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Note to the Paper by Guasch *et al.* (2002) Detailed Architecture of a DNA Translocating Machine: The High-resolution Structure of the Bacteriophage φ29 Connector Particle

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The recent paper by Guasch *et al.*[1] describing the structure of the φ29 bacteriophage head–tail connector at 2.1 Å resolution (PDB code 1h5w), makes reference to the original 3.2 Å resolution structure (PDB code 1fou) published by Simpson *et al.*[2] and used by Guasch *et al.* to solve the 1h5w structure by molecular replacement. The Guasch paper states that there are marked differences between the 1h5w and 1fou structures in the chain tracing and the side-chain positioning in the wide domain. As these and a number of other statements in the Guasch paper may have led to the impression that these differences are larger than they really are, we give here Tables summarizing the similarities and differences (Tables 1 and 2).

Another paper by Simpson *et al.*,[3] which was accidentally omitted from the text of the Guasch *et al.* paper, reports two additional structures of the φ29 connector: at 3.2 Å resolution and at 2.9 Å resolution (PDB codes 1jnb and 1ijg, respectively).

The 2.9 Å resolution structure shows no significant differences from the structure subsequently reported by Guasch *et al.* (Figure 1; Tables 1 and 2).

References

1. Guasch, A., Pous, J., Ibarra, B., Gomis-Rüth, F. X., Valpuesta, J. M., Sousa, N. *et al.* (2002). Detailed architecture of a DNA translocating machine: the high-resolution structure of the bacteriophage φ29 connector particle. *J. Mol. Biol.* **315**, 663–676.
2. Simpson, A. A., Tao, Y., Leiman, P. G., Badasso, M. O., He, Y., Jardine, P. J. *et al.* (2000). Structure of the bacteriophage φ29 DNA packaging motor. *Nature*, **408**, 745–750.
3. Simpson, A. A., Leiman, P. G., Tao, Y., He, Y., Badasso, M. O., Jardine, P. J. *et al.* (2001). Structure determination of the head–tail connector of bacteriophage φ29. *Acta Crystallog. sect. D*, **57**, 1260–1269.

Edited by P. Wright

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Table 1. Statistical comparison of the φ29 connector wide domains in different structures

	RMS deviation		Maximum deviation		
	C^α atoms	All atoms	C^α atoms	All atoms	Number of C^α atoms deviating more than 2 Å
1h5w *versus* 1fou	1.1	2.2	4.9	10.6	15
1h5w *versus* 1jnb	1.2	2.0	5.2	11.1	10
1h5w *versus* 1ijg	0.8	1.6	6.4	11.4	5

The wide domain is defined as residues 38–128 and 247–284. All distances are in Å and correspond to comparisons of the A monomers in all structures.

Table 2. Superposition of the entire monomers in the four reported structures

	RMS deviation		Maximum deviation		
	C^α atoms	All atoms	C^α atoms	All atoms	Number of C^α atoms deviating more than 2 Å
1h5w *versus* 1fou	1.1	1.8	4.9	10.6	20
1h5w *versus* 1jnb	1.1	1.8	5.1	11.3	19
1h5w *versus* 1ijg	0.9	1.3	7.0	11.6	9[a]
1ijg *versus* 1jnb	1.1	1.9	6.0	11.8	18
Chain A *versus* chain B in 1ijg	0.9	1.5	7.5	13.8	6
Chain A *versus* chain B in 1h5w	0.5	0.8	4.4	6.5	2

The number of the aligned C^α atoms is 251. All distances are in Å.
[a] The number of differences greater than 2 Å varies from 1 to 9 depending on which of the 12 monomers are being compared.

Figure 1. Stereo diagram showing the superposition of the C^α backbone of monomer A in the 2.1 Å resolution structure 1h5w (green) and the 2.9 Å resolution 1ijg structure (red).