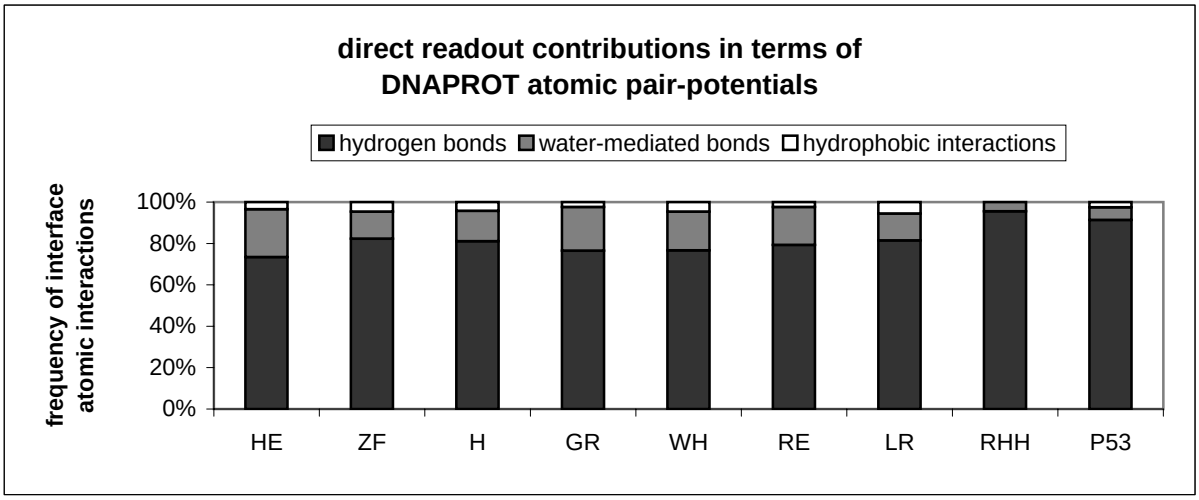
Supplementary Figure 1

summary of interface atomic scores (ONLYPOSITSCORES=1):

superfamily	H	w	V
HE	0.73356722	0.23157362	0.03485916
ZF	0.82303562	0.13018411	0.04678027
H	0.81088752	0.14630893	0.04280355
GR	0.7647404	0.21158003	0.02367956
WH	0.76642279	0.18728079	0.04629642
RE	0.79296197	0.1831407	0.02389733
LR	0.81452773	0.12967354	0.05579873
RHH	0.95531291	0.04468709	0
P53	0.9131538	0.06157813	0.02526808



Supplementary File 2

Sample output of DNAPROT program: the MunI restriction enzyme (PDB:1d02_B)

```
# parameters: dnaprot v3.01 -e 1 -W 0.01 -D 0.5 -t 1 -I 1d02_B.het.pdb -p
1d02_B.prot.pdb -d 1d02_B.dna.pdb

# strand1 (D) contains 10 bases
# strand2 (C) contains 10 bases
# duplex pair DG D0001 == DC C0010
# duplex pair DC D0002 == DG C0009
# duplex pair DC D0003 == DG C0008
# duplex pair DA D0004 == DT C0007
# duplex pair DA D0005 == DT C0006
# duplex pair DT D0006 == DA C0005
# duplex pair DT D0007 == DA C0004
# duplex pair DG D0008 == DC C0003
# duplex pair DG D0009 == DC C0002
# duplex pair DC D0010 == DG C0001
# DNA sequence complementary region:
GCCAATTGGC
||||||||||
CGGTTAACCG

# number of interface water molecules = 1
# Using Hbond matrix: HB50 ...
# Using water matrix: WM50 ...
# Using VdW matrix: VW50 ...

# generate_and_parse_DNAgeometry: running X3DNA in temporary directory ...
# Calculating protein-dna interface scores...

# Original PDB DNA sequence...
# Original interface contacts:
: w : LYS   NZ  B0045 <- 6.06 ->  DC   O2 D0010 : score 1.753
: H : ARG   NE  B0115 <- 2.77 ->  DG   O6 C0008 : score 3.212
: H : ARG  NH2  B0115 <- 2.99 ->  DG   N7 C0008 : score 4.798
: H : ASN  OD1  B0117 <- 2.80 ->  DA   N6 D0004 : score 4.58
: H : ASN  OD1  B0117 <- 2.86 ->  DA   N6 D0005 : score 4.58
: H : ASN  ND2  B0117 <- 3.19 ->  DA   N7 D0004 : score 4.58
: H : ARG  NH1  B0121 <- 3.04 ->  DA   N7 C0005 : score 0.874
: V : GLN   CG  B0102 <- 3.89 ->  DT   C7 C0006 : score 2.749

seq orig PDB 0 gcCAATtggC

: indirect readout interface 0000000000
A |  31.00 11.00 28.00 29.00 36.00 31.00 28.00 27.00 16.00 20.00
C |  19.00 37.00 28.00 24.00  0.00 34.00 19.00 14.00 29.00 25.00
G |  32.00 32.00  9.00 14.00 26.00  0.00 21.00 28.00 29.00 27.00
T |  14.00 16.00 31.00 29.00 34.00 31.00 28.00 27.00 22.00 24.00
                              ↑       ↑
                           DNA helical kink
                           reported by
                           Deibert et al. (1999)


: H hydrogen bonds interface 0111110000
A |  24.00  5.00  0.00 95.00 96.00 17.00 24.00 24.00 24.00 24.00
C |  24.00  5.00 95.00  0.00  0.00 17.00 24.00 24.00 24.00 24.00
G |  24.00  5.00  0.00  1.00  0.00 20.00 24.00 24.00 24.00 24.00
T |  24.00 81.00  1.00  0.00  0.00 42.00 24.00 24.00 24.00 24.00
```

Supplementary File 3

Fri May 15 15:03:12 2009

SCOP superfamily	PDB_chain
Homeodomain-like	1b72_A
Homeodomain-like	1b8i_A
Homeodomain-like	1b8i_B
Homeodomain-like	1bl0_A
Homeodomain-like	1fjl_C
Homeodomain-like	1gdt_A
Homeodomain-like	1h89_C
Homeodomain-like	1h8a_C
Homeodomain-like	1hlv_A
Homeodomain-like	1ig7_A
Homeodomain-like	1ign_A
Homeodomain-like	1jgg_B
Homeodomain-like	1jko_C
Homeodomain-like	1jt0_C
Homeodomain-like	1k78_A
Homeodomain-like	1le8_A
Homeodomain-like	1mnm_C
Homeodomain-like	1nk3_P
Homeodomain-like	1pdn_C
Homeodomain-like	1puf_A
Homeodomain-like	1puf_B
Homeodomain-like	1qpi_A
Homeodomain-like	1tc3_C
Homeodomain-like	1w0t_B
Homeodomain-like	1w0u_B
Homeodomain-like	1xpx_A
Homeodomain-like	1yz8_P
Homeodomain-like	1zq3_P
Homeodomain-like	2glo_A
Homeodomain-like	2h1k_B
Homeodomain-like	2hdd_A
Homeodomain-like	2kdz_A
Homeodomain-like	2qhb_A
Homeodomain-like	2r5y_A
Homeodomain-like	2yvh_C
Homeodomain-like	3cmy_A
Homeodomain-like	6pax_A
Homeodomain-like	9ant_B
Winged_helix	1awc_A
Winged_helix	1bc8_C
Winged_helix	1cf7_A
Winged_helix	1cf7_B
Winged_helix	1dp7_P
Winged_helix	1dux_C
Winged_helix	1f4k_B
Winged_helix	1f5t_A
Winged_helix	1h9t_B
Winged_helix	1if1_A
Winged_helix	1k78_F
Winged_helix	1pp7_U
Winged_helix	1pue_F
Winged_helix	1rep_C

Winged_helix	1sax_B
Winged_helix	1u8r_B
Winged_helix	1xsd_A
Winged_helix	1yo5_C
Winged_helix	1z9c_A
Winged_helix	1zrf_A
Winged_helix	2c6y_A
Winged_helix	2e1c_A
Winged_helix	2hdc_A
Winged_helix	2irf_L
Winged_helix	2isz_B
Winged_helix	2nra_C
Winged_helix	2o8k_A
Winged_helix	2p5l_G
Winged_helix	2p7c_B
Winged_helix	2pi0_C
Winged_helix	2qby_A
Winged_helix	2uzk_C
Winged_helix	2ve9_C
Winged_helix	3bpy_A
Winged_helix	3co6_C
Winged_helix	3e6c_C
Winged_helix	3ere_D
Winged_helix	3g73_B
Glucocorticoid_recep	1a6y_A
Glucocorticoid_recep	1cit_A
Glucocorticoid_recep	1dsz_A
Glucocorticoid_recep	1dsz_B
Glucocorticoid_recep	1hcq_F
Glucocorticoid_recep	1kb2_A
Glucocorticoid_recep	1lat_B
Glucocorticoid_recep	1lo1_A
Glucocorticoid_recep	1r4i_B
Glucocorticoid_recep	1r4o_A
Glucocorticoid_recep	2a66_A
Glucocorticoid_recep	2c7a_A
Glucocorticoid_recep	2ff0_A
Glucocorticoid_recep	2han_A
Glucocorticoid_recep	2han_B
Glucocorticoid_recep	2kae_A
Glucocorticoid_recep	2nll_B
Glucocorticoid_recep	3cbb_B
Glucocorticoid_recep	3dfx_B
Glucocorticoid_recep	3e00_D
Glucocorticoid_recep	3g9m_A
Glucocorticoid_recep	3gat_A
p53-like	1a3q_B
p53-like	1a66_A
p53-like	1bf5_A
p53-like	1bvo_A
p53-like	1gji_B
p53-like	1h6f_B
p53-like	1h9d_C
p53-like	1imh_C
p53-like	1mnn_A
p53-like	1nfk_B

p53-like	1p7h_N
p53-like	1xbr_A
p53-like	2ac0_D
p53-like	2v2t_A
p53-like	3brd_A
p53-like	3brg_C
p53-like	3exj_A
lambda_repressor-like	1efa_A
lambda_repressor-like	1lmb_4
lambda_repressor-like	1per_R
lambda_repressor-like	1qpz_A
lambda_repressor-like	1rzr_A
lambda_repressor-like	1zs4_C
lambda_repressor-like	2o4a_A
lambda_repressor-like	2r1j_L
lambda_repressor-like	3bdn_A
lambda_repressor-like	3clc_D
lambda_repressor-like	3cro_L
lambda_repressor-like	3dnv_B
Restriction_endonucle	1cl8_A
Restriction_endonucle	1d02_B
Restriction_endonucle	1dc1_A
Restriction_endonucle	1dfm_B
Restriction_endonucle	1dmu_A
Restriction_endonucle	1fiu_D
Restriction_endonucle	1iaw_A
Restriction_endonucle	1sa3_A
Restriction_endonucle	1sx5_B
Restriction_endonucle	1wte_A
Restriction_endonucle	2aor_A
Restriction_endonucle	2gig_B
Restriction_endonucle	2p0j_A
Restriction_endonucle	3bam_A
Restriction_endonucle	3dvo_B
Restriction_endonucle	3pvi_A
C2H2_and_C2HC_zi	1a1h_A
C2H2_and_C2HC_zi	1f2i_J
C2H2_and_C2HC_zi	1g2d_C
C2H2_and_C2HC_zi	1g2f_C
C2H2_and_C2HC_zi	1llm_C
C2H2_and_C2HC_zi	1mey_C
C2H2_and_C2HC_zi	1tf6_A
C2H2_and_C2HC_zi	1ubd_C
C2H2_and_C2HC_zi	1yuj_A
C2H2_and_C2HC_zi	2drp_A
C2H2_and_C2HC_zi	2gli_A
C2H2_and_C2HC_zi	2i13_A
C2H2_and_C2HC_zi	2prt_A
Homing_endonucleas	1lwt_A
Homing_endonucleas	1mow_D
Homing_endonucleas	1t9i_A
Homing_endonucleas	2ex5_A
Homing_endonucleas	2fld_A
Homing_endonucleas	2qoj_Z
Homing_endonucleas	2vbl_A
Homing_endonucleas	2vbl_B

Homing_endonucleas	2vs7_D
Homing_endonucleas	3c0w_A
Homing_endonucleas	3e54_B
Ribbon-helix-helix	1b01_B
Ribbon-helix-helix	1bdt_A
Ribbon-helix-helix	1mjo_C
Ribbon-helix-helix	2bnw_C
Ribbon-helix-helix	2bsq_G
Ribbon-helix-helix	2hzv_F
Ribbon-helix-helix	2rbf_A
Ribbon-helix-helix	3fmt_A

Homeodomain-like	H
Winged_helix	WH
Glucocorticoid_receptor-like	GR
p53-like	P53
lambda_repressor-like	LR
Restriction_endonuclease-like	RE
C2H2_and_C2HC_zinc_fingers	ZF
Homing_endonucleases	HE
Ribbon-helix-helix	RHH

total complexes 175

complexes skipped for containing two DNA-binding domains from different superfamilies:
1au7_B:lambda_repressor-like_DNA-binding_domains;Homeodomain-like;
1e3o_C:lambda_repressor-like_DNA-binding_domains;Homeodomain-like;
1ic8_A:lambda_repressor-like_DNA-binding_domains;Homeodomain-like;
2d5v_B:lambda_repressor-like_DNA-binding_domains;Homeodomain-like;
2h8r_A:lambda_repressor-like_DNA-binding_domains;Homeodomain-like;
1fok_A:Restriction_endonuclease-like;"Winged_helix"_DNA-binding_domain;
2o61_A:p53-like_transcription_factors;"Winged_helix"_DNA-binding_domain;