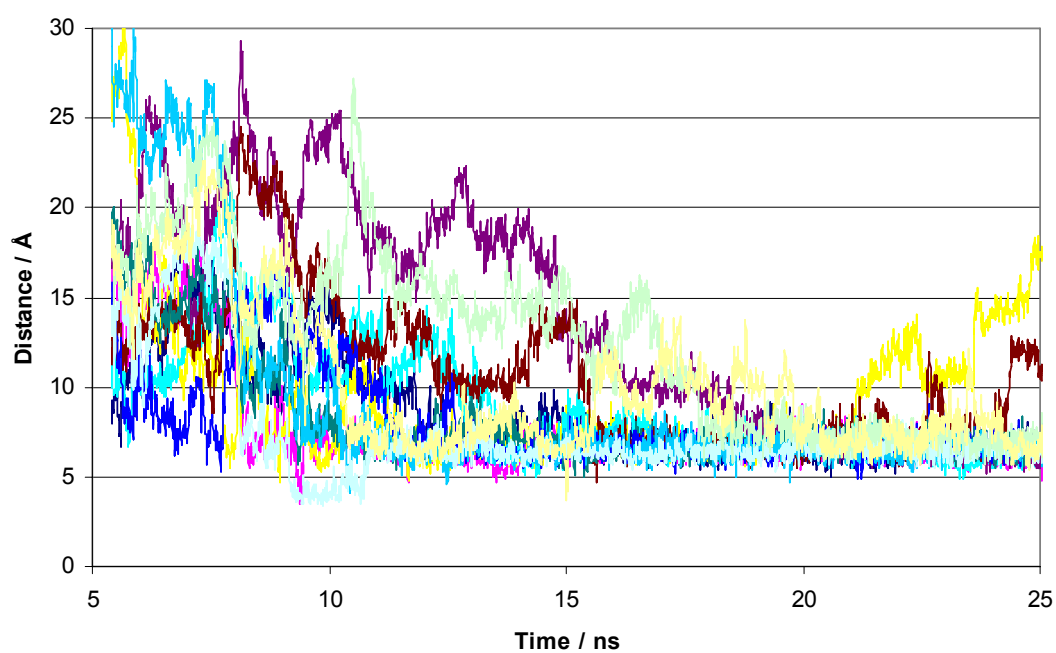
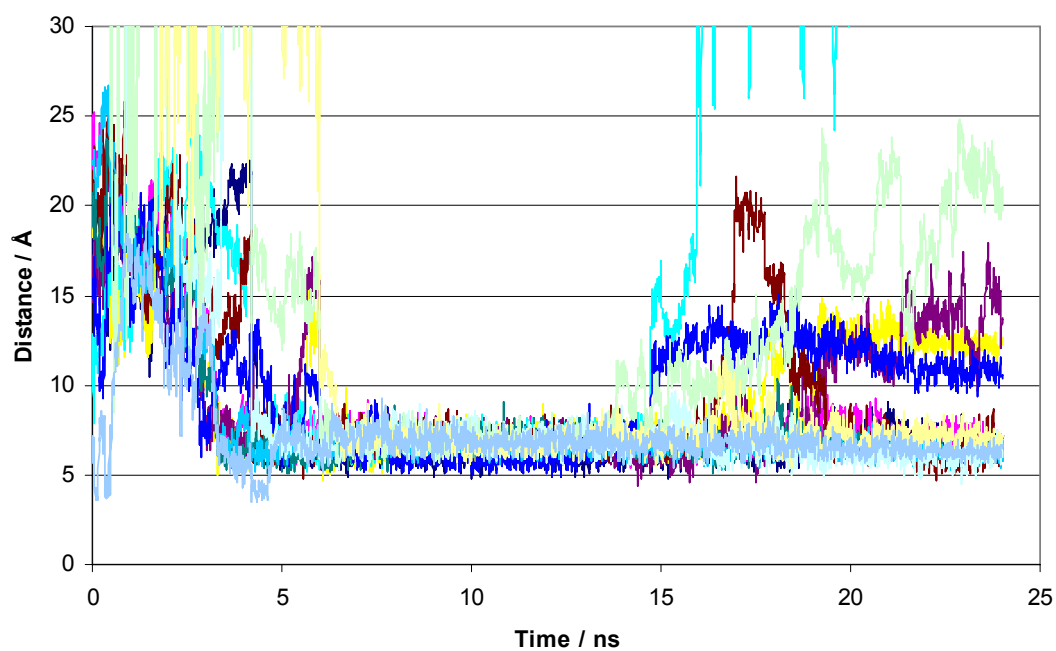
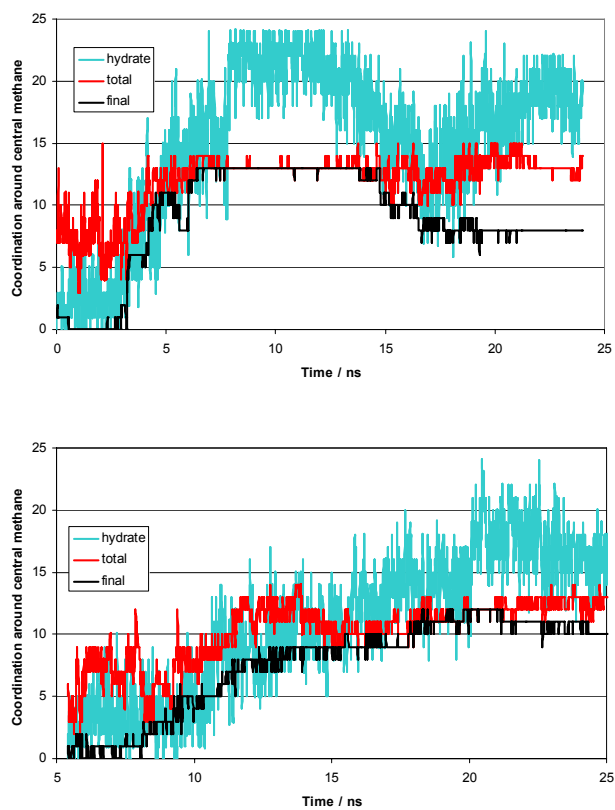


Distance from surrounding methane molecules to the central methane for the first 5¹² cage in B (top) and C (bottom).



Distance from surrounding methane molecules to the central methane for the first $5^{12}C^2$ cage in A (top) and C (bottom).



Number of methane molecules coordinating the methane at the centre of the first $5^{12}6^2$ cage for system A (top) and C (bottom). 'Total' shows the total coordination number, 'final' shows only the contribution from the methane molecules that coordinate the complete cage.

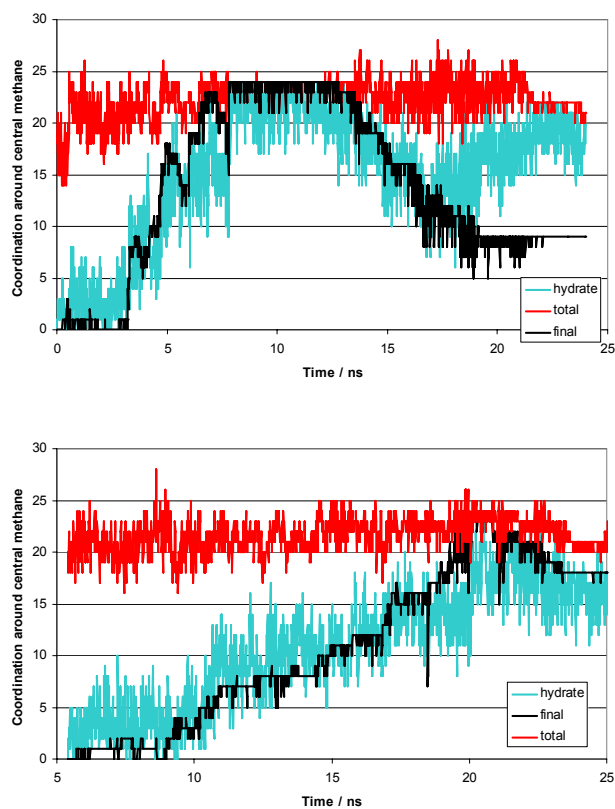


Fig. 16 Number of water molecules coordinating the methane at the centre of the first $5^{12}6^2$ cage for system A (top) C (bottom). 'Total' shows the total coordination number, 'final' shows only the contribution from the methane molecules that coordinate the complete cage. 'Hydrate' shows the total number of water molecules in the solvation shell that were assigned to the hydrate local phase.