Nucleotide binding in $\beta\alpha\beta$ - $\beta\alpha\beta$ 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like it pointed out that they were not the first people to identify a similarity between ATC and NDK, an observation originally made by Professor Joel Janin.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 |
| 5 | 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 <u>+</u> 0.45 | 5.00 |
| | Angle | 30.6 ± 3.02 | 20.9 |
| | Improper | 6.56 <u>+</u> 1.1 | 4.31 |
| | NCS | 10.6 <u>+</u> 1.8 | 7.40 |
| | Lennard-Jones | -307.2 <u>+</u> 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 |

¹The 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°.

²The average structure is the average coordinates of the 20 structures after energy minimization with experimental restraints. ³Upper 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 \pm 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 roonst value of 4.0 kcal mol⁻¹ Å⁴. 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⁻¹rad⁻², $K_{bond} = 1000$ kcal mol⁻¹ Å⁻², and $K_{angle'}/K_{impropers} = 500$ kcal mol⁻¹rad⁻².