Molecular Mechanics Descriptions of Non-covalent Interactions: a Critical Evaluation

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Supporting Information

JSCH-2005 data set: Results with infinite non-bonded cut-offs (opt = geometry optimization, const = constrained optimization)

MM2*

Complex		Monomer A (kJ/mol)	MonomerB (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Guanine : Cytosine (WC)	*opt*	-132.20	-93.99	-254.95	28.76	0.8160
Methylguanine : Methylcytosine (WC)	*opt*	-68.99	-122.18	-220.87	29.71	0.8900
Adenine : Thymine (WC)	*opt*	105.64	-331.71	-255.47	29.40	2.9370
Methyladenine : Methylthymine (planar)	*opt*	105.64	-331.53	-255.76	29.87	2.4960
8-Oxoguanine : Cytosine (WC planar)	*opt*	-325.52	-93.99	-448.15	28.64	0.8840
Inosine : Cytosine (WC planar)	*opt*	-93.99	18.96	-102.75	27.72	0.8980
Guanine : Uracil (wobble)	*opt*	-132.20	-346.86	-521.45	42.39	0.3420
Cytosine : CytosineH+	*opt*	-93.99	-426.38	-557.92	37.55	1.3970
Uracil dimer (Calcutta planar)	*opt*	-346.99	-346.86	-717.17	23.31	0.2850
Uracil dimer (planar)	*opt*	-346.99	-346.99	-734.35	40.37	0.1670
6-Thioguanine : Cytosine (WC planar)	*opt*	-93.99	-89.85	-211.80	27.96	0.9000
Adenine : 4-Thiouracil (WC)	*opt*	95.54	-253.85	-164.87	6.56	3.8880
2-aminoadenine : Thymine	*opt*	69.14	-366.01	-320.70	23.83	2.2030
2-aminoadenine : Thymine (planar)	*opt*	69.02	-366.01	-311.35	14.37	0.5060
Adenine : Difluorotoluene	*opt*	95.54	-16.59	55.30	23.66	2.9630
Guanine : 4-Thiouracil	*opt*	-132.20	-253.85	-430.29	44.24	0.2840
Guanine : 2-Thiouracil	*opt*	-132.20	-216.84	-375.31	26.27	0.6730
Adenine : Cytosine (planar)	*opt*	-93.99	95.54	-11.28	12.83	0.8620
Guanine dimer (planar)	*opt*	-132.20	-132.20	-290.42	26.02	0.7040
Guanine 6-Thioguanine (planar)	*opt*	-132.20	-89.85	-236.96	14.91	0.4050
6-Thioguanine : Guanine (planar)	*opt*	-89.85	-132.20	-249.34	27.29	0.7520
Guanine : Adenine 1	*opt*	-132.20	95.54	-59.88	23.23	2.1250
Guanine : Adenine 1 (planar)	*opt*	95.54	-132.20	-48.84	12.19	0.7730
Guanine : Adenine 2	*opt*	-132.20	95.54	-62.06	25.40	2.4620
Guanine : Adenine 2 (planar)	*opt*	-132.19	95.54	-43.92	7.27	0.4870
Guanine : Adenine 3	*opt*	-132.20	95.54	-62.65	25.99	2.4220
Guanine : Adenine 4	*opt*	-132.20	95.54	-62.57	25.91	3.6680
Adenine dimer 1 (planar)	*opt*	95.54	95.54	186.04	5.05	0.5620
Adenine dimer 2 (planar)	*opt*	95.54	95.54	169.30	21.78	2.9620
Adenine dimer 3 (planar)	*opt*	95.54	95.54	170.09	21.00	2.5830
8-Oxoguanine : Guanine	*opt*	-132.20	-325.52	-501.66	43.94	0.4380
2-Thiouracil dimer (planar)	*opt*	-216.87	-216.87	-459.80	26.06	0.4550
Adenine : Thymine (WC)	*const*	105.96	-331.71	-212.21	-13.53	0.1580
Guanine : Cytosine (WC)	*const*	-68.95	-122.17	-190.04	-1.09	0.2080
Adenine : thymine (WC)	*const*	105.76	-331.71	-208.60	-17.35	0.1750
Guanine : adenine (HB)	*const*	-132.20	95.56	-26.37	-10.27	0.1690
Cytosine : Guanine (WC)	*const*	-93.71	-132.20	-229.04	3.13	0.1310
Guanine : Cytosine (WC)	*const*	-132.20	-93.72	-228.42	2.50	0.1180
Cytosine : guanine (interstrand)	*const*	-132.20	-93.99	-229.70	3.51	0.1050
Adenine : thymine (interstrand)	*const*	-366.01	95.54	-271.82	1.35	0.1040
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-185.34	-2.64	0.1050
Guanine dimer (interstrand)	*const*	-132.20	-132.20	-264.33	-0.07	0.1080
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-189.17	1.19	0.1020
Guanine dimer (interstrand)	*const*	-132.20	-132.20	-272.71	8.31	0.1100
Adenine : cytosine (interstrand)	*const*	95.54	-93.99	-0.75	2.31	0.1010
Thymine : guanine (interstrand)	*const*	-366.01	-132.20	-495.83	-2.38	0.1050
Thymine : guanine (interstrand)	*const*	-132.20	-366.01	-498.84	0.63	0.1050
Thymine : cytosine (interstrand)	*const*	95.54	-93.99	-0.96	2.51	0.1010
Adenine : guanine (interstrand)	*const*	95.54	-132.20	-46.52	9.86	0.1030
Thymine : cytosine (interstrand)	*const*	-366.01	-93.99	-461.08	1.08	0.1030
Cytosine : Adenine (interstrand)	*const*	-366.01	-93.99	-458.30	-1.70	0.1030
Adenine : guanine (interstrand)	*const*	95.54	-132.20	-36.84	0.18	0.1040
Thymine dimer (interstrand)	*const*	-366.01	-366.01	-729.46	-2.56	0.1170
Adenine dimer (interstrand)	*const*	95.54	95.54	189.24	1.85	0.0990
Adenine dimer (interstrand)	*const*	95.54	95.54	188.69	2.40	0.1100
Thymine dimer (interstrand)	*const*	-366.01	-366.01	-730.36	-1.65	0.1100
Adenine : thymine (interstrand)	*const*	95.54	-366.01	-273.31	2.84	0.0910
Thymine : adenine (interstrand)	*const*	95.54	-366.01	-269.97	-0.50	0.0930
Adenine dimer (interstrand)	*const*	105.73	105.73	208.00	3.46	0.1790
Thymine dimer (interstrand)	*const*	-331.71	-331.71	-659.70	-3.72	0.1610
Guanine dimer (interstrand)	*const*	-122.17	-122.17	-259.73	15.38	0.2410
Cytosine dimer (interstrand)	*const*	-68.99	-68.99	-139.73	1.76	0.1190
Adenine : Guanine (interstrand)	*const*	105.73	-122.17	-17.92	1.48	0.2290
Thymine : Cytosine (interstrand)	*const*	-68.99	-331.71	-397.52	-3.18	0.3210
Cytosine : Adenine (interstrand)	*const*	-93.99	95.54	0.04	1.51	0.1330
Guanine dimer (interstrand)	*const*	-132.20	-132.20	-268.39	3.99	0.1180
Guanine dimer (interstrand)	*const*	-132.20	-132.20	-267.50	3.10	0.1220
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-184.07	-3.91	0.1080
Guanine : Cytosine (stacked)	*opt*	-132.20	-93.99	-251.78	25.59	0.8360
Methylguanine : Methylcytosine (stacked)	*opt*	-122.18	-68.99	-219.72	28.56	1.0990
Adenine : Thymine (stacked)	*opt*	95.54	-366.16	-294.56	23.94	0.6750
Methyladenine : Methylthymine (stacked)	*opt*	105.73	-331.71	-255.39	29.41	0.4880
Cytosine dimer 1 (stacked)	*const*	-93.99	-93.99	-193.91	5.94	0.0930
Cytosine dimer 2 (stacked)	*const*	-93.99	-93.99	-204.89	16.91	0.1020
Cytosine dimer 3 (stacked)	*const*	-93.99	-93.99	-203.55	15.58	0.1010
Cytosine dimer 4 (stacked)	*const*	-93.99	-93.99	-205.78	17.81	0.1050
Cytosine dimer 5 (stacked)	*const*	-93.99	-93.99	-196.38	8.40	0.0950

Cytosine dimer 6 (stacked)	*const*	-93.99	-93.99	-195.57	7.60	0.0930
Cytosine dimer 7 (stacked)	*const*	-93.99	-93.99	-201.60	13.62	0.0970
Cytosine dimer 8 (stacked)	*const*	-93.99	-93.99	-201.09	13.11	0.1190
Cytosine dimer 9 (stacked)	*const*	-93.99	-93.99	-207.24	19.27	0.1000
Cytosine dimer 10 (stacked)	*const*	-93.99	-93.99	-207.35	19.38	0.1050
Cytosine dimer 11 (stacked)	*const*	-93.99	-93.99	-204.83	16.86	0.1030
Cytosine dimer 12 (stacked)	*const*	-93.99	-93.99	-201.33	13.36	0.0980
Cytosine dimer 13 (stacked)	*const*	-93.99	-93.99	-207.57	19.59	0.1010
Cytosine dimer 14 (stacked)	*const*	-93.99	-93.99	-203.72	15.74	0.1030
Adenine dimer (stacked)	*const*	95.35	95.35	172.86	17.84	0.1050
guanine dimer (stacked)	*const*	-132.20	-132.20	-287.24	22.84	0.1100
Adenine : cytosine (stacked)	*const*	95.35	-93.99	-18.46	19.82	0.1020
Guanine : Adenine (stacked)	*const*	-132.20	95.35	-58.22	21.37	0.1060
Cytosine dimer (stacked)	*const*	-93.99	-93.99	-206.66	18.68	0.0990
Adenine : Uracil (stacked)	*const*	95.35	-346.86	-270.99	19.48	0.0930
Guanine : Cytosine (stacked)	*const*	-132.20	-93.99	-243.77	17.58	0.1090
Cytosine : Uracil (stacked)	*const*	-93.99	-346.86	-457.76	16.91	0.1120
Uracil dimer (Stacked)	*const*	-346.86	-346.86	-710.86	17.13	0.1130
Guanine : Uracil (stacked)	*const*	-132.20	-346.86	-496.96	17.89	0.0980
Guanine dimer (stacked)	*const*	-93.99	-93.99	-202.69	14.71	0.1050
Cytosine dimer (stacked)	*const*	-93.99	-132.20	-229.41	3.22	0.1080
Adenine dimer (stacked)	*const*	95.54	95.54	179.09	12.00	0.0990
Thymine dimer (stacked)	*const*	95.54	-366.01	-272.95	2.49	0.1080
Guanine : cytosine (stacked)	*const*	-93.99	-132.20	-243.55	17.36	0.1060
Guanine : cytosine (stacked)	*const*	-93.99	-132.20	-237.94	11.75	0.1070
Adenine : guanine (stacked)	*const*	95.54	-132.20	-55.14	18.48	0.1060
Thymine : cytosine (stacked)	*const*	-366.01	-93.99	-478.53	18.53	0.0970
Adenine : guanine (stacked)	*const*	95.54	-132.20	-46.94	10.28	0.1040
Thymine : cytosine (stacked)	*const*	-366.01	-93.99	-474.73	14.73	0.2010
Thymine : guanine (stacked)	*const*	-366.01	-132.20	-512.13	13.92	0.1090
Adenine : cytosine (stacked)	*const*	95.54	-93.99	-9.83	11.39	0.1050
Thymine : guanine (stacked)	*const*	-366.01	-132.20	-511.63	13.42	0.2050
Adenine : cytosine (stacked)	*const*	95.54	-93.99	-13.34	14.90	0.0990
Adenine : thymine (stacked)	*const*	95.54	-366.01	-285.30	14.84	0.1750
Adenine : thymine (stacked)	*const*	95.54	-366.01	-289.02	18.56	0.1310
Adenine dimer (stacked)	*const*	95.54	95.54	178.43	12.66	0.0990
Thymine dimer (stacked)	*const*	-366.01	-366.01	-748.50	16.49	0.2160
Adenine : Thymine (stacked)	*const*	105.73	-331.71	-247.80	21.82	0.1910
Guanine : Cytosine (stacked)	*const*	-68.99	-122.17	-204.43	13.27	0.1910
Adenine : Cytosine (stacked)	*const*	105.73	-68.99	18.32	18.42	0.3390
Thymine : Guanine (stacked)	*const*	-331.71	-122.17	-473.57	19.69	0.2100
guanine : Cytosine (stacked)	*const*	-93.99	-132.20	-241.99	15.80	0.1150
Adenine : Guanine (stacked)	*const*	95.54	-132.20	-50.42	13.77	0.1360
Cytosine : guanine (stacked)	*const*	-132.20	-93.99	-241.59	15.40	0.1070
Guanine : Cytosine (stacked)	*const*	-132.20	-93.99	-246.02	19.83	0.1290
Phe30 : Lys46 (1RB9)	*const*	86.44	94.44	172.06	8.81	0.1170
Phe30 : Leu33 (1RB9)	*const*	86.46	84.59	152.89	18.16	0.1670
Phe30 : Tyr13 (1RB9)	*const*	86.44	81.66	154.76	13.34	0.1130
Phe30 : Phe49 (1RB9)	*const*	85.69	86.44	164.26	7.87	0.1290
Phe30 : Tyr4 (1RB9)	*const*	86.44	87.91	156.97	17.38	0.1390
Phe49 : Cys39 (1RB9)	*const*	85.73	66.51	147.76	4.47	0.1280
Phe49 : Cys6 (1RB9)	*const*	85.75	66.60	137.39	14.96	0.1330
Phe49 : Lys46 (1RB9)	*const*	89.21	89.64	170.73	8.13	0.1160
Phe49 : Val5 (1RB9)	*const*	86.20	84.01	151.03	19.18	0.1580
Phe49 : Tyr37 (1RB9)	*const*	88.37	119.14	204.17	3.33	0.1320
Phe49 : Tyr4 (1RB9)	*const*	85.67	86.92	161.32	11.27	0.1300
Phe49 : Peptide bond (1RB9)	*const*	88.43	-91.75	-9.21	5.89	0.1630
Phe49 : Peptide bond (1RB9)	*const*	85.87	-91.75	-29.42	23.54	0.1820
Glu47 : Lys6 (PDB:1IU5)	*const*	245.74	74.90	-9.86	330.49	0.1390
Glu49 : Lys6 (PDB:1BQ9)	*const*	245.09	78.61	-138.06	461.76	0.1770
Glu54 : Lys2 (PDB:1SMM)	*const*	275.00	79.68	-19.00	373.68	0.1910
Glu50 : LysK30 (PDB:1BRF)	*const*	240.57	61.22	49.82	251.97	0.1770
Glu50 : Lys52 (PDB:1BRF)	*const*	241.15	85.24	-49.98	376.37	0.1400
Glu49 : Lys6 (PDB:1BRF)	*const*	248.59	78.24	50.81	276.02	0.1700

MM2* (explicit lone pairs)

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-132.20	-93.99	-254.95	28.76	0.8160
Methylguanine : Methylcytosine (WC)	*opt*	-68.99	-122.18	-220.87	29.71	0.8900
Adenine : Thymine (WC)	*opt*	105.64	-331.71	-255.47	29.40	2.9370
Methyladenine : Methylthymine (planar)	*opt*	105.64	-331.53	-255.76	29.87	2.4960
8-Oxoguanine : Cytosine (WC planar)	*opt*	-325.52	-93.99	-448.15	28.64	0.8840
Inosine : Cytosine (WC planar)	*opt*	-93.99	18.96	-102.75	27.72	0.8980
Guanine : Uracil (wobble)	*opt*	-132.20	-346.86	-521.45	42.39	0.3420
Cytosine : CytosineH+	*opt*	-93.99	-426.38	-557.92	37.55	1.3970
Uracil dimer (Calcutta planar)	*opt*	-346.99	-346.86	-717.17	23.31	0.2850
Uracil dimer (planar)	*opt*	-346.99	-346.99	-734.35	40.37	0.1670
6-Thioguanine : Cytosine (WC planar)	*opt*	-93.99	-89.85	-211.80	27.96	0.9000
Adenine : 4-Thiouracil (WC)	*opt*	95.54	-253.85	-164.87	6.56	3.8880
2-aminoadenine : Thymine	*opt*	69.14	-366.01	-320.70	23.83	2.2030
2-aminoadenine : Thymine (planar)	*opt*	69.02	-366.01	-311.35	14.37	0.5060
Adenine : Difluorotoluene	*opt*	95.54	-16.59	55.30	23.66	2.9630
Guanine : 4-Thiouracil	*opt*	-132.20	-253.85	-430.29	44.24	0.2840
Guanine : 2-Thiouracil	*opt*	-132.20	-216.84	-375.31	26.27	0.6730
Adenine : Cytosine (planar)	*opt*	-93.99	95.54	-11.28	12.83	0.8620
Guanine dimer (planar)	*opt*	-132.20	-132.20	-290.42	26.02	0.7040
Guanine 6-Thioguanine (planar)	*opt*	-132.20	-89.85	-236.96	14.91	0.4050

6-Thioguanine : Guanine (planar)	*opt*	-89.85	-132.20	-249.34	27.29	0.7520
Guanine : Adenine 1	*opt*	-132.20	95.54	-59.88	23.23	2.1250
Guanine : Adenine 1 (planar)	*opt*	95.54	-132.20	-48.84	12.19	0.7730
Guanine : Adenine 2	*opt*	-132.20	95.54	-62.06	25.40	2.4620
Guanine : Adenine 2 (planar)	*opt*	-132.19	95.54	-43.92	7.27	0.4870
Guanine : Adenine 3	*opt*	-132.20	95.54	-62.65	25.99	2.4220
Guanine : Adenine 4	*opt*	-132.20	95.54	-62.57	25.91	3.6680
Adenine dimer 1 (planar)	*opt*	95.54	95.54	186.04	5.05	0.5620
Adenine dimer 2 (planar)	*opt*	95.54	95.54	169.30	21.78	2.9620
Adenine dimer 3 (planar)	*opt*	95.54	95.54	170.09	21.00	2.5830
8-Oxoguanine : Guanine	*opt*	-132.20	-325.52	-501.66	43.94	0.4380
2-Thiouracil dimer (planar)	*opt*	-216.87	-216.87	-459.80	26.06	0.4550
Adenine : Thymine (WC)	*const*	105.96	-331.71	-212.21	-13.53	0.1580
Guanine : Cytosine (WC)	*const*	-68.95	-122.17	-190.04	-1.09	0.2080
Adenine : thymine (WC)	*const*	105.76	-331.71	-208.60	-17.35	0.1750
Guanine : adenine (HB)	*const*	-132.20	95.56	-26.37	-10.27	0.1690
Cytosine : Guanine (WC)	*const*	-93.71	-132.20	-229.04	3.13	0.1310
Guanine : Cytosine (WC)	*const*	-132.20	-93.72	-228.42	2.50	0.1180
Cytosine : guanine (interstrand)	*const*	-132.20	-93.99	-229.70	3.51	0.1050
Adenine : thymine (interstrand)	*const*	-366.01	95.54	-271.82	1.35	0.1040
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-185.34	-2.64	0.1050
Guanine dimer (interstrand)	*const*	-132.20	-132.20	-264.33	-0.07	0.1080
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-189.17	1.19	0.1020
Guanine dimer (interstrand)	*const*	-132.20	-132.20	-272.71	8.31	0.1100
Adenine : cytosine (interstrand)	*const*	95.54	-93.99	-0.75	2.31	0.1010
Thymine : guanine (interstrand)	*const*	-366.01	-132.20	-495.83	-2.38	0.1050
Thymine : guanine (interstrand)	*const*	-132.20	-366.01	-498.84	0.63	0.1050
Thymine : cytosine (interstrand)	*const*	95.54	-93.99	-0.96	2.51	0.1010
Adenine : guanine (interstrand)	*const*	95.54	-132.20	-46.52	9.86	0.1030
Thymine : cytosine (interstrand)	*const*	-366.01	-93.99	-461.08	1.08	0.1030
Cytosine : Adenine (interstrand)	*const*	-366.01	-93.99	-458.30	-1.70	0.1030
Adenine : guanine (interstrand)	*const*	95.54	-132.20	-36.84	0.18	0.1040
Thymine dimer (interstrand)	*const*	-366.01	-366.01	-729.46	-2.56	0.1170
Adenine dimer (interstrand)	*const*	95.54	95.54	189.24	1.85	0.0990
Adenine dimer (interstrand)	*const*	95.54	95.54	188.69	2.40	0.1100
Thymine dimer (interstrand)	*const*	-366.01	-366.01	-730.36	-1.65	0.1100
Adenine : thymine (interstrand)	*const*	95.54	-366.01	-273.31	2.84	0.0910
Thymine : adenine (interstrand)	*const*	95.54	-366.01	-269.97	-0.50	0.0930
Adenine dimer (interstrand)	*const*	105.73	105.73	208.00	3.46	0.1790
Thymine dimer (interstrand)	*const*	-331.71	-331.71	-659.70	-3.72	0.1610
Guanine dimer (interstrand)	*const*	-122.17	-122.17	-259.73	15.38	0.2410
Cytosine dimer (interstrand)	*const*	-68.99	-68.99	-139.73	1.76	0.1190
Adenine : Guanine (interstrand)	*const*	105.73	-122.17	-17.92	1.48	0.2290
Thymine : Cytosine (interstrand)	*const*	-68.99	-331.71	-397.52	-3.18	0.3210
Cytosine : Adenine (interstrand)	*const*	-93.99	95.54	0.04	1.51	0.1330
Guanine dimer (interstrand)	*const*	-132.20	-132.20	-268.39	3.99	0.1180
Guanine dimer (interstrand)	*const*	-132.20	-132.20	-267.50	3.10	0.1220
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-184.07	-3.91	0.1080
Guanine : Cytosine (stacked)	*opt*	-132.20	-93.99	-251.78	25.59	0.8360
Methylguanine : Methylcytosine (stacked)	*opt*	-122.18	-68.99	-219.72	28.56	1.0990
Adenine : Thymine (stacked)	*opt*	95.54	-366.16	-294.56	23.94	0.6750
Methyladenine : Methylthymine (stacked)	*opt*	105.73	-331.71	-255.39	29.41	0.4880
Cytosine dimer 1 (stacked)	*const*	-93.99	-93.99	-193.91	5.94	0.0930
Cytosine dimer 2 (stacked)	*const*	-93.99	-93.99	-204.89	16.91	0.1020
Cytosine dimer 3 (stacked)	*const*	-93.99	-93.99	-203.55	15.58	0.1010
Cytosine dimer 4 (stacked)	*const*	-93.99	-93.99	-205.78	17.81	0.1050
Cytosine dimer 5 (stacked)	*const*	-93.99	-93.99	-196.38	8.40	0.0950
Cytosine dimer 6 (stacked)	*const*	-93.99	-93.99	-195.57	7.60	0.0930
Cytosine dimer 7 (stacked)	*const*	-93.99	-93.99	-201.60	13.62	0.0970
Cytosine dimer 8 (stacked)	*const*	-93.99	-93.99	-201.09	13.11	0.1190
Cytosine dimer 9 (stacked)	*const*	-93.99	-93.99	-207.24	19.27	0.1000
Cytosine dimer 10 (stacked)	*const*	-93.99	-93.99	-207.35	19.38	0.1050
Cytosine dimer 11 (stacked)	*const*	-93.99	-93.99	-204.83	16.86	0.1030
Cytosine dimer 12 (stacked)	*const*	-93.99	-93.99	-201.33	13.36	0.0980
Cytosine dimer 13 (stacked)	*const*	-93.99	-93.99	-207.57	19.59	0.1010
Cytosine dimer 14 (stacked)	*const*	-93.99	-93.99	-203.72	15.74	0.1030
Adenine dimer (stacked)	*const*	95.35	95.35	172.86	17.84	0.1050
guanine dimer (stacked)	*const*	-132.20	-132.20	-287.24	22.84	0.1100
Adenine : cytosine (stacked)	*const*	95.35	-93.99	-18.46	19.82	0.1020
Guanine : Adenine (stacked)	*const*	-132.20	95.35	-58.22	21.37	0.1060
Cytosine dimer (stacked)	*const*	-93.99	-93.99	-206.66	18.68	0.0990
Adenine : Uracil (stacked)	*const*	95.35	-346.86	-270.99	19.48	0.0930
Guanine : Cytosine (stacked)	*const*	-132.20	-93.99	-243.77	17.58	0.1090
Cytosine : Uracil (stacked)	*const*	-93.99	-346.86	-457.76	16.91	0.1120
Uracil dimer (Stacked)	*const*	-346.86	-346.86	-710.86	17.13	0.1130
Guanine : Uracil (stacked)	*const*	-132.20	-346.86	-496.96	17.89	0.0980
Guanine dimer (stacked)	*const*	-93.99	-93.99	-202.69	14.71	0.1050
Cytosine dimer (stacked)	*const*	-93.99	-132.20	-229.41	3.22	0.1080
Adenine dimer (stacked)	*const*	95.54	95.54	179.09	12.00	0.0990
Thymine dimer (stacked)	*const*	95.54	-366.01	-272.95	2.49	0.1080
Guanine : cytosine (stacked)	*const*	-93.99	-132.20	-243.55	17.36	0.1060
Guanine : cytosine (stacked)	*const*	-93.99	-132.20	-237.94	11.75	0.1070
Adenine : guanine (stacked)	*const*	95.54	-132.20	-55.14	18.48	0.1060
Thymine : cytosine (stacked)	*const*	-366.01	-93.99	-478.53	18.53	0.0970
Adenine : guanine (stacked)	*const*	95.54	-132.20	-46.94	10.28	0.1040
Thymine : cytosine (stacked)	*const*	-366.01	-93.99	-474.73	14.73	0.2010
Thymine : guanine (stacked)	*const*	-366.01	-132.20	-512.13	13.92	0.1090
Adenine : cytosine (stacked)	*const*	95.54	-93.99	-9.83	11.39	0.1050

Thymine : guanine (stacked)	*const*	-366.01	-132.20	-511.63	13.42	0.2050
Adenine : cytosine (stacked)	*const*	95.54	-93.99	-13.34	14.90	0.0990
Adenine : thymine (stacked)	*const*	95.54	-366.01	-285.30	14.84	0.1750
Adenine : thymine (stacked)	*const*	95.54	-366.01	-289.02	18.56	0.1310
Adenine dimer (stacked)	*const*	95.54	95.54	178.43	12.66	0.0990
Thymine dimer (stacked)	*const*	-366.01	-366.01	-748.50	16.49	0.2160
Adenine : Thymine (stacked)	*const*	105.73	-331.71	-247.80	21.82	0.1910
Guanine : Cytosine (stacked)	*const*	-68.99	-122.17	-204.43	13.27	0.1910
Adenine : Cytosine (stacked)	*const*	105.73	-68.99	18.32	18.42	0.3390
Thymine : Guanine (stacked)	*const*	-331.71	-122.17	-473.57	19.69	0.2100
guanine : Cytosine (stacked)	*const*	-93.99	-132.20	-241.99	15.80	0.1150
Adenine : Guanine (stacked)	*const*	95.54	-132.20	-50.42	13.77	0.1360
Cytosine : guanine (stacked)	*const*	-132.20	-93.99	-241.59	15.40	0.1070
Guanine : Cytosine (stacked)	*const*	-132.20	-93.99	-246.02	19.83	0.1290
Phe30 : Lys46 (1RB9)	*const*	42.78	56.85	90.96	8.67	0.1200
Phe30 : Leu33 (1RB9)	*const*	42.82	41.93	63.53	21.22	0.1710
Phe30 : Tyr13 (1RB9)	*const*	42.76	34.35	63.20	13.91	0.1080
Phe30 : Phe49 (1RB9)	*const*	38.98	42.79	74.10	7.67	0.1380
Phe30 : Tyr4 (1RB9)	*const*	42.76	40.77	66.67	16.86	0.1260
Phe49 : Cys39 (1RB9)	*const*	39.04	8.39	42.96	4.47	0.1420
Phe49 : Cys6 (1RB9)	*const*	38.95	9.75	32.75	15.95	0.1500
Phe49 : Lys46 (1RB9)	*const*	41.61	45.48	76.83	10.26	0.1080
Phe49 : Val5 (1RB9)	*const*	39.39	40.98	60.95	19.43	0.1680
Phe49 : Tyr37 (1RB9)	*const*	40.94	72.13	110.34	2.73	0.1280
Phe49 : Tyr4 (1RB9)	*const*	38.94	40.23	68.23	10.94	0.1490
Phe49 : Peptide bond (1RB9)	*const*	40.99	-91.75	-56.08	5.32	0.1610
Phe49 : Peptide bond (1RB9)	*const*	39.09	-91.75	-76.82	24.16	0.1650
Glu47 : Lys6 (PDB:1IU5)	*const*	200.91	12.38	-118.24	331.53	0.3430
Glu49 : Lys6 (PDB:1BQ9)	*const*	200.77	27.61	-227.16	455.55	0.1890
Glu54 : Lys2 (PDB:1SMM)	*const*	217.82	24.89	-113.25	355.96	0.1960
Glu50 : LysK30 (PDB:1BRF)	*const*	194.34	4.24	-50.04	248.62	0.2020
Glu50 : Lys52 (PDB:1BRF)	*const*	194.76	28.32	-146.74	369.81	0.1520
Glu49 : Lys6 (PDB:1BRF)	*const*	204.55	27.20	-45.14	276.89	0.1510

MM3*

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-849.38	-416.21	-1282.91	17.33	0.9530
Methylguanine : Methylcytosine (WC)	*opt*	-368.79	-817.36	-1204.26	18.11	1.1200
Adenine : Thymine (WC)	*opt*	-211.62	-642.41	-869.39	15.37	0.7120
Methyladenine : Methylthymine (planar)	*opt*	-210.95	-642.41	-886.67	33.31	2.4190
8-Oxoguanine : Cytosine (WC planar)	*opt*	-877.98	-416.21	-1321.30	27.11	2.7520
Inosine : Cytosine (WC planar)	*opt*	-416.21	-260.63	-696.09	19.25	0.4940
Guanine : Uracil (wobble)	*opt*	-849.48	-705.99	-1568.82	13.35	0.4710
Cytosine : CytosineH+	*opt*	Missing params				
Uracil dimer (Calcutta planar)	*opt*	-705.99	-705.99	-1424.80	12.82	0.2110
Uracil dimer (planar)	*opt*	-705.99	-705.99	-1427.34	15.36	0.1350
6-Thioguanine : Cytosine (WC planar)	*opt*	Missing params				
Adenine : 4-Thiouracil (WC)	*opt*	Missing params				
2-aminoadenine : Thymine	*opt*	-600.43	-707.54	-1324.70	16.73	0.4580
2-aminoadenine : Thymine (planar)	*opt*	-600.83	-707.54	-1325.09	16.73	0.4520
Adenine : Difluorotoluene	*opt*	-243.35	-45.26	-307.93	19.32	1.7870
Guanine : 4-Thiouracil	*opt*	Missing params				
Guanine : 2-Thiouracil	*opt*	Missing params				
Adenine : Cytosine (planar)	*opt*	-416.27	-243.05	-690.41	31.09	2.4160
Guanine dimer (planar)	*opt*	-849.48	-849.48	-1717.92	18.97	1.0310
Guanine 6-Thioguanine (planar)	*opt*	Missing params				
6-Thioguanine : Guanine (planar)	*opt*	Missing params				
Guanine : Adenine 1	*opt*	-849.48	-243.05	-1106.34	13.81	0.9120
Guanine : Adenine 1 (planar)	*opt*	-243.11	-849.51	-1106.46	13.84	0.7220
Guanine : Adenine 2	*opt*	-849.48	-243.05	-1136.25	43.71	2.4390
Guanine : Adenine 2 (planar)	*opt*	-849.47	-243.37	-1136.50	43.66	2.6930
Guanine : Adenine 3	*opt*	-849.48	-243.05	-1125.23	32.69	2.6880
Guanine : Adenine 4	*opt*	-849.48	-243.05	-1107.94	15.40	1.6340
Adenine dimer 1 (planar)	*opt*	-243.05	-243.05	-517.80	31.70	3.1410
Adenine dimer 2 (planar)	*opt*	-243.05	-243.13	-529.59	43.40	3.3880
Adenine dimer 3 (planar)	*opt*	-243.05	-242.33	-533.48	48.10	2.4630
8-Oxoguanine : Guanine	*opt*	-849.82	-877.98	-1753.44	25.64	0.5650
2-Thiouracil dimer (planar)	*opt*	Missing params				
Adenine : Thymine (WC)	*const*	-210.34	-642.41	-855.47	2.72	0.1980
Guanine : Cytosine (WC)	*const*	-368.85	-816.85	-1185.86	0.15	0.3380
Adenine : thymine (WC)	*const*	-210.67	-642.41	-853.58	0.50	0.1650
Guanine : adenine (HB)	*const*	-849.38	-243.03	-1099.36	6.95	0.3950
Cytosine : Guanine (WC)	*const*	-416.27	-849.38	-1271.38	5.73	0.2700
Guanine : Cytosine (WC)	*const*	-849.38	-416.21	-1268.47	2.88	0.3000
Cytosine : guanine (interstrand)	*const*	-849.48	-416.21	-1275.97	10.28	0.3760
Adenine : thymine (interstrand)	*const*	-707.54	-243.05	-959.16	8.57	0.2020
Cytosine dimer (interstrand)	*const*	-416.21	-416.21	-830.28	-2.14	0.2860
Guanine dimer (interstrand)	*const*	-849.48	-849.48	-1706.22	7.27	0.5590
Cytosine dimer (interstrand)	*const*	-416.21	-416.21	-835.89	3.48	0.2640
Guanine dimer (interstrand)	*const*	-849.48	-849.48	-1704.08	5.13	0.3280
Adenine : cytosine (interstrand)	*const*	-243.05	-416.21	-661.86	2.60	0.2830
Thymine : guanine (interstrand)	*const*	-707.54	-849.48	-1558.65	1.64	0.3450
Thymine : guanine (interstrand)	*const*	-849.48	-707.54	-1566.87	9.85	0.3490
Thymine : cytosine (interstrand)	*const*	-243.05	-416.21	-665.19	5.93	0.3060
Adenine : guanine (interstrand)	*const*	-243.05	-849.48	-1104.23	11.70	0.3150
Thymine : cytosine (interstrand)	*const*	-707.54	-416.21	-1129.04	5.29	0.2490
Cytosine : Adenine (interstrand)	*const*	-707.54	-416.21	-1124.82	1.07	0.2030

Adenine : guanine (interstrand)	*const*	-243.05	-849.48	-1102.43	9.90	0.4320
Thymine dimer (interstrand)	*const*	-707.54	-707.54	-1416.82	1.74	0.0860
Adenine dimer (interstrand)	*const*	-243.05	-243.05	-486.04	-0.07	0.2190
Adenine dimer (interstrand)	*const*	-243.05	-243.05	-488.58	2.47	0.2570
Thymine dimer (interstrand)	*const*	-707.54	-707.54	-1415.81	0.73	0.1090
Adenine : thymine (interstrand)	*const*	-243.05	-707.54	-956.77	6.18	0.2080
Thymine : adenine (interstrand)	*const*	-243.05	-707.54	-957.51	6.92	0.2140
Adenine dimer (interstrand)	*const*	-210.74	-210.40	-421.38	0.23	0.2590
Thymine dimer (interstrand)	*const*	-642.41	-642.41	-1286.32	1.50	0.1560
Guanine dimer (interstrand)	*const*	-816.95	-816.95	-1646.01	12.11	0.5240
Cytosine dimer (interstrand)	*const*	-368.85	-368.85	-741.72	4.01	0.2390
Adenine : Guanine (interstrand)	*const*	-210.68	-816.83	-1034.06	6.56	0.3990
Thymine : Cytosine (interstrand)	*const*	-368.85	-642.41	-1012.41	1.15	0.3520
Cytosine : Adenine (interstrand)	*const*	-416.27	-243.03	-661.45	2.16	0.2430
Guanine dimer (interstrand)	*const*	-849.38	-849.38	-1706.47	7.72	0.4070
Guanine dimer (interstrand)	*const*	-849.38	-849.38	-1706.14	7.39	0.5230
Cytosine dimer (interstrand)	*const*	-416.27	-416.21	-830.42	-2.06	0.2650
Guanine : Cytosine (stacked)	*opt*	-849.48	-416.21	-1289.86	24.18	0.8760
Methylguanine : Methylcytosine (stacked)	*opt*	-817.37	-368.79	-1213.23	27.07	0.8220
Adenine : Thymine (stacked)	*opt*	-242.69	-707.54	-982.28	32.05	0.6100
Methyladenine : Methylthymine (stacked)	*opt*	-211.19	-642.41	-887.21	33.62	1.2240
Cytosine dimer 1 (stacked)	*const*	-416.21	-416.21	-830.77	-1.65	0.1480
Cytosine dimer 2 (stacked)	*const*	-416.21	-416.21	-847.14	14.72	0.3300
Cytosine dimer 3 (stacked)	*const*	-416.21	-416.21	-851.97	19.56	0.2840
Cytosine dimer 4 (stacked)	*const*	-416.21	-416.21	-851.73	19.31	0.2580
Cytosine dimer 5 (stacked)	*const*	-416.21	-416.21	-841.53	9.11	0.2540
Cytosine dimer 6 (stacked)	*const*	-416.21	-416.21	-842.75	10.33	0.2770
Cytosine dimer 7 (stacked)	*const*	-416.21	-416.21	-846.72	14.30	0.2350
Cytosine dimer 8 (stacked)	*const*	-416.21	-416.21	-852.17	19.75	0.2960
Cytosine dimer 9 (stacked)	*const*	-416.21	-416.21	-852.68	20.26	0.2600
Cytosine dimer 10 (stacked)	*const*	-416.21	-416.21	-854.26	21.84	0.2360
Cytosine dimer 11 (stacked)	*const*	-416.21	-416.21	-849.35	16.93	0.2470
Cytosine dimer 12 (stacked)	*const*	-416.21	-416.21	-842.93	10.51	0.3140
Cytosine dimer 13 (stacked)	*const*	-416.21	-416.21	-854.71	22.29	0.2160
Cytosine dimer 14 (stacked)	*const*	-416.21	-416.21	-845.21	12.79	0.1800
Adenine dimer (stacked)	*const*	-242.36	-243.08	-529.10	43.66	0.3050
guanine dimer (stacked)	*const*	-849.48	-849.48	-1722.88	23.92	0.3960
Adenine : cytosine (stacked)	*const*	-243.08	-416.21	-691.71	32.42	0.3100
Guanine : Adenine (stacked)	*const*	-849.48	-242.36	-1129.88	38.04	0.3460
Cytosine dimer (stacked)	*const*	-416.21	-416.21	-849.96	17.54	0.2360
Adenine : Uracil (stacked)	*const*	-242.36	-705.99	-974.59	26.24	0.1980
Guanine : Cytosine (stacked)	*const*	-849.48	-416.21	-1285.08	19.40	0.4240
Cytosine : Uracil (stacked)	*const*	-416.21	-705.99	-1143.42	21.22	0.2480
Uracil dimer (Stacked)	*const*	-705.99	-705.99	-1432.30	20.31	0.0900
Guanine : Uracil (stacked)	*const*	-849.48	-705.99	-1583.07	27.60	0.3370
Guanine dimer (stacked)	*const*	-416.21	-416.21	-844.23	11.81	0.2810
Cytosine dimer (stacked)	*const*	-416.21	-849.48	-1273.40	7.71	0.4420
Adenine dimer (stacked)	*const*	-242.33	-243.05	-495.95	10.57	0.2790
Thymine dimer (stacked)	*const*	-243.05	-707.54	-956.68	6.08	0.1960
Guanine : cytosine (stacked)	*const*	-416.21	-849.48	-1280.57	14.88	0.3660
Guanine : cytosine (stacked)	*const*	-416.21	-849.48	-1284.54	18.85	0.4710
Adenine : guanine (stacked)	*const*	-242.33	-849.48	-1112.95	21.14	0.3970
Thymine : cytosine (stacked)	*const*	-707.54	-416.21	-1133.83	10.08	0.1290
Adenine : guanine (stacked)	*const*	-243.05	-849.48	-1116.54	24.01	0.4120
Thymine : cytosine (stacked)	*const*	-707.54	-416.21	-1139.73	15.98	0.2920
Thymine : guanine (stacked)	*const*	-707.54	-849.48	-1570.70	13.69	0.3750
Adenine : cytosine (stacked)	*const*	-242.33	-416.21	-671.34	12.80	0.2780
Thymine : guanine (stacked)	*const*	-707.54	-849.48	-1573.48	16.46	0.3480
Adenine : cytosine (stacked)	*const*	-242.33	-416.21	-668.65	10.11	0.4070
Adenine : thymine (stacked)	*const*	-243.05	-707.54	-967.93	17.34	0.2710
Adenine : thymine (stacked)	*const*	-242.33	-707.54	-959.96	10.09	0.2350
Adenine dimer (stacked)	*const*	-242.33	-242.33	-500.24	15.58	0.2980
Thymine dimer (stacked)	*const*	-707.54	-707.54	-1428.74	13.66	0.1870
Adenine : Thymine (stacked)	*const*	-210.29	-642.41	-866.40	13.70	0.2150
Guanine : Cytosine (stacked)	*const*	-368.85	-816.91	-1204.49	18.73	0.4630
Adenine : Cytosine (stacked)	*const*	-210.64	-368.85	-590.79	11.29	0.4550
Thymine : Guanine (stacked)	*const*	-642.41	-816.87	-1476.62	17.34	0.3430
guanine : Cytosine (stacked)	*const*	-416.27	-849.37	-1290.19	24.55	0.4460
Adenine : Guanine (stacked)	*const*	-243.03	-849.37	-1117.07	24.67	0.4460
Cytosine : guanine (stacked)	*const*	-849.37	-416.27	-1283.32	17.68	0.3660
Guanine : Cytosine (stacked)	*const*	-849.37	-416.21	-1280.99	15.41	0.4500
Phe30 : Lys46 (1RB9)	*const*	107.30	67.15	168.21	6.24	0.1160
Phe30 : Leu33 (1RB9)	*const*	107.47	57.45	153.84	11.09	0.1500
Phe30 : Tyr13 (1RB9)	*const*	107.32	79.43	176.28	10.48	0.1170
Phe30 : Phe49 (1RB9)	*const*	98.22	107.47	198.57	7.11	0.1240
Phe30 : Tyr4 (1RB9)	*const*	107.31	84.20	181.24	10.27	0.1290
Phe49 : Cys39 (1RB9)	*const*	98.46	92.11	190.64	-0.07	0.1260
Phe49 : Cys6 (1RB9)	*const*	98.29	89.89	177.55	10.64	0.1260
Phe49 : Lys46 (1RB9)	*const*	105.17	61.81	160.63	6.35	0.1140
Phe49 : Val5 (1RB9)	*const*	98.91	59.87	144.70	14.07	0.1540
Phe49 : Tyr37 (1RB9)	*const*	104.63	166.06	269.47	1.22	0.1210
Phe49 : Tyr4 (1RB9)	*const*	98.23	81.27	173.60	5.90	0.1140
Phe49 : Peptide bond (1RB9)	*const*	104.65	-39.18	63.29	2.18	0.1720
Phe49 : Peptide bond (1RB9)	*const*	98.54	-39.18	41.36	18.00	0.1880
Glu47 : Lys6 (PDB:1IU5)	*const*	74.46	2.00	-258.70	335.15	0.1450
Glu49 : Lys6 (PDB:1BQ9)	*const*	79.14	34.48	-370.17	483.79	0.1320
Glu54 : Lys2 (PDB:1SMM)	*const*	108.11	38.11	-246.39	392.61	0.2180
Glu50 : LysK30 (PDB:1BRF)	*const*	72.83	-8.43	-200.73	265.14	0.1580

Glu50 : Lys52 (PDB:1BRF)	*const*	73.83	35.34	-307.59	416.77	0.1220
Glu49 : Lys6 (PDB:1BRF)	*const*	84.86	33.98	-172.55	291.38	0.3440

AMBER*

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-361.60	-331.02	-785.84	93.23	0.0850
Methylguanine : Methylcytosine (WC)	*opt*	-325.84	-363.44	-783.64	94.37	0.1290
Adenine : Thymine (WC)	*opt*	-362.20	-627.86	-1036.84	46.78	0.4140
Methyladenine : Methylthymine (planar)	*opt*	-362.20	-627.86	-1039.89	49.83	0.1990
8-Oxoguanine : Cytosine (WC planar)	*opt*	-205.56	-331.02	-602.77	66.19	0.0710
Inosine : Cytosine (WC planar)	*opt*	-331.02	-27.76	-415.44	56.66	0.1570
Guanine : Uracil (wobble)	*opt*	-361.60	-336.61	-747.81	49.61	0.1230
Cytosine : CytosineH+	*opt*	-331.02	-70.06	-483.24	82.17	0.1160
Uracil dimer (Calcutta planar)	*opt*	-336.61	-336.61	-699.72	26.51	0.1970
Uracil dimer (planar)	*opt*	-336.61	-336.61	-713.13	39.92	0.0550
6-Thioguanine : Cytosine (WC planar)	*opt*	-331.02	-179.73	-553.79	43.04	0.1080
Adenine : 4-Thiouracil (WC)	*opt*	-363.92	-186.26	-570.51	20.33	3.8870
2-aminoadenine : Thymine	*opt*	-458.78	-631.08	-1154.11	64.25	0.2880
2-aminoadenine : Thymine (planar)	*opt*	-458.78	-630.94	-1154.01	64.29	0.0530
Adenine : Difluorotoluene	*opt*	-364.94	-11.91	-418.12	41.26	2.7550
Guanine : 4-Thiouracil	*opt*	-361.60	-186.26	-592.94	45.08	0.2120
Guanine : 2-Thiouracil	*opt*	-361.60	-186.87	-600.97	52.51	1.9760
Adenine : Cytosine (planar)	*opt*	-331.02	-363.92	-752.91	57.97	0.0710
Guanine dimer (planar)	*opt*	-361.60	-361.60	-788.86	65.66	0.1730
Guanine 6-Thioguanine (planar)	*opt*	-361.60	-179.73	-584.30	42.97	0.2040
6-Thioguanine : Guanine (planar)	*opt*	-179.73	-361.60	-579.44	38.11	0.1630
Guanine : Adenine 1	*opt*	-361.60	-363.92	-783.62	58.10	0.1600
Guanine : Adenine 1 (planar)	*opt*	-364.94	-361.60	-784.41	57.87	0.0310
Guanine : Adenine 2	*opt*	-361.60	-363.92	-773.19	47.67	0.3140
Guanine : Adenine 2 (planar)	*opt*	-361.60	-363.92	-771.85	46.33	0.1020
Guanine : Adenine 3	*opt*	-361.60	-363.92	-779.55	54.03	0.7460
Guanine : Adenine 4	*opt*	-361.60	-363.92	-776.39	50.87	0.4090
Adenine dimer 1 (planar)	*opt*	-363.92	-363.92	-778.14	50.30	0.0480
Adenine dimer 2 (planar)	*opt*	-363.92	-364.94	-776.01	47.14	0.4860
Adenine dimer 3 (planar)	*opt*	-363.92	-363.92	-774.22	46.38	1.2210
8-Oxoguanine : Guanine	*opt*	-361.60	-205.56	-616.54	49.39	0.2060
2-Thiouracil dimer (planar)	*opt*	-186.87	-186.87	-391.73	17.99	0.3550
Adenine : Thymine (WC)	*const*	-362.20	-627.86	-1035.87	45.81	0.3750
Guanine : Cytosine (WC)	*const*	-325.84	-363.44	-783.23	93.96	0.4070
Adenine : thymine (WC)	*const*	-362.20	-627.86	-1034.72	44.66	0.3480
Guanine : adenine (HB)	*const*	-361.60	-364.94	-772.00	45.45	0.0960
Cytosine : Guanine (WC)	*const*	-331.02	-361.60	-784.75	92.13	0.0730
Guanine : Cytosine (WC)	*const*	-361.60	-331.02	-785.76	93.14	0.0670
Cytosine : guanine (interstrand)	*const*	-361.60	-331.02	-710.71	18.09	0.1200
Adenine : thymine (interstrand)	*const*	-631.08	-363.92	-1006.85	11.85	0.2090
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-654.00	-8.04	0.1060
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-723.00	-0.20	0.0790
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-658.65	-3.39	0.1130
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-746.77	23.58	0.0930
Adenine : cytosine (interstrand)	*const*	-363.92	-331.02	-696.66	1.72	0.0990
Thymine : guanine (interstrand)	*const*	-631.08	-361.60	-994.29	1.61	0.1870
Thymine : guanine (interstrand)	*const*	-361.60	-631.08	-1001.39	8.71	0.1830
Thymine : cytosine (interstrand)	*const*	-363.92	-331.02	-697.70	2.76	0.1000
Adenine : guanine (interstrand)	*const*	-363.92	-361.60	-745.63	20.11	0.0830
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-966.34	4.24	0.1940
Cytosine : Adenine (interstrand)	*const*	-631.08	-331.02	-962.18	0.08	0.1910
Adenine : guanine (interstrand)	*const*	-363.92	-361.60	-744.83	19.31	0.1020
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1262.59	0.42	0.2460
Adenine dimer (interstrand)	*const*	-363.92	-363.92	-734.80	6.96	0.0920
Adenine dimer (interstrand)	*const*	-363.92	-363.92	-741.27	13.43	0.0980
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1261.99	-0.17	0.2650
Adenine : thymine (interstrand)	*const*	-363.92	-631.08	-1003.29	8.29	0.1820
Thymine : adenine (interstrand)	*const*	-363.92	-631.08	-1002.19	7.19	0.1950
Adenine dimer (interstrand)	*const*	-362.20	-362.20	-733.11	8.70	0.3370
Thymine dimer (interstrand)	*const*	-627.86	-627.86	-1255.86	0.15	0.4350
Guanine dimer (interstrand)	*const*	-363.44	-363.44	-757.59	30.72	0.4090
Cytosine dimer (interstrand)	*const*	-325.84	-325.84	-649.81	-1.86	0.4330
Adenine : Guanine (interstrand)	*const*	-362.20	-363.44	-744.92	19.28	0.3010
Thymine : Cytosine (interstrand)	*const*	-325.84	-627.86	-953.76	0.07	0.3470
Cytosine : Adenine (interstrand)	*const*	-331.02	-364.94	-715.40	19.43	0.1660
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-742.30	19.10	0.0960
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-728.59	5.40	0.1100
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-654.17	-7.87	0.0950
Guanine : Cytosine (stacked)	*opt*	-361.60	-331.02	-745.63	53.01	0.3540
Methylguanine : Methylcytosine (stacked)	*opt*	-363.44	-325.84	-744.58	55.31	0.3810
Adenine : Thymine (stacked)	*opt*	-364.94	-631.08	-1040.71	44.68	0.4270
Methyladenine : Methylthymine (stacked)	*opt*	-362.20	-627.86	-1039.32	49.26	0.5470
Cytosine dimer 1 (stacked)	*const*	-331.02	-331.02	-664.16	2.12	0.0750
Cytosine dimer 2 (stacked)	*const*	-331.02	-331.02	-682.80	20.76	0.1170
Cytosine dimer 3 (stacked)	*const*	-331.02	-331.02	-704.62	42.58	0.1200
Cytosine dimer 4 (stacked)	*const*	-331.02	-331.02	-711.97	49.93	0.0940
Cytosine dimer 5 (stacked)	*const*	-331.02	-331.02	-668.18	6.14	0.0990
Cytosine dimer 6 (stacked)	*const*	-331.02	-331.02	-666.97	4.93	0.1060
Cytosine dimer 7 (stacked)	*const*	-331.02	-331.02	-669.87	7.83	0.1160
Cytosine dimer 8 (stacked)	*const*	-331.02	-331.02	-707.49	45.45	0.1010
Cytosine dimer 9 (stacked)	*const*	-331.02	-331.02	-710.87	48.83	0.0850
Cytosine dimer 10 (stacked)	*const*	-331.02	-331.02	-708.54	46.50	0.0870

Cytosine dimer 11 (stacked)	*const*	-331.02	-331.02	-712.42	50.38	0.0970
Cytosine dimer 12 (stacked)	*const*	-331.02	-331.02	-695.39	33.35	0.1010
Cytosine dimer 13 (stacked)	*const*	-331.02	-331.02	-703.00	40.96	0.0930
Cytosine dimer 14 (stacked)	*const*	-331.02	-331.02	-709.86	47.82	0.1120
Adenine dimer (stacked)	*const*	-363.92	-363.92	-771.78	43.94	0.0990
guanine dimer (stacked)	*const*	-361.60	-361.60	-781.44	58.24	0.0960
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-738.37	43.43	0.0940
Guanine : Adenine (stacked)	*const*	-361.60	-363.92	-777.61	52.09	0.0840
Cytosine dimer (stacked)	*const*	-331.02	-331.02	-712.60	50.56	0.0870
Adenine : Uracil (stacked)	*const*	-363.92	-336.61	-743.33	42.80	0.0840
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-745.30	52.68	0.1100
Cytosine : Uracil (stacked)	*const*	-331.02	-336.61	-712.96	45.33	0.0990
Uracil dimer (Stacked)	*const*	-336.61	-336.61	-706.39	33.18	0.0720
Guanine : Uracil (stacked)	*const*	-361.60	-336.61	-750.61	52.40	0.0830
Guanine dimer (stacked)	*const*	-331.02	-331.02	-670.38	8.34	0.1040
Cytosine dimer (stacked)	*const*	-331.02	-361.60	-710.21	17.59	0.1100
Adenine dimer (stacked)	*const*	-363.92	-363.92	-764.72	36.88	0.0950
Thymine dimer (stacked)	*const*	-363.92	-631.08	-1003.67	8.67	0.1790
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-743.11	50.50	0.1180
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-729.25	36.63	0.1070
Adenine : guanine (stacked)	*const*	-363.92	-361.60	-773.46	47.94	0.1010
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-986.57	24.47	0.1900
Adenine : guanine (stacked)	*const*	-363.92	-361.60	-766.55	41.03	0.0990
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-989.42	27.32	0.2440
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1022.55	29.87	0.1670
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-725.63	30.69	0.0950
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1024.89	32.21	0.1970
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-722.43	27.49	0.1010
Adenine : thymine (stacked)	*const*	-363.92	-631.08	-1026.88	31.88	0.1730
Adenine : thymine (stacked)	*const*	-363.92	-631.08	-1024.45	29.44	0.2740
Adenine dimer (stacked)	*const*	-363.92	-363.92	-765.20	37.36	0.0960
Thymine dimer (stacked)	*const*	-631.08	-631.08	-1287.46	25.30	0.2440
Adenine : Thymine (stacked)	*const*	-362.20	-627.86	-1025.29	35.23	0.2960
Guanine : Cytosine (stacked)	*const*	-325.84	-363.44	-720.03	30.76	0.3870
Adenine : Cytosine (stacked)	*const*	-362.20	-325.84	-719.82	31.78	0.1190
Thymine : Guanine (stacked)	*const*	-627.86	-363.44	-1024.91	33.62	0.3680
guanine : Cytosine (stacked)	*const*	-331.02	-361.60	-732.63	40.02	0.1090
Adenine : Guanine (stacked)	*const*	-364.94	-361.60	-765.79	39.24	0.1110
Cytosine : guanine (stacked)	*const*	-361.60	-331.02	-743.09	50.47	0.1310
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-743.89	51.27	0.1350
Phe30 : Lys46 (1RB9)	*const*	37.39	29.65	59.48	7.56	0.1360
Phe30 : Leu33 (1RB9)	*const*	37.52	8.44	25.70	20.26	0.2360
Phe30 : Tyr13 (1RB9)	*const*	37.40	20.25	47.56	10.10	0.1350
Phe30 : Phe49 (1RB9)	*const*	13.64	37.60	40.41	10.82	0.1410
Phe30 : Tyr4 (1RB9)	*const*	37.37	25.74	45.03	18.08	0.1550
Phe49 : Cys39 (1RB9)	*const*	13.48	15.01	25.94	2.55	0.1550
Phe49 : Cys6 (1RB9)	*const*	13.41	8.04	12.28	9.17	0.1520
Phe49 : Lys46 (1RB9)	*const*	25.09	29.17	40.79	13.47	0.1350
Phe49 : Val5 (1RB9)	*const*	13.94	11.40	4.12	21.22	0.1570
Phe49 : Tyr37 (1RB9)	*const*	25.08	-13.21	7.37	4.50	0.1320
Phe49 : Tyr4 (1RB9)	*const*	13.53	18.92	26.91	5.54	0.1210
Phe49 : Peptide bond (1RB9)	*const*	25.35	-69.99	-53.33	8.70	0.3320
Phe49 : Peptide bond (1RB9)	*const*	13.72	-69.99	-82.10	25.84	0.2990
Glu47 : Lys6 (PDB:1IU5)	*const*	184.30	-86.30	-212.54	310.53	0.1180
Glu49 : Lys6 (PDB:1BQ9)	*const*	178.57	-90.00	-344.97	433.54	0.1440
Glu54 : Lys2 (PDB:1SMM)	*const*	160.80	-73.41	-244.83	332.22	0.1920
Glu50 : LysK30 (PDB:1BRF)	*const*	177.17	-87.96	-151.76	240.96	0.1720
Glu50 : Lys52 (PDB:1BRF)	*const*	178.14	-89.50	-285.79	374.43	0.1490
Glu49 : Lys6 (PDB:1BRF)	*const*	203.11	-90.08	-174.16	287.19	0.3830

AMBER* (10,12-H bonding potential)

Complex		Monomer A (kJ/mol)	MonomerB (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Guanine : Cytosine (WC)	*opt*	-361.60	-331.02	-782.05	89.44	0.0910
Methylguanine : Methylcytosine (WC)	*opt*	-325.84	-363.44	-779.61	90.34	0.1320
Adenine : Thymine (WC)	*opt*	-361.87	-627.86	-1035.57	45.85	0.3980
Methyladenine : Methylthymine (planar)	*opt*	-361.87	-627.86	-1040.01	50.29	0.1780
8-Oxoguanine : Cytosine (WC planar)	*opt*	-205.56	-331.02	-601.96	65.38	0.0690
Inosine : Cytosine (WC planar)	*opt*	-331.02	-27.76	-414.65	55.87	0.1400
Guanine : Uracil (wobble)	*opt*	-361.60	-336.61	-745.97	47.77	0.1560
Cytosine : CytosineH+	*opt*	-331.02	-70.06	-482.96	81.88	0.1450
Uracil dimer (Calcutta planar)	*opt*	-336.61	-336.61	-699.08	25.87	0.1850
Uracil dimer (planar)	*opt*	-336.61	-336.61	-712.02	38.81	0.0820
6-Thioguanine : Cytosine (WC planar)	*opt*	-331.02	-179.73	-560.57	49.82	1.0980
Adenine : 4-Thiouracil (WC)	*opt*	-363.58	-186.26	-569.84	20.00	3.8870
2-aminoadenine : Thymine	*opt*	-458.44	-631.08	-1151.76	62.24	0.2880
2-aminoadenine : Thymine (planar)	*opt*	-458.44	-630.94	-1151.68	62.30	0.0470
Adenine : Difluorotoluene	*opt*	-364.61	-11.91	-417.78	41.26	2.7550
Guanine : 4-Thiouracil	*opt*	-361.60	-186.26	-592.97	45.11	0.3010
Guanine : 2-Thiouracil	*opt*	-361.60	-186.87	-600.98	52.51	1.9850
Adenine : Cytosine (planar)	*opt*	-331.02	-363.58	-754.31	59.71	0.0790
Guanine dimer (planar)	*opt*	-361.60	-361.60	-789.21	66.01	0.1340
Guanine 6-Thioguanine (planar)	*opt*	-361.60	-179.73	-583.58	42.25	0.1810
6-Thioguanine : Guanine (planar)	*opt*	-179.73	-361.60	-579.46	38.13	0.1200
Guanine : Adenine 1	*opt*	-361.60	-363.58	-781.64	56.46	0.1590
Guanine : Adenine 1 (planar)	*opt*	-364.61	-361.60	-782.03	55.83	0.0510
Guanine : Adenine 2	*opt*	-361.60	-363.58	-774.93	49.75	0.3320
Guanine : Adenine 2 (planar)	*opt*	-361.60	-363.58	-773.64	48.45	0.0960

Guanine : Adenine 3	*opt*	-361.60	-363.58	-779.43	54.25	0.8100
Guanine : Adenine 4	*opt*	-361.60	-363.58	-778.12	52.94	0.4030
Adenine dimer 1 (planar)	*opt*	-363.58	-363.58	-779.48	52.31	0.0760
Adenine dimer 2 (planar)	*opt*	-363.58	-364.61	-778.66	50.47	0.5010
Adenine dimer 3 (planar)	*opt*	-363.58	-363.58	-776.39	49.23	1.1580
8-Oxoguanine : Guanine	*opt*	-361.60	-205.56	-615.28	48.13	0.2200
2-Thiouracil dimer (planar)	*opt*	-186.87	-186.87	-391.48	17.74	0.3720
Adenine : Thymine (WC)	*const*	-361.87	-627.86	-1035.12	45.40	0.3720
Guanine : Cytosine (WC)	*const*	-325.84	-363.44	-779.40	90.13	0.4070
Adenine : thymine (WC)	*const*	-361.87	-627.86	-1034.62	44.90	0.3500
Guanine : adenine (HB)	*const*	-361.60	-364.61	-773.33	47.13	0.0960
Cytosine : Guanine (WC)	*const*	-331.02	-361.60	-781.18	88.56	0.0790
Guanine : Cytosine (WC)	*const*	-361.60	-331.02	-781.83	89.21	0.0710
Cytosine : guanine (interstrand)	*const*	-361.60	-331.02	-710.38	17.76	0.1200
Adenine : thymine (interstrand)	*const*	-631.08	-363.58	-1006.70	12.04	0.2100
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-654.00	-8.04	0.1060
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-723.00	-0.20	0.0790
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-658.65	-3.39	0.1130
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-746.65	23.45	0.0930
Adenine : cytosine (interstrand)	*const*	-363.58	-331.02	-696.32	1.72	0.0990
Thymine : guanine (interstrand)	*const*	-631.08	-361.60	-994.26	1.58	0.1870
Thymine : guanine (interstrand)	*const*	-361.60	-631.08	-1001.39	8.71	0.1830
Thymine : cytosine (interstrand)	*const*	-363.58	-331.02	-697.27	2.67	0.1000
Adenine : guanine (interstrand)	*const*	-363.58	-361.60	-745.24	20.06	0.0830
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-966.28	4.18	0.1950
Cytosine : Adenine (interstrand)	*const*	-631.08	-331.02	-962.18	0.08	0.1910
Adenine : guanine (interstrand)	*const*	-363.58	-361.60	-744.28	19.10	0.1040
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1262.59	0.42	0.2460
Adenine dimer (interstrand)	*const*	-363.58	-363.58	-733.97	6.80	0.0920
Adenine dimer (interstrand)	*const*	-363.58	-363.58	-740.60	13.43	0.0980
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1261.99	-0.17	0.2650
Adenine : thymine (interstrand)	*const*	-363.58	-631.08	-1002.81	8.14	0.1820
Thymine : adenine (interstrand)	*const*	-363.58	-631.08	-1001.68	7.02	0.1950
Adenine dimer (interstrand)	*const*	-361.87	-361.87	-732.31	8.58	0.3360
Thymine dimer (interstrand)	*const*	-627.86	-627.86	-1255.86	0.15	0.4350
Guanine dimer (interstrand)	*const*	-363.44	-363.44	-757.51	30.64	0.4100
Cytosine dimer (interstrand)	*const*	-325.84	-325.84	-649.81	-1.86	0.4330
Adenine : Guanine (interstrand)	*const*	-361.87	-363.44	-744.28	18.98	0.3010
Thymine : Cytosine (interstrand)	*const*	-325.84	-627.86	-953.76	0.07	0.3470
Cytosine : Adenine (interstrand)	*const*	-331.02	-364.61	-715.02	19.39	0.1660
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-742.22	19.02	0.0970
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-728.50	5.30	0.1100
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-654.17	-7.87	0.0950
Guanine : Cytosine (stacked)	*opt*	-361.60	-331.02	-745.20	52.58	0.3650
Methylguanine : Methylcytosine (stacked)	*opt*	-363.44	-325.84	-744.37	55.10	0.4090
Adenine : Thymine (stacked)	*opt*	-364.61	-631.08	-1040.29	44.60	0.4280
Methyladenine : Methylthymine (stacked)	*opt*	-361.87	-627.86	-1038.90	49.18	0.5480
Cytosine dimer 1 (stacked)	*const*	-331.02	-331.02	-664.16	2.12	0.0750
Cytosine dimer 2 (stacked)	*const*	-331.02	-331.02	-682.67	20.63	0.1170
Cytosine dimer 3 (stacked)	*const*	-331.02	-331.02	-704.62	42.58	0.1200
Cytosine dimer 4 (stacked)	*const*	-331.02	-331.02	-711.88	49.84	0.0950
Cytosine dimer 5 (stacked)	*const*	-331.02	-331.02	-668.18	6.14	0.0990
Cytosine dimer 6 (stacked)	*const*	-331.02	-331.02	-666.93	4.89	0.1050
Cytosine dimer 7 (stacked)	*const*	-331.02	-331.02	-669.65	7.61	0.1150
Cytosine dimer 8 (stacked)	*const*	-331.02	-331.02	-707.49	45.45	0.1010
Cytosine dimer 9 (stacked)	*const*	-331.02	-331.02	-710.87	48.83	0.0850
Cytosine dimer 10 (stacked)	*const*	-331.02	-331.02	-708.42	46.38	0.0870
Cytosine dimer 11 (stacked)	*const*	-331.02	-331.02	-712.42	50.38	0.0970
Cytosine dimer 12 (stacked)	*const*	-331.02	-331.02	-695.39	33.35	0.1010
Cytosine dimer 13 (stacked)	*const*	-331.02	-331.02	-702.86	40.82	0.0930
Cytosine dimer 14 (stacked)	*const*	-331.02	-331.02	-709.86	47.82	0.1120
Adenine dimer (stacked)	*const*	-363.58	-363.58	-770.75	43.58	0.0990
guanine dimer (stacked)	*const*	-361.60	-361.60	-781.29	58.09	0.0950
Adenine : cytosine (stacked)	*const*	-363.58	-331.02	-738.03	43.43	0.0940
Guanine : Adenine (stacked)	*const*	-361.60	-363.58	-777.12	51.94	0.0840
Cytosine dimer (stacked)	*const*	-331.02	-331.02	-712.60	50.56	0.0870
Adenine : Uracil (stacked)	*const*	-363.58	-336.61	-742.91	42.72	0.0840
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-744.86	52.24	0.1100
Cytosine : Uracil (stacked)	*const*	-331.02	-336.61	-712.84	45.22	0.0990
Uracil dimer (Stacked)	*const*	-336.61	-336.61	-706.39	33.18	0.0720
Guanine : Uracil (stacked)	*const*	-361.60	-336.61	-750.41	52.21	0.0830
Guanine dimer (stacked)	*const*	-331.02	-331.02	-670.38	8.34	0.1040
Cytosine dimer (stacked)	*const*	-331.02	-361.60	-710.07	17.45	0.1100
Adenine dimer (stacked)	*const*	-363.58	-363.58	-763.89	36.73	0.0950
Thymine dimer (stacked)	*const*	-363.58	-631.08	-1003.14	8.48	0.1790
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-742.81	50.19	0.1180
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-729.25	36.63	0.1070
Adenine : guanine (stacked)	*const*	-363.58	-361.60	-772.84	47.66	0.1000
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-986.30	24.20	0.1890
Adenine : guanine (stacked)	*const*	-363.58	-361.60	-766.20	41.02	0.0990
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-989.42	27.32	0.2440
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1022.55	29.87	0.1670
Adenine : cytosine (stacked)	*const*	-363.58	-331.02	-725.29	30.69	0.0950
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1024.85	32.17	0.1970
Adenine : cytosine (stacked)	*const*	-363.58	-331.02	-721.89	27.29	0.1020
Adenine : thymine (stacked)	*const*	-363.58	-631.08	-1026.33	31.67	0.1730
Adenine : thymine (stacked)	*const*	-363.58	-631.08	-1023.82	29.16	0.2740
Adenine dimer (stacked)	*const*	-363.58	-363.58	-764.35	37.19	0.0950

Thymine dimer (stacked)	*const*	-631.08	-631.08	-1287.46	25.30	0.2440
Adenine : Thymine (stacked)	*const*	-361.87	-627.86	-1024.76	35.04	0.2970
Guanine : Cytosine (stacked)	*const*	-325.84	-363.44	-720.03	30.76	0.3870
Adenine : Cytosine (stacked)	*const*	-361.87	-325.84	-719.48	31.78	0.1190
Thymine : Guanine (stacked)	*const*	-627.86	-363.44	-1024.91	33.62	0.3680
guanine : Cytosine (stacked)	*const*	-331.02	-361.60	-732.58	39.96	0.1090
Adenine : Guanine (stacked)	*const*	-364.61	-361.60	-765.39	39.19	0.1100
Cytosine : guanine (stacked)	*const*	-361.60	-331.02	-743.02	50.40	0.1320
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-743.51	50.89	0.1350
Phe30 : Lys46 (1RB9)	*const*	37.39	29.72	59.57	7.54	0.1360
Phe30 : Leu33 (1RB9)	*const*	37.52	8.37	25.12	20.77	0.2370
Phe30 : Tyr13 (1RB9)	*const*	37.40	20.10	47.53	9.97	0.1370
Phe30 : Phe49 (1RB9)	*const*	13.42	37.60	40.22	10.80	0.1420
Phe30 : Tyr4 (1RB9)	*const*	37.37	25.59	44.85	18.10	0.1590
Phe49 : Cys39 (1RB9)	*const*	13.27	14.99	25.88	2.38	0.1540
Phe49 : Cys6 (1RB9)	*const*	13.20	8.05	12.29	8.95	0.1520
Phe49 : Lys46 (1RB9)	*const*	25.05	29.18	40.75	13.48	0.1350
Phe49 : Val5 (1RB9)	*const*	13.74	11.15	3.76	21.13	0.1590
Phe49 : Tyr37 (1RB9)	*const*	13.23	-13.26	-5.99	5.96	0.3590
Phe49 : Tyr4 (1RB9)	*const*	13.32	18.83	26.70	5.45	0.1190
Phe49 : Peptide bond (1RB9)	*const*	13.38	-69.99	-66.12	9.51	0.5130
Phe49 : Peptide bond (1RB9)	*const*	13.51	-69.99	-82.30	25.81	0.3010
Glu47 : Lys6 (PDB:1IU5)	*const*	184.30	-86.26	-212.41	310.45	0.1170
Glu49 : Lys6 (PDB:1BQ9)	*const*	178.57	-90.29	-344.92	433.20	0.1440
Glu54 : Lys2 (PDB:1SMM)	*const*	161.30	-73.28	-244.08	332.10	0.1910
Glu50 : LysK30 (PDB:1BRF)	*const*	176.97	-84.08	-152.10	244.99	0.1700
Glu50 : Lys52 (PDB:1BRF)	*const*	177.95	-89.81	-285.63	373.76	0.1480
Glu49 : Lys6 (PDB:1BRF)	*const*	203.11	-90.35	-174.13	286.89	0.3860

AMBER* explicit lone pairs)

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-361.60	-331.02	-785.84	93.23	0.0850
Methylguanine : Methylcytosine (WC)	*opt*	-325.84	-363.44	-783.64	94.37	0.1290
Adenine : Thymine (WC)	*opt*	-362.20	-627.86	-1036.84	46.78	0.4140
Methyladenine : Methylthymine (planar)	*opt*	-362.20	-627.86	-1039.89	49.83	0.1990
8-Oxoguanine : Cytosine (WC planar)	*opt*	-205.56	-331.02	-602.77	66.19	0.0710
Inosine : Cytosine (WC planar)	*opt*	-331.02	-27.76	-415.44	56.66	0.1570
Guanine : Uracil (wobble)	*opt*	-361.60	-336.61	-747.81	49.61	0.1230
Cytosine : CytosineH+	*opt*	-331.02	-70.06	-483.24	82.17	0.1160
Uracil dimer (Calcutta planar)	*opt*	-336.61	-336.61	-699.72	26.51	0.1970
Uracil dimer (planar)	*opt*	-336.61	-336.61	-713.13	39.92	0.0550
6-Thioguanine : Cytosine (WC planar)	*opt*	-331.02	-158.27	-539.87	50.58	0.4140
Adenine : 4-Thiouracil (WC)	*opt*	-363.92	-220.01	-614.96	31.03	4.1460
2-aminoadenine : Thymine	*opt*	-458.78	-631.08	-1154.11	64.25	0.2880
2-aminoadenine : Thymine (planar)	*opt*	-458.78	-630.94	-1154.01	64.29	0.0530
Adenine : Difluorotoluene	*opt*	-364.94	-11.91	-418.12	41.26	2.7550
Guanine : 4-Thiouracil	*opt*	-361.60	-186.26	-592.94	45.08	0.2120
Guanine : 2-Thiouracil	*opt*	-361.60	-186.87	-600.97	52.51	1.9760
Adenine : Cytosine (planar)	*opt*	-331.02	-363.92	-752.91	57.97	0.0710
Guanine dimer (planar)	*opt*	-361.60	-361.60	-788.86	65.66	0.1730
Guanine 6-Thioguanine (planar)	*opt*	-361.60	-158.27	-572.46	52.59	1.8570
6-Thioguanine : Guanine (planar)	*opt*	-158.27	-361.60	-565.22	45.35	1.7170
Guanine : Adenine 1	*opt*	-361.60	-363.92	-783.62	58.10	0.1600
Guanine : Adenine 1 (planar)	*opt*	-364.94	-361.60	-784.41	57.87	0.0310
Guanine : Adenine 2	*opt*	-361.60	-363.92	-773.19	47.67	0.3140
Guanine : Adenine 2 (planar)	*opt*	-361.60	-363.92	-771.85	46.33	0.1020
Guanine : Adenine 3	*opt*	-361.60	-363.92	-779.55	54.03	0.7460
Guanine : Adenine 4	*opt*	-361.60	-363.92	-776.39	50.87	0.4090
Adenine dimer 1 (planar)	*opt*	-363.92	-363.92	-778.14	50.30	0.0480
Adenine dimer 2 (planar)	*opt*	-363.92	-364.94	-776.01	47.14	0.4860
Adenine dimer 3 (planar)	*opt*	-363.92	-363.92	-774.22	46.38	1.2210
8-Oxoguanine : Guanine	*opt*	-361.60	-205.56	-616.54	49.39	0.2060
2-Thiouracil dimer (planar)	*opt*	-98.91	-98.91	-237.60	39.79	2.3160
Adenine : Thymine (WC)	*const*	-362.20	-627.86	-1035.87	45.81	0.3750
Guanine : Cytosine (WC)	*const*	-325.84	-363.44	-783.23	93.96	0.4070
Adenine : thymine (WC)	*const*	-362.20	-627.86	-1034.72	44.66	0.3480
Guanine : adenine (HB)	*const*	-361.60	-364.94	-772.00	45.45	0.0960
Cytosine : Guanine (WC)	*const*	-331.02	-361.60	-784.75	92.13	0.0730
Guanine : Cytosine (WC)	*const*	-361.60	-331.02	-785.76	93.14	0.0670
Cytosine : guanine (interstrand)	*const*	-361.60	-331.02	-710.71	18.09	0.1200
Adenine : thymine (interstrand)	*const*	-631.08	-363.92	-1006.85	11.85	0.2090
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-654.00	-8.04	0.1060
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-723.00	-0.20	0.0790
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-658.65	-3.39	0.1130
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-746.77	23.58	0.0930
Adenine : cytosine (interstrand)	*const*	-363.92	-331.02	-696.66	1.72	0.0990
Thymine : guanine (interstrand)	*const*	-631.08	-361.60	-994.29	1.61	0.1870
Thymine : guanine (interstrand)	*const*	-361.60	-631.08	-1001.39	8.71	0.1830
Thymine : cytosine (interstrand)	*const*	-363.92	-331.02	-697.70	2.76	0.1000
Adenine : guanine (interstrand)	*const*	-363.92	-361.60	-745.63	20.11	0.0830
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-966.34	4.24	0.1940
Cytosine : Adenine (interstrand)	*const*	-631.08	-331.02	-962.18	0.08	0.1910
Adenine : guanine (interstrand)	*const*	-363.92	-361.60	-744.83	19.31	0.1020
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1262.59	0.42	0.2460
Adenine dimer (interstrand)	*const*	-363.92	-363.92	-734.80	6.96	0.0920
Adenine dimer (interstrand)	*const*	-363.92	-363.92	-741.27	13.43	0.0980
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1261.99	-0.17	0.2650

Adenine : thymine (interstrand)	*const*	-363.92	-631.08	-1003.29	8.29	0.1820
Thymine : adenine (interstrand)	*const*	-363.92	-631.08	-1002.19	7.19	0.1950
Adenine dimer (interstrand)	*const*	-362.20	-362.20	-733.11	8.70	0.3370
Thymine dimer (interstrand)	*const*	-627.86	-627.86	-1255.86	0.15	0.4350
Guanine dimer (interstrand)	*const*	-363.44	-363.44	-757.59	30.72	0.4090
Cytosine dimer (interstrand)	*const*	-325.84	-325.84	-649.81	-1.86	0.4330
Adenine : Guanine (interstrand)	*const*	-362.20	-363.44	-744.92	19.28	0.3010
Thymine : Cytosine (interstrand)	*const*	-325.84	-627.86	-953.76	0.07	0.3470
Cytosine : Adenine (interstrand)	*const*	-331.02	-364.94	-715.40	19.43	0.1660
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-742.30	19.10	0.0960
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-728.59	5.40	0.1100
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-654.17	-7.87	0.0950
Guanine : Cytosine (stacked)	*opt*	-361.60	-331.02	-745.63	53.01	0.3540
Methylguanine : Methylcytosine (stacked)	*opt*	-363.44	-325.84	-744.58	55.31	0.3810
Adenine : Thymine (stacked)	*opt*	-364.94	-631.08	-1040.71	44.68	0.4270
Methyladenine : Methylthymine (stacked)	*opt*	-362.20	-627.86	-1039.32	49.26	0.5470
Cytosine dimer 1 (stacked)	*const*	-331.02	-331.02	-664.16	2.12	0.0750
Cytosine dimer 2 (stacked)	*const*	-331.02	-331.02	-682.80	20.76	0.1170
Cytosine dimer 3 (stacked)	*const*	-331.02	-331.02	-704.62	42.58	0.1200
Cytosine dimer 4 (stacked)	*const*	-331.02	-331.02	-711.97	49.93	0.0940
Cytosine dimer 5 (stacked)	*const*	-331.02	-331.02	-668.18	6.14	0.0990
Cytosine dimer 6 (stacked)	*const*	-331.02	-331.02	-666.97	4.93	0.1060
Cytosine dimer 7 (stacked)	*const*	-331.02	-331.02	-669.87	7.83	0.1160
Cytosine dimer 8 (stacked)	*const*	-331.02	-331.02	-707.49	45.45	0.1010
Cytosine dimer 9 (stacked)	*const*	-331.02	-331.02	-710.87	48.83	0.0850
Cytosine dimer 10 (stacked)	*const*	-331.02	-331.02	-708.54	46.50	0.0870
Cytosine dimer 11 (stacked)	*const*	-331.02	-331.02	-712.42	50.38	0.0970
Cytosine dimer 12 (stacked)	*const*	-331.02	-331.02	-695.39	33.35	0.1010
Cytosine dimer 13 (stacked)	*const*	-331.02	-331.02	-703.00	40.96	0.0930
Cytosine dimer 14 (stacked)	*const*	-331.02	-331.02	-709.86	47.82	0.1120
Adenine dimer (stacked)	*const*	-363.92	-363.92	-771.78	43.94	0.0990
guanine dimer (stacked)	*const*	-361.60	-361.60	-781.44	58.24	0.0960
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-738.37	43.43	0.0940
Guanine : Adenine (stacked)	*const*	-361.60	-363.92	-777.61	52.09	0.0840
Cytosine dimer (stacked)	*const*	-331.02	-331.02	-712.60	50.56	0.0870
Adenine : Uracil (stacked)	*const*	-363.92	-336.61	-743.33	42.80	0.0840
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-745.30	52.68	0.1100
Cytosine : Uracil (stacked)	*const*	-331.02	-336.61	-712.96	45.33	0.0990
Uracil dimer (Stacked)	*const*	-336.61	-336.61	-706.39	33.18	0.0720
Guanine : Uracil (stacked)	*const*	-361.60	-336.61	-750.61	52.40	0.0830
Guanine dimer (stacked)	*const*	-331.02	-331.02	-670.38	8.34	0.1040
Cytosine dimer (stacked)	*const*	-331.02	-361.60	-710.21	17.59	0.1100
Adenine dimer (stacked)	*const*	-363.92	-363.92	-764.72	36.88	0.0950
Thymine dimer (stacked)	*const*	-363.92	-631.08	-1003.67	8.67	0.1790
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-743.11	50.50	0.1180
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-729.25	36.63	0.1070
Adenine : guanine (stacked)	*const*	-363.92	-361.60	-773.46	47.94	0.1010
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-986.57	24.47	0.1900
Adenine : guanine (stacked)	*const*	-363.92	-361.60	-766.55	41.03	0.0990
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-989.42	27.32	0.2440
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1022.55	29.87	0.1670
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-725.63	30.69	0.0950
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1024.89	32.21	0.1970
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-722.43	27.49	0.1010
Adenine : thymine (stacked)	*const*	-363.92	-631.08	-1026.88	31.88	0.1730
Adenine : thymine (stacked)	*const*	-363.92	-631.08	-1024.45	29.44	0.2740
Adenine dimer (stacked)	*const*	-363.92	-363.92	-765.20	37.36	0.0960
Thymine dimer (stacked)	*const*	-631.08	-631.08	-1287.46	25.30	0.2440
Adenine : Thymine (stacked)	*const*	-362.20	-627.86	-1025.29	35.23	0.2960
Guanine : Cytosine (stacked)	*const*	-325.84	-363.44	-720.03	30.76	0.3870
Adenine : Cytosine (stacked)	*const*	-362.20	-325.84	-719.82	31.78	0.1190
Thymine : Guanine (stacked)	*const*	-627.86	-363.44	-1024.91	33.62	0.3680
guanine : Cytosine (stacked)	*const*	-331.02	-361.60	-732.63	40.02	0.1090
Adenine : Guanine (stacked)	*const*	-364.94	-361.60	-765.79	39.24	0.1110
Cytosine : guanine (stacked)	*const*	-361.60	-331.02	-743.09	50.47	0.1310
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-743.89	51.27	0.1350
Phe30 : Lys46 (1RB9)	*const*	37.39	29.65	59.48	7.56	0.1360
Phe30 : Leu33 (1RB9)	*const*	37.52	8.44	25.70	20.26	0.2360
Phe30 : Tyr13 (1RB9)	*const*	37.40	20.25	47.56	10.10	0.1350
Phe30 : Phe49 (1RB9)	*const*	13.64	37.60	40.41	10.82	0.1410
Phe30 : Tyr4 (1RB9)	*const*	37.37	25.74	45.03	18.08	0.1550
Phe49 : Cys39 (1RB9)	*const*	13.48	15.01	25.94	2.55	0.1550
Phe49 : Cys6 (1RB9)	*const*	13.41	8.04	12.28	9.17	0.1520
Phe49 : Lys46 (1RB9)	*const*	25.09	29.17	40.79	13.47	0.1350
Phe49 : Val5 (1RB9)	*const*	13.94	11.40	4.12	21.22	0.1570
Phe49 : Tyr37 (1RB9)	*const*	25.08	-13.21	7.37	4.50	0.1320
Phe49 : Tyr4 (1RB9)	*const*	13.53	18.92	26.91	5.54	0.1210
Phe49 : Peptide bond (1RB9)	*const*	25.35	-69.99	-53.33	8.70	0.3320
Phe49 : Peptide bond (1RB9)	*const*	13.72	-69.99	-82.10	25.84	0.2990
Glu47 : Lys6 (PDB:1IU5)	*const*	184.30	-86.30	-212.54	310.53	0.1180
Glu49 : Lys6 (PDB:1BQ9)	*const*	178.57	-90.00	-344.97	433.54	0.1440
Glu54 : Lys2 (PDB:1SMM)	*const*	160.80	-73.41	-244.83	332.22	0.1920
Glu50 : LysK30 (PDB:1BRF)	*const*	177.17	-87.96	-151.76	240.96	0.1720
Glu50 : Lys52 (PDB:1BRF)	*const*	178.14	-89.50	-285.79	374.43	0.1490
Glu49 : Lys6 (PDB:1BRF)	*const*	203.11	-90.08	-174.16	287.19	0.3830

OPLS*

Complex		**Monomer A**	**MonomerB**	**Complex**	**Interaction**	**RMS geometry**

		(kJ/mol)	(kJ/mol)	(kJ/mol)	(kJ/mol)	(Å)
Guanine : Cytosine (WC)	*opt*	-123.97	-169.82	-389.92	96.13	0.0730
Methylguanine : Methylcytosine (WC)	*opt*	-151.25	-131.51	-380.12	97.37	0.1320
Adenine : Thymine (WC)	*opt*	-92.88	-186.54	-324.41	44.99	0.3660
Methyladenine : Methylthymine (planar)	*opt*	-92.88	-186.54	-325.84	46.43	0.0750
8-Oxoguanine : Cytosine (WC planar)	*opt*	-448.58	-169.82	-692.69	74.30	0.0810
Inosine : Cytosine (WC planar)	*opt*	-169.82	-125.66	-359.37	63.89	0.0970
Guanine : Uracil (wobble)	*opt*	-123.97	-171.76	-347.71	51.98	0.1250
Cytosine : CytosineH+	*opt*	-169.82	-130.53	-388.85	88.50	0.1320
Uracil dimer (Calcutta planar)	*opt*	-171.76	-171.76	-372.42	28.89	0.2000
Uracil dimer (planar)	*opt*	-171.76	-171.76	-381.91	38.38	0.0570
6-Thioguanine : Cytosine (WC planar)	*opt*	-169.82	-254.84	-480.20	55.55	0.1090
Adenine : 4-Thiouracil (WC)	*opt*	-89.55	-323.73	-447.44	34.16	3.8870
2-aminoadenine : Thymine	*opt*	-199.28	-201.01	-455.22	54.93	0.2650
2-aminoadenine : Thymine (planar)	*opt*	-199.28	-201.01	-455.22	54.93	0.0430
Adenine : Difluorotoluene	*opt*	-89.55	-0.29	-123.19	33.35	2.8440
Guanine : 4-Thiouracil	*opt*	-123.97	-323.73	-511.54	63.85	0.0810
Guanine : 2-Thiouracil	*opt*	-123.97	-254.12	-407.27	29.18	0.3580
Adenine : Cytosine (planar)	*opt*	-169.82	-89.55	-301.41	42.03	0.0650
Guanine dimer (planar)	*opt*	-123.97	-123.97	-322.57	74.64	0.1470
Guanine 6-Thioguanine (planar)	*opt*	-123.97	-254.84	-422.66	43.85	0.1820
6-Thioguanine : Guanine (planar)	*opt*	-254.84	-123.97	-430.65	51.84	0.1710
Guanine : Adenine 1	*opt*	-123.97	-89.55	-265.48	51.96	0.5750
Guanine : Adenine 1 (planar)	*opt*	-89.55	-123.97	-258.85	45.33	0.0590
Guanine : Adenine 2	*opt*	-123.97	-89.55	-251.62	38.10	0.5620
Guanine : Adenine 2 (planar)	*opt*	-123.97	-89.55	-246.27	32.75	0.0380
Guanine : Adenine 3	*opt*	-123.97	-89.55	-260.56	47.04	0.6840
Guanine : Adenine 4	*opt*	-123.97	-89.55	-253.23	39.71	0.4230
Adenine dimer 1 (planar)	*opt*	-89.55	-89.55	-212.70	33.59	0.0760
Adenine dimer 2 (planar)	*opt*	-89.55	-89.55	-212.36	33.25	0.9340
Adenine dimer 3 (planar)	*opt*	-89.55	-89.55	-211.75	32.65	1.0920
8-Oxoguanine : Guanine	*opt*	-123.97	-448.58	-646.06	73.52	0.1920
2-Thiouracil dimer (planar)	*opt*	-254.12	-254.12	-535.92	27.67	0.2350
Adenine : Thymine (WC)	*const*	-92.88	-186.54	-323.54	44.12	0.3450
Guanine : Cytosine (WC)	*const*	-151.25	-131.51	-379.56	96.81	0.4080
Adenine : thymine (WC)	*const*	-92.88	-186.54	-323.47	44.05	0.3010
Guanine : adenine (HB)	*const*	-123.97	-89.55	-248.09	34.57	0.0890
Cytosine : Guanine (WC)	*const*	-169.82	-123.97	-388.42	94.64	0.0760
Guanine : Cytosine (WC)	*const*	-123.97	-169.82	-389.89	96.10	0.0660
Cytosine : guanine (interstrand)	*const*	-123.97	-169.82	-314.12	20.34	0.1310
Adenine : thymine (interstrand)	*const*	-201.01	-89.55	-301.76	11.19	0.1110
Cytosine dimer (interstrand)	*const*	-169.82	-169.82	-327.37	-12.27	0.1060
Guanine dimer (interstrand)	*const*	-123.97	-123.97	-248.32	0.39	0.0860
Cytosine dimer (interstrand)	*const*	-169.82	-169.82	-334.12	-5.52	0.1130
Guanine dimer (interstrand)	*const*	-123.97	-123.97	-270.80	22.87	0.0980
Adenine : cytosine (interstrand)	*const*	-89.55	-169.82	-265.08	5.71	0.0860
Thymine : guanine (interstrand)	*const*	-201.01	-123.97	-326.34	1.36	0.1000
Thymine : guanine (interstrand)	*const*	-123.97	-201.01	-334.77	9.79	0.0930
Thymine : cytosine (interstrand)	*const*	-89.55	-169.82	-262.30	2.93	0.1040
Adenine : guanine (interstrand)	*const*	-89.55	-123.97	-237.26	23.74	0.0980
Thymine : cytosine (interstrand)	*const*	-201.01	-169.82	-376.58	5.75	0.1020
Cytosine : Adenine (interstrand)	*const*	-201.01	-169.82	-370.59	-0.24	0.0850
Adenine : guanine (interstrand)	*const*	-89.55	-123.97	-230.03	16.51	0.1060
Thymine dimer (interstrand)	*const*	-201.01	-201.01	-402.51	0.48	0.1050
Adenine dimer (interstrand)	*const*	-89.55	-89.55	-185.52	6.41	0.0970
Adenine dimer (interstrand)	*const*	-89.55	-89.55	-190.79	11.68	0.0860
Thymine dimer (interstrand)	*const*	-201.01	-201.01	-401.91	-0.12	0.1080
Adenine : thymine (interstrand)	*const*	-89.55	-201.01	-301.74	11.17	0.1080
Thymine : adenine (interstrand)	*const*	-89.55	-201.01	-298.78	8.22	0.1060
Adenine dimer (interstrand)	*const*	-92.88	-92.88	-192.02	6.27	0.3430
Thymine dimer (interstrand)	*const*	-186.54	-186.54	-373.50	0.42	0.3470
Guanine dimer (interstrand)	*const*	-131.51	-131.51	-290.69	27.67	0.4040
Cytosine dimer (interstrand)	*const*	-151.25	-151.25	-296.76	-5.73	0.4310
Adenine : Guanine (interstrand)	*const*	-92.88	-131.51	-244.33	19.95	0.3030
Thymine : Cytosine (interstrand)	*const*	-151.25	-186.54	-337.96	0.18	0.3180
Cytosine : Adenine (interstrand)	*const*	-169.82	-89.55	-274.83	15.45	0.1590
Guanine dimer (interstrand)	*const*	-123.97	-123.97	-270.23	22.29	0.1080
Guanine dimer (interstrand)	*const*	-123.97	-123.97	-254.15	6.22	0.1100
Cytosine dimer (interstrand)	*const*	-169.82	-169.82	-328.15	-11.49	0.0980
Guanine : Cytosine (stacked)	*opt*	-123.97	-169.82	-389.92	96.13	2.5290
Methylguanine : Methylcytosine (stacked)	*opt*	-131.51	-151.25	-359.32	76.57	2.1450
Adenine : Thymine (stacked)	*opt*	-89.55	-201.01	-331.52	40.95	0.3220
Methyladenine : Methylthymine (stacked)	*opt*	-92.88	-186.54	-326.52	47.10	0.4320
Cytosine dimer 1 (stacked)	*const*	-169.82	-169.82	-328.66	-10.98	0.1050
Cytosine dimer 2 (stacked)	*const*	-169.82	-169.82	-350.74	11.10	0.1180
Cytosine dimer 3 (stacked)	*const*	-169.82	-169.82	-378.33	38.69	0.1170
Cytosine dimer 4 (stacked)	*const*	-169.82	-169.82	-388.42	48.78	0.1020
Cytosine dimer 5 (stacked)	*const*	-169.82	-169.82	-331.74	-7.90	0.1040
Cytosine dimer 6 (stacked)	*const*	-169.82	-169.82	-329.76	-9.88	0.1060
Cytosine dimer 7 (stacked)	*const*	-169.82	-169.82	-340.63	0.99	0.1100
Cytosine dimer 8 (stacked)	*const*	-169.82	-169.82	-384.00	44.36	0.1120
Cytosine dimer 9 (stacked)	*const*	-169.82	-169.82	-387.65	48.01	0.1020
Cytosine dimer 10 (stacked)	*const*	-169.82	-169.82	-387.08	47.44	0.1030
Cytosine dimer 11 (stacked)	*const*	-169.82	-169.82	-388.81	49.17	0.1080
Cytosine dimer 12 (stacked)	*const*	-169.82	-169.82	-369.87	30.23	0.1100
Cytosine dimer 13 (stacked)	*const*	-169.82	-169.82	-384.41	44.77	0.1000
Cytosine dimer 14 (stacked)	*const*	-169.82	-169.82	-384.59	44.95	0.1030
Adenine dimer (stacked)	*const*	-89.55	-89.55	-213.51	34.40	0.0950

guanine dimer (stacked)	*const*	-123.97	-123.97	-299.00	51.07	0.0930
Adenine : cytosine (stacked)	*const*	-89.55	-169.82	-302.09	42.72	0.1040
Guanine : Adenine (stacked)	*const*	-123.97	-89.55	-256.54	43.02	0.0920
Cytosine dimer (stacked)	*const*	-169.82	-169.82	-388.81	49.17	0.1040
Adenine : Uracil (stacked)	*const*	-89.55	-171.76	-298.65	37.34	0.0880
Guanine : Cytosine (stacked)	*const*	-123.97	-169.82	-343.77	49.98	0.1120
Cytosine : Uracil (stacked)	*const*	-169.82	-171.76	-377.69	36.11	0.1000
Uracil dimer (Stacked)	*const*	-171.76	-171.76	-371.91	28.38	0.1020
Guanine : Uracil (stacked)	*const*	-123.97	-171.76	-339.85	44.13	0.0840
Guanine dimer (stacked)	*const*	-169.82	-169.82	-337.77	-1.87	0.1060
Cytosine dimer (stacked)	*const*	-169.82	-123.97	-315.72	21.93	0.1150
Adenine dimer (stacked)	*const*	-89.55	-89.55	-202.67	23.56	0.0970
Thymine dimer (stacked)	*const*	-89.55	-201.01	-305.05	14.49	0.1100
Guanine : cytosine (stacked)	*const*	-169.82	-123.97	-332.18	38.39	0.1120
Guanine : cytosine (stacked)	*const*	-169.82	-123.97	-317.18	23.39	0.1000
Adenine : guanine (stacked)	*const*	-89.55	-123.97	-246.40	32.88	0.0940
Thymine : cytosine (stacked)	*const*	-201.01	-169.82	-387.39	16.56	0.1030
Adenine : guanine (stacked)	*const*	-89.55	-123.97	-241.91	28.39	0.0820
Thymine : cytosine (stacked)	*const*	-201.01	-169.82	-391.52	20.68	0.1530
Thymine : guanine (stacked)	*const*	-201.01	-123.97	-343.32	18.34	0.0970
Adenine : cytosine (stacked)	*const*	-89.55	-169.82	-270.06	10.69	0.0930
Thymine : guanine (stacked)	*const*	-201.01	-123.97	-348.61	23.63	0.1540
Adenine : cytosine (stacked)	*const*	-89.55	-169.82	-277.47	18.09	0.0900
Adenine : thymine (stacked)	*const*	-89.55	-201.01	-319.34	28.77	0.1320
Adenine : thymine (stacked)	*const*	-89.55	-201.01	-307.27	16.71	0.1230
Adenine dimer (stacked)	*const*	-89.55	-89.55	-202.49	23.38	0.0890
Thymine dimer (stacked)	*const*	-201.01	-201.01	-420.31	18.28	0.2020
Adenine : Thymine (stacked)	*const*	-92.88	-186.54	-315.61	36.19	0.3060
Guanine : Cytosine (stacked)	*const*	-151.25	-131.51	-312.63	29.88	0.4310
Adenine : Cytosine (stacked)	*const*	-92.88	-151.25	-268.29	24.17	0.0870
Thymine : Guanine (stacked)	*const*	-186.54	-131.51	-353.17	35.12	0.4140
guanine : Cytosine (stacked)	*const*	-169.82	-123.97	-325.81	32.02	0.1240
Adenine : Guanine (stacked)	*const*	-89.55	-123.97	-242.60	29.08	0.1190
Cytosine : guanine (stacked)	*const*	-123.97	-169.82	-330.58	36.80	0.1210
Guanine : Cytosine (stacked)	*const*	-123.97	-169.82	-334.72	40.94	0.1390
Phe30 : Lys46 (1RB9)	*const*	56.38	45.85	92.83	9.39	0.1520
Phe30 : Leu33 (1RB9)	*const*	56.84	14.61	54.02	17.43	0.1730
Phe30 : Tyr13 (1RB9)	*const*	56.39	5.94	47.24	15.08	0.1330
Phe30 : Phe49 (1RB9)	*const*	30.99	56.51	78.37	9.13	0.1720
Phe30 : Tyr4 (1RB9)	*const*	56.35	11.61	47.65	20.31	0.1430
Phe49 : Cys39 (1RB9)	*const*	31.06	29.59	56.06	4.59	0.1600
Phe49 : Cys6 (1RB9)	*const*	31.17	23.17	40.89	13.45	0.1670
Phe49 : Lys46 (1RB9)	*const*	44.87	42.69	67.67	19.89	0.1480
Phe49 : Val5 (1RB9)	*const*	31.70	32.35	41.74	22.31	0.1670
Phe49 : Tyr37 (1RB9)	*const*	44.36	14.20	53.89	4.67	0.1290
Phe49 : Tyr4 (1RB9)	*const*	31.19	-3.32	12.54	15.33	0.1600
Phe49 : Peptide bond (1RB9)	*const*	44.54	-65.28	-34.67	13.93	0.1760
Phe49 : Peptide bond (1RB9)	*const*	31.50	-65.28	-58.43	24.65	0.1650
Glu47 : Lys6 (PDB:1IU5)	*const*	42.14	-14.95	-302.60	329.79	0.1690
Glu49 : Lys6 (PDB:1BQ9)	*const*	31.51	-23.18	-456.43	464.77	0.1690
Glu54 : Lys2 (PDB:1SMM)	*const*	7.32	21.56	-361.15	390.02	0.1870
Glu50 : LysK30 (PDB:1BRF)	*const*	5.39	-32.90	-278.07	250.55	0.1940
Glu50 : Lys52 (PDB:1BRF)	*const*	6.31	-19.21	-422.01	409.11	0.1690
Glu49 : Lys6 (PDB:1BRF)	*const*	52.91	-23.32	-246.91	276.50	0.3820

OPLSAA

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-110.63	-146.31	-352.35	95.41	0.0750
Methylguanine : Methylcytosine (WC)	*opt*	-147.04	-106.42	-351.05	97.58	0.1360
Adenine : Thymine (WC)	*opt*	-68.95	-172.98	-285.65	43.72	0.3730
Methyladenine : Methylthymine (planar)	*opt*	-68.95	-172.98	-287.07	45.14	0.1120
8-Oxoguanine : Cytosine (WC planar)	*opt*	-193.05	-146.31	-422.23	82.87	0.2550
Inosine : Cytosine (WC planar)	*opt*	-146.31	43.47	-177.00	74.17	0.1080
Guanine : Uracil (wobble)	*opt*	-110.63	-146.10	-308.38	51.65	0.1360
Cytosine : CytosineH+	*opt*	-146.31	122.33	-157.50	133.52	0.2130
Uracil dimer (Calcutta planar)	*opt*	-146.10	-146.10	-321.38	29.18	0.2340
Uracil dimer (planar)	*opt*	-146.10	-146.10	-331.16	38.96	0.0630
6-Thioguanine : Cytosine (WC planar)	*opt*	-146.31	-54.40	-272.84	72.13	0.3360
Adenine : 4-Thiouracil (WC)	*opt*	-75.96	-78.17	-195.35	41.22	3.8870
2-aminoadenine : Thymine	*opt*	-172.53	-168.26	-392.64	51.85	0.2660
2-aminoadenine : Thymine (planar)	*opt*	-172.53	-168.26	-392.64	51.85	0.0360
Adenine : Difluorotoluene	*opt*	-75.96	-2.27	-98.85	20.63	1.8910
Guanine : 4-Thiouracil	*opt*	-110.63	-78.17	-251.91	63.11	0.0900
Guanine : 2-Thiouracil	*opt*	-110.63	-56.33	-212.51	45.54	0.3120
Adenine : Cytosine (planar)	*opt*	-146.31	-75.96	-264.40	42.12	0.0710
Guanine dimer (planar)	*opt*	-110.63	-110.63	-294.83	73.58	0.1590
Guanine 6-Thioguanine (planar)	*opt*	-110.63	-54.40	-222.28	57.25	0.8350
6-Thioguanine : Guanine (planar)	*opt*	-54.40	-110.63	-229.51	64.48	1.2710
Guanine : Adenine 1	*opt*	-110.63	-75.96	-238.08	51.49	0.4920
Guanine : Adenine 1 (planar)	*opt*	-75.96	-110.63	-231.95	45.36	0.0690
Guanine : Adenine 2	*opt*	-110.63	-75.96	-224.38	37.79	0.5380
Guanine : Adenine 2 (planar)	*opt*	-110.63	-75.96	-218.73	32.14	0.0430
Guanine : Adenine 3	*opt*	-110.63	-75.96	-232.81	46.22	0.6440
Guanine : Adenine 4	*opt*	-110.63	-75.96	-226.13	39.54	0.3970
Adenine dimer 1 (planar)	*opt*	-75.96	-75.96	-185.95	34.02	0.5710
Adenine dimer 2 (planar)	*opt*	-75.96	-75.96	-184.86	32.94	0.9130
Adenine dimer 3 (planar)	*opt*	-75.96	-75.96	-184.04	32.11	1.1230

8-Oxoguanine : Guanine	*opt*	-110.63	-193.05	-368.29	64.61	0.1910
2-Thiouracil dimer (planar)	*opt*	-56.33	-56.33	-151.40	38.73	0.1510
Adenine : Thymine (WC)	*const*	-68.95	-172.98	-284.69	42.76	0.3380
Guanine : Cytosine (WC)	*const*	-147.04	-106.42	-350.47	97.01	0.4080
Adenine : thymine (WC)	*const*	-68.95	-172.98	-284.71	42.78	0.3030
Guanine : adenine (HB)	*const*	-110.63	-75.96	-221.98	35.39	0.1060
Cytosine : Guanine (WC)	*const*	-146.31	-110.63	-351.12	94.18	0.0800
Guanine : Cytosine (WC)	*const*	-110.63	-146.31	-352.29	95.35	0.0640
Cytosine : guanine (interstrand)	*const*	-110.63	-146.31	-280.63	23.69	0.1980
Adenine : thymine (interstrand)	*const*	-168.26	-75.96	-256.85	12.62	0.1350
Cytosine dimer (interstrand)	*const*	-146.31	-146.31	-280.79	-11.84	0.1090
Guanine dimer (interstrand)	*const*	-110.63	-110.63	-221.18	-0.07	0.0900
Cytosine dimer (interstrand)	*const*	-146.31	-146.31	-287.54	-5.09	0.1150
Guanine dimer (interstrand)	*const*	-110.63	-110.63	-243.12	21.86	0.1000
Adenine : cytosine (interstrand)	*const*	-75.96	-146.31	-228.78	6.50	0.1090
Thymine : guanine (interstrand)	*const*	-168.26	-110.63	-280.14	1.25	0.0940
Thymine : guanine (interstrand)	*const*	-110.63	-168.26	-288.85	9.96	0.0920
Thymine : cytosine (interstrand)	*const*	-75.96	-146.31	-225.47	3.20	0.1100
Adenine : guanine (interstrand)	*const*	-75.96	-110.63	-210.50	23.91	0.1390
Thymine : cytosine (interstrand)	*const*	-168.26	-146.31	-320.57	5.99	0.1080
Cytosine : Adenine (interstrand)	*const*	-168.26	-146.31	-314.57	0.00	0.0820
Adenine : guanine (interstrand)	*const*	-75.96	-110.63	-204.32	17.73	0.1620
Thymine dimer (interstrand)	*const*	-168.26	-168.26	-337.48	0.95	0.1030
Adenine dimer (interstrand)	*const*	-75.96	-75.96	-158.20	6.28	0.1050
Adenine dimer (interstrand)	*const*	-75.96	-75.96	-163.64	11.72	0.0880
Thymine dimer (interstrand)	*const*	-168.26	-168.26	-336.40	-0.13	0.1050
Adenine : thymine (interstrand)	*const*	-75.96	-168.26	-255.89	11.67	0.1080
Thymine : adenine (interstrand)	*const*	-75.96	-168.26	-252.76	8.54	0.1150
Adenine dimer (interstrand)	*const*	-68.95	-68.95	-143.76	5.85	0.3430
Thymine dimer (interstrand)	*const*	-172.98	-172.98	-346.43	0.47	0.3490
Guanine dimer (interstrand)	*const*	-106.42	-106.42	-240.36	27.51	0.4220
Cytosine dimer (interstrand)	*const*	-147.04	-147.04	-289.54	-4.55	0.4320
Adenine : Guanine (interstrand)	*const*	-68.95	-106.42	-195.50	20.13	0.3160
Thymine : Cytosine (interstrand)	*const*	-147.04	-172.98	-319.23	-0.79	0.3160
Cytosine : Adenine (interstrand)	*const*	-146.31	-75.96	-238.39	16.11	0.1710
Guanine dimer (interstrand)	*const*	-110.63	-110.63	-246.08	24.82	0.1600
Guanine dimer (interstrand)	*const*	-110.63	-110.63	-226.98	5.72	0.1100
Cytosine dimer (interstrand)	*const*	-146.31	-146.31	-281.49	-11.14	0.1020
Guanine : Cytosine (stacked)	*opt*	-110.63	-146.31	-352.35	95.41	2.5380
Methylguanine : Methylcytosine (stacked)	*opt*	-106.42	-147.04	-331.36	77.90	2.2480
Adenine : Thymine (stacked)	*opt*	-75.96	-168.26	-285.50	41.27	0.3840
Methyladenine : Methylthymine (stacked)	*opt*	-68.95	-172.98	-293.32	51.39	1.4800
Cytosine dimer 1 (stacked)	*const*	-146.31	-146.31	-284.09	-8.54	0.1150
Cytosine dimer 2 (stacked)	*const*	-146.31	-146.31	-305.50	12.87	0.1240
Cytosine dimer 3 (stacked)	*const*	-146.31	-146.31	-333.19	40.57	0.1440
Cytosine dimer 4 (stacked)	*const*	-146.31	-146.31	-341.78	49.15	0.1030
Cytosine dimer 5 (stacked)	*const*	-146.31	-146.31	-286.97	-5.66	0.1130
Cytosine dimer 6 (stacked)	*const*	-146.31	-146.31	-285.15	-7.47	0.1170
Cytosine dimer 7 (stacked)	*const*	-146.31	-146.31	-296.43	3.80	0.1620
Cytosine dimer 8 (stacked)	*const*	-146.31	-146.31	-337.23	44.61	0.1370
Cytosine dimer 9 (stacked)	*const*	-146.31	-146.31	-341.74	49.11	0.0960
Cytosine dimer 10 (stacked)	*const*	-146.31	-146.31	-341.13	48.50	0.1030
Cytosine dimer 11 (stacked)	*const*	-146.31	-146.31	-341.83	49.20	0.0970
Cytosine dimer 12 (stacked)	*const*	-146.31	-146.31	-322.01	29.38	0.1190
Cytosine dimer 13 (stacked)	*const*	-146.31	-146.31	-339.37	46.74	0.1160
Cytosine dimer 14 (stacked)	*const*	-146.31	-146.31	-337.60	44.97	0.0990
Adenine dimer (stacked)	*const*	-75.96	-75.96	-188.10	36.17	0.1110
guanine dimer (stacked)	*const*	-110.63	-110.63	-272.89	51.64	0.1150
Adenine : cytosine (stacked)	*const*	-75.96	-146.31	-265.58	43.30	0.1080
Guanine : Adenine (stacked)	*const*	-110.63	-75.96	-230.33	43.74	0.0930
Cytosine dimer (stacked)	*const*	-146.31	-146.31	-342.19	49.56	0.0910
Adenine : Uracil (stacked)	*const*	-75.96	-146.10	-261.20	39.13	0.0930
Guanine : Cytosine (stacked)	*const*	-110.63	-146.31	-310.02	53.08	0.1720
Cytosine : Uracil (stacked)	*const*	-146.31	-146.10	-329.04	36.62	0.0970
Uracil dimer (Stacked)	*const*	-146.10	-146.10	-323.09	30.89	0.0970
Guanine : Uracil (stacked)	*const*	-110.63	-146.10	-301.65	44.92	0.0940
Guanine dimer (stacked)	*const*	-146.31	-146.31	-292.36	-0.27	0.1100
Cytosine dimer (stacked)	*const*	-146.31	-110.63	-279.36	22.42	0.1270
Adenine dimer (stacked)	*const*	-75.96	-75.96	-176.26	24.33	0.0980
Thymine dimer (stacked)	*const*	-75.96	-168.26	-258.28	14.05	0.1090
Guanine : cytosine (stacked)	*const*	-146.31	-110.63	-298.95	42.01	0.1740
Guanine : cytosine (stacked)	*const*	-146.31	-110.63	-280.94	24.00	0.1170
Adenine : guanine (stacked)	*const*	-75.96	-110.63	-220.16	33.57	0.1000
Thymine : cytosine (stacked)	*const*	-168.26	-146.31	-331.62	17.04	0.1010
Adenine : guanine (stacked)	*const*	-75.96	-110.63	-215.26	28.67	0.0910
Thymine : cytosine (stacked)	*const*	-168.26	-146.31	-336.35	21.77	0.1500
Thymine : guanine (stacked)	*const*	-168.26	-110.63	-296.33	17.44	0.0970
Adenine : cytosine (stacked)	*const*	-75.96	-146.31	-233.37	11.10	0.0990
Thymine : guanine (stacked)	*const*	-168.26	-110.63	-303.35	24.46	0.1450
Adenine : cytosine (stacked)	*const*	-75.96	-146.31	-242.47	20.20	0.0960
Adenine : thymine (stacked)	*const*	-75.96	-168.26	-273.63	29.41	0.1290
Adenine : thymine (stacked)	*const*	-75.96	-168.26	-266.26	22.03	0.1060
Adenine dimer (stacked)	*const*	-75.96	-75.96	-176.31	24.39	0.0970
Thymine dimer (stacked)	*const*	-168.26	-168.26	-355.70	19.17	0.1820
Adenine : Thymine (stacked)	*const*	-68.95	-172.98	-274.68	32.75	0.2850
Guanine : Cytosine (stacked)	*const*	-147.04	-106.42	-277.20	23.74	0.3930
Adenine : Cytosine (stacked)	*const*	-68.95	-147.04	-238.79	22.79	0.1010
Thymine : Guanine (stacked)	*const*	-172.98	-106.42	-308.75	29.35	0.3690

guanine : Cytosine (stacked)	*const*	-146.31	-110.63	-291.44	34.49	0.1300
Adenine : Guanine (stacked)	*const*	-75.96	-110.63	-217.10	30.51	0.1240
Cytosine : guanine (stacked)	*const*	-110.63	-146.31	-297.55	40.61	0.1540
Guanine : Cytosine (stacked)	*const*	-110.63	-146.31	-300.59	43.65	0.1940
Phe30 : Lys46 (1RB9)	*const*	16.18	3.84	12.05	7.97	0.1570
Phe30 : Leu33 (1RB9)	*const*	16.24	-16.63	-21.81	21.42	0.2320
Phe30 : Tyr13 (1RB9)	*const*	16.17	-29.12	-24.05	11.09	0.1370
Phe30 : Phe49 (1RB9)	*const*	4.07	16.39	10.80	9.67	0.1550
Phe30 : Tyr4 (1RB9)	*const*	16.13	-15.57	-14.15	14.71	0.1490
Phe49 : Cys39 (1RB9)	*const*	4.07	-29.94	-31.33	5.45	0.1530
Phe49 : Cys6 (1RB9)	*const*	4.09	-39.71	-46.80	11.18	0.1490
Phe49 : Lys46 (1RB9)	*const*	10.68	5.09	-2.21	17.98	0.1440
Phe49 : Val5 (1RB9)	*const*	4.16	-36.49	-50.14	17.81	0.1450
Phe49 : Tyr37 (1RB9)	*const*	10.44	-47.04	-42.22	5.62	0.1230
Phe49 : Tyr4 (1RB9)	*const*	4.06	-21.99	-27.60	9.66	0.1340
Phe49 : Peptide bond (1RB9)	*const*	10.60	-68.79	-66.97	8.78	0.1990
Phe49 : Peptide bond (1RB9)	*const*	4.14	-68.79	-97.43	32.79	0.1780
Glu47 : Lys6 (PDB:1IU5)	*const*	95.88	-79.25	-309.87	326.51	0.1560
Glu49 : Lys6 (PDB:1BQ9)	*const*	97.06	-71.12	-448.02	473.95	0.1550
Glu54 : Lys2 (PDB:1SMM)	*const*	88.44	-59.37	-346.61	375.67	0.1930
Glu50 : LysK30 (PDB:1BRF)	*const*	71.07	-94.89	-286.39	262.57	0.1680
Glu50 : Lys52 (PDB:1BRF)	*const*	71.84	-70.91	-406.83	407.77	0.1650
Glu49 : Lys6 (PDB:1BRF)	*const*	112.59	-70.70	-254.52	296.42	0.3780

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Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-306.48	-371.70	-769.31	91.12	0.3240
Methylguanine : Methylcytosine (WC)	*opt*	-320.01	-287.69	-701.11	93.41	0.4130
Adenine : Thymine (WC)	*opt*	-2.58	-357.21	-407.48	47.68	0.3670
Methyladenine : Methylthymine (planar)	*opt*	-2.58	-357.21	-412.86	53.07	0.3780
8-Oxoguanine : Cytosine (WC planar)	*opt*	-656.49	-371.70	-1116.85	88.66	0.3450
Inosine : Cytosine (WC planar)	*opt*	-371.70	-31.84	-479.07	75.53	0.2440
Guanine : Uracil (wobble)	*opt*	-306.48	-403.79	-770.47	60.20	0.2020
Cytosine : CytosineH+	*opt*	-371.70	-380.62	-852.41	100.08	0.2590
Uracil dimer (Calcutta planar)	*opt*	-403.79	-403.79	-844.23	36.66	0.2190
Uracil dimer (planar)	*opt*	-403.79	-403.79	-859.07	51.50	0.1070
6-Thioguanine : Cytosine (WC planar)	*opt*	-371.70	-290.04	-732.41	70.67	0.2550
Adenine : 4-Thiouracil (WC)	*opt*	-21.25	-327.31	-385.94	37.39	3.8870
2-aminoadenine : Thymine	*opt*	-354.91	-396.10	-810.85	59.84	0.0740
2-aminoadenine : Thymine (planar)	*opt*	-354.91	-396.10	-810.85	59.84	0.3140
Adenine : Difluorotoluene	*opt*	-21.25	28.40	-6.32	13.46	0.8780
Guanine : 4-Thiouracil	*opt*	-306.48	-327.31	-695.55	61.76	0.1360
Guanine : 2-Thiouracil	*opt*	-306.48	-315.87	-659.87	37.52	0.4260
Adenine : Cytosine (planar)	*opt*	-371.70	-21.25	-432.49	39.54	0.5250
Guanine dimer (planar)	*opt*	-306.48	-306.48	-687.80	74.83	0.5620
Guanine 6-Thioguanine (planar)	*opt*	-306.48	-290.04	-659.48	62.95	0.8630
6-Thioguanine : Guanine (planar)	*opt*	-290.04	-306.48	-668.95	72.43	0.8120
Guanine : Adenine 1	*opt*	-306.48	-21.25	-380.02	52.29	0.2950
Guanine : Adenine 1 (planar)	*opt*	-21.25	-306.48	-380.02	52.29	0.6220
Guanine : Adenine 2	*opt*	-306.48	-21.25	-369.63	41.89	0.4200
Guanine : Adenine 2 (planar)	*opt*	-306.48	-21.25	-370.49	42.76	0.5890
Guanine : Adenine 3	*opt*	-306.48	-21.25	-386.26	58.53	0.2180
Guanine : Adenine 4	*opt*	-306.48	-21.25	-363.43	35.69	0.3510
Adenine dimer 1 (planar)	*opt*	-21.25	-21.25	-71.37	28.87	0.6790
Adenine dimer 2 (planar)	*opt*	-21.25	-21.25	-75.95	33.45	0.6040
Adenine dimer 3 (planar)	*opt*	-21.25	-21.25	-76.26	33.76	0.6160
8-Oxoguanine : Guanine	*opt*	-306.48	-656.49	-1026.07	63.10	0.2090
2-Thiouracil dimer (planar)	*opt*	-315.87	-315.87	-667.87	36.14	0.3040
Adenine : Thymine (WC)	*const*	-2.58	-357.21	-406.86	47.06	0.2640
Guanine : Cytosine (WC)	*const*	-320.01	-287.69	-697.24	89.54	0.3020
Adenine : thymine (WC)	*const*	-2.58	-357.21	-406.24	46.45	0.1130
Guanine : adenine (HB)	*const*	-306.48	-21.25	-369.56	41.83	0.1320
Cytosine : Guanine (WC)	*const*	-371.70	-306.48	-768.94	90.76	0.0970
Guanine : Cytosine (WC)	*const*	-306.48	-371.70	-766.52	88.33	0.1010
Cytosine : guanine (interstrand)	*const*	-306.48	-371.70	-706.68	28.49	0.2180
Adenine : thymine (interstrand)	*const*	-396.10	-21.25	-432.44	15.08	0.1460
Cytosine dimer (interstrand)	*const*	-371.70	-371.70	-733.78	-9.63	0.1710
Guanine dimer (interstrand)	*const*	-306.48	-306.48	-609.52	-3.44	0.1360
Cytosine dimer (interstrand)	*const*	-371.70	-371.70	-741.09	-2.32	0.1820
Guanine dimer (interstrand)	*const*	-306.48	-306.48	-635.94	22.98	0.1550
Adenine : cytosine (interstrand)	*const*	-21.25	-371.70	-400.77	7.81	0.1800
Thymine : guanine (interstrand)	*const*	-396.10	-306.48	-698.98	-3.61	0.1390
Thymine : guanine (interstrand)	*const*	-306.48	-396.10	-715.44	12.86	0.2150
Thymine : cytosine (interstrand)	*const*	-21.25	-371.70	-403.11	10.16	0.2000
Adenine : guanine (interstrand)	*const*	-21.25	-306.48	-348.28	20.55	0.1450
Thymine : cytosine (interstrand)	*const*	-396.10	-371.70	-777.10	9.29	0.1510
Cytosine : Adenine (interstrand)	*const*	-396.10	-371.70	-767.42	-0.39	0.1520
Adenine : guanine (interstrand)	*const*	-21.25	-306.48	-342.78	15.05	0.1620
Thymine dimer (interstrand)	*const*	-396.10	-396.10	-788.03	-4.17	0.1090
Adenine dimer (interstrand)	*const*	-21.25	-21.25	-45.97	3.47	0.1340
Adenine dimer (interstrand)	*const*	-21.25	-21.25	-44.65	2.15	0.1400
Thymine dimer (interstrand)	*const*	-396.10	-396.10	-788.90	-3.30	0.1050
Adenine : thymine (interstrand)	*const*	-21.25	-396.10	-428.43	11.08	0.1370
Thymine : adenine (interstrand)	*const*	-21.25	-396.10	-427.18	9.83	0.1530
Adenine dimer (interstrand)	*const*	-2.58	-2.58	-13.78	8.62	0.3600
Thymine dimer (interstrand)	*const*	-357.21	-357.21	-709.52	-4.91	0.1650
Guanine dimer (interstrand)	*const*	-287.69	-287.69	-605.13	29.74	0.4270

Cytosine dimer (interstrand)	*const*	-320.01	-320.01	-637.09	-2.92	0.2560
Adenine : Guanine (interstrand)	*const*	-2.58	-287.69	-306.70	16.43	0.3340
Thymine : Cytosine (interstrand)	*const*	-320.01	-357.21	-676.91	-0.30	0.2630
Cytosine : Adenine (interstrand)	*const*	-371.70	-21.25	-409.72	16.77	0.2330
Guanine dimer (interstrand)	*const*	-306.48	-306.48	-640.66	27.70	0.1600
Guanine dimer (interstrand)	*const*	-306.48	-306.48	-613.33	0.36	0.1200
Cytosine dimer (interstrand)	*const*	-371.70	-371.70	-734.54	-8.87	0.1810
Guanine : Cytosine (stacked)	*opt*	-306.48	-371.70	-769.31	91.12	2.3130
Methylguanine : Methylcytosine (stacked)	*opt*	-287.69	-320.01	-701.11	93.41	2.8000
Adenine : Thymine (stacked)	*opt*	-21.25	-396.10	-470.55	53.20	2.2970
Methyladenine : Methylthymine (stacked)	*opt*	-2.58	-357.21	-412.86	53.07	2.5650
Cytosine dimer 1 (stacked)	*const*	-371.70	-371.70	-725.65	-17.76	0.1450
Cytosine dimer 2 (stacked)	*const*	-371.70	-371.70	-759.52	16.11	0.2350
Cytosine dimer 3 (stacked)	*const*	-371.70	-371.70	-780.21	36.80	0.2380
Cytosine dimer 4 (stacked)	*const*	-371.70	-371.70	-775.20	31.79	0.1590
Cytosine dimer 5 (stacked)	*const*	-371.70	-371.70	-742.90	-0.50	0.2400
Cytosine dimer 6 (stacked)	*const*	-371.70	-371.70	-740.88	-2.52	0.2150
Cytosine dimer 7 (stacked)	*const*	-371.70	-371.70	-754.94	11.53	0.2260
Cytosine dimer 8 (stacked)	*const*	-371.70	-371.70	-779.82	36.42	0.2490
Cytosine dimer 9 (stacked)	*const*	-371.70	-371.70	-775.94	32.53	0.2080
Cytosine dimer 10 (stacked)	*const*	-371.70	-371.70	-778.92	35.51	0.1690
Cytosine dimer 11 (stacked)	*const*	-371.70	-371.70	-776.63	33.23	0.1930
Cytosine dimer 12 (stacked)	*const*	-371.70	-371.70	-767.72	24.31	0.2170
Cytosine dimer 13 (stacked)	*const*	-371.70	-371.70	-779.53	36.12	0.1640
Cytosine dimer 14 (stacked)	*const*	-371.70	-371.70	-767.17	23.76	0.1370
Adenine dimer (stacked)	*const*	-21.25	-21.25	-68.77	26.27	0.1680
guanine dimer (stacked)	*const*	-306.48	-306.48	-665.97	53.00	0.2010
Adenine : cytosine (stacked)	*const*	-21.25	-371.70	-429.18	36.22	0.1670
Guanine : Adenine (stacked)	*const*	-306.48	-21.25	-363.97	36.23	0.1690
Cytosine dimer (stacked)	*const*	-371.70	-371.70	-777.73	34.32	0.2090
Adenine : Uracil (stacked)	*const*	-21.25	-403.79	-453.62	28.58	0.1210
Guanine : Cytosine (stacked)	*const*	-306.48	-371.70	-730.30	52.11	0.2120
Cytosine : Uracil (stacked)	*const*	-371.70	-403.79	-805.34	29.85	0.1560
Uracil dimer (Stacked)	*const*	-403.79	-403.79	-826.14	18.56	0.0930
Guanine : Uracil (stacked)	*const*	-306.48	-403.79	-755.94	45.67	0.1860
Guanine dimer (stacked)	*const*	-371.70	-371.70	-745.78	2.37	0.1870
Cytosine dimer (stacked)	*const*	-371.70	-306.48	-705.72	27.54	0.2130
Adenine dimer (stacked)	*const*	-21.25	-21.25	-56.94	14.44	0.1440
Thymine dimer (stacked)	*const*	-21.25	-396.10	-430.82	13.47	0.1220
Guanine : cytosine (stacked)	*const*	-371.70	-306.48	-729.52	51.33	0.2430
Guanine : cytosine (stacked)	*const*	-371.70	-306.48	-705.63	27.44	0.2420
Adenine : guanine (stacked)	*const*	-21.25	-306.48	-353.83	26.09	0.1730
Thymine : cytosine (stacked)	*const*	-396.10	-371.70	-780.02	12.22	0.1170
Adenine : guanine (stacked)	*const*	-21.25	-306.48	-348.65	20.91	0.1470
Thymine : cytosine (stacked)	*const*	-396.10	-371.70	-787.10	19.29	0.1860
Thymine : guanine (stacked)	*const*	-396.10	-306.48	-715.14	12.56	0.1400
Adenine : cytosine (stacked)	*const*	-21.25	-371.70	-403.71	10.76	0.1480
Thymine : guanine (stacked)	*const*	-396.10	-306.48	-716.64	14.06	0.1880
Adenine : cytosine (stacked)	*const*	-21.25	-371.70	-415.84	22.88	0.1840
Adenine : thymine (stacked)	*const*	-21.25	-396.10	-433.95	16.59	0.1590
Adenine : thymine (stacked)	*const*	-21.25	-396.10	-425.24	7.89	0.1280
Adenine dimer (stacked)	*const*	-21.25	-21.25	-58.71	16.21	0.1400
Thymine dimer (stacked)	*const*	-396.10	-396.10	-797.68	5.48	0.1320
Adenine : Thymine (stacked)	*const*	-2.58	-357.21	-375.52	15.73	0.2240
Guanine : Cytosine (stacked)	*const*	-320.01	-287.69	-633.69	25.99	0.3450
Adenine : Cytosine (stacked)	*const*	-2.58	-320.01	-349.28	26.69	0.2380
Thymine : Guanine (stacked)	*const*	-357.21	-287.69	-668.74	23.84	0.3040
guanine : Cytosine (stacked)	*const*	-371.70	-306.48	-707.07	28.88	0.2140
Adenine : Guanine (stacked)	*const*	-21.25	-306.48	-360.26	32.52	0.1810
Cytosine : guanine (stacked)	*const*	-306.48	-371.70	-732.07	53.89	0.2720
Guanine : Cytosine (stacked)	*const*	-306.48	-371.70	-727.98	49.80	0.2450
Phe30 : Lys46 (1RB9)	*const*	281.02	153.34	428.41	5.95	0.1320
Phe30 : Leu33 (1RB9)	*const*	281.08	154.39	422.50	12.97	0.2200
Phe30 : Tyr13 (1RB9)	*const*	281.14	212.77	485.05	8.85	0.1160
Phe30 : Phe49 (1RB9)	*const*	266.22	281.62	540.58	7.27	0.1450
Phe30 : Tyr4 (1RB9)	*const*	281.25	226.66	501.98	5.93	0.1280
Phe49 : Cys39 (1RB9)	*const*	266.18	203.07	470.34	-1.09	0.1450
Phe49 : Cys6 (1RB9)	*const*	266.41	200.79	457.08	10.12	0.1540
Phe49 : Lys46 (1RB9)	*const*	273.42	143.65	409.59	7.48	0.1260
Phe49 : Val5 (1RB9)	*const*	266.76	161.06	400.11	27.70	0.1790
Phe49 : Tyr37 (1RB9)	*const*	272.73	236.89	509.09	0.54	0.1250
Phe49 : Tyr4 (1RB9)	*const*	266.27	221.04	487.48	-0.17	0.1510
Phe49 : Peptide bond (1RB9)	*const*	272.79	-103.13	164.83	4.83	0.3730
Phe49 : Peptide bond (1RB9)	*const*	266.51	-103.13	135.89	27.49	0.3180
Glu47 : Lys6 (PDB:1IU5)	*const*	163.76	106.59	-48.89	319.23	0.1470
Glu49 : Lys6 (PDB:1BQ9)	*const*	161.16	120.06	-170.78	452.00	0.1670
Glu54 : Lys2 (PDB:1SMM)	*const*	168.25	129.62	-60.13	358.00	0.2050
Glu50 : LysK30 (PDB:1BRF)	*const*	151.06	91.30	-12.47	254.82	0.3320
Glu50 : Lys52 (PDB:1BRF)	*const*	151.85	120.03	-119.42	391.30	0.1420
Glu49 : Lys6 (PDB:1BRF)	*const*	171.22	120.79	9.44	282.58	0.3510

MMFF94s

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-303.93	-369.34	-765.47	92.19	0.0680
Methylguanine : Methylcytosine (WC)	*opt*	-318.58	-285.07	-698.06	94.41	0.3230
Adenine : Thymine (WC)	*opt*	0.44	-360.59	-408.55	48.40	0.2450
Methyladenine : Methylthymine (planar)	*opt*	0.44	-360.59	-413.00	52.85	0.2820

8-Oxoguanine : Cytosine (WC planar)	*opt*	-655.95	-369.34	-1115.36	90.07	0.0560
Inosine : Cytosine (WC planar)	*opt*	-369.34	-32.39	-477.98	76.24	0.0560
Guanine : Uracil (wobble)	*opt*	-303.93	-406.12	-771.13	61.08	0.1840
Cytosine : CytosineH+	*opt*	-369.34	-377.93	-847.75	100.48	0.1320
Uracil dimer (Calcutta planar)	*opt*	-406.12	-406.12	-848.90	36.66	0.2190
Uracil dimer (planar)	*opt*	-406.12	-406.12	-863.73	51.50	0.1070
6-Thioguanine : Cytosine (WC planar)	*opt*	-369.34	-286.62	-729.83	73.87	0.1410
Adenine : 4-Thiouracil (WC)	*opt*	-18.30	-328.99	-384.67	37.38	3.8870
2-aminoadenine : Thymine	*opt*	-345.32	-398.43	-804.61	60.86	0.2630
2-aminoadenine : Thymine (planar)	*opt*	-345.32	-398.43	-804.61	60.86	0.0440
Adenine : Difluorotoluene	*opt*	-18.30	28.40	-2.90	12.99	0.6370
Guanine : 4-Thiouracil	*opt*	-303.93	-328.99	-695.59	62.66	0.1410
Guanine : 2-Thiouracil	*opt*	-303.93	-316.91	-658.95	38.11	0.4170
Adenine : Cytosine (planar)	*opt*	-369.34	-18.30	-423.57	35.92	0.1200
Guanine dimer (planar)	*opt*	-303.93	-303.93	-683.25	75.38	0.1090
Guanine 6-Thioguanine (planar)	*opt*	-303.93	-286.62	-652.85	62.30	0.1040
6-Thioguanine : Guanine (planar)	*opt*	-286.62	-303.93	-659.68	69.12	0.1140
Guanine : Adenine 1	*opt*	-303.93	-18.30	-367.98	45.74	0.3520
Guanine : Adenine 1 (planar)	*opt*	-18.30	-303.93	-361.24	39.01	0.1010
Guanine : Adenine 2	*opt*	-303.93	-18.30	-362.82	40.58	0.2840
Guanine : Adenine 2 (planar)	*opt*	-303.93	-18.30	-360.64	38.41	0.0780
Guanine : Adenine 3	*opt*	-303.93	-18.30	-373.58	51.35	0.2910
Guanine : Adenine 4	*opt*	-303.93	-18.30	-358.10	35.87	0.2360
Adenine dimer 1 (planar)	*opt*	-18.30	-18.30	-65.26	28.66	0.0940
Adenine dimer 2 (planar)	*opt*	-18.30	-18.30	-67.53	30.93	0.5110
Adenine dimer 3 (planar)	*opt*	-18.30	-18.30	-68.32	31.72	0.6650
8-Oxoguanine : Guanine	*opt*	-303.93	-655.95	-1024.14	64.26	0.2450
2-Thiouracil dimer (planar)	*opt*	-316.91	-316.91	-669.96	36.14	0.3040
Adenine : Thymine (WC)	*const*	0.44	-360.59	-407.44	47.29	0.2570
Guanine : Cytosine (WC)	*const*	-318.58	-285.07	-697.17	93.53	0.3010
Adenine : thymine (WC)	*const*	0.44	-360.59	-407.26	47.11	0.0950
Guanine : adenine (HB)	*const*	-303.93	-18.30	-359.60	37.36	0.0930
Cytosine : Guanine (WC)	*const*	-369.34	-303.93	-764.17	90.89	0.0790
Guanine : Cytosine (WC)	*const*	-303.93	-369.34	-765.45	92.17	0.0630
Cytosine : guanine (interstrand)	*const*	-303.93	-369.34	-690.67	17.39	0.1350
Adenine : thymine (interstrand)	*const*	-398.43	-18.30	-426.03	9.30	0.1180
Cytosine dimer (interstrand)	*const*	-369.34	-369.34	-727.32	-11.36	0.1030
Guanine dimer (interstrand)	*const*	-303.93	-303.93	-600.87	-7.00	0.0830
Cytosine dimer (interstrand)	*const*	-369.34	-369.34	-733.62	-5.06	0.1070
Guanine dimer (interstrand)	*const*	-303.93	-303.93	-624.30	16.43	0.0890
Adenine : cytosine (interstrand)	*const*	-18.30	-369.34	-394.07	6.43	0.1020
Thymine : guanine (interstrand)	*const*	-398.43	-303.93	-698.37	-4.00	0.0750
Thymine : guanine (interstrand)	*const*	-303.93	-398.43	-703.93	1.57	0.1030
Thymine : cytosine (interstrand)	*const*	-18.30	-369.34	-391.71	4.07	0.1040
Adenine : guanine (interstrand)	*const*	-18.30	-303.93	-340.37	18.13	0.0870
Thymine : cytosine (interstrand)	*const*	-398.43	-369.34	-773.31	5.53	0.1030
Cytosine : Adenine (interstrand)	*const*	-398.43	-369.34	-767.23	-0.55	0.0970
Adenine : guanine (interstrand)	*const*	-18.30	-303.93	-330.65	8.41	0.0920
Thymine dimer (interstrand)	*const*	-398.43	-398.43	-792.69	-4.17	0.1100
Adenine dimer (interstrand)	*const*	-18.30	-18.30	-40.65	4.05	0.1090
Adenine dimer (interstrand)	*const*	-18.30	-18.30	-36.35	-0.25	0.0870
Thymine dimer (interstrand)	*const*	-398.43	-398.43	-793.55	-3.31	0.1080
Adenine : thymine (interstrand)	*const*	-18.30	-398.43	-427.83	11.09	0.1060
Thymine : adenine (interstrand)	*const*	-18.30	-398.43	-422.17	5.44	0.1090
Adenine dimer (interstrand)	*const*	0.44	0.44	-2.21	3.08	0.3360
Thymine dimer (interstrand)	*const*	-360.59	-360.59	-716.27	-4.92	0.1530
Guanine dimer (interstrand)	*const*	-285.07	-285.07	-590.30	20.16	0.4030
Cytosine dimer (interstrand)	*const*	-318.58	-318.58	-631.60	-5.56	0.1270
Adenine : Guanine (interstrand)	*const*	0.44	-285.07	-297.35	12.72	0.3020
Thymine : Cytosine (interstrand)	*const*	-318.58	-360.59	-678.34	-0.83	0.3180
Cytosine : Adenine (interstrand)	*const*	-369.34	-18.30	-396.87	9.23	0.1690
Guanine dimer (interstrand)	*const*	-303.93	-303.93	-629.68	21.82	0.1050
Guanine dimer (interstrand)	*const*	-303.93	-303.93	-605.22	-2.65	0.0930
Cytosine dimer (interstrand)	*const*	-369.34	-369.34	-727.74	-10.94	0.1020
Guanine : Cytosine (stacked)	*opt*	-303.93	-369.34	-765.47	92.19	2.5210
Methylguanine : Methylcytosine (stacked)	*opt*	-285.07	-318.58	-698.06	94.41	3.0810
Adenine : Thymine (stacked)	*opt*	-18.30	-398.43	-469.79	53.06	2.4500
Methyladenine : Methylthymine (stacked)	*opt*	0.44	-360.59	-396.64	36.49	0.5640
Cytosine dimer 1 (stacked)	*const*	-369.34	-369.34	-724.76	-13.93	0.1050
Cytosine dimer 2 (stacked)	*const*	-369.34	-369.34	-743.22	4.54	0.1160
Cytosine dimer 3 (stacked)	*const*	-369.34	-369.34	-763.65	24.97	0.1210
Cytosine dimer 4 (stacked)	*const*	-369.34	-369.34	-769.41	30.72	0.0900
Cytosine dimer 5 (stacked)	*const*	-369.34	-369.34	-727.26	-11.42	0.1060
Cytosine dimer 6 (stacked)	*const*	-369.34	-369.34	-725.94	-12.75	0.1080
Cytosine dimer 7 (stacked)	*const*	-369.34	-369.34	-736.48	-2.20	0.1240
Cytosine dimer 8 (stacked)	*const*	-369.34	-369.34	-766.83	28.14	0.1050
Cytosine dimer 9 (stacked)	*const*	-369.34	-369.34	-768.77	30.08	0.1000
Cytosine dimer 10 (stacked)	*const*	-369.34	-369.34	-769.34	30.65	0.0890
Cytosine dimer 11 (stacked)	*const*	-369.34	-369.34	-770.77	32.09	0.0920
Cytosine dimer 12 (stacked)	*const*	-369.34	-369.34	-759.59	20.91	0.1130
Cytosine dimer 13 (stacked)	*const*	-369.34	-369.34	-769.02	30.33	0.0900
Cytosine dimer 14 (stacked)	*const*	-369.34	-369.34	-765.85	27.17	0.0920
Adenine dimer (stacked)	*const*	-18.30	-18.30	-59.13	22.53	0.1000
guanine dimer (stacked)	*const*	-303.93	-303.93	-651.42	43.55	0.0940
Adenine : cytosine (stacked)	*const*	-18.30	-369.34	-420.07	32.43	0.0940
Guanine : Adenine (stacked)	*const*	-303.93	-18.30	-355.08	32.84	0.0870
Cytosine dimer (stacked)	*const*	-369.34	-369.34	-770.77	32.08	0.0990
Adenine : Uracil (stacked)	*const*	-18.30	-406.12	-451.83	27.41	0.0960

Guanine : Cytosine (stacked)	*const*	-303.93	-369.34	-714.65	41.37	0.1170
Cytosine : Uracil (stacked)	*const*	-369.34	-406.12	-802.20	26.74	0.0940
Uracil dimer (Stacked)	*const*	-406.12	-406.12	-830.61	18.37	0.0950
Guanine : Uracil (stacked)	*const*	-303.93	-406.12	-748.90	38.85	0.0960
Guanine dimer (stacked)	*const*	-369.34	-369.34	-733.57	-5.11	0.0990
Cytosine dimer (stacked)	*const*	-369.34	-303.93	-694.44	21.16	0.1170
Adenine dimer (stacked)	*const*	-18.30	-18.30	-46.13	9.53	0.1000
Thymine dimer (stacked)	*const*	-18.30	-398.43	-430.92	14.18	0.1070
Guanine : cytosine (stacked)	*const*	-369.34	-303.93	-706.76	33.49	0.1320
Guanine : cytosine (stacked)	*const*	-369.34	-303.93	-690.25	16.97	0.0970
Adenine : guanine (stacked)	*const*	-18.30	-303.93	-341.42	19.18	0.1010
Thymine : cytosine (stacked)	*const*	-398.43	-369.34	-780.74	12.96	0.1010
Adenine : guanine (stacked)	*const*	-18.30	-303.93	-340.33	18.10	0.0890
Thymine : cytosine (stacked)	*const*	-398.43	-369.34	-782.59	14.81	0.1070
Thymine : guanine (stacked)	*const*	-398.43	-303.93	-714.94	12.57	0.0890
Adenine : cytosine (stacked)	*const*	-18.30	-369.34	-395.70	8.06	0.0930
Thymine : guanine (stacked)	*const*	-398.43	-303.93	-709.78	7.42	0.1090
Adenine : cytosine (stacked)	*const*	-18.30	-369.34	-400.71	13.06	0.1090
Adenine : thymine (stacked)	*const*	-18.30	-398.43	-430.24	13.50	0.1030
Adenine : thymine (stacked)	*const*	-18.30	-398.43	-421.94	5.21	0.1010
Adenine dimer (stacked)	*const*	-18.30	-18.30	-48.97	12.37	0.0980
Thymine dimer (stacked)	*const*	-398.43	-398.43	-802.33	5.46	0.1330
Adenine : Thymine (stacked)	*const*	0.44	-360.59	-378.25	18.10	0.2340
Guanine : Cytosine (stacked)	*const*	-318.58	-285.07	-623.72	20.07	0.3010
Adenine : Cytosine (stacked)	*const*	0.44	-318.58	-333.09	14.94	0.3150
Thymine : Guanine (stacked)	*const*	-360.59	-285.07	-662.67	17.01	0.2750
guanine : Cytosine (stacked)	*const*	-369.34	-303.93	-692.97	19.69	0.1300
Adenine : Guanine (stacked)	*const*	-18.30	-303.93	-337.06	14.83	0.1100
Cytosine : guanine (stacked)	*const*	-303.93	-369.34	-708.21	34.94	0.1490
Guanine : Cytosine (stacked)	*const*	-303.93	-369.34	-709.78	36.50	0.1480
Phe30 : Lys46 (1RB9)	*const*	281.02	153.34	428.41	5.95	0.1320
Phe30 : Leu33 (1RB9)	*const*	281.08	154.39	422.50	12.97	0.2200
Phe30 : Tyr13 (1RB9)	*const*	281.14	212.77	485.05	8.85	0.1160
Phe30 : Phe49 (1RB9)	*const*	266.22	281.62	540.58	7.27	0.1450
Phe30 : Tyr4 (1RB9)	*const*	281.25	226.66	501.98	5.93	0.1280
Phe49 : Cys39 (1RB9)	*const*	266.18	203.07	470.34	-1.09	0.1450
Phe49 : Cys6 (1RB9)	*const*	266.41	200.79	457.08	10.12	0.1540
Phe49 : Lys46 (1RB9)	*const*	273.42	143.65	409.59	7.48	0.1260
Phe49 : Val5 (1RB9)	*const*	266.76	161.06	400.11	27.70	0.1790
Phe49 : Tyr37 (1RB9)	*const*	272.73	236.89	509.09	0.54	0.1250
Phe49 : Tyr4 (1RB9)	*const*	266.27	221.04	487.48	-0.17	0.1510
Phe49 : Peptide bond (1RB9)	*const*	272.80	-105.67	163.52	3.61	0.2160
Phe49 : Peptide bond (1RB9)	*const*	266.54	-105.67	133.00	27.87	0.2550
Glu47 : Lys6 (PDB:1IU5)	*const*	163.76	106.59	-48.89	319.23	0.1470
Glu49 : Lys6 (PDB:1BQ9)	*const*	161.16	120.06	-170.78	452.00	0.1670
Glu54 : Lys2 (PDB:1SMM)	*const*	168.25	129.62	-60.13	358.00	0.2050
Glu50 : LysK30 (PDB:1BRF)	*const*	151.06	91.30	-12.47	254.82	0.3320
Glu50 : Lys52 (PDB:1BRF)	*const*	151.85	120.03	-119.42	391.30	0.1420
Glu49 : Lys6 (PDB:1BRF)	*const*	171.23	120.79	9.44	282.58	0.3510

JSCH-2005 data set: Results with default non-bonded cut-offs (opt = geometry optimization, const = constrained optimization)

MM2*

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-132.19	-93.99	-254.63	28.45	0.8200
Methylguanine : Methylcytosine (WC)	*opt*	-68.98	-122.16	-220.51	29.38	0.8940
Adenine : Thymine (WC)	*opt*	105.65	-331.71	-255.36	29.30	2.9350
Methyladenine : Methylthymine (planar)	*opt*	105.65	-331.53	-255.64	29.77	2.4940
8-Oxoguanine : Cytosine (WC planar)	*opt*	-325.51	-93.99	-447.80	28.30	0.8870
Inosine : Cytosine (WC planar)	*opt*	-93.99	18.96	-102.45	27.43	0.9010
Guanine : Uracil (wobble)	*opt*	-132.19	-346.86	-521.15	42.09	0.3420
Cytosine : CytosineH+	*opt*	-93.99	-426.38	-557.94	37.57	1.4020
Uracil dimer (Calcutta planar)	*opt*	-346.99	-346.86	-716.95	23.10	0.2870
Uracil dimer (planar)	*opt*	-346.99	-346.99	-734.15	40.16	0.1670
6-Thioguanine : Cytosine (WC planar)	*opt*	-93.99	-89.84	-213.11	29.28	0.8940
Adenine : 4-Thiouracil (WC)	*opt*	95.54	-253.85	-164.53	6.22	3.8880
2-aminoadenine : Thymine	*opt*	69.15	-366.01	-320.53	23.67	2.1460
2-aminoadenine : Thymine (planar)	*opt*	69.03	-366.01	-311.51	14.54	0.5130
Adenine : Difluorotoluene	*opt*	95.54	-16.59	55.35	23.61	2.9630
Guanine : 4-Thiouracil	*opt*	-132.19	-253.85	-429.91	43.86	0.2840
Guanine : 2-Thiouracil	*opt*	-132.19	-216.84	-375.34	26.30	0.6740
Adenine : Cytosine (planar)	*opt*	-93.99	95.54	-10.99	12.55	0.8690
Guanine dimer (planar)	*opt*	-132.19	-132.19	-285.37	20.99	0.7040
Guanine 6-Thioguanine (planar)	*opt*	-132.19	-89.84	-238.68	16.65	0.4060
6-Thioguanine : Guanine (planar)	*opt*	-89.84	-132.19	-245.69	23.65	0.7460
Guanine : Adenine 1	*opt*	-132.19	95.54	-59.70	23.05	2.0990
Guanine : Adenine 1 (planar)	*opt*	95.54	-132.19	-44.94	8.29	0.7870
Guanine : Adenine 2	*opt*	-132.19	95.54	-61.97	25.32	2.4620
Guanine : Adenine 2 (planar)	*opt*	-132.18	95.54	-43.52	6.88	0.4840
Guanine : Adenine 3	*opt*	-132.19	95.54	-62.53	25.88	2.4130
Guanine : Adenine 4	*opt*	-132.19	95.54	-62.48	25.83	3.6690
Adenine dimer 1 (planar)	*opt*	95.54	95.54	191.85	-0.76	0.5660
Adenine dimer 2 (planar)	*opt*	95.54	95.54	169.17	21.92	2.8460
Adenine dimer 3 (planar)	*opt*	95.54	95.54	181.80	9.28	1.3450
8-Oxoguanine : Guanine	*opt*	-132.19	-325.51	-497.74	40.03	0.4420
2-Thiouracil dimer (planar)	*opt*	-216.87	-216.87	-459.50	25.76	0.4570

Adenine : Thymine (WC)	*const*	105.98	-331.71	-211.94	-13.78	0.1580
Guanine : Cytosine (WC)	*const*	-68.95	-122.15	-189.64	-1.46	0.2080
Adenine : thymine (WC)	*const*	105.77	-331.71	-208.33	-17.61	0.1750
Guanine : adenine (HB)	*const*	-132.19	95.56	-26.01	-10.62	0.1690
Cytosine : Guanine (WC)	*const*	-93.71	-132.19	-228.78	2.87	0.1310
Guanine : Cytosine (WC)	*const*	-132.19	-93.72	-228.16	2.25	0.1180
Cytosine : guanine (interstrand)	*const*	-132.19	-93.99	-229.40	3.22	0.1050
Adenine : thymine (interstrand)	*const*	-366.01	95.54	-274.20	3.74	0.1050
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-185.02	-2.95	0.1050
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-266.82	2.43	0.1080
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-190.68	2.70	0.1020
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-272.45	8.07	0.1100
Adenine : cytosine (interstrand)	*const*	95.54	-93.99	-0.46	2.01	0.1010
Thymine : guanine (interstrand)	*const*	-366.01	-132.19	-497.86	-0.34	0.1040
Thymine : guanine (interstrand)	*const*	-132.19	-366.01	-498.62	0.42	0.1060
Thymine : cytosine (interstrand)	*const*	95.54	-93.99	-3.63	5.19	0.1010
Adenine : guanine (interstrand)	*const*	95.54	-132.19	-46.26	9.61	0.1030
Thymine : cytosine (interstrand)	*const*	-366.01	-93.99	-462.56	2.56	0.1030
Thymine : cytosine (interstrand)	*const*	-366.01	-93.99	-457.97	-2.03	0.1030
Adenine : guanine (interstrand)	*const*	95.54	-132.19	-39.87	3.22	0.1040
Thymine dimer (interstrand)	*const*	-366.01	-366.01	-729.09	-2.93	0.1160
Adenine dimer (interstrand)	*const*	95.54	95.54	189.85	1.24	0.0990
Adenine dimer (interstrand)	*const*	95.54	95.54	188.96	2.12	0.1100
Thymine dimer (interstrand)	*const*	-366.01	-366.01	-731.13	-0.89	0.1100
Adenine : thymine (interstrand)	*const*	95.54	-366.01	-273.09	2.62	0.0910
Thymine : adenine (interstrand)	*const*	95.54	-366.01	-271.62	1.16	0.0940
Adenine dimer (interstrand)	*const*	105.74	105.74	207.65	3.83	0.1800
Thymine dimer (interstrand)	*const*	-331.71	-331.71	-659.20	-4.21	0.1620
Guanine dimer (interstrand)	*const*	-122.16	-122.16	-259.32	15.00	0.2410
Cytosine dimer (interstrand)	*const*	-68.98	-68.98	-141.89	3.93	0.1190
Adenine : Guanine (interstrand)	*const*	105.74	-122.16	-19.06	2.65	0.2290
Thymine : Cytosine (interstrand)	*const*	-68.98	-331.71	-397.04	-3.64	0.3210
Cytosine dimer (interstrand)	*const*	-93.99	95.54	0.37	1.19	0.1330
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-264.89	0.50	0.1180
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-271.05	6.66	0.1210
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-183.76	-4.21	0.1080
Guanine : Cytosine (stacked)	*opt*	-132.19	-93.99	-251.71	25.53	0.8380
Methylguanine : Methylcytosine (stacked)	*opt*	-122.16	-68.98	-219.50	28.37	1.1140
Adenine : Thymine (stacked)	*opt*	95.54	-366.16	-294.51	23.90	0.6750
Methyladenine : Methylthymine (stacked)	*opt*	105.74	-331.71	-255.28	29.32	0.4880
Cytosine dimer 1 (stacked)	*const*	-93.99	-93.99	-193.91	5.93	0.0930
Cytosine dimer 2 (stacked)	*const*	-93.99	-93.99	-204.88	16.90	0.1020
Cytosine dimer 3 (stacked)	*const*	-93.99	-93.99	-203.55	15.57	0.1010
Cytosine dimer 4 (stacked)	*const*	-93.99	-93.99	-205.77	17.80	0.1050
Cytosine dimer 5 (stacked)	*const*	-93.99	-93.99	-196.36	8.39	0.0950
Cytosine dimer 6 (stacked)	*const*	-93.99	-93.99	-195.55	7.57	0.0930
Cytosine dimer 7 (stacked)	*const*	-93.99	-93.99	-201.51	13.54	0.0970
Cytosine dimer 8 (stacked)	*const*	-93.99	-93.99	-201.07	13.09	0.1190
Cytosine dimer 9 (stacked)	*const*	-93.99	-93.99	-207.23	19.25	0.1000
Cytosine dimer 10 (stacked)	*const*	-93.99	-93.99	-207.34	19.36	0.1050
Cytosine dimer 11 (stacked)	*const*	-93.99	-93.99	-204.81	16.83	0.1030
Cytosine dimer 12 (stacked)	*const*	-93.99	-93.99	-201.21	13.23	0.0980
Cytosine dimer 13 (stacked)	*const*	-93.99	-93.99	-207.53	19.55	0.1010
Cytosine dimer 14 (stacked)	*const*	-93.99	-93.99	-203.71	15.74	0.1030
Adenine dimer (stacked)	*const*	95.35	95.35	172.93	17.77	0.1050
guanine dimer (stacked)	*const*	-132.19	-132.19	-287.17	22.78	0.1100
Adenine : cytosine (stacked)	*const*	95.35	-93.99	-18.43	19.79	0.1020
Guanine : Adenine (stacked)	*const*	-132.19	95.35	-58.15	21.31	0.1060
Cytosine dimer (stacked)	*const*	-93.99	-93.99	-206.64	18.67	0.0990
Adenine : Uracil (stacked)	*const*	95.35	-346.86	-270.98	19.47	0.0930
Guanine : Cytosine (stacked)	*const*	-132.19	-93.99	-243.71	17.53	0.1090
Cytosine : Uracil (stacked)	*const*	-93.99	-346.86	-457.76	16.91	0.1120
Uracil dimer (Stacked)	*const*	-346.86	-346.86	-710.85	17.12	0.1130
Guanine : Uracil (stacked)	*const*	-132.19	-346.86	-496.93	17.87	0.0980
Guanine dimer (stacked)	*const*	-93.99	-93.99	-202.63	14.65	0.1050
Cytosine dimer (stacked)	*const*	-93.99	-132.19	-231.98	5.79	0.1080
Adenine dimer (stacked)	*const*	95.54	95.54	179.14	11.95	0.0980
Thymine dimer (stacked)	*const*	95.54	-366.01	-272.71	2.25	0.1090
Guanine : cytosine (stacked)	*const*	-93.99	-132.19	-243.52	17.34	0.1060
Guanine : cytosine (stacked)	*const*	-93.99	-132.19	-237.81	11.63	0.1070
Adenine : guanine (stacked)	*const*	95.54	-132.19	-55.09	18.45	0.1060
Thymine : cytosine (stacked)	*const*	-366.01	-93.99	-478.45	18.45	0.0970
Adenine : guanine (stacked)	*const*	95.54	-132.19	-46.83	10.19	0.1040
Thymine : cytosine (stacked)	*const*	-366.01	-93.99	-474.68	14.68	0.2010
Thymine : guanine (stacked)	*const*	-366.01	-132.19	-511.93	13.73	0.1090
Adenine : cytosine (stacked)	*const*	95.54	-93.99	-9.75	11.31	0.1050
Thymine : guanine (stacked)	*const*	-366.01	-132.19	-511.57	13.37	0.2050
Adenine : cytosine (stacked)	*const*	95.54	-93.99	-13.31	14.86	0.0990
Adenine : thymine (stacked)	*const*	95.54	-366.01	-285.27	14.80	0.1750
Adenine : thymine (stacked)	*const*	95.54	-366.01	-288.99	18.53	0.1310
Adenine dimer (stacked)	*const*	95.54	95.54	178.51	12.58	0.0990
Thymine dimer (stacked)	*const*	-366.01	-366.01	-748.41	16.40	0.2160
Adenine : Thymine (stacked)	*const*	105.74	-331.71	-247.70	21.74	0.1910
Guanine : Cytosine (stacked)	*const*	-68.98	-122.16	-204.13	13.00	0.1910
Adenine : Cytosine (stacked)	*const*	105.74	-68.98	18.41	18.36	0.3390
Thymine : Guanine (stacked)	*const*	-331.71	-122.16	-473.43	19.57	0.2100
guanine : Cytosine (stacked)	*const*	-93.99	-132.19	-241.96	15.77	0.1150
Adenine : Guanine (stacked)	*const*	95.54	-132.19	-50.36	13.71	0.1360

Cytosine : guanine (stacked)	*const*	-132.19	-93.99	-241.55	15.36	0.1070
Guanine : Cytosine (stacked)	*const*	-132.19	-93.99	-245.97	19.79	0.1290
Phe30 : Lys46 (1RB9)	*const*	86.48	94.48	169.62	11.34	0.1170
Phe30 : Leu33 (1RB9)	*const*	86.51	84.60	153.59	17.51	0.1670
Phe30 : Tyr13 (1RB9)	*const*	86.48	81.71	155.75	12.44	0.1120
Phe30 : Phe49 (1RB9)	*const*	85.78	86.48	164.72	7.55	0.1290
Phe30 : Tyr4 (1RB9)	*const*	86.48	88.01	157.71	16.78	0.1400
Phe49 : Cys39 (1RB9)	*const*	85.83	66.51	153.88	-1.54	0.1280
Phe49 : Cys6 (1RB9)	*const*	85.83	66.60	137.81	14.62	0.1330
Phe49 : Lys46 (1RB9)	*const*	89.31	89.70	170.34	8.66	0.1140
Phe49 : Val5 (1RB9)	*const*	86.30	84.01	151.63	18.68	0.1570
Phe49 : Tyr37 (1RB9)	*const*	88.48	119.21	205.88	1.81	0.1330
Phe49 : Tyr4 (1RB9)	*const*	85.77	87.03	162.31	10.49	0.1300
Phe49 : Peptide bond (1RB9)	*const*	88.52	-91.75	-8.88	5.65	0.1630
Phe49 : Peptide bond (1RB9)	*const*	85.96	-91.75	-29.22	23.43	0.1820
Glu47 : Lys6 (PDB:1IU5)	*const*	245.78	74.90	-9.47	330.16	0.1390
Glu49 : Lys6 (PDB:1BQ9)	*const*	245.10	78.61	-137.63	461.35	0.1770
Glu54 : Lys2 (PDB:1SMM)	*const*	275.01	79.69	-20.81	375.50	0.1910
Glu50 : LysK30 (PDB:1BRF)	*const*	240.61	61.23	50.53	251.32	0.1760
Glu50 : Lys52 (PDB:1BRF)	*const*	241.21	79.38	-49.61	370.20	0.1400
Glu49 : Lys6 (PDB:1BRF)	*const*	248.63	78.24	51.24	275.63	0.1700

MM2* (explicit lone pairs)

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-132.19	-93.99	-254.63	28.45	0.8200
Methylguanine : Methylcytosine (WC)	*opt*	-68.98	-122.16	-220.51	29.38	0.8940
Adenine : Thymine (WC)	*opt*	105.65	-331.71	-255.36	29.30	2.9350
Methyladenine : Methylthymine (planar)	*opt*	105.65	-331.53	-255.64	29.77	2.4940
8-Oxoguanine : Cytosine (WC planar)	*opt*	-325.51	-93.99	-447.80	28.30	0.8870
Inosine : Cytosine (WC planar)	*opt*	-93.99	18.96	-102.45	27.43	0.9010
Guanine : Uracil (wobble)	*opt*	-132.19	-346.86	-521.15	42.09	0.3420
Cytosine : CytosineH+	*opt*	-93.99	-426.38	-557.94	37.57	1.4020
Uracil dimer (Calcutta planar)	*opt*	-346.99	-346.86	-716.95	23.10	0.2870
Uracil dimer (planar)	*opt*	-346.99	-346.99	-734.15	40.16	0.1670
6-Thioguanine : Cytosine (WC planar)	*opt*	-93.99	-89.84	-213.11	29.28	0.8940
Adenine : 4-Thiouracil (WC)	*opt*	95.54	-253.85	-164.53	6.22	3.8880
2-aminoadenine : Thymine	*opt*	69.15	-366.01	-320.53	23.67	2.1460
2-aminoadenine : Thymine (planar)	*opt*	69.03	-366.01	-311.51	14.54	0.5130
Adenine : Difluorotoluene	*opt*	95.54	-16.59	55.35	23.61	2.9630
Guanine : 4-Thiouracil	*opt*	-132.19	-253.85	-429.91	43.86	0.2840
Guanine : 2-Thiouracil	*opt*	-132.19	-216.84	-375.34	26.30	0.6740
Adenine : Cytosine (planar)	*opt*	-93.99	95.54	-10.99	12.55	0.8690
Guanine dimer (planar)	*opt*	-132.19	-132.19	-285.37	20.99	0.7040
Guanine 6-Thioguanine (planar)	*opt*	-132.19	-89.84	-238.68	16.65	0.4060
6-Thioguanine : Guanine (planar)	*opt*	-89.84	-132.19	-245.69	23.65	0.7460
Guanine : Adenine 1	*opt*	-132.19	95.54	-59.70	23.05	2.0990
Guanine : Adenine 1 (planar)	*opt*	95.54	-132.19	-44.94	8.29	0.7870
Guanine : Adenine 2	*opt*	-132.19	95.54	-61.97	25.32	2.4620
Guanine : Adenine 2 (planar)	*opt*	-132.18	95.54	-43.52	6.88	0.4840
Guanine : Adenine 3	*opt*	-132.19	95.54	-62.53	25.88	2.4130
Guanine : Adenine 4	*opt*	-132.19	95.54	-62.48	25.83	3.6690
Adenine dimer 1 (planar)	*opt*	95.54	95.54	191.85	-0.76	0.5660
Adenine dimer 2 (planar)	*opt*	95.54	95.54	169.17	21.92	2.8460
Adenine dimer 3 (planar)	*opt*	95.54	95.54	181.80	9.28	1.3450
8-Oxoguanine : Guanine	*opt*	-132.19	-325.51	-497.74	40.03	0.4420
2-Thiouracil dimer (planar)	*opt*	-216.87	-216.87	-459.50	25.76	0.4570
Adenine : Thymine (WC)	*const*	105.98	-331.71	-211.94	-13.78	0.1580
Guanine : Cytosine (WC)	*const*	-68.95	-122.15	-189.64	-1.46	0.2080
Adenine : thymine (WC)	*const*	105.77	-331.71	-208.33	-17.61	0.1750
Guanine : adenine (HB)	*const*	-132.19	95.56	-26.01	-10.62	0.1690
Cytosine : Guanine (WC)	*const*	-93.71	-132.19	-228.78	2.87	0.1310
Guanine : Cytosine (WC)	*const*	-132.19	-93.72	-228.16	2.25	0.1180
Cytosine : guanine (interstrand)	*const*	-132.19	-93.99	-229.40	3.22	0.1050
Adenine : thymine (interstrand)	*const*	-366.01	95.54	-274.20	3.74	0.1050
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-185.02	-2.95	0.1050
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-266.82	2.43	0.1080
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-190.68	2.70	0.1020
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-272.45	8.07	0.1100
Adenine : cytosine (interstrand)	*const*	95.54	-93.99	-0.46	2.01	0.1010
Thymine : guanine (interstrand)	*const*	-366.01	-132.19	-497.86	-0.34	0.1040
Thymine : guanine (interstrand)	*const*	-132.19	-366.01	-498.62	0.42	0.1060
Thymine : cytosine (interstrand)	*const*	95.54	-93.99	-3.63	5.19	0.1010
Adenine : guanine (interstrand)	*const*	95.54	-132.19	-46.26	9.61	0.1030
Thymine : cytosine (interstrand)	*const*	-366.01	-93.99	-462.56	2.56	0.1030
Thymine : cytosine (interstrand)	*const*	-366.01	-93.99	-457.97	-2.03	0.1030
Adenine : guanine (interstrand)	*const*	95.54	-132.19	-39.87	3.22	0.1040
Thymine dimer (interstrand)	*const*	-366.01	-366.01	-729.09	-2.93	0.1160
Adenine dimer (interstrand)	*const*	95.54	95.54	189.85	1.24	0.0990
Adenine dimer (interstrand)	*const*	95.54	95.54	188.96	2.12	0.1100
Thymine dimer (interstrand)	*const*	-366.01	-366.01	-731.13	-0.89	0.1100
Adenine : thymine (interstrand)	*const*	95.54	-366.01	-273.09	2.62	0.0910
Thymine : adenine (interstrand)	*const*	95.54	-366.01	-271.62	1.16	0.0940
Adenine dimer (interstrand)	*const*	105.74	105.74	207.65	3.83	0.1800
Thymine dimer (interstrand)	*const*	-331.71	-331.71	-659.20	-4.21	0.1620
Guanine dimer (interstrand)	*const*	-122.16	-122.16	-259.32	15.00	0.2410
Cytosine dimer (interstrand)	*const*	-68.98	-68.98	-141.89	3.93	0.1190
Adenine : Guanine (interstrand)	*const*	105.74	-122.16	-19.06	2.65	0.2290

Thymine : Cytosine (interstrand)	*const*	-68.98	-331.71	-397.04	-3.64	0.3210
Cytosine dimer (interstrand)	*const*	-93.99	95.54	0.37	1.19	0.1330
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-264.89	0.50	0.1180
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-271.05	6.66	0.1210
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-183.76	-4.21	0.1080
Guanine : Cytosine (stacked)	*opt*	-132.19	-93.99	-251.71	25.53	0.8380
Methylguanine : Methylcytosine (stacked)	*opt*	-122.16	-68.98	-219.50	28.37	1.1140
Adenine : Thymine (stacked)	*opt*	95.54	-366.16	-294.51	23.90	0.6750
Methyladenine : Methylthymine (stacked)	*opt*	105.74	-331.71	-255.28	29.32	0.4880
Cytosine dimer 1 (stacked)	*const*	-93.99	-93.99	-193.91	5.93	0.0930
Cytosine dimer 2 (stacked)	*const*	-93.99	-93.99	-204.88	16.90	0.1020
Cytosine dimer 3 (stacked)	*const*	-93.99	-93.99	-203.55	15.57	0.1010
Cytosine dimer 4 (stacked)	*const*	-93.99	-93.99	-205.77	17.80	0.1050
Cytosine dimer 5 (stacked)	*const*	-93.99	-93.99	-196.36	8.39	0.0950
Cytosine dimer 6 (stacked)	*const*	-93.99	-93.99	-195.55	7.57	0.0930
Cytosine dimer 7 (stacked)	*const*	-93.99	-93.99	-201.51	13.54	0.0970
Cytosine dimer 8 (stacked)	*const*	-93.99	-93.99	-201.07	13.09	0.1190
Cytosine dimer 9 (stacked)	*const*	-93.99	-93.99	-207.23	19.25	0.1000
Cytosine dimer 10 (stacked)	*const*	-93.99	-93.99	-207.34	19.36	0.1050
Cytosine dimer 11 (stacked)	*const*	-93.99	-93.99	-204.81	16.83	0.1030
Cytosine dimer 12 (stacked)	*const*	-93.99	-93.99	-201.21	13.23	0.0980
Cytosine dimer 13 (stacked)	*const*	-93.99	-93.99	-207.53	19.55	0.1010
Cytosine dimer 14 (stacked)	*const*	-93.99	-93.99	-203.71	15.74	0.1030
Adenine dimer (stacked)	*const*	95.35	95.35	172.93	17.77	0.1050
guanine dimer (stacked)	*const*	-132.19	-132.19	-287.17	22.78	0.1100
Adenine : cytosine (stacked)	*const*	95.35	-93.99	-18.43	19.79	0.1020
Guanine : Adenine (stacked)	*const*	-132.19	95.35	-58.15	21.31	0.1060
Cytosine dimer (stacked)	*const*	-93.99	-93.99	-206.64	18.67	0.0990
Adenine : Uracil (stacked)	*const*	95.35	-346.86	-270.98	19.47	0.0930
Guanine : Cytosine (stacked)	*const*	-132.19	-93.99	-243.71	17.53	0.1090
Cytosine : Uracil (stacked)	*const*	-93.99	-346.86	-457.76	16.91	0.1120
Uracil dimer (Stacked)	*const*	-346.86	-346.86	-710.85	17.12	0.1130
Guanine : Uracil (stacked)	*const*	-132.19	-346.86	-496.93	17.87	0.0980
Guanine dimer (stacked)	*const*	-93.99	-93.99	-202.63	14.65	0.1050
Cytosine dimer (stacked)	*const*	-93.99	-132.19	-231.98	5.79	0.1080
Adenine dimer (stacked)	*const*	95.54	95.54	179.14	11.95	0.0980
Thymine dimer (stacked)	*const*	95.54	-366.01	-272.71	2.25	0.1090
Guanine : cytosine (stacked)	*const*	-93.99	-132.19	-243.52	17.34	0.1060
Guanine : cytosine (stacked)	*const*	-93.99	-132.19	-237.81	11.63	0.1070
Adenine : guanine (stacked)	*const*	95.54	-132.19	-55.09	18.45	0.1060
Thymine : cytosine (stacked)	*const*	-366.01	-93.99	-478.45	18.45	0.0970
Adenine : guanine (stacked)	*const*	95.54	-132.19	-46.83	10.19	0.1040
Thymine : cytosine (stacked)	*const*	-366.01	-93.99	-474.68	14.68	0.2010
Thymine : guanine (stacked)	*const*	-366.01	-132.19	-511.93	13.73	0.1090
Adenine : cytosine (stacked)	*const*	95.54	-93.99	-9.75	11.31	0.1050
Thymine : guanine (stacked)	*const*	-366.01	-132.19	-511.57	13.37	0.2050
Adenine : cytosine (stacked)	*const*	95.54	-93.99	-13.31	14.86	0.0990
Adenine : thymine (stacked)	*const*	95.54	-366.01	-285.27	14.80	0.1750
Adenine : thymine (stacked)	*const*	95.54	-366.01	-288.99	18.53	0.1310
Adenine dimer (stacked)	*const*	95.54	95.54	178.51	12.58	0.0990
Thymine dimer (stacked)	*const*	-366.01	-366.01	-748.41	16.40	0.2160
Adenine : Thymine (stacked)	*const*	105.74	-331.71	-247.70	21.74	0.1910
Guanine : Cytosine (stacked)	*const*	-68.98	-122.16	-204.13	13.00	0.1910
Adenine : Cytosine (stacked)	*const*	105.74	-68.98	18.41	18.36	0.3390
Thymine : Guanine (stacked)	*const*	-331.71	-122.16	-473.43	19.57	0.2100
guanine : Cytosine (stacked)	*const*	-93.99	-132.19	-241.96	15.77	0.1150
Adenine : Guanine (stacked)	*const*	95.54	-132.19	-50.36	13.71	0.1360
Cytosine : guanine (stacked)	*const*	-132.19	-93.99	-241.55	15.36	0.1070
Guanine : Cytosine (stacked)	*const*	-132.19	-93.99	-245.97	19.79	0.1290
Phe30 : Lys46 (1RB9)	*const*	42.83	56.90	89.70	10.03	0.0860
Phe30 : Leu33 (1RB9)	*const*	42.86	41.95	64.24	20.57	0.1030
Phe30 : Tyr13 (1RB9)	*const*	42.80	34.40	64.29	12.91	0.0840
Phe30 : Phe49 (1RB9)	*const*	39.06	42.84	74.31	7.59	0.0900
Phe30 : Tyr4 (1RB9)	*const*	42.80	40.89	67.47	16.23	0.0940
Phe49 : Cys39 (1RB9)	*const*	39.13	8.40	48.91	-1.38	0.0980
Phe49 : Cys6 (1RB9)	*const*	39.03	9.75	33.18	15.60	0.0990
Phe49 : Lys46 (1RB9)	*const*	41.70	45.54	76.23	11.02	0.0860
Phe49 : Val5 (1RB9)	*const*	39.49	40.99	61.55	18.92	0.1020
Phe49 : Tyr37 (1RB9)	*const*	41.05	72.20	113.20	0.06	0.0910
Phe49 : Tyr4 (1RB9)	*const*	39.04	40.36	69.28	10.12	0.0960
Phe49 : Peptide bond (1RB9)	*const*	41.08	-91.75	-55.74	5.07	0.1010
Phe49 : Peptide bond (1RB9)	*const*	39.18	-91.75	-76.62	24.06	0.1030
Glu47 : Lys6 (PDB:1IU5)	*const*	200.96	12.39	-117.85	331.19	0.1660
Glu49 : Lys6 (PDB:1BQ9)	*const*	200.78	27.62	-226.76	455.16	0.1170
Glu54 : Lys2 (PDB:1SMM)	*const*	217.83	24.82	-114.81	357.46	0.1240
Glu50 : LysK30 (PDB:1BRF)	*const*	194.39	4.24	-49.53	248.17	0.1210
Glu50 : Lys52 (PDB:1BRF)	*const*	194.82	28.32	-146.37	369.51	0.1040
Glu49 : Lys6 (PDB:1BRF)	*const*	204.59	27.18	-44.72	276.48	0.1090

MM3*

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-849.37	-416.21	-1282.61	17.02	0.8970
Methylguanine : Methylcytosine (WC)	*opt*	-368.79	-817.35	-1203.79	17.65	1.0250
Adenine : Thymine (WC)	*opt*	-211.61	-642.41	-876.13	22.11	0.6350
Methyladenine : Methylthymine (planar)	*opt*	-210.94	-642.41	-886.53	33.18	2.4170
8-Oxoguanine : Cytosine (WC planar)	*opt*	-877.97	-416.21	-1312.01	17.83	1.4060
Inosine : Cytosine (WC planar)	*opt*	-416.21	-260.63	-699.73	22.90	0.4930

Guanine : Uracil (wobble)	*opt*	-849.47	-705.99	-1570.93	15.47	0.4810
Cytosine : CytosineH+	*opt*	Missing params				
Uracil dimer (Calcutta planar)	*opt*	-705.99	-705.99	-1424.34	12.36	0.2140
Uracil dimer (planar)	*opt*	-705.99	-705.99	-1427.10	15.12	0.1360
6-Thioguanine : Cytosine (WC planar)	*opt*	Missing params				
Adenine : 4-Thiouracil (WC)	*opt*	Missing params				
2-aminoadenine : Thymine	*opt*	-600.42	-707.54	-1327.28	19.31	0.4810
2-aminoadenine : Thymine (planar)	*opt*	-600.82	-707.54	-1328.19	19.83	0.4840
Adenine : Difluorotoluene	*opt*	-243.35	-45.26	-307.65	19.04	1.8100
Guanine : 4-Thiouracil	*opt*	Missing params				
Guanine : 2-Thiouracil	*opt*	Missing params				
Adenine : Cytosine (planar)	*opt*	-416.27	-243.05	-690.37	31.06	2.4140
Guanine dimer (planar)	*opt*	-849.47	-849.47	-1730.13	31.19	2.0280
Guanine 6-Thioguanine (planar)	*opt*	Missing params				
6-Thioguanine : Guanine (planar)	*opt*	Missing params				
Guanine : Adenine 1	*opt*	-849.47	-243.05	-1107.20	14.68	1.6060
Guanine : Adenine 1 (planar)	*opt*	-243.11	-849.51	-1116.61	24.00	2.7120
Guanine : Adenine 2	*opt*	-849.48	-243.05	-1136.13	43.60	2.4390
Guanine : Adenine 2 (planar)	*opt*	-849.47	-243.37	-1136.38	43.54	2.6930
Guanine : Adenine 3	*opt*	-849.48	-243.05	-1125.09	32.56	2.6880
Guanine : Adenine 4	*opt*	-849.48	-243.05	-1101.22	8.69	0.8130
Adenine dimer 1 (planar)	*opt*	-243.05	-243.05	-517.75	31.65	3.1400
Adenine dimer 2 (planar)	*opt*	-243.05	-243.13	-529.48	43.30	3.3880
Adenine dimer 3 (planar)	*opt*	-243.05	-243.05	-536.60	50.50	2.3110
8-Oxoguanine : Guanine	*opt*	-849.82	-877.97	-1757.28	29.49	0.5870
2-Thiouracil dimer (planar)	*opt*	Missing params				
Adenine : Thymine (WC)	*const*	-210.34	-642.41	-857.77	5.02	0.1980
Guanine : Cytosine (WC)	*const*	-368.85	-816.84	-1187.87	2.18	0.3380
Adenine : thymine (WC)	*const*	-210.66	-642.41	-855.74	2.67	0.1650
Guanine : adenine (HB)	*const*	-849.37	-243.03	-1098.93	6.53	0.3950
Cytosine : Guanine (WC)	*const*	-416.27	-849.37	-1272.43	6.79	0.2700
Guanine : Cytosine (WC)	*const*	-849.37	-416.21	-1269.69	4.11	0.3000
Cytosine : guanine (interstrand)	*const*	-849.48	-416.21	-1276.74	11.05	0.3760
Adenine : thymine (interstrand)	*const*	-707.54	-243.05	-965.86	15.27	0.2020
Cytosine dimer (interstrand)	*const*	-416.21	-416.21	-830.92	-1.50	0.2880
Guanine dimer (interstrand)	*const*	-849.47	-849.47	-1708.08	9.14	0.5590
Cytosine dimer (interstrand)	*const*	-416.21	-416.21	-839.87	7.45	0.2640
Guanine dimer (interstrand)	*const*	-849.47	-849.47	-1704.85	5.91	0.3280
Adenine : cytosine (interstrand)	*const*	-243.05	-416.21	-662.72	3.46	0.2820
Thymine : guanine (interstrand)	*const*	-707.54	-849.47	-1564.40	7.39	0.3450
Thymine : guanine (interstrand)	*const*	-849.47	-707.54	-1568.49	11.48	0.3490
Thymine : cytosine (interstrand)	*const*	-243.05	-416.21	-670.11	10.85	0.3070
Adenine : guanine (interstrand)	*const*	-243.05	-849.47	-1104.83	12.31	0.3150
Thymine : cytosine (interstrand)	*const*	-707.54	-416.21	-1133.80	10.05	0.2480
Thymine : cytosine (interstrand)	*const*	-707.54	-416.21	-1125.95	2.20	0.2040
Adenine : guanine (interstrand)	*const*	-243.05	-849.48	-1107.40	14.87	0.4240
Thymine dimer (interstrand)	*const*	-707.54	-707.54	-1416.86	1.78	0.0860
Adenine dimer (interstrand)	*const*	-243.05	-243.05	-497.52	11.42	0.2200
Adenine dimer (interstrand)	*const*	-243.05	-243.05	-489.40	3.30	0.2570
Thymine dimer (interstrand)	*const*	-707.54	-707.54	-1419.56	4.48	0.1100
Adenine : thymine (interstrand)	*const*	-243.05	-707.54	-958.39	7.80	0.2080
Thymine : adenine (interstrand)	*const*	-243.05	-707.54	-963.32	12.73	0.2140
Adenine dimer (interstrand)	*const*	-210.73	-210.39	-432.16	11.04	0.2590
Thymine dimer (interstrand)	*const*	-642.41	-642.41	-1286.33	1.52	0.1550
Guanine dimer (interstrand)	*const*	-816.94	-816.94	-1645.88	12.00	0.5240
Cytosine dimer (interstrand)	*const*	-368.85	-368.85	-747.47	9.76	0.2430
Adenine : Guanine (interstrand)	*const*	-210.66	-816.81	-1043.75	16.28	0.3990
Thymine : Cytosine (interstrand)	*const*	-368.85	-642.41	-1012.98	1.72	0.3510
Cytosine dimer (interstrand)	*const*	-416.27	-243.03	-661.44	2.14	0.2430
Guanine dimer (interstrand)	*const*	-849.37	-849.37	-1708.66	9.91	0.4070
Guanine dimer (interstrand)	*const*	-849.37	-849.37	-1708.23	9.49	0.5230
Cytosine dimer (interstrand)	*const*	-416.27	-416.21	-831.90	-0.58	0.2650
Guanine : Cytosine (stacked)	*opt*	-849.47	-416.21	-1289.82	24.14	0.8770
Methylguanine : Methylcytosine (stacked)	*opt*	-817.36	-368.79	-1213.13	26.98	0.8240
Adenine : Thymine (stacked)	*opt*	-242.69	-707.54	-982.24	32.01	0.6110
Methyladenine : Methylthymine (stacked)	*opt*	-211.18	-642.41	-887.08	33.49	1.2270
Cytosine dimer 1 (stacked)	*const*	-416.21	-416.21	-830.76	-1.66	0.1480
Cytosine dimer 2 (stacked)	*const*	-416.21	-416.21	-847.13	14.72	0.3300
Cytosine dimer 3 (stacked)	*const*	-416.21	-416.21	-851.97	19.55	0.2840
Cytosine dimer 4 (stacked)	*const*	-416.21	-416.21	-851.73	19.31	0.2580
Cytosine dimer 5 (stacked)	*const*	-416.21	-416.21	-841.51	9.10	0.2540
Cytosine dimer 6 (stacked)	*const*	-416.21	-416.21	-842.72	10.30	0.2770
Cytosine dimer 7 (stacked)	*const*	-416.21	-416.21	-846.63	14.22	0.2350
Cytosine dimer 8 (stacked)	*const*	-416.21	-416.21	-852.16	19.74	0.2960
Cytosine dimer 9 (stacked)	*const*	-416.21	-416.21	-852.67	20.25	0.2600
Cytosine dimer 10 (stacked)	*const*	-416.21	-416.21	-854.25	21.83	0.2360
Cytosine dimer 11 (stacked)	*const*	-416.21	-416.21	-849.33	16.92	0.2470
Cytosine dimer 12 (stacked)	*const*	-416.21	-416.21	-842.83	10.41	0.3140
Cytosine dimer 13 (stacked)	*const*	-416.21	-416.21	-854.66	22.25	0.2160
Cytosine dimer 14 (stacked)	*const*	-416.21	-416.21	-845.21	12.79	0.1800
Adenine dimer (stacked)	*const*	-242.36	-243.08	-529.02	43.58	0.3050
guanine dimer (stacked)	*const*	-849.47	-849.48	-1722.82	23.87	0.3960
Adenine : cytosine (stacked)	*const*	-243.08	-416.21	-691.68	32.39	0.3100
Guanine : Adenine (stacked)	*const*	-849.47	-242.36	-1129.81	37.98	0.3460
Cytosine dimer (stacked)	*const*	-416.21	-416.21	-849.95	17.53	0.2350
Adenine : Uracil (stacked)	*const*	-242.36	-705.99	-974.58	26.23	0.1980
Guanine : Cytosine (stacked)	*const*	-849.47	-416.21	-1285.02	19.34	0.4240
Cytosine : Uracil (stacked)	*const*	-416.21	-705.99	-1143.42	21.21	0.2480

Uracil dimer (Stacked)	*const*	-705.99	-705.99	-1432.28	20.30	0.0900
Guanine : Uracil (stacked)	*const*	-849.48	-705.99	-1583.06	27.59	0.3370
Guanine dimer (stacked)	*const*	-416.21	-416.21	-844.17	11.75	0.2810
Cytosine dimer (stacked)	*const*	-416.21	-849.47	-1280.45	14.77	0.4420
Adenine dimer (stacked)	*const*	-242.33	-243.05	-495.90	10.52	0.2790
Thymine dimer (stacked)	*const*	-243.05	-707.54	-957.76	7.17	0.1960
Guanine : cytosine (stacked)	*const*	-416.21	-849.47	-1280.55	14.87	0.3660
Guanine : cytosine (stacked)	*const*	-416.21	-849.48	-1284.42	18.73	0.4710
Adenine : guanine (stacked)	*const*	-242.33	-849.47	-1112.90	21.10	0.3970
Thymine : cytosine (stacked)	*const*	-707.54	-416.21	-1133.75	10.00	0.1290
Adenine : guanine (stacked)	*const*	-243.05	-849.48	-1116.45	23.92	0.4120
Thymine : cytosine (stacked)	*const*	-707.54	-416.21	-1139.69	15.94	0.2920
Thymine : guanine (stacked)	*const*	-707.54	-849.47	-1570.50	13.49	0.3750
Adenine : cytosine (stacked)	*const*	-242.33	-416.21	-671.26	12.71	0.2780
Thymine : guanine (stacked)	*const*	-707.54	-849.47	-1573.42	16.41	0.3480
Adenine : cytosine (stacked)	*const*	-242.33	-416.21	-668.61	10.07	0.4070
Adenine : thymine (stacked)	*const*	-243.05	-707.54	-967.90	17.30	0.2710
Adenine : thymine (stacked)	*const*	-242.33	-707.54	-959.93	10.06	0.2350
Adenine dimer (stacked)	*const*	-242.33	-242.33	-500.16	15.50	0.2980
Thymine dimer (stacked)	*const*	-707.54	-707.54	-1428.66	13.58	0.1870
Adenine : Thymine (stacked)	*const*	-210.28	-642.41	-866.31	13.62	0.2150
Guanine : Cytosine (stacked)	*const*	-368.85	-816.90	-1204.22	18.47	0.4620
Adenine : Cytosine (stacked)	*const*	-210.63	-368.85	-590.71	11.23	0.4550
Thymine : Guanine (stacked)	*const*	-642.41	-816.87	-1476.51	17.23	0.3440
guanine : Cytosine (stacked)	*const*	-416.27	-849.37	-1290.16	24.53	0.4460
Adenine : Guanine (stacked)	*const*	-243.03	-849.37	-1117.01	24.61	0.4460
Cytosine : guanine (stacked)	*const*	-849.37	-416.27	-1283.29	17.65	0.3660
Guanine : Cytosine (stacked)	*const*	-849.37	-416.21	-1280.95	15.37	0.4500
Phe30 : Lys46 (1RB9)	*const*	107.34	67.19	165.37	9.16	0.1160
Phe30 : Leu33 (1RB9)	*const*	107.52	57.47	154.51	10.47	0.1490
Phe30 : Tyr13 (1RB9)	*const*	107.37	79.48	177.35	9.51	0.1170
Phe30 : Phe49 (1RB9)	*const*	98.33	107.52	197.20	8.65	0.1250
Phe30 : Tyr4 (1RB9)	*const*	107.35	84.32	181.67	10.00	0.1290
Phe49 : Cys39 (1RB9)	*const*	98.55	92.11	191.24	-0.58	0.1260
Phe49 : Cys6 (1RB9)	*const*	98.39	89.89	177.97	10.31	0.1270
Phe49 : Lys46 (1RB9)	*const*	105.27	61.86	160.94	6.19	0.1140
Phe49 : Val5 (1RB9)	*const*	99.00	59.87	145.27	13.60	0.1540
Phe49 : Tyr37 (1RB9)	*const*	104.74	166.14	278.55	-7.68	0.1210
Phe49 : Tyr4 (1RB9)	*const*	98.33	81.40	174.07	5.66	0.1140
Phe49 : Peptide bond (1RB9)	*const*	104.74	-39.18	63.63	1.93	0.1720
Phe49 : Peptide bond (1RB9)	*const*	98.63	-39.18	41.56	17.90	0.1880
Glu47 : Lys6 (PDB:1IU5)	*const*	74.53	2.00	-258.29	334.82	0.1450
Glu49 : Lys6 (PDB:1BQ9)	*const*	79.17	34.49	-369.71	483.36	0.1320
Glu54 : Lys2 (PDB:1SMM)	*const*	108.12	38.12	-249.10	395.34	0.2180
Glu50 : LysK30 (PDB:1BRF)	*const*	72.94	-8.42	-195.04	259.56	0.1580
Glu50 : Lys52 (PDB:1BRF)	*const*	73.91	35.36	-307.17	416.44	0.1220
Glu49 : Lys6 (PDB:1BRF)	*const*	84.94	33.94	-172.35	291.23	0.3560

AMBER*

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-361.60	-331.02	-786.33	93.72	0.0850
Methylguanine : Methylcytosine (WC)	*opt*	-325.83	-363.43	-786.83	97.57	0.1290
Adenine : Thymine (WC)	*opt*	-362.20	-627.86	-1043.25	53.19	0.4130
Methyladenine : Methylthymine (planar)	*opt*	-362.20	-627.86	-1039.29	49.24	0.2010
8-Oxoguanine : Cytosine (WC planar)	*opt*	-205.55	-331.02	-596.69	60.12	0.0710
Inosine : Cytosine (WC planar)	*opt*	-331.02	-27.76	-416.04	57.26	0.1580
Guanine : Uracil (wobble)	*opt*	-361.60	-336.61	-749.36	51.16	0.1240
Cytosine : CytosineH+	*opt*	-331.02	-70.06	-483.05	81.98	0.1160
Uracil dimer (Calcutta planar)	*opt*	-336.61	-336.61	-699.21	25.99	0.1980
Uracil dimer (planar)	*opt*	-336.61	-336.61	-712.87	39.66	0.0550
6-Thioguanine : Cytosine (WC planar)	*opt*	-331.02	-179.73	-556.07	45.32	0.1080
Adenine : 4-Thiouracil (WC)	*opt*	-363.92	-186.26	-570.11	19.93	3.8870
2-aminoadenine : Thymine	*opt*	-458.77	-631.08	-1156.67	66.82	0.2910
2-aminoadenine : Thymine (planar)	*opt*	-458.77	-630.94	-1156.45	66.73	0.0530
Adenine : Difluorotoluene	*opt*	-364.94	-11.91	-418.09	41.24	2.7530
Guanine : 4-Thiouracil	*opt*	-361.60	-186.26	-594.47	46.61	0.2090
Guanine : 2-Thiouracil	*opt*	-361.60	-186.87	-602.19	53.72	1.9750
Adenine : Cytosine (planar)	*opt*	-331.02	-363.92	-754.71	59.77	0.0710
Guanine dimer (planar)	*opt*	-361.60	-361.60	-781.23	58.03	0.1740
Guanine 6-Thioguanine (planar)	*opt*	-361.60	-179.73	-585.73	44.40	0.2090
6-Thioguanine : Guanine (planar)	*opt*	-179.73	-361.60	-573.16	31.83	0.1600
Guanine : Adenine 1	*opt*	-361.60	-363.92	-792.75	67.24	0.1810
Guanine : Adenine 1 (planar)	*opt*	-364.94	-361.60	-793.36	66.83	0.0310
Guanine : Adenine 2	*opt*	-361.60	-363.92	-772.64	47.13	0.3090
Guanine : Adenine 2 (planar)	*opt*	-361.60	-363.92	-771.50	45.98	0.0990
Guanine : Adenine 3	*opt*	-361.60	-363.92	-779.19	53.67	0.7170
Guanine : Adenine 4	*opt*	-361.60	-363.92	-764.23	38.72	0.4100
Adenine dimer 1 (planar)	*opt*	-363.92	-363.92	-785.70	57.86	0.0490
Adenine dimer 2 (planar)	*opt*	-363.92	-364.94	-773.78	44.92	0.3570
Adenine dimer 3 (planar)	*opt*	-363.92	-363.92	-773.77	45.93	1.2080
8-Oxoguanine : Guanine	*opt*	-361.60	-205.55	-603.32	36.18	0.2130
2-Thiouracil dimer (planar)	*opt*	-186.87	-186.87	-391.80	18.06	0.3600
Adenine : Thymine (WC)	*const*	-362.20	-627.86	-1042.00	51.95	0.3750
Guanine : Cytosine (WC)	*const*	-325.83	-363.43	-786.26	96.99	0.4080
Adenine : thymine (WC)	*const*	-362.20	-627.86	-1040.69	50.63	0.3480
Guanine : adenine (HB)	*const*	-361.60	-364.94	-771.45	44.91	0.0960
Cytosine : Guanine (WC)	*const*	-331.02	-361.60	-785.10	92.48	0.0730

Guanine : Cytosine (WC)	*const*	-361.60	-331.02	-786.22	93.60	0.0670
Cytosine : guanine (interstrand)	*const*	-361.60	-331.02	-711.22	18.61	0.1200
Adenine : thymine (interstrand)	*const*	-631.08	-363.92	-1011.84	16.84	0.2110
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-654.77	-7.27	0.1060
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-725.90	2.71	0.0790
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-662.35	0.31	0.1130
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-746.56	23.36	0.0940
Adenine : cytosine (interstrand)	*const*	-363.92	-331.02	-696.75	1.81	0.0990
Thymine : guanine (interstrand)	*const*	-631.08	-361.60	-998.61	5.93	0.1900
Thymine : guanine (interstrand)	*const*	-361.60	-631.08	-1006.05	13.37	0.1830
Thymine : cytosine (interstrand)	*const*	-363.92	-331.02	-701.21	6.27	0.1000
Adenine : guanine (interstrand)	*const*	-363.92	-361.60	-745.41	19.89	0.0830
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-971.46	9.36	0.1990
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-968.23	6.13	0.1940
Adenine : guanine (interstrand)	*const*	-363.92	-361.60	-748.62	23.10	0.1020
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1266.24	4.07	0.2460
Adenine dimer (interstrand)	*const*	-363.92	-363.92	-740.59	12.75	0.0920
Adenine dimer (interstrand)	*const*	-363.92	-363.92	-741.09	13.25	0.0980
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1267.37	5.21	0.2700
Adenine : thymine (interstrand)	*const*	-363.92	-631.08	-1008.10	13.10	0.1830
Thymine : adenine (interstrand)	*const*	-363.92	-631.08	-1006.76	11.76	0.1990
Adenine dimer (interstrand)	*const*	-362.20	-362.20	-742.08	17.69	0.3360
Thymine dimer (interstrand)	*const*	-627.86	-627.86	-1261.26	5.55	0.4360
Guanine dimer (interstrand)	*const*	-363.43	-363.43	-757.19	30.33	0.4090
Cytosine dimer (interstrand)	*const*	-325.83	-325.83	-657.86	6.19	0.4330
Adenine : Guanine (interstrand)	*const*	-362.20	-363.43	-753.76	28.13	0.3030
Thymine : Cytosine (interstrand)	*const*	-325.83	-627.86	-958.67	4.98	0.3460
Cytosine dimer (interstrand)	*const*	-331.02	-364.94	-715.36	19.39	0.1660
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-738.69	15.50	0.0960
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-731.92	8.73	0.1100
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-656.09	-5.95	0.0950
Guanine : Cytosine (stacked)	*opt*	-361.60	-331.02	-745.60	52.98	0.3540
Methylguanine : Methylcytosine (stacked)	*opt*	-363.43	-325.83	-744.54	55.28	0.3810
Adenine : Thymine (stacked)	*opt*	-364.94	-631.08	-1040.69	44.67	0.4270
Methyladenine : Methylthymine (stacked)	*opt*	-362.20	-627.86	-1039.27	49.22	0.5470
Cytosine dimer 1 (stacked)	*const*	-331.02	-331.02	-664.15	2.11	0.0750
Cytosine dimer 2 (stacked)	*const*	-331.02	-331.02	-682.80	20.76	0.1170
Cytosine dimer 3 (stacked)	*const*	-331.02	-331.02	-704.62	42.58	0.1200
Cytosine dimer 4 (stacked)	*const*	-331.02	-331.02	-711.96	49.92	0.0940
Cytosine dimer 5 (stacked)	*const*	-331.02	-331.02	-668.17	6.13	0.0990
Cytosine dimer 6 (stacked)	*const*	-331.02	-331.02	-666.95	4.91	0.1060
Cytosine dimer 7 (stacked)	*const*	-331.02	-331.02	-669.77	7.73	0.1160
Cytosine dimer 8 (stacked)	*const*	-331.02	-331.02	-707.49	45.45	0.1010
Cytosine dimer 9 (stacked)	*const*	-331.02	-331.02	-710.86	48.82	0.0850
Cytosine dimer 10 (stacked)	*const*	-331.02	-331.02	-708.54	46.50	0.0870
Cytosine dimer 11 (stacked)	*const*	-331.02	-331.02	-712.40	50.36	0.0960
Cytosine dimer 12 (stacked)	*const*	-331.02	-331.02	-695.30	33.26	0.1010
Cytosine dimer 13 (stacked)	*const*	-331.02	-331.02	-702.97	40.93	0.0930
Cytosine dimer 14 (stacked)	*const*	-331.02	-331.02	-709.86	47.82	0.1120
Adenine dimer (stacked)	*const*	-363.92	-363.92	-771.73	43.89	0.0990
guanine dimer (stacked)	*const*	-361.60	-361.60	-781.39	58.19	0.0960
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-738.36	43.42	0.0940
Guanine : Adenine (stacked)	*const*	-361.60	-363.92	-777.55	52.03	0.0840
Cytosine dimer (stacked)	*const*	-331.02	-331.02	-712.59	50.55	0.0870
Adenine : Uracil (stacked)	*const*	-363.92	-336.61	-743.33	42.80	0.0840
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-745.24	52.63	0.1100
Cytosine : Uracil (stacked)	*const*	-331.02	-336.61	-712.96	45.33	0.0990
Uracil dimer (Stacked)	*const*	-336.61	-336.61	-706.38	33.17	0.0720
Guanine : Uracil (stacked)	*const*	-361.60	-336.61	-750.59	52.39	0.0830
Guanine dimer (stacked)	*const*	-331.02	-331.02	-670.34	8.30	0.1040
Cytosine dimer (stacked)	*const*	-331.02	-361.60	-713.82	21.21	0.1100
Adenine dimer (stacked)	*const*	-363.92	-363.92	-764.68	36.84	0.0950
Thymine dimer (stacked)	*const*	-363.92	-631.08	-1008.65	13.65	0.1780
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-743.10	50.48	0.1180
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-729.13	36.52	0.1070
Adenine : guanine (stacked)	*const*	-363.92	-361.60	-773.42	47.90	0.1010
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-986.51	24.40	0.1890
Adenine : guanine (stacked)	*const*	-363.92	-361.60	-766.46	40.94	0.0990
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-989.39	27.29	0.2440
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1022.36	29.69	0.1670
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-725.57	30.63	0.0950
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1024.86	32.18	0.1970
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-722.42	27.48	0.1010
Adenine : thymine (stacked)	*const*	-363.92	-631.08	-1026.86	31.86	0.1740
Adenine : thymine (stacked)	*const*	-363.92	-631.08	-1024.42	29.42	0.2740
Adenine dimer (stacked)	*const*	-363.92	-363.92	-765.14	37.30	0.0960
Thymine dimer (stacked)	*const*	-631.08	-631.08	-1287.39	25.23	0.2440
Adenine : Thymine (stacked)	*const*	-362.20	-627.86	-1025.24	35.19	0.2960
Guanine : Cytosine (stacked)	*const*	-325.83	-363.43	-719.80	30.54	0.3870
Adenine : Cytosine (stacked)	*const*	-362.20	-325.83	-719.78	31.75	0.1190
Thymine : Guanine (stacked)	*const*	-627.86	-363.43	-1024.83	33.54	0.3680
guanine : Cytosine (stacked)	*const*	-331.02	-361.60	-732.62	40.00	0.1090
Adenine : Guanine (stacked)	*const*	-364.94	-361.60	-765.73	39.19	0.1110
Cytosine : guanine (stacked)	*const*	-361.60	-331.02	-743.08	50.46	0.1310
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-743.86	51.24	0.1350
Phe30 : Lys46 (1RB9)	*const*	37.41	29.69	55.56	11.55	0.1350
Phe30 : Leu33 (1RB9)	*const*	37.55	8.45	26.26	19.73	0.2360
Phe30 : Tyr13 (1RB9)	*const*	37.43	20.30	48.52	9.20	0.1350

Phe30 : Phe49 (1RB9)	*const*	13.71	37.63	39.04	12.29	0.1410
Phe30 : Tyr4 (1RB9)	*const*	37.40	25.85	45.42	17.82	0.1550
Phe49 : Cys39 (1RB9)	*const*	13.58	15.01	43.33	-14.74	0.1550
Phe49 : Cys6 (1RB9)	*const*	13.50	8.03	12.59	8.94	0.1520
Phe49 : Lys46 (1RB9)	*const*	25.18	29.20	37.07	17.31	0.1350
Phe49 : Val5 (1RB9)	*const*	14.02	11.40	4.57	20.85	0.1570
Phe49 : Tyr37 (1RB9)	*const*	25.18	-13.15	4.26	7.77	0.1320
Phe49 : Tyr4 (1RB9)	*const*	13.61	19.04	27.33	5.32	0.1210
Phe49 : Peptide bond (1RB9)	*const*	25.44	-69.99	-53.04	8.49	0.3320
Phe49 : Peptide bond (1RB9)	*const*	13.81	-69.99	-81.95	25.77	0.2990
Glu47 : Lys6 (PDB:1IU5)	*const*	184.34	-86.30	-212.21	310.25	0.1180
Glu49 : Lys6 (PDB:1BQ9)	*const*	178.58	-89.98	-344.59	433.18	0.1440
Glu54 : Lys2 (PDB:1SMM)	*const*	160.81	-73.45	-245.15	332.51	0.1910
Glu50 : LysK30 (PDB:1BRF)	*const*	177.23	-88.33	-166.36	255.25	0.1720
Glu50 : Lys52 (PDB:1BRF)	*const*	178.20	-89.49	-285.47	374.18	0.1490
Glu49 : Lys6 (PDB:1BRF)	*const*	203.14	-90.07	-173.77	286.84	0.3830

AMBER* (10,12-H bonding potential)

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-361.60	-331.02	-782.69	90.08	0.0910
Methylguanine : Methylcytosine (WC)	*opt*	-325.83	-363.43	-783.25	93.99	0.1330
Adenine : Thymine (WC)	*opt*	-361.86	-627.86	-1042.04	52.32	0.3990
Methyladenine : Methylthymine (planar)	*opt*	-361.86	-627.86	-1039.42	49.70	0.1790
8-Oxoguanine : Cytosine (WC planar)	*opt*	-205.55	-331.02	-595.28	58.72	0.0690
Inosine : Cytosine (WC planar)	*opt*	-331.02	-27.76	-415.27	56.49	0.1400
Guanine : Uracil (wobble)	*opt*	-361.60	-336.61	-747.79	49.59	0.1570
Cytosine : CytosineH+	*opt*	-331.02	-70.06	-482.76	81.68	0.1450
Uracil dimer (Calcutta planar)	*opt*	-336.61	-336.61	-698.43	25.22	0.1860
Uracil dimer (planar)	*opt*	-336.61	-336.61	-711.75	38.54	0.0830
6-Thioguanine : Cytosine (WC planar)	*opt*	-331.02	-179.73	-561.18	50.43	1.0990
Adenine : 4-Thiouracil (WC)	*opt*	-363.58	-186.26	-569.44	19.59	3.8870
2-aminoadenine : Thymine	*opt*	-458.44	-631.08	-1154.73	65.21	0.2920
2-aminoadenine : Thymine (planar)	*opt*	-458.44	-630.94	-1154.37	64.98	0.0470
Adenine : Difluorotoluene	*opt*	-364.61	-11.91	-417.75	41.24	2.7540
Guanine : 4-Thiouracil	*opt*	-361.60	-186.26	-594.33	46.47	0.3000
Guanine : 2-Thiouracil	*opt*	-361.60	-186.87	-602.11	53.65	1.9850
Adenine : Cytosine (planar)	*opt*	-331.02	-363.58	-756.15	61.55	0.0790
Guanine dimer (planar)	*opt*	-361.60	-361.60	-782.29	59.09	0.1360
Guanine 6-Thioguanine (planar)	*opt*	-361.60	-179.73	-585.51	44.18	0.1850
6-Thioguanine : Guanine (planar)	*opt*	-179.73	-361.60	-574.13	32.81	0.1180
Guanine : Adenine 1	*opt*	-361.60	-363.58	-790.64	65.46	0.2050
Guanine : Adenine 1 (planar)	*opt*	-364.61	-361.60	-790.05	63.85	0.0500
Guanine : Adenine 2	*opt*	-361.60	-363.58	-774.38	49.21	0.3270
Guanine : Adenine 2 (planar)	*opt*	-361.60	-363.58	-773.30	48.12	0.0940
Guanine : Adenine 3	*opt*	-361.60	-363.58	-779.13	53.95	0.7790
Guanine : Adenine 4	*opt*	-361.60	-363.58	-765.90	40.72	0.4060
Adenine dimer 1 (planar)	*opt*	-363.58	-363.58	-787.07	59.91	0.0770
Adenine dimer 2 (planar)	*opt*	-363.58	-364.61	-777.33	49.14	0.4400
Adenine dimer 3 (planar)	*opt*	-363.58	-363.58	-775.96	48.79	1.1490
8-Oxoguanine : Guanine	*opt*	-361.60	-205.55	-600.39	33.25	0.2240
2-Thiouracil dimer (planar)	*opt*	-186.87	-186.87	-391.72	17.98	0.3760
Adenine : Thymine (WC)	*const*	-361.86	-627.86	-1041.45	51.74	0.3720
Guanine : Cytosine (WC)	*const*	-325.83	-363.43	-782.76	93.50	0.4080
Adenine : thymine (WC)	*const*	-361.86	-627.86	-1040.76	51.04	0.3500
Guanine : adenine (HB)	*const*	-361.60	-364.61	-772.79	46.59	0.0960
Cytosine : Guanine (WC)	*const*	-331.02	-361.60	-781.64	89.02	0.0790
Guanine : Cytosine (WC)	*const*	-361.60	-331.02	-782.42	89.80	0.0710
Cytosine : guanine (interstrand)	*const*	-361.60	-331.02	-710.90	18.29	0.1200
Adenine : thymine (interstrand)	*const*	-631.08	-363.58	-1011.68	17.02	0.2120
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-654.77	-7.27	0.1060
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-725.90	2.71	0.0790
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-662.35	0.31	0.1130
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-746.43	23.24	0.0930
Adenine : cytosine (interstrand)	*const*	-363.58	-331.02	-696.42	1.81	0.0990
Thymine : guanine (interstrand)	*const*	-631.08	-361.60	-998.58	5.90	0.1910
Thymine : guanine (interstrand)	*const*	-361.60	-631.08	-1006.05	13.37	0.1830
Thymine : cytosine (interstrand)	*const*	-363.58	-331.02	-700.79	6.19	0.1000
Adenine : guanine (interstrand)	*const*	-363.58	-361.60	-745.02	19.84	0.0820
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-971.41	9.31	0.1990
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-968.23	6.13	0.1940
Adenine : guanine (interstrand)	*const*	-363.58	-361.60	-748.00	22.82	0.1030
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1266.24	4.07	0.2460
Adenine dimer (interstrand)	*const*	-363.58	-363.58	-739.76	12.60	0.0920
Adenine dimer (interstrand)	*const*	-363.58	-363.58	-740.42	13.26	0.0980
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1267.37	5.21	0.2700
Adenine : thymine (interstrand)	*const*	-363.58	-631.08	-1007.61	12.95	0.1840
Thymine : adenine (interstrand)	*const*	-363.58	-631.08	-1006.26	11.59	0.1990
Adenine dimer (interstrand)	*const*	-361.86	-361.86	-741.29	17.57	0.3350
Thymine dimer (interstrand)	*const*	-627.86	-627.86	-1261.26	5.55	0.4360
Guanine dimer (interstrand)	*const*	-363.43	-363.43	-757.11	30.25	0.4090
Cytosine dimer (interstrand)	*const*	-325.83	-325.83	-657.88	6.21	0.4330
Adenine : Guanine (interstrand)	*const*	-361.86	-363.43	-753.12	27.83	0.3020
Thymine : Cytosine (interstrand)	*const*	-325.83	-627.86	-958.67	4.98	0.3460
Cytosine dimer (interstrand)	*const*	-331.02	-364.61	-714.98	19.35	0.1660
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-738.61	15.41	0.0960
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-731.82	8.63	0.1100
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-656.09	-5.95	0.0950

Guanine : Cytosine (stacked)	*opt*	-361.60	-331.02	-745.17	52.55	0.3650
Methylguanine : Methylcytosine (stacked)	*opt*	-363.43	-325.83	-744.32	55.06	0.4030
Adenine : Thymine (stacked)	*opt*	-364.61	-631.08	-1040.27	44.59	0.4280
Methyladenine : Methylthymine (stacked)	*opt*	-361.86	-627.86	-1038.85	49.14	0.5480
Cytosine dimer 1 (stacked)	*const*	-331.02	-331.02	-664.15	2.11	0.0750
Cytosine dimer 2 (stacked)	*const*	-331.02	-331.02	-682.67	20.63	0.1170
Cytosine dimer 3 (stacked)	*const*	-331.02	-331.02	-704.62	42.58	0.1200
Cytosine dimer 4 (stacked)	*const*	-331.02	-331.02	-711.87	49.83	0.0950
Cytosine dimer 5 (stacked)	*const*	-331.02	-331.02	-668.17	6.13	0.0990
Cytosine dimer 6 (stacked)	*const*	-331.02	-331.02	-666.91	4.87	0.1050
Cytosine dimer 7 (stacked)	*const*	-331.02	-331.02	-669.55	7.51	0.1150
Cytosine dimer 8 (stacked)	*const*	-331.02	-331.02	-707.49	45.45	0.1010
Cytosine dimer 9 (stacked)	*const*	-331.02	-331.02	-710.86	48.82	0.0850
Cytosine dimer 10 (stacked)	*const*	-331.02	-331.02	-708.41	46.37	0.0870
Cytosine dimer 11 (stacked)	*const*	-331.02	-331.02	-712.40	50.36	0.0960
Cytosine dimer 12 (stacked)	*const*	-331.02	-331.02	-695.30	33.26	0.1010
Cytosine dimer 13 (stacked)	*const*	-331.02	-331.02	-702.84	40.80	0.0930
Cytosine dimer 14 (stacked)	*const*	-331.02	-331.02	-709.86	47.82	0.1120
Adenine dimer (stacked)	*const*	-363.58	-363.58	-770.70	43.53	0.0990
guanine dimer (stacked)	*const*	-361.60	-361.60	-781.24	58.04	0.0950
Adenine : cytosine (stacked)	*const*	-363.58	-331.02	-738.01	43.41	0.0940
Guanine : Adenine (stacked)	*const*	-361.60	-363.58	-777.06	51.88	0.0840
Cytosine dimer (stacked)	*const*	-331.02	-331.02	-712.59	50.55	0.0870
Adenine : Uracil (stacked)	*const*	-363.58	-336.61	-742.91	42.72	0.0840
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-744.80	52.18	0.1100
Cytosine : Uracil (stacked)	*const*	-331.02	-336.61	-712.84	45.22	0.0990
Uracil dimer (Stacked)	*const*	-336.61	-336.61	-706.38	33.17	0.0720
Guanine : Uracil (stacked)	*const*	-361.60	-336.61	-750.40	52.20	0.0830
Guanine dimer (stacked)	*const*	-331.02	-331.02	-670.34	8.30	0.1040
Cytosine dimer (stacked)	*const*	-331.02	-361.60	-713.68	21.07	0.1100
Adenine dimer (stacked)	*const*	-363.58	-363.58	-763.85	36.69	0.0950
Thymine dimer (stacked)	*const*	-363.58	-631.08	-1008.13	13.46	0.1780
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-742.79	50.18	0.1180
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-729.13	36.52	0.1070
Adenine : guanine (stacked)	*const*	-363.58	-361.60	-772.80	47.62	0.1000
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-986.24	24.14	0.1890
Adenine : guanine (stacked)	*const*	-363.58	-361.60	-766.11	40.93	0.0990
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-989.39	27.29	0.2440
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1022.36	29.69	0.1670
Adenine : cytosine (stacked)	*const*	-363.58	-331.02	-725.23	30.63	0.0950
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1024.82	32.14	0.1970
Adenine : cytosine (stacked)	*const*	-363.58	-331.02	-721.87	27.27	0.1020
Adenine : thymine (stacked)	*const*	-363.58	-631.08	-1026.30	31.64	0.1730
Adenine : thymine (stacked)	*const*	-363.58	-631.08	-1023.80	29.14	0.2740
Adenine dimer (stacked)	*const*	-363.58	-363.58	-764.29	37.13	0.0950
Thymine dimer (stacked)	*const*	-631.08	-631.08	-1287.39	25.23	0.2440
Adenine : Thymine (stacked)	*const*	-361.86	-627.86	-1024.72	35.00	0.2960
Guanine : Cytosine (stacked)	*const*	-325.83	-363.43	-719.80	30.54	0.3870
Adenine : Cytosine (stacked)	*const*	-361.86	-325.83	-719.44	31.75	0.1190
Thymine : Guanine (stacked)	*const*	-627.86	-363.43	-1024.83	33.54	0.3680
guanine : Cytosine (stacked)	*const*	-331.02	-361.60	-732.56	39.95	0.1090
Adenine : Guanine (stacked)	*const*	-364.61	-361.60	-765.34	39.14	0.1100
Cytosine : guanine (stacked)	*const*	-361.60	-331.02	-743.01	50.39	0.1320
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-743.48	50.86	0.1350
Phe30 : Lys46 (1RB9)	*const*	37.42	29.76	55.62	11.56	0.1350
Phe30 : Leu33 (1RB9)	*const*	37.54	8.37	25.68	20.24	0.2370
Phe30 : Tyr13 (1RB9)	*const*	37.43	20.15	48.51	9.06	0.1370
Phe30 : Phe49 (1RB9)	*const*	13.49	37.63	38.88	12.24	0.1420
Phe30 : Tyr4 (1RB9)	*const*	37.40	25.70	45.25	17.84	0.1590
Phe49 : Cys39 (1RB9)	*const*	13.38	14.99	43.28	-14.92	0.1540
Phe49 : Cys6 (1RB9)	*const*	13.28	8.05	12.61	8.72	0.1520
Phe49 : Lys46 (1RB9)	*const*	25.14	29.21	36.99	17.36	0.1350
Phe49 : Val5 (1RB9)	*const*	13.82	11.15	4.20	20.77	0.1590
Phe49 : Tyr37 (1RB9)	*const*	13.32	-13.20	-4.55	4.67	0.3590
Phe49 : Tyr4 (1RB9)	*const*	13.41	18.95	27.11	5.24	0.1190
Phe49 : Peptide bond (1RB9)	*const*	13.46	-69.99	-65.82	9.29	0.5130
Phe49 : Peptide bond (1RB9)	*const*	13.59	-69.99	-82.14	25.75	0.3010
Glu47 : Lys6 (PDB:1IU5)	*const*	184.34	-86.25	-212.08	310.17	0.1170
Glu49 : Lys6 (PDB:1BQ9)	*const*	178.58	-90.27	-344.54	432.84	0.1440
Glu54 : Lys2 (PDB:1SMM)	*const*	161.31	-73.33	-244.41	332.38	0.1910
Glu50 : LysK30 (PDB:1BRF)	*const*	177.03	-84.13	-166.83	259.73	0.1700
Glu50 : Lys52 (PDB:1BRF)	*const*	178.00	-89.80	-285.32	373.52	0.1480
Glu49 : Lys6 (PDB:1BRF)	*const*	203.14	-90.34	-173.73	286.54	0.3860

AMBER* explicit lone pairs)

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-361.60	-331.02	-786.33	93.72	0.0850
Methylguanine : Methylcytosine (WC)	*opt*	-325.83	-363.43	-786.83	97.57	0.1290
Adenine : Thymine (WC)	*opt*	-362.20	-627.86	-1043.25	53.19	0.4130
Methyladenine : Methylthymine (planar)	*opt*	-362.20	-627.86	-1039.29	49.24	0.2010
8-Oxoguanine : Cytosine (WC planar)	*opt*	-205.55	-331.02	-596.69	60.12	0.0710
Inosine : Cytosine (WC planar)	*opt*	-331.02	-27.76	-416.04	57.26	0.1580
Guanine : Uracil (wobble)	*opt*	-361.60	-336.61	-749.36	51.16	0.1240
Cytosine : CytosineH+	*opt*	-331.02	-70.06	-483.05	81.98	0.1160
Uracil dimer (Calcutta planar)	*opt*	-336.61	-336.61	-699.21	25.99	0.1980
Uracil dimer (planar)	*opt*	-336.61	-336.61	-712.87	39.66	0.0550
6-Thioguanine : Cytosine (WC planar)	*opt*	-331.02	-158.27	-540.57	51.28	0.4120

Adenine : 4-Thiouracil (WC)	*opt*	-363.92	-220.01	-614.73	30.80	4.1470
2-aminoadenine : Thymine	*opt*	-458.77	-631.08	-1156.67	66.82	0.2910
2-aminoadenine : Thymine (planar)	*opt*	-458.77	-630.94	-1156.45	66.73	0.0530
Adenine : Difluorotoluene	*opt*	-364.94	-11.91	-418.09	41.24	2.7530
Guanine : 4-Thiouracil	*opt*	-361.60	-186.26	-594.47	46.61	0.2090
Guanine : 2-Thiouracil	*opt*	-361.60	-186.87	-602.19	53.72	1.9750
Adenine : Cytosine (planar)	*opt*	-331.02	-363.92	-754.71	59.77	0.0710
Guanine dimer (planar)	*opt*	-361.60	-361.60	-781.23	58.03	0.1740
Guanine 6-Thioguanine (planar)	*opt*	-361.60	-158.27	-571.59	51.73	1.5320
6-Thioguanine : Guanine (planar)	*opt*	-158.27	-361.60	-554.10	34.23	0.6450
Guanine : Adenine 1	*opt*	-361.60	-363.92	-792.75	67.24	0.1810
Guanine : Adenine 1 (planar)	*opt*	-364.94	-361.60	-793.36	66.83	0.0310
Guanine : Adenine 2	*opt*	-361.60	-363.92	-772.64	47.13	0.3090
Guanine : Adenine 2 (planar)	*opt*	-361.60	-363.92	-771.50	45.98	0.0990
Guanine : Adenine 3	*opt*	-361.60	-363.92	-779.19	53.67	0.7170
Guanine : Adenine 4	*opt*	-361.60	-363.92	-764.23	38.72	0.4100
Adenine dimer 1 (planar)	*opt*	-363.92	-363.92	-785.70	57.86	0.0490
Adenine dimer 2 (planar)	*opt*	-363.92	-364.94	-773.78	44.92	0.3570
Adenine dimer 3 (planar)	*opt*	-363.92	-363.92	-773.77	45.93	1.2080
8-Oxoguanine : Guanine	*opt*	-361.60	-205.55	-603.32	36.18	0.2130
2-Thiouracil dimer (planar)	*opt*	-98.91	-98.91	-237.60	39.78	2.3160
Adenine : Thymine (WC)	*const*	-362.20	-627.86	-1042.00	51.95	0.3750
Guanine : Cytosine (WC)	*const*	-325.83	-363.43	-786.26	96.99	0.4080
Adenine : thymine (WC)	*const*	-362.20	-627.86	-1040.69	50.63	0.3480
Guanine : adenine (HB)	*const*	-361.60	-364.94	-771.45	44.91	0.0960
Cytosine : Guanine (WC)	*const*	-331.02	-361.60	-785.10	92.48	0.0730
Guanine : Cytosine (WC)	*const*	-361.60	-331.02	-786.22	93.60	0.0670
Cytosine : guanine (interstrand)	*const*	-361.60	-331.02	-711.22	18.61	0.1200
Adenine : thymine (interstrand)	*const*	-631.08	-363.92	-1011.84	16.84	0.2110
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-654.77	-7.27	0.1060
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-725.90	2.71	0.0790
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-662.35	0.31	0.1130
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-746.56	23.36	0.0940
Adenine : cytosine (interstrand)	*const*	-363.92	-331.02	-696.75	1.81	0.0990
Thymine : guanine (interstrand)	*const*	-631.08	-361.60	-998.61	5.93	0.1900
Thymine : guanine (interstrand)	*const*	-361.60	-631.08	-1006.05	13.37	0.1830
Thymine : cytosine (interstrand)	*const*	-363.92	-331.02	-701.21	6.27	0.1000
Adenine : guanine (interstrand)	*const*	-363.92	-361.60	-745.41	19.89	0.0830
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-971.46	9.36	0.1990
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-968.23	6.13	0.1940
Adenine : guanine (interstrand)	*const*	-363.92	-361.60	-748.62	23.10	0.1020
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1266.24	4.07	0.2460
Adenine dimer (interstrand)	*const*	-363.92	-363.92	-740.59	12.75	0.0920
Adenine dimer (interstrand)	*const*	-363.92	-363.92	-741.09	13.25	0.0980
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1267.37	5.21	0.2700
Adenine : thymine (interstrand)	*const*	-363.92	-631.08	-1008.10	13.10	0.1830
Thymine : adenine (interstrand)	*const*	-363.92	-631.08	-1006.76	11.76	0.1990
Adenine dimer (interstrand)	*const*	-362.20	-362.20	-742.08	17.69	0.3360
Thymine dimer (interstrand)	*const*	-627.86	-627.86	-1261.26	5.55	0.4360
Guanine dimer (interstrand)	*const*	-363.43	-363.43	-757.19	30.33	0.4090
Cytosine dimer (interstrand)	*const*	-325.83	-325.83	-657.86	6.19	0.4330
Adenine : Guanine (interstrand)	*const*	-362.20	-363.43	-753.76	28.13	0.3030
Thymine : Cytosine (interstrand)	*const*	-325.83	-627.86	-958.67	4.98	0.3460
Cytosine dimer (interstrand)	*const*	-331.02	-364.94	-715.36	19.39	0.1660
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-738.69	15.50	0.0960
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-731.92	8.73	0.1100
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-656.09	-5.95	0.0950
Guanine : Cytosine (stacked)	*opt*	-361.60	-331.02	-745.60	52.98	0.3540
Methylguanine : Methylcytosine (stacked)	*opt*	-363.43	-325.83	-744.54	55.28	0.3810
Adenine : Thymine (stacked)	*opt*	-364.94	-631.08	-1040.69	44.67	0.4270
Methyladenine : Methylthymine (stacked)	*opt*	-362.20	-627.86	-1039.27	49.22	0.5470
Cytosine dimer 1 (stacked)	*const*	-331.02	-331.02	-664.15	2.11	0.0750
Cytosine dimer 2 (stacked)	*const*	-331.02	-331.02	-682.80	20.76	0.1170
Cytosine dimer 3 (stacked)	*const*	-331.02	-331.02	-704.62	42.58	0.1200
Cytosine dimer 4 (stacked)	*const*	-331.02	-331.02	-711.96	49.92	0.0940
Cytosine dimer 5 (stacked)	*const*	-331.02	-331.02	-668.17	6.13	0.0990
Cytosine dimer 6 (stacked)	*const*	-331.02	-331.02	-666.95	4.91	0.1060
Cytosine dimer 7 (stacked)	*const*	-331.02	-331.02	-669.77	7.73	0.1160
Cytosine dimer 8 (stacked)	*const*	-331.02	-331.02	-707.49	45.45	0.1010
Cytosine dimer 9 (stacked)	*const*	-331.02	-331.02	-710.86	48.82	0.0850
Cytosine dimer 10 (stacked)	*const*	-331.02	-331.02	-708.54	46.50	0.0870
Cytosine dimer 11 (stacked)	*const*	-331.02	-331.02	-712.40	50.36	0.0960
Cytosine dimer 12 (stacked)	*const*	-331.02	-331.02	-695.30	33.26	0.1010
Cytosine dimer 13 (stacked)	*const*	-331.02	-331.02	-702.97	40.93	0.0930
Cytosine dimer 14 (stacked)	*const*	-331.02	-331.02	-709.86	47.82	0.1120
Adenine dimer (stacked)	*const*	-363.92	-363.92	-771.73	43.89	0.0990
guanine dimer (stacked)	*const*	-361.60	-361.60	-781.39	58.19	0.0960
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-738.36	43.42	0.0940
Guanine : Adenine (stacked)	*const*	-361.60	-363.92	-777.55	52.03	0.0840
Cytosine dimer (stacked)	*const*	-331.02	-331.02	-712.59	50.55	0.0870
Adenine : Uracil (stacked)	*const*	-363.92	-336.61	-743.33	42.80	0.0840
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-745.24	52.63	0.1100
Cytosine : Uracil (stacked)	*const*	-331.02	-336.61	-712.96	45.33	0.0990
Uracil dimer (Stacked)	*const*	-336.61	-336.61	-706.38	33.17	0.0720
Guanine : Uracil (stacked)	*const*	-361.60	-336.61	-750.59	52.39	0.0830
Guanine dimer (stacked)	*const*	-331.02	-331.02	-670.34	8.30	0.1040
Cytosine dimer (stacked)	*const*	-331.02	-361.60	-713.82	21.21	0.1100
Adenine dimer (stacked)	*const*	-363.92	-363.92	-764.68	36.84	0.0950

Thymine dimer (stacked)	*const*	-363.92	-631.08	-1008.65	13.65	0.1780
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-743.10	50.48	0.1180
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-729.13	36.52	0.1070
Adenine : guanine (stacked)	*const*	-363.92	-361.60	-773.42	47.90	0.1010
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-986.51	24.40	0.1890
Adenine : guanine (stacked)	*const*	-363.92	-361.60	-766.46	40.94	0.0990
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-989.39	27.29	0.2440
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1022.36	29.69	0.1670
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-725.57	30.63	0.0950
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1024.86	32.18	0.1970
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-722.42	27.48	0.1010
Adenine : thymine (stacked)	*const*	-363.92	-631.08	-1026.86	31.86	0.1740
Adenine : thymine (stacked)	*const*	-363.92	-631.08	-1024.42	29.42	0.2740
Adenine dimer (stacked)	*const*	-363.92	-363.92	-765.14	37.30	0.0960
Thymine dimer (stacked)	*const*	-631.08	-631.08	-1287.39	25.23	0.2440
Adenine : Thymine (stacked)	*const*	-362.20	-627.86	-1025.24	35.19	0.2960
Guanine : Cytosine (stacked)	*const*	-325.83	-363.43	-719.80	30.54	0.3870
Adenine : Cytosine (stacked)	*const*	-362.20	-325.83	-719.78	31.75	0.1190
Thymine : Guanine (stacked)	*const*	-627.86	-363.43	-1024.83	33.54	0.3680
guanine : Cytosine (stacked)	*const*	-331.02	-361.60	-732.62	40.00	0.1090
Adenine : Guanine (stacked)	*const*	-364.94	-361.60	-765.73	39.19	0.1110
Cytosine : guanine (stacked)	*const*	-361.60	-331.02	-743.08	50.46	0.1310
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-743.86	51.24	0.1350
Phe30 : Lys46 (1RB9)	*const*	37.41	29.69	55.56	11.55	0.1350
Phe30 : Leu33 (1RB9)	*const*	37.55	8.45	26.26	19.73	0.2360
Phe30 : Tyr13 (1RB9)	*const*	37.43	20.30	48.52	9.20	0.1350
Phe30 : Phe49 (1RB9)	*const*	13.71	37.63	39.04	12.29	0.1410
Phe30 : Tyr4 (1RB9)	*const*	37.40	25.85	45.42	17.82	0.1550
Phe49 : Cys39 (1RB9)	*const*	13.58	15.01	43.33	-14.74	0.1550
Phe49 : Cys6 (1RB9)	*const*	13.50	8.03	12.59	8.94	0.1520
Phe49 : Lys46 (1RB9)	*const*	25.18	29.20	37.07	17.31	0.1350
Phe49 : Val5 (1RB9)	*const*	14.02	11.40	4.57	20.85	0.1570
Phe49 : Tyr37 (1RB9)	*const*	25.18	-13.15	4.26	7.77	0.1320
Phe49 : Tyr4 (1RB9)	*const*	13.61	19.04	27.33	5.32	0.1210
Phe49 : Peptide bond (1RB9)	*const*	25.44	-69.99	-53.04	8.49	0.3320
Phe49 : Peptide bond (1RB9)	*const*	13.81	-69.99	-81.95	25.77	0.2990
Glu47 : Lys6 (PDB:1IU5)	*const*	184.34	-86.30	-212.21	310.25	0.1180
Glu49 : Lys6 (PDB:1BQ9)	*const*	178.58	-89.98	-344.59	433.18	0.1440
Glu54 : Lys2 (PDB:1SMM)	*const*	160.81	-73.45	-245.15	332.51	0.1910
Glu50 : LysK30 (PDB:1BRF)	*const*	177.23	-88.33	-166.36	255.25	0.1720
Glu50 : Lys52 (PDB:1BRF)	*const*	178.20	-89.49	-285.47	374.18	0.1490
Glu49 : Lys6 (PDB:1BRF)	*const*	203.14	-90.07	-173.77	286.84	0.3830

OPLS*

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-123.96	-169.82	-392.07	98.29	0.0730
Methylguanine : Methylcytosine (WC)	*opt*	-151.25	-131.50	-383.38	100.63	0.1310
Adenine : Thymine (WC)	*opt*	-92.87	-186.54	-329.96	50.55	0.3660
Methyladenine : Methylthymine (planar)	*opt*	-92.87	-186.54	-325.89	46.48	0.0760
8-Oxoguanine : Cytosine (WC planar)	*opt*	-448.57	-169.82	-685.84	67.45	0.0790
Inosine : Cytosine (WC planar)	*opt*	-169.82	-125.66	-360.00	64.52	0.0970
Guanine : Uracil (wobble)	*opt*	-123.96	-171.76	-350.32	54.59	0.1260
Cytosine : CytosineH+	*opt*	-169.82	-130.53	-388.70	88.35	0.1320
Uracil dimer (Calcutta planar)	*opt*	-171.76	-171.76	-371.90	28.38	0.2010
Uracil dimer (planar)	*opt*	-171.76	-171.76	-381.60	38.08	0.0580
6-Thioguanine : Cytosine (WC planar)	*opt*	-169.82	-254.84	-481.84	57.19	0.1090
Adenine : 4-Thiouracil (WC)	*opt*	-89.55	-323.73	-446.99	33.71	3.8870
2-aminoadenine : Thymine	*opt*	-199.27	-201.01	-460.20	59.91	0.2640
2-aminoadenine : Thymine (planar)	*opt*	-199.27	-201.01	-460.20	59.91	0.0420
Adenine : Difluorotoluene	*opt*	-89.55	-0.28	-123.14	33.30	2.8380
Guanine : 4-Thiouracil	*opt*	-123.96	-323.73	-514.13	66.44	0.0810
Guanine : 2-Thiouracil	*opt*	-123.96	-254.12	-410.27	32.18	0.3470
Adenine : Cytosine (planar)	*opt*	-169.82	-89.55	-305.95	46.58	0.0650
Guanine dimer (planar)	*opt*	-123.96	-123.96	-313.51	65.58	0.1470
Guanine 6-Thioguanine (planar)	*opt*	-123.96	-254.84	-417.39	38.59	0.1860
6-Thioguanine : Guanine (planar)	*opt*	-254.84	-123.96	-423.29	44.49	0.1690
Guanine : Adenine 1	*opt*	-123.96	-89.55	-279.73	66.21	0.7000
Guanine : Adenine 1 (planar)	*opt*	-89.55	-123.96	-270.27	56.76	0.0600
Guanine : Adenine 2	*opt*	-123.96	-89.55	-250.94	37.42	0.5570
Guanine : Adenine 2 (planar)	*opt*	-123.96	-89.55	-244.03	30.51	0.0360
Guanine : Adenine 3	*opt*	-123.96	-89.55	-262.25	48.73	0.6830
Guanine : Adenine 4	*opt*	-123.96	-89.55	-235.24	21.72	0.3620
Adenine dimer 1 (planar)	*opt*	-89.55	-89.55	-223.64	44.53	0.7030
Adenine dimer 2 (planar)	*opt*	-89.55	-89.55	-216.90	37.79	0.9460
Adenine dimer 3 (planar)	*opt*	-89.55	-89.55	-211.23	32.12	1.0810
8-Oxoguanine : Guanine	*opt*	-123.96	-448.57	-634.08	61.55	0.1920
2-Thiouracil dimer (planar)	*opt*	-254.12	-254.12	-535.52	27.27	0.2410
Adenine : Thymine (WC)	*const*	-92.87	-186.54	-329.01	49.60	0.3450
Guanine : Cytosine (WC)	*const*	-151.25	-131.50	-382.63	99.89	0.4080
Adenine : thymine (WC)	*const*	-92.87	-186.54	-328.87	49.47	0.3010
Guanine : adenine (HB)	*const*	-123.96	-89.55	-247.41	33.89	0.0890
Cytosine : Guanine (WC)	*const*	-169.82	-123.96	-390.11	96.33	0.0760
Guanine : Cytosine (WC)	*const*	-123.96	-169.82	-391.97	98.19	0.0660
Cytosine : guanine (interstrand)	*const*	-123.96	-169.82	-316.04	22.25	0.1310
Adenine : thymine (interstrand)	*const*	-201.01	-89.55	-313.76	23.20	0.1100
Cytosine dimer (interstrand)	*const*	-169.82	-169.82	-327.94	-11.70	0.1060
Guanine dimer (interstrand)	*const*	-123.96	-123.96	-260.64	12.72	0.0880

Cytosine dimer (interstrand)	*const*	-169.82	-169.82	-340.49	0.85	0.1120
Guanine dimer (interstrand)	*const*	-123.96	-123.96	-273.61	25.68	0.0980
Adenine : cytosine (interstrand)	*const*	-89.55	-169.82	-266.79	7.42	0.1020
Thymine : guanine (interstrand)	*const*	-201.01	-123.96	-336.06	11.08	0.1030
Thymine : guanine (interstrand)	*const*	-123.96	-201.01	-339.66	14.68	0.0930
Thymine : cytosine (interstrand)	*const*	-89.55	-169.82	-272.52	13.15	0.1040
Adenine : guanine (interstrand)	*const*	-89.55	-123.96	-239.97	26.45	0.0980
Thymine : cytosine (interstrand)	*const*	-201.01	-169.82	-383.75	12.92	0.1010
Thymine : cytosine (interstrand)	*const*	-201.01	-169.82	-373.85	3.02	0.0850
Adenine : guanine (interstrand)	*const*	-89.55	-123.96	-243.03	29.51	0.1060
Thymine dimer (interstrand)	*const*	-201.01	-201.01	-403.74	1.72	0.1050
Adenine dimer (interstrand)	*const*	-89.55	-89.55	-197.63	18.53	0.0980
Adenine dimer (interstrand)	*const*	-89.55	-89.55	-192.56	13.45	0.0860
Thymine dimer (interstrand)	*const*	-201.01	-201.01	-410.10	8.08	0.1110
Adenine : thymine (interstrand)	*const*	-89.55	-201.01	-306.54	15.98	0.1090
Thymine : adenine (interstrand)	*const*	-89.55	-201.01	-309.43	18.86	0.1040
Adenine dimer (interstrand)	*const*	-92.87	-92.87	-205.84	20.11	0.3420
Thymine dimer (interstrand)	*const*	-186.54	-186.54	-375.97	2.89	0.3470
Guanine dimer (interstrand)	*const*	-131.50	-131.50	-290.98	27.98	0.4040
Cytosine dimer (interstrand)	*const*	-151.25	-151.25	-305.23	2.73	0.4310
Adenine : Guanine (interstrand)	*const*	-92.87	-131.50	-258.26	33.90	0.3030
Thymine : Cytosine (interstrand)	*const*	-151.25	-186.54	-340.16	2.38	0.3180
Cytosine dimer (interstrand)	*const*	-169.82	-89.55	-275.06	15.69	0.1590
Guanine dimer (interstrand)	*const*	-123.96	-123.96	-268.19	20.26	0.1080
Guanine dimer (interstrand)	*const*	-123.96	-123.96	-266.99	19.06	0.1100
Cytosine dimer (interstrand)	*const*	-169.82	-169.82	-329.45	-10.19	0.0980
Guanine : Cytosine (stacked)	*opt*	-123.96	-169.82	-392.07	98.29	2.5290
Methylguanine : Methylcytosine (stacked)	*opt*	-131.50	-151.25	-358.76	76.02	2.1620
Adenine : Thymine (stacked)	*opt*	-89.55	-201.01	-331.49	40.93	0.3220
Methyladenine : Methylthymine (stacked)	*opt*	-92.87	-186.54	-326.40	46.99	0.4340
Cytosine dimer 1 (stacked)	*const*	-169.82	-169.82	-328.66	-10.98	0.1050
Cytosine dimer 2 (stacked)	*const*	-169.82	-169.82	-350.74	11.10	0.1180
Cytosine dimer 3 (stacked)	*const*	-169.82	-169.82	-378.33	38.69	0.1170
Cytosine dimer 4 (stacked)	*const*	-169.82	-169.82	-388.41	48.77	0.1020
Cytosine dimer 5 (stacked)	*const*	-169.82	-169.82	-331.73	-7.91	0.1040
Cytosine dimer 6 (stacked)	*const*	-169.82	-169.82	-329.75	-9.89	0.1060
Cytosine dimer 7 (stacked)	*const*	-169.82	-169.82	-340.52	0.88	0.1100
Cytosine dimer 8 (stacked)	*const*	-169.82	-169.82	-383.99	44.35	0.1120
Cytosine dimer 9 (stacked)	*const*	-169.82	-169.82	-387.64	48.00	0.1020
Cytosine dimer 10 (stacked)	*const*	-169.82	-169.82	-387.07	47.43	0.1030
Cytosine dimer 11 (stacked)	*const*	-169.82	-169.82	-388.80	49.16	0.1080
Cytosine dimer 12 (stacked)	*const*	-169.82	-169.82	-369.78	30.14	0.1100
Cytosine dimer 13 (stacked)	*const*	-169.82	-169.82	-384.39	44.75	0.1000
Cytosine dimer 14 (stacked)	*const*	-169.82	-169.82	-384.59	44.95	0.1030
Adenine dimer (stacked)	*const*	-89.55	-89.55	-213.42	34.31	0.0950
guanine dimer (stacked)	*const*	-123.96	-123.96	-298.93	51.00	0.0940
Adenine : cytosine (stacked)	*const*	-89.55	-169.82	-302.06	42.69	0.1040
Guanine : Adenine (stacked)	*const*	-123.96	-89.55	-256.47	42.95	0.0920
Cytosine dimer (stacked)	*const*	-169.82	-169.82	-388.80	49.16	0.1040
Adenine : Uracil (stacked)	*const*	-89.55	-171.76	-298.65	37.33	0.0880
Guanine : Cytosine (stacked)	*const*	-123.96	-169.82	-343.70	49.92	0.1120
Cytosine : Uracil (stacked)	*const*	-169.82	-171.76	-377.69	36.11	0.1000
Uracil dimer (Stacked)	*const*	-171.76	-171.76	-371.89	28.37	0.1020
Guanine : Uracil (stacked)	*const*	-123.96	-171.76	-339.84	44.11	0.0840
Guanine dimer (stacked)	*const*	-169.82	-169.82	-337.71	-1.93	0.1060
Cytosine dimer (stacked)	*const*	-169.82	-123.96	-325.78	31.99	0.1150
Adenine dimer (stacked)	*const*	-89.55	-89.55	-202.61	23.50	0.0970
Thymine dimer (stacked)	*const*	-89.55	-201.01	-309.88	19.31	0.1100
Guanine : cytosine (stacked)	*const*	-169.82	-123.96	-332.16	38.38	0.1120
Guanine : cytosine (stacked)	*const*	-169.82	-123.96	-317.05	23.26	0.0990
Adenine : guanine (stacked)	*const*	-89.55	-123.96	-246.35	32.83	0.0940
Thymine : cytosine (stacked)	*const*	-201.01	-169.82	-387.29	16.45	0.1030
Adenine : guanine (stacked)	*const*	-89.55	-123.96	-241.81	28.29	0.0820
Thymine : cytosine (stacked)	*const*	-201.01	-169.82	-391.47	20.64	0.1530
Thymine : guanine (stacked)	*const*	-201.01	-123.96	-343.05	18.07	0.0970
Adenine : cytosine (stacked)	*const*	-89.55	-169.82	-269.98	10.61	0.0930
Thymine : guanine (stacked)	*const*	-201.01	-123.96	-348.54	23.57	0.1540
Adenine : cytosine (stacked)	*const*	-89.55	-169.82	-277.43	18.06	0.0900
Adenine : thymine (stacked)	*const*	-89.55	-201.01	-319.31	28.74	0.1320
Adenine : thymine (stacked)	*const*	-89.55	-201.01	-307.25	16.68	0.1220
Adenine dimer (stacked)	*const*	-89.55	-89.55	-202.41	23.30	0.0890
Thymine dimer (stacked)	*const*	-201.01	-201.01	-420.19	18.17	0.2020
Adenine : Thymine (stacked)	*const*	-92.87	-186.54	-315.52	36.11	0.3060
Guanine : Cytosine (stacked)	*const*	-151.25	-131.50	-312.33	29.59	0.4310
Adenine : Cytosine (stacked)	*const*	-92.87	-151.25	-268.23	24.12	0.0870
Thymine : Guanine (stacked)	*const*	-186.54	-131.50	-353.02	34.98	0.4140
guanine : Cytosine (stacked)	*const*	-169.82	-123.96	-325.79	32.01	0.1240
Adenine : Guanine (stacked)	*const*	-89.55	-123.96	-242.54	29.02	0.1180
Cytosine : guanine (stacked)	*const*	-123.96	-169.82	-330.57	36.78	0.1210
Guanine : Cytosine (stacked)	*const*	-123.96	-169.82	-334.68	40.89	0.1390
Phe30 : Lys46 (1RB9)	*const*	56.41	45.90	89.42	12.89	0.1520
Phe30 : Leu33 (1RB9)	*const*	56.88	14.62	54.93	16.58	0.1720
Phe30 : Tyr13 (1RB9)	*const*	56.43	6.00	48.66	13.77	0.1330
Phe30 : Phe49 (1RB9)	*const*	31.10	56.55	75.88	11.77	0.1730
Phe30 : Tyr4 (1RB9)	*const*	56.40	11.79	48.83	19.36	0.1430
Phe49 : Cys39 (1RB9)	*const*	31.18	29.59	75.38	-14.61	0.1590
Phe49 : Cys6 (1RB9)	*const*	31.28	23.17	41.39	13.07	0.1670
Phe49 : Lys46 (1RB9)	*const*	45.00	42.74	64.53	23.21	0.1480

Phe49 : Val5 (1RB9)	*const*	31.82	32.35	42.48	21.69	0.1660
Phe49 : Tyr37 (1RB9)	*const*	44.47	14.27	48.55	10.19	0.1300
Phe49 : Tyr4 (1RB9)	*const*	31.31	-3.15	16.31	11.85	0.1590
Phe49 : Peptide bond (1RB9)	*const*	44.64	-65.28	-34.25	13.61	0.1760
Phe49 : Peptide bond (1RB9)	*const*	31.61	-65.28	-58.21	24.54	0.1650
Glu47 : Lys6 (PDB:1IU5)	*const*	42.20	-14.95	-302.05	329.30	0.1690
Glu49 : Lys6 (PDB:1BQ9)	*const*	31.52	-23.16	-455.81	464.16	0.1690
Glu54 : Lys2 (PDB:1SMM)	*const*	7.33	21.56	-361.96	390.85	0.1880
Glu50 : LysK30 (PDB:1BRF)	*const*	5.46	-32.88	-283.35	255.93	0.1970
Glu50 : Lys52 (PDB:1BRF)	*const*	6.38	-19.20	-421.51	408.70	0.1690
Glu49 : Lys6 (PDB:1BRF)	*const*	52.95	-23.31	-246.26	275.89	0.3820

OPLSAA

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-110.63	-146.31	-354.62	97.68	0.0740
Methylguanine : Methylcytosine (WC)	*opt*	-147.04	-106.41	-363.00	109.55	0.1360
Adenine : Thymine (WC)	*opt*	-68.95	-172.97	-300.33	58.41	0.3720
Methyladenine : Methylthymine (planar)	*opt*	-68.95	-172.97	-289.86	47.94	0.1120
8-Oxoguanine : Cytosine (WC planar)	*opt*	-193.04	-146.31	-417.41	78.06	0.2460
Inosine : Cytosine (WC planar)	*opt*	-146.31	43.47	-178.02	75.18	0.1080
Guanine : Uracil (wobble)	*opt*	-110.63	-146.10	-311.26	54.53	0.1370
Cytosine : CytosineH+	*opt*	-146.31	122.33	-157.27	133.29	0.2130
Uracil dimer (Calcutta planar)	*opt*	-146.10	-146.10	-320.91	28.70	0.2340
Uracil dimer (planar)	*opt*	-146.10	-146.10	-330.80	38.60	0.0650
6-Thioguanine : Cytosine (WC planar)	*opt*	-146.31	-54.40	-274.22	73.50	0.3360
Adenine : 4-Thiouracil (WC)	*opt*	-75.96	-78.17	-194.87	40.74	3.8870
2-aminoadenine : Thymine	*opt*	-172.53	-168.26	-397.78	57.00	0.2660
2-aminoadenine : Thymine (planar)	*opt*	-172.53	-168.26	-397.78	57.00	0.0360
Adenine : Difluorotoluene	*opt*	-75.96	-2.27	-98.50	20.28	1.8670
Guanine : 4-Thiouracil	*opt*	-110.63	-78.17	-254.88	66.09	0.0900
Guanine : 2-Thiouracil	*opt*	-110.63	-56.33	-215.06	48.10	0.3140
Adenine : Cytosine (planar)	*opt*	-146.31	-75.96	-269.10	46.82	0.0710
Guanine dimer (planar)	*opt*	-110.63	-110.63	-285.96	64.71	0.1590
Guanine 6-Thioguanine (planar)	*opt*	-110.63	-54.40	-215.31	50.28	0.5820
6-Thioguanine : Guanine (planar)	*opt*	-54.40	-110.63	-234.54	69.51	0.9210
Guanine : Adenine 1	*opt*	-110.63	-75.96	-252.33	65.74	0.6920
Guanine : Adenine 1 (planar)	*opt*	-75.96	-110.63	-241.63	55.04	0.0700
Guanine : Adenine 2	*opt*	-110.63	-75.96	-223.72	37.14	0.5340
Guanine : Adenine 2 (planar)	*opt*	-110.63	-75.96	-216.50	29.92	0.0410
Guanine : Adenine 3	*opt*	-110.63	-75.96	-235.00	48.42	0.6570
Guanine : Adenine 4	*opt*	-110.63	-75.96	-207.83	21.24	0.3410
Adenine dimer 1 (planar)	*opt*	-75.96	-75.96	-196.87	44.94	0.6680
Adenine dimer 2 (planar)	*opt*	-75.96	-75.96	-190.43	38.50	0.9280
Adenine dimer 3 (planar)	*opt*	-75.96	-75.96	-183.51	31.59	1.1090
8-Oxoguanine : Guanine	*opt*	-110.63	-193.04	-362.43	58.77	0.2010
2-Thiouracil dimer (planar)	*opt*	-56.33	-56.33	-150.96	38.29	0.1530
Adenine : Thymine (WC)	*const*	-68.95	-172.97	-298.90	56.99	0.3380
Guanine : Cytosine (WC)	*const*	-147.04	-106.41	-361.94	108.49	0.4100
Adenine : thymine (WC)	*const*	-68.95	-172.97	-298.52	56.60	0.3030
Guanine : adenine (HB)	*const*	-110.63	-75.96	-221.34	34.75	0.1070
Cytosine : Guanine (WC)	*const*	-146.31	-110.63	-352.89	95.95	0.0800
Guanine : Cytosine (WC)	*const*	-110.63	-146.31	-354.45	97.51	0.0640
Cytosine : guanine (interstrand)	*const*	-110.63	-146.31	-282.55	25.62	0.1980
Adenine : thymine (interstrand)	*const*	-168.26	-75.96	-268.96	24.74	0.1340
Cytosine dimer (interstrand)	*const*	-146.31	-146.31	-281.34	-11.28	0.1090
Guanine dimer (interstrand)	*const*	-110.63	-110.63	-233.70	12.45	0.0910
Cytosine dimer (interstrand)	*const*	-146.31	-146.31	-293.73	1.11	0.1150
Guanine dimer (interstrand)	*const*	-110.63	-110.63	-245.98	24.73	0.1000
Adenine : cytosine (interstrand)	*const*	-75.96	-146.31	-230.58	8.30	0.1090
Thymine : guanine (interstrand)	*const*	-168.26	-110.63	-289.85	10.96	0.0960
Thymine : guanine (interstrand)	*const*	-110.63	-168.26	-293.72	14.83	0.0920
Thymine : cytosine (interstrand)	*const*	-75.96	-146.31	-235.65	13.38	0.1100
Adenine : guanine (interstrand)	*const*	-75.96	-110.63	-213.07	26.48	0.1390
Thymine : cytosine (interstrand)	*const*	-168.26	-146.31	-327.87	13.29	0.1070
Thymine : cytosine (interstrand)	*const*	-168.26	-146.31	-317.80	3.23	0.0820
Adenine : guanine (interstrand)	*const*	-75.96	-110.63	-217.64	31.05	0.1610
Thymine dimer (interstrand)	*const*	-168.26	-168.26	-338.78	2.25	0.1040
Adenine dimer (interstrand)	*const*	-75.96	-75.96	-169.66	17.74	0.1060
Adenine dimer (interstrand)	*const*	-75.96	-75.96	-165.47	13.55	0.0870
Thymine dimer (interstrand)	*const*	-168.26	-168.26	-344.41	7.89	0.1080
Adenine : thymine (interstrand)	*const*	-75.96	-168.26	-260.73	16.51	0.1090
Thymine : adenine (interstrand)	*const*	-75.96	-168.26	-263.54	19.31	0.1140
Adenine dimer (interstrand)	*const*	-68.95	-68.95	-152.20	14.31	0.3400
Thymine dimer (interstrand)	*const*	-172.97	-172.97	-351.80	5.85	0.3490
Guanine dimer (interstrand)	*const*	-106.41	-106.41	-241.05	28.23	0.4220
Cytosine dimer (interstrand)	*const*	-147.04	-147.04	-300.35	6.27	0.4320
Adenine : Guanine (interstrand)	*const*	-68.95	-106.41	-206.72	31.37	0.3140
Thymine : Cytosine (interstrand)	*const*	-147.04	-172.97	-324.24	4.22	0.3150
Cytosine dimer (interstrand)	*const*	-146.31	-75.96	-238.70	16.42	0.1710
Guanine dimer (interstrand)	*const*	-110.63	-110.63	-243.67	22.42	0.1600
Guanine dimer (interstrand)	*const*	-110.63	-110.63	-239.52	18.27	0.1110
Cytosine dimer (interstrand)	*const*	-146.31	-146.31	-282.78	-9.85	0.1020
Guanine : Cytosine (stacked)	*opt*	-110.63	-146.31	-354.62	97.68	2.5380
Methylguanine : Methylcytosine (stacked)	*opt*	-106.41	-147.04	-330.47	77.02	2.5000
Adenine : Thymine (stacked)	*opt*	-75.96	-168.26	-285.48	41.25	0.3850
Methyladenine : Methylthymine (stacked)	*opt*	-68.95	-172.97	-293.16	51.24	1.4890
Cytosine dimer 1 (stacked)	*const*	-146.31	-146.31	-284.08	-8.54	0.1150

Cytosine dimer 2 (stacked)	*const*	-146.31	-146.31	-305.49	12.87	0.1240
Cytosine dimer 3 (stacked)	*const*	-146.31	-146.31	-333.19	40.57	0.1440
Cytosine dimer 4 (stacked)	*const*	-146.31	-146.31	-341.77	49.14	0.1030
Cytosine dimer 5 (stacked)	*const*	-146.31	-146.31	-286.96	-5.67	0.1130
Cytosine dimer 6 (stacked)	*const*	-146.31	-146.31	-285.14	-7.49	0.1170
Cytosine dimer 7 (stacked)	*const*	-146.31	-146.31	-296.29	3.67	0.1620
Cytosine dimer 8 (stacked)	*const*	-146.31	-146.31	-337.23	44.60	0.1370
Cytosine dimer 9 (stacked)	*const*	-146.31	-146.31	-341.73	49.10	0.0960
Cytosine dimer 10 (stacked)	*const*	-146.31	-146.31	-341.12	48.50	0.1030
Cytosine dimer 11 (stacked)	*const*	-146.31	-146.31	-341.82	49.19	0.0970
Cytosine dimer 12 (stacked)	*const*	-146.31	-146.31	-321.90	29.28	0.1190
Cytosine dimer 13 (stacked)	*const*	-146.31	-146.31	-339.34	46.71	0.1160
Cytosine dimer 14 (stacked)	*const*	-146.31	-146.31	-337.60	44.97	0.0990
Adenine dimer (stacked)	*const*	-75.96	-75.96	-188.00	36.08	0.1100
guanine dimer (stacked)	*const*	-110.63	-110.63	-272.82	51.57	0.1150
Adenine : cytosine (stacked)	*const*	-75.96	-146.31	-265.54	43.27	0.1080
Guanine : Adenine (stacked)	*const*	-110.63	-75.96	-230.25	43.67	0.0930
Cytosine dimer (stacked)	*const*	-146.31	-146.31	-342.18	49.55	0.0910
Adenine : Uracil (stacked)	*const*	-75.96	-146.10	-261.19	39.13	0.0930
Guanine : Cytosine (stacked)	*const*	-110.63	-146.31	-309.94	53.00	0.1720
Cytosine : Uracil (stacked)	*const*	-146.31	-146.10	-329.04	36.62	0.0970
Uracil dimer (Stacked)	*const*	-146.10	-146.10	-323.08	30.87	0.0970
Guanine : Uracil (stacked)	*const*	-110.63	-146.10	-301.62	44.90	0.0940
Guanine dimer (stacked)	*const*	-146.31	-146.31	-292.30	-0.33	0.1100
Cytosine dimer (stacked)	*const*	-146.31	-110.63	-289.42	32.48	0.1270
Adenine dimer (stacked)	*const*	-75.96	-75.96	-176.20	24.28	0.0980
Thymine dimer (stacked)	*const*	-75.96	-168.26	-263.01	18.78	0.1090
Guanine : cytosine (stacked)	*const*	-146.31	-110.63	-298.93	41.99	0.1740
Guanine : cytosine (stacked)	*const*	-146.31	-110.63	-280.80	23.86	0.1160
Adenine : guanine (stacked)	*const*	-75.96	-110.63	-220.10	33.51	0.1000
Thymine : cytosine (stacked)	*const*	-168.26	-146.31	-331.50	16.93	0.1010
Adenine : guanine (stacked)	*const*	-75.96	-110.63	-215.16	28.57	0.0910
Thymine : cytosine (stacked)	*const*	-168.26	-146.31	-336.29	21.72	0.1500
Thymine : guanine (stacked)	*const*	-168.26	-110.63	-296.07	17.18	0.0960
Adenine : cytosine (stacked)	*const*	-75.96	-146.31	-233.28	11.00	0.0990
Thymine : guanine (stacked)	*const*	-168.26	-110.63	-303.28	24.39	0.1450
Adenine : cytosine (stacked)	*const*	-75.96	-146.31	-242.43	20.16	0.0960
Adenine : thymine (stacked)	*const*	-75.96	-168.26	-273.59	29.37	0.1290
Adenine : thymine (stacked)	*const*	-75.96	-168.26	-266.23	22.00	0.1060
Adenine dimer (stacked)	*const*	-75.96	-75.96	-176.23	24.31	0.0970
Thymine dimer (stacked)	*const*	-168.26	-168.26	-355.57	19.05	0.1820
Adenine : Thymine (stacked)	*const*	-68.95	-172.97	-274.58	32.66	0.2850
Guanine : Cytosine (stacked)	*const*	-147.04	-106.41	-276.88	23.43	0.3930
Adenine : Cytosine (stacked)	*const*	-68.95	-147.04	-238.72	22.74	0.1010
Thymine : Guanine (stacked)	*const*	-172.97	-106.41	-308.58	29.20	0.3690
guanine : Cytosine (stacked)	*const*	-146.31	-110.63	-291.42	34.48	0.1300
Adenine : Guanine (stacked)	*const*	-75.96	-110.63	-217.03	30.44	0.1240
Cytosine : guanine (stacked)	*const*	-110.63	-146.31	-297.53	40.59	0.1540
Guanine : Cytosine (stacked)	*const*	-110.63	-146.31	-300.54	43.61	0.1940
Phe30 : Lys46 (1RB9)	*const*	16.21	3.88	10.02	10.06	0.1560
Phe30 : Leu33 (1RB9)	*const*	16.27	-16.62	-21.09	20.74	0.2320
Phe30 : Tyr13 (1RB9)	*const*	16.20	-29.07	-22.88	10.00	0.1370
Phe30 : Phe49 (1RB9)	*const*	4.17	16.42	11.58	9.00	0.1550
Phe30 : Tyr4 (1RB9)	*const*	16.16	-15.45	-13.69	14.40	0.1490
Phe49 : Cys39 (1RB9)	*const*	4.16	-29.94	-11.59	-14.19	0.1550
Phe49 : Cys6 (1RB9)	*const*	4.18	-39.71	-46.36	10.84	0.1490
Phe49 : Lys46 (1RB9)	*const*	10.79	5.14	-5.09	21.02	0.1440
Phe49 : Val5 (1RB9)	*const*	4.26	-36.49	-49.54	17.31	0.1450
Phe49 : Tyr37 (1RB9)	*const*	10.54	-46.97	-46.73	10.31	0.1240
Phe49 : Tyr4 (1RB9)	*const*	4.15	-21.86	-25.24	7.53	0.1340
Phe49 : Peptide bond (1RB9)	*const*	10.69	-68.79	-66.59	8.49	0.1990
Phe49 : Peptide bond (1RB9)	*const*	4.21	-68.79	-97.24	32.66	0.1770
Glu47 : Lys6 (PDB:1IU5)	*const*	95.92	-79.24	-309.38	326.07	0.1560
Glu49 : Lys6 (PDB:1BQ9)	*const*	97.06	-71.11	-447.47	473.42	0.1550
Glu54 : Lys2 (PDB:1SMM)	*const*	88.46	-59.37	-346.91	376.00	0.1930
Glu50 : LysK30 (PDB:1BRF)	*const*	71.14	-94.82	-299.38	275.70	0.1680
Glu50 : Lys52 (PDB:1BRF)	*const*	71.91	-70.89	-406.39	407.41	0.1650
Glu49 : Lys6 (PDB:1BRF)	*const*	112.64	-70.68	-253.95	295.90	0.3780

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Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-306.48	-371.70	-770.66	92.47	0.3280
Methylguanine : Methylcytosine (WC)	*opt*	-320.01	-287.69	-703.85	96.15	0.4170
Adenine : Thymine (WC)	*opt*	-2.58	-357.21	-411.09	51.29	0.3780
Methyladenine : Methylthymine (planar)	*opt*	-2.58	-357.21	-412.93	53.14	0.3780
8-Oxoguanine : Cytosine (WC planar)	*opt*	-656.49	-371.70	-1110.71	82.52	0.3320
Inosine : Cytosine (WC planar)	*opt*	-371.70	-31.84	-480.76	77.21	0.2470
Guanine : Uracil (wobble)	*opt*	-306.48	-403.79	-773.83	63.56	0.2020
Cytosine : CytosineH+	*opt*	-371.70	-380.62	-852.39	100.06	0.2590
Uracil dimer (Calcutta planar)	*opt*	-403.79	-403.79	-843.91	36.33	0.2190
Uracil dimer (planar)	*opt*	-403.79	-403.79	-859.04	51.47	0.1070
6-Thioguanine : Cytosine (WC planar)	*opt*	-371.70	-290.04	-735.85	74.10	0.2590
Adenine : 4-Thiouracil (WC)	*opt*	-21.25	-327.31	-385.90	37.34	3.8870
2-aminoadenine : Thymine	*opt*	-354.91	-396.10	-812.88	61.86	0.0750
2-aminoadenine : Thymine (planar)	*opt*	-354.91	-396.10	-812.88	61.86	0.3150
Adenine : Difluorotoluene	*opt*	-21.25	28.40	-6.57	13.72	1.0640
Guanine : 4-Thiouracil	*opt*	-306.48	-327.31	-698.98	65.19	0.1360

Guanine : 2-Thiouracil	*opt*	-306.48	-315.87	-663.82	41.47	0.4270
Adenine : Cytosine (planar)	*opt*	-371.70	-21.25	-435.71	42.75	0.5290
Guanine dimer (planar)	*opt*	-306.48	-306.48	-682.75	69.79	0.4530
Guanine 6-Thioguanine (planar)	*opt*	-306.48	-290.04	-661.22	64.70	0.8700
6-Thioguanine : Guanine (planar)	*opt*	-290.04	-306.48	-662.03	65.50	0.6780
Guanine : Adenine 1	*opt*	-306.48	-21.25	-397.34	69.61	0.2980
Guanine : Adenine 1 (planar)	*opt*	-21.25	-306.48	-397.34	69.60	0.6270
Guanine : Adenine 2	*opt*	-306.48	-21.25	-369.55	41.82	0.4160
Guanine : Adenine 2 (planar)	*opt*	-306.48	-21.25	-369.77	42.04	0.5860
Guanine : Adenine 3	*opt*	-306.48	-21.25	-389.09	61.36	0.2210
Guanine : Adenine 4	*opt*	-306.48	-21.25	-347.93	20.19	0.2920
Adenine dimer 1 (planar)	*opt*	-21.25	-21.25	-81.44	38.94	0.8410
Adenine dimer 2 (planar)	*opt*	-21.25	-21.25	-78.33	35.83	0.6160
Adenine dimer 3 (planar)	*opt*	-21.25	-21.25	-76.62	34.12	0.6170
8-Oxoguanine : Guanine	*opt*	-306.48	-656.49	-1012.99	50.03	0.2200
2-Thiouracil dimer (planar)	*opt*	-315.87	-315.87	-668.12	36.38	0.3040
Adenine : Thymine (WC)	*const*	-2.58	-357.21	-410.97	51.18	0.2630
Guanine : Cytosine (WC)	*const*	-320.01	-287.69	-701.02	93.32	0.3020
Adenine : thymine (WC)	*const*	-2.58	-357.21	-410.36	50.57	0.1130
Guanine : adenine (HB)	*const*	-306.48	-21.25	-369.47	41.74	0.1320
Cytosine : Guanine (WC)	*const*	-371.70	-306.48	-770.57	92.39	0.0970
Guanine : Cytosine (WC)	*const*	-306.48	-371.70	-768.71	90.52	0.1020
Cytosine : guanine (interstrand)	*const*	-306.48	-371.70	-708.88	30.69	0.2180
Adenine : thymine (interstrand)	*const*	-396.10	-21.25	-441.77	24.41	0.1440
Cytosine dimer (interstrand)	*const*	-371.70	-371.70	-736.24	-7.17	0.1710
Guanine dimer (interstrand)	*const*	-306.48	-306.48	-617.51	4.55	0.1370
Cytosine dimer (interstrand)	*const*	-371.70	-371.70	-749.79	6.38	0.1830
Guanine dimer (interstrand)	*const*	-306.48	-306.48	-637.17	24.21	0.1550
Adenine : cytosine (interstrand)	*const*	-21.25	-371.70	-402.94	9.98	0.1800
Thymine : guanine (interstrand)	*const*	-396.10	-306.48	-706.48	3.89	0.1400
Thymine : guanine (interstrand)	*const*	-306.48	-396.10	-718.61	16.03	0.2150
Thymine : cytosine (interstrand)	*const*	-21.25	-371.70	-412.42	19.46	0.2010
Adenine : guanine (interstrand)	*const*	-21.25	-306.48	-349.66	21.93	0.1450
Thymine : cytosine (interstrand)	*const*	-396.10	-371.70	-784.10	16.30	0.1510
Thymine : cytosine (interstrand)	*const*	-396.10	-371.70	-770.29	2.48	0.1520
Adenine : guanine (interstrand)	*const*	-21.25	-306.48	-351.64	23.90	0.1620
Thymine dimer (interstrand)	*const*	-396.10	-396.10	-789.12	-3.09	0.1090
Adenine dimer (interstrand)	*const*	-21.25	-21.25	-60.64	18.14	0.1300
Adenine dimer (interstrand)	*const*	-21.25	-21.25	-45.95	3.45	0.1400
Thymine dimer (interstrand)	*const*	-396.10	-396.10	-797.45	5.25	0.0980
Adenine : thymine (interstrand)	*const*	-21.25	-396.10	-431.22	13.87	0.1370
Thymine : adenine (interstrand)	*const*	-21.25	-396.10	-435.53	18.18	0.1520
Adenine dimer (interstrand)	*const*	-2.58	-2.58	-30.64	25.48	0.3610
Thymine dimer (interstrand)	*const*	-357.21	-357.21	-711.08	-3.34	0.1650
Guanine dimer (interstrand)	*const*	-287.69	-287.69	-605.57	30.18	0.4270
Cytosine dimer (interstrand)	*const*	-320.01	-320.01	-648.83	8.82	0.2580
Adenine : Guanine (interstrand)	*const*	-2.58	-287.69	-322.27	31.99	0.3330
Thymine : Cytosine (interstrand)	*const*	-320.01	-357.21	-679.01	1.79	0.2620
Cytosine dimer (interstrand)	*const*	-371.70	-21.25	-410.48	17.52	0.2330
Guanine dimer (interstrand)	*const*	-306.48	-306.48	-636.46	23.49	0.1600
Guanine dimer (interstrand)	*const*	-306.48	-306.48	-621.96	8.99	0.1200
Cytosine dimer (interstrand)	*const*	-371.70	-371.70	-737.21	-6.20	0.1810
Guanine : Cytosine (stacked)	*opt*	-306.48	-371.70	-770.67	92.48	2.3120
Methylguanine : Methylcytosine (stacked)	*opt*	-287.69	-320.01	-703.87	96.17	2.7960
Adenine : Thymine (stacked)	*opt*	-21.25	-396.10	-470.61	53.26	2.2980
Methyladenine : Methylthymine (stacked)	*opt*	-2.58	-357.21	-412.93	53.13	2.5670
Cytosine dimer 1 (stacked)	*const*	-371.70	-371.70	-725.65	-17.76	0.1450
Cytosine dimer 2 (stacked)	*const*	-371.70	-371.70	-759.52	16.11	0.2350
Cytosine dimer 3 (stacked)	*const*	-371.70	-371.70	-780.21	36.80	0.2380
Cytosine dimer 4 (stacked)	*const*	-371.70	-371.70	-775.20	31.79	0.1590
Cytosine dimer 5 (stacked)	*const*	-371.70	-371.70	-742.90	-0.50	0.2400
Cytosine dimer 6 (stacked)	*const*	-371.70	-371.70	-740.88	-2.52	0.2150
Cytosine dimer 7 (stacked)	*const*	-371.70	-371.70	-754.94	11.53	0.2260
Cytosine dimer 8 (stacked)	*const*	-371.70	-371.70	-779.82	36.42	0.2490
Cytosine dimer 9 (stacked)	*const*	-371.70	-371.70	-775.94	32.53	0.2080
Cytosine dimer 10 (stacked)	*const*	-371.70	-371.70	-778.92	35.51	0.1690
Cytosine dimer 11 (stacked)	*const*	-371.70	-371.70	-776.63	33.23	0.1930
Cytosine dimer 12 (stacked)	*const*	-371.70	-371.70	-767.72	24.31	0.2170
Cytosine dimer 13 (stacked)	*const*	-371.70	-371.70	-779.53	36.12	0.1640
Cytosine dimer 14 (stacked)	*const*	-371.70	-371.70	-767.17	23.76	0.1370
Adenine dimer (stacked)	*const*	-21.25	-21.25	-68.77	26.27	0.1680
guanine dimer (stacked)	*const*	-306.48	-306.48	-665.97	53.00	0.2010
Adenine : cytosine (stacked)	*const*	-21.25	-371.70	-429.18	36.22	0.1670
Guanine : Adenine (stacked)	*const*	-306.48	-21.25	-363.97	36.23	0.1690
Cytosine dimer (stacked)	*const*	-371.70	-371.70	-777.73	34.32	0.2090
Adenine : Uracil (stacked)	*const*	-21.25	-403.79	-453.62	28.58	0.1210
Guanine : Cytosine (stacked)	*const*	-306.48	-371.70	-730.30	52.11	0.2120
Cytosine : Uracil (stacked)	*const*	-371.70	-403.79	-805.34	29.85	0.1560
Uracil dimer (Stacked)	*const*	-403.79	-403.79	-826.14	18.56	0.0930
Guanine : Uracil (stacked)	*const*	-306.48	-403.79	-755.94	45.67	0.1860
Guanine dimer (stacked)	*const*	-371.70	-371.70	-745.78	2.37	0.1870
Cytosine dimer (stacked)	*const*	-371.70	-306.48	-714.56	36.37	0.2130
Adenine dimer (stacked)	*const*	-21.25	-21.25	-56.94	14.44	0.1440
Thymine dimer (stacked)	*const*	-21.25	-396.10	-433.66	16.30	0.1230
Guanine : cytosine (stacked)	*const*	-371.70	-306.48	-729.52	51.33	0.2430
Guanine : cytosine (stacked)	*const*	-371.70	-306.48	-705.63	27.44	0.2420
Adenine : guanine (stacked)	*const*	-21.25	-306.48	-353.83	26.09	0.1730
Thymine : cytosine (stacked)	*const*	-396.10	-371.70	-780.02	12.22	0.1170

Adenine : guanine (stacked)	*const*	-21.25	-306.48	-348.64	20.91	0.1470
Thymine : cytosine (stacked)	*const*	-396.10	-371.70	-787.10	19.29	0.1860
Thymine : guanine (stacked)	*const*	-396.10	-306.48	-715.13	12.54	0.1400
Adenine : cytosine (stacked)	*const*	-21.25	-371.70	-403.71	10.76	0.1480
Thymine : guanine (stacked)	*const*	-396.10	-306.48	-716.64	14.06	0.1880
Adenine : cytosine (stacked)	*const*	-21.25	-371.70	-415.84	22.88	0.1840
Adenine : thymine (stacked)	*const*	-21.25	-396.10	-433.95	16.59	0.1590
Adenine : thymine (stacked)	*const*	-21.25	-396.10	-425.24	7.89	0.1280
Adenine dimer (stacked)	*const*	-21.25	-21.25	-58.71	16.21	0.1400
Thymine dimer (stacked)	*const*	-396.10	-396.10	-797.68	5.48	0.1320
Adenine : Thymine (stacked)	*const*	-2.58	-357.21	-375.52	15.73	0.2240
Guanine : Cytosine (stacked)	*const*	-320.01	-287.69	-633.67	25.97	0.3450
Adenine : Cytosine (stacked)	*const*	-2.58	-320.01	-349.28	26.69	0.2380
Thymine : Guanine (stacked)	*const*	-357.21	-287.69	-668.74	23.83	0.3040
guanine : Cytosine (stacked)	*const*	-371.70	-306.48	-707.07	28.88	0.2140
Adenine : Guanine (stacked)	*const*	-21.25	-306.48	-360.26	32.52	0.1810
Cytosine : guanine (stacked)	*const*	-306.48	-371.70	-732.07	53.89	0.2720
Guanine : Cytosine (stacked)	*const*	-306.48	-371.70	-727.98	49.80	0.2450
Phe30 : Lys46 (1RB9)	*const*	281.02	153.35	425.23	9.15	0.1310
Phe30 : Leu33 (1RB9)	*const*	281.08	154.39	422.62	12.85	0.2200
Phe30 : Tyr13 (1RB9)	*const*	281.14	212.77	485.23	8.67	0.1160
Phe30 : Phe49 (1RB9)	*const*	266.23	281.62	533.29	14.56	0.1450
Phe30 : Tyr4 (1RB9)	*const*	281.25	226.67	502.05	5.87	0.1280
Phe49 : Cys39 (1RB9)	*const*	266.18	203.07	489.09	-19.84	0.1450
Phe49 : Cys6 (1RB9)	*const*	266.41	200.79	457.10	10.10	0.1540
Phe49 : Lys46 (1RB9)	*const*	273.43	143.65	406.75	10.33	0.1260
Phe49 : Val5 (1RB9)	*const*	266.76	161.06	400.17	27.65	0.1790
Phe49 : Tyr37 (1RB9)	*const*	272.77	236.90	511.02	-1.35	0.1260
Phe49 : Tyr4 (1RB9)	*const*	266.27	221.05	487.89	-0.57	0.1500
Phe49 : Peptide bond (1RB9)	*const*	272.79	-103.13	164.83	4.83	0.3730
Phe49 : Peptide bond (1RB9)	*const*	266.51	-103.13	135.89	27.49	0.3180
Glu47 : Lys6 (PDB:1IU5)	*const*	163.76	106.59	-48.87	319.22	0.1470
Glu49 : Lys6 (PDB:1BQ9)	*const*	161.16	120.06	-170.73	451.95	0.1670
Glu54 : Lys2 (PDB:1SMM)	*const*	168.24	129.62	-63.79	361.65	0.2050
Glu50 : LysK30 (PDB:1BRF)	*const*	151.06	91.28	-17.74	260.08	0.3290
Glu50 : Lys52 (PDB:1BRF)	*const*	151.85	120.03	-119.41	391.29	0.1420
Glu49 : Lys6 (PDB:1BRF)	*const*	171.23	120.79	9.49	282.52	0.3510

MMFF94s

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-303.93	-369.34	-767.89	94.61	0.0680
Methylguanine : Methylcytosine (WC)	*opt*	-318.58	-285.07	-702.15	98.50	0.3230
Adenine : Thymine (WC)	*opt*	0.44	-360.59	-412.88	52.72	0.2450
Methyladenine : Methylthymine (planar)	*opt*	0.44	-360.59	-413.48	53.33	0.2820
8-Oxoguanine : Cytosine (WC planar)	*opt*	-655.95	-369.34	-1106.84	81.55	0.0550
Inosine : Cytosine (WC planar)	*opt*	-369.34	-32.39	-480.12	78.38	0.0560
Guanine : Uracil (wobble)	*opt*	-303.93	-406.12	-774.49	64.44	0.1840
Cytosine : CytosineH+	*opt*	-369.34	-377.93	-847.74	100.47	0.1320
Uracil dimer (Calcutta planar)	*opt*	-406.12	-406.12	-848.57	36.33	0.2190
Uracil dimer (planar)	*opt*	-406.12	-406.12	-863.70	51.47	0.1070
6-Thioguanine : Cytosine (WC planar)	*opt*	-369.34	-286.62	-734.15	78.18	0.1410
Adenine : 4-Thiouracil (WC)	*opt*	-18.30	-328.99	-384.62	37.33	3.8870
2-aminoadenine : Thymine	*opt*	-345.32	-398.43	-807.22	63.46	0.2620
2-aminoadenine : Thymine (planar)	*opt*	-345.32	-398.43	-807.22	63.46	0.0440
Adenine : Difluorotoluene	*opt*	-18.30	28.40	-4.98	15.07	0.7010
Guanine : 4-Thiouracil	*opt*	-303.93	-328.99	-699.02	66.09	0.1410
Guanine : 2-Thiouracil	*opt*	-303.93	-316.91	-662.92	42.08	0.4170
Adenine : Cytosine (planar)	*opt*	-369.34	-18.30	-429.41	41.76	0.1180
Guanine dimer (planar)	*opt*	-303.93	-303.93	-678.13	70.26	0.1110
Guanine 6-Thioguanine (planar)	*opt*	-303.93	-286.62	-648.18	57.63	0.1070
6-Thioguanine : Guanine (planar)	*opt*	-286.62	-303.93	-653.98	63.43	0.1160
Guanine : Adenine 1	*opt*	-303.93	-18.30	-383.70	61.47	0.4010
Guanine : Adenine 1 (planar)	*opt*	-18.30	-303.93	-380.17	57.94	0.0980
Guanine : Adenine 2	*opt*	-303.93	-18.30	-362.21	39.98	0.2790
Guanine : Adenine 2 (planar)	*opt*	-303.93	-18.30	-359.16	36.92	0.0790
Guanine : Adenine 3	*opt*	-303.93	-18.30	-376.34	54.11	0.3070
Guanine : Adenine 4	*opt*	-303.93	-18.30	-336.89	14.66	0.2050
Adenine dimer 1 (planar)	*opt*	-18.30	-18.30	-84.41	47.81	0.0900
Adenine dimer 2 (planar)	*opt*	-18.30	-18.30	-69.67	33.06	0.5260
Adenine dimer 3 (planar)	*opt*	-18.30	-18.30	-68.72	32.11	0.6680
8-Oxoguanine : Guanine	*opt*	-303.93	-655.95	-1007.45	47.57	0.2480
2-Thiouracil dimer (planar)	*opt*	-316.91	-316.91	-670.20	36.38	0.3050
Adenine : Thymine (WC)	*const*	0.44	-360.59	-411.62	51.46	0.2570
Guanine : Cytosine (WC)	*const*	-318.58	-285.07	-701.08	97.44	0.3010
Adenine : thymine (WC)	*const*	0.44	-360.59	-411.43	51.27	0.0950
Guanine : adenine (HB)	*const*	-303.93	-18.30	-359.50	37.27	0.0930
Cytosine : Guanine (WC)	*const*	-369.34	-303.93	-766.17	92.89	0.0790
Guanine : Cytosine (WC)	*const*	-303.93	-369.34	-767.82	94.55	0.0630
Cytosine : guanine (interstrand)	*const*	-303.93	-369.34	-692.86	19.58	0.1350
Adenine : thymine (interstrand)	*const*	-398.43	-18.30	-435.46	18.72	0.1180
Cytosine dimer (interstrand)	*const*	-369.34	-369.34	-729.60	-9.09	0.1030
Guanine dimer (interstrand)	*const*	-303.93	-303.93	-608.83	0.97	0.0850
Cytosine dimer (interstrand)	*const*	-369.34	-369.34	-742.09	3.40	0.1070
Guanine dimer (interstrand)	*const*	-303.93	-303.93	-625.76	17.90	0.0890
Adenine : cytosine (interstrand)	*const*	-18.30	-369.34	-396.25	8.60	0.1020
Thymine : guanine (interstrand)	*const*	-398.43	-303.93	-705.89	3.52	0.0850
Thymine : guanine (interstrand)	*const*	-303.93	-398.43	-707.00	4.63	0.1030

Thymine : cytosine (interstrand)	*const*	-18.30	-369.34	-401.42	13.78	0.1040
Adenine : guanine (interstrand)	*const*	-18.30	-303.93	-341.76	19.53	0.0870
Thymine : cytosine (interstrand)	*const*	-398.43	-369.34	-781.00	13.23	0.1030
Thymine : cytosine (interstrand)	*const*	-398.43	-369.34	-770.12	2.34	0.0970
Adenine : guanine (interstrand)	*const*	-18.30	-303.93	-339.38	17.14	0.0900
Thymine dimer (interstrand)	*const*	-398.43	-398.43	-793.78	-3.09	0.1100
Adenine dimer (interstrand)	*const*	-18.30	-18.30	-58.28	21.68	0.1100
Adenine dimer (interstrand)	*const*	-18.30	-18.30	-37.67	1.07	0.0870
Thymine dimer (interstrand)	*const*	-398.43	-398.43	-802.04	5.17	0.1000
Adenine : thymine (interstrand)	*const*	-18.30	-398.43	-430.68	13.94	0.1060
Thymine : adenine (interstrand)	*const*	-18.30	-398.43	-430.44	13.70	0.1080
Adenine dimer (interstrand)	*const*	0.44	0.44	-20.35	21.22	0.3350
Thymine dimer (interstrand)	*const*	-360.59	-360.59	-717.83	-3.35	0.1520
Guanine dimer (interstrand)	*const*	-285.07	-285.07	-590.81	20.67	0.4040
Cytosine dimer (interstrand)	*const*	-318.58	-318.58	-643.19	6.03	0.1320
Adenine : Guanine (interstrand)	*const*	0.44	-285.07	-312.85	28.22	0.3020
Thymine : Cytosine (interstrand)	*const*	-318.58	-360.59	-680.44	1.27	0.3180
Cytosine dimer (interstrand)	*const*	-369.34	-18.30	-397.74	10.10	0.1690
Guanine dimer (interstrand)	*const*	-303.93	-303.93	-625.75	17.89	0.1050
Guanine dimer (interstrand)	*const*	-303.93	-303.93	-613.88	6.02	0.0930
Cytosine dimer (interstrand)	*const*	-369.34	-369.34	-730.59	-8.10	0.1020
Guanine : Cytosine (stacked)	*opt*	-303.93	-369.34	-767.89	94.61	2.5200
Methylguanine : Methylcytosine (stacked)	*opt*	-285.07	-318.58	-702.15	98.50	3.0330
Adenine : Thymine (stacked)	*opt*	-18.30	-398.43	-470.05	53.31	2.4500
Methyladenine : Methylthymine (stacked)	*opt*	0.44	-360.59	-396.64	36.48	0.5640
Cytosine dimer 1 (stacked)	*const*	-369.34	-369.34	-724.76	-13.93	0.1050
Cytosine dimer 2 (stacked)	*const*	-369.34	-369.34	-743.22	4.54	0.1160
Cytosine dimer 3 (stacked)	*const*	-369.34	-369.34	-763.65	24.97	0.1210
Cytosine dimer 4 (stacked)	*const*	-369.34	-369.34	-769.41	30.72	0.0900
Cytosine dimer 5 (stacked)	*const*	-369.34	-369.34	-727.26	-11.42	0.1060
Cytosine dimer 6 (stacked)	*const*	-369.34	-369.34	-725.94	-12.75	0.1080
Cytosine dimer 7 (stacked)	*const*	-369.34	-369.34	-736.48	-2.21	0.1240
Cytosine dimer 8 (stacked)	*const*	-369.34	-369.34	-766.83	28.14	0.1050
Cytosine dimer 9 (stacked)	*const*	-369.34	-369.34	-768.77	30.08	0.1000
Cytosine dimer 10 (stacked)	*const*	-369.34	-369.34	-769.34	30.65	0.0890
Cytosine dimer 11 (stacked)	*const*	-369.34	-369.34	-770.77	32.09	0.0920
Cytosine dimer 12 (stacked)	*const*	-369.34	-369.34	-759.59	20.90	0.1130
Cytosine dimer 13 (stacked)	*const*	-369.34	-369.34	-769.02	30.33	0.0900
Cytosine dimer 14 (stacked)	*const*	-369.34	-369.34	-765.85	27.17	0.0920
Adenine dimer (stacked)	*const*	-18.30	-18.30	-59.13	22.53	0.1000
guanine dimer (stacked)	*const*	-303.93	-303.93	-651.42	43.55	0.0940
Adenine : cytosine (stacked)	*const*	-18.30	-369.34	-420.07	32.43	0.0940
Guanine : Adenine (stacked)	*const*	-303.93	-18.30	-355.08	32.84	0.0870
Cytosine dimer (stacked)	*const*	-369.34	-369.34	-770.77	32.08	0.0990
Adenine : Uracil (stacked)	*const*	-18.30	-406.12	-451.83	27.41	0.0960
Guanine : Cytosine (stacked)	*const*	-303.93	-369.34	-714.65	41.37	0.1170
Cytosine : Uracil (stacked)	*const*	-369.34	-406.12	-802.20	26.74	0.0940
Uracil dimer (Stacked)	*const*	-406.12	-406.12	-830.61	18.37	0.0950
Guanine : Uracil (stacked)	*const*	-303.93	-406.12	-748.90	38.85	0.0960
Guanine dimer (stacked)	*const*	-369.34	-369.34	-733.57	-5.11	0.0990
Cytosine dimer (stacked)	*const*	-369.34	-303.93	-703.59	30.31	0.1170
Adenine dimer (stacked)	*const*	-18.30	-18.30	-46.13	9.53	0.1000
Thymine dimer (stacked)	*const*	-18.30	-398.43	-433.75	17.02	0.1060
Guanine : cytosine (stacked)	*const*	-369.34	-303.93	-706.76	33.49	0.1320
Guanine : cytosine (stacked)	*const*	-369.34	-303.93	-690.24	16.97	0.0970
Adenine : guanine (stacked)	*const*	-18.30	-303.93	-341.42	19.18	0.1010
Thymine : cytosine (stacked)	*const*	-398.43	-369.34	-780.74	12.96	0.1010
Adenine : guanine (stacked)	*const*	-18.30	-303.93	-340.33	18.10	0.0890
Thymine : cytosine (stacked)	*const*	-398.43	-369.34	-782.59	14.81	0.1070
Thymine : guanine (stacked)	*const*	-398.43	-303.93	-714.93	12.56	0.0890
Adenine : cytosine (stacked)	*const*	-18.30	-369.34	-395.70	8.06	0.0930
Thymine : guanine (stacked)	*const*	-398.43	-303.93	-709.78	7.42	0.1090
Adenine : cytosine (stacked)	*const*	-18.30	-369.34	-400.71	13.06	0.1090
Adenine : thymine (stacked)	*const*	-18.30	-398.43	-430.24	13.50	0.1030
Adenine : thymine (stacked)	*const*	-18.30	-398.43	-421.94	5.21	0.1010
Adenine dimer (stacked)	*const*	-18.30	-18.30	-48.97	12.37	0.0980
Thymine dimer (stacked)	*const*	-398.43	-398.43	-802.33	5.46	0.1320
Adenine : Thymine (stacked)	*const*	0.44	-360.59	-378.25	18.09	0.2340
Guanine : Cytosine (stacked)	*const*	-318.58	-285.07	-623.70	20.06	0.3020
Adenine : Cytosine (stacked)	*const*	0.44	-318.58	-333.09	14.94	0.3140
Thymine : Guanine (stacked)	*const*	-360.59	-285.07	-662.67	17.01	0.2750
guanine : Cytosine (stacked)	*const*	-369.34	-303.93	-692.97	19.69	0.1300
Adenine : Guanine (stacked)	*const*	-18.30	-303.93	-337.06	14.83	0.1100
Cytosine : guanine (stacked)	*const*	-303.93	-369.34	-708.21	34.94	0.1490
Guanine : Cytosine (stacked)	*const*	-303.93	-369.34	-709.78	36.50	0.1480
Phe30 : Lys46 (1RB9)	*const*	281.02	153.35	425.23	9.15	0.1310
Phe30 : Leu33 (1RB9)	*const*	281.08	154.39	422.62	12.85	0.2200
Phe30 : Tyr13 (1RB9)	*const*	281.14	212.77	485.23	8.67	0.1160
Phe30 : Phe49 (1RB9)	*const*	266.23	281.62	533.29	14.56	0.1450
Phe30 : Tyr4 (1RB9)	*const*	281.25	226.67	502.05	5.87	0.1280
Phe49 : Cys39 (1RB9)	*const*	266.18	203.07	489.09	-19.84	0.1450
Phe49 : Cys6 (1RB9)	*const*	266.41	200.79	457.10	10.10	0.1540
Phe49 : Lys46 (1RB9)	*const*	273.43	143.65	406.75	10.33	0.1260
Phe49 : Val5 (1RB9)	*const*	266.76	161.06	400.17	27.65	0.1790
Phe49 : Tyr37 (1RB9)	*const*	272.77	236.90	511.02	-1.35	0.1260
Phe49 : Tyr4 (1RB9)	*const*	266.27	221.05	487.89	-0.57	0.1500
Phe49 : Peptide bond (1RB9)	*const*	272.81	-105.67	163.53	3.61	0.2160
Phe49 : Peptide bond (1RB9)	*const*	266.54	-105.67	133.01	27.87	0.2550

Glu47 : Lys6 (PDB:1IU5)	*const*	163.76	106.59	-48.87	319.22	0.1470
Glu49 : Lys6 (PDB:1BQ9)	*const*	161.16	120.06	-170.73	451.95	0.1670
Glu54 : Lys2 (PDB:1SMM)	*const*	168.24	129.62	-63.79	361.65	0.2050
Glu50 : LysK30 (PDB:1BRF)	*const*	151.06	91.28	-17.74	260.08	0.3290
Glu50 : Lys52 (PDB:1BRF)	*const*	151.85	120.03	-119.41	391.29	0.1420
Glu49 : Lys6 (PDB:1BRF)	*const*	171.23	120.79	9.49	282.52	0.3510

JSCH-2005 data set: Results with default bond dipole cut-offs (BDCOs) (opt = geometry optimization, const = constrained optimization)

MM2*

Complex		Monomer A (kJ/mol)	MonomerB (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Guanine : Cytosine (WC)	*opt*	-132.19	-93.99	-254.63	28.44	0.8200
Methylguanine : Methylcytosine (WC)	*opt*	-68.98	-122.16	-220.42	29.29	0.8950
Adenine : Thymine (WC)	*opt*	105.65	-331.71	-255.36	29.30	2.9340
Methyladenine : Methylthymine (planar)	*opt*	105.65	-331.53	-255.64	29.77	2.4940
8-Oxoguanine : Cytosine (WC planar)	*opt*	-325.51	-93.99	-447.80	28.30	0.8880
Inosine : Cytosine (WC planar)	*opt*	-93.99	18.96	-102.45	27.43	0.9020
Guanine : Uracil (wobble)	*opt*	-132.19	-346.86	-521.15	42.09	0.3420
Cytosine : CytosineH+	*opt*	-93.99	-426.38	-557.65	37.29	1.4050
Uracil dimer (Calcutta planar)	*opt*	-346.99	-346.86	-716.95	23.10	0.2870
Uracil dimer (planar)	*opt*	-346.99	-346.99	-734.15	40.16	0.1670
6-Thioguanine : Cytosine (WC planar)	*opt*	-93.99	-89.84	-211.46	27.63	0.9100
Adenine : 4-Thiouracil (WC)	*opt*	95.54	-253.85	-164.53	6.22	3.8880
2-aminoadenine : Thymine	*opt*	69.15	-366.01	-320.54	23.68	2.1620
2-aminoadenine : Thymine (planar)	*opt*	69.03	-366.01	-310.99	14.01	0.5160
Adenine : Difluorotoluene	*opt*	95.54	-16.59	55.36	23.60	2.9510
Guanine : 4-Thiouracil	*opt*	-132.19	-253.85	-429.91	43.86	0.2850
Guanine : 2-Thiouracil	*opt*	-132.19	-216.84	-374.94	25.91	0.6740
Adenine : Cytosine (planar)	*opt*	-93.99	95.54	-10.99	12.55	0.8700
Guanine dimer (planar)	*opt*	-132.19	-132.19	-289.98	25.59	0.7100
Guanine 6-Thioguanine (planar)	*opt*	-132.19	-89.84	-236.45	14.42	0.4020
6-Thioguanine : Guanine (planar)	*opt*	-89.84	-132.19	-248.81	26.78	0.7560
Guanine : Adenine 1	*opt*	-132.19	95.54	-59.70	23.05	2.0880
Guanine : Adenine 1 (planar)	*opt*	95.54	-132.19	-48.50	11.85	0.7820
Guanine : Adenine 2	*opt*	-132.19	95.54	-61.97	25.32	2.4620
Guanine : Adenine 2 (planar)	*opt*	-132.18	95.54	-43.52	6.88	0.4840
Guanine : Adenine 3	*opt*	-132.19	95.54	-62.53	25.89	2.4140
Guanine : Adenine 4	*opt*	-132.19	95.54	-62.48	25.83	3.6690
Adenine dimer 1 (planar)	*opt*	95.54	95.54	186.37	4.72	0.5630
Adenine dimer 2 (planar)	*opt*	95.54	95.54	169.37	21.72	2.9190
Adenine dimer 3 (planar)	*opt*	95.54	95.54	174.66	16.43	2.2650
8-Oxoguanine : Guanine	*opt*	-132.19	-325.51	-501.33	43.63	0.4380
2-Thiouracil dimer (planar)	*opt*	-216.87	-216.87	-459.50	25.76	0.4570
Adenine : Thymine (WC)	*const*	105.98	-331.71	-211.77	-13.96	0.1580
Guanine : Cytosine (WC)	*const*	-68.95	-122.15	-189.64	-1.46	0.2080
Adenine : thymine (WC)	*const*	105.77	-331.71	-208.16	-17.78	0.1750
Guanine : adenine (HB)	*const*	-132.19	95.56	-26.01	-10.62	0.1690
Cytosine : Guanine (WC)	*const*	-93.71	-132.19	-228.78	2.87	0.1310
Guanine : Cytosine (WC)	*const*	-132.19	-93.72	-228.16	2.25	0.1180
Cytosine : guanine (interstrand)	*const*	-132.19	-93.99	-229.40	3.22	0.1050
Adenine : thymine (interstrand)	*const*	-366.01	95.54	-271.46	1.00	0.1060
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-185.02	-2.95	0.1050
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-263.96	-0.43	0.1080
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-188.88	0.90	0.1020
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-272.46	8.07	0.1100
Adenine : cytosine (interstrand)	*const*	95.54	-93.99	-0.45	2.01	0.1010
Thymine : guanine (interstrand)	*const*	-366.01	-132.19	-495.42	-2.79	0.1040
Thymine : guanine (interstrand)	*const*	-132.19	-366.01	-498.50	0.29	0.1060
Thymine : cytosine (interstrand)	*const*	95.54	-93.99	-0.65	2.20	0.1010
Adenine : guanine (interstrand)	*const*	95.54	-132.19	-46.26	9.61	0.1030
Thymine : cytosine (interstrand)	*const*	-366.01	-93.99	-460.74	0.75	0.1030
Thymine : cytosine (interstrand)	*const*	-366.01	-93.99	-457.97	-2.03	0.1030
Adenine : guanine (interstrand)	*const*	95.54	-132.19	-36.50	-0.15	0.1040
Thymine dimer (interstrand)	*const*	-366.01	-366.01	-729.09	-2.93	0.1160
Adenine dimer (interstrand)	*const*	95.54	95.54	189.49	1.60	0.0990
Adenine dimer (interstrand)	*const*	95.54	95.54	188.96	2.13	0.1100
Thymine dimer (interstrand)	*const*	-366.01	-366.01	-729.95	-2.07	0.1080
Adenine : thymine (interstrand)	*const*	95.54	-366.01	-272.96	2.49	0.0910
Thymine : adenine (interstrand)	*const*	95.54	-366.01	-269.60	-0.87	0.0900
Adenine dimer (interstrand)	*const*	105.74	105.74	208.33	3.16	0.1800
Thymine dimer (interstrand)	*const*	-331.71	-331.71	-659.20	-4.21	0.1620
Guanine dimer (interstrand)	*const*	-122.16	-122.16	-259.31	15.00	0.2410
Cytosine dimer (interstrand)	*const*	-68.98	-68.98	-139.52	1.57	0.1190
Adenine : Guanine (interstrand)	*const*	105.74	-122.16	-17.58	1.17	0.2290
Thymine : Cytosine (interstrand)	*const*	-68.98	-331.71	-397.04	-3.64	0.3210
Cytosine dimer (interstrand)	*const*	-93.99	95.54	0.37	1.19	0.1330
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-267.95	3.56	0.1180
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-267.15	2.76	0.1220
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-183.77	-4.21	0.1080
Guanine : Cytosine (stacked)	*opt*	-132.19	-93.99	-251.71	25.53	0.8380
Methylguanine : Methylcytosine (stacked)	*opt*	-122.16	-68.98	-219.50	28.37	1.1140
Adenine : Thymine (stacked)	*opt*	95.54	-366.16	-294.51	23.90	0.6750
Methyladenine : Methylthymine (stacked)	*opt*	105.74	-331.71	-255.28	29.32	0.4880
Cytosine dimer 1 (stacked)	*const*	-93.99	-93.99	-193.91	5.93	0.0930
Cytosine dimer 2 (stacked)	*const*	-93.99	-93.99	-204.88	16.90	0.1020
Cytosine dimer 3 (stacked)	*const*	-93.99	-93.99	-203.55	15.57	0.1010

Cytosine dimer 4 (stacked)	*const*	-93.99	-93.99	-205.77	17.80	0.1050
Cytosine dimer 5 (stacked)	*const*	-93.99	-93.99	-196.36	8.39	0.0950
Cytosine dimer 6 (stacked)	*const*	-93.99	-93.99	-195.55	7.58	0.0930
Cytosine dimer 7 (stacked)	*const*	-93.99	-93.99	-201.51	13.54	0.0970
Cytosine dimer 8 (stacked)	*const*	-93.99	-93.99	-201.07	13.09	0.1190
Cytosine dimer 9 (stacked)	*const*	-93.99	-93.99	-207.23	19.25	0.1000
Cytosine dimer 10 (stacked)	*const*	-93.99	-93.99	-207.34	19.36	0.1050
Cytosine dimer 11 (stacked)	*const*	-93.99	-93.99	-204.81	16.84	0.1030
Cytosine dimer 12 (stacked)	*const*	-93.99	-93.99	-201.21	13.23	0.0980
Cytosine dimer 13 (stacked)	*const*	-93.99	-93.99	-207.53	19.55	0.1010
Cytosine dimer 14 (stacked)	*const*	-93.99	-93.99	-203.71	15.74	0.1030
Adenine dimer (stacked)	*const*	95.35	95.35	172.93	17.77	0.1050
guanine dimer (stacked)	*const*	-132.19	-132.19	-287.17	22.78	0.1100
Adenine : cytosine (stacked)	*const*	95.35	-93.99	-18.43	19.79	0.1020
Guanine : Adenine (stacked)	*const*	-132.19	95.35	-58.15	21.31	0.1060
Cytosine dimer (stacked)	*const*	-93.99	-93.99	-206.64	18.67	0.0990
Adenine : Uracil (stacked)	*const*	95.35	-346.86	-270.98	19.47	0.0930
Guanine : Cytosine (stacked)	*const*	-132.19	-93.99	-243.71	17.53	0.1090
Cytosine : Uracil (stacked)	*const*	-93.99	-346.86	-457.76	16.91	0.1120
Uracil dimer (Stacked)	*const*	-346.86	-346.86	-710.85	17.12	0.1130
Guanine : Uracil (stacked)	*const*	-132.19	-346.86	-496.93	17.87	0.0980
Guanine dimer (stacked)	*const*	-93.99	-93.99	-202.63	14.65	0.1050
Cytosine dimer (stacked)	*const*	-93.99	-132.19	-229.05	2.87	0.1080
Adenine dimer (stacked)	*const*	95.54	95.54	179.14	11.95	0.0980
Thymine dimer (stacked)	*const*	95.54	-366.01	-272.61	2.15	0.1090
Guanine : cytosine (stacked)	*const*	-93.99	-132.19	-243.52	17.34	0.1060
Guanine : cytosine (stacked)	*const*	-93.99	-132.19	-237.81	11.63	0.1070
Adenine : guanine (stacked)	*const*	95.54	-132.19	-55.09	18.45	0.1060
Thymine : cytosine (stacked)	*const*	-366.01	-93.99	-478.45	18.45	0.0970
Adenine : guanine (stacked)	*const*	95.54	-132.19	-46.84	10.19	0.1040
Thymine : cytosine (stacked)	*const*	-366.01	-93.99	-474.68	14.68	0.2010
Thymine : guanine (stacked)	*const*	-366.01	-132.19	-511.93	13.73	0.1090
Adenine : cytosine (stacked)	*const*	95.54	-93.99	-9.75	11.31	0.1050
Thymine : guanine (stacked)	*const*	-366.01	-132.19	-511.57	13.37	0.2050
Adenine : cytosine (stacked)	*const*	95.54	-93.99	-13.31	14.86	0.0990
Adenine : thymine (stacked)	*const*	95.54	-366.01	-285.27	14.80	0.1750
Adenine : thymine (stacked)	*const*	95.54	-366.01	-288.99	18.53	0.1310
Adenine dimer (stacked)	*const*	95.54	95.54	178.51	12.58	0.0990
Thymine dimer (stacked)	*const*	-366.01	-366.01	-748.41	16.40	0.2160
Adenine : Thymine (stacked)	*const*	105.74	-331.71	-247.70	21.74	0.1910
Guanine : Cytosine (stacked)	*const*	-68.98	-122.16	-204.13	13.00	0.1910
Adenine : Cytosine (stacked)	*const*	105.74	-68.98	18.40	18.36	0.3390
Thymine : Guanine (stacked)	*const*	-331.71	-122.16	-473.43	19.57	0.2100
guanine : Cytosine (stacked)	*const*	-93.99	-132.19	-241.96	15.78	0.1150
Adenine : Guanine (stacked)	*const*	95.54	-132.19	-50.36	13.71	0.1360
Cytosine : guanine (stacked)	*const*	-132.19	-93.99	-241.55	15.37	0.1070
Guanine : Cytosine (stacked)	*const*	-132.19	-93.99	-245.97	19.79	0.1290
Phe30 : Lys46 (1RB9)	*const*	86.48	94.48	172.84	8.12	0.1170
Phe30 : Leu33 (1RB9)	*const*	86.51	84.60	153.59	17.51	0.1670
Phe30 : Tyr13 (1RB9)	*const*	86.48	81.71	155.75	12.43	0.1120
Phe30 : Phe49 (1RB9)	*const*	85.78	86.48	165.07	7.19	0.1290
Phe30 : Tyr4 (1RB9)	*const*	86.48	88.01	157.79	16.70	0.1400
Phe49 : Cys39 (1RB9)	*const*	85.83	66.51	148.24	4.10	0.1280
Phe49 : Cys6 (1RB9)	*const*	85.83	66.60	137.81	14.62	0.1330
Phe49 : Lys46 (1RB9)	*const*	89.31	89.70	171.58	7.42	0.1140
Phe49 : Val5 (1RB9)	*const*	86.30	84.01	151.63	18.68	0.1570
Phe49 : Tyr37 (1RB9)	*const*	88.46	119.21	205.13	2.53	0.1330
Phe49 : Tyr4 (1RB9)	*const*	85.77	87.03	162.31	10.49	0.1300
Phe49 : Peptide bond (1RB9)	*const*	88.52	-91.75	-8.87	5.65	0.1630
Phe49 : Peptide bond (1RB9)	*const*	85.96	-91.75	-29.22	23.43	0.1820
Glu47 : Lys6 (PDB:1IU5)	*const*	245.78	74.90	-9.47	330.16	0.1390
Glu49 : Lys6 (PDB:1BQ9)	*const*	245.11	78.61	-137.63	461.35	0.1770
Glu54 : Lys2 (PDB:1SMM)	*const*	275.01	79.68	-18.52	373.22	0.1910
Glu50 : LysK30 (PDB:1BRF)	*const*	240.64	61.23	50.15	251.73	0.1770
Glu50 : Lys52 (PDB:1BRF)	*const*	241.21	85.25	-49.61	376.07	0.1400
Glu49 : Lys6 (PDB:1BRF)	*const*	248.63	78.24	51.24	275.63	0.1700

MM2* (explicit lone pairs)

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-132.19	-93.99	-254.63	28.44	0.7320
Methylguanine : Methylcytosine (WC)	*opt*	-68.98	-122.16	-220.42	29.29	2.9330
Adenine : Thymine (WC)	*opt*	105.65	-331.71	-255.36	29.30	2.6030
Methyladenine : Methylthymine (planar)	*opt*	105.65	-331.53	-255.64	29.77	2.0690
8-Oxoguanine : Cytosine (WC planar)	*opt*	-325.51	-93.99	-447.80	28.30	0.8040
Inosine : Cytosine (WC planar)	*opt*	-93.99	18.96	-102.45	27.43	2.7860
Guanine : Uracil (wobble)	*opt*	-132.19	-346.86	-521.15	42.09	0.3010
Cytosine : CytosineH+	*opt*	-93.99	-426.38	-557.65	37.29	2.8350
Uracil dimer (Calcutta planar)	*opt*	-346.99	-346.86	-716.95	23.10	0.2670
Uracil dimer (planar)	*opt*	-346.99	-346.99	-734.15	40.16	0.1650
6-Thioguanine : Cytosine (WC planar)	*opt*	-93.99	-89.84	-211.46	27.63	2.9310
Adenine : 4-Thiouracil (WC)	*opt*	95.54	-253.85	-164.53	6.22	3.3280
2-aminoadenine : Thymine	*opt*	69.15	-366.01	-320.54	23.68	1.6640
2-aminoadenine : Thymine (planar)	*opt*	69.03	-366.01	-310.99	14.01	2.8670
Adenine : Difluorotoluene	*opt*	95.54	-16.59	55.36	23.60	2.3890
Guanine : 4-Thiouracil	*opt*	-132.19	-253.85	-429.91	43.86	0.2460
Guanine : 2-Thiouracil	*opt*	-132.19	-216.84	-374.94	25.91	0.5790
Adenine : Cytosine (planar)	*opt*	-93.99	95.54	-10.99	12.55	2.6010

Guanine dimer (planar)	*opt*	-132.19	-132.19	-289.98	25.59	3.0770
Guanine 6-Thioguanine (planar)	*opt*	-132.19	-89.84	-236.45	14.42	2.8390
6-Thioguanine : Guanine (planar)	*opt*	-89.84	-132.19	-248.81	26.78	3.5100
Guanine : Adenine 1	*opt*	-132.19	95.54	-59.70	23.05	1.8370
Guanine : Adenine 1 (planar)	*opt*	95.54	-132.19	-48.50	11.85	0.6770
Guanine : Adenine 2	*opt*	-132.19	95.54	-61.97	25.32	2.2900
Guanine : Adenine 2 (planar)	*opt*	-132.18	95.54	-43.52	6.88	2.9840
Guanine : Adenine 3	*opt*	-132.19	95.54	-62.53	25.89	2.0890
Guanine : Adenine 4	*opt*	-132.19	95.54	-62.48	25.83	3.3050
Adenine dimer 1 (planar)	*opt*	95.54	95.54	186.37	4.72	0.4900
Adenine dimer 2 (planar)	*opt*	95.54	95.54	169.37	21.72	2.5700
Adenine dimer 3 (planar)	*opt*	95.54	95.54	174.66	16.43	2.1730
8-Oxoguanine : Guanine	*opt*	-132.19	-325.51	-501.33	43.63	0.3640
2-Thiouracil dimer (planar)	*opt*	-216.87	-216.87	-459.50	25.76	0.4740
Adenine : Thymine (WC)	*const*	105.98	-331.71	-211.77	-13.96	0.1580
Guanine : Cytosine (WC)	*const*	-68.95	-122.15	-189.64	-1.46	0.2080
Adenine : thymine (WC)	*const*	105.77	-331.71	-208.16	-17.78	0.1750
Guanine : adenine (HB)	*const*	-132.19	95.56	-26.01	-10.62	0.1690
Cytosine : Guanine (WC)	*const*	-93.71	-132.19	-228.78	2.87	0.1310
Guanine : Cytosine (WC)	*const*	-132.19	-93.72	-228.16	2.25	0.1180
Cytosine : guanine (interstrand)	*const*	-132.19	-93.99	-229.40	3.22	0.0920
Adenine : thymine (interstrand)	*const*	-366.01	95.54	-271.46	1.00	0.0840
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-185.02	-2.95	0.0950
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-263.96	-0.43	0.0920
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-188.88	0.90	0.0950
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-272.46	8.07	0.0910
Adenine : cytosine (interstrand)	*const*	95.54	-93.99	-0.45	2.01	0.0900
Thymine : guanine (interstrand)	*const*	-366.01	-132.19	-495.42	-2.79	0.0880
Thymine : guanine (interstrand)	*const*	-132.19	-366.01	-498.50	0.29	0.0890
Thymine : cytosine (interstrand)	*const*	95.54	-93.99	-0.65	2.20	0.0910
Adenine : guanine (interstrand)	*const*	95.54	-132.19	-46.26	9.61	0.0870
Thymine : cytosine (interstrand)	*const*	-366.01	-93.99	-460.74	0.75	0.0890
Thymine : cytosine (interstrand)	*const*	-366.01	-93.99	-457.97	-2.03	0.0910
Adenine : guanine (interstrand)	*const*	95.54	-132.19	-36.50	-0.15	0.0890
Thymine dimer (interstrand)	*const*	-366.01	-366.01	-729.09	-2.93	0.0940
Adenine dimer (interstrand)	*const*	95.54	95.54	189.49	1.60	0.0860
Adenine dimer (interstrand)	*const*	95.54	95.54	188.96	2.13	0.0880
Thymine dimer (interstrand)	*const*	-366.01	-366.01	-729.95	-2.07	0.0870
Adenine : thymine (interstrand)	*const*	95.54	-366.01	-272.96	2.49	0.0760
Thymine : adenine (interstrand)	*const*	95.54	-366.01	-269.60	-0.87	0.0770
Adenine dimer (interstrand)	*const*	105.74	105.74	208.33	3.16	0.4240
Thymine dimer (interstrand)	*const*	-331.71	-331.71	-659.20	-4.21	0.0990
Guanine dimer (interstrand)	*const*	-122.16	-122.16	-259.31	15.00	0.1110
Cytosine dimer (interstrand)	*const*	-68.98	-68.98	-139.52	1.57	0.0930
Adenine : Guanine (interstrand)	*const*	105.74	-122.16	-17.58	1.17	0.1100
Thymine : Cytosine (interstrand)	*const*	-68.98	-331.71	-397.04	-3.64	0.1390
Cytosine dimer (interstrand)	*const*	-93.99	95.54	0.37	1.19	0.2750
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-267.95	3.56	0.0930
Guanine dimer (interstrand)	*const*	-132.19	-132.19	-267.15	2.76	0.0920
Cytosine dimer (interstrand)	*const*	-93.99	-93.99	-183.77	-4.21	0.0960
Guanine : Cytosine (stacked)	*opt*	-132.19	-93.99	-251.71	25.53	0.7700
Methylguanine : Methylcytosine (stacked)	*opt*	-122.16	-68.98	-219.50	28.37	0.9330
Adenine : Thymine (stacked)	*opt*	95.54	-366.16	-294.51	23.90	0.6370
Methyladenine : Methylthymine (stacked)	*opt*	105.74	-331.71	-255.28	29.32	0.4300
Cytosine dimer 1 (stacked)	*const*	-93.99	-93.99	-193.91	5.93	0.0890
Cytosine dimer 2 (stacked)	*const*	-93.99	-93.99	-204.88	16.90	0.0910
Cytosine dimer 3 (stacked)	*const*	-93.99	-93.99	-203.55	15.57	0.0910
Cytosine dimer 4 (stacked)	*const*	-93.99	-93.99	-205.77	17.80	0.0890
Cytosine dimer 5 (stacked)	*const*	-93.99	-93.99	-196.36	8.39	0.0900
Cytosine dimer 6 (stacked)	*const*	-93.99	-93.99	-195.55	7.58	0.0890
Cytosine dimer 7 (stacked)	*const*	-93.99	-93.99	-201.51	13.54	0.0900
Cytosine dimer 8 (stacked)	*const*	-93.99	-93.99	-201.07	13.09	0.0930
Cytosine dimer 9 (stacked)	*const*	-93.99	-93.99	-207.23	19.25	0.0900
Cytosine dimer 10 (stacked)	*const*	-93.99	-93.99	-207.34	19.36	0.0900
Cytosine dimer 11 (stacked)	*const*	-93.99	-93.99	-204.81	16.84	0.0890
Cytosine dimer 12 (stacked)	*const*	-93.99	-93.99	-201.21	13.23	0.0900
Cytosine dimer 13 (stacked)	*const*	-93.99	-93.99	-207.53	19.55	0.0900
Cytosine dimer 14 (stacked)	*const*	-93.99	-93.99	-203.71	15.74	0.0940
Adenine dimer (stacked)	*const*	95.35	95.35	172.93	17.77	0.0890
guanine dimer (stacked)	*const*	-132.19	-132.19	-287.17	22.78	0.0900
Adenine : cytosine (stacked)	*const*	95.35	-93.99	-18.43	19.79	0.0870
Guanine : Adenine (stacked)	*const*	-132.19	95.35	-58.15	21.31	0.0910
Cytosine dimer (stacked)	*const*	-93.99	-93.99	-206.64	18.67	0.0890
Adenine : Uracil (stacked)	*const*	95.35	-346.86	-270.98	19.47	0.0830
Guanine : Cytosine (stacked)	*const*	-132.19	-93.99	-243.71	17.53	0.0910
Cytosine : Uracil (stacked)	*const*	-93.99	-346.86	-457.76	16.91	0.0930
Uracil dimer (Stacked)	*const*	-346.86	-346.86	-710.85	17.12	0.0910
Guanine : Uracil (stacked)	*const*	-132.19	-346.86	-496.93	17.87	0.0880
Guanine dimer (stacked)	*const*	-93.99	-93.99	-202.63	14.65	0.0960
Cytosine dimer (stacked)	*const*	-93.99	-132.19	-229.05	2.87	0.0930
Adenine dimer (stacked)	*const*	95.54	95.54	179.14	11.95	0.0850
Thymine dimer (stacked)	*const*	95.54	-366.01	-272.61	2.15	0.0880
Guanine : cytosine (stacked)	*const*	-93.99	-132.19	-243.52	17.34	0.0920
Guanine : cytosine (stacked)	*const*	-93.99	-132.19	-237.81	11.63	0.0920
Adenine : guanine (stacked)	*const*	95.54	-132.19	-55.09	18.45	0.0880
Thymine : cytosine (stacked)	*const*	-366.01	-93.99	-478.45	18.45	0.0810
Adenine : guanine (stacked)	*const*	95.54	-132.19	-46.84	10.19	0.0870
Thymine : cytosine (stacked)	*const*	-366.01	-93.99	-474.68	14.68	0.1100

Thymine : guanine (stacked)	*const*	-366.01	-132.19	-511.93	13.73	0.0910
Adenine : cytosine (stacked)	*const*	95.54	-93.99	-9.75	11.31	0.0920
Thymine : guanine (stacked)	*const*	-366.01	-132.19	-511.57	13.37	0.1070
Adenine : cytosine (stacked)	*const*	95.54	-93.99	-13.31	14.86	0.0880
Adenine : thymine (stacked)	*const*	95.54	-366.01	-285.27	14.80	0.0970
Adenine : thymine (stacked)	*const*	95.54	-366.01	-288.99	18.53	0.0980
Adenine dimer (stacked)	*const*	95.54	95.54	178.51	12.58	0.0850
Thymine dimer (stacked)	*const*	-366.01	-366.01	-748.41	16.40	0.1120
Adenine : Thymine (stacked)	*const*	105.74	-331.71	-247.70	21.74	0.1010
Guanine : Cytosine (stacked)	*const*	-68.98	-122.16	-204.13	13.00	0.1040
Adenine : Cytosine (stacked)	*const*	105.74	-68.98	18.40	18.36	0.1460
Thymine : Guanine (stacked)	*const*	-331.71	-122.16	-473.43	19.57	0.1090
guanine : Cytosine (stacked)	*const*	-93.99	-132.19	-241.96	15.78	0.0950
Adenine : Guanine (stacked)	*const*	95.54	-132.19	-50.36	13.71	0.0950
Cytosine : guanine (stacked)	*const*	-132.19	-93.99	-241.55	15.37	0.0890
Guanine : Cytosine (stacked)	*const*	-132.19	-93.99	-245.97	19.79	0.0920
Phe30 : Lys46 (1RB9)	*const*	42.83	56.90	91.76	7.97	0.0860
Phe30 : Leu33 (1RB9)	*const*	42.86	41.95	64.24	20.57	0.1030
Phe30 : Tyr13 (1RB9)	*const*	42.80	34.40	64.23	12.97	0.0840
Phe30 : Phe49 (1RB9)	*const*	39.08	42.84	74.93	6.99	0.0910
Phe30 : Tyr4 (1RB9)	*const*	42.80	40.89	67.54	16.15	0.0940
Phe49 : Cys39 (1RB9)	*const*	39.10	8.40	43.58	3.91	0.0960
Phe49 : Cys6 (1RB9)	*const*	39.03	9.75	33.18	15.60	0.0990
Phe49 : Lys46 (1RB9)	*const*	41.70	45.54	77.70	9.54	0.0850
Phe49 : Val5 (1RB9)	*const*	39.49	40.99	61.55	18.92	0.1020
Phe49 : Tyr37 (1RB9)	*const*	41.03	72.20	111.35	1.88	0.0910
Phe49 : Tyr4 (1RB9)	*const*	39.04	40.36	69.28	10.12	0.0960
Phe49 : Peptide bond (1RB9)	*const*	41.08	-91.75	-55.74	5.07	0.1010
Phe49 : Peptide bond (1RB9)	*const*	39.18	-91.75	-76.62	24.06	0.1030
Glu47 : Lys6 (PDB:1IU5)	*const*	200.96	12.39	-117.85	331.19	0.1660
Glu49 : Lys6 (PDB:1BQ9)	*const*	200.78	27.62	-226.76	455.16	0.1170
Glu54 : Lys2 (PDB:1SMM)	*const*	217.84	24.81	-112.77	355.42	0.1240
Glu50 : LysK30 (PDB:1BRF)	*const*	194.45	4.24	-49.60	248.29	0.1210
Glu50 : Lys52 (PDB:1BRF)	*const*	194.82	28.32	-146.37	369.51	0.1040
Glu49 : Lys6 (PDB:1BRF)	*const*	204.59	27.18	-44.72	276.48	0.1090

MM3*

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-849.37	-416.21	-1282.60	17.02	0.8970
Methylguanine : Methylcytosine (WC)	*opt*	-368.79	-817.35	-1203.79	17.64	1.0250
Adenine : Thymine (WC)	*opt*	-211.61	-642.41	-869.00	14.98	0.7190
Methyladenine : Methylthymine (planar)	*opt*	-210.94	-642.41	-886.53	33.18	2.4160
8-Oxoguanine : Cytosine (WC planar)	*opt*	-877.97	-416.21	-1312.06	17.88	1.4500
Inosine : Cytosine (WC planar)	*opt*	-416.21	-260.63	-695.80	18.96	0.4970
Guanine : Uracil (wobble)	*opt*	-849.47	-705.99	-1568.46	13.00	0.4720
Cytosine : CytosineH+	*opt*	Missing params				
Uracil dimer (Calcutta planar)	*opt*	-705.99	-705.99	-1424.56	12.57	0.2140
Uracil dimer (planar)	*opt*	-705.99	-705.99	-1427.11	15.12	0.1360
6-Thioguanine : Cytosine (WC planar)	*opt*	Missing params				
Adenine : 4-Thiouracil (WC)	*opt*	Missing params				
2-aminoadenine : Thymine	*opt*	-600.42	-707.54	-1324.33	16.36	0.4580
2-aminoadenine : Thymine (planar)	*opt*	-600.82	-707.54	-1324.72	16.36	0.4420
Adenine : Difluorotoluene	*opt*	-243.35	-45.26	-307.65	19.04	1.8150
Guanine : 4-Thiouracil	*opt*	Missing params				
Guanine : 2-Thiouracil	*opt*	Missing params				
Adenine : Cytosine (planar)	*opt*	-416.27	-243.05	-690.37	31.06	2.4140
Guanine dimer (planar)	*opt*	-849.47	-849.47	-1717.48	18.54	1.0040
Guanine 6-Thioguanine (planar)	*opt*	Missing params				
6-Thioguanine : Guanine (planar)	*opt*	Missing params				
Guanine : Adenine 1	*opt*	-849.47	-243.05	-1106.32	13.80	0.8870
Guanine : Adenine 1 (planar)	*opt*	-243.11	-849.51	-1106.44	13.82	0.6840
Guanine : Adenine 2	*opt*	-849.48	-243.05	-1136.13	43.60	2.4390
Guanine : Adenine 2 (planar)	*opt*	-849.47	-243.37	-1136.38	43.55	2.6940
Guanine : Adenine 3	*opt*	-849.48	-243.05	-1125.09	32.56	2.6880
Guanine : Adenine 4	*opt*	-849.48	-243.05	-1106.82	14.29	1.0840
Adenine dimer 1 (planar)	*opt*	-243.05	-243.05	-517.75	31.65	3.1400
Adenine dimer 2 (planar)	*opt*	-243.05	-243.13	-529.48	43.30	3.3880
Adenine dimer 3 (planar)	*opt*	-243.05	-243.05	-529.42	43.32	2.3450
8-Oxoguanine : Guanine	*opt*	-849.82	-877.97	-1753.04	25.25	0.5580
2-Thiouracil dimer (planar)	*opt*	Missing params				
Adenine : Thymine (WC)	*const*	-210.34	-642.41	-855.01	2.27	0.1980
Guanine : Cytosine (WC)	*const*	-368.85	-816.84	-1185.44	-0.25	0.3380
Adenine : thymine (WC)	*const*	-210.66	-642.41	-853.11	0.05	0.1650
Guanine : adenine (HB)	*const*	-849.37	-243.03	-1098.94	6.53	0.3950
Cytosine : Guanine (WC)	*const*	-416.27	-849.37	-1271.09	5.45	0.2700
Guanine : Cytosine (WC)	*const*	-849.37	-416.21	-1268.18	2.59	0.3000
Cytosine : guanine (interstrand)	*const*	-849.48	-416.21	-1275.63	9.94	0.3760
Adenine : thymine (interstrand)	*const*	-707.54	-243.05	-958.77	8.18	0.2030
Cytosine dimer (interstrand)	*const*	-416.21	-416.21	-829.90	-2.52	0.2880
Guanine dimer (interstrand)	*const*	-849.47	-849.47	-1705.79	6.85	0.5590
Cytosine dimer (interstrand)	*const*	-416.21	-416.21	-835.56	3.14	0.2640
Guanine dimer (interstrand)	*const*	-849.47	-849.47	-1703.81	4.87	0.3280
Adenine : cytosine (interstrand)	*const*	-243.05	-416.21	-661.54	2.28	0.2820
Thymine : guanine (interstrand)	*const*	-707.54	-849.47	-1558.19	1.18	0.3440
Thymine : guanine (interstrand)	*const*	-849.47	-707.54	-1566.50	9.49	0.3500
Thymine : cytosine (interstrand)	*const*	-243.05	-416.21	-664.83	5.57	0.3060
Adenine : guanine (interstrand)	*const*	-243.05	-849.47	-1103.95	11.42	0.3150

Thymine : cytosine (interstrand)	*const*	-707.54	-416.21	-1128.66	4.91	0.2480
Thymine : cytosine (interstrand)	*const*	-707.54	-416.21	-1124.44	0.69	0.2050
Adenine : guanine (interstrand)	*const*	-243.05	-849.47	-1102.04	9.52	0.4320
Thymine dimer (interstrand)	*const*	-707.54	-707.54	-1416.43	1.35	0.0860
Adenine dimer (interstrand)	*const*	-243.05	-243.05	-485.87	-0.24	0.2190
Adenine dimer (interstrand)	*const*	-243.05	-243.05	-488.29	2.18	0.2570
Thymine dimer (interstrand)	*const*	-707.54	-707.54	-1415.35	0.27	0.1100
Adenine : thymine (interstrand)	*const*	-243.05	-707.54	-956.41	5.81	0.2080
Thymine : adenine (interstrand)	*const*	-243.05	-707.54	-957.11	6.52	0.2150
Adenine dimer (interstrand)	*const*	-210.73	-210.40	-421.15	0.02	0.2590
Thymine dimer (interstrand)	*const*	-642.41	-642.41	-1285.79	0.97	0.1550
Guanine dimer (interstrand)	*const*	-816.94	-816.94	-1645.59	11.70	0.5240
Cytosine dimer (interstrand)	*const*	-368.85	-368.85	-741.52	3.82	0.2440
Adenine : Guanine (interstrand)	*const*	-210.67	-816.82	-1033.83	6.34	0.3990
Thymine : Cytosine (interstrand)	*const*	-368.85	-642.41	-1011.90	0.64	0.3510
Cytosine dimer (interstrand)	*const*	-416.27	-243.03	-661.07	1.77	0.2430
Guanine dimer (interstrand)	*const*	-849.37	-849.37	-1705.98	7.23	0.4070
Guanine dimer (interstrand)	*const*	-849.37	-849.37	-1705.72	6.97	0.5230
Cytosine dimer (interstrand)	*const*	-416.27	-416.21	-830.08	-2.40	0.2660
Guanine : Cytosine (stacked)	*opt*	-849.47	-416.21	-1289.82	24.14	0.8770
Methylguanine : Methylcytosine (stacked)	*opt*	-817.36	-368.79	-1213.13	26.98	0.8240
Adenine : Thymine (stacked)	*opt*	-242.69	-707.54	-982.24	32.01	0.6100
Methyladenine : Methylthymine (stacked)	*opt*	-211.18	-642.41	-887.08	33.49	1.2260
Cytosine dimer 1 (stacked)	*const*	-416.21	-416.21	-830.76	-1.66	0.1480
Cytosine dimer 2 (stacked)	*const*	-416.21	-416.21	-847.13	14.72	0.3300
Cytosine dimer 3 (stacked)	*const*	-416.21	-416.21	-851.97	19.55	0.2840
Cytosine dimer 4 (stacked)	*const*	-416.21	-416.21	-851.73	19.31	0.2580
Cytosine dimer 5 (stacked)	*const*	-416.21	-416.21	-841.51	9.10	0.2540
Cytosine dimer 6 (stacked)	*const*	-416.21	-416.21	-842.72	10.30	0.2770
Cytosine dimer 7 (stacked)	*const*	-416.21	-416.21	-846.63	14.22	0.2350
Cytosine dimer 8 (stacked)	*const*	-416.21	-416.21	-852.16	19.74	0.2960
Cytosine dimer 9 (stacked)	*const*	-416.21	-416.21	-852.67	20.25	0.2600
Cytosine dimer 10 (stacked)	*const*	-416.21	-416.21	-854.25	21.83	0.2360
Cytosine dimer 11 (stacked)	*const*	-416.21	-416.21	-849.33	16.92	0.2470
Cytosine dimer 12 (stacked)	*const*	-416.21	-416.21	-842.83	10.41	0.3140
Cytosine dimer 13 (stacked)	*const*	-416.21	-416.21	-854.66	22.25	0.2160
Cytosine dimer 14 (stacked)	*const*	-416.21	-416.21	-845.21	12.79	0.1800
Adenine dimer (stacked)	*const*	-242.36	-243.08	-529.02	43.58	0.3050
guanine dimer (stacked)	*const*	-849.47	-849.48	-1722.82	23.87	0.3960
Adenine : cytosine (stacked)	*const*	-243.08	-416.21	-691.68	32.39	0.3100
Guanine : Adenine (stacked)	*const*	-849.47	-242.36	-1129.81	37.98	0.3460
Cytosine dimer (stacked)	*const*	-416.21	-416.21	-849.95	17.53	0.2350
Adenine : Uracil (stacked)	*const*	-242.36	-705.99	-974.58	26.23	0.1980
Guanine : Cytosine (stacked)	*const*	-849.47	-416.21	-1285.02	19.34	0.4240
Cytosine : Uracil (stacked)	*const*	-416.21	-705.99	-1143.42	21.21	0.2480
Uracil dimer (Stacked)	*const*	-705.99	-705.99	-1432.28	20.30	0.0900
Guanine : Uracil (stacked)	*const*	-849.48	-705.99	-1583.06	27.59	0.3370
Guanine dimer (stacked)	*const*	-416.21	-416.21	-844.17	11.75	0.2810
Cytosine dimer (stacked)	*const*	-416.21	-849.47	-1272.99	7.31	0.4420
Adenine dimer (stacked)	*const*	-242.33	-243.05	-495.90	10.52	0.2790
Thymine dimer (stacked)	*const*	-243.05	-707.54	-956.29	5.70	0.1960
Guanine : cytosine (stacked)	*const*	-416.21	-849.47	-1280.55	14.87	0.3660
Guanine : cytosine (stacked)	*const*	-416.21	-849.48	-1284.42	18.73	0.4710
Adenine : guanine (stacked)	*const*	-242.33	-849.47	-1112.90	21.10	0.3970
Thymine : cytosine (stacked)	*const*	-707.54	-416.21	-1133.75	10.00	0.1290
Adenine : guanine (stacked)	*const*	-243.05	-849.48	-1116.45	23.92	0.4120
Thymine : cytosine (stacked)	*const*	-707.54	-416.21	-1139.69	15.94	0.2920
Thymine : guanine (stacked)	*const*	-707.54	-849.47	-1570.51	13.49	0.3750
Adenine : cytosine (stacked)	*const*	-242.33	-416.21	-671.25	12.71	0.2780
Thymine : guanine (stacked)	*const*	-707.54	-849.47	-1573.42	16.41	0.3480
Adenine : cytosine (stacked)	*const*	-242.33	-416.21	-668.61	10.07	0.4070
Adenine : thymine (stacked)	*const*	-243.05	-707.54	-967.90	17.30	0.2710
Adenine : thymine (stacked)	*const*	-242.33	-707.54	-959.93	10.06	0.2350
Adenine dimer (stacked)	*const*	-242.33	-242.33	-500.16	15.50	0.2980
Thymine dimer (stacked)	*const*	-707.54	-707.54	-1428.66	13.58	0.1870
Adenine : Thymine (stacked)	*const*	-210.28	-642.41	-866.31	13.62	0.2150
Guanine : Cytosine (stacked)	*const*	-368.85	-816.90	-1204.22	18.47	0.4620
Adenine : Cytosine (stacked)	*const*	-210.63	-368.85	-590.71	11.23	0.4550
Thymine : Guanine (stacked)	*const*	-642.41	-816.87	-1476.51	17.23	0.3440
guanine : Cytosine (stacked)	*const*	-416.27	-849.37	-1290.16	24.53	0.4460
Adenine : Guanine (stacked)	*const*	-243.03	-849.37	-1117.01	24.61	0.4460
Cytosine : guanine (stacked)	*const*	-849.37	-416.27	-1283.29	17.65	0.3660
Guanine : Cytosine (stacked)	*const*	-849.37	-416.21	-1280.95	15.37	0.4500
Phe30 : Lys46 (1RB9)	*const*	107.34	67.19	168.94	5.60	0.1160
Phe30 : Leu33 (1RB9)	*const*	107.52	57.47	154.51	10.47	0.1490
Phe30 : Tyr13 (1RB9)	*const*	107.37	79.48	177.34	9.51	0.1170
Phe30 : Phe49 (1RB9)	*const*	98.31	107.52	199.37	6.46	0.1240
Phe30 : Tyr4 (1RB9)	*const*	107.35	84.32	182.10	9.57	0.1290
Phe49 : Cys39 (1RB9)	*const*	98.55	92.12	191.14	-0.47	0.1260
Phe49 : Cys6 (1RB9)	*const*	98.39	89.89	177.97	10.31	0.1270
Phe49 : Lys46 (1RB9)	*const*	105.27	61.86	161.37	5.77	0.1140
Phe49 : Val5 (1RB9)	*const*	99.00	59.87	145.27	13.60	0.1540
Phe49 : Tyr37 (1RB9)	*const*	104.72	166.14	270.37	0.48	0.1210
Phe49 : Tyr4 (1RB9)	*const*	98.33	81.40	174.66	5.07	0.1140
Phe49 : Peptide bond (1RB9)	*const*	104.74	-39.18	63.63	1.93	0.1720
Phe49 : Peptide bond (1RB9)	*const*	98.63	-39.18	41.55	17.90	0.1880
Glu47 : Lys6 (PDB:1IU5)	*const*	74.53	2.00	-258.29	334.82	0.1450
Glu49 : Lys6 (PDB:1BQ9)	*const*	79.17	34.49	-369.71	483.36	0.1320

Glu54 : Lys2 (PDB:1SMM)	*const*	108.13	38.12	-245.85	392.10	0.2180
Glu50 : LysK30 (PDB:1BRF)	*const*	72.94	-8.42	-200.22	264.74	0.1580
Glu50 : Lys52 (PDB:1BRF)	*const*	73.91	35.36	-307.17	416.44	0.1220
Glu49 : Lys6 (PDB:1BRF)	*const*	84.91	33.98	-172.08	290.97	0.3440

AMBER*

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-361.60	-331.02	-785.51	92.89	0.0850
Methylguanine : Methylcytosine (WC)	*opt*	-325.83	-363.43	-783.20	93.94	0.1290
Adenine : Thymine (WC)	*opt*	-362.20	-627.86	-1036.46	46.40	0.4140
Methyladenine : Methylthymine (planar)	*opt*	-362.20	-627.86	-1039.37	49.31	0.2000
8-Oxoguanine : Cytosine (WC planar)	*opt*	-205.55	-331.02	-602.29	65.72	0.0710
Inosine : Cytosine (WC planar)	*opt*	-331.02	-27.76	-415.11	56.33	0.1580
Guanine : Uracil (wobble)	*opt*	-361.60	-336.61	-747.39	49.18	0.1250
Cytosine : CytosineH+	*opt*	-331.02	-70.06	-483.05	81.98	0.1160
Uracil dimer (Calcutta planar)	*opt*	-336.61	-336.61	-699.42	26.21	0.1980
Uracil dimer (planar)	*opt*	-336.61	-336.61	-712.87	39.66	0.0550
6-Thioguanine : Cytosine (WC planar)	*opt*	-331.02	-179.73	-553.38	42.63	0.1080
Adenine : 4-Thiouracil (WC)	*opt*	-363.92	-186.26	-570.13	19.95	3.8870
2-aminoadenine : Thymine	*opt*	-458.77	-631.08	-1153.71	63.86	0.2880
2-aminoadenine : Thymine (planar)	*opt*	-458.77	-630.94	-1153.61	63.89	0.0520
Adenine : Difluorotoluene	*opt*	-364.94	-11.91	-418.09	41.24	2.7540
Guanine : 4-Thiouracil	*opt*	-361.60	-186.26	-592.47	44.62	0.2070
Guanine : 2-Thiouracil	*opt*	-361.60	-186.87	-600.53	52.06	1.9750
Adenine : Cytosine (planar)	*opt*	-331.02	-363.92	-752.51	57.57	0.0710
Guanine dimer (planar)	*opt*	-361.60	-361.60	-788.29	65.09	0.1730
Guanine 6-Thioguanine (planar)	*opt*	-361.60	-179.73	-583.61	42.29	0.2040
6-Thioguanine : Guanine (planar)	*opt*	-179.73	-361.60	-578.83	37.51	0.1620
Guanine : Adenine 1	*opt*	-361.60	-363.92	-783.28	57.76	0.1590
Guanine : Adenine 1 (planar)	*opt*	-364.94	-361.60	-784.07	57.53	0.0310
Guanine : Adenine 2	*opt*	-361.60	-363.92	-772.64	47.13	0.3090
Guanine : Adenine 2 (planar)	*opt*	-361.60	-363.92	-771.29	45.78	0.0990
Guanine : Adenine 3	*opt*	-361.60	-363.92	-779.09	53.57	0.7200
Guanine : Adenine 4	*opt*	-361.60	-363.92	-775.76	50.24	0.4090
Adenine dimer 1 (planar)	*opt*	-363.92	-363.92	-777.80	49.96	0.0480
Adenine dimer 2 (planar)	*opt*	-363.92	-364.94	-775.48	46.62	0.3890
Adenine dimer 3 (planar)	*opt*	-363.92	-363.92	-773.77	45.93	1.2070
8-Oxoguanine : Guanine	*opt*	-361.60	-205.55	-616.06	48.91	0.2110
2-Thiouracil dimer (planar)	*opt*	-186.87	-186.87	-391.37	17.63	0.3610
Adenine : Thymine (WC)	*const*	-362.20	-627.86	-1035.48	45.43	0.3730
Guanine : Cytosine (WC)	*const*	-325.83	-363.43	-782.80	93.54	0.4070
Adenine : thymine (WC)	*const*	-362.20	-627.86	-1034.34	44.28	0.3470
Guanine : adenine (HB)	*const*	-361.60	-364.94	-771.45	44.91	0.0960
Cytosine : Guanine (WC)	*const*	-331.02	-361.60	-784.42	91.80	0.0740
Guanine : Cytosine (WC)	*const*	-361.60	-331.02	-785.42	92.80	0.0670
Cytosine : guanine (interstrand)	*const*	-361.60	-331.02	-710.28	17.67	0.1200
Adenine : thymine (interstrand)	*const*	-631.08	-363.92	-1006.42	11.41	0.2100
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-653.53	-8.51	0.1060
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-722.45	-0.75	0.0790
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-658.23	-3.81	0.1140
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-746.41	23.21	0.0940
Adenine : cytosine (interstrand)	*const*	-363.92	-331.02	-696.24	1.30	0.0990
Thymine : guanine (interstrand)	*const*	-631.08	-361.60	-993.73	1.05	0.1880
Thymine : guanine (interstrand)	*const*	-361.60	-631.08	-1000.94	8.26	0.1840
Thymine : cytosine (interstrand)	*const*	-363.92	-331.02	-697.27	2.33	0.1000
Adenine : guanine (interstrand)	*const*	-363.92	-361.60	-745.25	19.74	0.0830
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-965.87	3.77	0.1940
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-961.74	-0.36	0.1910
Adenine : guanine (interstrand)	*const*	-363.92	-361.60	-744.34	18.82	0.1040
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1262.20	0.04	0.2460
Adenine dimer (interstrand)	*const*	-363.92	-363.92	-734.40	6.56	0.0920
Adenine dimer (interstrand)	*const*	-363.92	-363.92	-740.89	13.05	0.0980
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1261.46	-0.70	0.2660
Adenine : thymine (interstrand)	*const*	-363.92	-631.08	-1002.86	7.85	0.1820
Thymine : adenine (interstrand)	*const*	-363.92	-631.08	-1001.70	6.70	0.1950
Adenine dimer (interstrand)	*const*	-362.20	-362.20	-732.88	8.48	0.3360
Thymine dimer (interstrand)	*const*	-627.86	-627.86	-1255.34	-0.37	0.4330
Guanine dimer (interstrand)	*const*	-363.43	-363.43	-757.12	30.26	0.4090
Cytosine dimer (interstrand)	*const*	-325.83	-325.83	-649.81	-1.86	0.4340
Adenine : Guanine (interstrand)	*const*	-362.20	-363.43	-744.65	19.02	0.3020
Thymine : Cytosine (interstrand)	*const*	-325.83	-627.86	-953.20	-0.49	0.3490
Cytosine dimer (interstrand)	*const*	-331.02	-364.94	-714.92	18.96	0.1660
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-741.63	18.44	0.0960
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-728.07	4.88	0.1100
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-653.73	-8.31	0.0960
Guanine : Cytosine (stacked)	*opt*	-361.60	-331.02	-745.60	52.98	0.3540
Methylguanine : Methylcytosine (stacked)	*opt*	-363.43	-325.83	-744.54	55.28	0.3810
Adenine : Thymine (stacked)	*opt*	-364.94	-631.08	-1040.69	44.67	0.4270
Methyladenine : Methylthymine (stacked)	*opt*	-362.20	-627.86	-1039.27	49.22	0.5470
Cytosine dimer 1 (stacked)	*const*	-331.02	-331.02	-664.15	2.11	0.0750
Cytosine dimer 2 (stacked)	*const*	-331.02	-331.02	-682.80	20.76	0.1170
Cytosine dimer 3 (stacked)	*const*	-331.02	-331.02	-704.62	42.58	0.1200
Cytosine dimer 4 (stacked)	*const*	-331.02	-331.02	-711.96	49.92	0.0940
Cytosine dimer 5 (stacked)	*const*	-331.02	-331.02	-668.17	6.13	0.0990
Cytosine dimer 6 (stacked)	*const*	-331.02	-331.02	-666.95	4.91	0.1060
Cytosine dimer 7 (stacked)	*const*	-331.02	-331.02	-669.77	7.73	0.1160
Cytosine dimer 8 (stacked)	*const*	-331.02	-331.02	-707.49	45.45	0.1010

Cytosine dimer 9 (stacked)	*const*	-331.02	-331.02	-710.86	48.82	0.0850
Cytosine dimer 10 (stacked)	*const*	-331.02	-331.02	-708.54	46.50	0.0870
Cytosine dimer 11 (stacked)	*const*	-331.02	-331.02	-712.40	50.36	0.0960
Cytosine dimer 12 (stacked)	*const*	-331.02	-331.02	-695.30	33.26	0.1010
Cytosine dimer 13 (stacked)	*const*	-331.02	-331.02	-702.97	40.93	0.0930
Cytosine dimer 14 (stacked)	*const*	-331.02	-331.02	-709.86	47.82	0.1120
Adenine dimer (stacked)	*const*	-363.92	-363.92	-771.73	43.89	0.0990
guanine dimer (stacked)	*const*	-361.60	-361.60	-781.39	58.19	0.0960
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-738.36	43.42	0.0940
Guanine : Adenine (stacked)	*const*	-361.60	-363.92	-777.55	52.03	0.0840
Cytosine dimer (stacked)	*const*	-331.02	-331.02	-712.59	50.55	0.0870
Adenine : Uracil (stacked)	*const*	-363.92	-336.61	-743.33	42.80	0.0840
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-745.24	52.63	0.1100
Cytosine : Uracil (stacked)	*const*	-331.02	-336.61	-712.96	45.33	0.0990
Uracil dimer (Stacked)	*const*	-336.61	-336.61	-706.38	33.17	0.0720
Guanine : Uracil (stacked)	*const*	-361.60	-336.61	-750.59	52.39	0.0830
Guanine dimer (stacked)	*const*	-331.02	-331.02	-670.34	8.30	0.1040
Cytosine dimer (stacked)	*const*	-331.02	-361.60	-709.73	17.12	0.1110
Adenine dimer (stacked)	*const*	-363.92	-363.92	-764.68	36.84	0.0950
Thymine dimer (stacked)	*const*	-363.92	-631.08	-1003.25	8.25	0.1790
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-743.10	50.48	0.1180
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-729.13	36.52	0.1070
Adenine : guanine (stacked)	*const*	-363.92	-361.60	-773.42	47.90	0.1010
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-986.51	24.40	0.1890
Adenine : guanine (stacked)	*const*	-363.92	-361.60	-766.46	40.94	0.0990
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-989.39	27.29	0.2440
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1022.36	29.69	0.1670
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-725.57	30.63	0.0950
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1024.86	32.18	0.1970
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-722.42	27.48	0.1010
Adenine : thymine (stacked)	*const*	-363.92	-631.08	-1026.86	31.86	0.1740
Adenine : thymine (stacked)	*const*	-363.92	-631.08	-1024.42	29.42	0.2730
Adenine dimer (stacked)	*const*	-363.92	-363.92	-765.14	37.30	0.0960
Thymine dimer (stacked)	*const*	-631.08	-631.08	-1287.39	25.23	0.2440
Adenine : Thymine (stacked)	*const*	-362.20	-627.86	-1025.24	35.19	0.2960
Guanine : Cytosine (stacked)	*const*	-325.83	-363.43	-719.80	30.54	0.3870
Adenine : Cytosine (stacked)	*const*	-362.20	-325.83	-719.78	31.75	0.1190
Thymine : Guanine (stacked)	*const*	-627.86	-363.43	-1024.83	33.54	0.3680
guanine : Cytosine (stacked)	*const*	-331.02	-361.60	-732.62	40.00	0.1090
Adenine : Guanine (stacked)	*const*	-364.94	-361.60	-765.73	39.19	0.1110
Cytosine : guanine (stacked)	*const*	-361.60	-331.02	-743.08	50.46	0.1310
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-743.86	51.24	0.1350
Phe30 : Lys46 (1RB9)	*const*	37.42	29.67	60.06	7.03	0.1350
Phe30 : Leu33 (1RB9)	*const*	37.55	8.44	26.27	19.73	0.2360
Phe30 : Tyr13 (1RB9)	*const*	37.43	20.30	48.55	9.17	0.1350
Phe30 : Phe49 (1RB9)	*const*	13.71	37.63	41.19	10.15	0.1410
Phe30 : Tyr4 (1RB9)	*const*	37.40	25.85	45.79	17.46	0.1550
Phe49 : Cys39 (1RB9)	*const*	13.57	15.01	26.32	2.26	0.1550
Phe49 : Cys6 (1RB9)	*const*	13.50	8.03	12.60	8.94	0.1520
Phe49 : Lys46 (1RB9)	*const*	25.18	29.21	41.45	12.93	0.1350
Phe49 : Val5 (1RB9)	*const*	14.02	11.40	4.57	20.85	0.1570
Phe49 : Tyr37 (1RB9)	*const*	25.17	-13.15	8.72	3.30	0.1320
Phe49 : Tyr4 (1RB9)	*const*	13.62	19.05	27.88	4.78	0.1200
Phe49 : Peptide bond (1RB9)	*const*	25.44	-69.99	-53.04	8.49	0.3320
Phe49 : Peptide bond (1RB9)	*const*	13.81	-69.99	-81.95	25.77	0.2990
Glu47 : Lys6 (PDB:1IU5)	*const*	184.34	-86.30	-212.21	310.25	0.1180
Glu49 : Lys6 (PDB:1BQ9)	*const*	178.58	-89.98	-344.59	433.18	0.1440
Glu54 : Lys2 (PDB:1SMM)	*const*	160.82	-73.43	-244.45	331.84	0.1910
Glu50 : LysK30 (PDB:1BRF)	*const*	177.22	-87.99	-151.07	240.31	0.1720
Glu50 : Lys52 (PDB:1BRF)	*const*	178.20	-89.49	-285.47	374.18	0.1490
Glu49 : Lys6 (PDB:1BRF)	*const*	203.14	-90.07	-173.77	286.84	0.3830

AMBER* (10,12-H bonding potential)

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-361.60	-331.02	-781.72	89.10	0.0910
Methylguanine : Methylcytosine (WC)	*opt*	-325.83	-363.43	-779.17	89.90	0.1330
Adenine : Thymine (WC)	*opt*	-361.86	-627.86	-1035.19	45.47	0.4000
Methyladenine : Methylthymine (planar)	*opt*	-361.86	-627.86	-1039.49	49.77	0.1780
8-Oxoguanine : Cytosine (WC planar)	*opt*	-205.55	-331.02	-601.46	64.89	0.0690
Inosine : Cytosine (WC planar)	*opt*	-331.02	-27.76	-414.32	55.54	0.1400
Guanine : Uracil (wobble)	*opt*	-361.60	-336.61	-745.54	47.34	0.1570
Cytosine : CytosineH+	*opt*	-331.02	-70.06	-482.76	81.68	0.1450
Uracil dimer (Calcutta planar)	*opt*	-336.61	-336.61	-698.79	25.57	0.1860
Uracil dimer (planar)	*opt*	-336.61	-336.61	-711.75	38.53	0.0830
6-Thioguanine : Cytosine (WC planar)	*opt*	-331.02	-179.73	-560.20	49.45	1.0970
Adenine : 4-Thiouracil (WC)	*opt*	-363.58	-186.26	-569.46	19.62	3.8870
2-aminoadenine : Thymine	*opt*	-458.44	-631.08	-1151.38	61.86	0.2880
2-aminoadenine : Thymine (planar)	*opt*	-458.44	-630.94	-1151.29	61.91	0.0470
Adenine : Difluorotoluene	*opt*	-364.61	-11.91	-417.75	41.24	2.7540
Guanine : 4-Thiouracil	*opt*	-361.60	-186.26	-592.52	44.66	0.3000
Guanine : 2-Thiouracil	*opt*	-361.60	-186.87	-600.54	52.07	1.9850
Adenine : Cytosine (planar)	*opt*	-331.02	-363.58	-753.93	59.33	0.0800
Guanine dimer (planar)	*opt*	-361.60	-361.60	-788.64	65.45	0.1340
Guanine 6-Thioguanine (planar)	*opt*	-361.60	-179.73	-582.89	41.57	0.1810
6-Thioguanine : Guanine (planar)	*opt*	-179.73	-361.60	-578.79	37.47	0.1200
Guanine : Adenine 1	*opt*	-361.60	-363.58	-781.29	56.11	0.1500
Guanine : Adenine 1 (planar)	*opt*	-364.61	-361.60	-781.88	55.67	0.0510

Guanine : Adenine 2	*opt*	-361.60	-363.58	-774.39	49.21	0.3260
Guanine : Adenine 2 (planar)	*opt*	-361.60	-363.58	-773.09	47.91	0.0940
Guanine : Adenine 3	*opt*	-361.60	-363.58	-778.98	53.80	0.7840
Guanine : Adenine 4	*opt*	-361.60	-363.58	-777.50	52.32	0.4020
Adenine dimer 1 (planar)	*opt*	-363.58	-363.58	-779.17	52.00	0.0760
Adenine dimer 2 (planar)	*opt*	-363.58	-364.61	-778.01	49.82	0.0930
Adenine dimer 3 (planar)	*opt*	-363.58	-363.58	-775.96	48.79	1.1480
8-Oxoguanine : Guanine	*opt*	-361.60	-205.55	-614.84	47.70	0.2220
2-Thiouracil dimer (planar)	*opt*	-186.87	-186.87	-391.12	17.38	0.3770
Adenine : Thymine (WC)	*const*	-361.86	-627.86	-1034.73	45.02	0.3700
Guanine : Cytosine (WC)	*const*	-325.83	-363.43	-778.96	89.70	0.4070
Adenine : thymine (WC)	*const*	-361.86	-627.86	-1034.25	44.54	0.3470
Guanine : adenine (HB)	*const*	-361.60	-364.61	-772.79	46.59	0.0960
Cytosine : Guanine (WC)	*const*	-331.02	-361.60	-780.83	88.21	0.0790
Guanine : Cytosine (WC)	*const*	-361.60	-331.02	-781.49	88.88	0.0720
Cytosine : guanine (interstrand)	*const*	-361.60	-331.02	-709.96	17.34	0.1200
Adenine : thymine (interstrand)	*const*	-631.08	-363.58	-1006.27	11.60	0.2110
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-653.53	-8.51	0.1060
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-722.45	-0.75	0.0790
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-658.23	-3.81	0.1140
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-746.28	23.09	0.0930
Adenine : cytosine (interstrand)	*const*	-363.58	-331.02	-695.91	1.30	0.0990
Thymine : guanine (interstrand)	*const*	-631.08	-361.60	-993.69	1.01	0.1870
Thymine : guanine (interstrand)	*const*	-361.60	-631.08	-1000.94	8.26	0.1840
Thymine : cytosine (interstrand)	*const*	-363.58	-331.02	-696.85	2.25	0.1000
Adenine : guanine (interstrand)	*const*	-363.58	-361.60	-744.86	19.68	0.0820
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-965.81	3.71	0.1940
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-961.74	-0.36	0.1910
Adenine : guanine (interstrand)	*const*	-363.58	-361.60	-743.79	18.62	0.1050
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1262.20	0.04	0.2460
Adenine dimer (interstrand)	*const*	-363.58	-363.58	-733.56	6.40	0.0920
Adenine dimer (interstrand)	*const*	-363.58	-363.58	-740.22	13.06	0.0980
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1261.46	-0.70	0.2660
Adenine : thymine (interstrand)	*const*	-363.58	-631.08	-1002.37	7.71	0.1820
Thymine : adenine (interstrand)	*const*	-363.58	-631.08	-1001.19	6.53	0.1950
Adenine dimer (interstrand)	*const*	-361.86	-361.86	-732.09	8.37	0.3360
Thymine dimer (interstrand)	*const*	-627.86	-627.86	-1255.34	-0.37	0.4330
Guanine dimer (interstrand)	*const*	-363.43	-363.43	-757.04	30.18	0.4090
Cytosine dimer (interstrand)	*const*	-325.83	-325.83	-649.81	-1.86	0.4340
Adenine : Guanine (interstrand)	*const*	-361.86	-363.43	-744.01	18.73	0.3010
Thymine : Cytosine (interstrand)	*const*	-325.83	-627.86	-953.20	-0.49	0.3490
Cytosine dimer (interstrand)	*const*	-331.02	-364.61	-714.54	18.92	0.1660
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-741.55	18.36	0.0960
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-727.98	4.79	0.1100
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-653.73	-8.31	0.0960
Guanine : Cytosine (stacked)	*opt*	-361.60	-331.02	-745.17	52.55	0.3650
Methylguanine : Methylcytosine (stacked)	*opt*	-363.43	-325.83	-744.33	55.06	0.4070
Adenine : Thymine (stacked)	*opt*	-364.61	-631.08	-1040.27	44.59	0.4280
Methyladenine : Methylthymine (stacked)	*opt*	-361.86	-627.86	-1038.85	49.14	0.5480
Cytosine dimer 1 (stacked)	*const*	-331.02	-331.02	-664.15	2.11	0.0750
Cytosine dimer 2 (stacked)	*const*	-331.02	-331.02	-682.67	20.63	0.1170
Cytosine dimer 3 (stacked)	*const*	-331.02	-331.02	-704.62	42.58	0.1200
Cytosine dimer 4 (stacked)	*const*	-331.02	-331.02	-711.87	49.83	0.0950
Cytosine dimer 5 (stacked)	*const*	-331.02	-331.02	-668.17	6.13	0.0990
Cytosine dimer 6 (stacked)	*const*	-331.02	-331.02	-666.91	4.87	0.1050
Cytosine dimer 7 (stacked)	*const*	-331.02	-331.02	-669.55	7.51	0.1150
Cytosine dimer 8 (stacked)	*const*	-331.02	-331.02	-707.49	45.45	0.1010
Cytosine dimer 9 (stacked)	*const*	-331.02	-331.02	-710.86	48.82	0.0850
Cytosine dimer 10 (stacked)	*const*	-331.02	-331.02	-708.41	46.37	0.0870
Cytosine dimer 11 (stacked)	*const*	-331.02	-331.02	-712.40	50.36	0.0960
Cytosine dimer 12 (stacked)	*const*	-331.02	-331.02	-695.30	33.26	0.1010
Cytosine dimer 13 (stacked)	*const*	-331.02	-331.02	-702.84	40.80	0.0930
Cytosine dimer 14 (stacked)	*const*	-331.02	-331.02	-709.86	47.82	0.1120
Adenine dimer (stacked)	*const*	-363.58	-363.58	-770.70	43.53	0.0990
guanine dimer (stacked)	*const*	-361.60	-361.60	-781.24	58.04	0.0950
Adenine : cytosine (stacked)	*const*	-363.58	-331.02	-738.01	43.41	0.0940
Guanine : Adenine (stacked)	*const*	-361.60	-363.58	-777.06	51.88	0.0840
Cytosine dimer (stacked)	*const*	-331.02	-331.02	-712.59	50.55	0.0870
Adenine : Uracil (stacked)	*const*	-363.58	-336.61	-742.91	42.72	0.0840
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-744.80	52.18	0.1100
Cytosine : Uracil (stacked)	*const*	-331.02	-336.61	-712.84	45.22	0.0990
Uracil dimer (Stacked)	*const*	-336.61	-336.61	-706.38	33.17	0.0720
Guanine : Uracil (stacked)	*const*	-361.60	-336.61	-750.40	52.20	0.0830
Guanine dimer (stacked)	*const*	-331.02	-331.02	-670.34	8.30	0.1040
Cytosine dimer (stacked)	*const*	-331.02	-361.60	-709.59	16.98	0.1110
Adenine dimer (stacked)	*const*	-363.58	-363.58	-763.85	36.69	0.0950
Thymine dimer (stacked)	*const*	-363.58	-631.08	-1002.72	8.06	0.1790
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-742.79	50.18	0.1180
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-729.13	36.52	0.1070
Adenine : guanine (stacked)	*const*	-363.58	-361.60	-772.80	47.62	0.1000
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-986.24	24.14	0.1890
Adenine : guanine (stacked)	*const*	-363.58	-361.60	-766.11	40.93	0.0990
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-989.39	27.29	0.2440
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1022.36	29.69	0.1670
Adenine : cytosine (stacked)	*const*	-363.58	-331.02	-725.23	30.63	0.0950
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1024.82	32.14	0.1970
Adenine : cytosine (stacked)	*const*	-363.58	-331.02	-721.87	27.27	0.1020
Adenine : thymine (stacked)	*const*	-363.58	-631.08	-1026.30	31.64	0.1730

Adenine : thymine (stacked)	*const*	-363.58	-631.08	-1023.80	29.14	0.2730
Adenine dimer (stacked)	*const*	-363.58	-363.58	-764.29	37.13	0.0950
Thymine dimer (stacked)	*const*	-631.08	-631.08	-1287.39	25.23	0.2440
Adenine : Thymine (stacked)	*const*	-361.86	-627.86	-1024.72	35.00	0.2960
Guanine : Cytosine (stacked)	*const*	-325.83	-363.43	-719.80	30.54	0.3870
Adenine : Cytosine (stacked)	*const*	-361.86	-325.83	-719.44	31.75	0.1190
Thymine : Guanine (stacked)	*const*	-627.86	-363.43	-1024.83	33.54	0.3680
guanine : Cytosine (stacked)	*const*	-331.02	-361.60	-732.56	39.95	0.1090
Adenine : Guanine (stacked)	*const*	-364.61	-361.60	-765.34	39.14	0.1100
Cytosine : guanine (stacked)	*const*	-361.60	-331.02	-743.01	50.39	0.1320
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-743.48	50.86	0.1350
Phe30 : Lys46 (1RB9)	*const*	37.42	29.74	60.15	7.01	0.1350
Phe30 : Leu33 (1RB9)	*const*	37.55	8.37	25.68	20.24	0.2370
Phe30 : Tyr13 (1RB9)	*const*	37.43	20.15	48.53	9.04	0.1370
Phe30 : Phe49 (1RB9)	*const*	13.49	37.64	41.01	10.12	0.1420
Phe30 : Tyr4 (1RB9)	*const*	37.40	25.70	45.61	17.48	0.1590
Phe49 : Cys39 (1RB9)	*const*	13.36	14.99	26.25	2.10	0.1530
Phe49 : Cys6 (1RB9)	*const*	13.29	8.05	12.61	8.72	0.1520
Phe49 : Lys46 (1RB9)	*const*	25.15	29.21	41.41	12.95	0.1350
Phe49 : Val5 (1RB9)	*const*	13.82	11.15	4.20	20.77	0.1590
Phe49 : Tyr37 (1RB9)	*const*	13.31	-13.20	-5.21	5.32	0.3600
Phe49 : Tyr4 (1RB9)	*const*	13.41	18.97	27.68	4.70	0.1190
Phe49 : Peptide bond (1RB9)	*const*	13.46	-69.99	-65.83	9.30	0.5130
Phe49 : Peptide bond (1RB9)	*const*	13.59	-69.99	-82.14	25.75	0.3010
Glu47 : Lys6 (PDB:1IU5)	*const*	184.34	-86.25	-212.09	310.17	0.1170
Glu49 : Lys6 (PDB:1BQ9)	*const*	178.58	-90.27	-344.54	432.84	0.1440
Glu54 : Lys2 (PDB:1SMM)	*const*	161.31	-73.30	-243.70	331.71	0.1910
Glu50 : LysK30 (PDB:1BRF)	*const*	177.03	-84.08	-151.41	244.36	0.1700
Glu50 : Lys52 (PDB:1BRF)	*const*	178.00	-89.80	-285.31	373.52	0.1480
Glu49 : Lys6 (PDB:1BRF)	*const*	203.14	-90.34	-173.74	286.54	0.3860

AMBER* explicit lone pairs)

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-361.60	-331.02	-785.51	92.89	0.0850
Methylguanine : Methylcytosine (WC)	*opt*	-325.83	-363.43	-783.20	93.94	0.1290
Adenine : Thymine (WC)	*opt*	-362.20	-627.86	-1036.46	46.40	0.4140
Methyladenine : Methylthymine (planar)	*opt*	-362.20	-627.86	-1039.37	49.31	0.2000
8-Oxoguanine : Cytosine (WC planar)	*opt*	-205.55	-331.02	-602.29	65.72	0.0710
Inosine : Cytosine (WC planar)	*opt*	-331.02	-27.76	-415.11	56.33	0.1580
Guanine : Uracil (wobble)	*opt*	-361.60	-336.61	-747.39	49.18	0.1250
Cytosine : CytosineH+	*opt*	-331.02	-70.06	-483.05	81.98	0.1160
Uracil dimer (Calcutta planar)	*opt*	-336.61	-336.61	-699.42	26.21	0.1980
Uracil dimer (planar)	*opt*	-336.61	-336.61	-712.87	39.66	0.0550
6-Thioguanine : Cytosine (WC planar)	*opt*	-331.02	-158.27	-539.51	50.22	0.4100
Adenine : 4-Thiouracil (WC)	*opt*	-363.92	-220.01	-614.75	30.82	4.1470
2-aminoadenine : Thymine	*opt*	-458.77	-631.08	-1153.71	63.86	0.2870
2-aminoadenine : Thymine (planar)	*opt*	-458.77	-630.94	-1153.61	63.89	0.0520
Adenine : Difluorotoluene	*opt*	-364.94	-11.91	-418.09	41.24	2.7540
Guanine : 4-Thiouracil	*opt*	-361.60	-186.26	-592.47	44.62	0.2070
Guanine : 2-Thiouracil	*opt*	-361.60	-186.87	-600.53	52.06	1.9750
Adenine : Cytosine (planar)	*opt*	-331.02	-363.92	-752.51	57.57	0.0710
Guanine dimer (planar)	*opt*	-361.60	-361.60	-788.29	65.09	0.1730
Guanine 6-Thioguanine (planar)	*opt*	-361.60	-158.27	-571.87	52.01	1.7830
6-Thioguanine : Guanine (planar)	*opt*	-158.27	-361.60	-564.57	44.70	1.6360
Guanine : Adenine 1	*opt*	-361.60	-363.92	-783.28	57.76	0.1590
Guanine : Adenine 1 (planar)	*opt*	-364.94	-361.60	-784.07	57.53	0.0310
Guanine : Adenine 2	*opt*	-361.60	-363.92	-772.64	47.13	0.3090
Guanine : Adenine 2 (planar)	*opt*	-361.60	-363.92	-771.29	45.78	0.0990
Guanine : Adenine 3	*opt*	-361.60	-363.92	-779.09	53.57	0.7200
Guanine : Adenine 4	*opt*	-361.60	-363.92	-775.76	50.24	0.4090
Adenine dimer 1 (planar)	*opt*	-363.92	-363.92	-777.80	49.96	0.0480
Adenine dimer 2 (planar)	*opt*	-363.92	-364.94	-775.48	46.62	0.3890
Adenine dimer 3 (planar)	*opt*	-363.92	-363.92	-773.77	45.93	1.2070
8-Oxoguanine : Guanine	*opt*	-361.60	-205.55	-616.06	48.91	0.2110
2-Thiouracil dimer (planar)	*opt*	-98.91	-98.91	-237.60	39.78	2.3160
Adenine : Thymine (WC)	*const*	-362.20	-627.86	-1035.48	45.43	0.3730
Guanine : Cytosine (WC)	*const*	-325.83	-363.43	-782.80	93.54	0.4070
Adenine : thymine (WC)	*const*	-362.20	-627.86	-1034.34	44.28	0.3470
Guanine : adenine (HB)	*const*	-361.60	-364.94	-771.45	44.91	0.0960
Cytosine : Guanine (WC)	*const*	-331.02	-361.60	-784.42	91.80	0.0740
Guanine : Cytosine (WC)	*const*	-361.60	-331.02	-785.42	92.80	0.0670
Cytosine : guanine (interstrand)	*const*	-361.60	-331.02	-710.28	17.67	0.1200
Adenine : thymine (interstrand)	*const*	-631.08	-363.92	-1006.42	11.41	0.2100
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-653.53	-8.51	0.1060
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-722.45	-0.75	0.0790
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-658.23	-3.81	0.1140
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-746.41	23.21	0.0940
Adenine : cytosine (interstrand)	*const*	-363.92	-331.02	-696.24	1.30	0.0990
Thymine : guanine (interstrand)	*const*	-631.08	-361.60	-993.73	1.05	0.1880
Thymine : guanine (interstrand)	*const*	-361.60	-631.08	-1000.94	8.26	0.1840
Thymine : cytosine (interstrand)	*const*	-363.92	-331.02	-697.27	2.33	0.1000
Adenine : guanine (interstrand)	*const*	-363.92	-361.60	-745.25	19.74	0.0830
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-965.87	3.77	0.1940
Thymine : cytosine (interstrand)	*const*	-631.08	-331.02	-961.74	-0.36	0.1910
Adenine : guanine (interstrand)	*const*	-363.92	-361.60	-744.34	18.82	0.1040
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1262.20	0.04	0.2450
Adenine dimer (interstrand)	*const*	-363.92	-363.92	-734.40	6.56	0.0920

Adenine dimer (interstrand)	*const*	-363.92	-363.92	-740.89	13.05	0.0980
Thymine dimer (interstrand)	*const*	-631.08	-631.08	-1261.46	-0.70	0.2660
Adenine : thymine (interstrand)	*const*	-363.92	-631.08	-1002.86	7.85	0.1820
Thymine : adenine (interstrand)	*const*	-363.92	-631.08	-1001.70	6.70	0.1950
Adenine dimer (interstrand)	*const*	-362.20	-362.20	-732.88	8.48	0.3360
Thymine dimer (interstrand)	*const*	-627.86	-627.86	-1255.34	-0.37	0.4330
Guanine dimer (interstrand)	*const*	-363.43	-363.43	-757.12	30.26	0.4090
Cytosine dimer (interstrand)	*const*	-325.83	-325.83	-649.81	-1.86	0.4340
Adenine : Guanine (interstrand)	*const*	-362.20	-363.43	-744.65	19.02	0.3020
Thymine : Cytosine (interstrand)	*const*	-325.83	-627.86	-953.20	-0.49	0.3490
Cytosine dimer (interstrand)	*const*	-331.02	-364.94	-714.92	18.96	0.1660
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-741.63	18.44	0.0960
Guanine dimer (interstrand)	*const*	-361.60	-361.60	-728.07	4.88	0.1100
Cytosine dimer (interstrand)	*const*	-331.02	-331.02	-653.73	-8.31	0.0960
Guanine : Cytosine (stacked)	*opt*	-361.60	-331.02	-745.60	52.98	0.3540
Methylguanine : Methylcytosine (stacked)	*opt*	-363.43	-325.83	-744.54	55.28	0.3810
Adenine : Thymine (stacked)	*opt*	-364.94	-631.08	-1040.69	44.67	0.4270
Methyladenine : Methylthymine (stacked)	*opt*	-362.20	-627.86	-1039.27	49.22	0.5470
Cytosine dimer 1 (stacked)	*const*	-331.02	-331.02	-664.15	2.11	0.0750
Cytosine dimer 2 (stacked)	*const*	-331.02	-331.02	-682.80	20.76	0.1170
Cytosine dimer 3 (stacked)	*const*	-331.02	-331.02	-704.62	42.58	0.1200
Cytosine dimer 4 (stacked)	*const*	-331.02	-331.02	-711.96	49.92	0.0940
Cytosine dimer 5 (stacked)	*const*	-331.02	-331.02	-668.17	6.13	0.0990
Cytosine dimer 6 (stacked)	*const*	-331.02	-331.02	-666.95	4.91	0.1060
Cytosine dimer 7 (stacked)	*const*	-331.02	-331.02	-669.77	7.73	0.1160
Cytosine dimer 8 (stacked)	*const*	-331.02	-331.02	-707.49	45.45	0.1010
Cytosine dimer 9 (stacked)	*const*	-331.02	-331.02	-710.86	48.82	0.0850
Cytosine dimer 10 (stacked)	*const*	-331.02	-331.02	-708.54	46.50	0.0870
Cytosine dimer 11 (stacked)	*const*	-331.02	-331.02	-712.40	50.36	0.0960
Cytosine dimer 12 (stacked)	*const*	-331.02	-331.02	-695.30	33.26	0.1010
Cytosine dimer 13 (stacked)	*const*	-331.02	-331.02	-702.97	40.93	0.0930
Cytosine dimer 14 (stacked)	*const*	-331.02	-331.02	-709.86	47.82	0.1120
Adenine dimer (stacked)	*const*	-363.92	-363.92	-771.73	43.89	0.0990
guanine dimer (stacked)	*const*	-361.60	-361.60	-781.39	58.19	0.0960
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-738.36	43.42	0.0940
Guanine : Adenine (stacked)	*const*	-361.60	-363.92	-777.55	52.03	0.0840
Cytosine dimer (stacked)	*const*	-331.02	-331.02	-712.59	50.55	0.0870
Adenine : Uracil (stacked)	*const*	-363.92	-336.61	-743.33	42.80	0.0840
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-745.24	52.63	0.1100
Cytosine : Uracil (stacked)	*const*	-331.02	-336.61	-712.96	45.33	0.0990
Uracil dimer (Stacked)	*const*	-336.61	-336.61	-706.38	33.17	0.0720
Guanine : Uracil (stacked)	*const*	-361.60	-336.61	-750.59	52.39	0.0830
Guanine dimer (stacked)	*const*	-331.02	-331.02	-670.34	8.30	0.1040
Cytosine dimer (stacked)	*const*	-331.02	-361.60	-709.73	17.12	0.1110
Adenine dimer (stacked)	*const*	-363.92	-363.92	-764.68	36.84	0.0950
Thymine dimer (stacked)	*const*	-363.92	-631.08	-1003.25	8.25	0.1800
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-743.10	50.48	0.1180
Guanine : cytosine (stacked)	*const*	-331.02	-361.60	-729.13	36.52	0.1070
Adenine : guanine (stacked)	*const*	-363.92	-361.60	-773.42	47.90	0.1010
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-986.51	24.40	0.1890
Adenine : guanine (stacked)	*const*	-363.92	-361.60	-766.46	40.94	0.0990
Thymine : cytosine (stacked)	*const*	-631.08	-331.02	-989.39	27.29	0.2440
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1022.36	29.69	0.1670
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-725.57	30.63	0.0950
Thymine : guanine (stacked)	*const*	-631.08	-361.60	-1024.86	32.18	0.1970
Adenine : cytosine (stacked)	*const*	-363.92	-331.02	-722.42	27.48	0.1010
Adenine : thymine (stacked)	*const*	-363.92	-631.08	-1026.86	31.86	0.1730
Adenine : thymine (stacked)	*const*	-363.92	-631.08	-1024.42	29.42	0.2730
Adenine dimer (stacked)	*const*	-363.92	-363.92	-765.14	37.30	0.0960
Thymine dimer (stacked)	*const*	-631.08	-631.08	-1287.39	25.23	0.2440
Adenine : Thymine (stacked)	*const*	-362.20	-627.86	-1025.24	35.19	0.2960
Guanine : Cytosine (stacked)	*const*	-325.83	-363.43	-719.80	30.54	0.3870
Adenine : Cytosine (stacked)	*const*	-362.20	-325.83	-719.78	31.75	0.1190
Thymine : Guanine (stacked)	*const*	-627.86	-363.43	-1024.83	33.54	0.3680
guanine : Cytosine (stacked)	*const*	-331.02	-361.60	-732.62	40.00	0.1090
Adenine : Guanine (stacked)	*const*	-364.94	-361.60	-765.73	39.19	0.1110
Cytosine : guanine (stacked)	*const*	-361.60	-331.02	-743.08	50.46	0.1310
Guanine : Cytosine (stacked)	*const*	-361.60	-331.02	-743.86	51.24	0.1350
Phe30 : Lys46 (1RB9)	*const*	37.42	29.67	60.06	7.03	0.1350
Phe30 : Leu33 (1RB9)	*const*	37.55	8.44	26.27	19.73	0.2360
Phe30 : Tyr13 (1RB9)	*const*	37.43	20.30	48.55	9.17	0.1350
Phe30 : Phe49 (1RB9)	*const*	13.71	37.63	41.19	10.15	0.1410
Phe30 : Tyr4 (1RB9)	*const*	37.40	25.85	45.79	17.46	0.1550
Phe49 : Cys39 (1RB9)	*const*	13.60	30.43	43.50	0.53	0.1410
Phe49 : Cys6 (1RB9)	*const*	13.62	24.64	29.55	8.71	0.1380
Phe49 : Lys46 (1RB9)	*const*	25.18	29.21	41.45	12.93	0.1350
Phe49 : Val5 (1RB9)	*const*	14.02	11.40	4.57	20.85	0.1570
Phe49 : Tyr37 (1RB9)	*const*	25.17	-13.15	8.72	3.30	0.1320
Phe49 : Tyr4 (1RB9)	*const*	13.62	19.05	27.88	4.78	0.1200
Phe49 : Peptide bond (1RB9)	*const*	25.44	-69.99	-53.04	8.49	0.3330
Phe49 : Peptide bond (1RB9)	*const*	13.81	-69.99	-81.95	25.77	0.2990
Glu47 : Lys6 (PDB:1IU5)	*const*	184.34	-86.30	-212.21	310.25	0.1180
Glu49 : Lys6 (PDB:1BQ9)	*const*	178.58	-89.98	-344.59	433.18	0.1440
Glu54 : Lys2 (PDB:1SMM)	*const*	160.82	-73.43	-244.45	331.84	0.1910
Glu50 : LysK30 (PDB:1BRF)	*const*	177.22	-87.99	-151.07	240.31	0.1720
Glu50 : Lys52 (PDB:1BRF)	*const*	178.20	-89.49	-285.47	374.18	0.1490
Glu49 : Lys6 (PDB:1BRF)	*const*	203.14	-90.07	-173.77	286.84	0.3830

OPLS*

Complex		Monomer A (kJ/mol)	MonomerB (kJ/mol)	Complex (kJ/mol)	Interaction (kJ/mol)	RMS geometry (Å)
Guanine : Cytosine (WC)	*opt*	-123.96	-169.82	-389.54	95.75	0.0730
Methylguanine : Methylcytosine (WC)	*opt*	-151.25	-131.50	-379.52	96.78	0.1320
Adenine : Thymine (WC)	*opt*	-92.87	-186.54	-323.76	44.35	0.3660
Methyladenine : Methylthymine (planar)	*opt*	-92.87	-186.54	-325.06	45.65	0.0760
8-Oxoguanine : Cytosine (WC planar)	*opt*	-448.57	-169.82	-692.12	73.74	0.0800
Inosine : Cytosine (WC planar)	*opt*	-169.82	-125.66	-358.99	63.52	0.0980
Guanine : Uracil (wobble)	*opt*	-123.96	-171.76	-347.20	51.48	0.1270
Cytosine : CytosineH+	*opt*	-169.82	-130.53	-388.69	88.35	0.1320
Uracil dimer (Calcutta planar)	*opt*	-171.76	-171.76	-372.08	28.56	0.2010
Uracil dimer (planar)	*opt*	-171.76	-171.76	-381.60	38.08	0.0580
6-Thioguanine : Cytosine (WC planar)	*opt*	-169.82	-254.84	-479.76	55.10	0.1090
Adenine : 4-Thiouracil (WC)	*opt*	-89.55	-323.73	-447.04	33.76	3.8870
2-aminoadenine : Thymine	*opt*	-199.27	-201.01	-454.73	54.44	0.2640
2-aminoadenine : Thymine (planar)	*opt*	-199.27	-201.01	-454.73	54.44	0.0430
Adenine : Difluorotoluene	*opt*	-89.55	-0.28	-123.14	33.30	2.8400
Guanine : 4-Thiouracil	*opt*	-123.96	-323.73	-510.98	63.29	0.0810
Guanine : 2-Thiouracil	*opt*	-123.96	-254.12	-406.77	28.68	0.3680
Adenine : Cytosine (planar)	*opt*	-169.82	-89.55	-300.95	41.58	0.0660
Guanine dimer (planar)	*opt*	-123.96	-123.96	-322.25	74.33	0.1460
Guanine 6-Thioguanine (planar)	*opt*	-123.96	-254.84	-422.08	43.28	0.1830
6-Thioguanine : Guanine (planar)	*opt*	-254.84	-123.96	-430.12	51.32	0.1710
Guanine : Adenine 1	*opt*	-123.96	-89.55	-265.13	51.61	0.5540
Guanine : Adenine 1 (planar)	*opt*	-89.55	-123.96	-259.04	45.52	0.0600
Guanine : Adenine 2	*opt*	-123.96	-89.55	-250.94	37.42	0.5570
Guanine : Adenine 2 (planar)	*opt*	-123.96	-89.55	-245.58	32.06	0.0360
Guanine : Adenine 3	*opt*	-123.96	-89.55	-259.99	46.48	0.6610
Guanine : Adenine 4	*opt*	-123.96	-89.55	-252.53	39.01	0.4190
Adenine dimer 1 (planar)	*opt*	-89.55	-89.55	-213.01	33.90	0.6050
Adenine dimer 2 (planar)	*opt*	-89.55	-89.55	-211.75	32.64	0.9220
Adenine dimer 3 (planar)	*opt*	-89.55	-89.55	-211.23	32.12	1.0790
8-Oxoguanine : Guanine	*opt*	-123.96	-448.57	-645.54	73.01	0.1930
2-Thiouracil dimer (planar)	*opt*	-254.12	-254.12	-535.52	27.27	0.2410
Adenine : Thymine (WC)	*const*	-92.87	-186.54	-322.90	43.49	0.3450
Guanine : Cytosine (WC)	*const*	-151.25	-131.50	-378.96	96.21	0.4080
Adenine : thymine (WC)	*const*	-92.87	-186.54	-322.82	43.42	0.3010
Guanine : adenine (HB)	*const*	-123.96	-89.55	-247.41	33.89	0.0890
Cytosine : Guanine (WC)	*const*	-169.82	-123.96	-388.04	94.25	0.0760
Guanine : Cytosine (WC)	*const*	-123.96	-169.82	-389.51	95.72	0.0660
Cytosine : guanine (interstrand)	*const*	-123.96	-169.82	-313.66	19.88	0.1310
Adenine : thymine (interstrand)	*const*	-201.01	-89.55	-301.16	10.59	0.1110
Cytosine dimer (interstrand)	*const*	-169.82	-169.82	-326.88	-12.76	0.1060
Guanine dimer (interstrand)	*const*	-123.96	-123.96	-247.83	-0.10	0.0860
Cytosine dimer (interstrand)	*const*	-169.82	-169.82	-333.66	-5.98	0.1130
Guanine dimer (interstrand)	*const*	-123.96	-123.96	-270.38	22.46	0.0980
Adenine : cytosine (interstrand)	*const*	-89.55	-169.82	-264.66	5.29	0.1020
Thymine : guanine (interstrand)	*const*	-201.01	-123.96	-325.58	0.60	0.0980
Thymine : guanine (interstrand)	*const*	-123.96	-201.01	-334.18	9.20	0.0940
Thymine : cytosine (interstrand)	*const*	-89.55	-169.82	-261.84	2.47	0.1040
Adenine : guanine (interstrand)	*const*	-89.55	-123.96	-236.86	23.34	0.0980
Thymine : cytosine (interstrand)	*const*	-201.01	-169.82	-376.00	5.16	0.1020
Thymine : cytosine (interstrand)	*const*	-201.01	-169.82	-370.06	-0.78	0.0860
Adenine : guanine (interstrand)	*const*	-89.55	-123.96	-229.61	16.10	0.1060
Thymine dimer (interstrand)	*const*	-201.01	-201.01	-401.86	-0.16	0.1050
Adenine dimer (interstrand)	*const*	-89.55	-89.55	-185.29	6.18	0.0970
Adenine dimer (interstrand)	*const*	-89.55	-89.55	-190.42	11.31	0.0860
Thymine dimer (interstrand)	*const*	-201.01	-201.01	-401.14	-0.88	0.1090
Adenine : thymine (interstrand)	*const*	-89.55	-201.01	-301.19	10.63	0.1080
Thymine : adenine (interstrand)	*const*	-89.55	-201.01	-298.13	7.56	0.1060
Adenine dimer (interstrand)	*const*	-92.87	-92.87	-191.72	5.98	0.3430
Thymine dimer (interstrand)	*const*	-186.54	-186.54	-372.60	-0.48	0.3470
Guanine dimer (interstrand)	*const*	-131.50	-131.50	-289.96	26.96	0.4040
Cytosine dimer (interstrand)	*const*	-151.25	-151.25	-296.62	-5.87	0.4320
Adenine : Guanine (interstrand)	*const*	-92.87	-131.50	-244.00	19.64	0.3030
Thymine : Cytosine (interstrand)	*const*	-151.25	-186.54	-337.18	-0.60	0.3180
Cytosine dimer (interstrand)	*const*	-169.82	-89.55	-274.29	14.92	0.1590
Guanine dimer (interstrand)	*const*	-123.96	-123.96	-269.43	21.51	0.1080
Guanine dimer (interstrand)	*const*	-123.96	-123.96	-253.65	5.72	0.1100
Cytosine dimer (interstrand)	*const*	-169.82	-169.82	-327.69	-11.95	0.0980
Guanine : Cytosine (stacked)	*opt*	-123.96	-169.82	-389.54	95.75	2.5300
Methylguanine : Methylcytosine (stacked)	*opt*	-131.50	-151.25	-358.76	76.02	2.1630
Adenine : Thymine (stacked)	*opt*	-89.55	-201.01	-331.49	40.93	0.3220
Methyladenine : Methylthymine (stacked)	*opt*	-92.87	-186.54	-326.40	46.99	0.4340
Cytosine dimer 1 (stacked)	*const*	-169.82	-169.82	-328.66	-10.98	0.1050
Cytosine dimer 2 (stacked)	*const*	-169.82	-169.82	-350.74	11.10	0.1180
Cytosine dimer 3 (stacked)	*const*	-169.82	-169.82	-378.33	38.69	0.1170
Cytosine dimer 4 (stacked)	*const*	-169.82	-169.82	-388.41	48.77	0.1020
Cytosine dimer 5 (stacked)	*const*	-169.82	-169.82	-331.73	-7.91	0.1040
Cytosine dimer 6 (stacked)	*const*	-169.82	-169.82	-329.75	-9.89	0.1060
Cytosine dimer 7 (stacked)	*const*	-169.82	-169.82	-340.53	0.88	0.1100
Cytosine dimer 8 (stacked)	*const*	-169.82	-169.82	-383.99	44.35	0.1120
Cytosine dimer 9 (stacked)	*const*	-169.82	-169.82	-387.64	48.00	0.1020
Cytosine dimer 10 (stacked)	*const*	-169.82	-169.82	-387.07	47.43	0.1030
Cytosine dimer 11 (stacked)	*const*	-169.82	-169.82	-388.80	49.16	0.1080
Cytosine dimer 12 (stacked)	*const*	-169.82	-169.82	-369.78	30.14	0.1100
Cytosine dimer 13 (stacked)	*const*	-169.82	-169.82	-384.39	44.75	0.1000

Cytosine dimer 14 (stacked)	*const*	-169.82	-169.82	-384.59	44.95	0.1030
Adenine dimer (stacked)	*const*	-89.55	-89.55	-213.42	34.31	0.0950
guanine dimer (stacked)	*const*	-123.96	-123.96	-298.93	51.00	0.0930
Adenine : cytosine (stacked)	*const*	-89.55	-169.82	-302.06	42.69	0.1040
Guanine : Adenine (stacked)	*const*	-123.96	-89.55	-256.47	42.95	0.0920
Cytosine dimer (stacked)	*const*	-169.82	-169.82	-388.80	49.16	0.1040
Adenine : Uracil (stacked)	*const*	-89.55	-171.76	-298.65	37.33	0.0880
Guanine : Cytosine (stacked)	*const*	-123.96	-169.82	-343.70	49.92	0.1120
Cytosine : Uracil (stacked)	*const*	-169.82	-171.76	-377.69	36.11	0.1000
Uracil dimer (Stacked)	*const*	-171.76	-171.76	-371.89	28.37	0.1020
Guanine : Uracil (stacked)	*const*	-123.96	-171.76	-339.84	44.11	0.0840
Guanine dimer (stacked)	*const*	-169.82	-169.82	-337.71	-1.93	0.1060
Cytosine dimer (stacked)	*const*	-169.82	-123.96	-315.19	21.41	0.1150
Adenine dimer (stacked)	*const*	-89.55	-89.55	-202.61	23.50	0.0970
Thymine dimer (stacked)	*const*	-89.55	-201.01	-304.58	14.01	0.1100
Guanine : cytosine (stacked)	*const*	-169.82	-123.96	-332.16	38.38	0.1120
Guanine : cytosine (stacked)	*const*	-169.82	-123.96	-317.05	23.26	0.0990
Adenine : guanine (stacked)	*const*	-89.55	-123.96	-246.35	32.83	0.0940
Thymine : cytosine (stacked)	*const*	-201.01	-169.82	-387.29	16.45	0.1030
Adenine : guanine (stacked)	*const*	-89.55	-123.96	-241.81	28.29	0.0820
Thymine : cytosine (stacked)	*const*	-201.01	-169.82	-391.47	20.64	0.1530
Thymine : guanine (stacked)	*const*	-201.01	-123.96	-343.05	18.07	0.0970
Adenine : cytosine (stacked)	*const*	-89.55	-169.82	-269.98	10.61	0.0930
Thymine : guanine (stacked)	*const*	-201.01	-123.96	-348.54	23.57	0.1540
Adenine : cytosine (stacked)	*const*	-89.55	-169.82	-277.43	18.06	0.0900
Adenine : thymine (stacked)	*const*	-89.55	-201.01	-319.31	28.74	0.1320
Adenine : thymine (stacked)	*const*	-89.55	-201.01	-307.25	16.68	0.1220
Adenine dimer (stacked)	*const*	-89.55	-89.55	-202.41	23.30	0.0890
Thymine dimer (stacked)	*const*	-201.01	-201.01	-420.19	18.17	0.2020
Adenine : Thymine (stacked)	*const*	-92.87	-186.54	-315.52	36.11	0.3060
Guanine : Cytosine (stacked)	*const*	-151.25	-131.50	-312.33	29.59	0.4310
Adenine : Cytosine (stacked)	*const*	-92.87	-151.25	-268.23	24.12	0.0870
Thymine : Guanine (stacked)	*const*	-186.54	-131.50	-353.02	34.98	0.4140
guanine : Cytosine (stacked)	*const*	-169.82	-123.96	-325.79	32.01	0.1240
Adenine : Guanine (stacked)	*const*	-89.55	-123.96	-242.54	29.02	0.1180
Cytosine : guanine (stacked)	*const*	-123.96	-169.82	-330.57	36.78	0.1210
Guanine : Cytosine (stacked)	*const*	-123.96	-169.82	-334.68	40.89	0.1390
Phe30 : Lys46 (1RB9)	*const*	56.41	45.89	93.88	8.42	0.1520
Phe30 : Leu33 (1RB9)	*const*	56.88	14.62	54.93	16.58	0.1720
Phe30 : Tyr13 (1RB9)	*const*	56.43	6.00	48.66	13.76	0.1330
Phe30 : Phe49 (1RB9)	*const*	31.10	56.55	79.50	8.16	0.1720
Phe30 : Tyr4 (1RB9)	*const*	56.40	11.79	48.83	19.36	0.1430
Phe49 : Cys39 (1RB9)	*const*	31.17	29.59	56.85	3.92	0.1600
Phe49 : Cys6 (1RB9)	*const*	31.28	23.17	41.39	13.07	0.1670
Phe49 : Lys46 (1RB9)	*const*	45.00	42.74	68.79	18.95	0.1490
Phe49 : Val5 (1RB9)	*const*	31.82	32.35	42.48	21.69	0.1660
Phe49 : Tyr37 (1RB9)	*const*	44.47	14.28	55.39	3.36	0.1290
Phe49 : Tyr4 (1RB9)	*const*	31.31	-3.15	14.00	14.16	0.1590
Phe49 : Peptide bond (1RB9)	*const*	44.64	-65.28	-34.25	13.61	0.1760
Phe49 : Peptide bond (1RB9)	*const*	31.61	-65.28	-58.21	24.54	0.1650
Glu47 : Lys6 (PDB:1IU5)	*const*	42.20	-14.95	-302.05	329.30	0.1690
Glu49 : Lys6 (PDB:1BQ9)	*const*	31.52	-23.16	-455.81	464.16	0.1690
Glu54 : Lys2 (PDB:1SMM)	*const*	7.34	21.56	-360.34	389.24	0.1870
Glu50 : LysK30 (PDB:1BRF)	*const*	5.46	-32.90	-277.65	250.20	0.1950
Glu50 : Lys52 (PDB:1BRF)	*const*	6.38	-19.20	-421.52	408.70	0.1690
Glu49 : Lys6 (PDB:1BRF)	*const*	52.95	-23.31	-246.26	275.90	0.3820

OPLSAA

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-110.63	-146.31	-351.95	95.01	0.0750
Methylguanine : Methylcytosine (WC)	*opt*	-147.04	-106.41	-350.53	97.07	0.1360
Adenine : Thymine (WC)	*opt*	-68.95	-172.97	-285.25	43.33	0.3730
Methyladenine : Methylthymine (planar)	*opt*	-68.95	-172.97	-286.35	44.43	0.1130
8-Oxoguanine : Cytosine (WC planar)	*opt*	-193.04	-146.31	-421.64	82.28	0.2530
Inosine : Cytosine (WC planar)	*opt*	-146.31	43.47	-176.63	73.79	0.1080
Guanine : Uracil (wobble)	*opt*	-110.63	-146.10	-307.85	51.13	0.1370
Cytosine : CytosineH+	*opt*	-146.31	122.33	-157.27	133.29	0.2130
Uracil dimer (Calcutta planar)	*opt*	-146.10	-146.10	-320.98	28.78	0.2350
Uracil dimer (planar)	*opt*	-146.10	-146.10	-330.80	38.60	0.0650
6-Thioguanine : Cytosine (WC planar)	*opt*	-146.31	-54.40	-272.42	71.71	0.3350
Adenine : 4-Thiouracil (WC)	*opt*	-75.96	-78.17	-194.92	40.79	3.8870
2-aminoadenine : Thymine	*opt*	-172.53	-168.26	-392.19	51.40	0.2660
2-aminoadenine : Thymine (planar)	*opt*	-172.53	-168.26	-392.19	51.40	0.0360
Adenine : Difluorotoluene	*opt*	-75.96	-2.27	-98.50	20.28	1.8620
Guanine : 4-Thiouracil	*opt*	-110.63	-78.17	-251.30	62.51	0.0910
Guanine : 2-Thiouracil	*opt*	-110.63	-56.33	-211.96	45.01	0.3140
Adenine : Cytosine (planar)	*opt*	-146.31	-75.96	-263.91	41.64	0.0720
Guanine dimer (planar)	*opt*	-110.63	-110.63	-294.54	73.29	0.1580
Guanine 6-Thioguanine (planar)	*opt*	-110.63	-54.40	-221.92	56.90	0.7800
6-Thioguanine : Guanine (planar)	*opt*	-54.40	-110.63	-228.91	63.89	1.1300
Guanine : Adenine 1	*opt*	-110.63	-75.96	-237.71	51.13	0.4730
Guanine : Adenine 1 (planar)	*opt*	-75.96	-110.63	-232.37	45.78	0.0710
Guanine : Adenine 2	*opt*	-110.63	-75.96	-223.72	37.14	0.5340
Guanine : Adenine 2 (planar)	*opt*	-110.63	-75.96	-218.07	31.48	0.0420
Guanine : Adenine 3	*opt*	-110.63	-75.96	-232.25	45.67	0.6150
Guanine : Adenine 4	*opt*	-110.63	-75.96	-225.47	38.89	0.3890
Adenine dimer 1 (planar)	*opt*	-75.96	-75.96	-185.94	34.01	0.5690

Adenine dimer 2 (planar)	*opt*	-75.96	-75.96	-184.28	32.36	0.9010
Adenine dimer 3 (planar)	*opt*	-75.96	-75.96	-183.51	31.59	1.1090
8-Oxoguanine : Guanine	*opt*	-110.63	-193.04	-368.03	64.37	0.1870
2-Thiouracil dimer (planar)	*opt*	-56.33	-56.33	-150.96	38.29	0.1530
Adenine : Thymine (WC)	*const*	-68.95	-172.97	-284.30	42.38	0.3390
Guanine : Cytosine (WC)	*const*	-147.04	-106.41	-349.95	96.50	0.4080
Adenine : thymine (WC)	*const*	-68.95	-172.97	-284.31	42.39	0.3030
Guanine : adenine (HB)	*const*	-110.63	-75.96	-221.34	34.75	0.1070
Cytosine : Guanine (WC)	*const*	-146.31	-110.63	-350.71	93.77	0.0800
Guanine : Cytosine (WC)	*const*	-110.63	-146.31	-351.88	94.94	0.0640
Cytosine : guanine (interstrand)	*const*	-110.63	-146.31	-280.16	23.22	0.1980
Adenine : thymine (interstrand)	*const*	-168.26	-75.96	-256.27	12.05	0.1350
Cytosine dimer (interstrand)	*const*	-146.31	-146.31	-280.24	-12.39	0.1090
Guanine dimer (interstrand)	*const*	-110.63	-110.63	-220.73	-0.52	0.0900
Cytosine dimer (interstrand)	*const*	-146.31	-146.31	-287.01	-5.62	0.1160
Guanine dimer (interstrand)	*const*	-110.63	-110.63	-242.72	21.47	0.1000
Adenine : cytosine (interstrand)	*const*	-75.96	-146.31	-228.34	6.06	0.1100
Thymine : guanine (interstrand)	*const*	-168.26	-110.63	-279.41	0.52	0.0930
Thymine : guanine (interstrand)	*const*	-110.63	-168.26	-288.28	9.39	0.0930
Thymine : cytosine (interstrand)	*const*	-75.96	-146.31	-224.99	2.72	0.1100
Adenine : guanine (interstrand)	*const*	-75.96	-110.63	-210.13	23.54	0.1390
Thymine : cytosine (interstrand)	*const*	-168.26	-146.31	-319.93	5.36	0.1090
Thymine : cytosine (interstrand)	*const*	-168.26	-146.31	-314.01	-0.56	0.0830
Adenine : guanine (interstrand)	*const*	-75.96	-110.63	-203.94	17.36	0.1620
Thymine dimer (interstrand)	*const*	-168.26	-168.26	-336.86	0.33	0.1040
Adenine dimer (interstrand)	*const*	-75.96	-75.96	-158.00	6.08	0.1060
Adenine dimer (interstrand)	*const*	-75.96	-75.96	-163.29	11.37	0.0870
Thymine dimer (interstrand)	*const*	-168.26	-168.26	-335.62	-0.90	0.1060
Adenine : thymine (interstrand)	*const*	-75.96	-168.26	-255.38	11.15	0.1080
Thymine : adenine (interstrand)	*const*	-75.96	-168.26	-252.18	7.96	0.1150
Adenine dimer (interstrand)	*const*	-68.95	-68.95	-144.06	6.17	0.3430
Thymine dimer (interstrand)	*const*	-172.97	-172.97	-345.57	-0.38	0.3490
Guanine dimer (interstrand)	*const*	-106.41	-106.41	-239.65	26.84	0.4640
Cytosine dimer (interstrand)	*const*	-147.04	-147.04	-289.98	-4.11	0.4320
Adenine : Guanine (interstrand)	*const*	-68.95	-106.41	-195.75	20.40	0.3170
Thymine : Cytosine (interstrand)	*const*	-147.04	-172.97	-318.42	-1.60	0.3170
Cytosine dimer (interstrand)	*const*	-146.31	-75.96	-237.82	15.54	0.1710
Guanine dimer (interstrand)	*const*	-110.63	-110.63	-245.34	24.09	0.1600
Guanine dimer (interstrand)	*const*	-110.63	-110.63	-226.52	5.27	0.1100
Cytosine dimer (interstrand)	*const*	-146.31	-146.31	-280.96	-11.66	0.1020
Guanine : Cytosine (stacked)	*opt*	-110.63	-146.31	-351.95	95.01	2.5380
Methylguanine : Methylcytosine (stacked)	*opt*	-106.41	-147.04	-330.47	77.02	2.5000
Adenine : Thymine (stacked)	*opt*	-75.96	-168.26	-285.48	41.25	0.3840
Methyladenine : Methylthymine (stacked)	*opt*	-68.95	-172.97	-293.16	51.24	1.4870
Cytosine dimer 1 (stacked)	*const*	-146.31	-146.31	-284.08	-8.54	0.1150
Cytosine dimer 2 (stacked)	*const*	-146.31	-146.31	-305.49	12.87	0.1240
Cytosine dimer 3 (stacked)	*const*	-146.31	-146.31	-333.19	40.57	0.1440
Cytosine dimer 4 (stacked)	*const*	-146.31	-146.31	-341.77	49.14	0.1030
Cytosine dimer 5 (stacked)	*const*	-146.31	-146.31	-286.96	-5.67	0.1130
Cytosine dimer 6 (stacked)	*const*	-146.31	-146.31	-285.14	-7.49	0.1170
Cytosine dimer 7 (stacked)	*const*	-146.31	-146.31	-296.29	3.67	0.1620
Cytosine dimer 8 (stacked)	*const*	-146.31	-146.31	-337.23	44.60	0.1370
Cytosine dimer 9 (stacked)	*const*	-146.31	-146.31	-341.73	49.10	0.0960
Cytosine dimer 10 (stacked)	*const*	-146.31	-146.31	-341.12	48.50	0.1030
Cytosine dimer 11 (stacked)	*const*	-146.31	-146.31	-341.82	49.19	0.0960
Cytosine dimer 12 (stacked)	*const*	-146.31	-146.31	-321.90	29.28	0.1190
Cytosine dimer 13 (stacked)	*const*	-146.31	-146.31	-339.34	46.71	0.1160
Cytosine dimer 14 (stacked)	*const*	-146.31	-146.31	-337.60	44.97	0.0990
Adenine dimer (stacked)	*const*	-75.96	-75.96	-188.00	36.08	0.1100
guanine dimer (stacked)	*const*	-110.63	-110.63	-272.82	51.57	0.1150
Adenine : cytosine (stacked)	*const*	-75.96	-146.31	-265.54	43.27	0.1080
Guanine : Adenine (stacked)	*const*	-110.63	-75.96	-230.25	43.67	0.0930
Cytosine dimer (stacked)	*const*	-146.31	-146.31	-342.18	49.55	0.0910
Adenine : Uracil (stacked)	*const*	-75.96	-146.10	-261.19	39.13	0.0930
Guanine : Cytosine (stacked)	*const*	-110.63	-146.31	-309.94	53.00	0.1720
Cytosine : Uracil (stacked)	*const*	-146.31	-146.10	-329.04	36.62	0.0970
Uracil dimer (Stacked)	*const*	-146.10	-146.10	-323.08	30.87	0.0970
Guanine : Uracil (stacked)	*const*	-110.63	-146.10	-301.62	44.90	0.0940
Guanine dimer (stacked)	*const*	-146.31	-146.31	-292.30	-0.33	0.1100
Cytosine dimer (stacked)	*const*	-146.31	-110.63	-278.81	21.87	0.1270
Adenine dimer (stacked)	*const*	-75.96	-75.96	-176.20	24.28	0.0980
Thymine dimer (stacked)	*const*	-75.96	-168.26	-257.83	13.61	0.1090
Guanine : cytosine (stacked)	*const*	-146.31	-110.63	-298.93	41.99	0.1740
Guanine : cytosine (stacked)	*const*	-146.31	-110.63	-280.80	23.86	0.1160
Adenine : guanine (stacked)	*const*	-75.96	-110.63	-220.10	33.51	0.1000
Thymine : cytosine (stacked)	*const*	-168.26	-146.31	-331.50	16.93	0.1010
Adenine : guanine (stacked)	*const*	-75.96	-110.63	-215.16	28.57	0.0910
Thymine : cytosine (stacked)	*const*	-168.26	-146.31	-336.29	21.72	0.1500
Thymine : guanine (stacked)	*const*	-168.26	-110.63	-296.07	17.18	0.0960
Adenine : cytosine (stacked)	*const*	-75.96	-146.31	-233.28	11.00	0.0990
Thymine : guanine (stacked)	*const*	-168.26	-110.63	-303.28	24.39	0.1450
Adenine : cytosine (stacked)	*const*	-75.96	-146.31	-242.43	20.16	0.0960
Adenine : thymine (stacked)	*const*	-75.96	-168.26	-273.59	29.37	0.1290
Adenine : thymine (stacked)	*const*	-75.96	-168.26	-266.23	22.00	0.1060
Adenine dimer (stacked)	*const*	-75.96	-75.96	-176.23	24.31	0.0970
Thymine dimer (stacked)	*const*	-168.26	-168.26	-355.57	19.05	0.1820
Adenine : Thymine (stacked)	*const*	-68.95	-172.97	-274.58	32.66	0.2850
Guanine : Cytosine (stacked)	*const*	-147.04	-106.41	-276.88	23.43	0.3930

Adenine : Cytosine (stacked)	*const*	-68.95	-147.04	-238.72	22.74	0.1010
Thymine : Guanine (stacked)	*const*	-172.97	-106.41	-308.58	29.20	0.3690
guanine : Cytosine (stacked)	*const*	-146.31	-110.63	-291.42	34.48	0.1300
Adenine : Guanine (stacked)	*const*	-75.96	-110.63	-217.03	30.44	0.1240
Cytosine : guanine (stacked)	*const*	-110.63	-146.31	-297.53	40.59	0.1540
Guanine : Cytosine (stacked)	*const*	-110.63	-146.31	-300.54	43.61	0.1940
Phe30 : Lys46 (1RB9)	*const*	16.21	3.88	12.82	7.27	0.1560
Phe30 : Leu33 (1RB9)	*const*	16.27	-16.62	-21.09	20.74	0.2320
Phe30 : Tyr13 (1RB9)	*const*	16.20	-29.07	-22.90	10.03	0.1370
Phe30 : Phe49 (1RB9)	*const*	4.17	16.43	11.64	8.96	0.1550
Phe30 : Tyr4 (1RB9)	*const*	16.16	-15.45	-13.21	13.92	0.1490
Phe49 : Cys39 (1RB9)	*const*	4.16	-29.94	-30.83	5.05	0.1540
Phe49 : Cys6 (1RB9)	*const*	4.18	-39.71	-46.36	10.84	0.1490
Phe49 : Lys46 (1RB9)	*const*	10.79	5.14	-1.37	17.29	0.1440
Phe49 : Val5 (1RB9)	*const*	4.26	-36.49	-49.54	17.31	0.1450
Phe49 : Tyr37 (1RB9)	*const*	10.54	-46.97	-41.23	4.80	0.1230
Phe49 : Tyr4 (1RB9)	*const*	4.15	-21.86	-26.43	8.72	0.1340
Phe49 : Peptide bond (1RB9)	*const*	10.69	-68.79	-66.59	8.49	0.1990
Phe49 : Peptide bond (1RB9)	*const*	4.21	-68.79	-97.24	32.66	0.1770
Glu47 : Lys6 (PDB:1IU5)	*const*	95.92	-79.24	-309.38	326.07	0.1560
Glu49 : Lys6 (PDB:1BQ9)	*const*	97.06	-71.11	-447.47	473.42	0.1550
Glu54 : Lys2 (PDB:1SMM)	*const*	88.46	-59.37	-346.01	375.10	0.1930
Glu50 : LysK30 (PDB:1BRF)	*const*	71.14	-94.89	-285.85	262.10	0.1680
Glu50 : Lys52 (PDB:1BRF)	*const*	71.91	-70.89	-406.39	407.41	0.1650
Glu49 : Lys6 (PDB:1BRF)	*const*	112.64	-70.68	-253.95	295.90	0.3780

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Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-306.48	-371.70	-769.27	91.08	0.3230
Methylguanine : Methylcytosine (WC)	*opt*	-320.01	-287.69	-701.02	93.32	0.4120
Adenine : Thymine (WC)	*opt*	-2.58	-357.21	-407.37	47.57	0.3660
Methyladenine : Methylthymine (planar)	*opt*	-2.58	-357.21	-412.74	52.95	0.3770
8-Oxoguanine : Cytosine (WC planar)	*opt*	-656.49	-371.70	-1116.57	88.38	0.3440
Inosine : Cytosine (WC planar)	*opt*	-371.70	-31.84	-479.03	75.49	0.2440
Guanine : Uracil (wobble)	*opt*	-306.48	-403.79	-770.40	60.13	0.2020
Cytosine : CytosineH+	*opt*	-371.70	-380.62	-852.39	100.06	0.2590
Uracil dimer (Calcutta planar)	*opt*	-403.79	-403.79	-844.19	36.61	0.2190
Uracil dimer (planar)	*opt*	-403.79	-403.79	-859.04	51.47	0.1070
6-Thioguanine : Cytosine (WC planar)	*opt*	-371.70	-290.04	-732.39	70.65	0.2550
Adenine : 4-Thiouracil (WC)	*opt*	-21.25	-327.31	-385.95	37.39	3.8870
2-aminoadenine : Thymine	*opt*	-354.91	-396.10	-810.79	59.78	0.0740
2-aminoadenine : Thymine (planar)	*opt*	-354.91	-396.10	-810.79	59.78	0.3140
Adenine : Difluorotoluene	*opt*	-21.25	28.40	-6.23	13.38	0.8380
Guanine : 4-Thiouracil	*opt*	-306.48	-327.31	-695.44	61.66	0.1360
Guanine : 2-Thiouracil	*opt*	-306.48	-315.87	-659.87	37.53	0.4270
Adenine : Cytosine (planar)	*opt*	-371.70	-21.25	-432.44	39.48	0.5250
Guanine dimer (planar)	*opt*	-306.48	-306.48	-688.15	75.19	0.5770
Guanine 6-Thioguanine (planar)	*opt*	-306.48	-290.04	-659.60	63.07	0.8380
6-Thioguanine : Guanine (planar)	*opt*	-290.04	-306.48	-669.27	72.74	0.8290
Guanine : Adenine 1	*opt*	-306.48	-21.25	-380.42	52.69	0.2950
Guanine : Adenine 1 (planar)	*opt*	-21.25	-306.48	-380.42	52.69	0.6230
Guanine : Adenine 2	*opt*	-306.48	-21.25	-369.55	41.82	0.4160
Guanine : Adenine 2 (planar)	*opt*	-306.48	-21.25	-370.40	42.67	0.5890
Guanine : Adenine 3	*opt*	-306.48	-21.25	-386.23	58.50	0.2180
Guanine : Adenine 4	*opt*	-306.48	-21.25	-363.12	35.39	0.3450
Adenine dimer 1 (planar)	*opt*	-21.25	-21.25	-71.53	29.03	0.6790
Adenine dimer 2 (planar)	*opt*	-21.25	-21.25	-75.91	33.41	0.6030
Adenine dimer 3 (planar)	*opt*	-21.25	-21.25	-76.19	33.69	0.6140
8-Oxoguanine : Guanine	*opt*	-306.48	-656.49	-1026.45	63.48	0.2090
2-Thiouracil dimer (planar)	*opt*	-315.87	-315.87	-667.78	36.05	0.3050
Adenine : Thymine (WC)	*const*	-2.58	-357.21	-406.75	46.95	0.2640
Guanine : Cytosine (WC)	*const*	-320.01	-287.69	-697.15	89.45	0.3010
Adenine : thymine (WC)	*const*	-2.58	-357.21	-406.14	46.34	0.1130
Guanine : adenine (HB)	*const*	-306.48	-21.25	-369.47	41.74	0.1320
Cytosine : Guanine (WC)	*const*	-371.70	-306.48	-768.90	90.72	0.0970
Guanine : Cytosine (WC)	*const*	-306.48	-371.70	-766.48	88.29	0.1010
Cytosine : guanine (interstrand)	*const*	-306.48	-371.70	-706.65	28.46	0.2180
Adenine : thymine (interstrand)	*const*	-396.10	-21.25	-432.41	15.06	0.1460
Cytosine dimer (interstrand)	*const*	-371.70	-371.70	-733.71	-9.70	0.1700
Guanine dimer (interstrand)	*const*	-306.48	-306.48	-609.54	-3.43	0.1360
Cytosine dimer (interstrand)	*const*	-371.70	-371.70	-741.07	-2.34	0.1820
Guanine dimer (interstrand)	*const*	-306.48	-306.48	-635.93	22.97	0.1550
Adenine : cytosine (interstrand)	*const*	-21.25	-371.70	-400.75	7.80	0.1810
Thymine : guanine (interstrand)	*const*	-396.10	-306.48	-698.95	-3.64	0.1390
Thymine : guanine (interstrand)	*const*	-306.48	-396.10	-715.45	12.86	0.2150
Thymine : cytosine (interstrand)	*const*	-21.25	-371.70	-403.11	10.15	0.2000
Adenine : guanine (interstrand)	*const*	-21.25	-306.48	-348.27	20.54	0.1450
Thymine : cytosine (interstrand)	*const*	-396.10	-371.70	-777.01	9.20	0.1510
Thymine : cytosine (interstrand)	*const*	-396.10	-371.70	-767.38	-0.43	0.1520
Adenine : guanine (interstrand)	*const*	-21.25	-306.48	-342.80	15.07	0.1620
Thymine dimer (interstrand)	*const*	-396.10	-396.10	-787.94	-4.26	0.1090
Adenine dimer (interstrand)	*const*	-21.25	-21.25	-46.10	3.60	0.1350
Adenine dimer (interstrand)	*const*	-21.25	-21.25	-44.64	2.14	0.1400
Thymine dimer (interstrand)	*const*	-396.10	-396.10	-788.80	-3.41	0.1060
Adenine : thymine (interstrand)	*const*	-21.25	-396.10	-428.39	11.04	0.1370
Thymine : adenine (interstrand)	*const*	-21.25	-396.10	-427.14	9.79	0.1530
Adenine dimer (interstrand)	*const*	-2.58	-2.58	-14.01	8.84	0.3610

Thymine dimer (interstrand)	*const*	-357.21	-357.21	-709.36	-5.07	0.1650
Guanine dimer (interstrand)	*const*	-287.69	-287.69	-605.05	29.66	0.4270
Cytosine dimer (interstrand)	*const*	-320.01	-320.01	-637.53	-2.48	0.2560
Adenine : Guanine (interstrand)	*const*	-2.58	-287.69	-306.94	16.66	0.3330
Thymine : Cytosine (interstrand)	*const*	-320.01	-357.21	-676.78	-0.44	0.2620
Cytosine dimer (interstrand)	*const*	-371.70	-21.25	-409.64	16.68	0.2330
Guanine dimer (interstrand)	*const*	-306.48	-306.48	-640.58	27.62	0.1600
Guanine dimer (interstrand)	*const*	-306.48	-306.48	-613.34	0.37	0.1200
Cytosine dimer (interstrand)	*const*	-371.70	-371.70	-734.50	-8.91	0.1800
Guanine : Cytosine (stacked)	*opt*	-306.48	-371.70	-769.27	91.08	2.3140
Methylguanine : Methylcytosine (stacked)	*opt*	-287.69	-320.01	-701.02	93.32	2.8010
Adenine : Thymine (stacked)	*opt*	-21.25	-396.10	-470.48	53.13	2.2980
Methyladenine : Methylthymine (stacked)	*opt*	-2.58	-357.21	-412.74	52.95	2.5680
Cytosine dimer 1 (stacked)	*const*	-371.70	-371.70	-725.65	-17.76	0.1450
Cytosine dimer 2 (stacked)	*const*	-371.70	-371.70	-759.52	16.11	0.2350
Cytosine dimer 3 (stacked)	*const*	-371.70	-371.70	-780.21	36.80	0.2380
Cytosine dimer 4 (stacked)	*const*	-371.70	-371.70	-775.20	31.79	0.1590
Cytosine dimer 5 (stacked)	*const*	-371.70	-371.70	-742.90	-0.50	0.2400
Cytosine dimer 6 (stacked)	*const*	-371.70	-371.70	-740.88	-2.52	0.2150
Cytosine dimer 7 (stacked)	*const*	-371.70	-371.70	-754.94	11.53	0.2260
Cytosine dimer 8 (stacked)	*const*	-371.70	-371.70	-779.82	36.42	0.2490
Cytosine dimer 9 (stacked)	*const*	-371.70	-371.70	-775.94	32.53	0.2080
Cytosine dimer 10 (stacked)	*const*	-371.70	-371.70	-778.92	35.51	0.1690
Cytosine dimer 11 (stacked)	*const*	-371.70	-371.70	-776.63	33.23	0.1930
Cytosine dimer 12 (stacked)	*const*	-371.70	-371.70	-767.72	24.31	0.2170
Cytosine dimer 13 (stacked)	*const*	-371.70	-371.70	-779.53	36.12	0.1640
Cytosine dimer 14 (stacked)	*const*	-371.70	-371.70	-767.17	23.76	0.1370
Adenine dimer (stacked)	*const*	-21.25	-21.25	-68.77	26.27	0.1680
guanine dimer (stacked)	*const*	-306.48	-306.48	-665.97	53.00	0.2010
Adenine : cytosine (stacked)	*const*	-21.25	-371.70	-429.18	36.22	0.1670
Guanine : Adenine (stacked)	*const*	-306.48	-21.25	-363.97	36.23	0.1690
Cytosine dimer (stacked)	*const*	-371.70	-371.70	-777.73	34.32	0.2090
Adenine : Uracil (stacked)	*const*	-21.25	-403.79	-453.62	28.58	0.1210
Guanine : Cytosine (stacked)	*const*	-306.48	-371.70	-730.30	52.11	0.2120
Cytosine : Uracil (stacked)	*const*	-371.70	-403.79	-805.34	29.85	0.1560
Uracil dimer (Stacked)	*const*	-403.79	-403.79	-826.14	18.56	0.0930
Guanine : Uracil (stacked)	*const*	-306.48	-403.79	-755.94	45.67	0.1860
Guanine dimer (stacked)	*const*	-371.70	-371.70	-745.78	2.37	0.1870
Cytosine dimer (stacked)	*const*	-371.70	-306.48	-705.70	27.51	0.2130
Adenine dimer (stacked)	*const*	-21.25	-21.25	-56.94	14.44	0.1440
Thymine dimer (stacked)	*const*	-21.25	-396.10	-430.83	13.48	0.1220
Guanine : cytosine (stacked)	*const*	-371.70	-306.48	-729.52	51.33	0.2430
Guanine : cytosine (stacked)	*const*	-371.70	-306.48	-705.63	27.44	0.2420
Adenine : guanine (stacked)	*const*	-21.25	-306.48	-353.83	26.09	0.1730
Thymine : cytosine (stacked)	*const*	-396.10	-371.70	-780.02	12.22	0.1170
Adenine : guanine (stacked)	*const*	-21.25	-306.48	-348.64	20.91	0.1470
Thymine : cytosine (stacked)	*const*	-396.10	-371.70	-787.10	19.29	0.1860
Thymine : guanine (stacked)	*const*	-396.10	-306.48	-715.13	12.54	0.1400
Adenine : cytosine (stacked)	*const*	-21.25	-371.70	-403.71	10.76	0.1480
Thymine : guanine (stacked)	*const*	-396.10	-306.48	-716.64	14.06	0.1880
Adenine : cytosine (stacked)	*const*	-21.25	-371.70	-415.84	22.88	0.1840
Adenine : thymine (stacked)	*const*	-21.25	-396.10	-433.95	16.59	0.1590
Adenine : thymine (stacked)	*const*	-21.25	-396.10	-425.24	7.89	0.1280
Adenine dimer (stacked)	*const*	-21.25	-21.25	-58.71	16.21	0.1400
Thymine dimer (stacked)	*const*	-396.10	-396.10	-797.68	5.48	0.1320
Adenine : Thymine (stacked)	*const*	-2.58	-357.21	-375.52	15.73	0.2240
Guanine : Cytosine (stacked)	*const*	-320.01	-287.69	-633.67	25.97	0.3450
Adenine : Cytosine (stacked)	*const*	-2.58	-320.01	-349.28	26.69	0.2380
Thymine : Guanine (stacked)	*const*	-357.21	-287.69	-668.74	23.83	0.3040
guanine : Cytosine (stacked)	*const*	-371.70	-306.48	-707.07	28.88	0.2140
Adenine : Guanine (stacked)	*const*	-21.25	-306.48	-360.26	32.52	0.1810
Cytosine : guanine (stacked)	*const*	-306.48	-371.70	-732.07	53.89	0.2720
Guanine : Cytosine (stacked)	*const*	-306.48	-371.70	-727.98	49.80	0.2450
Phe30 : Lys46 (1RB9)	*const*	281.02	153.34	428.77	5.59	0.1320
Phe30 : Leu33 (1RB9)	*const*	281.08	154.39	422.62	12.85	0.2200
Phe30 : Tyr13 (1RB9)	*const*	281.14	212.77	485.23	8.67	0.1160
Phe30 : Phe49 (1RB9)	*const*	266.22	281.62	540.97	6.87	0.1450
Phe30 : Tyr4 (1RB9)	*const*	281.25	226.67	502.07	5.85	0.1280
Phe49 : Cys39 (1RB9)	*const*	266.18	203.08	470.32	-1.07	0.1450
Phe49 : Cys6 (1RB9)	*const*	266.41	200.79	457.10	10.10	0.1540
Phe49 : Lys46 (1RB9)	*const*	273.42	143.65	409.70	7.38	0.1260
Phe49 : Val5 (1RB9)	*const*	266.76	161.06	400.17	27.65	0.1790
Phe49 : Tyr37 (1RB9)	*const*	272.73	236.90	509.21	0.41	0.1250
Phe49 : Tyr4 (1RB9)	*const*	266.27	221.05	487.56	-0.24	0.1500
Phe49 : Peptide bond (1RB9)	*const*	272.79	-103.13	164.83	4.83	0.3730
Phe49 : Peptide bond (1RB9)	*const*	266.51	-103.13	135.89	27.49	0.3180
Glu47 : Lys6 (PDB:1IU5)	*const*	163.76	106.59	-48.87	319.22	0.1470
Glu49 : Lys6 (PDB:1BQ9)	*const*	161.16	120.06	-170.73	451.95	0.1670
Glu54 : Lys2 (PDB:1SMM)	*const*	168.25	129.62	-59.97	357.85	0.2050
Glu50 : LysK30 (PDB:1BRF)	*const*	151.06	91.30	-12.28	254.63	0.3320
Glu50 : Lys52 (PDB:1BRF)	*const*	151.85	120.03	-119.41	391.29	0.1420
Glu49 : Lys6 (PDB:1BRF)	*const*	171.23	120.79	9.49	282.52	0.3510

MMFF94s

Complex		**Monomer A (kJ/mol)**	**MonomerB (kJ/mol)**	**Complex (kJ/mol)**	**Interaction (kJ/mol)**	**RMS geometry (Å)**
Guanine : Cytosine (WC)	*opt*	-303.93	-369.34	-765.42	92.14	0.0680
Methylguanine : Methylcytosine (WC)	*opt*	-318.58	-285.07	-697.97	94.32	0.3230

Adenine : Thymine (WC)	*opt*	0.44	-360.59	-408.44	48.29	0.2450
Methyladenine : Methylthymine (planar)	*opt*	0.44	-360.59	-412.89	52.74	0.2820
8-Oxoguanine : Cytosine (WC planar)	*opt*	-655.95	-369.34	-1115.08	89.80	0.0560
Inosine : Cytosine (WC planar)	*opt*	-369.34	-32.39	-477.94	76.20	0.0560
Guanine : Uracil (wobble)	*opt*	-303.93	-406.12	-771.06	61.01	0.1840
Cytosine : CytosineH+	*opt*	-369.34	-377.93	-847.74	100.47	0.1320
Uracil dimer (Calcutta planar)	*opt*	-406.12	-406.12	-848.85	36.61	0.2190
Uracil dimer (planar)	*opt*	-406.12	-406.12	-863.70	51.47	0.1070
6-Thioguanine : Cytosine (WC planar)	*opt*	-369.34	-286.62	-729.82	73.85	0.1410
Adenine : 4-Thiouracil (WC)	*opt*	-18.30	-328.99	-384.67	37.38	3.8870
2-aminoadenine : Thymine	*opt*	-345.32	-398.43	-804.55	60.79	0.2630
2-aminoadenine : Thymine (planar)	*opt*	-345.32	-398.43	-804.55	60.79	0.0440
Adenine : Difluorotoluene	*opt*	-18.30	28.40	-2.86	12.96	0.6230
Guanine : 4-Thiouracil	*opt*	-303.93	-328.99	-695.48	62.55	0.1410
Guanine : 2-Thiouracil	*opt*	-303.93	-316.91	-658.95	38.11	0.4170
Adenine : Cytosine (planar)	*opt*	-369.34	-18.30	-423.56	35.91	0.1200
Guanine dimer (planar)	*opt*	-303.93	-303.93	-683.48	75.62	0.1080
Guanine 6-Thioguanine (planar)	*opt*	-303.93	-286.62	-653.02	62.46	0.1040
6-Thioguanine : Guanine (planar)	*opt*	-286.62	-303.93	-659.80	69.25	0.1140
Guanine : Adenine 1	*opt*	-303.93	-18.30	-368.37	46.14	0.3530
Guanine : Adenine 1 (planar)	*opt*	-18.30	-303.93	-362.13	39.89	0.1010
Guanine : Adenine 2	*opt*	-303.93	-18.30	-362.72	40.49	0.2840
Guanine : Adenine 2 (planar)	*opt*	-303.93	-18.30	-360.54	38.30	0.0790
Guanine : Adenine 3	*opt*	-303.93	-18.30	-373.55	51.32	0.2900
Guanine : Adenine 4	*opt*	-303.93	-18.30	-357.46	35.23	0.2350
Adenine dimer 1 (planar)	*opt*	-18.30	-18.30	-66.18	29.57	0.0940
Adenine dimer 2 (planar)	*opt*	-18.30	-18.30	-67.45	30.85	0.5110
Adenine dimer 3 (planar)	*opt*	-18.30	-18.30	-68.25	31.64	0.6630
8-Oxoguanine : Guanine	*opt*	-303.93	-655.95	-1024.61	64.73	0.2460
2-Thiouracil dimer (planar)	*opt*	-316.91	-316.91	-669.86	36.05	0.3050
Adenine : Thymine (WC)	*const*	0.44	-360.59	-407.34	47.18	0.2570
Guanine : Cytosine (WC)	*const*	-318.58	-285.07	-697.08	93.44	0.3020
Adenine : thymine (WC)	*const*	0.44	-360.59	-407.16	47.00	0.0950
Guanine : adenine (HB)	*const*	-303.93	-18.30	-359.50	37.27	0.0930
Cytosine : Guanine (WC)	*const*	-369.34	-303.93	-764.11	90.84	0.0780
Guanine : Cytosine (WC)	*const*	-303.93	-369.34	-765.40	92.12	0.0630
Cytosine : guanine (interstrand)	*const*	-303.93	-369.34	-690.64	17.36	0.1350
Adenine : thymine (interstrand)	*const*	-398.43	-18.30	-426.01	9.27	0.1180
Cytosine dimer (interstrand)	*const*	-369.34	-369.34	-727.26	-11.43	0.1030
Guanine dimer (interstrand)	*const*	-303.93	-303.93	-600.88	-6.99	0.0830
Cytosine dimer (interstrand)	*const*	-369.34	-369.34	-733.56	-5.13	0.1070
Guanine dimer (interstrand)	*const*	-303.93	-303.93	-624.29	16.42	0.0890
Adenine : cytosine (interstrand)	*const*	-18.30	-369.34	-394.06	6.41	0.1020
Thymine : guanine (interstrand)	*const*	-398.43	-303.93	-698.34	-4.03	0.0740
Thymine : guanine (interstrand)	*const*	-303.93	-398.43	-703.93	1.57	0.1030
Thymine : cytosine (interstrand)	*const*	-18.30	-369.34	-391.74	4.10	0.1040
Adenine : guanine (interstrand)	*const*	-18.30	-303.93	-340.36	18.12	0.0870
Thymine : cytosine (interstrand)	*const*	-398.43	-369.34	-773.26	5.49	0.1030
Thymine : cytosine (interstrand)	*const*	-398.43	-369.34	-767.19	-0.59	0.0970
Adenine : guanine (interstrand)	*const*	-18.30	-303.93	-330.67	8.43	0.0920
Thymine dimer (interstrand)	*const*	-398.43	-398.43	-792.60	-4.26	0.1100
Adenine dimer (interstrand)	*const*	-18.30	-18.30	-40.79	4.18	0.1090
Adenine dimer (interstrand)	*const*	-18.30	-18.30	-36.34	-0.26	0.0870
Thymine dimer (interstrand)	*const*	-398.43	-398.43	-793.45	-3.42	0.1090
Adenine : thymine (interstrand)	*const*	-18.30	-398.43	-427.79	11.05	0.1060
Thymine : adenine (interstrand)	*const*	-18.30	-398.43	-422.18	5.44	0.1090
Adenine dimer (interstrand)	*const*	0.44	0.44	-2.42	3.29	0.3360
Thymine dimer (interstrand)	*const*	-360.59	-360.59	-716.10	-5.08	0.1530
Guanine dimer (interstrand)	*const*	-285.07	-285.07	-590.22	20.08	0.4030
Cytosine dimer (interstrand)	*const*	-318.58	-318.58	-632.03	-5.13	0.1280
Adenine : Guanine (interstrand)	*const*	0.44	-285.07	-297.58	12.95	0.3020
Thymine : Cytosine (interstrand)	*const*	-318.58	-360.59	-678.20	-0.97	0.3180
Cytosine dimer (interstrand)	*const*	-369.34	-18.30	-396.80	9.15	0.1690
Guanine dimer (interstrand)	*const*	-303.93	-303.93	-629.60	21.73	0.1050
Guanine dimer (interstrand)	*const*	-303.93	-303.93	-605.23	-2.64	0.0930
Cytosine dimer (interstrand)	*const*	-369.34	-369.34	-727.70	-10.99	0.1020
Guanine : Cytosine (stacked)	*opt*	-303.93	-369.34	-765.42	92.14	2.5210
Methylguanine : Methylcytosine (stacked)	*opt*	-285.07	-318.58	-697.97	94.32	3.0330
Adenine : Thymine (stacked)	*opt*	-18.30	-398.43	-469.73	53.00	2.4500
Methyladenine : Methylthymine (stacked)	*opt*	0.44	-360.59	-396.64	36.48	0.5640
Cytosine dimer 1 (stacked)	*const*	-369.34	-369.34	-724.76	-13.93	0.1050
Cytosine dimer 2 (stacked)	*const*	-369.34	-369.34	-743.22	4.54	0.1160
Cytosine dimer 3 (stacked)	*const*	-369.34	-369.34	-763.65	24.97	0.1210
Cytosine dimer 4 (stacked)	*const*	-369.34	-369.34	-769.41	30.72	0.0900
Cytosine dimer 5 (stacked)	*const*	-369.34	-369.34	-727.26	-11.42	0.1060
Cytosine dimer 6 (stacked)	*const*	-369.34	-369.34	-725.94	-12.75	0.1080
Cytosine dimer 7 (stacked)	*const*	-369.34	-369.34	-736.48	-2.21	0.1240
Cytosine dimer 8 (stacked)	*const*	-369.34	-369.34	-766.83	28.14	0.1050
Cytosine dimer 9 (stacked)	*const*	-369.34	-369.34	-768.77	30.08	0.1000
Cytosine dimer 10 (stacked)	*const*	-369.34	-369.34	-769.34	30.65	0.0890
Cytosine dimer 11 (stacked)	*const*	-369.34	-369.34	-770.77	32.09	0.0920
Cytosine dimer 12 (stacked)	*const*	-369.34	-369.34	-759.59	20.90	0.1130
Cytosine dimer 13 (stacked)	*const*	-369.34	-369.34	-769.02	30.33	0.0900
Cytosine dimer 14 (stacked)	*const*	-369.34	-369.34	-765.85	27.17	0.0920
Adenine dimer (stacked)	*const*	-18.30	-18.30	-59.13	22.53	0.1000
guanine dimer (stacked)	*const*	-303.93	-303.93	-651.42	43.55	0.0940
Adenine : cytosine (stacked)	*const*	-18.30	-369.34	-420.07	32.43	0.0940
Guanine : Adenine (stacked)	*const*	-303.93	-18.30	-355.08	32.84	0.0870

Cytosine dimer (stacked)	*const*	-369.34	-369.34	-770.77	32.08	0.0990
Adenine : Uracil (stacked)	*const*	-18.30	-406.12	-451.83	27.41	0.0960
Guanine : Cytosine (stacked)	*const*	-303.93	-369.34	-714.65	41.37	0.1170
Cytosine : Uracil (stacked)	*const*	-369.34	-406.12	-802.20	26.74	0.0940
Uracil dimer (Stacked)	*const*	-406.12	-406.12	-830.61	18.37	0.0950
Guanine : Uracil (stacked)	*const*	-303.93	-406.12	-748.90	38.85	0.0960
Guanine dimer (stacked)	*const*	-369.34	-369.34	-733.57	-5.11	0.0990
Cytosine dimer (stacked)	*const*	-369.34	-303.93	-694.41	21.13	0.1170
Adenine dimer (stacked)	*const*	-18.30	-18.30	-46.13	9.53	0.1000
Thymine dimer (stacked)	*const*	-18.30	-398.43	-430.93	14.20	0.1070
Guanine : cytosine (stacked)	*const*	-369.34	-303.93	-706.76	33.49	0.1320
Guanine : cytosine (stacked)	*const*	-369.34	-303.93	-690.24	16.97	0.0970
Adenine : guanine (stacked)	*const*	-18.30	-303.93	-341.42	19.18	0.1010
Thymine : cytosine (stacked)	*const*	-398.43	-369.34	-780.74	12.96	0.1010
Adenine : guanine (stacked)	*const*	-18.30	-303.93	-340.33	18.10	0.0890
Thymine : cytosine (stacked)	*const*	-398.43	-369.34	-782.59	14.81	0.1070
Thymine : guanine (stacked)	*const*	-398.43	-303.93	-714.93	12.56	0.0890
Adenine : cytosine (stacked)	*const*	-18.30	-369.34	-395.70	8.06	0.0930
Thymine : guanine (stacked)	*const*	-398.43	-303.93	-709.78	7.42	0.1090
Adenine : cytosine (stacked)	*const*	-18.30	-369.34	-400.71	13.06	0.1090
Adenine : thymine (stacked)	*const*	-18.30	-398.43	-430.24	13.50	0.1030
Adenine : thymine (stacked)	*const*	-18.30	-398.43	-421.94	5.21	0.1010
Adenine dimer (stacked)	*const*	-18.30	-18.30	-48.97	12.37	0.0980
Thymine dimer (stacked)	*const*	-398.43	-398.43	-802.33	5.46	0.1320
Adenine : Thymine (stacked)	*const*	0.44	-360.59	-378.25	18.09	0.2340
Guanine : Cytosine (stacked)	*const*	-318.58	-285.07	-623.70	20.06	0.3020
Adenine : Cytosine (stacked)	*const*	0.44	-318.58	-333.09	14.94	0.3140
Thymine : Guanine (stacked)	*const*	-360.59	-285.07	-662.67	17.01	0.2750
guanine : Cytosine (stacked)	*const*	-369.34	-303.93	-692.97	19.69	0.1300
Adenine : Guanine (stacked)	*const*	-18.30	-303.93	-337.06	14.83	0.1100
Cytosine : guanine (stacked)	*const*	-303.93	-369.34	-708.21	34.94	0.1490
Guanine : Cytosine (stacked)	*const*	-303.93	-369.34	-709.78	36.50	0.1480
Phe30 : Lys46 (1RB9)	*const*	281.02	153.34	428.77	5.59	0.1320
Phe30 : Leu33 (1RB9)	*const*	281.08	154.39	422.62	12.85	0.2200
Phe30 : Tyr13 (1RB9)	*const*	281.14	212.77	485.23	8.67	0.1160
Phe30 : Phe49 (1RB9)	*const*	266.22	281.62	540.97	6.87	0.1450
Phe30 : Tyr4 (1RB9)	*const*	281.25	226.67	502.07	5.85	0.1280
Phe49 : Cys39 (1RB9)	*const*	266.18	203.08	470.32	-1.07	0.1450
Phe49 : Cys6 (1RB9)	*const*	266.41	200.79	457.10	10.10	0.1540
Phe49 : Lys46 (1RB9)	*const*	273.42	143.65	409.70	7.38	0.1260
Phe49 : Val5 (1RB9)	*const*	266.76	161.06	400.17	27.65	0.1790
Phe49 : Tyr37 (1RB9)	*const*	272.73	236.90	509.21	0.41	0.1250
Phe49 : Tyr4 (1RB9)	*const*	266.27	221.05	487.56	-0.24	0.1500
Phe49 : Peptide bond (1RB9)	*const*	272.81	-105.67	163.53	3.61	0.2160
Phe49 : Peptide bond (1RB9)	*const*	266.54	-105.67	133.01	27.87	0.2550
Glu47 : Lys6 (PDB:1IU5)	*const*	163.76	106.59	-48.87	319.22	0.1470
Glu49 : Lys6 (PDB:1BQ9)	*const*	161.16	120.06	-170.73	451.95	0.1670
Glu54 : Lys2 (PDB:1SMM)	*const*	168.25	129.62	-59.97	357.85	0.2050
Glu50 : LysK30 (PDB:1BRF)	*const*	151.06	91.30	-12.28	254.63	0.3320
Glu50 : Lys52 (PDB:1BRF)	*const*	151.85	120.03	-119.41	391.29	0.1420
Glu49 : Lys6 (PDB:1BRF)	*const*	171.23	120.79	9.49	282.52	0.3510