7o ,1e8o ,3bsu ,1ser ,4ifd ,1a9n ,4b3o

S9.3 Complete dataset (2464 files)

URL: https://drive.google.com/open?id=0Bz9N3h6Uh7BYd0hHRmIyUlA3S0E

X-ray crystal structures with resolution less than 3.5Å (1873 files

2xpj ,3hga ,3ok4 ,4ejt ,1rxa ,3wzi ,4ang ,3ahu ,2x1a ,1mdg ,1laj ,1osu ,2c4z ,2c50 ,2c51 ,1p79 ,2fz2 ,4afy ,4alp ,2xnr ,4qvc ,4lq3 ,4jiy ,4n2s ,333d ,3u2e ,2x1f ,1h2c ,1eqq ,4oi0 ,4oi1 ,4ohy ,4n2q ,3qjp ,2r7u ,2r7v ,4yoe ,4qu6 ,4lmz ,2r7s ,3o8c ,3mj0 ,4r3i ,4qvd ,3hsb ,4ms9 ,4ohz ,2r7r ,2r7t ,283d ,3pf4 ,4rcm ,3qsu ,3gpq ,3rtj ,2vop ,1g2j ,3b0u ,3nj6 ,4dwa ,3qg9 ,3q0q ,3q0r ,3q0s ,3af6 ,4s2y ,5bud ,2a1r ,4jzv ,4jvh ,3k5q ,3k5y ,3k5z ,3k61 ,3k62 ,3k64 ,4tu0 ,3t3n ,3pf5 ,1h2d ,3rc8 ,3t3o ,4x9e ,1b2m ,2voo ,4i67 ,2xs7 ,4rby ,4rbz ,4rc0 ,4rkv ,3qgb ,3qgc ,4s2x ,1l3z ,4jzu ,1kq2 ,4hot ,4hos ,3avt ,4nku ,4lj0 ,2asb ,4j7m ,4qu7 ,3nna ,2g91 ,4u3p ,4xk0 ,1n1h ,4rj1 ,413d ,3o8r ,3v71 ,5bte ,3v6y ,2xs2 ,3bsb ,4j7l ,4oau ,1nb7 ,4hor ,1fxl ,2bbv ,1si3 ,4nl3 ,3nma ,1i5l ,1pgl ,3mij ,3nmr ,4jab ,255d ,2q66 ,2r7w ,4oav ,3t5n ,3v74 ,3l26 ,4tyw ,4tz0 ,4tz6 ,1uvk ,4rcj ,1g2e ,4kre ,3nnc ,1wrq ,4d26 ,4d25 ,1uvi ,3ice ,3gib ,2c0b ,2po1 ,4ola ,4olb ,3pey ,2q1r ,3g9y ,2vnu ,4am3 ,3mdg ,3mdi ,4e59 ,4u35 ,2v7r ,4u34 ,4u37 ,259d ,402d ,4u3l ,4u3o ,4u3r ,4u47 ,4u78 ,4cs1 ,3iev ,1wpu ,3sqw ,3sqx ,1uvj ,2jea ,3czw ,4fte ,4fts ,3pew ,4tyy ,4kxt ,1cwp ,4wkr ,4e78 ,2xs5 ,4c8y ,4g9z ,3r1e ,4al7 ,1rxb ,3nd3 ,3nd4 ,3q0o ,3i61 ,3i62 ,3i5x ,3i5y ,1wmq ,1av6 ,3o3i ,2a8v ,4qm6 ,4ii9 ,4mdx ,2xgj ,4krf ,4wal ,4c8z ,4u6m ,4u6l ,2vuq ,2a0p ,3p4c ,3p4d ,4c40 ,4f1n ,3o6e ,4ht8 ,2xzo ,2b2d ,2r7y ,3jxr ,4gv3 ,4gv6 ,3oin ,4al6 ,2xli ,1kd3 ,1kd4 ,1kd5 ,438d ,1kfo ,3ie1 ,1uvm ,3q0m ,3q0p ,2bx2 ,1ddl ,3o7v ,2jlu ,2jlw ,2vrt ,4g0a ,3bx3 ,2g4b ,3aev ,3er9 ,2von ,1n38 ,4wtk ,4wtl ,4wtm ,4wti ,4wtj ,4gv9 ,3kmq ,2xlj ,2f8k ,3knc ,4o8j ,3d0m ,3rer ,1uvl ,5c0y ,1pvo ,4ngg ,4ba2 ,4jvy ,4fsj ,2vod ,1zse ,4iqx ,1zdj ,4e58 ,2gxb ,3gvn ,421d ,479d ,4msr ,2r7x ,3q0n ,1m8x ,3bnt ,1bmv ,4nh5 ,3g0h ,4ht9 ,4n48 ,3bx2 ,4dzs ,4b3g ,4ftb ,3klv ,3kms ,3kna ,3nl0 ,422d ,472d ,3jxq ,1efo ,1dqf ,1dqh ,4jrd ,377d ,3ibk ,3q0l ,1m8y ,4ngb ,4ngc ,4ngd ,3qrr ,3bsx ,4nha ,4f3t ,2bs1 ,3uld ,3vnu ,1wne ,2g8f ,2g8h ,2g8k ,2g8u ,2g8v ,2g8w ,2gun ,165d ,2y8y ,439d ,4l8h ,3eqt ,2g92 ,1g4q ,1fix ,404d ,2ykg ,205d ,2r21 ,2r22 ,4nh3 ,2jly ,2jlz ,1xpo ,1xpr ,1xpu ,1knz ,3fht ,4wta ,4wtc ,4wtf ,4wtg ,2izn ,2iz8 ,2c4q ,2c4y ,4wte ,4wtd ,2y8w ,4zld ,3avu ,2v6w ,4fvu ,3l25 ,2dqo ,2dqp ,2dqq ,4bpb ,3zd6 ,4j39 ,1j8g ,3pkm ,4jk0 ,2jlv ,4w5n ,3qjj ,3qjl ,4x2b ,1yty ,1zh5 ,3qrp ,3adl ,1jb8 ,1i9x ,4jgn ,1j6s ,4nh6 ,4j5v ,2jlx ,3d2s ,2atw ,3twh ,1n35 ,2g8i ,1uvn ,1ytu ,4nmg ,3vnv ,4nxh ,4nlf ,3fs0 ,1lnt ,3vyx ,157d ,3cjz ,4jrt ,4knq ,2yjy ,4ed5 ,2ix1 ,4wzq ,354d ,3avv ,4e6b ,3dw4 ,3dw6 ,480d ,2pjp ,1pjg ,1pjo ,2r1s ,2r20 ,433d ,4pei ,4f02 ,2bs0 ,4qpx ,3bso ,2ab4 ,3zd7 ,430d ,1fuf ,3boy ,2py9 ,3m85 ,3q2t ,3bsn ,3cgp ,3cgq ,3cgr ,3cgs ,3ssf ,437d ,1rna ,4kyy ,3k1v ,2gje ,3dd2 ,3m7n ,3nnh ,2ann ,2e9r ,4wzm ,3h5x ,3h5y ,1a34 ,4c9d ,4w5r ,3s7c ,3s8u ,3dvz ,3dw5 ,3dw7 ,483d ,3adi ,1l3d ,1l2x ,3q51 ,4h5p ,1b7f ,2e9z ,387d ,4tv0 ,3hxm ,5amr ,3r2d ,1q9a ,4ay2 ,1msy ,353d ,1csl ,2a43 ,2h1m ,464d ,466d ,434d ,435d ,405d ,3q50 ,4pmw ,1f8v ,2izm ,1k8w ,3avw ,1mhk ,397d ,4gha ,2val ,1m8w ,4peh ,3r2c ,2anr ,1zl3 ,4bw0 ,1zbi ,1zdh ,4oq8 ,3avx ,2bgg ,3ncu ,3lrr ,4fnj ,3k49 ,3k4e ,3avy ,2j0s ,7msf ,4u6k ,1zdi ,3ho1 ,3tmi ,2xsl ,4pcj ,1ik5 ,2w89 ,420d ,3og8 ,3iem ,2bny ,1aq3 ,2xlk ,1jid ,2oe6 ,2oe8 ,3gca ,1jzv ,4w5t ,3oij ,2iz9 ,4ato ,4kji ,3hm9

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,3sn2 ,4h8k ,1f1t ,1j9h ,3p6y ,4bwm ,1aq4 ,2dr5 ,2zy6 ,2jlt ,4m59 ,4oe1 ,4w5q ,2b2e ,3gm7 ,2bu1 ,3glp ,2dr7 ,2oe5 ,4m7d ,4w5o ,2b2g ,1u1y
,2e9t ,3hjf ,1f27 ,2dr9 ,2zh1 ,2zh7 ,2zh9 ,3lrn ,3tzr ,4wcq ,4wcs ,3sj2 ,1o9m ,2ao5 ,3r9w ,2db3 ,4oo1 ,2j0q ,4m7a ,4ill ,1t0k ,2drb ,2zh2 ,2zh3
,2zh4 ,2zh5 ,2zh8 ,2zhb ,4qil ,4pgy ,2ec0 ,1e7k ,1sa9 ,2hw8 ,4f8v ,4wcr ,1saq ,4pdb ,4e5c ,4ijs ,3mqk ,2xdb ,3szx ,4j50 ,4yn6 ,1t0e ,4p20 ,4fxd
,4k32 ,4ghl ,3ex7 ,2bq5 ,5msf ,4jah ,2dr8 ,299d ,361d ,3syw ,301d ,1j7t ,4gpx ,1lc4 ,1mwl ,3dvv ,3bnl ,4qqb ,6msf ,5amq ,2dvi ,2dra ,2zha ,3ova
,1q29 ,2fqn ,2az0 ,2az2 ,2g5k ,3td0 ,4k31 ,2grb ,4jng ,2hyi ,3bt7 ,1zbh ,2zh6 ,1xok ,1zdk ,2f4s ,2f4u ,2o3x ,4gpw ,3td1 ,3s4p ,2be0 ,2bee ,4gpy
,2pwt ,4ktg ,3mei ,3c44 ,2qek ,4bhh ,4wan ,4u8t ,1br3 ,1ec6 ,1di2 ,4jnx ,300d ,359d ,1nta ,1ntb ,4hkq ,1nyi ,4oog ,3wru ,1z7f ,4pmi ,2et4 ,2et5
,2o3w ,2et3 ,2et8 ,2o3v ,2o3y ,1yrj ,4kq0 ,1rc7 ,2oiy ,2oj0 ,4lg2 ,409d ,1duh ,1sds ,3rzo ,1yzd ,1z79 ,4nfp ,4nfq ,1q2r ,4gg4 ,4nfo ,4qik ,2esj
,2zi0 ,3far ,1nlc ,1y90 ,2awe ,2gic ,3ptx ,3pu0 ,3pu4 ,379d ,4iqs ,3s1m ,3s1n ,3rzd ,2f8s ,4f8u ,4pdq ,3bnp ,2zko ,5bs3 ,2b8r ,1xpf ,1xp7 ,1xpe
,280d ,4j1g ,1gtn ,1gtf ,4phy ,2esi ,4o41 ,4mce ,1rpu ,2qk9 ,2fcx ,2fcy ,2fd0 ,4erd ,1o3z ,3erc ,4lgt ,3mj3 ,3mja ,3mjb ,3npn ,4en5 ,3loa ,1ze2
,2oij ,1yz9 ,3ks8 ,4rwp ,3vrs ,4s3n ,1xjr ,4enc ,2nue ,1y6s ,1wvd ,1y6t ,1y73 ,1y95 ,1y99 ,4rne ,3p4b ,3pu1 ,3zc0 ,1qcu ,4r8i ,3agv ,4wsb ,3r9x
,4wsa ,4wrt ,3b31 ,4py5 ,4zcf ,3lqx ,2b8s ,1y3o ,1y3s ,1yxp ,3ftm ,1kh6 ,1utd ,3s1r ,1yy0 ,1q2s ,3ts0 ,1dfu ,429d ,2pn3 ,4ig8 ,1r9f ,2q1o ,4k27
,3s2h ,3s2d ,2pxl ,4ena ,1rlg ,4enb ,3wbm ,4oji ,2f8t ,1yyk ,3hhz ,3ts2 ,2i91 ,3s14 ,2uwm ,3fte ,2ply ,462d ,1sdr ,1yyo ,2xb2 ,4a3b ,3s49 ,3s15
,3ftf ,2pxb ,2pxe ,2pxu ,2nug ,2pxd ,2pxf ,2pxk ,2pxp ,2pxq ,2pxt ,2pxv ,1hq1 ,4tux ,4rwn ,4rwo ,3s16 ,3vyy ,1i6h ,4enn ,2f4t ,3s1q ,3r1d ,2qkb
,4p97 ,3s17 ,1dul ,3e5e ,3e5f ,3e5c ,1zbl ,4qoz ,4l8r ,2b3j ,1qln ,2fk6 ,4u38 ,4msb ,488d ,3nvi ,4m2z ,3nj7 ,4v4f ,1c9s ,3po3 ,1mzp ,4m30 ,2nuf
,3t5q ,4a3g ,4gcw ,1jbs ,4m4o ,1m8v ,2w2h ,1s77 ,1yvp ,3hvr ,1jbt ,4xw7 ,4xwf ,2ez6 ,4kz2 ,3fo4 ,3ok2 ,1msw ,4e48 ,3f73 ,1r3e ,4q5v ,4tuw
,1f7y ,4c7o ,1e8o ,1kuq ,3bsu ,1zz5 ,2a04 ,1ser ,3gog ,4ifd ,1s76 ,1a9n ,1dk1 ,4b3o ,3gs5 ,5c7w ,3gao ,2xnz ,3fo6 ,4fe5 ,3g4m ,3ger ,1urn ,3iab
,4wcp ,1ooa ,3r4f ,2b57 ,3ges ,3got ,2ees ,2eet ,2eeu ,2eev ,2eew ,3hov ,4a3c ,5c7u ,4fej ,4fel ,2g9c ,4fen ,4feo ,4fep ,3snp ,4a3e ,4pqv ,2oeu
,1kxk ,4bxx ,3siu ,4g6s ,4g6p ,3bbm ,1vtq ,3b5a ,3b5s ,3la5 ,4tzx ,4tzy ,1cvj ,2bh2 ,3hoy ,4a3d ,4a3k ,4ycp ,3b5f ,3b91 ,3bbk ,3b58 ,2oue ,4lx6
,4lx5 ,4q5s ,4x4v ,1p6v ,3egz ,357d ,364d ,1t0d ,3l0u ,1yfg ,4tna ,4xnr ,3nvk ,1hys ,4boc ,4a3l ,1wsu ,1ehz ,3tra ,3hk2 ,6tna ,1tn2 ,1i9v ,3bbi
,1mji ,2tra ,1y27 ,1y26 ,4n0t ,2det ,2du3 ,2du4 ,4g6r ,1x9c ,1tn1 ,1zev ,2hop ,1zft ,1vc5 ,1tra ,3moj ,1gsg ,2nqp ,2du6 ,2du5 ,1jbr ,4arc ,4pkd
,2d2l ,4a3f ,3cw5 ,3cw6 ,4tra ,1gts ,1h4s ,1qc0 ,1evv ,4ngf ,2nvt ,4x4s ,2d2k ,1f7v ,1zfv ,2bcy ,2fgp ,3gs8 ,2p7f ,1fir ,4c4w ,4x4q ,2npy ,1x9k
,1vfg ,1qtq ,1zfx ,1vc6 ,4qei ,4jf2 ,3vjr ,4ol8 ,2ake ,4a93 ,2dlc ,4nyg ,3ovs ,3ov7 ,1zjw ,2oih ,2oj3 ,2bcz ,1vbx ,1vby ,1vc0 ,3tup ,1u0b ,1vbz
,1h4q ,2hom ,4yvi ,4yvj ,4yvk ,4x0b ,4wc3 ,3ouy ,2npz ,2rd2 ,1euq ,3gs1 ,1f7u ,4x4o ,1exd ,2ozb ,1sjf ,1sj3 ,1sj4 ,3e2e ,2hok ,1qu3 ,4nyb ,4nyc
,1ffy ,1qu2 ,4nyd ,2g3s ,4jxx ,1euy ,4kr2 ,4jyz ,4jxz ,1gtr ,2re8 ,4pr6 ,2hoj ,2hol ,1j1u ,1i6u ,2bj6 ,3x1l ,4wc4 ,2dr2 ,4wc5 ,4x4r ,3ovb ,3wqz
,1o0c ,3wqy ,2hoo ,4wj4 ,4zc7 ,1q93 ,4wc6 ,4wc2 ,4wc7 ,3po2 ,4k4t ,3bnn ,4prf ,1ob2 ,4kr3 ,4by7 ,3bno ,1qf6 ,2vum ,1q96 ,3a3a ,4xjn ,1b23
,2rfk ,1o0b ,1c0a ,4k4s ,3amt ,3amu ,4kr9 ,2zuf ,4k4w ,1mme ,1qrt ,4ari ,4p5j ,3u56 ,3umy ,2hvy ,1eiy ,1drz ,4rdx ,1qru ,2zue ,1qrs ,5btm
,4mcf ,4qi2 ,2zzm ,3lwv ,3cz3 ,4lvw ,4lvx ,4lvy ,4lvz ,4db2 ,2e2j ,4kr6 ,3lwr ,2gjw ,3hjw ,4as1 ,4qvi ,3u4m ,4qg3 ,4lw0 ,3gtj ,2iy5 ,3gtl ,4kr7
,4k4u ,3lwq ,3lwo ,3lwp ,1qbp ,3sd3 ,4x4u ,3am1 ,3hax ,4lvv ,4q9q ,4q9r ,2yu9 ,2e2i ,2nvq ,1r9t ,4y52 ,4y7n ,3m3y ,1h3e ,3qsy ,1k9w ,4aob
,3iqp ,2gis ,2i82 ,3iqn ,2ydh ,4b5r ,3iqr ,3zju ,1feu ,3dh3 ,3al0 ,4rum ,3bnq ,2nok ,1s03 ,2pn4 ,3gx6 ,3gx7 ,4kze ,3gx2 ,2fcz ,3gx3 ,3gx5 ,3hl2
,4x4n ,4kzd ,4ts2 ,3fu2 ,1d4r ,4yb1 ,4yhw ,1zci ,4l81 ,4oqu ,3zjt ,1tfy ,3bns ,4wkj ,1tfw ,4o26 ,4puo ,4ts0 ,4q0b ,3suh ,3sux ,3suy ,1nuj ,1nuv
,3p59 ,1z43 ,3zla ,3irw ,3muv ,4rzd ,1lng ,3htx ,3ciy ,1yyw ,3mut ,3zjv ,3mxh ,3mum ,3mur ,3bnr ,2vpl ,4w92 ,4pwd ,4x4t ,1u63 ,3hou ,4pqu
,1ykq ,1ykv ,3ucu ,4w90 ,3w3s ,1yls ,3ucz ,3ud4 ,3ud3 ,4wfl ,1duq ,4qlm ,3f30 ,3f2t ,3f2x ,3f2y ,3f2w ,3f2q ,3nmu ,2xdd ,1egk ,3a6p ,4jrc ,4qyz
,3f4h ,3f4e ,3f4g ,4qk9 ,2yif ,4kqy ,4tvx ,4qln ,1qa6 ,4g7o ,1zx7 ,2yie ,5btp ,4qka ,4csf ,4mgm ,1y39 ,4qk8 ,1hc8 ,5axw ,5czz ,1mms ,4x4p ,4un5
,4un3 ,4un4 ,1un6 ,4ilm ,3trz ,3rw6 ,3skr ,1l9a ,3ds7 ,3skw ,3skl ,3skt ,4p3e ,1mfq ,4znp ,3ivn ,3icq ,2o5i ,4k4x ,3slm ,2oiu ,3slq ,3skz ,406d
,2qus ,4meg ,1ddy ,3siv ,3ski ,1hmh ,3b4c ,2o5j ,2ppb ,4uyk ,4u7u ,3epk ,3epj ,3ndb ,3b4a ,2ho6 ,2gcv ,2h0w ,5cd4 ,3eph ,2quw ,2zzn ,4meh
,3b4b ,2ho7 ,2gcs ,2h0x ,4zt0 ,1h38 ,4zt9 ,2der ,2zni ,4k4z ,2zxu ,2zm5 ,3pla ,3npq ,2azx ,1efw ,1il2 ,2qbz ,2wj8 ,3wfs ,2qux ,3foz ,2deu ,1u9s
,1j2b ,2y9h ,1asy ,2cky ,2csx ,2ct8 ,1g59 ,3d2x ,3d2g ,3d2v ,2cv0 ,3q3z ,2qwy ,2d6f ,1asz ,1zho ,2byt ,2cv1 ,2cv2 ,1n78 ,1gax ,1ivs ,2v0g ,4erj
,4erl ,3d0x ,3d0u ,2fmt ,3ol8 ,1s0v ,2bte ,2dxi ,1n77 ,3ol6 ,4aq7 ,2gdi ,4nya ,3ol7 ,4gxy ,4frg ,2r8s ,4rgf ,4rge ,3olb ,3ol9 ,4cqn ,4yb0 ,3rg5 ,4yaz
,3zgz ,3dig ,3dis ,3dj0 ,3dil ,3diz ,3diq ,3dix ,3dim ,3dir ,3dj2 ,3dio ,3diy ,3oxj ,3owz ,1et4 ,1wz2 ,2qkk ,3oxb ,3oxd ,3oww ,3owi ,3ox0 ,3oxe
,3oxm ,3k0j ,1g1x ,4y1m ,3add ,3adc ,3adb ,4p9r ,3cun ,3iwn ,4p95 ,3ktw ,4k50 ,3cul ,4xco ,3p22 ,4frn ,2v3c ,4y1i ,4y1j ,4wfm ,2gtt ,4v9e
,2xd0 ,4yco ,4plx ,4uyj ,1m5o ,1ttt ,1m5k ,1ob5 ,1u6b ,3bo3 ,1m5v ,1m5p ,4eya ,1zzn ,3bo2 ,4v99 ,4oo8 ,2czj ,4m6d ,3v7e ,2il9 ,3ivk ,3rkf
,4pjo ,1nbs ,3hhn ,3r1l ,3r1h ,3r1c ,4qjd ,2a64 ,3akz ,3wfr ,1l8v ,3kfu ,1kog ,1hr2 ,1gid ,3pdr ,4mgn ,4oq9 ,4nia ,3bwp ,4lck ,3eoh ,4fax ,4fau
,4e8p ,4e8r ,4e8q ,4e8n ,4fb0 ,4e8m ,3eog ,4faq ,4e8k ,3igi ,4faw ,3g78 ,4far ,4e8t ,1fg0 ,3g9c ,3g96 ,3g8s ,3g8t ,3l3c ,2nz4 ,4v8i ,4v8h ,4v7x
,4v7z ,4v7y ,4v7w ,4v8g ,1fka ,4v6c ,4v7u ,4v7v ,4v7s ,4v7t ,2uxd ,4u1u ,4u1v ,4u20 ,4u25 ,4u27 ,4u26 ,4u24 ,4v84 ,4v85 ,4wf1 ,4v83 ,2hhh
,2zm6 ,4yhh ,4v95 ,4lf6 ,4ji3 ,4dv7 ,4dr3 ,4khp ,4lf9 ,1ibk ,4lfb ,4ji1 ,4lf4 ,1hr0 ,4lf7 ,4lf8 ,1i94 ,4duy ,4dr2 ,4dv6 ,4ji0 ,1hnz ,1hnw ,1hnx ,1fjg
,1j5e ,4ji7 ,1xnq ,2vqe ,4gkk ,2uxb ,1xmo ,2vqf ,1xnr ,1xmq ,4gkj ,4k0k ,4jv5 ,2e5l ,2uxc ,1n33 ,1ibm ,2uub ,2uuc ,3t1h ,3t1y ,4b3s ,2uua ,2uu9
,4aqy ,4b3r ,4jya ,4b3t ,4dr5 ,1ibl ,1n32 ,4b3m ,4v6a ,4v9s ,4v9r ,4dr6 ,4v9a ,1vy6 ,4v9n ,1vy7 ,4v90 ,4v9h ,1vvj ,4l47 ,4lsk ,4lnt ,4lt8 ,4tue
,4w2h ,4v5a ,4v9k ,4v9l ,4woi ,4v9c ,4v64 ,4v4h ,4v4q ,4v54 ,4v52 ,4v57 ,4v5e ,4v9b ,4v5j ,4v8x ,4v67 ,4v50 ,4v63 ,4v7j ,4wu1 ,4v5k ,4wzd
,4v51 ,4v6g ,4v7m ,4wzo ,4v7l ,1vy4 ,4wro ,1vy5 ,4w2i ,4wsd ,4wt1 ,4v9i ,4wqr ,4w2g ,4w2f ,4v5d ,4v5c ,4wq1 ,4v5l ,4u4z ,4u3m ,4u53 ,4u4y
,4u4q ,4u56 ,4u3n ,4u55 ,4u4n ,4u51 ,4u4u ,4u52 ,4u50 ,4u4r ,4u3u ,4v8n ,4v5s ,4v5q ,4v8b ,4v5p ,4v5r ,4wr6 ,4v8d ,4wsm ,4wra ,4u6f ,4v88
,1p9x ,2o44 ,2ogm ,1ond ,2aar ,1jzx ,1j5a ,1k01 ,1jzy ,3pip ,1njp ,3pio ,2d3o ,3dll ,2zjq ,3cf5 ,2zjr ,4io9 ,4ioa ,4z8c ,1ffk ,1y69 ,2qa4 ,3g4s ,3ccj
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,1w2b ,2qex ,1n8r ,3ow2 ,1yjn ,3ccr ,1yjw ,1yj9 ,3g6e ,1yi2 ,2otl ,1yit ,3i56 ,1nji ,3ccs ,1k73 ,2otj ,1s72 ,1yij ,3cc2 ,1jj2 ,3cc7 ,3ccl ,3ccq ,3cc4 ,3cce ,3ccv ,3ccu ,3ccm ,1kc8 ,1k8a ,1k9m ,1q81 ,1q82 ,1kd1 ,1m1k ,1m90 ,1vqo ,3g71 ,1vqk ,1yhq ,3cpw ,1vq8 ,1vq9 ,3cd6 ,1vq6 ,3cme ,3cxc ,1kqs ,1vq4 ,1vq5 ,1q86 ,3cma ,1vqn ,1vq7 ,1vql ,1vqp ,1vqm ,1xbp ,1sm1 ,1nwx ,1nkw ,1qvg ,1nwy ,1qvf ,4v9f ,4v8a ,4zer ,4v9q ,4v9p ,4v9o ,4wqy ,4www ,4wqf ,4y4p ,4y4o ,4wqu ,4wpo ,4z3q ,4z3s ,4z3r ,4v8q ,4wt8 ,4v6f ,4v8c ,4v87 ,4v8f ,4v8e ,4w2e ,4ybb ,4v9d

Solution NMR structures (591 files)

124d, 176d, 17ra, 1a1t, 1a3m, 1a4d, 1a4t, 1a51, 1a60, 1a9l, 1ac3, 1afx, 1ajf, 1ajl, 1ajt, 1aju, 1akx, 1al5, 1am0, 1anr, 1aqo, 1arj, 1ato, 1atv, 1atw, 1aud, 1b36, 1bau, 1bgz, 1biv, 1bj2, 1bn0, 1bvj, 1byj, 1bz2, 1bz3, 1bzt, 1bzu, 1c0o, 1c2q, 1c4l, 1cq5, 1cql, 1cx5, 1d0t, 1d0u, 1d6k, 1drr, 1dz5, 1e4p, 1e95, 1ebq, 1ebr, 1ebs, 1efs, 1eht, 1ei2, 1ejz, 1eka, 1ekd, 1ekz, 1elh, 1esh, 1esy, 1etf, 1etg, 1exy, 1f5g, 1f5h, 1f5u, 1f6u, 1f6x, 1f6z, 1f78, 1f79, 1f7f, 1f7g, 1f7h, 1f7i, 1f84, 1f85, 1f9l, 1feq, 1fhk, 1fje, 1fl8, 1fmn, 1fnx, 1fqz, 1fyo, 1fyp, 1g3a, 1g70, 1guc, 1h0q, 1hg9, 1hji, 1hlx, 1hs1, 1hs2, 1hs3, 1hs4, 1hs8, 1hwq, 1i3x, 1i3y, 1i46, 1i4b, 1i4c, 1i9f, 1i9k, 1idv, 1ie1, 1ie2, 1ik1, 1ikd, 1j4y, 1jo7, 1jox, 1jp0, 1jtj, 1jtw, 1ju1, 1ju7, 1jur, 1jwc, 1jzc, 1k1g, 1k2g, 1k4a, 1k4b, 1k5i, 1k6g, 1k6h, 1k8s, 1kaj, 1kis, 1kka, 1kks, 1koc, 1kod, 1kos, 1kp7, 1kpd, 1kpy, 1kpz, 1l1c, 1l1w, 1lc6, 1ldz, 1lmv, 1lpw, 1luu, 1lux, 1lvj, 1m5l, 1m82, 1me1, 1mfj, 1mfk, 1mfy, 1mis, 1mnb, 1mnx, 1mt4, 1muv, 1mv1, 1mv2, 1mv6, 1mwg, 1my9, 1n53, 1n66, 1n8x, 1na2, 1nbk, 1nbr, 1nc0, 1nem, 1ntq, 1nts, 1ntt, 1nxr, 1nyb, 1nz1, 1o15, 1okf, 1oln, 1oo7, 1oq0, 1osw, 1ow9, 1p5m, 1p5n, 1p5o, 1p5p, 1pbl, 1pbm, 1pbr, 1pjy, 1q75, 1q8n, 1qc8, 1qd3, 1qes, 1qet, 1qfq, 1qwa, 1qwb, 1r2p, 1r3x, 1r4h, 1r7w, 1r7z, 1rau, 1raw, 1rfr, 1rgo, 1rht, 1rkj, 1rng, 1rnk, 1roq, 1rrd, 1rrr, 1s2f, 1s34, 1s9l, 1s9s, 1scl, 1slo, 1slp, 1sy4, 1syz, 1szy, 1t28, 1t2r, 1t4l, 1t4x, 1tbk, 1tfn, 1tjz, 1tlr, 1tob, 1tut, 1txs, 1u2a, 1u3k, 1u6p, 1ull, 1uts, 1uud, 1uui, 1uuu, 1vop, 1wks, 1wts, 1wtt, 1wwd, 1wwe, 1wwf, 1wwg, 1xhp, 1xsg, 1xsh, 1xst, 1xsu, 1xv0, 1xv6, 1xwp, 1xwu, 1yfv, 1yg3, 1yg4, 1ylg, 1ymo, 1yn1, 1yn2, 1ync, 1yne, 1yng, 1ysv, 1z2j, 1z30, 1z31, 1zbn, 1zc5, 1zif, 1zig, 1zih, 219d, 28sp, 28sr, 2a9l, 2a9x, 2ad9, 2adb, 2adc, 2adt, 2aht, 2ap0, 2ap5, 2au4, 2awq, 2b6g, 2b7g, 2bj2, 2c06, 2cd1, 2cd3, 2cd5, 2cd6, 2cjk, 2d17, 2d18, 2d19, 2d1a, 2d1b, 2dd1, 2dd2, 2dd3, 2err, 2es5, 2ese, 2euy, 2evy, 2f4x, 2f87, 2f88, 2fdt, 2fey, 2fy1, 2g1g, 2g1w, 2gbh, 2gio, 2gip, 2gm0, 2grw, 2gv3, 2gv4, 2gvo, 2h49, 2hem, 2hgh, 2hns, 2hua, 2i2y, 2i7e, 2i7z, 2ihx, 2irn, 2iro, 2ixy, 2ixz, 2jpp, 2jq7, 2jr4, 2jrg, 2jrq, 2jse, 2jsg, 2jtp, 2juk, 2jwv, 2jxq, 2jxs, 2jxv, 2jyf, 2jyh, 2jyj, 2jym, 2k3z, 2k41, 2k4c, 2k5z, 2k65, 2k66, 2k7e, 2k95, 2k96, 2kbp, 2kd4, 2kd8, 2kdq, 2ke6, 2kez, 2kf0, 2kfy, 2kg0, 2kg1, 2kgp, 2kh9, 2khy, 2km8, 2kmj, 2koc, 2kp3, 2kp4, 2kpc, 2kpd, 2kpv, 2krl, 2krp, 2krq, 2krv, 2krw, 2kry, 2krz, 2ktz, 2ku0, 2kur, 2kuu, 2kuv, 2kuw, 2kvn, 2kwg, 2kx5, 2kx8, 2kxm, 2kxn, 2kxz, 2ky0, 2ky1, 2ky2, 2kyd, 2kye, 2kzl, 2l1f, 2l1v, 2l2j, 2l2k, 2l3c, 2l3e, 2l3j, 2l41, 2l5d, 2l5z, 2l6i, 2l8c, 2l8f, 2l8h, 2l8u, 2l8w, 2l94, 2l9e, 2la5, 2la9, 2lac, 2lar, 2lb4, 2lbj, 2lbk, 2lbl, 2lbq, 2lbr, 2lbs, 2lc8, 2ldl, 2ldt, 2ldz, 2leb, 2lec, 2lhp, 2li4, 2li8, 2ljj, 2lk3, 2lkr, 2lp9, 2lpa, 2lps, 2lpt, 2lqz, 2lu0, 2lub, 2lun, 2lup, 2lv0, 2lvy, 2lwk, 2lx1, 2m12, 2m18, 2m1o, 2m1v, 2m21, 2m22, 2m23, 2m24, 2m39, 2m4q, 2m4w, 2m57, 2m58, 2m5u, 2m8d, 2m8k, 2mb0, 2meq, 2mer, 2mf0, 2mf1, 2mfc, 2mfd, 2mfe, 2mff, 2mfg, 2mfh, 2mgz, 2mhi, 2mi0, 2mis, 2miy, 2mjh, 2mki, 2mkk, 2mkn, 2mn0, 2mnc, 2mqt, 2mqv, 2ms0, 2ms1, 2ms5, 2mtj, 2mtk, 2mtv, 2mvs, 2mxj, 2mxk, 2mxl, 2mxy, 2mz1, 2n1q, 2n2o, 2n2p, 2n3q, 2n3r, 2n4j, 2o32, 2o33, 2o81, 2o83, 2oj7, 2oj8, 2oom, 2p89, 2pcv, 2pcw, 2pn9, 2qh2, 2qh3, 2qh4, 2rlu, 2rn1, 2ro2, 2rp0, 2rp1, 2rpk, 2rpt, 2rqc, 2rqj, 2rra, 2rrc, 2rs2, 2rsk, 2ru3, 2ru7, 2tob, 2tpk, 2u2a, 2xc7, 2xeb, 2xfm, 2y95, 2yh1, 3php, 484d, 4a4r, 4a4s, 4a4t, 4a4u, 4b8t, 4bs2, 4by9, 4cio, 5a17, 5a18, 8drh, 8psh

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