that rhodopsin has an additional, previously unrecognized function, perhaps a role in circadian rhythms^{10,11}, unrelated to light absorption.

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Chirality errors in nucleic acid structures

The prevalence of errors as opposed to true anomalies in protein structures was discussed in Correspondence last year¹. We have analysed the nucleic acid structures in the Brookhaven Protein Data Bank using a simple automatic procedure (program available at <http://www.mbi.ucla.edu/people/peter/chiral.html>) to determine the configurations at tetrahedral chiral centres. It appears that a number of structures containing significant “chirality errors that no-one would argue with”² have made their way into the data bank.

Of 562 data bank files containing nucleic acid coordinates, we found that 34 contained reversed configurations (Table 1) of at least one chiral centre (Fig. 1). Incorrect configurations at C1', C3' and C4' are detectable in both NMR and crystal structures. C2' represents a special case for DNA structures where H2' and H2'' are included. Errors in the naming of H2'/H2'' atoms would be irrelevant in X-ray structures but are significant in NMR structures of DNA because H2' and H2'' are almost always stereospecifically assigned. In the case of RNA, the correct chirality of C2' would be equally significant in both X-ray and NMR structures.

In 25 further coordinate files, not listed

Table 1 Chirality problems in nucleic acid coordinate sets from the Brookhaven Protein Data Bank

PDB entry code	Total number of nucleosides	Chirality errors			Method	PDB entry code	Total number of nucleosides	Chirality errors			Method
		1', 3', 4'	2'					1', 3', 4'	2'		
106D	96	0	8		NMR	1DSD	16	0	1		NMR
108D	640	0	20*		NMR	1HRY	16	2	1		NMR
143D	132	21	20		NMR	1HRZ	560	70	35		NMR
149D	294	0	147		NMR	1LBG	84	7	0		X-ray
170D	22	0	10		NMR	1QDF	15	7	15		NMR
171D	24	0	12		NMR	1QDG	15	7	0		Theory
173D	16	1	0		X-ray	1QDH	15	7	0		NMR
186D	168	9	5		NMR	1RCS	600	36	0		NMR
1ARA	136	34	87†		NMR	1URN	55	0	2†		X-ray
1BUF	12	2	0		NMR	203D	640	0	60*		NMR
1D31	26	1	0		X-ray	204D	640	20	40*		NMR
1D42	80	1	0		NMR	228D	88	9	73		NMR
1D70	64	1	0		NMR	229D	14	2	7		NMR
1D98	24	1	0		X-ray	28DN	8	1	0		X-ray
1D99	24	1	0		X-ray	2DA8	96	0	2		NMR
1DDP	200	0	20*		NMR	5BNA	24	1	0		X-ray
1DSC	16	0	1		NMR	5ZNA	32	0	16		Theory

A chiral centre was designated wrong if the dihedral angle defined by its four ligands – or three ligands and the central atom in cases where no hydrogen coordinates are given – was found to have the opposite sign of the correct configuration. A complete, detailed table of chirality problems is available at <http://www.mbi.ucla.edu/people/peter/chiral.html>.

*In these cases the majority of H2'/H2'' configurations are inconsistent with the convention as given in ref. 3. The number given represents configurations opposite to the nomenclature used within these entries. Coordinate files where all H2'/H2'' configurations are reversed throughout are not listed.

†RNA, number of flipped O2' atoms.

in Table 1, the naming of H2'/H2'' was reversed throughout compared with the IUPAC-IUB convention^{3,4}. Whether these cases are merely in discrepancy with the convention in a particular file or inconsistent with the underlying experimental data would depend on whether the same nomenclature was used for the determination of the stereospecific resonance assignment in each case.

We also observed inconsistencies in the naming of the amino protons, which are distinguishable even when they are not involved in hydrogen bonds simply by their *cis/trans* positions with respect to other base atoms. We disregarded inconsistencies in the naming of the diastereotopic atom pairs H5'/H5'' and O1P/O2P as they are generally not relevant to the experimental results in either NMR or X-ray structures. However, these atoms should be consistently named for accurate structure comparisons by root mean square deviations of atomic positions.

The overall topology of most affected structures would probably not change substantially on correction of their chirality problems and re-refinement. Nevertheless, these errors are significant both because the structures are stereochemically wrong and because of the importance of ion and hydrogen bonding interactions with the phosphodiester backbone which stabilize the structures of nucleic acids.

We note that current refinement programs and their parametrization for nucleic acids do not always prevent this type of avoidable error, especially when high-temperature simulated annealing protocols are used. The higher number of errors found in

Figure 1 Stereochemical nomenclature of a nucleotide. Carbon atoms are numbered from that bound to the base.

the NMR structures compared with the X-ray structures does not reflect a weakness of NMR experiments, but rather depends on problems in the refinement protocols.

It might be reasonable to test all structures for rigorous adherence to the existing conventions of stereochemical nomenclature^{3,4} at the time of deposition into the data bank.

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