Supplementary Information

3DNA: A Software Package for the Analysis, Rebuilding, and Visualization of Three-dimensional Nucleic Acid Structures

Xiang-Jun Lu and Wilma K. Olson*

Department of Chemistry & Chemical Biology
Rutgers, the State University of New Jersey
Wright-Rieman Laboratories
610 Taylor Road
Piscataway, NJ 08854-8087, USA

* To whom correspondence should be addressed.
Tel: 732-445-3993; Fax: 732-445-5958; E-mail: olson@rutchem.rutgers.edu.

Table S-1. Base-pair parameters and hydrogen bond characteristics of a representative crystallographic example of each of the classic nucleic acid base pairs with two or more hydrogen bonds between bases.

	Base-pair Identity†	NDB_ID*	Base IDs#	Shear (Å)	Shift (Å)	Stagger (Å)	Buckle (deg)	Prop. (deg)	Open (deg)	Hydrogen bonds§ Atom IDs	Length (Å)	
	Homo purine pairs (7)											
I.	A+A N1···HN6H sym. WC/WC *trans*	rr0033	A204·A436	–1.45	–1.36	–0.56	–4.0	–16.3	175.0	N6···N1	N1···N6	
										2.88	3.01	
II.	A+A N7···HN6H sym. H/H *trans*	rr0033	A161·A174	6.05	–5.01	–0.05	15.5	6.4	175.7	N7···N6	N6···N7	
										2.76	2.99	
III.	G+G N1···C=O6 sym. WC/WC *trans*	rr0025	G1383·G1481	–0.34	–1.03	2.32	29.6	–4.0	165.5	O6···N1	N1···O6	
										3.37	2.89	
IV.	G+G N3···HN2H sym. S/S *trans*	rr0033	G32·G456	3.06	8.04	–0.98	–13.6	8.7	175.3	N2···N3	N3···N2	
										2.94	3.10	
V.	A–A N1···HN6H, HN6H···N7 WC/H *trans*	rr0033	A455·A460	3.94	1.36	1.37	13.0	15.5	–108.9	N6···N7	N1···N6	
										2.90	3.01	
VI.	G+G N1···O6=C, HN2H···N7 WC/H *cis*	rr0033	G56·G84	2.16	3.07	0.34	–13.1	–4.0	–85.3	N1···O6	N2···N7	
										2.76	2.75	
VII.	G–G N1···N7, HN2H···O6=C WC/H *trans*	rr0033	G2082·G535	5.55	–0.51	0.34	5.3	20.7	–101.1	N1···N7	N2···O6	
										3.08	2.53	
	Hetero purine pairs (4)											
VIII.	A–G N1···N1, HN6H···O6=C WC/WC *cis*	rr0033	A2596·G2582	0.39	1.47	–0.11	7.5	–8.3	–14.4	N6···O6	N1···N1	
										2.95	2.83	
IX.	A+G N7···N1, HN6H···O6=C H/WC *cis*	rr0020	A665·G724	0.56	–4.95	0.49	–7.5	–1.9	95.7	N7···N1	N6···O6	
										3.17	2.82	
X.	A+G HN6H···N3, N1···HN2H WC/S *trans*	rr0033	A629·G2070	–3.25	4.11	0.11	4.4	–10.0	69.4	N6···N3	N1···N2	(N6···O2′)
										3.14	2.94	2.93
XI.	A–G N7···HN2H, HN6H···N3 H/S *trans*	rr0033	A215·G225	–6.82	–4.21	–0.42	2.8	10.9	–2.2	N7···N2	N6···N3	(N6···O2′)
										2.95	3.08	2.99
	Homo pyrimidine pairs (5)											
XII.	U+U C=O4···N3 sym. WC/WC *trans*	rr0033	U1838·U2621	–1.62	1.43	–0.23	2.9	5.2	–175.4	N3···O4	O4···N3	
										2.78	2.96	
XIII.	U+U C=O2···N3 sym. WC/WC *trans*	rr0052	U956·U960	–1.95	–2.78	–0.19	–13.1	–1.3	–169.0	O2···N3	N3···O2	(O2···O4)
										2.85	3.23	3.20

Table S-1- continued

	Base-pair	Identity†	NDB_ID*	Base IDs#	Shear (Å)	Shift (Å)	Stagger (Å)	Buckle (deg)	Prop. (deg)	Open (deg)	Hydrogen bonds§ Atom IDs Length (Å)		
XIV.	C+C	N3···HN4H sym. WC/WC *trans*	rr0014	C2105·C2536	2.01	–1.72	2.15	1.7	38.7	126.1	N3···N4 3.34	N4···N3 2.09	
XV.	C+C	C=O2···HN4H sym. WC/WC *trans*	pr0004	C16·C59	1.76	1.21	0.60	–3.4	16.5	176.7	O2···N4 3.19	N4···O2 2.84	(N3···N3) 2.96
XVI.	U–U	C=O2···N3, ·N3··O4=C WC/WC *cis*	rr0033	U391·U398	2.27	–1.79	0.27	6.5	–11.7	12.4	O2···N3 2.86	N3···O4 2.87	
				Hetero pyrimidine pairs (2)									
XVII.	C+U	N3···N3, HN4H···O2=C WC/WC *trans*	rr0033	C1394·U1432	1.81	1.47	–0.14	19.1	6.8	178.6	N3···N3 3.03	N4···O2 2.91	(O2···O4) 3.22
XVIII.	C–U	N3···N3, HN4H···O4=C WC/WC *cis*	rr0033	C1545·U1702	0.94	–1.61	0.29	5.9	–35.4	8.8	N3···N3 3.17	N4···O4 3.16	
				Purine-pyrimidine pairs (10)									
XIX.	G–C	Watson-Crick WC/WC *cis*	rr0033	G13·C530	–0.41	0.01	–0.15	0.0	2.2	1.3	O6···N4 3.11	N1···N3 3.06	N2···O2 2.88
XX.	A–U	Watson-Crick WC/WC *cis*	rr0033	A16·U527	0.06	–0.20	0.26	3.6	–11.1	–0.6	N6···O4 2.84	N1···N3 2.76	
XXI.	A+U	reverse Watson-Crick WC/WC *trans*	rr0033	A2301·U2306	0.27	1.25	–0.34	15.5	4.9	167.3	N6···O2 2.76	N1···N3 2.72	
XXII.	G+C	reverse Watson-Crick WC/WC *trans*	rr0033	G1683·C1377	0.02	4.11	0.33	1.7	5.7	147.5	N1···O2 2.72	N2···N3 3.10	
XXIII.	A+U	Hoogsteen H/WC *cis*	rr0033	A2793·U2791	0.56	–3.49	0.01	–7.7	0.6	71.8	N7···N3 2.94	N6···O4 2.79	(O2P···O2) 3.27
XXIV.	A–U	reverse Hoogsteen H/WC *trans*	rr0033	A160·U176	–4.22	–2.06	–0.63	–1.1	–14.0	–98.7	N7···N3 2.83	N6···O2 2.95	
XXV.	A–C	reverse Hoogsteen H/WC *trans*	rr0033	A766·C896	–3.16	–0.84	–0.81	10.0	–13.3	–90.0	N7···N4 2.91	N6···N3 2.92	
XXVI.	A+C	reverse wobble WC/WC *trans*	rr0033	A1742·C2037	0.04	–1.54	–0.03	30.2	–6.5	163.0	N6···N3 3.02	N1···N4 2.97	
XXVII.	G+U	reverse wobble WC/WC *trans*	rr0033	G1970·U1966	0.34	–1.53	0.60	18.1	–9.3	157.3	O6···N3 2.84	N1···O4 2.95	
XXVIII.	G–U	wobble WC/WC *cis*	rr0033	G17·U526	–2.26	–0.67	0.14	4.3	–14.2	–1.5	O6···N3 2.71	N1···O2 2.67	

Footnotes to Table S-1

† Roman numerals refer to the base-pair identification code given by Saenger (1); other base pairs with *cis* and *trans* arrangements of a single bifurcated hydrogen bond (2, 3) and with potential steric conflicts (see the Image Library of Biological Macromolecules, IMB Jena for examples: http://www.imb-jena.de/ImgLibDoc/bp/gc.html) are omitted. The + and – symbols designate parallel and antiparallel orientations of the interacting bases; the base-pair names are adapted from the Tinoco compilation (4), where sym. is an abbreviation for symmetric, HNH denotes amino, and C=O or O=C stands for carbonyl, and from the proposed classification scheme of Leontis and Westhof (3), where WC, H, and S refer respectively to hydrogen-bonded atoms on the Watson-Crick, Hoogsteen, and sugar edges of a base.

* Of the 28 possible base-pair types, examples of 23 are found in the high resolution (2.4 Å) crystal structure of the large ribosomal subunit, NDB_ID: `rr0033` (5). The remaining five examples come from other, less well-resolved ribosomal structures—`rr0014` (6), `rr0020` (7), `rr0025` (8), `rr0052` (9)—and from the 2.6 Å resolution structure of the ternary complex of Cys-tRNA^{Cys} with the translation elongation factor EF-Tu and GTP, `pr0004` (10),

Base-pairs are identified using the `find_pair` utility program in `3DNA` with the `-p` option. The numerical values refer to the position of a given base in the nucleotide sequence.

§ The atoms comprising the hydrogen bonds associated with a given base-pair type are listed such that the atoms from the base preceding the + or – sign in column 2 appear first in each paired entry. Interactions within parentheses are not included in conventional descriptors of the given base-pair type but are identified by the program. Note the occurrence of potentially repulsive interactions between hydrogen-bond acceptors (O2···O4 and N3···N3) in some examples.

References to Table S-1

1. Saenger, W. (1984) *Principles of Nucleic Acid Structure*. Springer-Verlag, New York, Chpt. 6.
2. Auffinger, P. and Westhof, E. (1999) Singly and bifurcated hydrogen-bonded base-pairs in tRNA anticodon hairpins and ribozymes. *J. Mol. Biol.* **292**, 467-483.
3. Leontis, N.B. and Westhof, E. (2001) Geometric nomenclature and classification of RNA base pairs. *RNA* **7**, 499-512.
4. Tinoco, J., I. (1993) Appendix 1: structures of base pairs involving at least two hydrogen bonds. In Gesteland, R.F. and Atkins, J.F. (ed.), *The RNA World* Cold Spring Harbor Laboratory Press, Cold Spring Harbor, NY, pp. 603-607.
5. Klein, D.J., Schmeing, T.M., Moore, P.B. and Steitz, T.A. (2001) The kink-turn: a new RNA secondary structure motif. *EMBO J.* **20**, 4214-4221.
6. Nissen, P., Hansen, J., Ban, N., Moore, P.B. and Steitz, T.A. (2000) The structural basis of ribosome activity in peptide bond synthesis. *Science* **289**, 920-930.
7. Brodersen, D.E., Clemons Jr., W.M., Carter, A.P., Morgan-Warren, R.J., Wimberly, B.T. and Ramakrishnan, V. (2000) The structural basis for the action of the antibiotics tetracycline, pactamycin, and hygromycin B on the 30S ribosomal subunit. *Cell* **103**, 1143-1154.
8. Pioletti, M., Schluenzen, F., Harms, J., Zarivach, R., Gluehmann, M., Avila, H., Bashan, A., Bartels, H., Auerbach, T., Jacobi, C., et al. (2001) Crystal structures of complexes of the small ribosomal subunit with tetracycline, edeine and IF3. *EMBO J.* **20**, 1829-1839.
9. Wimberly, B.T., Brodersen, D.E., Clemons Jr., W.M., Morgan-Warren, R.J., Carter, A.P., Vonrhein, C., Hartsch, T. and Ramakrishnan, V. (2000) Structure of the 30S ribosomal subunit. *Nature* **407**, 327-339.
10. Nissen, P., Thirup, S., Kjeldgaard, M. and Nyborg, J. (1999) The crystal structure of Cys-tRNA^{Cys}-EF-Tu-GDPNP reveals general and specific features in the ternary complex and in tRNA. *Structure Fold. Des.* **7**, 143-156.