Nucleotide binding in βαβ-βαβ topologies

Swindells M.B. & Alexandrov N.N.
Nature structural Biology, **1** 677–678 (1994).

The content of this work was erroneously summarized in its strap line. The Correspondence reports a similarity between glutamine synthetase and both aspartate transcarbamylase (ATC) and nucleotide diphosphate kinase (NDK). The authors would like it pointed out that they were not the first people to identify a similarity between ATC and NDK, an observation originally made by Professor Joel Janin.

Solution structure of the tetrameric minimum transforming domain of p53

Arrowsmith, C. *et al.*
Nature structural Biology, **1** 877–888.

Table 2 was unfortunately omitted.

Table 2 Structure statistics for the 20 final simulated annealing structures.

Experimental restraints		**r.m.s.d. from experimental value (Å)**	
NOES:[1]		Average of 20	r.m.s.d of Avg. Structure[2]
all (457)		0.040 ± 0.002	0.035
A-B (73)		0.036 ± 0.001	0.032
A-C (18)		0.030 ± 0.001	0.018
A-D (33)		0.038 ± 0.002	0.031
ambiguous (6)		0.003 ± 0.000	0.000
not A (5)		0.013 ± 0.000	0.013
A-A:	intra (100)	0.038 ± 0.001	0.037
	sequential (98)	0.047 ± 0.002	0.045
	short range (65)	0.042 ± 0.002	0.034
	long range (23)	0.009 ± 0.002	0.000
H-bonds:	helix (26)[3]	0.039 ± 0.000	0.033
	sheet (10)[3]	0.018 ± 0.000	0.006
Dihedrals (38) (degrees)[4]		0.22 ± 0.23	0.598
r.m.s.d. from ideal geometry:			
bonds (Å)		0.002± 0.000	0.002
angles (degrees)		0.23 ± 0.02	0.192
impropers (Å)		0.196 ± 0.000	0.160
Energies:	Total[5]	107.7 ± 8.2	78.1
	Repel	15.8 ± 2.2	11.4
	NOE	36.7 ± 3.5	28.1
	Symmetry	1.02 ± 0.15	0.55
	Restrained Dihedral	0.18 ± 0.23	0.80
	Bond	7.0 ± 0.45	5.00
	Angle	30.6 ± 3.02	20.9
	Improper	6.56 ± 1.1	4.31
	NCS	10.6 ± 1.8	7.40
	Lennard-Jones	-307.2 ± 28.7	-243.3
Atomic RMSD from avg.		**Backbone atoms**	**All heavy atoms**
Sheet (326–334)		0.48	1.06
Helix (337–354)		0.48	0.83
All (325–355)		0.61	1.01

[1]The number of restraints per subunit in each category are listed in brackets. Each restraint wasused only once in the calculation and the symmetry restraints ensure that the other 3 symmetry-related distance and angular restraints are satisfied. NOE intensities were converted to distance restraints with upper-bounds of 2.7 Å for strong, 3.3 Å for medium, and 5.0 Å for weak NOEs. None of the structures has distance violations of more than 0.3 Å nor dihedral angle violations of greater than 5°.
[2]The average structure is the average coordinates of the 20 structures after energy minimization with experimental restraints.
[3] Upper bounds for hydrogen bond restraints were 2.3 Å for the NH-O distance and 3.3 Å for the N-O distance.
4 Dihedral angle restraints were implemented with minimum ranges of ± 20°. All ϕ and φ angles lie within the allowed regions of the Ramachandran plot.
[5] Energies(kcal mol^{-1}) are calculated with a repel value of 0.75 times the van der Waals radii and an rconst value of 4.0 kcal mol^{-1} Å^4. Force constants were as follows: K_{NCS} = 10.0, K_{NOE} = 50.0 kcal^{-1} mol Å^{-2} (including symmetry NOEs), $K_{dihedral}$ = 200.0 kcal mol^{-1}rad^{-2}, K_{bond}= 1000 kcal mol^{-1} Å^{-2}, and K_{angle}/$K_{impropers}$ = 500 kcal mol^{-1}rad^{-2}.