Supplementary Information

Protein-DNA coarse-grained docking with HADDOCK

Rodrigo V. Honorato[1,2] ‡, Jorge Roel-Touris[1] ‡, Alexandre M.J.J. Bonvin[1]*

[1]Bijvoet Center for Biomolecular Research, Faculty of Science – Chemistry, Utrecht University. The Netherlands.

[2]Brazilian Biosciences National Laboratory (LNBio), Brazilian Center for Research in Energy and Materials (CNPEM), Zip Code 13083-970, Campinas, São Paulo, Brazil.

‡Joint first authors as both contributed equally.

*To whom correspondence should be addressed. Email: a.m.j.j.bonvin@uu.nl

TABLE OF CONTENTS

SI-1. IMPLEMENTATION OF THE MARTINI FORCE FIELD FOR DNA IN HADDOCK

Converted force field parameters from the original work of *Uusitalo. et al* into CNS compatible format.

Table SI-1. Nucleotide particle types.

Nucleotide	Backbone	Side-chains	H-bonding
ADE	NB1-NB2-NB3	ANS1-ANS1-ANS3-ANS2	NH1-NH2
GUA	NB1-NB2-NB3	GNS1-GNS3-GNS4-GNS2	NH3-NH4
THY	NB1-NB2-NB3	TNS1-TNS4-TNS2	NH5-NH6
CYT	NB1-NB2-NB3	CNS1-CNS4-CNS3	NH7-NH8

Table SI-2. Nucleotide particle relations.

A) Adapted bond length parameters and corresponding force constants. D: Bond Length (Å). K: Force Constant (kcal.mol^{-1}).

Nucleotide	$D_{BB1-BB2}$ (K)	$D_{BB2-BB3}$ (K)	$D_{BB3-SC1}$ (K)	$D_{SC1-SC2}$ (K)	$D_{SC2-SC3}$ (K)	$D_{SC2-SC4}$ (K)	$D_{SC3-SC4}$ (K)	$D_{SC4-SC1}$ (K)
ADE	3.6 (47.87)	1.98 (191.479)	3.0 (71.805)	2.29 (500.0)	2.66 (500.0)	3.26 (47.87)	2.88 (500.0)	1.62 (500.0)
GUA	3.6 (47.87)	1.98 (191.479)	3.0 (71.805)	2.95 (500.0)	2.95 (500.0)	3.89 (47.87)	2.85 (500.0)	1.61 (500.0)
THY	3.6 (47.87)	1.98 (191.479)	2.7 (71.805)	2.17 (500.0)	3.22 (500.0)	-	-	2.65* (500.0)
CYT	3.6 (47.87)	1.98 (191.479)	2.7 (71.805)	2.2 (500.0)	2.85 (500.0)	-	-	2.68* (500.0)

*$D_{SC3-SC1}$

B) Adapted bond angle parameters and corresponding force constants. ϕ: Bond Angle (°). K: Force Constant (kcal.mol^{-1}).

Nucleotide	$\phi_{BB1-BB2-BB3}$ (K)	$\phi_{BB2-BB3-SC1}$ (K)	$\phi_{BB3-SC1-SC2}$ (K)	$\phi_{BB3-SC1-SC4}$ (K)	$\phi_{SC1-SC2-SC3}$ (K)	$\phi_{SC2-SC1-SC4}$ (K)	$\phi_{SC2-SC3-SC4}$ (K)	$\phi_{SC3-SC4-SC1}$ (K)
ADE	110 (47.87)	94 (59.84)	160 (47.87)	140 (47.87)	85 (47.87)	125 (47.87)	74 (47.87)	98 (47.87)
GUA	110 (47.87)	94 (59.84)	137 (71.8)	130 (59.84)	69 (47.87)	125 (47.87)	84 (47.87)	94 (47.87)
THY	110 (47.87)	92 (52.66)	107 (71.8)	145* (71.8)	55 (23.93)	83** (23.93)	42*** (23.93)	-
CYT	110 (47.87)	95 (50.26)	95 (71.8)	150* (71.8)	61 (47.87)	71** (47.87)	47*** (47.87)	-

*$\phi_{BB2-SC1-SC3}$, **$\phi_{SC2-SC1-SC3}$, ***$\phi_{SC2-SC3-SC1}$

C) Adapted bond dihedral parameters and corresponding force constants.
Ψ: Bond Dihedral (°). K: Force Constant (kcal.mol^{-1}).

Nucleotide	$\Psi_{BB1-BB2-BB3-SC1}$ (K)	$\Psi_{BB2-BB3-SC1-SC2}$ (K)	$\Psi_{BB2-BB3-SC1-SC4}$ (K)
ADE	-90 (0.05)	-116 (0.0)	98 (0.04)
GUA	-90 (0.05)	-117 (0.0)	92 (0.04)
THY	-75 (0.1)	-110 (0.04)	-145* (0.16)
CYT	-78 (0.05)	-90 (0.05)	-142* (0.12)

*$\Psi_{BB2-BB3-SC1-SC3}$

Table SI-3. Nucleotide particle relations for the special H-bonding beads.

For the sake of simplicity, regardless the nucleotide the special beads are displayed as NH1 and NH2.

A) Adapted bond length parameters and corresponding force constants.
D: Bond Length (Å). K: Force Constant (kcal.mol^{-1}).

Nucleotide	$D_{SC2-NH1}$ (K)	$D_{SC3-NH1}$ (K)	$D_{SC4-NH1}$ (K)	$D_{SC2-NH2}$ (K)	$D_{SC4-NH2}$ (K)	$D_{NH1-NH2}$ (K)
ADE	2.29 (500.0)	2.66 (500.0)	3.26 (47.87)	2.66 (500.0)	2.88 (500.0)	2.66 (500.0)
GUA	2.95 (500.0)	2.95 (500.0)	3.89 (47.87)	2.95 (500.0)	2.85 (500.0)	2.95 (500.0)
THY	2.17 (500.0)	3.22 (500.0)	-	2.65 (500.0)	3.22 (500.0)	3.22 (500.0)
CYT	2.2 (500.0)	2.85 (500.0)	-	2.68 (500.0)	2.85 (500.0)	2.85 (500.0)

B) Adapted bond angle parameters and corresponding force constants. ϕ: Bond Angle (°).
K: Force Constant (kcal.mol^{-1}).

Nucleotide	$\phi_{BB3-SC1-NH1}$ (K)	$\phi_{SC2-SC3-NH1}$ (K)	$\phi_{SC2-SC4-NH1}$ (K)	$\phi_{SC2-NH1-NH2}$ (K)	$\phi_{SC3-SC4-NH1}$ (K)	$\phi_{SC4-NH1-NH2}$ (K)	$\phi_{SC1-SC2-NH2}$ (K)	$\phi_{SC2-SC4-NH2}$ (K)
ADE	160 (47.87)	85 (47.87)	125 (47.87)	85 (47.87)	74 (47.87)	74 (47.87)	85 (47.87)	74 (47.87)
GUA	137 (71.80)	84 (47.87)	125 (47.87)	69 (47.87)	69 (47.87)	84 (47.87)	94 (47.87)	94 (47.87)
THY	107 (71.80)	83 (23.93)	55* (23.93)	83 (23.93)	-	42** (23.93)	83 (23.93)	55*** (23.93)
CYT	95 (71.80)	71 (47.87)	47* (47.87)	71 (47.87)	-	47** (47.87)	71 (47.87)	71*** (47.87)

*$\phi_{SC2-SC3-NH1}$, **$\phi_{SC3-NH1-NH2}$, ***$\phi_{SC2-SC3-NH2}$

C) Adapted bond dihedral parameters and corresponding force constants.
Ψ: Bond Dihedral (°). K: Force Constant (kcal.mol^{-1}).

Nucleotide	$\Psi_{BB2-BB3-SC1-NH1}$ (K)	$\Psi_{BB2-BB3-SC1-NH2}$ (K)
ADE	-116 (0.0)	-
GUA	-117 (0.0)	-
THY	-110 (0.0)	-145 (0.16)
CYT	-90 (0.05)	-142 (0.12)

SI-2. MODELING OF THE PRC1 UBIQUITYLATION MODULE BOUND TO THE NUCLEOSOME

Table SI-4. Ambiguous and unambiguous interaction restraints as defined in HADDOCK for the modeling of PRC1-nucleosome complex.

Type		Residue
Specific distance restraint		H2A: Cys85 (Atom SG) - PRC1: Lys118, Lys119 (Atom NZ). Distance range 0-2Å
Ambiguous Interaction Restraints (AIRs)	**Active**	62, 64, 97, 98
	Passive	38, 40, 52, 53, 56, 59, 64, 76, 77, 78, 80, 81, 86, 105, 115, 125, 129, 132, 134, 220, 221, 223, 224, 227, 231, 249, 252, 259, 260, 264, 267, 277, 284, 293, 294, 419, 422, 435, 436, 441, 468, 471, 472, 473, 474, 489, 491, 495, 498, 499, 509, 510, 513, 514, 516, 517, 518, 519, 628, 629, 631, 640, 644, 647, 648, 653, 654, 682, 696, 701, 702, 705, 706, 709, 712, 713, 716, 717, 719, 720, 722, 839, 852, 853, 856, 859, 864, 869, 876, 877, 880, 881, 886, 890, 915, 922, 925, 929, 932, 933, 934, 935, 1025, 1027, 1031, 1048, 1049, 1052, 1056, 1059, 1060, 1074, 1077, 1084, 1091, 1093, 1101, 1214, 1215, 1219, 1222, 1236, 1241, 1268, 1271, 1272, 1273, 1274, 1289, 1291, 1295, 1298, 1299, 1309, 1310, 1313, 1314, 1316, 1317, 1318, 1319, 1320, 1429, 1431, 1432, 1440, 1444, 1447, 1448, 1453, 1454, 1468, 1476, 1482, 1489, 1496, 1501, 1502, 1505, 1506, 1509, 1510, 1512, 1513, 1516, 1517, 1519, 1520, 1521

SI-3. DETAILED OVERVIEW OF THE SELECTED CASES FROM THE PROTEIN-DNA DOCKING BENCHMARK

Table SI-5. Atom/Bead count and computing time for the rigid-body and semi-flexible refinement stages (*it0* + *it1*) for the selected cases of the protein-DNA benchmark. CPU times are averaged values (seconds/model)[#]

Case	Atom count	Bead count	<AA time>	<CG time>
1AZP	1175	300	32	25
1PT3	1845	513	55	27
2IRF	1925	493	78	21
1QRV	2107	554	64	31
1HJC	2158	547	62	23
1VAS	2275	581	61	28
1K79	2459	631	67	30
1W0T	2476	614	93	35
1ZME	2558	654	92	29
1RPE	2558	643	89	45
1JJ4	2603	697	78	31
1R4O	2686	652	132	33
3CRO	2696	664	92	47
1QNE	2703	705	247	32
1CMA	2710	740	71	31
1BY4	2713	699	94	40
1EA4	3003	770	99	40
2FL3	3084	862	198	41
2OAA	3169	897	90	36
1TRO	3273	824	130	45
1BDT	3648	923	140	53
1B3T	3658	959	111	56
1MNN	3793	1058	157	57
1F4K	3827	995	125	56
7MHT	3957	1102	369	50
1EYU	3969	1078	311	57
1KSY	4236	1140	130	55
1A74	4439	1180	138	73
2C5R	4459	1280	304	84
1ZS4	4576	1163	198	51
1G9Z	4593	1248	316	77
1Z9C	4613	1190	168	66
1VRR	4633	1260	202	72
3BAM	4733	1354	174	64
2FIO	5038	1265	175	56
1DFM	5460	1540	182	67
1H9T	5577	1519	194	96
1KC6	5638	1616	263	98
1RVA	5761	1672	193	104
1O3T	5930	1551	201	60
1Z63	6022	1664	158	69
1FOK	6854	1900	291	110
1DDN	7611	1994	710	179
1JT0	9476	2704	262	179

The timing corresponds to the total time in seconds reported by CNS as measured on an AMD Opteron (tm) Processor 6344.