Supplementary Table I

Supplementary Table I. Summary of Selected Crystallographic Statistics

Data set	**Native**	**Peak**	**Inflection**	**Remote**
Data collection statistics				
Wavelength (Å)	0.97976	1.07206	1.07227	1.12051
Unique reflections	46030	7280	7292	7286
Total reflections	628458	69464	69383	60097
Resolution	50.0 – 1.50	50.0 – 2.80	50.0 – 2.80	50.0 – 2.80
(last shell) (Å)	1.55 – 1.50	2.90 – 2.80	2.90 – 2.80	2.90 – 2.80
Completeness (%)	99.7 (99.7)	99.2 (94.0)	99.3 (94.6)	98.9 (94.1)
R_{sym} (%)	10.1 (46.9)	5.7 (16.8)	5.8 (16.9)	5.4 (14.6)
$I/\sigma(I)$	43.4 (4.5)	14.0 (3.9)	13.9 (3.8)	15.4 (4.4)
Refinement statistics				
Resolution	45 – 1.50			
R_{factor}/R_{free} (%)	14.1/19.1			
Protein residues	205			
Non-protein residues	5			
Fe ions	3			
Solvent atoms	237			
rmsd				
Bond lengths (Å)	0.00809			
Bond angles (°)	2.07			
Ramachandran Plot				
Most favoured	92.7 %			
Additional allowed	7.3 %			
Generously allowed	0			
Disallowed	0			

Supplementary Table II

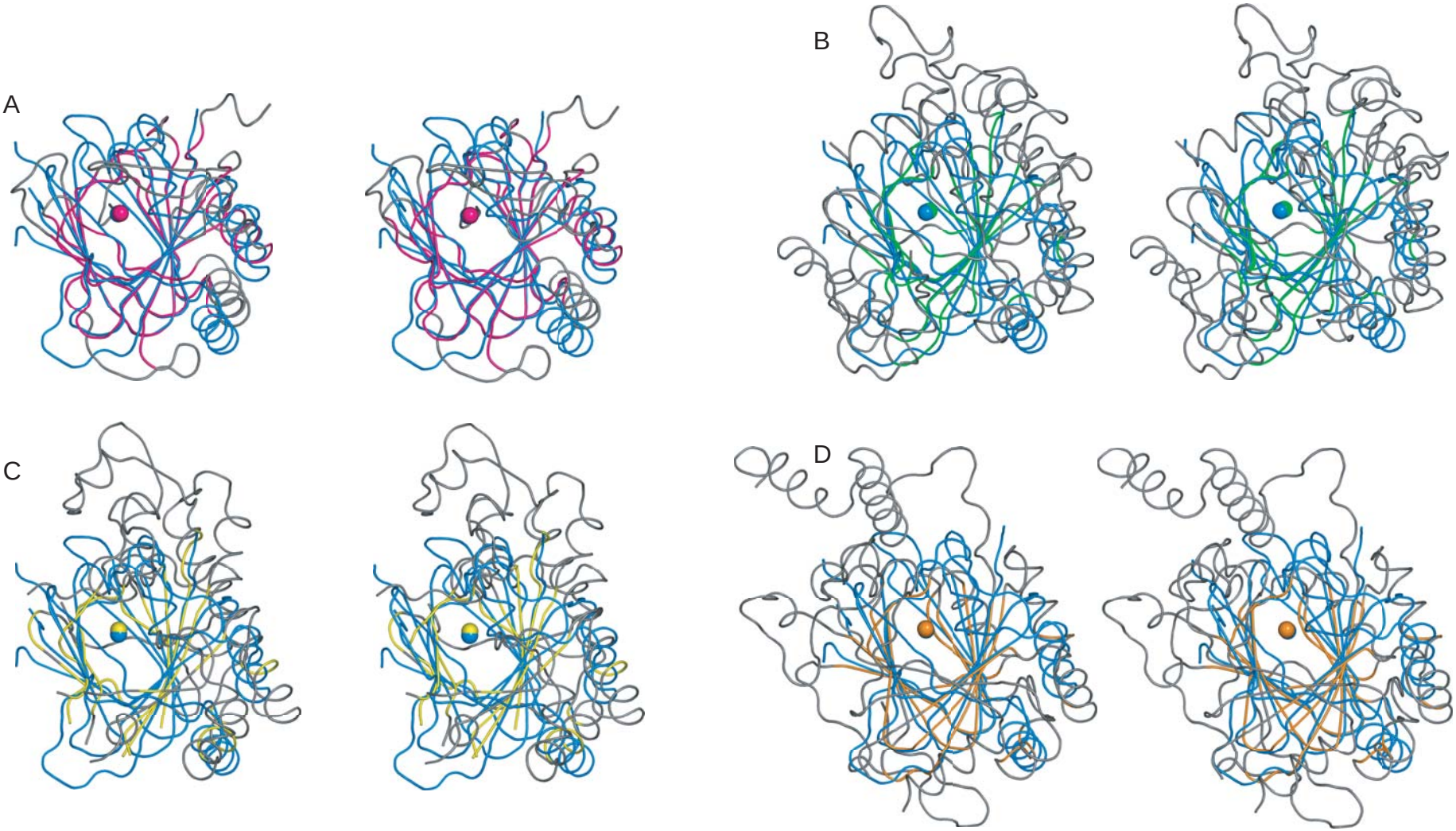
Table II. Pairwise sequence similarity between hABH2/3 and AlkB.

I / S (%)	hABH3	AlkB	
hABH2	32 / 46	21 / 35	Complete
	39 / 54	26 / 41	C-term (50%)
hABH3		18 / 34	Complete
		21 / 39	C-term (50%)

The table shows pairwise percentage sequence identity (I) and similarity (S) for aligned positions of the multiple alignment in Figure 2. Similar residues are defined as residue pairs with a positive score value in the Blosum62 log-odds matrix (Henikoff and Henikoff, 1992). The first line shows values for the complete alignment, the second line is for the C-terminal half of the alignment only. This shows that the C-terminal part is in general more conserved than the N-terminal part of these proteins.

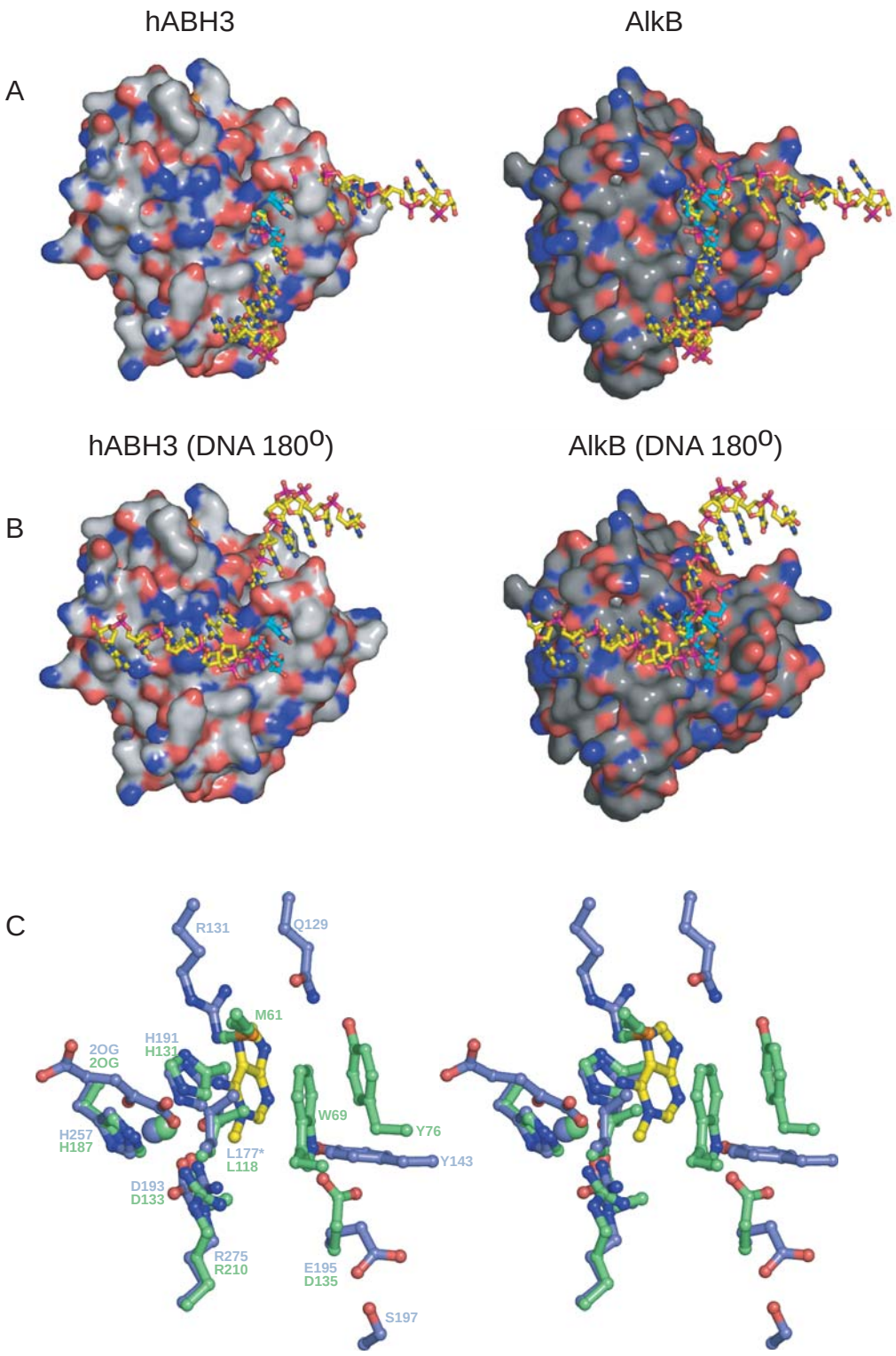
Henikoff, S. and Henikoff, J. G. (1992) Amino acid substitution matrices from protein blocks. Proc. Natl. Acad. Sci. USA 89: 10915-1091

Supplementary Figure 1



Supplementary Figure 1. Structure comparison of hABH3 and selected enzymes in the Fe(II)/2OG dependent dioxygenase family. hABH3 (coloured blue) superimposed onto AlkB (2FDJ) (A), ANS (1GP5) (B), DAOCS (1RXG) (C), and FIH (1MZF) (D). Regions that superimpose with hABH3 are coloured magenta, green, yellow and orange for AlkB, ANS, DAOCS and FIH, respectively. The other regions are coloured grey. The iron atoms are presented as spheres.

Supplementary Figure 2



Supplementary Figure 2. Docking models (A) The oligonucleotide substrate observed in the complex of AGT (Daniels et al., 2004) was manually docked onto hABH3 (left) and AlkB (right) after substitution of the flipped-out O(6)-meG by 1-meA and alignment to the 1-meA in the AlkB/T-1-meA-T complex. **(B)** As in (A), but the direction of the oligonucleotide has been rotated 180^{o}, keeping the 1-methyl group fixed. Significantly less steric interference between the model DNA and hABH3 is observed in the latter orientation. (C) Stereo pair representation similar to that of Figure 3A, illustrating that 180^{o} rotation of the DNA still allow binding of f 1-meA in the catalytic pocket.

Daniels, D.S., Woo, T.T., Luu, K.X., Noll, D.M., Clarke, N.D., Pegg, A.E. and Tainer, J.A. (2004) DNA binding and nucleotide flipping by the human DNA repair protein AGT.
Nat Struct Mol Biol, 11, 714-720.