Supplementary Materials for:

Homology modeling, molecular dynamics, and site-directed mutagenesis study of AlkB human homolog 1 (ALKBH1)

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Supplementary Table S1

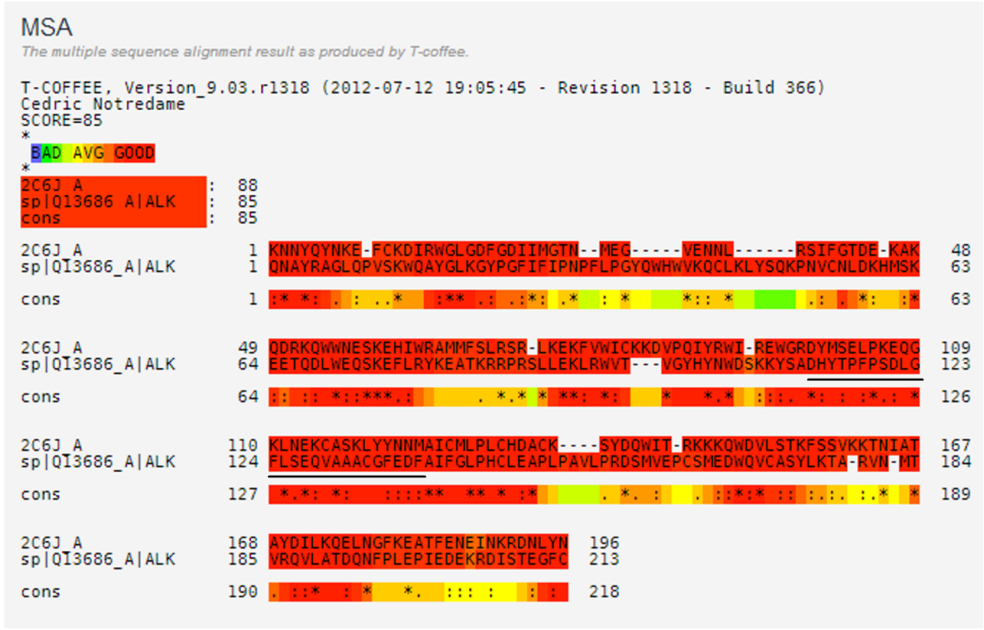
Primers and plasmids used to create ABH1 variants.

Plasmid	Variant	Primers	Based on plasmid
pABH175	H113A	for 5' CAGGTTACCAGTGGGCGTGGGTGAAACAGTGC 3' rev 5' GCACTGTTTCACCCACGCCCACTGGTAACCTG 3'	pBAR67
pABH136	C118A	for 5' GGCACTGGGTGAAACAGGCGCTTAAGTTATATTCCC 3' rev 5' GGGAATATAACTTAAGCGCCTGTTTCACCCAGTGCC 3'	pBAR67
pABH137	C129A	for 5' CCCAGAAACCTAATGTAGCGAACCTGGACAAACACATG 3' rev 5' CATGTGTTTGTCCAGGTTCGCTACATTAGGTTTCTGGG 3'	pBAR67
pABH190	H134A	for 5' GTATGTAACCTGGACAAAGCGATGTCTAAAGAAGAGACCC 3' rev 5' GGGTCTCTTCTTTAGACATCGCTTTGTCCAGGTTACATAC 3'	pBAR67
pABH191	H303A	for 5' GGAAGGCCTGCCTGCGTGCCTAGAGGCAC 3' rev 5' GTGCCTCTAGGCACGCAGGCAGGCCTTCC 3'	pBAR67
pABH139	C304A	for 5' GCCTGCCTCACGCGCTAGAGGCACCT 3' rev 5' AGGTGCCTCTAGCGCGTGAGGCAGGC 3'	pBAR67
pABH142	C371A	for 5' CATCAGTACAGAAGGTTTCGCGCATCTGGATGACCAGAATAG 3' rev 5' CTATTCTGGTCATCCAGATGCGCGAAACCTTCTGTACTGATG 3'	pBAR67
pABH192	H372A	for 5' GTACAGAAGGTTTCTGCGCGCTGGATGACCAGAATAG 3' rev 5' CTATTCTGGTCATCCAGCGCGCAGAAACCTTCTGTAC 3'	pBAR67
pABH187	H113A/C129A	for 5' CAGGTTACCAGTGGGCGTGGGTGAAACAGTGC 3' rev 5' GCACTGTTTCACCCACGCCCACTGGTAACCTG 3'	pABH137
pABH188	C118A/C129A	for 5' CCCAGAAACCTAATGTAGCGAACCTGGACAAACACATG 3' rev 5' CATGTGTTTGTCCAGGTTCGCTACATTAGGTTTCTGGG 3'	pABH136
pABH193	H113A/C118A	for 5' GGGCGTGGGTGAAACAGGCGCTTAAGTTATATTCCC 3' rev 5' GGGAATATAACTTAAGCGCCTGTTTCACCCACGCCC 3'	pABH175
pABH194	C129A/H134A	for 5' GTAGCGAACCTGGACAAAGCGATGTCTAAAGAAGAGAC 3' rev 5' GTCTCTTCTTTAGACATCGCTTTGTCCAGGTTCGCTAC 3'	pABH137
pABH195	H303A/C304A	for 5' GAAGGGGAAGGCCTGCCTGCGGCGCTAGAGGCACCTCTC 3' rev 5' GAGAGGTGCCTCTAGCGCCGCAGGCAGGCCTTCCCCTTC 3'	pABH139
pABH189	C304A/C371A	for 5' CATCAGTACAGAAGGTTTCGCGCATCTGGATGACCAGAATAG 3' rev 5' CTATTCTGGTCATCCAGATGCGCGAAACCTTCTGTACTGATG 3'	pABH139
pABH196	C371A/H372A	for 5' GTACAGAAGGTTTCGCGGCGCTGGATGACCAGAATAG 3' rev 5' CTATTCTGGTCATCCAGCGCCGCGAAACCTTCTGTAC 3'	pABH142
pABH203	H113A/C129A/H134A	for 5' CAGGTTACCAGTGGGCGTGGGTGAAACAGTGC 3' rev 5' GCACTGTTTCACCCACGCCCACTGGTAACCTG 3'	pABH194
pABH204	H113A/C118A/C129A/H134A	for 5' GGGCGTGGGTGAAACAGGCGCTTAAGTTATATTCCC 3' rev 5' GGGAATATAACTTAAGCGCCTGTTTCACCCACGCCC 3'	pABH203

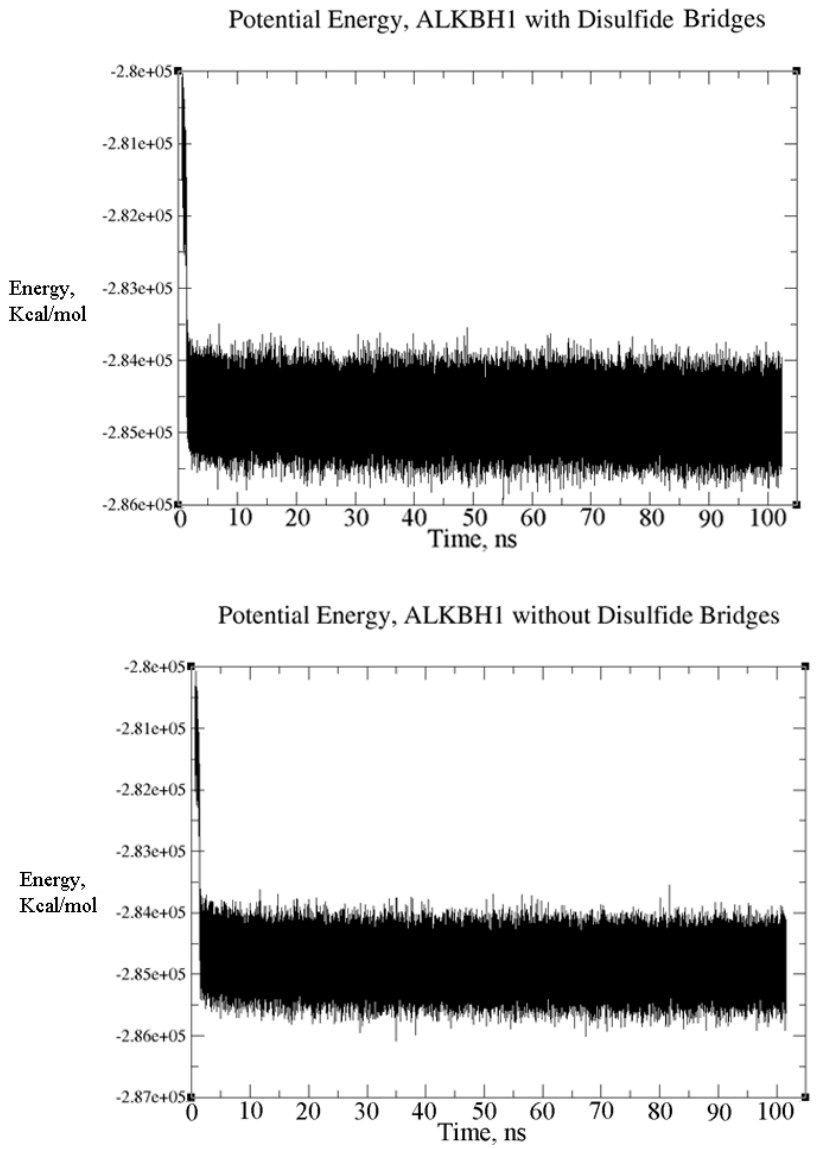
Supplementary Figure S1. Sequence alignments (a) between AlkB and the AlkB part of ALKBH1 (b) between DBL and the DBL part of ALKBH1. The residues introduced to the sequences and the overlapping regions are underlined.

a)

b)

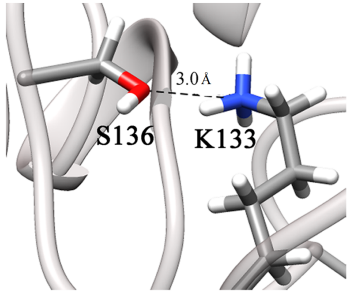


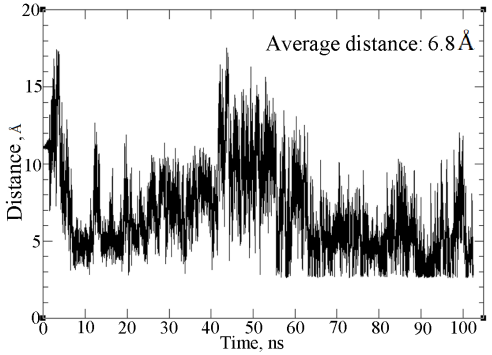
Supplementary Figure S2. Potential energy throughout the MD simulations.



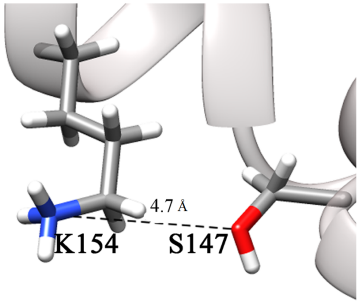
Supplementary Figure S3. Dynamics of distances between lysines and serines throughout the 100ns simulation with disulfide bridges are shown for the three pairs: (a) K133 and S136 (b) K154 and S147 (c) K182 and S181.

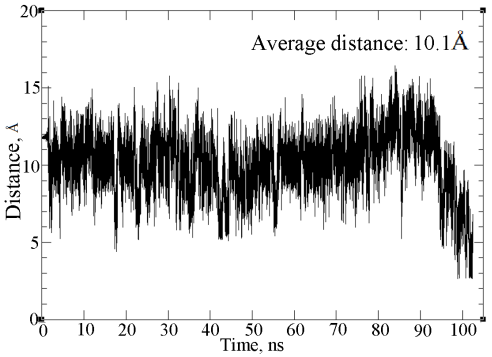
a)



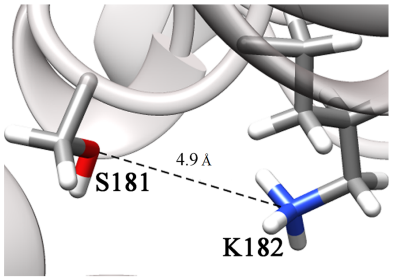


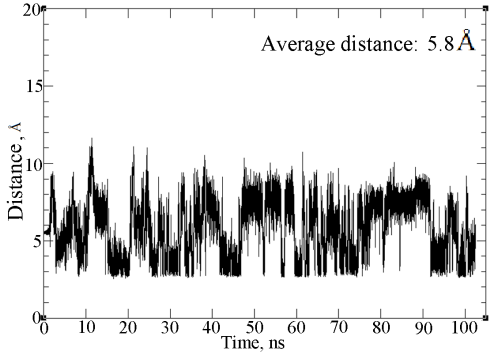
b)





c)





Supplementary Figure S4. Residues in proximity to K25. Shown are a snapshot at the 100th ns of the simulation with disulfide bridges and the dynamics of distances between the nitrogen of the amino group of K25 and the atoms in nearby residues.