Supplementary Information for "Binding Structures of tri-N-acetyl-β-glucosamine in Hen Egg White Lysozyme using Molecular Dynamics with a Polarizable Force Field"

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Atom Name	Atom Type	χ^a	$(\eta_i^\circ)^a/2$
C1	CTS	310	98
H1	HAS	295	251
O1	OHS	515	154
HO1	HOS	88	259
C2	CTS	310	98
H2	HAS	268	251
C5	CTS	290	98
H5	HAS	268	251
O5	OES	500	154
NT	NG1	557	149
HNT	HG	99	297
C7	CG	216	123
O7	OG	626	190
C8	CT3G	470	120
H81	HA3G	271	251
H82	HA3G	271	251
H83	HA3G	271	251

[a] Electronegativity χ and atomic hardness η are in units of $\frac{kcal/mol}{e}$ and $\frac{kcal/mol}{e^2}$, respectively. The values for η correspond identically to J_{ii} in the text discussion.

TABLE I:

Atom Name	Atom Type	χ^a	$(\eta_i^\circ)^a/2$
C3	CTS	310	98
H3	HAS	268	251
O3	OHS	550	154
HO3	HOS	86	259
C4	CTS	380	98
H4	HAS	268	251
O4	OHS	550	154
HO4	HOS	86	259
C6	CTS	320	104
H61	HAS	305	251
H62	HAS	305	251
O6	OHS	540	154
HO6	HOS	98	259

[a] Electronegativity χ and atomic hardness η are in units of $\frac{kcal/mol}{e}$ and $\frac{kcal/mol}{e^2}$, respectively. The values for η correspond identically to J_{ii} in the text discussion.

TABLE II:

Atom Type Unit	ϵ (CHEQ) (kcal/mol)	$R_{min}/2$ (CHEQ) (Å)	ϵ (PHLB) (kcal/mol)	$R_{min}/2$ (PHLB) (Å)
CTS	0.020	2.275	0.020	2.275
HAS	0.082	1.320	0.020	1.320
OHS	0.170	1.630	0.152	1.770
HOS	0.016	0.125	0.046	0.225
OES	0.070	1.803	0.152	1.770
NG1	0.120	1.880	0.200	1.850
HG	0.016	0.125	0.046	0.225
CG	0.160	2.225	0.110	2.000
OG	0.115	1.925	0.120	1.700
CT3G	0.073	2.020	0.080	2.060
HA3G	0.023	1.320	0.022	1.320
ON2	0.070	1.803	0.152	1.770

TABLE III:

Molecule	C22	CHEQ
Methanol	−7.05	−9.93
Ethanol	−7.09	−9.58
Propanol	−7.12	−8.48
Butanol	−7.05	−9.56
Acetamide	−10.81	−21.46
N-Methylacetamide	−9.39	−21.07
Formamide	−13.11	−24.65
N-Methylformamide	−13.42	−21.24
Methanethiol	−2.01	−6.82
Ethanethiol	−1.97	−4.67
Methylamine	−5.43	−6.20
Ethylamine	−3.89	−3.23
Propylamine	−4.58	−4.90
Butane	−1.19	−0.41

TABLE IV:

System	Model	S_∞(kcal/mol/K)	$A \times 10^{-4}$	n
$(NAG)_3$	C22	80.01(0.19)	3.43(4.16)	1.30(0.18)
	CHEQ	75.63(0.45)	3.43(14.85)	1.25(0.59)
$Protein_{WT}$	C22	1978.67(2.91)	9.71(0.28)	0.68(0.00)
	CHEQ	1868.48(34.61)	2.36(0.29)	0.48(0.02)
$Protein_{W62Y}$	C22	2030.23(16.84)	8.73(1.37)	0.66(0.03)
	CHEQ	1828.14(51.22)	3.01(0.64)	0.53(0.04)
$Complex_{WT}^{ABC}$	C22	2156.22(7.03)	6.19(0.39)	0.59(0.01)
	CHEQ	1885.26(40)	2.94(0.08)	0.51(0.04)
$Complex_{WT}^{BCD}$	C22	2122.13(10.88)	5.15(0.57)	0.57(0.02)
	CHEQ	2036.60(70.33)	0.89(0.22)	0.33(0.04)
$Complex_{W62Y}^{ABC}$	C22	2060.18(9.62)	9.68(0.88)	0.67(0.01)
	CHEQ	1897.44(17.73)	4.07(0.39)	0.56(0.02)

TABLE V:

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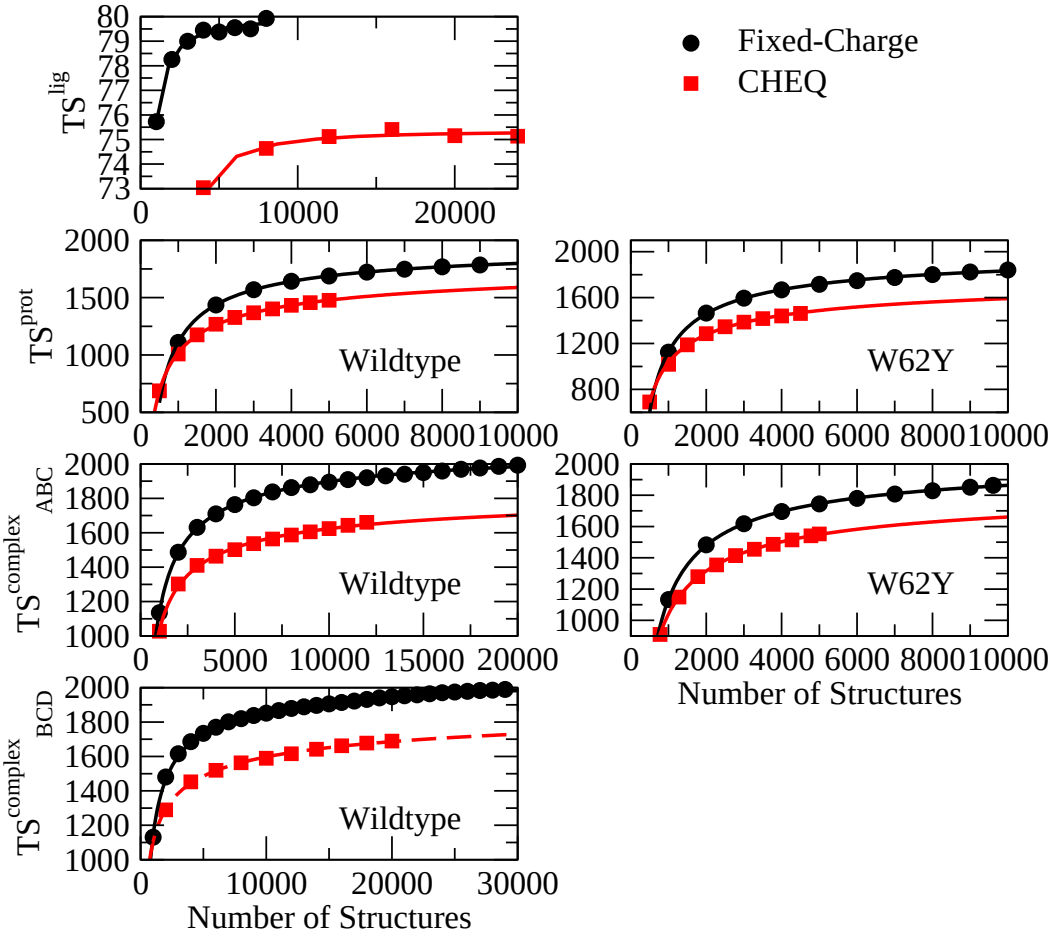
Fixed-Charge
CHEQ
TS lig
TS prot
TS complex ABC
TS complex BCD
Wildtype
W62Y
Number of Structures

FIG. 1:

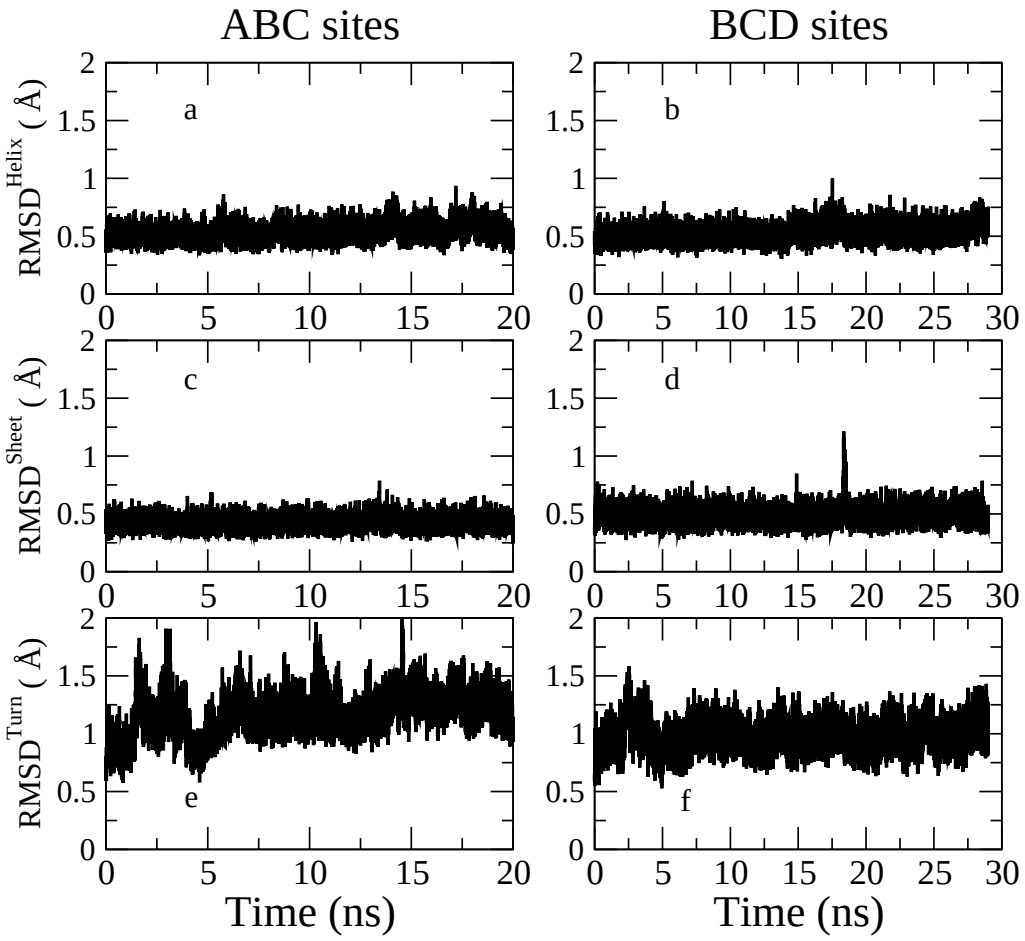
ABC sites
BCD sites
RMSD^Helix (Å)
RMSD^Sheet (Å)
RMSD^Turn (Å)
a
b
c
d
e
f
Time (ns)
Time (ns)

FIG. 2:

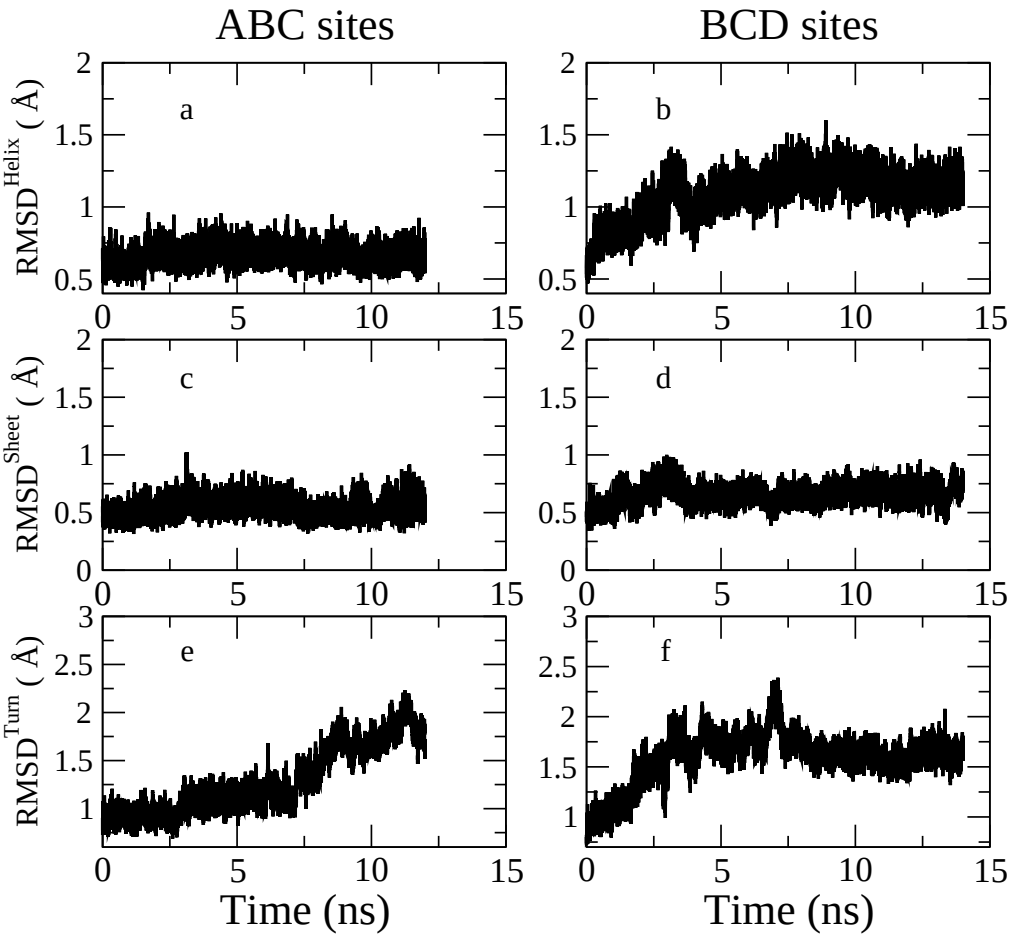
ABC sites
BCD sites
RMSD^Helix (Å)
RMSD^Sheet (Å)
RMSD^Turn (Å)
a
b
c
d
e
f
Time (ns)
Time (ns)

FIG. 3:

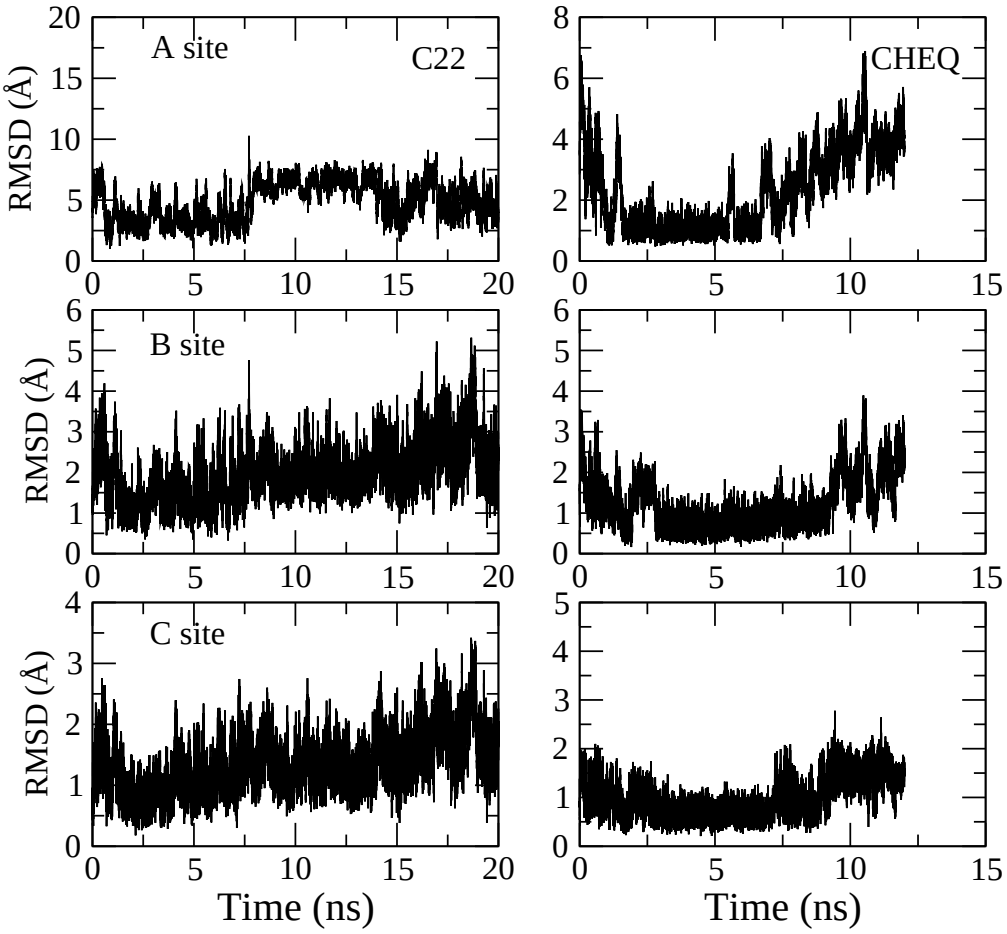

FIG. 4:

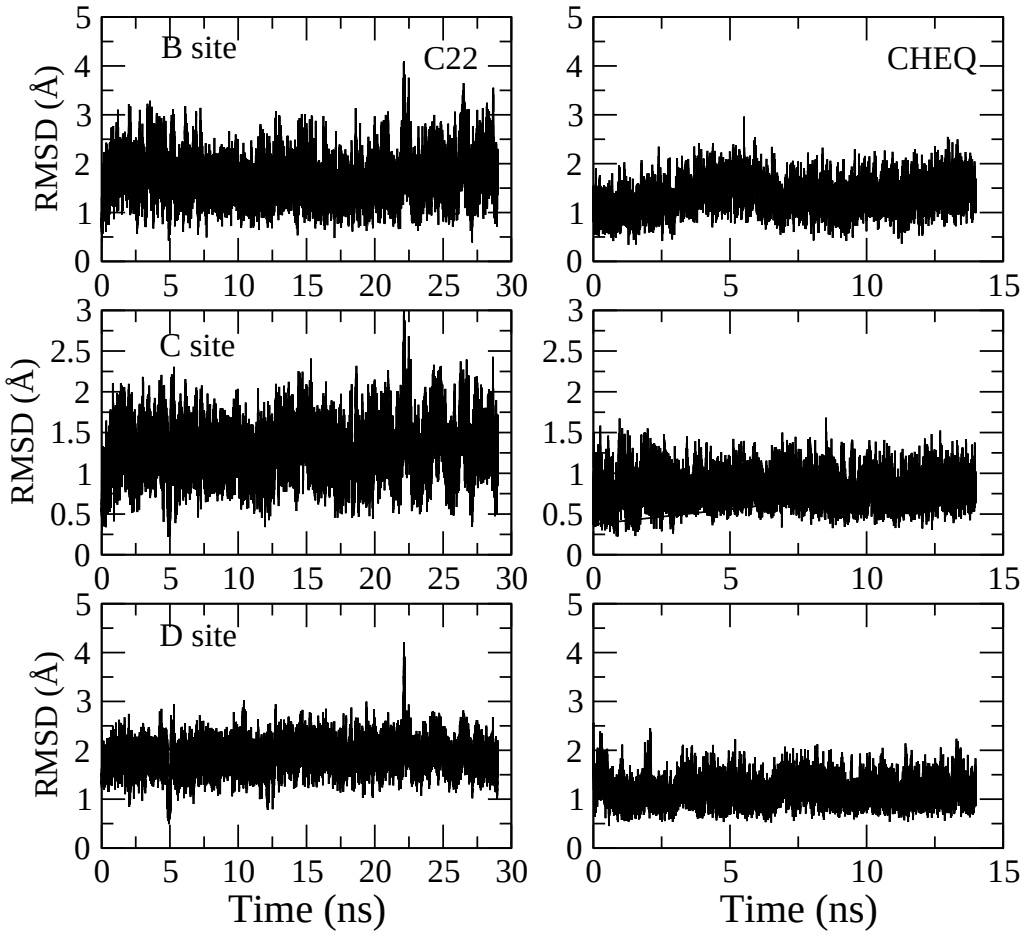

FIG. 5:

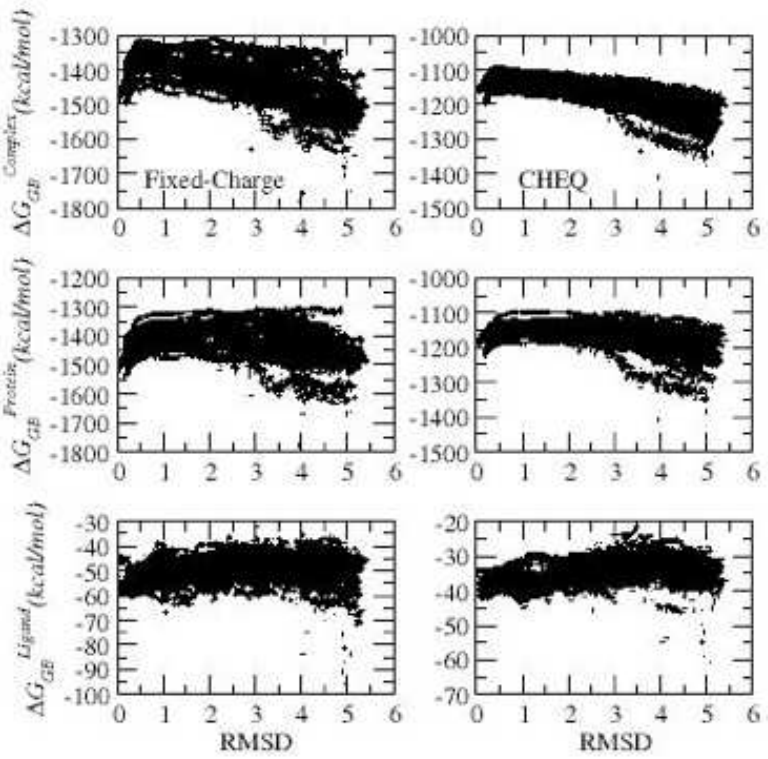
Fixed-Charge
CHEQ
$\Delta G_{GB}^{Complex}$ (kcal/mol)
$\Delta G_{GB}^{Protein}$ (kcal/mol)
ΔG_{GB}^{Ligand} (kcal/mol)
RMSD
RMSD

FIG. 6:

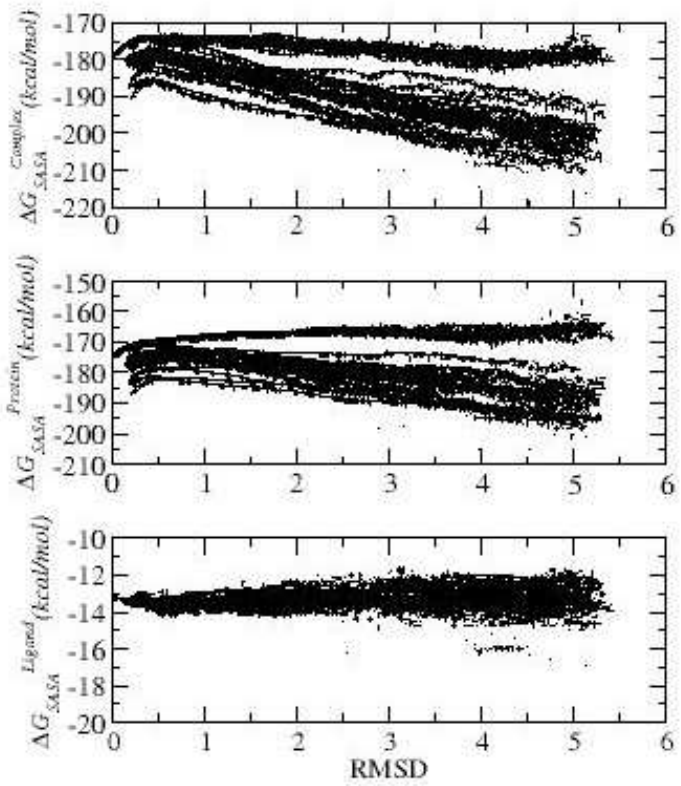
$\Delta G_{SASA}^{Complex}$ (kcal/mol)
-170
-180
-190
-200
-210
-220
$\Delta G_{SASA}^{Protein}$ (kcal/mol)
-150
-160
-170
-180
-190
-200
-210
ΔG_{SASA}^{Ligand} (kcal/mol)
-10
-12
-14
-16
-18
-20
0
1
2
3
4
5
6
RMSD

FIG. 7:

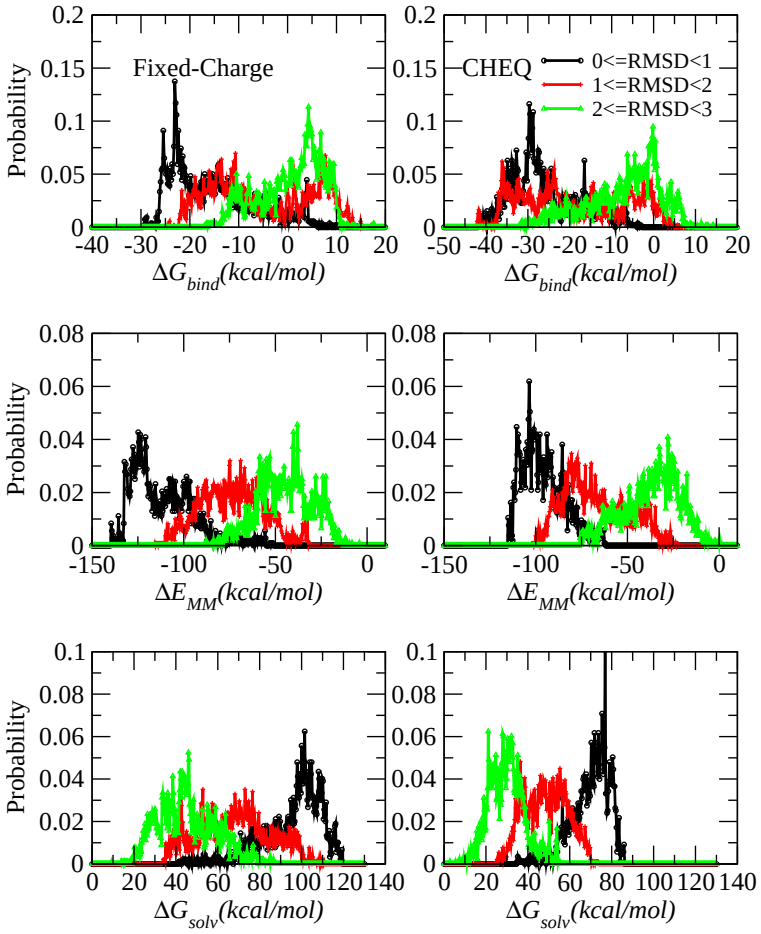
Fixed-Charge
CHEQ
0<=RMSD<1
1<=RMSD<2
2<=RMSD<3
Probability
ΔG_{bind}(kcal/mol)
ΔE_{MM}(kcal/mol)
ΔG_{solv}(kcal/mol)

FIG. 8: