SUPPLEMENTARY INFORMATION TO

Higher Order Structures Involving Post Transcriptionally Modified Nucleobases in RNA

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SECTION S1

Additional Computational Details

Using the 'Het Groups' option of PDBsum[1] database, a unique 3-letter code corresponding to each of the 15 modified residues participating in higher order interactions (Table 1) was used to retrieve the relevant list of PDB entries submitted till 18 July 2016. The retrieved crystal structures were further filtered according to their resolution, and structures with resolution better than 3.5 Å were selected for further analysis. Further, experimental or modelled (in absence of experimental structure) structures of unmodified counterparts of modified higher order interactions were also considered for this study. For geometry optimization of the base triples and quadruples that do not involve interaction of ribose sugar, the sugar moiety was removed and the C1' atoms of the participating nucleosides were replaced with hydrogen atoms. For the higher order interactions that involved base-nucleoside interactions, the ribose sugar of the nucleoside that interacts through its sugar-edge was retained, after replacing the 5'-OH group of its ribose sugar with a hydrogen atom. Further, in case of triples involving the dinucleotide platform interactions between adjacent nucleotides, the phosphate backbone joining the platform was retained after neutralizing it with a hydrogen atom. Geometry optimization of the modified base triples were carried out at the B3LYP/6-31G(d,p)[2, 3] level using Gaussian 09[4], which was selected in synchrony with previous studies on RNA base pairs[5-9]. The geometries of the corresponding unmodified triplet geometries were also optimized for comparison. Although we were able fully optimize all the triplet structures, only one (m^5U:G:A:A) of the three (m^5U:G:A:A, C:Gm:G:C and A:Gm:G:C) quadruples, as well as its unmodified counterpart could be fully optimized. However, the modification at the sugar edge of one of the nucleobases, and consequent requirement of inclusion of ribose sugar in the calculations prohibited the full optimization of C:Gm:G:C and A:Gm:G:Cquartets. Nevertheless,

we were successful in carrying out hydrogen-only optimization of the C:Gm:G:C quartet, while freezing the heavy atoms.

Comparison of geometries of select modified motifs optimized using different DFT functionals (B3LYP, M06-2X and PBE), basis sets (6-31G(d,p) and aug-cc-pVDZ) and quantum chemical methods (DFT and HF) reveals that change in functional changes the hydrogen bond donor-acceptor (D-A) distances change by only up to 0.05 Å, whereas the change in basis set has even less pronounced effect, where the D-A distances change only by 0.1 Å (Table S11). However, the change in quantum chemical method is a slightly greater effect, where D-A distances change by up to 0.14 Å between HF and B3LYP optimizations (Table S11)), mainly due to lack of proper description of electron correlation in HF calculations. Nevertheless, the B3LYP/6-31G(d,p) optimized geometries of hydrogen bonded structures compare very well with reference RIMP2/cc-pVTZ optimized structures, where a typical overestimation of the H-bond distances by only 0.01-0.05 Å is observed using B3LYP.[10]

The energy of interaction ($\Delta E_{A\text{-}BC}$) between the modified base A with other constituents (B and C) is defined as

$$\Delta E_{A\text{-}BC} = E_{ABC} - (E_A + E_{BC})$$

where E_{ABC} is the single-point energy of the B3LYP/6-31G(d,p) optimized base triple and E_A and E_{BC} are the single-point energies of modified base A and the rest of the constituents (BC) respectively, calculated at the RIMP2/aug-cc-pVDZ level [11, 12]. The interaction energies were corrected for basis set superposition error[13] using the Turbomole v6.2[14] suite of quantum chemical programs. Comparison of interaction energies of a selected modified motif calculated on the B3LYP/6-31G(d,p) optimized geometries using different basis sets and quantum chemical methods reveals that the change in basis set has a negligible effect on binding energies (Table

S11). However, due to inadequate description of dispersion interactions, B3LYP functional underestimates the binding energy by up to 2 kcal/mol compared to the RIMP2/aug-cc-pVDZ method used in the present work. However, interaction energies calculated at the M06-2X level with same basis set match very well with the RIMP2/aug-cc-pVDZ values. Further, (RI)MP2/aug-cc-pVDZ interaction energies of hydrogen bonded RNA nucleobases compare very well with reference MP2/CBS(T) interaction energies, where an underestimation of only up to 1.1 kcal/mol is observed compared to reference values.[15] Additionally, Morokuma decomposition[16] of interaction energies was carried out on the charged base pairs, at the HF/6-31G(d,p) level, to estimate the electrostatic contribution to interaction energies.

Twelve of the total seventeen modified higher order associations had the corresponding unmodified counterparts available in the crystal structure dataset. Geometry optimizations and binding energy calculations were carried out to on the unmodified motifs to understand the effect of modification on the structure and strength of these associations. However, for the six motifs that did not have the unmodified counterparts in the dataset, the structures of the corresponding unmodified motifs were modelled by carrying out geometry optimizations after replacing the modified base with the corresponding unmodified base.

E-Values of hydrogen bonds

To evaluate the relative goodness of hydrogen bonds within base pairs in their crystal occurrences as well as in optimized geometries, we have calculated a parameter called E-value, which is defined as:

$$E = \sum_i (d_i - 3.0)^2 + \frac{1}{2}\sum_j \left(\theta_j - \pi\right)^2$$

Here d is the heavy atom distance for each hydrogen bond between two bases under consideration and θ is a pseudo angle subtended by precursor atoms of both the bases[17]. This parameter was used, since the RNA crystal structures from which base pairs were extracted, did not contain

hydrogen atoms. The E-value parameter assess the quality of hydrogen bonds in the absence of hydrogen atom coordinates, and is useful in analyzing hydrogen bonds within the crystal occurrences of base pairs.

REFERENCES

1. R. A. Laskowski, *Nucleic Acids Res.*, 2009, 37, D355-D359.
2. A. D. Becke, *J. Chem. Phys.*, 1993, 98, 5648-5652.
3. C. Lee, W. Yang and R. G. Parr, *Physical Review B*, 1988, 37, 785-789.
4. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, N. J. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian, Inc., Wallingford, CT, USA, 2009.
5. A. Mládek, P. Sharma, A. Mitra, D. Bhattacharyya, J. Šponer and J. E. Šponer, *J. Phys. Chem. B*, 2009, 113, 1743-1755.
6. P. Sharma, J. E. Šponer, J. Šponer, S. Sharma, D. Bhattacharyya and A. Mitra, *J. Phys. Chem B*, 2010, 114, 10234-10234.
7. J. Šponer, P. Jurečka and P. Hobza, *J. Am. Chem. Soc.*, 2004, 126, 10142-10151.
8. J. E. Šponer, N. a. Špačková, P. Kulhánek, J. Leszczynski and J. Šponer, *J. Phys. Chem. A*, 2005, 109, 2292-2301.
9. J. E. Šponer, N. a. Špačková, J. Leszczynski and J. Šponer, *J. Phys. Chem. B*, 2005, 109, 11399-11410.
10. J. Šponer, P. Jurečka, P. Hobza, *J. Am. Chem. Soc.*, 2004, 126, 10142–10151.
11. R. Ahlrichs, S. D. Elliott and U. Huniar, *Berichte der Bunsengesellschaft für Physikalische Chemie*, 1998, 102, 795-804.
12. F. Weigend and M. Häser, *Theor. Chem. Acc.*, 1997, 97, 331-340.
13. S. F. Boys and F. Bernardi, *Mol. Phys.*, 1970, 19, 553-566.
14. U. o. Karlsruhe and F. GmbH, 2011, DOI: citeulike-article-id:10416537.
15. J. Šponer, M. Zgarbová, P. Jurečka, K. E. Riley, J. E. Šponer, P. Hobza, *J. Chem. Theory Comput.*, 2009, 5, 1166–1179.
16. K. Kitaura and K. Morokuma. *Int. J. Quantum Chem.*, 1976, 10, 325-331.
17. J. Das, S. Mukherjee, A. Mitra and D. Bhattacharyya, *J. Biomol. Struct. Dyn.*, 2006, 24, 149-161.

TABLE S1. Distribution of crystal structures based on type of RNA in the dataset.

Structure category	Structures with at least one modified base	Structures with at least one modified base pair	Structures with only unpaired modified bases
tRNA	50	49	1
16S rRNA	32	22	10
23S rRNA	48	46	2
RBP	32	8	24
Ribosomes	21	2	19
ribozyme	16	6	10
Others	8	2	6
Total	207	135	72

Table S2. List of Modified Base Triples and quadruples identified from the dataset.

Modified base	Modified base triple	f	PDB accession no.	Base Pair I	Base Pair II	Quadruple
Gm (56)	G2617:C2542:Gm2588:WWC–SSC	43	1s72, 1vq4, 1vq5, 1vq6, 1vq8, 1vq9, 1vqk, 1vql, 1vqm, 1vqn, 1vqo, 1vqp, 1yhq, 1yi2, 1yij, 1yit, 1yj9, 1yjn, 1yjw, 2otj, 2otl, 2qa4, 2qex, 3cc2, 3cc4, 3cc7, 3cce, 3ccj, 3ccl, 3ccm, 3ccq, 3ccr, 3ccs, 3ccu, 3ccv, 3cd6, 3cma, 3cme, 3g4s, 3g6e, 3g71, 3i55, 3i56,	OMG2588:G2617 S:SC		
	Gm2588:C75:G2617:WWC–SSC	12	1vq4, 1vq6, 1vqk, 1vql, 1vqm, 1vqn, 1vqo, 3cd6, 3cma, 3i55, 1vq5, 1vqp,	OMG2588:G2617 S:SC	OMG2588:C75 WWC	C2542
	Gm2588:A76:G2617:WWC–SSC	1	3cme	OMG2588:G2617 SSC	OMG2588:A76 WWC	
m^7G (31)	m^7G 527:C522:A535:WWC–swT	11	4ji0, 4dr2, 4dr5, 4dv6, 4dv7, 4ji1, 4ji3, 4ji7, 4lf6, 4lf7, 4lf8,	7MG527:C522 WWC	7MG527:A535 SWT	
	G22:C13: m^7G46:WWC–HWT:1ehz	20	1c0a, 1ob2, 1ob5, 1yfg, 1ehz, 1evv, 1fir, 1tn1, 1tn2, 1tra, 1ttt, 2y0u, 2y0w, 2y10, 2y18, 4tna, 4tra, 6tna, 1efw, 1qf6,	7MG46:G22 WHT		
Ψ (28)	Ψ516:A533:C519:WHT–SWC	22	4dr2, 4dr3, 4dr5, 4dr6, 4duy, 4dv6, 4dv7, 4ji0, 4ji1, 4ji3, 4ji7, 4lf4, 4lf6, 4lf7, 4lf8, 4lf9, 4lfb,	PSU516:A533 WHT		
	G22:Ψ13:A46:WWC–H+T	4	4x62, 4x64, 4x65, 4x66, 5br8, 1il2, 1asy, 1asz, 1il2,	PSU13:G22 WWC		
	Ψ4:A36:A1493:WWC–SSC	2	4jv5,4jya (1471 instead of 1493)	PSU4:A36 WWC	PSU4:A1493 SSC	
s^4U (13)	s^4U8:A14:A21:WHT–swT	12	1c0a, 1efw, 2xqd, 2y0y, 2y12, 2y14, 2y16, 3cw5, 3cw6, 4jyz, 2y10, 2y18,	4SU8:A14 WHT	4SU8:A21 SWT	
	s4U8:A14:A46:WHT–ssC	1	1b23	4SU8:A14 WHT	4SU8:A46 SSC	
m^5U (3)	G10: m5U1:A58:WWC–ssC	3	1t42, 1u6b, 1zzn,	5MU1:G10 WWC		A86
D (2)	G15:C48:D20:WWT–SWT	1	1ser	H2U:G SWT		
	G619:C656:D620:WWC–shC	1	1c0a	H2U:G HSC		
m^5C (2)	G1497:m^5C1404:A1518:WWC–swT	2	4lf7, 4lf8	5MC:G WWC		
$m^6{}_2A$ (1)	G2618:U2541:$m^6{}_2$A76:WWC–swT	1	1vq6	5AA:G WST		
Um (1)	Um2656:G2655:A2665:hsC–WHT	1	3dw5	OMU:G HSC	OMU2656:A2665 WHT	

Table S3. Root mean square deviation (RMSD) between heavy atoms with different structures of triples involving modified bases.

Higher order interactions	PDB	RMSD (Å)		
		Crystal	Crystal Vs. Optimized	Modified Vs. Unmodified
C:m^{7}G^{+}:A	4dv7	0.23	0.48	0.51
C:Gm:G	1vqn	0.19	0.98	0.21
A:Gm:G	3cme	–	0.85	0.45
A:s^{4}U:Aw	2xqd	1.07	1.06	0.32
A:s^{4}U:As	1b23	–	0.72	0.12
A:Ψ:C	4dv7	0.23	0.29	-
G:Um:A	3dw5	–	0.62	0.26
m$^{6}_{2}$A:G:U	1vq6	–	1.02	0.57
m^{7}G^{+}:G:C	6tna	0.70	0.16	0.15
Gm:G:C	1vqm	0.15	0.93	0.59
m^{5}C:G:A	4lf7	0.0	1.27	0.03
Ψ:G:A^{H+}	1asy	0.30	0.17	-
m^{5}U:G:A	1t42	0.23	0.80	0.02
Dw:G:C	1ser	–	1.05	0.20
Dh:G:C	1c0a	–	0.59	0.78

Table S4. Average base pair parameters observed in the crystal structures of modified base triples.

Modified Triples	f	Base Pair 1							Base Pair 2						
		BP1	Buckle	Open	Propeller	Stagger	Shear	Stretch	BP2	Buckle	Open	Propeller	Stagger	Shear	Stretch
C:m^{7}G$^+$:A	11	C: m^{7}G$^+$	9.4	8.2	7.5	–0.1	–0.1	2.8	m^{7}G$^+$:A	–35.6	33.9	–27.9	–0.6	–2.3	2.9
C:Gm:G	12	Gm:G	15.5	10.1	14.0	1.5	–2.5	3.1	Gm:C	8.0	–4.2	0.5	0.1	0.0	2.9
A:Gm:G	1	Gm:G	20.9	0.0	–3.4	1.1	–2.0	3.6	Gm:A	16.6	10.3	15.0	0.2	–0.3	2.5
A:s^{4}U:Aw	18	A:s^{4}U	9.6	–6.9	0.4	–0.1	–0.1	3.1	s^{4}U:A	10.6	–1.6	3.2	0.0	0.6	2.9
A:s^{4}U:As	1	A:s^{4}U	6.2	3.4	–11.6	1.0	0.5	3.0	s^{4}U:A	–19.8	–29.0	–12.2	–1.8	1.2	3.2
A:Ψ:C	22	A:Ψ	18.7	–0.5	4.7	–0.3	–0.1	2.9	Ψ:C	–33.8	16.4	–21.9	–0.5	–1.3	4.5
G:Um:A	1	Um:G	3.2	–5.2	3.5	–0.2	–1.2	3.3	Um:A	–18.9	–2.5	–6.2	0.1	–0.0	2.6
m$^6_2$A:G:U	1	G:m$^6_2$A	–37.8	13.1	3.4	0.8	1.3	3.0	G:U	5.5	–1.3	–12.1	–0.1	2.3	2.8
m^{7}G$^+$:G:C	20	m^{7}G$^+$:G	8.6	0.8	4.5	0.2	0.2	2.8	C:G	3.9	2.9	–5.7	0.0	0.1	3.0
Gm:G:C	43	Gm:G	–12.8	9.1	12.1	1.6	2.5	3.0	C:G	–9.4	–2.0	9.9	–0.1	0.2	2.9
m^{5}C:G:A	2	m^{5}C:G	6.5	–7.1	–2.5	–0.1	0.6	2.9	G:A	60.2	48.9	–32.1	–0.4	–3.3	3.0
Ψ:G:A^{H+}	4	Ψ:G	11.5	7.8	–4.2	0.0	2.2	2.8	G:A^{H+}	2.4	9.3	6.8	–0.1	2.2	2.7
m^{5}U:G:A	3	m^{5}U:G	0.0	–13.4	–7.5	0.7	–2.3	2.8	G:A	5.7	6.3	–44.3	–42.4	1.1	–2.4
Dw:G:C	1	Dw:G	29.6	0.7	39.8	0.1	–0.7	3.13	G:C	–7.0	3.1	10.0	0.0	–2.3	2.9
Dh:G:C	1	Dh:G	17.5	0.9	–7.6	–0.7	–0.2	3.13	G:C	–19.0	1.2	–10.5	0.3	–0.1	3.0

Table S5. Average base pair parameters observed in the optimized structures of modified base triples.

Modified Triples	f	Base Pair 1							Base Pair 2						
		BP1	Buckle	Open	Propeller	Stagger	Shear	Stretch	BP2	Buckle	Open	Propeller	Stagger	Shear	Stretch
C:m^{7}G$^+$:A	11	C:m^{7}G$^+$	1.7	0.5	–1.6	–0.0	0.2	2.9	m^{7}G$^+$:A	–38.4	–33.1	5.3	–0.6	1.9	3.0
C:Gm:G	12	Gm:G	33.7	–1.3	–4.7	1.1	–2.1	3.6	Gm:C	3.9	–2.5	–2.7	–0.1	–0.1	2.9
A:Gm:G	1	Gm:G	20.9	0.0	–3.4	1.1	–2.0	3.6	Gm:A	–2.0	–1.6	19.3	0.2	0.0	2.9
A:s^{4}U:Aw	18	A:s^{4}U	–9.0	–4.4	2.1	0.1	0.1	2.9	s^{4}U:A	–38.4	–51.9	–44.4	–0.1	0.3	4.2
A:s^{4}U:As	1	A:s^{4}U	–4.4	4.2	–2.7	–0.1	0.2	2.9	s^{4}U:A	–42.1	–38.9	–31.5	–0.2	0.6	4.3
A:Ψ:C	22	A:Ψ	3.1	–4.3	4.1	0.1	0.2	2.8	Ψ:C	–53.0	–36.6	–10.6	–1.1	0.5	4.5
G:Um:A	1	Um:G	27.2	–1.4	–10.1	–0.2	–0.6	3.6	Um:A	–2.1	–4.1	2.2	0.0	0.1	2.8
m$^6{}_2$A:G:U	1	G:m$^6{}_2$A	–67.6	–16.1	8.2	–0.5	1.6	3.3	G:U	–35.1	2.6	15.2	0.1	2.4	2.8
m^{7}G$^+$:G:C	20	m^{7}G$^+$:G	0.3	–3.0	–0.2	0.0	0.2	2.8	C:G	0.5	–0.1	–0.2	0.0	0.1	2.9
Gm:G:C	43	Gm:G	–44.7	–4.1	–3.0	1.4	2.1	3.5	C:G	–4.0	–4.5	–0.4	–0.1	0.0	3.0
m^{5}C:G:A	2	m^{5}C:G	–1.2	–4.2	–3.0	–0.1	0.1	2.9	G:A	–34.9	30.9	–24.0	–0.2	–0.0	3.8
Ψ:G:A^{H+}	4	Ψ:G	–0.1	7.0	0.1	0.0	2.2	2.9	G:A^{H+}	0.0	–1.6	–0.3	0.0	2.7	2.8
m^{5}U:G:A	3	m^{5}U:G	0.8	1.1	–1.9	–0.1	–2.4	2.8	G:A	–36.2	–38.8	–32.1	–0.3	–2.5	3.1
Dw:G:C	1	Dw:G	34.2	–15.0	–31.4	0.8	–0.2	2.8	G:C	43.8	7.6	61.8	–0.1	–1.8	2.9
Dh:G:C	1	Dh:G	19.3	6.3	–23.1	–0.4	–0.5	3.4	G:C	–2.3	–4.0	2.6	0.1	–0.1	2.9

Table S6. Comparison of base pair parameters between the geometries of modified base pairs present as a part of optimized geometries of motifs, and isolated geometries of modified base pairs.

Modified Triples	f	Base pair as part of triple							Isolated base pair						
		BP	Buckle	Open	Propeller	Stagger	Shear	Stretch	BP	Buckle	Open	Propeller	Stagger	Shear	Stretch
C:m^{7}G$^+$:A	11	C:m^{7}G$^+$	1.7	0.5	–1.6	–0.0	0.2	2.9	C:m^{7}G$^+$	–1.4	–3.7	–2.3	–0.1	0.1	2.9
		m^{7}G$^+$:A	–38.4	–33.1	5.3	–0.6	1.9	3.0	m^{7}G$^+$:A	–53.2	38.7	18.9	1.4	2.0	2.7
C:Gm:G	12	Gm:G	33.7	–1.3	–4.7	1.1	–2.1	3.6	Gm:G	–59.7	22.8	4.9	1.1	1.6	3.1
		Gm:C	3.9	–2.5	–2.7	–0.1	–0.1	2.9	Gm:C	–2.0	–3.4	1.9	0.0	–0.1	2.9
A:Gm:G	1	Gm:G	20.9	0.0	–3.4	1.1	–2.0	3.6	Gm:G	–59.7	22.8	4.9	1.1	1.6	3.1
		Gm:A	–2.0	–1.6	19.3	0.2	0.0	2.9	Gm:A	1.3	–2.4	20.2	–0.2	0.0	2.9
A:s^{4}U:Aw	18	A:s^{4}U	–9.0	–4.4	2.1	0.1	0.1	2.9	A:s^{4}U	0.4	2.8	1.0	0.0	0.1	2.9
		s^{4}U:A	–38.4	–51.9	–44.4	–0.1	0.3	4.2	s^{4}U:A	8.4	44.0	–13.9	0.8	0.7	4.1
A:s^{4}U:As	1	A:s^{4}U	–4.4	4.2	–2.7	–0.1	0.2	2.9	A:s^{4}U	0.4	2.8	1.0	0.0	0.1	2.9
		s^{4}U:A	–42.1	–38.9	–31.5	–0.2	0.6	4.3	s^{4}U:A	45.4	–35.9	–15.9	–0.9	–0.9	4.3
A:Ψ:C	22	A:Ψ	3.1	–4.3	4.1	0.1	0.2	2.8	A:Ψ	–0.1	–0.4	–0.1	0.0	–0.1	2.9
		Ψ:C	–53.0	–36.6	–10.6	–1.1	0.5	4.5	Ψ:C	38.8	17.6	–12.4	–0.7	0.4	4.4
G:Um:A	1	Um:G	27.2	–1.4	–10.1	–0.2	–0.6	3.6	Um:G	0.5	–1.9	27.9	0.6	0.4	3.4
		Um:A	–2.1	–4.1	2.2	0.0	0.1	2.8	Um:A	3.8	4.8	0.4	0.0	0.1	2.8
m$^6{}_2$A:G:U	1	G:m$^6{}_2$A	–67.6	–16.1	8.2	–0.5	1.6	3.3	G:m$^6{}_2$A	–67.0	–14.8	11.9	–0.4	1.5	3.3
m^{7}G$^+$:G:C	20	m^{7}G$^+$:G	0.3	–3.0	–0.2	0.0	0.2	2.8	m^{7}G$^+$:G	0.3	2.7	0.2	0.0	0.3	2.8
Gm:G:C	43	Gm:G	–44.7	–4.1	–3.0	1.4	2.1	3.5	Gm:G	–59.7	22.8	4.9	1.1	1.6	3.1
m^{5}C:G:A	2	m^{5}C:G	–1.2	–4.2	–3.0	–0.1	0.1	2.9	m^{5}C:G	0.0	–3.6	0.2	0.0	0.1	2.9
Ψ:G:A	4	Ψ:G	–0.1	7.0	0.1	0.0	2.2	2.9	Ψ:G	0.7	1.1	1.7	0.1	2.4	2.8
m^{5}U:G:A	3	U:G	0.8	1.1	–1.9	–0.1	–2.4	2.8	m^{5}U:G	3.3	1.5	0.5	0.1	–2.4	2.8
Dw:G:C	1	U:G	34.2	–15.0	–31.4	0.8	–0.2	2.8	Dw:G	17.6	–11.2	59.2	–0.1	–0.4	3.0
Dh:G:C	1	U:G	19.3	6.3	–23.1	–0.4	–0.5	3.4	Dh:G	–32.7	6.5	–10.5	0.2	0.9	3.3

Table S7. Comparison of base pair parameters between the base pairs present as a part of the modified and unmodified base triples.

Modified Triples	Base pair in modified triples							Unmodified base triples						
	Base pair	Buckle	Open	Propeller	Stagger	Shear	Stretch	Base pair	Buckle	Open	Propeller	Stagger	Shear	Stretch
C:m^{7}G$^+$:A	C:m^{7}G$^+$	1.7	0.5	–1.6	–0.0	0.2	2.9	C:G	1.7	–4.1	–3.9	–0.1	0.1	2.9
	m^{7}G$^+$:A	–38.4	–33.1	5.3	–0.6	1.9	3.0	G:A	–64.2	49.1	–46.6	–1.0	–2.1	2.7
C:Gm:G	Gm:G	33.7	–1.3	–4.7	1.1	–2.1	3.6	G:G	27.4	–5.3	–12.7	1.8	–2.1	3.3
	Gm:C	3.9	–2.5	–2.7	–0.1	–0.1	2.9	G:C	3.2	–2.5	–3.6	–0.1	–0.1	2.9
A:Gm:G	Gm:G	20.9	0.0	–3.4	1.1	–2.0	3.6	G:G	39.6	1.1	–4.9	0.5	–2.4	3.6
	Gm:A	–2.0	–1.6	19.3	0.2	0.0	2.9	G:A	1.7	–1.6	21.0	0.2	0.0	2.9
A:s^{4}U:Aw	A:s^{4}U	–9.0	–4.4	2.1	0.1	0.1	2.9	A:U	–14.2	6.1	–1.8	–0.1	0.2	2.8
	s^{4}U:A	–38.4	–51.9	–44.4	–0.1	0.3	4.2	U:A	–48.8	–47.8	–35.4	0.4	0.8	4.2
A:s^{4}U:As	A:s^{4}U	–4.4	4.2	–2.7	–0.1	0.2	2.9	A:U	–11.2	5.2	–1.8	–0.1	0.2	2.8
	s^{4}U:A	–42.1	–38.9	–31.5	–0.2	0.6	4.3	U:A	–44.4	–39.8	–29.2	–0.3	0.7	4.3
A:Ψ:C	A:Ψ	3.1	–4.3	4.1	0.1	0.2	2.8	A:U	4.2	6.4	3.0	0.1	0.1	2.8
	Ψ:C	–53.0	–36.6	–10.6	–1.1	0.5	4.5	U:C	–55.4	–34.6	–14.5	–1.4	0.4	4.3
G:Um:A	Um:G	27.2	–1.4	–10.1	–0.2	–0.6	3.6	U:G	–17.9	–0.9	–11.4	–0.1	0.7	3.6
	Um:A	–2.1	–4.1	2.2	0.0	0.1	2.8	U:A	1.0	–3.3	0.9	0.0	0.1	2.8
m$^6{}_2$A:G:U	G:m$^6{}_2$A	–67.6	–16.1	8.2	–0.5	1.6	3.3	G:A	–71.7	51.9	–40.9	–0.9	–2.3	2.6
m^{7}G$^+$:G:C	m^{7}G$^+$:G	0.3	–3.0	–0.2	0.0	0.2	2.8	G:G	6.2	–9.1	2.4	0.1	0.1	2.8
Gm:G:C	Gm:G	–44.7	–4.1	–3.0	1.4	2.1	3.5	G:G	–29.7	3.1	0.2	0.3	2.6	3.7
m^{5}C:G:A	m^{5}C:G	–1.2	–4.2	–3.0	–0.1	0.1	2.9	C:G	–1.1	–4.2	–2.4	–0.1	0.1	2.9
Ψ:G:A^{H+}	Ψ:G	–0.1	7.0	0.1	0.0	2.2	2.9	U:G	0.0	7.7	0.0	0.0	2.2	2.9
m^{5}U:G:A	m^{5}U:G	0.8	1.1	–1.9	–0.1	–2.4	2.8	U:G	1.2	0.9	–1.2	–0.1	–2.4	2.8
Dw:G:C	Dw:G	34.2	–15.0	–31.4	0.8	–0.2	2.8	U:G	27.4	-15.9	-56.6	0.9	–0.2	2.8
Dh:G:C	Dh:G	19.3	6.3	–23.1	–0.4	–0.5	3.4	U:G	29.7	0.6	–3.0	0.5	–0.7	3.5

Table S8. Comparison of E-values of the base pairs present as a part of the modified and unmodified base triples.

Modified Triples	f	modified triples			Unmodified base triples	
		BP	Crystal	Optimized	BP	Optimized
C:m^{7}G$^+$:A	11	C:m^{7}G$^+$	0.32	-	C:G	0.18
		m^{7}G$^+$:A	1.24	-	G:A	1.43
C:Gm:G	12	G:Gm	0.97	1.60	G:G	1.72
		Gm:C	0.25	0.18	G:C	0.18
A:Gm:G	1	G:Gm	1.13	1.45	G:G	0.40
		Gm:A	0.36	0.07	G:A	0.07
A:s^{4}U:Aw	18	A:s^{4}U	0.38	0.28	A:U	0.30
		s^{4}U:A	0.91	0.81	U:A	1.05
A:s^{4}U:As	1	A:s^{4}U	0.65	0.25	A:U	0.28
		s^{4}U:A	1.21	0.79	U:A	0.73
A:Ψ:C	22	A:Ψ	0.49	0.26	A:U	0.29
		Ψ:C	1.04	0.95	U:C	1.03
G:Um:A	1	Um:G	0.74	0.78	U:G	0.72
		Um:A	0.45	0.28	U:A	0.29
m$^6{}_2$A:G:U	1	G: m$^6{}_2$A	0.83	1.09	G:A	1.56
		G:U	0.17	0.33	G:U	0.15
m^{7}G$^+$:G:C	20	m^{7}G$^+$:G	0.59	0.28	G:G	0.31
		G:C	0.33	0.15	G:C	0.16
Gm:G:C	43	Gm:G	1.17	-	G:G	0.34
		G:C	0.25	0.15	G:C	0.17
m^{5}C:G:A	2	m^{5}C:G	0.35	0.17	C:G	0.18
		G:A	1.25	0.58	G:A	0.56
Ψ:G:A^{H+}	4	Ψ:G	0.17	-	U:G	0.20
		G:A^{H+}	0.53	-	G:A	0.17
m^{5}U:G:A	3	m^{5}U:G	0.34	-	U:G	0.06
		G:A	1.12	-	G:A	0.73
Dw:G:C	1	Dw:G	0.44	-	U:G	0.19
		G:C	0.28	-	G:C	0.24
Dh:G:C	1	Dh:G	0.64	0.65	U:G	0.77
		G:C	0.28	0.18	G:C	0.18

Table S9. Interaction energies (kcal/mol) of the base pairs within the optimized geometries of Modified Base Triples.

Higher order interactions	Contribution of third base to higher order motif			
	Modified		Unmodified	
	Base Pair 1	Base Pair 2	Base Pair 1	Base Pair 2
C:m^{7}G^{+}:A	–21.1	–35.9	–15.9	–29.5
C:Gm:G	–17.8	–31.7	–16.2	–31.3
A:Gm:G	–16.6	–18.7	–21.8	–19.0
A:s^{4}U:Aw	–29.1	–31.7	–26.6	–26.3
A:s^{4}U:As	–24.5	–20.4	–24.6	–20.0
A:Ψ:C	–20.6	–17.4	–22.5	–17.2
A:Ψ:A	–22.3	–23.1	–28.7	–29.8
G:Um:A	–15.6	–9.3	–17.0	–9.8
m$^{6}{}_{2}$A:G:U	–24.9	–	–23.5	–
m^{7}G^{+}:G:C	–30.7	–	–20.2	–
Gm:G:C	–35.9	–	–37.1	–
m^{5}C:G:A	–15.2	–	–15.2	–
Ψ:G:A^{H+}	–48.8	–	–48.8	–
m^{5}U:G:A	–23.9	–	–23.9	–
Dw:G:C	–20.6	–	–20.3	–
Dh:G:C	–27.7	–	–26.3	–

Table S10. Morokuma Decomposition of interaction energies (kcal/mol) of the charged modified base triples at the HF/6-31G(d,p) level.

Energy Components	m^7G^+:G:C	G:C:m^7G^+	Ψ:G:A^{H+}
Electrostatic energy	–81.52	–47.48	–35.74
Exchange repulsion energy	60.56	33.46	25.76
Polarization energy	–18.44	–12.90	–6.06
Charge transfer energy	–18.36	–10.97	–8.43
High order coupling energy	1.03	1.20	–0.53
Total interaction energy	–56.74	–36.70	–25.01

Table S11. Comparison of hydrogen bond donor-acceptor (D–A) distances, acceptor-hydrogen (A–H) distances and D–H–A angles for select modified triples optimized at different levels of theory.

motif	method/basis set	Hydrogen bond (D-H...A)	D-A (Å)	A-H (Å)	∠D-H-A (deg)
m5C:G:A	B3LYP/6-31G(d,p)	N4–H (m5C)···O6 (G)	2.77	1.74	178.7
		N1–H (G)···N3 (m5C)	2.94	1.91	177.1
		N6–H (G)···O2 (m5C)	2.95	1.93	177.4
		N6–H (G)···N3 (A)	3.19	2.19	166.2
		C2–H (A)···N3 (G)	3.23	2.29	143.6
		O2'–H (G)···N1 (A)	2.78	1.80	179.7
	M06/6-31G(d,p)	N4–H (m5C)···O6 (G)	2.75	1.72	178.7
		N1–H (G)···N3 (m5C)	2.94	1.91	171.9
		N6–H (G)···O2 (m5C)	3.07	2.08	165.6
		N6–H (G)···N3 (A)	2.99	2.27	126.6
		C2–H (A)···N3 (G)	3.70	4.15	58.5
		O2'–H (G)···N1 (A)	2.80	1.89	152.9
	PBE/6-31G(d,p)	N4–H (m5C)···O6 (G)	2.72	1.66	177.1
		N1–H (G)···N3 (m5C)	2.90	1.85	177.5
		N6–H (G)···O2 (m5C)	2.92	1.89	176.6
		N6–H (G)···N3 (A)	3.10	2.11	161.7
		C2–H (A)···N3 (G)	3.28	3.11	89.1
		O2'–H (G)···N1 (A)	2.67	1.69	161.3
	HF/6-31G(d,p)	N4–H (m5C)···O6 (G)	2.91	1.90	178.7
		N1–H (G)···N3 (m5C)	3.06	2.05	175.6
		N6–H (G)···O2 (m5C)	3.03	2.03	179.6
		N6–H (G)···N3 (A)	3.33	2.36	166.8
		C2–H (A)···N3 (G)	3.49	3.11	101.6
		O2'–H (G)···N1 (A)	2.87	1.94	166.0
	B3LYP/aug-cc-pVDZ	N4–H (m5C)···O6 (G)	2.76	1.71	179.1
		N1–H (G)···N3 (m5C)	2.93	1.89	176.3
		N6–H (G)···O2 (m5C)	2.94	1.91	177.4
		N6–H (G)···N3 (A)	3.20	2.20	165.8
		C2–H (A)···N3 (G)	3.22	2.28	143.4

		O2'–H (G)···N1 (A)	2.77	1.78	177.2
m7G:G:C		N1–H (m7G)···N7 (G)	2.75	1.69	174.2
		N2–H (m7G)···O6 (G)	2.84	1.83	164.9
	B3LYP/6-31G(d,p)	N4–H (C)···O6 (G)	2.92	1.89	178.6
		N1–H (G)···N3 (C)	2.92	1.88	179.4
		N2–H (G)···O2 (C)	2.83	1.80	180.0
		N1–H (m7G)···N7 (G)	2.70	1.63	172.1
		N2–H (m7G)···O6 (G)	2.86	1.86	165.5
	M06/6-31G(d,p)	N4–H (C)···O6 (G)	2.90	1.88	178.3
		N1–H (G)···N3 (C)	2.90	1.86	178.5
		N2–H (G)···O2 (C)	2.83	1.81	179.9
		N1–H (m7G)···N7 (G)	2.70	1.62	174.3
		N2–H (m7G)···O6 (G)	2.81	1.79	165.2
	PBE/6-31G(d,p)	N4–H (C)···O6 (G)	2.87	1.83	179.6
		N1–H (G)···N3 (C)	2.87	1.82	179.9
		N2–H (G)···O2 (C)	2.80	1.76	179.2
		N1–H (m7G)···N7 (G)	2.88	1.86	175.1
		N2–H (m7G)···O6 (G)	2.93	1.96	163.0
	HF/6-31G(d,p)	N4–H (C)···O6 (G)	3.06	2.06	176.3
		N1–H (G)···N3 (C)	3.03	2.02	177.8
		N2–H (G)···O2 (C)	2.92	1.92	178.7
		N1–H (m7G)···N7 (G)	2.77	1.71	174.7
		N2–H (m7G)···O6 (G)	2.83	1.82	164.6
	B3LYP/aug-cc-pVDZ	N4–H (C)···O6 (G)	2.83	1.82	164.6
		N1–H (G)···N3 (C)	2.93	1.88	178.8
		N2–H (G)···O2 (C)	2.83	1.80	179.7

Table S12. Comparison of binding energies (interaction energies, kcal/mol) of a selected modified triple calculated at different levels of theory, using the B3LYP/6-31G(d,p) optimized geometries.

motif	method	interaction energy (kcal/mol)	
		6-311+G(2df,p)	aug-cc-pvdz
m^7G:G:C	B3LYP	–36.0	–36.0
	M06	–38.0	–38.0
	MP2	–38.3	–38.0

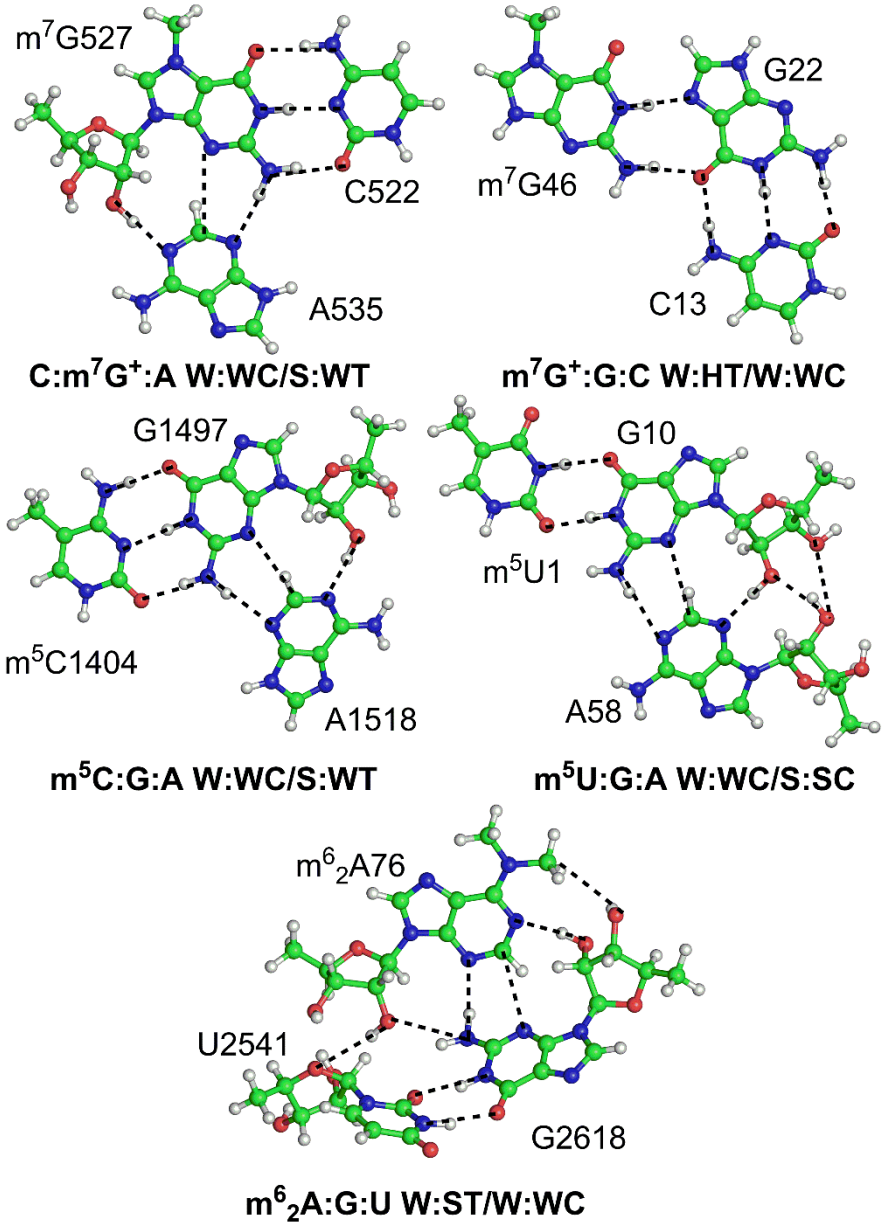

Figure S1. Schematic representation of optimized geometries of base triples involving methyl modified bases (m^7G, m^5C, m^5U and $m^6{}_2A$).

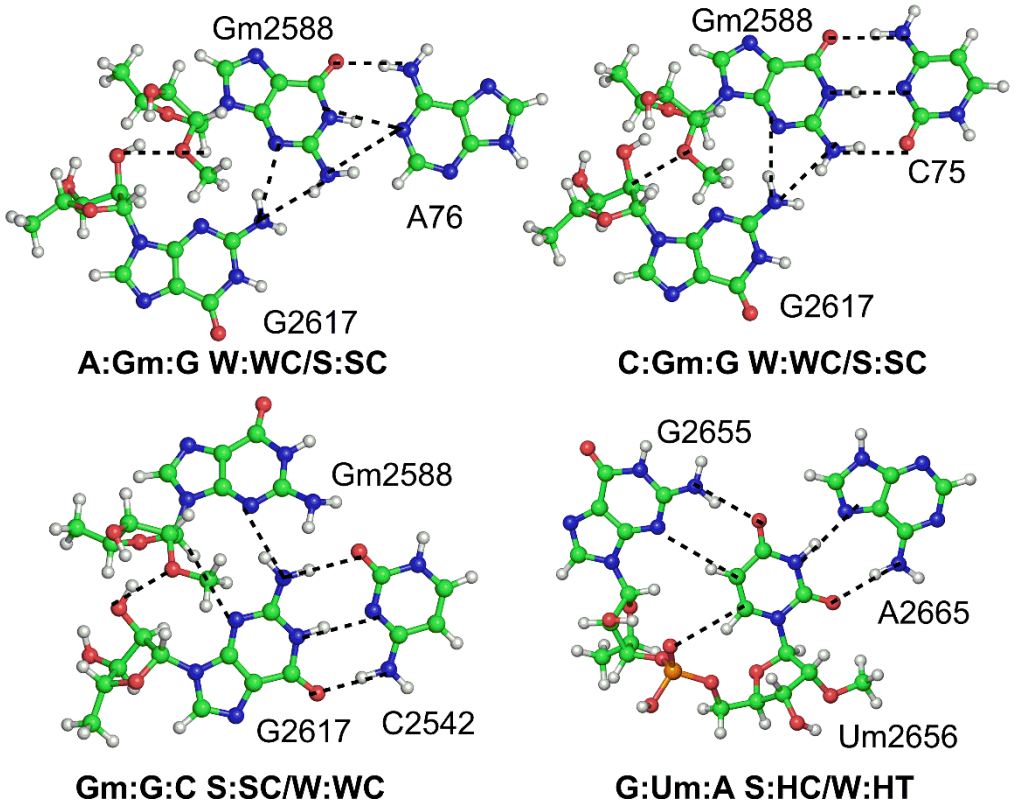

Figure S2. Schematic representation of base triples involving 2'–O–ribose methyl modified bases (Gm and Um).

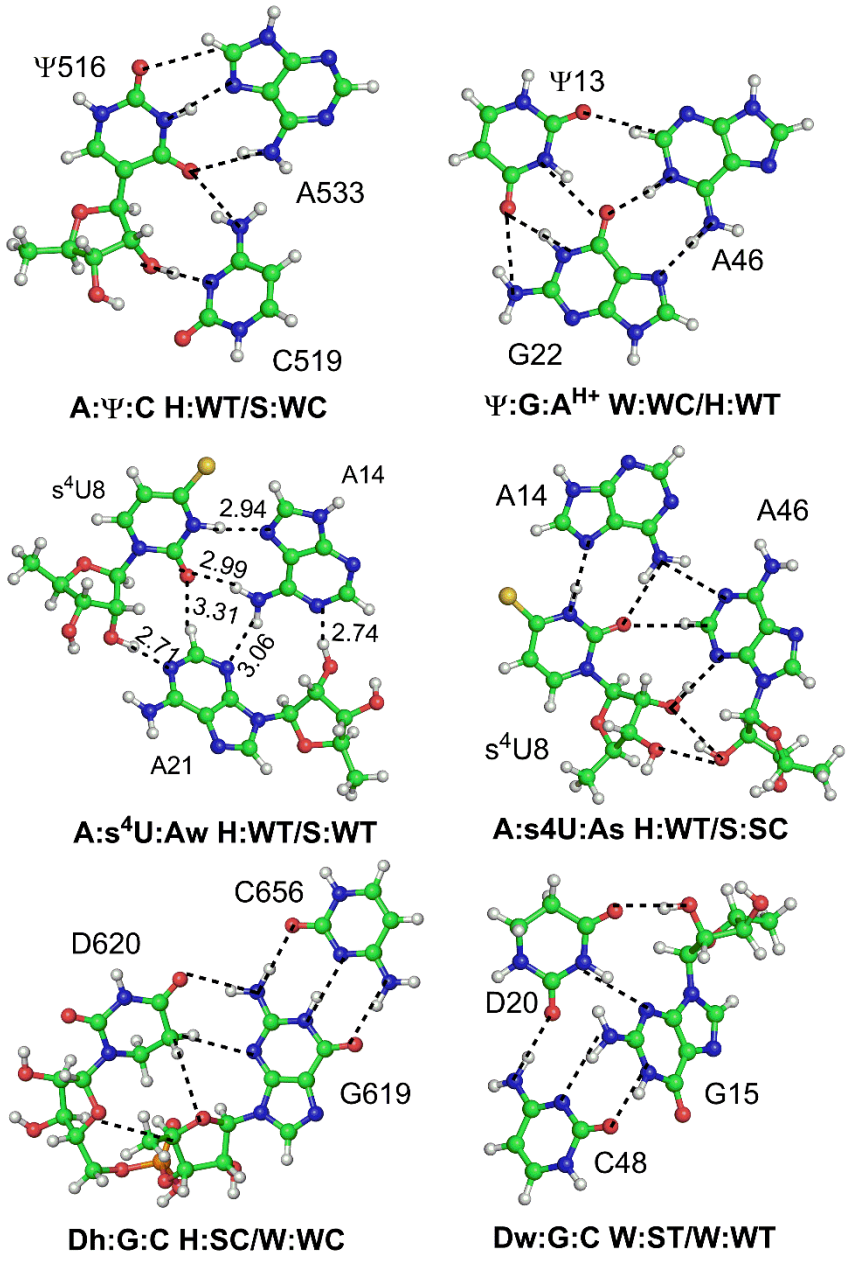

Figure S3. Schematic representation of optimized geometries of base triples involving modified bases Ψ, D and s^{4}U.

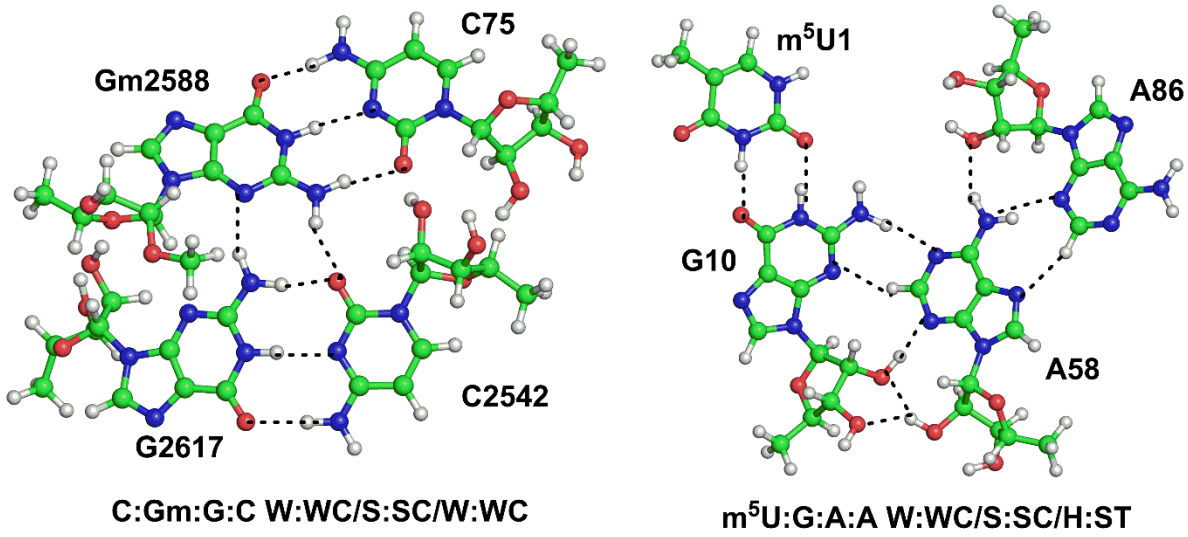

Figure S4. Schematic representation of modified base quadruples. Although the quadruple on the right was fully optimized, the quadruple on the right was hydrogen-only optimized.

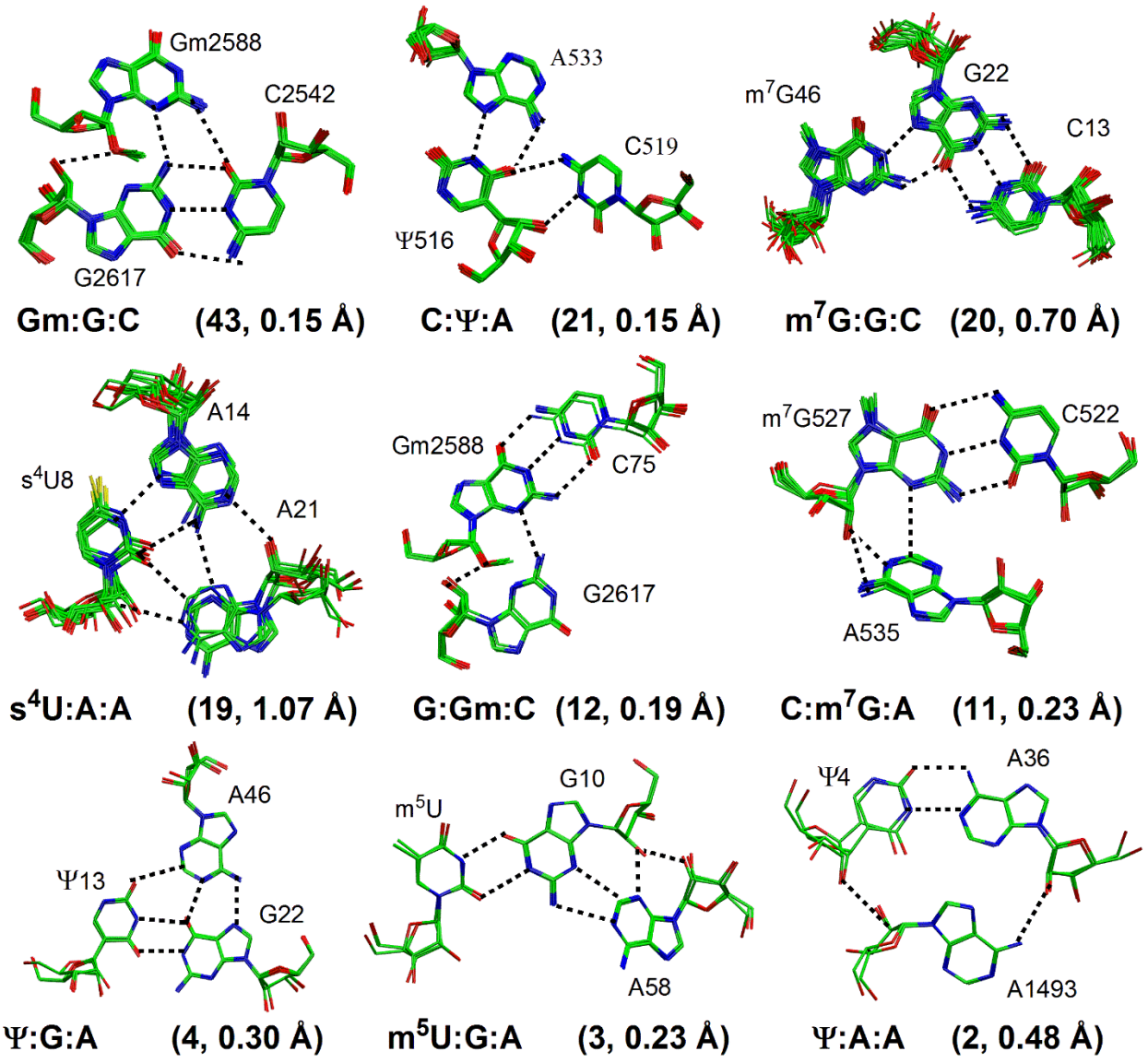

Figure S5. Structural alignment of crystal occurrences of modified base triples. Occurrence frequency and RMSD for each motif is given in parenthesis.

Table S13-29 Cartesian coordinates of geometry optimized modified base higher order interactions

Table S13 - C:m^{7}G$^+$:A

Total-atoms=64

Atoms	X	Y	Z
N	-6.44011	1.94691	-0.01234
C	-5.14554	1.41174	-0.08697
O	-4.20553	2.18078	-0.32091
N	-5.0079	0.07011	0.1047
C	-6.07797	-0.69803	0.35695
N	-5.87598	-2.009	0.53812
C	-7.40762	-0.15209	0.43469
C	-7.53781	1.18417	0.24059
C	5.10312	-4.39141	0.28115
C	4.69033	-3.0045	-0.1616
O	3.52625	-3.09634	-1.04204
C	4.24235	-2.04411	0.95534
O	5.29816	-1.42062	1.62959
C	3.35736	-1.0485	0.1699
O	4.23428	-0.14951	-0.46612
C	2.70176	-1.97532	-0.88389
N	1.35733	-2.49142	-0.46216
C	1.08637	-3.78978	-0.2114
N	-0.21094	-3.9508	0.0421
C	-0.8189	-2.70581	-0.05609
C	-2.18287	-2.28712	0.07922
O	-3.14967	-3.00815	0.34964
N	-2.30245	-0.91547	-0.13937
C	-1.2639	-0.05267	-0.453
N	-1.5691	1.22758	-0.62151
N	0.00842	-0.47143	-0.58915
C	0.16225	-1.77813	-0.38256
C	-0.88129	-5.21361	0.36837
N	0.515	5.41354	-0.02551
C	1.38435	6.3206	0.55305
N	2.59434	5.84635	0.71667
C	2.51971	4.56117	0.21729
C	3.4828	3.53418	0.11983
N	4.74283	3.68372	0.56347
N	3.09988	2.36057	-0.4336
C	1.83214	2.22224	-0.86176
N	0.83718	3.10524	-0.79995
C	1.23521	4.2678	-0.25158
H	-6.65183	-2.62189	0.72853
H	-8.26652	-0.77782	0.63772
H	-8.49097	1.6992	0.27554
H	4.306	-4.88054	0.85257
H	5.98162	-4.3108	0.92778
H	5.49858	-2.52592	-0.72725
H	3.64684	-2.5898	1.69816
H	5.56753	-0.69482	1.03996
H	2.61346	-0.5375	0.7901
H	3.86881	0.77605	-0.45525
H	2.54389	-1.4511	-1.83143
H	1.82607	-4.57176	-0.24513
H	-1.70298	-5.37418	-0.32934
H	-1.28169	-5.16294	1.38172
H	-0.15626	-6.02357	0.29113
H	1.05994	7.31451	0.82928
H	5.03733	4.57398	0.93331

H	1.5829	1.25449	-1.2829
H	-4.93166	-2.39892	0.48317
H	-3.27388	-0.53329	-0.05142
H	5.42311	2.9566	0.41171
H	5.36096	-5.0219	-0.57376
H	-0.81669	1.8992	-0.78962
H	-2.53551	1.56841	-0.51081
H	-6.5116	2.94422	-0.16289
H	-0.45595	5.56454	-0.2576

Table S14 - C:Gm:G

Total-atoms=80

Atoms	X	Y	Z
C	2.85775	-4.70227	-0.01341
C	2.43173	-3.40975	0.64962
O	1.75389	-2.55874	-0.32587
C	1.42007	-3.53967	1.80049
O	1.99393	-3.88966	3.03236
C	0.7607	-2.14666	1.79458
O	1.65675	-1.29492	2.49088
C	1.06611	-0.11168	3.02903
C	0.71266	-1.8045	0.28886
N	-0.55639	-2.18278	-0.33444
C	-0.86852	-3.34648	-1.03463
N	-2.12376	-3.41202	-1.39245
C	-2.68404	-2.24486	-0.90913
C	-4.02845	-1.75253	-0.96419
O	-5.02326	-2.2753	-1.48004
N	-4.14593	-0.50509	-0.31026
C	-3.12909	0.18449	0.29489
N	-3.43134	1.39406	0.82296
N	-1.87722	-0.26315	0.34685
C	-1.72671	-1.46808	-0.25505
C	8.02781	0.0006	-0.26395
C	6.5954	-0.47217	-0.41039
O	5.75882	0.1745	0.58035
C	5.92118	-0.1494	-1.75863
O	6.25216	-1.03551	-2.79769
C	4.43438	-0.19145	-1.36041
O	4.10827	-1.57045	-1.34093
C	4.46584	0.41852	0.06079
N	4.2385	1.87078	0.04699
C	5.20737	2.8637	-0.01814
N	4.70998	4.07132	-0.09188
C	3.34495	3.88109	-0.07747
C	2.28012	4.84718	-0.13564
O	2.29772	6.06338	-0.21323
N	1.0171	4.16622	-0.07859
C	0.81354	2.81363	0.03247
N	-0.48786	2.40635	0.17267
N	1.7965	1.93669	0.0661
C	3.02761	2.52402	0.01626
N	-8.36892	2.18306	0.56341
C	-7.05642	1.67909	0.49074
O	-6.15632	2.30994	1.05632
N	-6.8695	0.52473	-0.20145
C	-7.89737	-0.10753	-0.78469
N	-7.63732	-1.24114	-1.44192
C	-9.24378	0.40757	-0.71386

C	-9.42708	1.56076	-0.02448
H	3.36098	-5.33144	0.72696
H	3.55436	-4.50777	-0.83305
H	3.31193	-2.86686	1.01417
H	0.67342	-4.30305	1.55369
H	2.35921	-3.06286	3.38827
H	-0.23558	-2.12776	2.25071
H	0.2463	-0.36381	3.71476
H	1.85442	0.40367	3.58033
H	0.69351	0.54813	2.23986
H	0.8757	-0.73531	0.12035
H	-0.10668	-4.07504	-1.26426
H	-2.73067	1.79877	1.42535
H	8.41635	-0.22434	0.73309
H	8.65151	-0.51016	-1.00398
H	6.54201	-1.55873	-0.25684
H	6.19893	0.86025	-2.08203
H	5.67258	-1.80412	-2.66734
H	3.7783	0.37517	-2.03111
H	3.15849	-1.71533	-1.1697
H	3.6994	-0.02599	0.70499
H	6.25589	2.61576	0.02796
H	-0.66412	1.40225	0.12931
H	-8.38369	-1.75072	-1.88591
H	-10.07183	-0.1032	-1.18752
H	-10.39551	2.03408	0.09257
H	-8.47939	3.04225	1.08378
H	-6.67602	-1.62203	-1.47242
H	-5.10409	-0.10912	-0.28089
H	-4.4046	1.70333	0.92525
H	-1.19938	2.95864	-0.28566
H	0.22517	4.79669	-0.04862
H	8.10985	1.07954	-0.43168
H	1.99583	-5.25178	-0.40536

Table S15 - A:Gm:G

Total-atoms=82

Atoms	X	Y	Z
C	3.56538	-4.55097	-0.29509
C	3.09974	-3.31711	0.4476
O	2.24924	-2.51087	-0.42578
C	2.23238	-3.56171	1.6939
O	2.96127	-3.8856	2.84776
C	1.45435	-2.23547	1.79763
O	2.33652	-1.317	2.42354
C	1.69604	-0.20304	3.04508
C	1.22027	-1.8626	0.31586
N	-0.07439	-2.3185	-0.19025
C	-0.39789	-3.5481	-0.75696
N	-1.67409	-3.68176	-1.00853
C	-2.23637	-2.49288	-0.5896
C	-3.60249	-2.04887	-0.59132
O	-4.61182	-2.64302	-0.97007
N	-3.71109	-0.73707	-0.05946
C	-2.67716	0.00935	0.42183
N	-2.98612	1.26944	0.87743
N	-1.4166	-0.38737	0.43305
C	-1.26055	-1.63416	-0.08524
C	8.36188	0.21906	-0.70522

C	6.93474	-0.28167	-0.80437
O	6.16457	0.18585	0.33344
C	6.14256	0.20106	-2.03609
O	6.40744	-0.52063	-3.21218
C	4.69513	0.05558	-1.53077
O	4.40457	-1.32413	-1.67058
C	4.83537	0.47485	-0.04893
N	4.5993	1.91705	0.13446
C	5.55824	2.91731	0.21719
N	5.04835	4.12085	0.29141
C	3.68604	3.91919	0.25529
C	2.61021	4.87612	0.29285
O	2.6145	6.09159	0.37227
N	1.35383	4.18063	0.22887
C	1.16725	2.82407	0.16323
N	-0.13981	2.3892	0.21285
N	2.15683	1.959	0.11579
C	3.3833	2.5588	0.16862
N	-10.05901	2.02898	-0.22565
C	-10.75146	0.8418	-0.36105
N	-9.9713	-0.20971	-0.42468
C	-8.69542	0.3143	-0.32488
C	-7.41973	-0.30006	-0.34222
N	-7.25415	-1.62382	-0.46269
N	-6.3358	0.51106	-0.22127
C	-6.5247	1.84266	-0.12298
N	-7.66394	2.52699	-0.10093
C	-8.7223	1.70526	-0.20211
H	4.19165	-5.15078	0.37215
H	4.15731	-4.27555	-1.17169
H	3.96385	-2.70625	0.73527
H	1.53418	-4.38463	1.50362
H	3.30106	-3.04101	3.18579
H	0.51356	-2.31914	2.35409
H	1.1586	0.41151	2.31561
H	0.99937	-0.54078	3.8238
H	2.48661	0.39531	3.50027
H	1.27557	-0.77977	0.16921
H	0.36758	-4.27412	-0.98368
H	-2.2501	1.70458	1.41873
H	8.83871	-0.12806	0.21619
H	8.93429	-0.16125	-1.5576
H	6.92193	-1.37996	-0.80187
H	6.36997	1.25448	-2.23588
H	5.87026	-1.3268	-3.14309
H	3.97161	0.68282	-2.06426
H	3.49076	-1.53099	-1.39843
H	4.12626	-0.05693	0.59498
H	6.60841	2.67342	0.24646
H	-0.26379	1.38599	0.08517
H	-11.83174	0.82108	-0.40691
H	-8.07578	-2.18732	-0.61827
H	-5.61213	2.43418	-0.06087
H	-6.3258	-2.02542	-0.63412
H	-3.92237	1.40871	1.23082
H	-4.65779	-0.30338	-0.11172
H	2.7191	-5.16473	-0.61979
H	-0.81473	2.93922	-0.30321
H	0.55175	4.79162	0.32591
H	8.40184	1.31303	-0.72581

H	-10.44324	2.96	-0.16419

Table S16 - A:s^{4}U:Aw

Total-atoms=74

Atoms	X	Y	Z
N	-4.2615	0.10678	-0.50045
C	-3.10683	0.88235	-0.48137
N	-3.27916	2.20276	-0.12733
C	-4.47384	2.82474	0.1983
C	-5.62332	1.969	0.12233
C	-5.4857	0.66564	-0.22374
O	-2.00411	0.40465	-0.76039
S	-4.54633	4.43905	0.63261
C	-4.11949	-1.33361	-0.88889
C	-3.58925	-2.21435	0.27088
O	-2.87589	-3.32931	-0.21868
C	-4.89549	-2.78268	0.86308
C	-5.75329	-2.9543	-0.40379
O	-4.7078	-3.97053	1.5892
O	-5.3898	-1.82496	-1.24061
C	-7.2528	-2.97481	-0.18916
N	0.2215	5.66877	0.74939
C	-0.97954	5.03717	0.53946
N	-0.83377	3.81641	0.07374
C	0.53678	3.63837	-0.0276
C	1.33386	2.5502	-0.4606
N	0.81855	1.40087	-0.91129
N	2.67996	2.71426	-0.40952
C	3.19122	3.88145	0.03041
N	2.54349	4.96497	0.44505
C	1.21496	4.7836	0.39375
C	8.17844	-1.61869	0.27075
C	6.9598	-0.94613	-0.32464
O	5.97069	-1.94902	-0.64734
C	6.20906	0.02499	0.60303
O	6.78898	1.29909	0.69472
C	4.79957	0.05855	-0.04227
O	4.79246	1.0821	-1.01254
C	4.69749	-1.33939	-0.71809
N	3.74558	-2.25181	-0.07505
C	4.00481	-3.23899	0.85825
N	2.93733	-3.90707	1.2345
C	1.91563	-3.33264	0.50626
C	0.5292	-3.57985	0.45265
N	-0.08141	-4.52799	1.19164
N	-0.21735	-2.82765	-0.38692
C	0.37482	-1.86979	-1.12124
N	1.66259	-1.53293	-1.13959
C	2.39375	-2.30283	-0.31254
H	-6.59688	2.38579	0.33687
H	-6.32156	-0.01173	-0.32756

H	-3.43723	-1.35669	-1.74192
H	-2.99805	-1.62852	0.98341
H	-5.36352	-2.05327	1.53513
H	-5.43211	-3.87332	-0.91165
H	-7.59329	-2.07306	0.33133
H	-7.78714	-3.04988	-1.1401
H	-1.93874	5.49451	0.74231
H	1.42522	0.61795	-1.13436
H	4.27757	3.92746	0.04763
H	7.91101	-2.17391	1.17611
H	8.63539	-2.31305	-0.43968
H	7.23371	-0.40135	-1.24061
H	6.15988	-0.40543	1.61128
H	4.00039	0.20474	0.69286
H	4.36128	-1.20532	-1.75283
H	5.01319	-3.42218	1.19577
H	0.449	-5.04251	1.87576
H	-0.29427	-1.29201	-1.75126
H	-2.40416	2.76407	-0.09703
H	-0.18168	1.22506	-0.8583
H	8.9154	-0.85524	0.53668
H	-1.08834	-4.58812	1.17637
H	-1.91994	-3.08301	-0.37984
H	-7.5136	-3.84178	0.42522
H	-4.01201	-4.44129	1.10037
H	3.96724	1.62668	-0.89103
H	6.4056	1.7815	-0.06095
H	0.36305	6.60338	1.10264

Table S17 - A:s^{4}U:As

Total-atoms=74

Atoms	X	Y	Z
N	-1.44849	2.94293	0.48692
C	-2.23387	1.79292	0.44059
N	-3.51593	1.95792	-0.03579
C	-4.09348	3.14725	-0.45196
C	-3.2329	4.29284	-0.34641
C	-1.96788	4.16191	0.12008
O	-1.78659	0.70276	0.80247
S	-5.66488	3.22767	-1.01733
C	-0.06956	2.80101	1.05287
C	0.91985	2.09037	0.09407
O	1.92882	1.45278	0.84488
C	1.53605	3.29233	-0.63414
C	1.65684	4.30735	0.51499
O	2.7562	2.92244	-1.23841
O	0.45228	4.08864	1.29277
C	1.74289	5.76896	0.11872
N	-7.07733	-1.49238	-0.77006
C	-6.4091	-0.2999	-0.64538
N	-5.18324	-0.4507	-0.19411
C	-5.03994	-1.82058	-0.01271
C	-3.96824	-2.63003	0.43866
N	-2.79154	-2.12232	0.83131
N	-4.15269	-3.97026	0.47071

C	-5.34092	-4.46258	0.0919
N	-6.42789	-3.81196	-0.3386
C	-6.2111	-2.49072	-0.37095
C	7.76856	-1.38576	-1.35734
C	6.59417	-0.50952	-0.97394
O	5.3905	-1.00838	-1.61059
C	6.24787	-0.47855	0.52633
O	7.05032	0.38987	1.28439
C	4.76345	-0.06928	0.49587
O	4.75067	1.33674	0.38373
C	4.26377	-0.73565	-0.80857
N	3.56453	-2.01343	-0.56424
C	3.91108	-3.27064	-1.03134
N	3.04095	-4.2067	-0.72942
C	2.05871	-3.53503	-0.02987
C	0.83379	-3.95573	0.53264
N	0.40632	-5.23229	0.47673
N	0.06268	-3.03919	1.15624
C	0.47585	-1.7687	1.20399
N	1.59554	-1.24715	0.69024
C	2.36041	-2.17389	0.07893
H	-3.62129	5.26011	-0.63128
H	-1.29498	4.99703	0.2541
H	-0.16359	2.23766	1.9838
H	0.41025	1.39179	-0.57497
H	1.78377	0.46575	0.82635
H	0.81746	3.67054	-1.37855
H	2.52272	4.02817	1.1285
H	3.09006	3.66848	-1.75262
H	1.72626	6.41269	1.0021
H	2.68256	5.95798	-0.41206
H	-6.84619	0.65565	-0.90065
H	-2.60479	-1.1275	0.77199
H	-5.43061	-5.54638	0.14214
H	7.60664	-2.41916	-1.03322
H	7.92908	-1.38191	-2.43904
H	6.76312	0.5236	-1.30686
H	6.3513	-1.4868	0.94576
H	6.62757	1.261	1.19848
H	4.20148	-0.41595	1.37079
H	3.82067	1.63984	0.41369
H	3.5677	-0.06885	-1.33095
H	4.81985	-3.40976	-1.59555
H	-0.53624	-5.4405	0.77033
H	-0.1881	-1.0676	1.70125
H	-2.02902	-2.74773	1.07037
H	0.91271	-5.89734	-0.08576
H	8.67256	-1.00762	-0.87052
H	0.91311	6.05566	-0.53624
H	-4.09002	1.0858	-0.0721
H	-8.02162	-1.62766	-1.09776

Table S18 - A:Ψ:C

Total-atoms=56

Atoms	X	Y	Z
N	0.08241	-4.08656	-0.87508
C	1.30749	-3.43343	-0.90143
N	1.2873	-2.214	-0.25279
C	0.20751	-1.61354	0.37352

C	-1.04301	-2.35849	0.33283
C	-1.04218	-3.56728	-0.27994
O	2.29805	-3.90026	-1.44678
O	0.35244	-0.50792	0.92469
C	-2.27436	-1.78637	0.99083
C	-2.90639	-0.57774	0.24054
O	-3.24189	0.44261	1.15415
C	-4.21172	-1.17994	-0.33269
C	-4.55787	-2.22405	0.74091
O	-5.2067	-0.22487	-0.58054
O	-3.27926	-2.80933	1.05504
C	-5.52065	-3.31147	0.31231
N	-3.02916	4.78216	-1.02886
C	-3.38134	3.52759	-0.46583
O	-4.5618	3.2259	-0.37442
N	-2.33654	2.737	-0.06
C	-1.07156	3.13286	-0.18886
N	-0.10849	2.29719	0.23269
C	-0.71847	4.41074	-0.75568
C	-1.74441	5.20117	-1.16318
N	5.98409	-0.96225	-0.95516
C	4.772	-1.60443	-1.02206
N	3.8255	-0.95941	-0.37975
C	4.44318	0.16425	0.14142
C	3.98802	1.23249	0.94348
N	2.68972	1.37091	1.33107
N	4.87562	2.17296	1.31455
C	6.14782	2.05904	0.89977
N	6.70055	1.10614	0.14116
C	5.79887	0.18194	-0.204
H	-1.93849	-4.17393	-0.30958
H	-2.01688	-1.43713	1.99944
H	-2.25068	-0.19427	-0.54997
H	-4.00195	-1.70845	-1.27364
H	-4.94798	-1.69333	1.62291
H	-5.02525	0.51377	0.02896
H	-5.69491	-4.03163	1.11727
H	-6.47656	-2.85649	0.03647
H	-0.33882	1.37027	0.57872
H	0.31221	4.72455	-0.8542
H	-1.59462	6.18021	-1.60557
H	4.62141	-2.54181	-1.54078
H	2.04772	0.5823	1.25509
H	6.81708	2.85007	1.23058
H	2.19059	-1.69499	-0.25964
H	0.06328	-4.98902	-1.32794
H	2.53698	2.01397	2.09564
H	0.87248	2.50615	0.12263
H	-2.93542	1.30467	0.77551
H	-5.13021	-3.851	-0.55778
H	6.8566	-1.26521	-1.36155
H	-3.80803	5.35307	-1.32622

Table S19 - G:Um:A

Total-atoms=78

Atoms	X	Y	Z
C	5.5546	-1.4652	2.9495
C	4.3733	-1.202	2.0235
O	4.0945	0.2163	1.9979

C	4.6097	-1.6149	0.561
O	3.3234	-2.0944	0.0621
C	5.0164	-0.2804	-0.0901
O	5.0639	-0.1994	-1.479
C	4.0704	0.6897	0.6513
N	4.4597	2.0708	0.6134
C	5.6673	2.6313	1.0205
N	5.719	3.9235	0.8508
C	4.4909	4.2524	0.3066
C	3.9709	5.5291	-0.1043
O	4.4666	6.6433	-0.0918
N	2.6345	5.3615	-0.6008
C	1.9209	4.1887	-0.6842
N	0.6678	4.2651	-1.2105
N	2.4208	3.0239	-0.3139
C	3.6886	3.1221	0.1587
N	-1.4721	-1.4682	0.4105
C	-2.6751	-0.7664	0.4176
N	-2.5983	0.5414	0.0268
C	-1.4453	1.2397	-0.3348
C	-0.2273	0.4611	-0.2692
C	-0.2846	-0.8402	0.097
O	-3.7316	-1.3142	0.7525
O	-1.5308	2.4273	-0.6699
C	-1.5344	-2.8796	0.8829
C	-2.2199	-3.826	-0.1297
O	-2.8671	-4.8934	0.5457
C	-4.2314	-4.6457	0.8857
C	-1.0267	-4.4611	-0.8682
C	0.0328	-4.5133	0.2509
O	-1.3096	-5.7103	-1.4411
O	-0.2228	-3.3611	1.0763
C	1.477	-4.5009	-0.2055
N	-6.01	3.9713	-0.6661
C	-4.8123	3.3067	-0.584
N	-4.9511	2.0757	-0.1472
C	-6.3102	1.9188	0.0701
C	-7.1	0.8396	0.5333
N	-6.589	-0.3577	0.8786
N	-8.4324	1.0283	0.6321
C	-8.9435	2.2197	0.2884
N	-8.311	3.3099	-0.1612
C	-6.9938	3.0953	-0.2483
H	5.7002	-2.5403	3.0974
H	6.4809	-1.0393	2.5515
H	3.4836	-1.7241	2.3956
H	5.3455	-2.4118	0.4337
H	6.0353	-0.0718	0.2585
H	4.201	-0.4205	-1.8789
H	3.0604	0.6459	0.2269
H	6.4502	2.0248	1.4527
H	0.0321	3.4819	-1.0454
H	-2.0774	-2.8735	1.8318
H	-2.9152	-3.2983	-0.7892
H	-4.585	-5.5331	1.414
H	-4.8376	-4.4926	-0.0169
H	-4.3324	-3.7648	1.5271
H	-0.6825	-3.7936	-1.6628
H	-0.1205	-5.4254	0.8449
H	-1.9637	-6.1195	-0.85

H	1.7096	-5.4321	-0.6786
H	2.1172	-4.3609	0.6403
H	-3.8632	3.7507	-0.8509
H	-7.2386	-1.0593	1.1962
H	-10.0232	2.3077	0.3904
H	0.22	5.1687	-1.2189
H	2.2251	6.2262	-0.9322
H	5.3637	-1.0053	3.9222
H	-5.5986	-0.5753	0.8162
H	-3.5025	1.0704	-0.0004
H	0.5895	-1.4696	0.1754
H	0.7123	0.9489	-0.4971
H	-6.1607	4.9208	-0.9721
H	1.6246	-3.701	-0.9007
H	3.4704	-2.7518	-0.6218

Table S20 - $m^6{}_2$A:G:U

Total-atoms=97

Atoms	X	Y	Z
C	7.94926	-0.36462	-1.479
C	6.82339	0.03317	-0.54531
O	5.51927	-0.18505	-1.18134
C	6.75242	-0.7392	0.79055
O	7.57047	-0.19965	1.79739
C	5.24792	-0.68405	1.11241
O	4.93963	0.57296	1.72899
C	4.61027	-0.80586	-0.28094
N	4.34345	-2.20955	-0.69098
C	3.19643	-2.77458	-0.12997
O	2.6024	-2.16912	0.7719
N	2.80317	-3.98003	-0.63155
C	3.4563	-4.72051	-1.64846
O	3.02452	-5.79705	-2.01533
C	4.64119	-4.05276	-2.18064
C	5.01667	-2.8435	-1.718
C	-8.28561	-2.96662	-0.43333
C	-7.37792	-1.9254	0.1906
O	-6.4083	-2.57623	1.0376
C	-6.53837	-1.09474	-0.79666
O	-7.23453	-0.0031	-1.35649
C	-5.3588	-0.64695	0.09656
O	-5.77473	0.51405	0.8019
C	-5.19949	-1.83923	1.07028
N	-4.1118	-2.75111	0.69984
C	-4.20861	-4.03341	0.17014
N	-3.04741	-4.60729	-0.013
C	-2.12687	-3.67251	0.42044
C	-0.69366	-3.70547	0.45577
O	0.09064	-4.58906	0.08949
N	-0.18246	-2.50498	0.99524
C	-0.90692	-1.40913	1.38839
N	-0.18743	-0.35253	1.86128
N	-2.22843	-1.3642	1.34884
C	-2.76899	-2.51297	0.87061
C	4.2051	5.48501	0.4026
C	3.38876	4.25301	0.7357
O	2.01323	4.62114	0.8974
C	1.2061	3.45983	0.78563
N	-0.03846	3.84903	0.14397

C	-1.27368	3.26972	0.35082
N	-1.57885	2.3153	1.24354
C	-2.86211	1.96893	1.1672
N	-3.79855	2.45041	0.33597
C	-3.49082	3.42844	-0.55862
N	-4.48386	3.88701	-1.35195
C	-2.13712	3.88345	-0.56663
N	-1.44581	4.82543	-1.31467
C	-0.21515	4.77067	-0.87104
C	-4.26784	4.82052	-2.45488
C	-5.83366	3.33845	-1.224
C	2.03456	2.39265	-0.00875
O	2.23036	1.203	0.72474
C	3.33933	3.16921	-0.34997
H	7.93525	-1.4381	-1.69217
H	7.89259	0.18115	-2.42482
H	6.90032	1.10579	-0.32224
H	7.06009	-1.77995	0.63035
H	4.90577	-1.45724	1.79785
H	5.02538	1.28342	1.06027
H	3.64975	-0.29036	-0.30752
H	5.18295	-4.54367	-2.97747
H	5.84967	-2.28807	-2.12507
H	-8.81868	-3.53522	0.33364
H	-9.02119	-2.46917	-1.07283
H	-7.97077	-1.22734	0.80107
H	-6.18849	-1.72725	-1.61994
H	-7.24004	0.64967	-0.63404
H	-4.43621	-0.46298	-0.46031
H	-5.1579	1.25363	0.58957
H	-4.99487	-1.46287	2.07843
H	-5.17236	-4.47444	-0.02943
H	-0.68158	0.53597	1.88177
H	4.15716	6.2122	1.21676
H	5.25014	5.20278	0.24742
H	3.76411	3.79364	1.66582
H	0.9431	3.03978	1.76401
H	-3.18947	1.17398	1.83053
H	0.60119	5.3901	-1.21114
H	-4.95128	5.67099	-2.35525
H	-3.2435	5.18536	-2.45222
H	-4.47237	4.32612	-3.41276
H	-6.13722	3.30914	-0.17585
H	-6.51504	3.99248	-1.77064
H	-5.91204	2.32635	-1.6372
H	1.48847	2.09982	-0.9093
H	3.22444	3.65337	-1.32839
H	-7.70908	-3.6673	-1.0461
H	3.82896	5.95956	-0.50902
H	8.9049	-0.12795	-1.00112
H	1.8872	-4.33739	-0.29321
H	0.84029	-2.4573	1.04422
H	0.77178	-0.2672	1.54746
H	7.01961	0.44972	2.26511
H	3.00732	1.23734	1.31
O	4.53874	2.40822	-0.31926
H	4.59068	1.78868	-1.06688

Table S21 - m^7G^+:G:C

Total-atoms=49

Atoms	X	Y	Z
N	6.97396	-1.48812	0.00602
C	5.9657	-0.50918	-0.00111
O	6.30253	0.6784	-0.00768
N	4.67299	-0.94173	-0.00025
C	4.39058	-2.24932	0.00738
N	3.09716	-2.60488	0.0077
C	5.4196	-3.25591	0.01493
C	6.70511	-2.82045	0.01383
N	-0.23859	3.88199	0.00328
C	-1.33899	3.05647	0.00505
N	-1.00124	1.78902	0.00233
C	0.38309	1.77621	-0.00143
C	1.30901	0.69843	-0.00504
O	1.04857	-0.52934	-0.00583
N	2.62829	1.14166	-0.00778
C	3.01939	2.46975	-0.00713
N	4.33523	2.71415	-0.01063
N	2.15667	3.48527	-0.00356
C	0.88142	3.08141	-0.00089
N	-6.11851	-2.58433	-0.01273
C	-7.14586	-1.70459	-0.00484
N	-6.66164	-0.46629	0.00493
C	-5.27614	-0.54179	0.00373
C	-4.25513	0.47631	0.00645
O	-4.42256	1.69114	0.01206
N	-2.98608	-0.11873	0.00083
C	-2.73336	-1.46876	-0.00902
N	-1.45871	-1.86372	-0.01379
N	-3.69721	-2.40797	-0.01441
C	-4.91746	-1.88373	-0.00795
C	-7.44586	0.77563	0.02169
H	2.84154	-3.57823	0.01439
H	5.18315	-4.31165	0.02108
H	7.55822	-3.48934	0.01897
H	-2.35672	3.42021	0.00834
H	5.04886	1.97438	-0.01102
H	-8.19215	-1.96594	-0.00591
H	-1.30514	-2.86002	-0.02228
H	-8.50496	0.52251	-0.01982
H	-7.22245	1.32803	0.93465
H	-7.1654	1.38531	-0.83695
H	-6.20505	-3.59225	-0.02239
H	2.36559	-1.88719	0.0028
H	3.36251	0.40395	-0.01037
H	4.61231	3.68279	-0.00912
H	-2.17581	0.57014	0.00193
H	-0.6426	-1.23527	-0.01016
H	7.92267	-1.13785	0.00517
H	-0.23574	4.89175	0.00478

Table S22 - Gm:G:C

Total-atoms=80

Atoms	X	Y	Z
N	6.98553	0.38294	-0.09887
C	5.62015	0.06327	0.00121
O	4.80415	0.99464	0.0845

N	5.28119	-1.24954	-0.00126
C	6.21851	-2.20536	-0.10446
N	5.81786	-3.47784	-0.10635
C	7.6221	-1.8818	-0.20955
C	7.95544	-0.56866	-0.20321
C	-5.57078	2.28348	-0.3654
C	-4.3714	1.78315	0.41078
O	-3.23118	1.62735	-0.49209
C	-3.84921	2.71084	1.52083
O	-4.562	2.61883	2.72626
C	-2.37805	2.2662	1.63244
O	-2.39424	1.08599	2.41921
C	-1.1472	0.74851	3.02859
C	-2.0133	1.96173	0.16414
N	-1.42344	3.11909	-0.51891
C	-1.99991	3.96968	-1.45565
N	-1.17712	4.89091	-1.88979
C	0.00445	4.64674	-1.22065
C	1.28055	5.31539	-1.29177
O	1.64701	6.28163	-1.93516
N	2.21553	4.66219	-0.40994
C	1.97585	3.57356	0.38231
N	3.01202	3.1275	1.17073
N	0.8021	2.97505	0.4373
C	-0.12989	3.55361	-0.36867
C	-5.20338	-4.99658	-0.16434
C	-4.66814	-3.5846	-0.29255
O	-3.6328	-3.36102	0.69447
C	-3.99756	-3.24658	-1.63841
O	-4.89629	-2.93598	-2.67255
C	-3.09568	-2.06711	-1.2292
O	-3.96059	-0.94346	-1.19862
C	-2.64271	-2.48461	0.19023
N	-1.35827	-3.19604	0.1844
C	-1.15801	-4.57186	0.12794
N	0.10285	-4.91347	0.08881
C	0.78434	-3.71231	0.12285
C	2.18729	-3.43593	0.09529
O	3.13896	-4.22822	0.02418
N	2.43234	-2.05171	0.15873
C	1.48109	-1.06447	0.23956
N	1.95161	0.19858	0.3547
N	0.17626	-1.30531	0.244
C	-0.10417	-2.63178	0.18746
H	4.81156	-3.73233	-0.0478
H	8.37633	-2.65338	-0.29167
H	8.97717	-0.21422	-0.27891
H	-6.41504	2.397	0.32136
H	-5.85473	1.57392	-1.14705
H	-4.58495	0.79961	0.8454
H	-3.8953	3.7534	1.18611
H	-4.21524	1.82611	3.16784
H	-1.71767	3.02297	2.07065
H	-0.77048	1.58433	3.63274
H	-1.34339	-0.10729	3.67699
H	-0.39725	0.46577	2.28368
H	-1.31166	1.12432	0.09118
H	-3.0184	3.82694	-1.78073
H	2.76198	2.28269	1.67108
H	-5.61984	-5.17094	0.83158

H	-5.99483	-5.14948	-0.90445
H	-5.4765	-2.85953	-0.12467
H	-3.38614	-4.09361	-1.97086
H	-5.12312	-2.0014	-2.53362
H	-2.24241	-1.90905	-1.8976
H	-3.46462	-0.10705	-1.11859
H	-2.52903	-1.60853	0.8385
H	-1.9951	-5.25164	0.1522
H	1.29162	0.96727	0.28807
H	6.49847	-4.21581	-0.18978
H	3.42367	-1.76768	0.1345
H	3.90668	3.00159	0.70692
H	3.11435	5.12572	-0.35433
H	-5.36814	3.25503	-0.82734
H	-4.41604	-5.73612	-0.34412
H	2.93234	0.40202	0.16091
H	7.20993	1.36787	-0.10311

Table S23 - m^{5}C:G:A

Total-atoms=63

Atoms	X	Y	Z
N	-6.30617	1.87921	-0.10574
C	-4.9932	1.38732	-0.21312
O	-4.08901	2.17908	-0.50148
N	-4.81616	0.05924	0.01203
C	-5.84466	-0.73812	0.32527
N	-5.57845	-2.03092	0.53527
C	-7.20894	-0.24494	0.43914
C	-7.36821	1.08374	0.20797
C	-8.35464	-1.15303	0.7897
C	5.26374	-4.6897	-0.07251
C	4.85452	-3.24821	-0.30056
O	3.67733	-3.20301	-1.13721
C	4.46299	-2.45928	0.9629
O	5.55743	-1.95466	1.68807
C	3.57994	-1.34913	0.35819
O	4.48073	-0.37355	-0.13624
C	2.86265	-2.09602	-0.79481
N	1.53695	-2.60715	-0.4253
C	1.20468	-3.90717	-0.05501
N	-0.06945	-4.07061	0.18609
C	-0.6234	-2.82334	-0.03653
C	-1.97609	-2.36982	0.05587
O	-2.98752	-3.01475	0.37499
N	-2.08499	-1.00462	-0.26988
C	-1.05078	-0.17383	-0.63698
N	-1.37746	1.10354	-0.92266
N	0.20907	-0.59146	-0.72856
C	0.35511	-1.90083	-0.42062
N	0.9784	5.43293	-0.2463
C	1.86641	6.29655	0.3655
N	3.00397	5.7314	0.68729
C	2.85704	4.42245	0.26375
C	3.71226	3.30235	0.33183
N	4.94707	3.35959	0.87071
N	3.26581	2.13373	-0.17145
C	2.03505	2.07443	-0.7151
N	1.14075	3.05756	-0.82533

C	1.60314	4.21089	-0.31993
H	-6.31823	-2.66987	0.77334
H	-8.33601	1.57172	0.26177
H	-8.4762	-1.95781	0.05373
H	-9.29576	-0.59806	0.82462
H	-8.21538	-1.62366	1.77113
H	6.1612	-4.71478	0.55329
H	5.48496	-5.19113	-1.01886
H	5.66601	-2.70178	-0.80209
H	3.87552	-3.09689	1.63385
H	5.78397	-1.13457	1.21538
H	2.86215	-0.92138	1.06666
H	4.05179	0.51762	-0.14998
H	2.72981	-1.43083	-1.65503
H	1.95888	-4.67722	-0.0171
H	-2.32243	1.45532	-0.7576
H	1.61178	7.33227	0.5446
H	5.48824	2.51449	0.95942
H	1.71847	1.09688	-1.06862
H	4.47118	-5.2476	0.43712
H	-0.62917	1.77711	-1.04272
H	-3.0359	-0.60753	-0.1949
H	-4.60445	-2.38723	0.46626
H	5.26042	4.20818	1.31265
H	0.04684	5.64159	-0.57388
H	-6.42028	2.86731	-0.28108

Table S24 - Ψ:G:A

Total-atoms=44

Atoms	X	Y	Z
N	-2.17243	-4.64692	0.00217
C	-1.38265	-3.50441	0.00225
N	-2.10898	-2.32534	-0.00043
C	-3.49808	-2.20452	-0.00255
C	-4.22782	-3.45352	-0.00208
C	-3.54275	-4.62068	0.00017
O	-0.16376	-3.55272	0.00453
O	-4.02589	-1.08303	-0.0047
N	-1.05899	4.89627	0.00503
C	0.27498	4.56292	0.00532
N	0.46716	3.26532	0.0032
C	-0.80476	2.7143	0.00143
C	-1.24977	1.36245	-0.00092
O	-0.5721	0.30495	-0.00135
N	-2.63729	1.27826	-0.00287
C	-3.50605	2.34557	-0.00176
N	-4.8187	2.04102	-0.00421
N	-3.11129	3.60962	0.00114
C	-1.77463	3.72537	0.0024
N	5.87811	-1.63939	-0.00012
C	6.54422	-0.42934	-0.00468
N	5.73583	0.60436	-0.00626
C	4.48099	0.04053	-0.00263
C	3.20591	0.64663	-0.00202
N	3.00499	1.95541	-0.00521
N	2.16491	-0.24422	0.00208
C	2.34068	-1.60958	0.00583
N	3.49983	-2.2143	0.0057
C	4.54062	-1.35417	0.00128

H	-4.03097	-5.58842	0.00054
H	1.05187	5.31412	0.00702
H	-5.48326	2.79756	-0.00189
H	7.62414	-0.37711	-0.00663
H	2.06575	2.40178	-0.00206
H	1.42465	-2.19478	0.00911
H	-5.30779	-3.42206	-0.00367
H	-1.66322	-5.52059	0.00408
H	-1.54815	-1.46369	-0.00069
H	-3.05422	0.32923	-0.00559
H	-5.13768	1.08355	-0.00374
H	-1.45534	5.82566	0.00618
H	3.83228	2.53614	-0.00797
H	1.18123	0.09902	0.0017
H	6.28705	-2.564	0.00194

Table S25 - m^{5}U:G:A

Total-atoms=78

Atoms	X	Y	Z
C	-2.39374	5.85456	-0.37681
C	-2.38089	4.35313	-0.59322
O	-1.19169	3.99331	-1.32487
C	-2.29885	3.48432	0.67362
O	-3.52244	3.27927	1.34752
C	-1.77788	2.16378	0.09538
O	-2.86223	1.48544	-0.50385
C	-0.78811	2.67379	-0.99245
N	0.61007	2.72047	-0.56214
C	1.3074	3.80383	-0.03677
N	2.5554	3.53249	0.24203
C	2.70823	2.20666	-0.11495
C	3.84929	1.34072	-0.04919
O	4.99136	1.57597	0.35851
N	3.53313	0.05187	-0.53372
C	2.31488	-0.36075	-1.00489
N	2.24785	-1.65054	-1.44148
N	1.2585	0.4319	-1.07239
C	1.51425	1.68463	-0.61964
C	-8.48549	-1.87874	1.56474
C	-7.32498	-0.93006	1.34806
O	-6.10027	-1.55298	1.81262
C	-7.03054	-0.56011	-0.11683
O	-7.85682	0.45033	-0.63318
C	-5.5458	-0.1505	-0.04358
O	-5.5326	1.19362	0.38112
C	-5.00131	-1.0889	1.06277
N	-4.29312	-2.27069	0.52728
C	-4.59659	-3.60676	0.73194
N	-3.7063	-4.43581	0.2356
C	-2.75115	-3.60525	-0.31701
C	-1.52872	-3.86405	-0.97293
N	-1.07005	-5.11932	-1.16425
N	-0.78657	-2.82027	-1.40297
C	-1.24831	-1.57787	-1.19702
N	-2.3739	-1.21012	-0.57565
C	-3.0954	-2.2616	-0.14602
N	7.71799	-2.53197	0.01593
C	6.71532	-1.58348	-0.00869
N	7.09255	-0.34159	0.42066

C	8.37833	0.03246	0.87049
C	9.38435	-1.04334	0.86027
C	10.76845	-0.70209	1.32539
C	9.00912	-2.2676	0.43585
O	5.57807	-1.88269	-0.39806
O	8.60456	1.17365	1.23403
H	-3.31347	6.15438	0.13811
H	-2.36067	6.38282	-1.33335
H	-3.26805	4.0418	-1.16178
H	-1.53432	3.90356	1.34619
H	-1.26957	1.53949	0.83843
H	-0.83682	2.01724	-1.86728
H	0.83028	4.76463	0.07684
H	3.00979	-2.26601	-1.19822
H	-8.60734	-2.12047	2.62429
H	-9.40592	-1.40705	1.20768
H	-7.4804	0.0001	1.91125
H	-7.14513	-1.45088	-0.74704
H	-7.41798	1.27976	-0.37537
H	-5.01441	-0.28645	-0.9917
H	-4.29509	-0.54465	1.70126
H	-5.49184	-3.88555	1.26545
H	-0.25504	-5.25974	-1.73884
H	-0.6111	-0.77027	-1.5449
H	11.1927	0.10258	0.71619
H	10.74942	-0.33259	2.35579
H	11.43215	-1.56959	1.27458
H	9.68915	-3.11189	0.39779
H	6.3628	0.39968	0.41779
H	4.30584	-0.62748	-0.49734
H	1.33326	-2.07819	-1.55304
H	-1.66163	-5.90102	-0.93241
H	-4.64029	1.57012	0.22863
H	-2.66332	0.51197	-0.54307
H	-3.78467	4.10669	1.77016
H	-1.53591	6.17525	0.22346
H	-8.33544	-2.81085	1.00981
H	7.44928	-3.45043	-0.30356

Table S26 - Dw:G:C

Total-atoms=59

Atoms	X	Y	Z
C	6.43119	-1.77173	-1.24712
C	5.54972	-0.71624	-0.60991
O	4.34336	-0.54684	-1.3946
C	5.04997	-1.0394	0.81185
O	5.98378	-0.75893	1.8254
C	3.78013	-0.17355	0.88893
O	4.24132	1.12862	1.19318
C	3.24141	-0.26578	-0.55654
N	2.25353	-1.34236	-0.71228
C	2.44945	-2.57387	-1.3256
N	1.41118	-3.36497	-1.23826
C	0.47769	-2.6347	-0.53258
C	-0.84788	-3.00444	-0.09768
O	-1.47522	-4.03534	-0.27505
N	-1.42232	-1.94058	0.66443
C	-0.86691	-0.71677	0.89213
N	-1.62082	0.14999	1.63439

N	0.34197	-0.36441	0.46792
C	0.97488	-1.37503	-0.20341
N	-1.26315	4.24857	-0.7675
C	-1.02782	2.90646	-0.66392
O	-1.80401	2.05098	-1.07744
N	0.18139	2.54564	-0.05283
C	1.18971	3.41361	0.31508
O	2.22222	3.02711	0.84234
C	0.95512	4.87681	-0.01532
C	-0.52747	5.23545	0.01626
N	-6.14151	-1.88656	0.62761
C	-4.84627	-1.42881	0.94915
O	-4.1712	-2.07899	1.74745
N	-4.41806	-0.28426	0.34014
C	-5.17197	0.31548	-0.57635
N	-4.67383	1.41673	-1.17922
C	-6.49144	-0.15149	-0.92237
C	-6.93208	-1.26744	-0.2868
H	7.3452	-1.88177	-0.65536
H	6.70941	-1.4909	-2.26686
H	6.07792	0.24623	-0.57246
H	4.78884	-2.1016	0.88201
H	5.89359	0.19385	1.99274
H	3.0434	-0.53012	1.61797
H	3.48775	1.74389	1.21049
H	2.76874	0.67591	-0.85843
H	3.3759	-2.79307	-1.83178
H	-2.62288	0.10866	1.44716
H	1.36239	5.05051	-1.01933
H	-0.88916	5.26725	1.05461
H	-0.69366	6.22258	-0.42152
H	-5.14517	1.77845	-1.99268
H	-7.10248	0.35573	-1.65751
H	-7.90339	-1.71205	-0.47327
H	-3.68015	1.62478	-1.08145
H	-1.24039	1.08253	1.68572
H	-2.34397	-2.13222	1.07216
H	5.92263	-2.74079	-1.28041
H	0.34052	1.52218	0.07814
H	1.53409	5.4773	0.68814
H	-2.19291	4.47106	-1.0926
H	-6.42139	-2.74702	1.07862

Table S27 - Dh:G:C

Total-atoms=75

Atoms	X	Y	Z
C	-2.5636	-1.4377	3.1038
C	-2.0949	-1.6266	1.6729
O	-0.6639	-1.7074	1.6648
C	-2.5551	-2.9436	0.9988
O	-3.7128	-2.8138	0.1484
C	-1.2795	-3.4782	0.2694
O	-1.454	-3.7838	-1.0911
C	-0.2854	-2.3099	0.4251
N	1.1046	-2.6761	0.4677
C	1.6905	-3.9144	0.7408
N	2.992	-3.8962	0.6983

C	3.3101	-2.5833	0.3973
C	4.5806	-1.9519	0.2175
O	5.7096	-2.4625	0.2881
N	4.4351	-0.5833	-0.0657
C	3.2426	0.1024	-0.1615
N	3.3266	1.4182	-0.4295
N	2.0569	-0.4875	-0.0154
C	2.1601	-1.8032	0.2567
C	-5.9611	-0.918	0.0059
C	-5.7391	0.556	0.2765
O	-4.3747	0.809	0.6135
C	-6.0313	1.5331	-0.8815
O	-7.3996	1.7688	-1.0954
C	-4.204	2.2255	0.584
C	-5.2248	2.7812	-0.4525
O	-6.1335	3.6808	0.1676
N	-2.8131	2.5378	0.3456
C	-2.3705	3.73	0.8545
O	-3.0722	4.5321	1.4653
N	-1.0113	3.9918	0.6263
C	-0.0508	3.1141	0.1346
O	1.1276	3.4341	0.1192
C	-0.5961	1.7895	-0.3446
C	-2.0608	1.9075	-0.7498
N	8.2009	2.8425	-0.6066
C	6.9662	2.1664	-0.4922
O	5.9294	2.8291	-0.5709
N	7.0121	0.8208	-0.3013
C	8.1795	0.1709	-0.2228
N	8.1427	-1.1506	-0.028
C	9.4441	0.8596	-0.3434
C	9.3986	2.2012	-0.5348
H	-3.6545	-1.3577	3.1374
H	-2.1412	-0.5207	3.5223
H	-2.4294	-0.7869	1.0539
H	-2.8873	-3.6625	1.7515
H	-0.9195	-4.3461	0.8339
H	-0.4292	-1.609	-0.4047
H	1.0961	-4.7925	0.9437
H	2.4973	1.9928	-0.3187
H	-6.9995	-1.0934	-0.1837
H	-5.6529	-1.4874	0.8578
H	-6.398	0.8209	1.1223
H	-5.6052	1.116	-1.7992
H	-7.6249	2.5471	-0.56
H	-4.4609	2.6553	1.5583
H	-4.7178	3.2615	-1.2984
H	-5.6144	4.3842	0.5853
H	0.0216	1.4384	-1.1729
H	-0.4647	1.0579	0.4623
H	-2.1515	2.5121	-1.6645

H	-2.48	0.9233	-0.9471
H	7.2338	-1.6406	0.0798
H	10.3862	0.3306	-0.2823
H	10.2864	2.8157	-0.637
H	9.0001	-1.6728	0.0466
H	4.2305	1.8906	-0.4775
H	5.3197	-0.0589	-0.1681
H	-2.2487	-2.2785	3.73
H	-0.6785	4.8728	0.9994
H	-2.0111	-4.5686	-1.1777
H	8.1387	3.8409	-0.7481
H	-3.4299	-2.6754	-0.7585
H	-5.3878	-1.2143	-0.8476

Table S28 - m^5U:G:A:A
Total-atoms=109

Atoms	X	Y	Z
C	-7.1436	-4.93741	-0.16257
C	-5.7549	-4.44724	-0.52829
O	-5.86737	-3.19735	-1.24016
C	-4.82267	-4.11092	0.64846
O	-4.16453	-5.21494	1.2343
C	-3.80926	-3.18346	-0.0322
O	-2.89867	-3.97281	-0.76833
C	-4.72916	-2.38521	-0.99725
N	-5.19293	-1.10102	-0.4616
C	-6.4378	-0.80126	0.08332
N	-6.56524	0.45268	0.43086
C	-5.35259	1.02666	0.1001
C	-4.88661	2.3761	0.22374
O	-5.46751	3.36952	0.67589
N	-3.56549	2.5011	-0.25989
C	-2.79397	1.49535	-0.78455
N	-1.55073	1.85554	-1.20978
N	-3.21986	0.2496	-0.91002
C	-4.4874	0.08086	-0.4584
C	2.0366	-8.33665	1.15822
C	0.76401	-7.55286	0.91216
O	0.88132	-6.24157	1.51862
C	0.43549	-7.26267	-0.56352
O	-0.18271	-8.3298	-1.23573
C	-0.46323	-6.01641	-0.44535
O	-1.76032	-6.49683	-0.16933
C	0.13446	-5.29513	0.78681
N	1.04181	-4.18669	0.42686
C	2.35935	-4.016	0.81197
N	2.86145	-2.8521	0.46878
C	1.81868	-2.20362	-0.16824
C	1.68942	-0.90234	-0.72029
N	2.68224	-0.00692	-0.72756
N	0.4861	-0.55507	-1.25123
C	-0.50809	-1.44896	-1.24717
N	-0.50603	-2.68653	-0.74021
C	0.68336	-3.01609	-0.20002
C	6.34787	6.07551	-1.28091
C	5.4058	4.89113	-1.37884
O	6.1355	3.72271	-1.80996

C	4.73858	4.45807	-0.06716
O	3.56314	5.23092	0.15294
C	4.41591	2.97679	-0.34899
O	3.24069	2.90353	-1.14202
C	5.61082	2.54852	-1.2197
N	6.67603	1.91279	-0.43319
C	7.96876	2.37361	-0.23105
N	8.7192	1.55249	0.46318
C	7.88687	0.48015	0.72816
C	8.08679	-0.73592	1.41643
N	9.25986	-1.04002	2.0179
N	7.07192	-1.6168	1.49149
C	5.90245	-1.30214	0.91704
N	5.5834	-0.18221	0.24532
C	6.61668	0.67315	0.17705
N	-2.56655	7.33053	0.20559
C	-3.09355	6.05466	0.24849
N	-4.39627	5.98778	0.65683
C	-5.21448	7.07957	1.02073
C	-4.57042	8.40206	0.94019
C	-5.39384	9.59796	1.31415
C	-3.28479	8.46522	0.5369
O	-2.39853	5.07895	-0.06631
O	-6.36841	6.90579	1.37268
H	-7.08059	-5.90961	0.33943
H	-7.75823	-5.06423	-1.05795
H	-5.24521	-5.18309	-1.16542
H	-5.38636	-3.53404	1.39843
H	-3.29253	-2.52061	0.67014
H	-4.19128	-2.17942	-1.92854
H	-7.20266	-1.55825	0.15913
H	-1.21777	2.77152	-0.94869
H	1.94767	-9.32219	0.69114
H	2.89998	-7.82237	0.72302
H	-0.09656	-8.06978	1.35795
H	1.35885	-7.01065	-1.09966
H	-1.13062	-8.22388	-1.04426
H	-0.4411	-5.38327	-1.33886
H	-2.39292	-5.75049	-0.23271
H	-0.67164	-4.87876	1.40294
H	2.87734	-4.79441	1.3499
H	2.52261	0.91799	-1.10827
H	-1.44906	-1.11458	-1.67228
H	5.78825	6.96464	-0.97379
H	6.81233	6.27888	-2.24955
H	4.61027	5.10112	-2.10684
H	5.44263	4.54925	0.76961
H	3.35153	5.21109	1.09601
H	4.32622	2.35802	0.55237
H	2.69395	3.66244	-0.8736
H	5.28416	1.84313	-1.99164
H	8.28439	3.31883	-0.64491
H	9.37981	-1.97113	2.38446
H	5.10652	-2.03944	0.99424
H	-6.29075	9.65874	0.68946
H	-5.74278	9.51895	2.34887
H	-4.82423	10.52496	1.2047
H	-2.73999	9.39911	0.44928
H	-4.8312	5.04163	0.6954
H	-3.16383	3.44472	-0.18454

H	-0.845	1.13176	-1.33787
H	3.61457	-0.21843	-0.37045
H	10.06491	-0.45675	1.85704
H	-2.0199	-3.50149	-0.80265
H	-7.6486	-4.23155	0.50544
H	-4.81582	-5.74182	1.71464
H	2.21696	-8.47416	2.22808
H	7.14008	5.88947	-0.54822
H	-1.61077	7.39049	-0.11154

Table S29 - C:Gm:G:C
Total-atoms=125

Atoms	X	Y	Z
C	-6.58811	4.58713	0.37107
C	-5.75871	3.35424	0.59852
O	-4.75466	3.22622	-0.44094
C	-4.95584	3.32665	1.88606
O	-5.77303	2.9484	2.99013
C	-3.89529	2.28735	1.55495
O	-4.42537	0.97684	1.57921
C	-3.58125	2.6409	0.09975
N	-2.48839	3.61735	-0.01665
C	-1.16229	3.17933	0.12482
O	-0.94044	1.97436	0.31259
N	-0.15758	4.07953	0.04856
C	-0.43199	5.36709	-0.17319
N	0.59036	6.22299	-0.25577
C	-1.77099	5.83765	-0.32719
C	-2.75585	4.9372	-0.24677
C	6.97136	-3.8684	1.65601
C	6.01221	-2.72199	1.89483
O	5.22164	-2.47811	0.69342
C	4.98547	-2.9129	3.00467
O	5.54553	-2.56284	4.28701
C	3.89356	-1.9242	2.58104
O	4.23227	-0.5776	2.85966
C	3.1334	0.17253	3.36093
C	3.91127	-2.06625	1.05492
N	2.96478	-3.05002	0.53596
C	3.26483	-4.33343	0.14071
N	2.22474	-5.0053	-0.26357
C	1.16525	-4.11566	-0.13688
C	-0.21365	-4.28818	-0.43084
O	-0.78244	-5.28726	-0.87106
N	-0.94205	-3.14124	-0.16057
C	-0.41807	-1.96729	0.32213
N	-1.30333	-0.96504	0.51389
N	0.87408	-1.78749	0.59737
C	1.60117	-2.89773	0.34944
C	9.41141	1.20218	-3.04767
C	8.50674	0.19511	-2.3727
O	8.25798	0.58819	-0.99553
C	7.13153	0.0496	-3.00184
O	7.21258	-0.9262	-4.02854
C	6.28416	-0.41355	-1.82516
O	6.48813	-1.77386	-1.52316
C	6.88793	0.40513	-0.68262
N	6.29576	1.7301	-0.5065
C	6.96171	2.93144	-0.51356

N	6.17585	3.95055	-0.32386
C	4.9167	3.39398	-0.19098
C	3.67238	4.00791	0.02193
O	3.4168	5.21104	0.10779
N	2.65157	3.0711	0.12601
C	2.81062	1.72099	0.02178
N	1.70968	0.97662	0.17843
N	3.96451	1.13599	-0.20859
C	4.97175	2.02578	-0.29684
C	-10.4075	-2.29483	-0.34639
C	-9.35432	-1.21766	-0.32423
O	-8.20096	-1.65352	0.43888
C	-8.81874	-0.82185	-1.68822
O	-9.67875	0.1854	-2.23522
C	-7.42948	-0.2829	-1.3541
O	-7.47794	1.06407	-0.93066
C	-7.01926	-1.14362	-0.14914
N	-6.11328	-2.27762	-0.44972
C	-4.71256	-2.08892	-0.38805
O	-4.25271	-0.97123	-0.12401
N	-3.89859	-3.13701	-0.62183
C	-4.41465	-4.33293	-0.91622
N	-3.57093	-5.3476	-1.1025
C	-5.81981	-4.54591	-1.02078
C	-6.62435	-3.50529	-0.77881
H	-7.33281	4.66309	1.16902
H	-7.11669	4.54814	-0.58612
H	-6.39574	2.46503	0.59337
H	-4.50124	4.29555	2.11637
H	-5.84618	1.98195	2.93142
H	-3.00793	2.35759	2.19475
H	-3.28181	1.76345	-0.4791
H	1.56038	5.89861	-0.12293
H	-1.9823	6.88195	-0.52037
H	-3.79792	5.18119	-0.38763
H	7.59643	-4.00266	2.5436
H	7.6206	-3.65417	0.80279
H	6.5696	-1.80546	2.12491
H	4.58893	-3.9376	2.99569
H	4.87238	-2.74877	4.95395
H	2.91106	-2.18103	2.99422
H	2.28388	0.16839	2.66808
H	2.80448	-0.20544	4.34033
H	3.48652	1.19865	3.48108
H	3.70783	-1.09647	0.59344
H	4.27982	-4.69802	0.15254
H	-0.97339	-0.02902	0.70353
H	10.37295	1.28294	-2.53226
H	9.59918	0.88434	-4.07829
H	8.97594	-0.79601	-2.3622
H	6.74995	0.98582	-3.41867
H	7.08414	-1.77649	-3.57789
H	5.22067	-0.19039	-1.96482
H	5.90769	-2.02916	-0.7829
H	6.80209	-0.1352	0.26631
H	8.03103	2.96944	-0.64627
H	1.73708	-0.03444	0.14678
H	-10.72645	-2.56173	0.66464
H	-11.27927	-1.93163	-0.89892
H	-9.7534	-0.31068	0.14794

H	-8.76451	-1.66197	-2.3871
H	-9.32779	1.02448	-1.89467
H	-6.72823	-0.40175	-2.18662
H	-6.67407	1.51228	-1.22542
H	-6.47416	-0.51859	0.56127
H	-3.93892	-6.25944	-1.32333
H	-6.22367	-5.52078	-1.26363
H	-7.70315	-3.57439	-0.77541
H	1.69834	3.44389	0.21746
H	0.7944	1.41494	0.26006
H	8.9459	2.19283	-3.06878
H	-2.26793	-1.05844	0.20728
H	-1.9541	-3.15896	-0.34947
H	6.43694	-4.80445	1.46301
H	-2.53956	-5.25851	-1.02705
H	-10.04385	-3.20161	-0.84272
H	-5.97836	5.49695	0.39002
H	0.42453	7.20423	-0.40631
H	-4.163	0.39371	0.84543