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SI Structural stability of chromophore-grafted Ubiquitin mutants in vacuum. †

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1 Supplementary Figures

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† Electronic Supplementary Information (ESI) available: 10.5281/zenodo.15270985

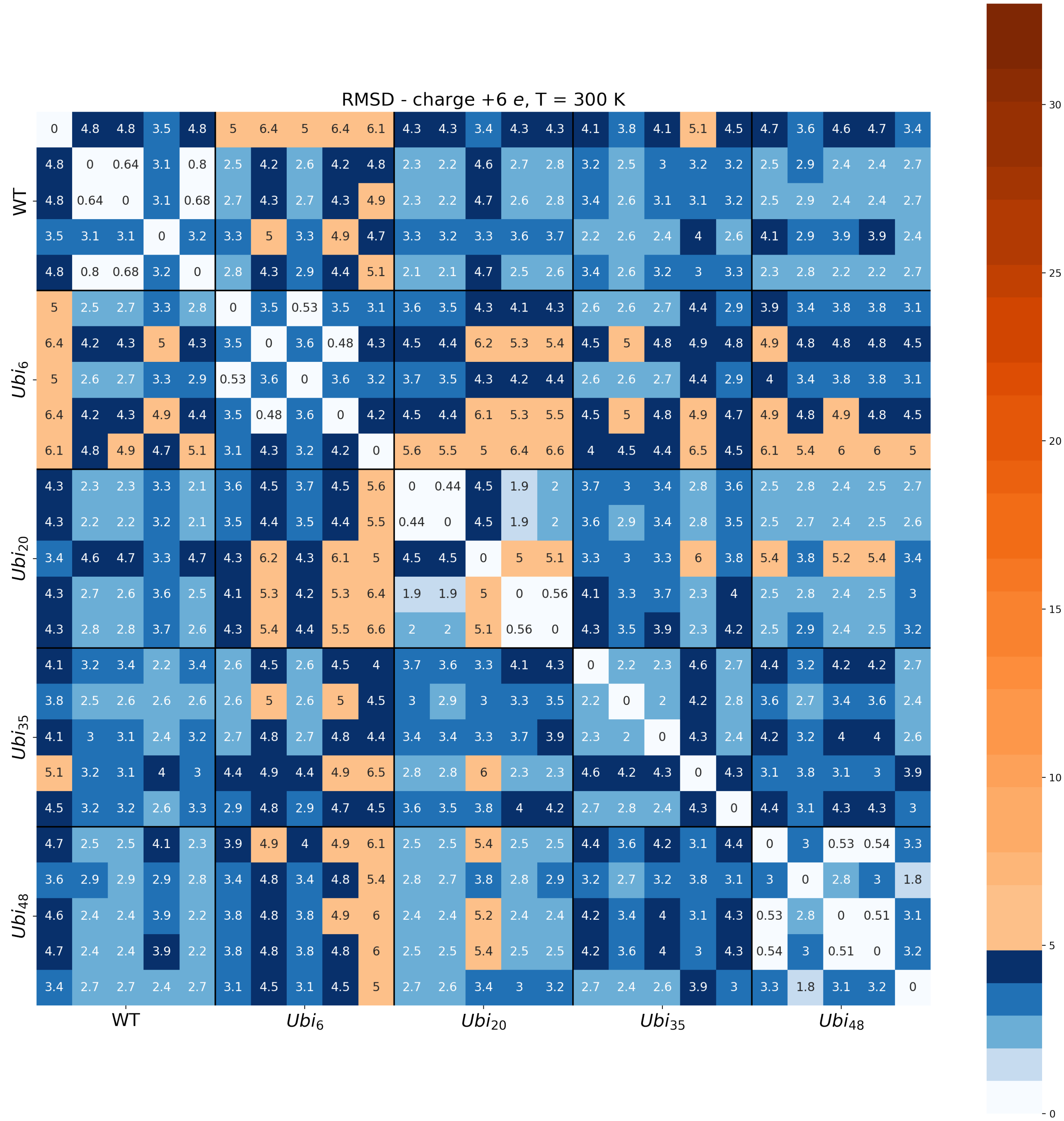

Fig. S1 Heatmap representation of pairwise RMSD values between ubiquitin variants, illustrating the structural variations. Each column corresponds to different simulation temperatures, while each row represents distinct net charges of the systems. The color gradient in the heatmap visualizes the magnitude of structural differences, with shades of blue indicating high similarity (RMSD < 5 Å) and shades of orange indicating significant divergence (RMSD > 5 Å). The RMSD values, expressed in units of Å, are computed as the mean value of pairwise comparisons among replica simulations.

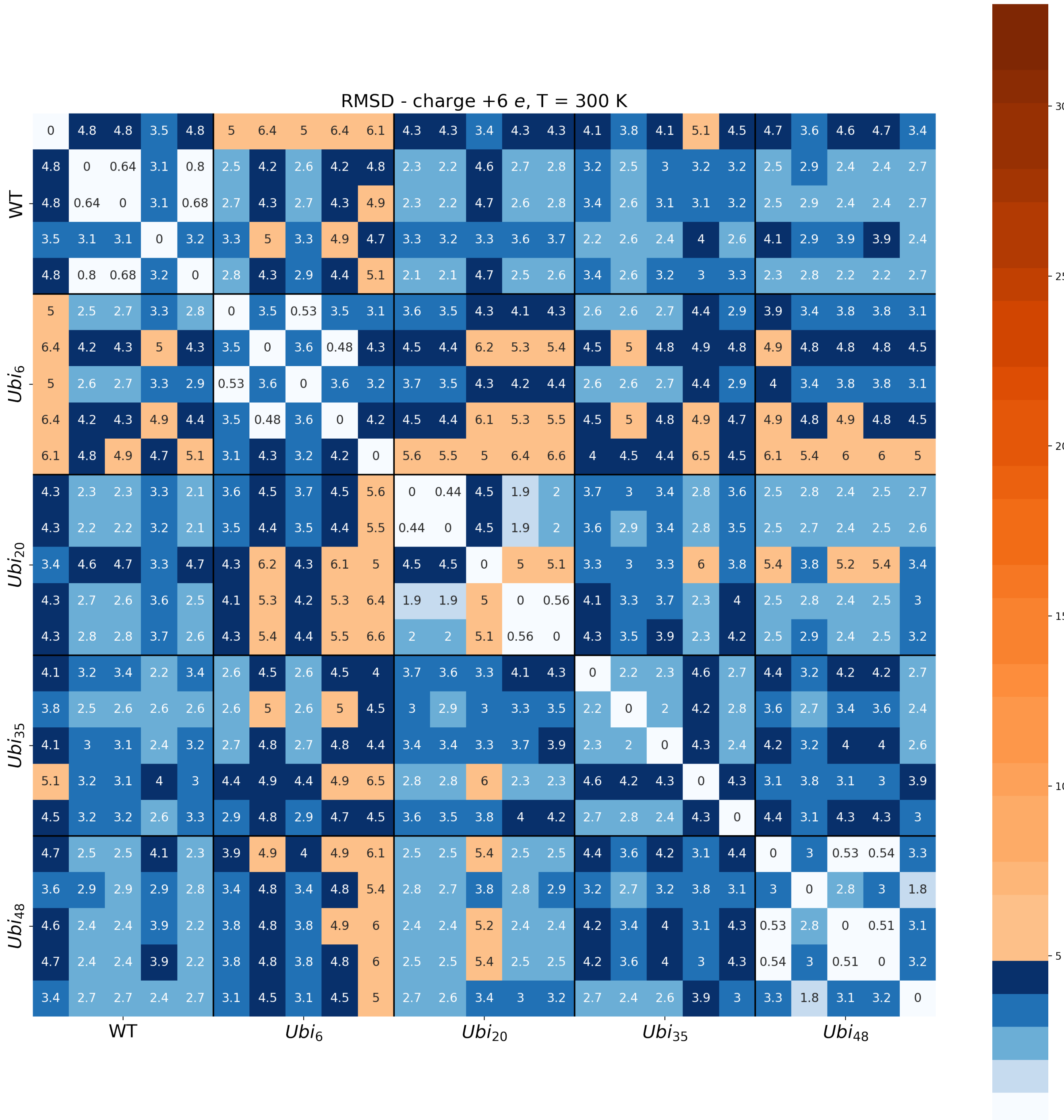

Fig. S2 RMSD matrix for simulations performed at 300 K for systems of net charge +6 e. The values are expressed in units of Å.

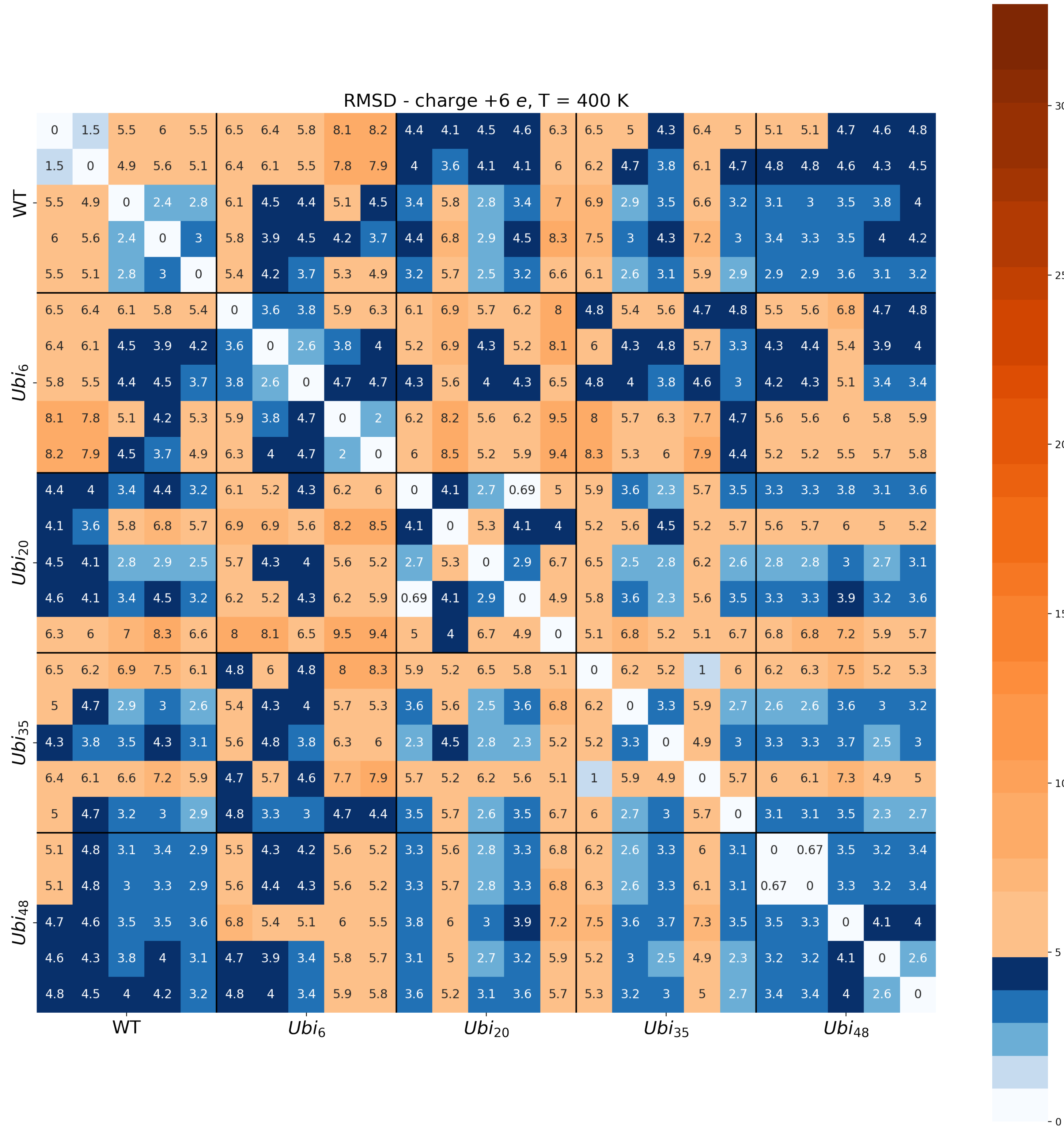

Fig. S3 RMSD matrix for simulations performed at 400 K for systems of net charge +6 e. The values are expressed in units of Å.

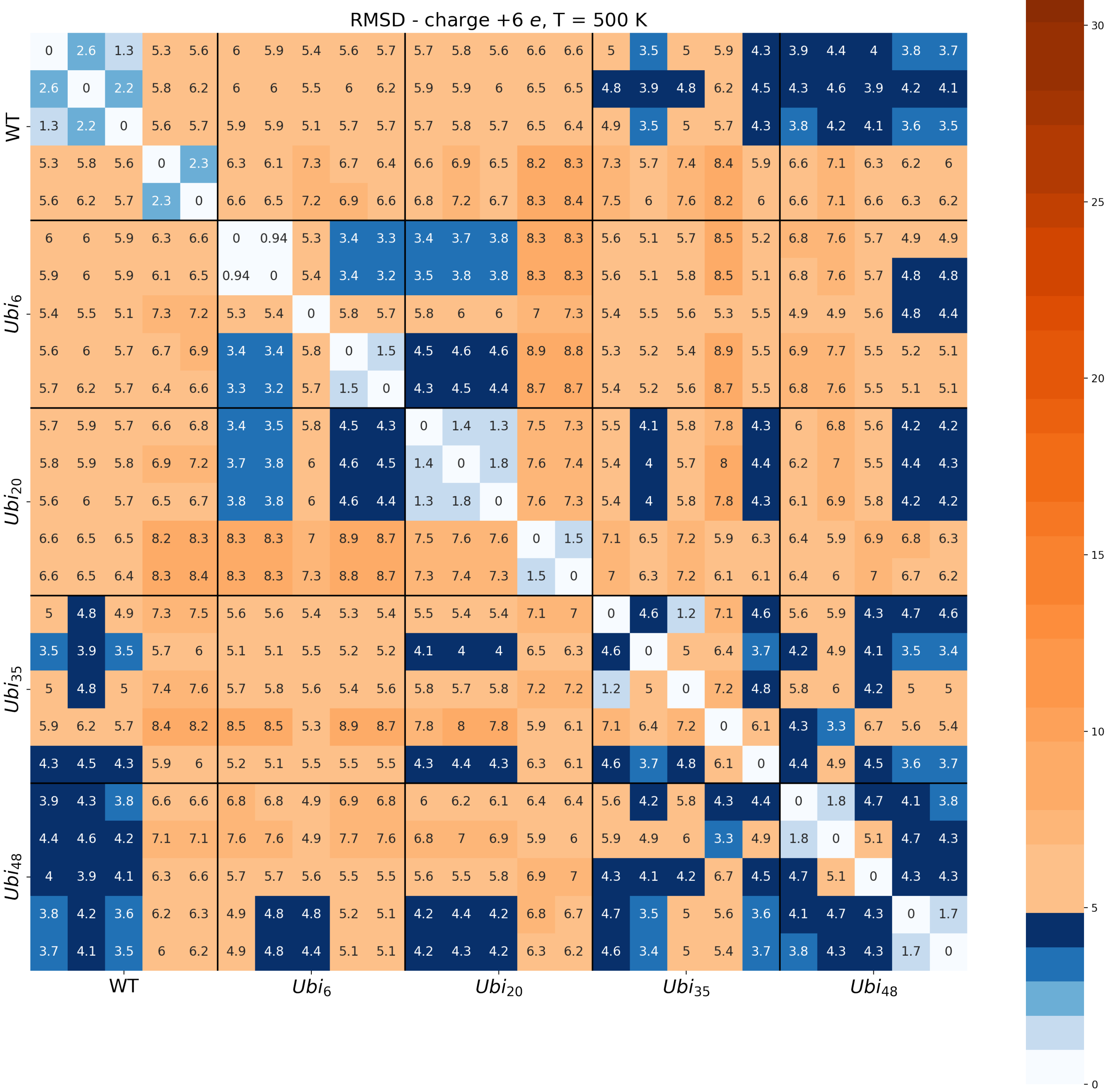

Fig. S4 RMSD matrix for simulations performed at 500 K for systems of net charge +6 *e*. The values are expressed in units of Å.

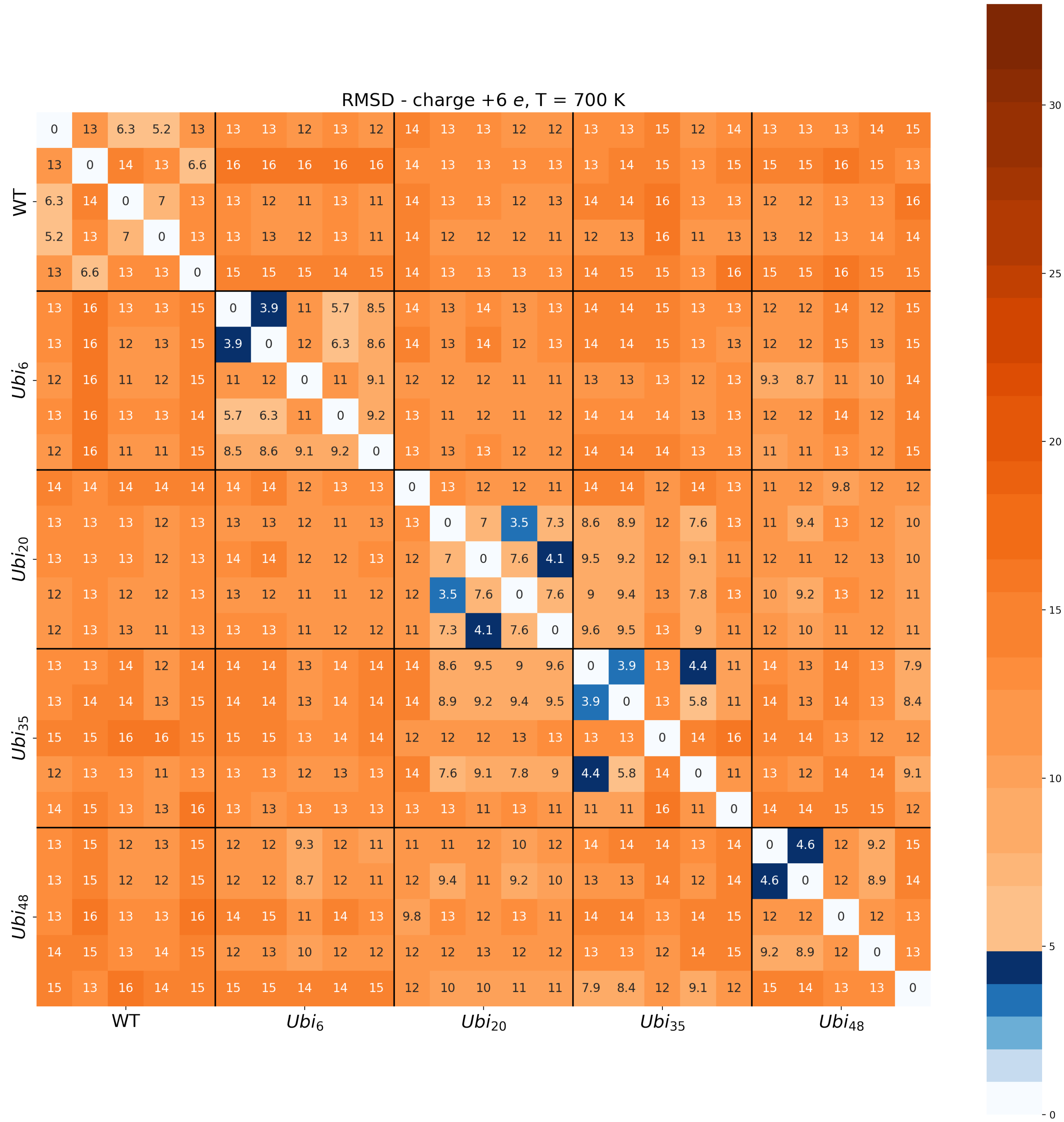

Fig. S5 RMSD matrix for simulations performed at 700 K for systems of net charge +6 *e*. The values are expressed in units of Å.

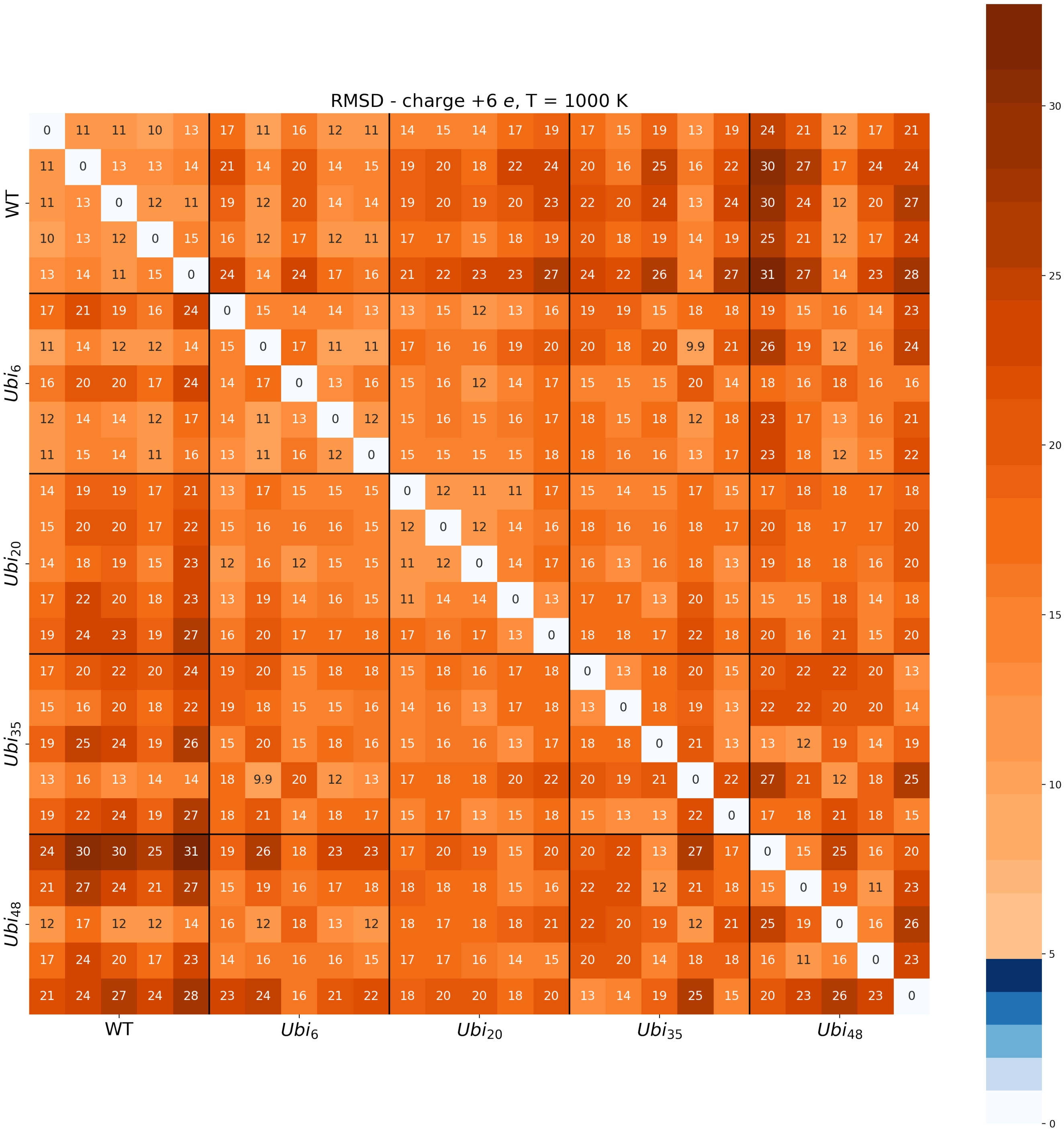

Fig. S6 RMSD matrix for simulations performed at 1000 K for systems of net charge +6 e. The values are expressed in units of Å.

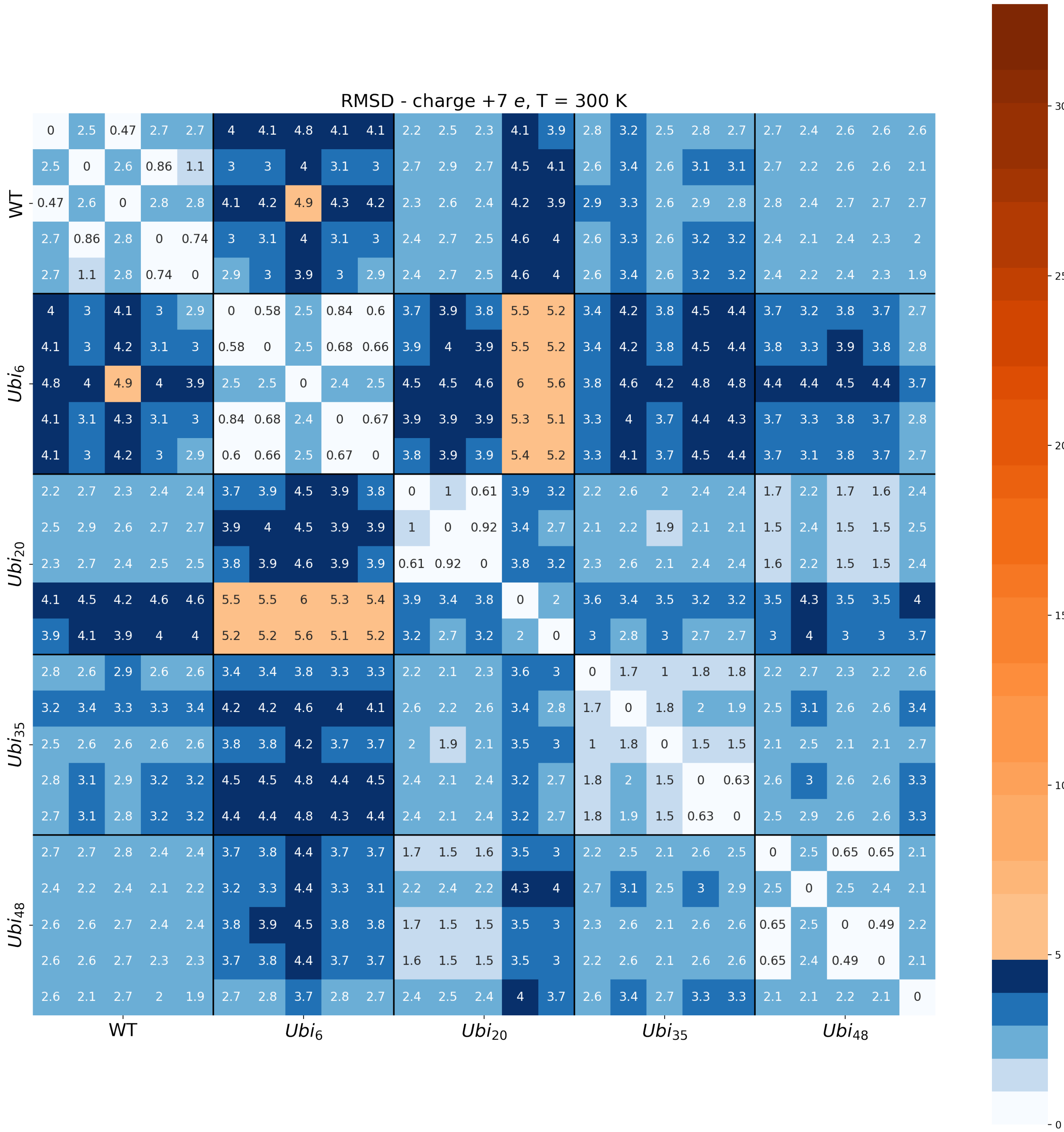

Fig. S7 RMSD matrix for simulations performed at 500 K for systems of net charge +7 *e*. The values are expressed in units of Å.

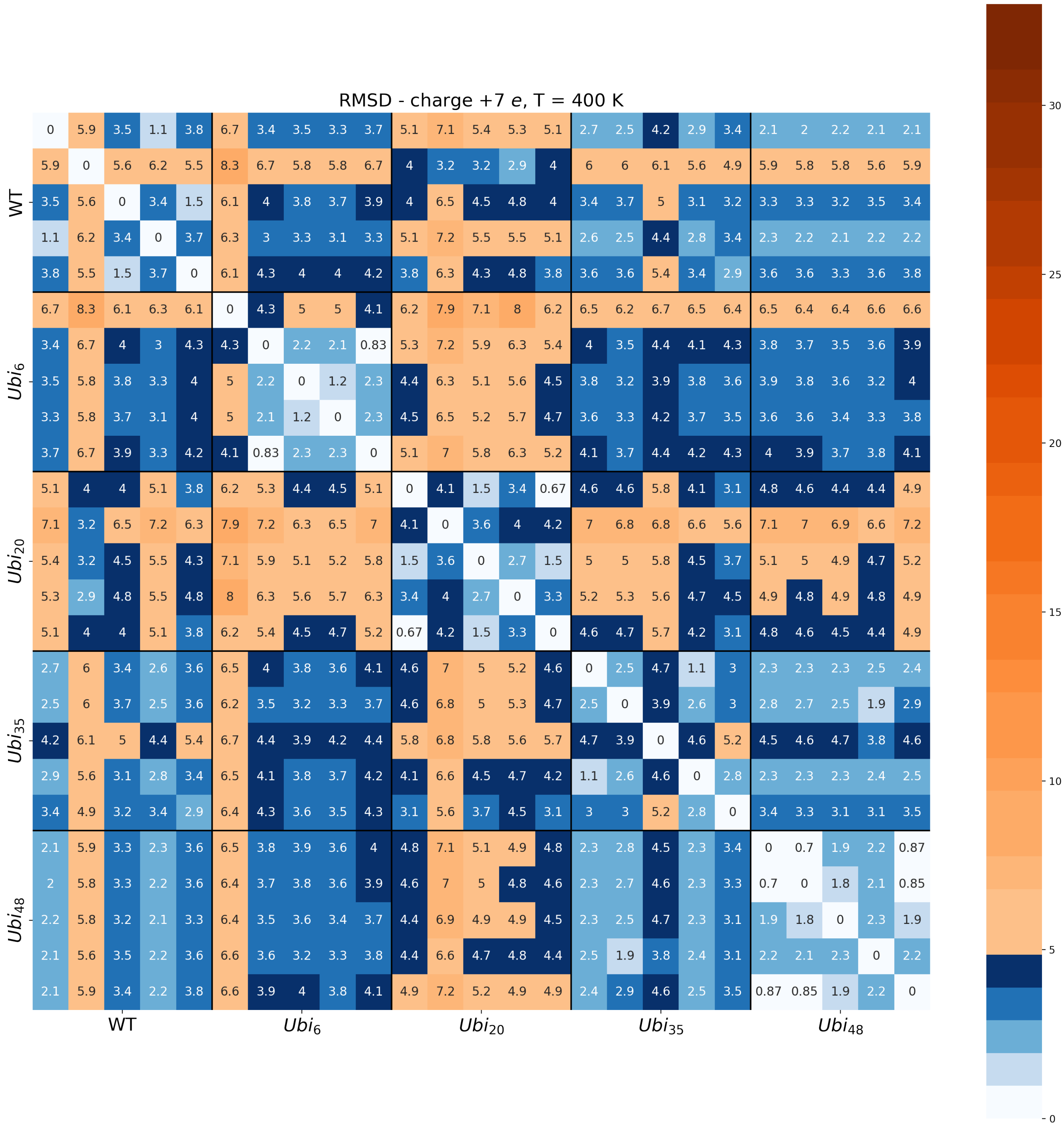

Fig. S8 RMSD matrix for simulations performed at 500 K for systems of net charge +7 *e*. The values are expressed in units of Å.

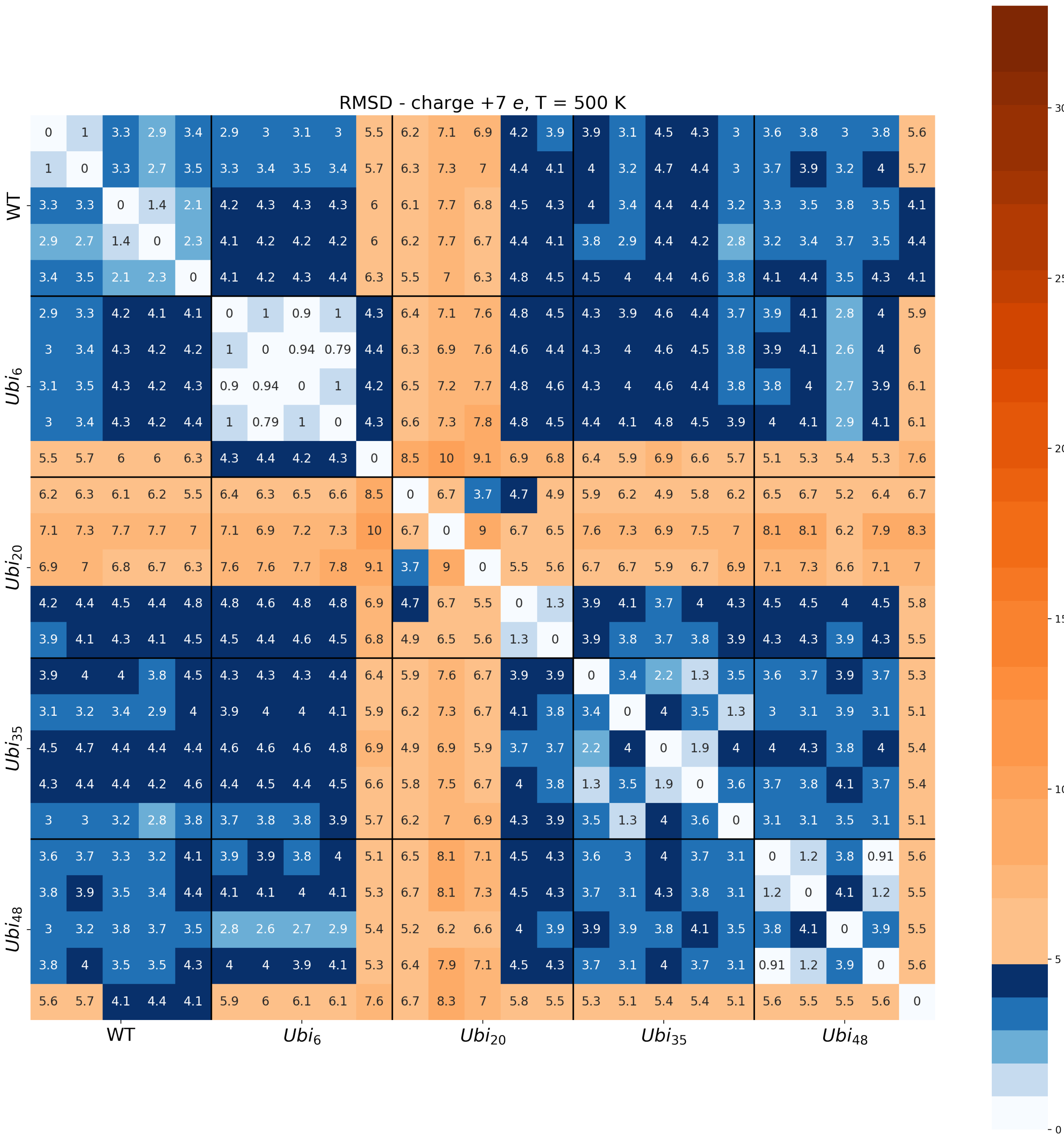

Fig. S9 RMSD matrix for simulations performed at 500 K for systems of net charge +7 e. The values are expressed in units of Å.

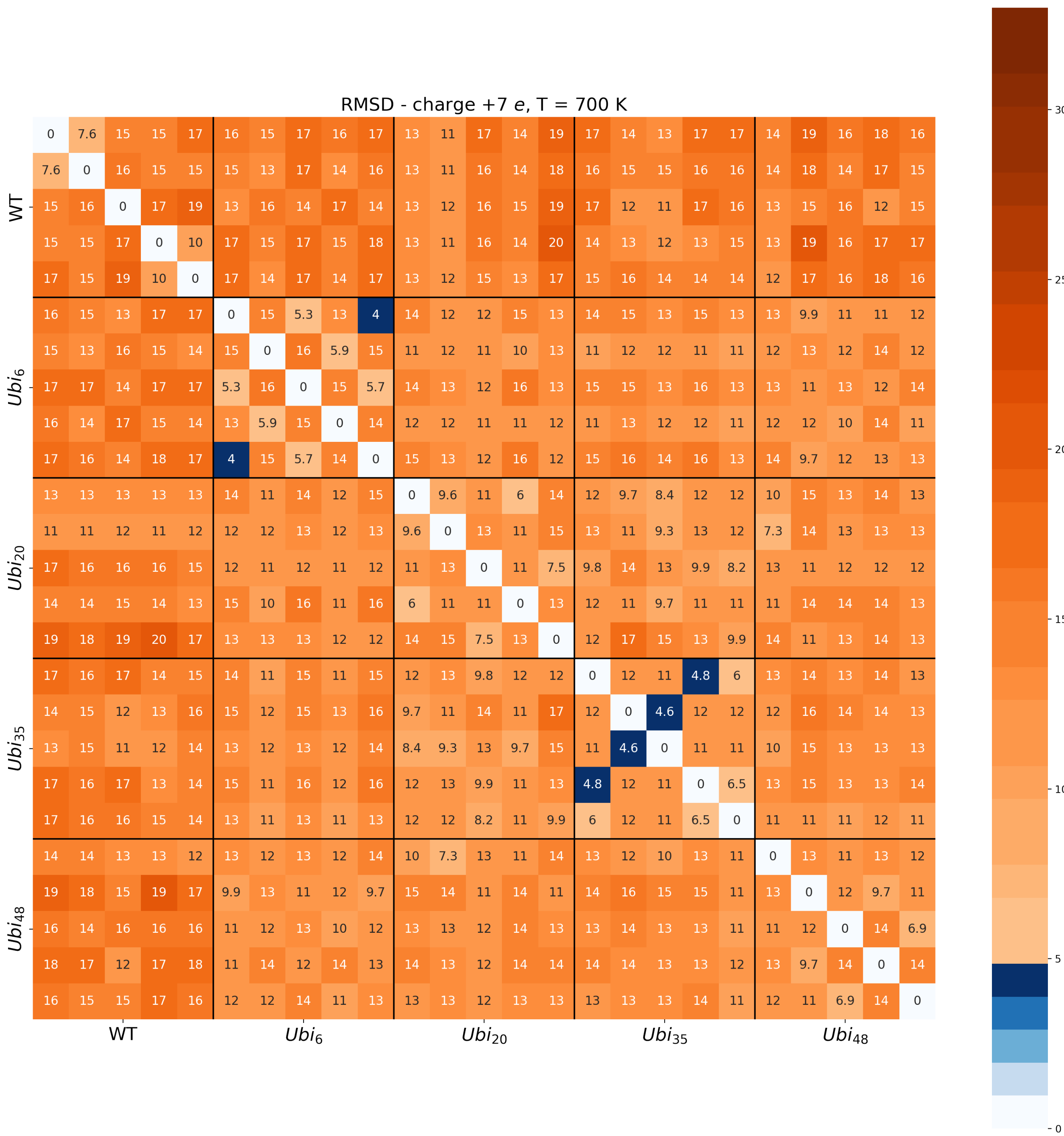

Fig. S10 RMSD matrix for simulations performed at 700 K for systems of net charge +7 e. The values are expressed in units of Å.

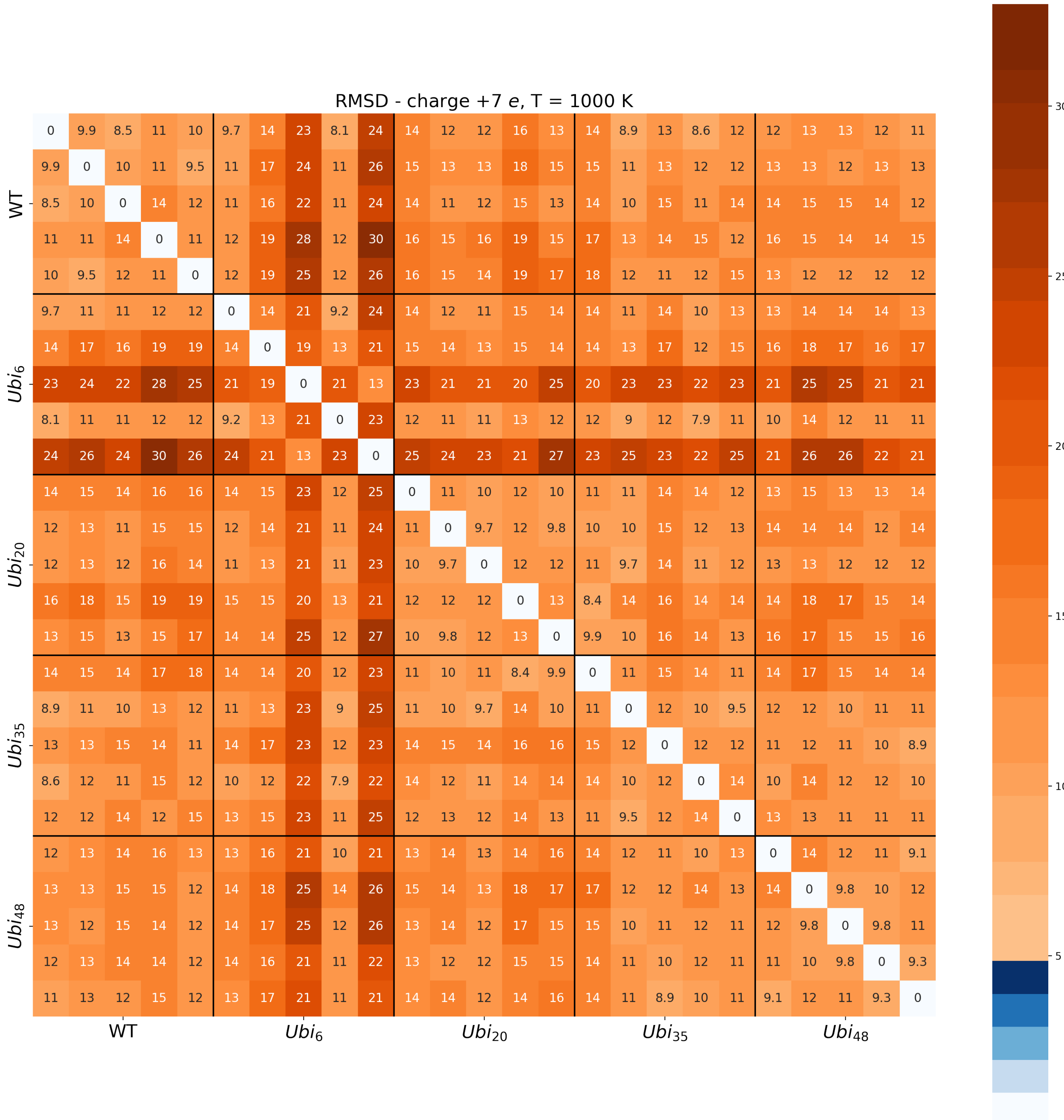

Fig. S11 RMSD matrix for simulations performed at 1000 K for systems of net charge +7 e. The values are expressed in units of Å.

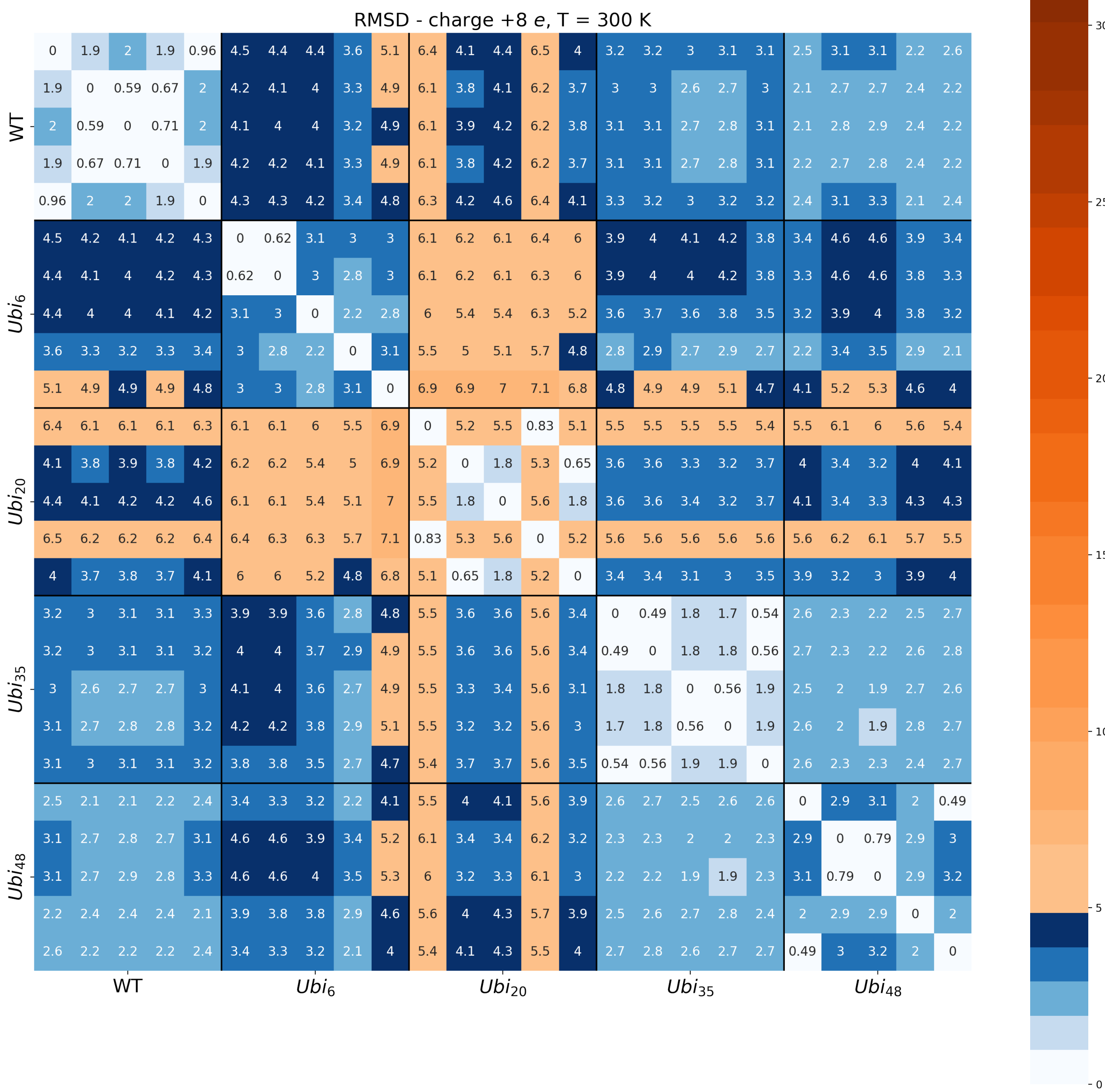

Fig. S12 RMSD matrix for simulations performed at 500 K for systems of net charge +8 e. The values are expressed in units of Å.

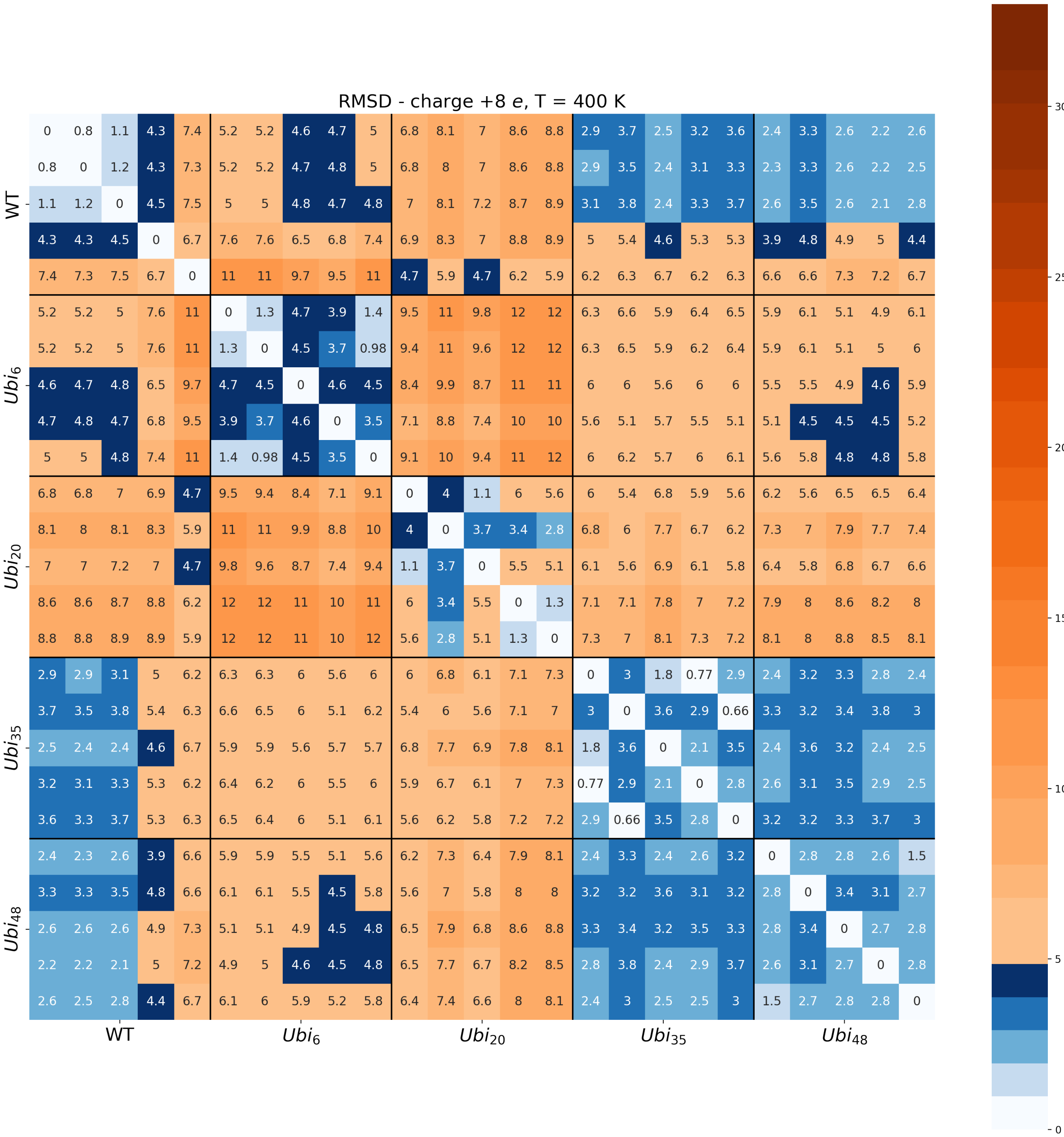

Fig. S13 RMSD matrix for simulations performed at 500 K for systems of net charge +8 e. The values are expressed in units of Å.

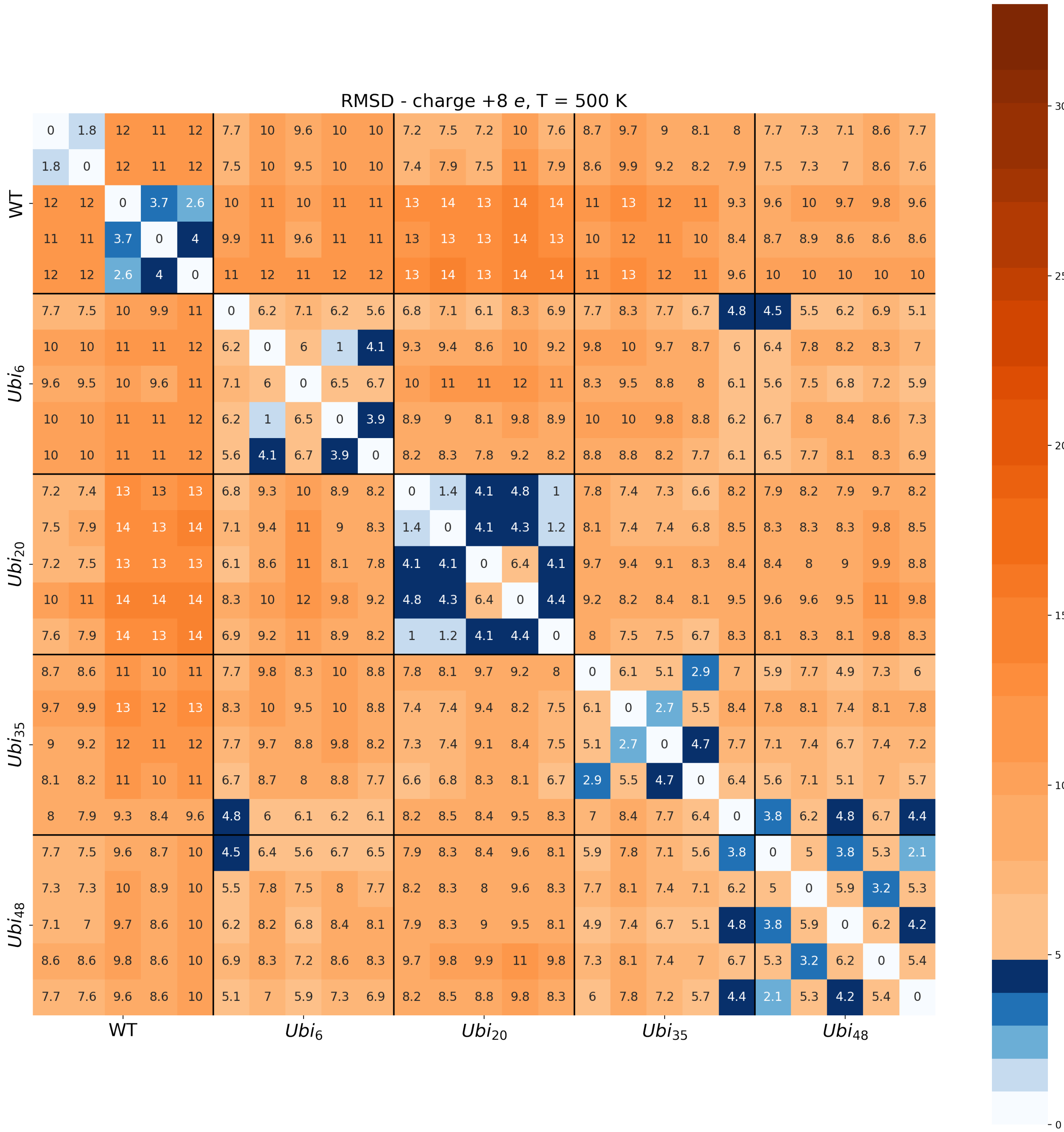

Fig. S14 RMSD matrix for simulations performed at 500 K for systems of net charge +8 *e*. The values are expressed in units of Å.

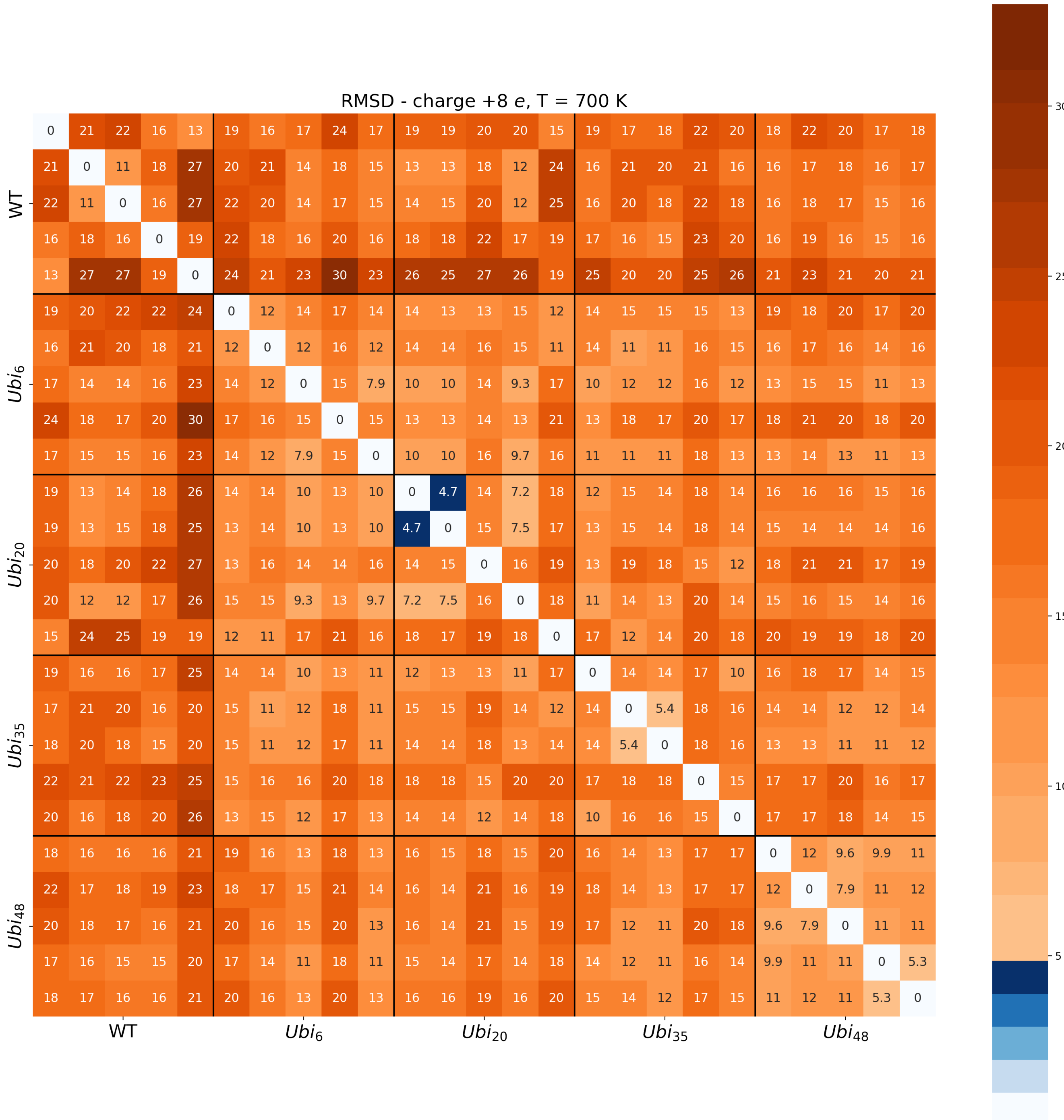

Fig. S15 RMSD matrix for simulations performed at 700 K for systems of net charge +8 *e*. The values are expressed in units of Å.

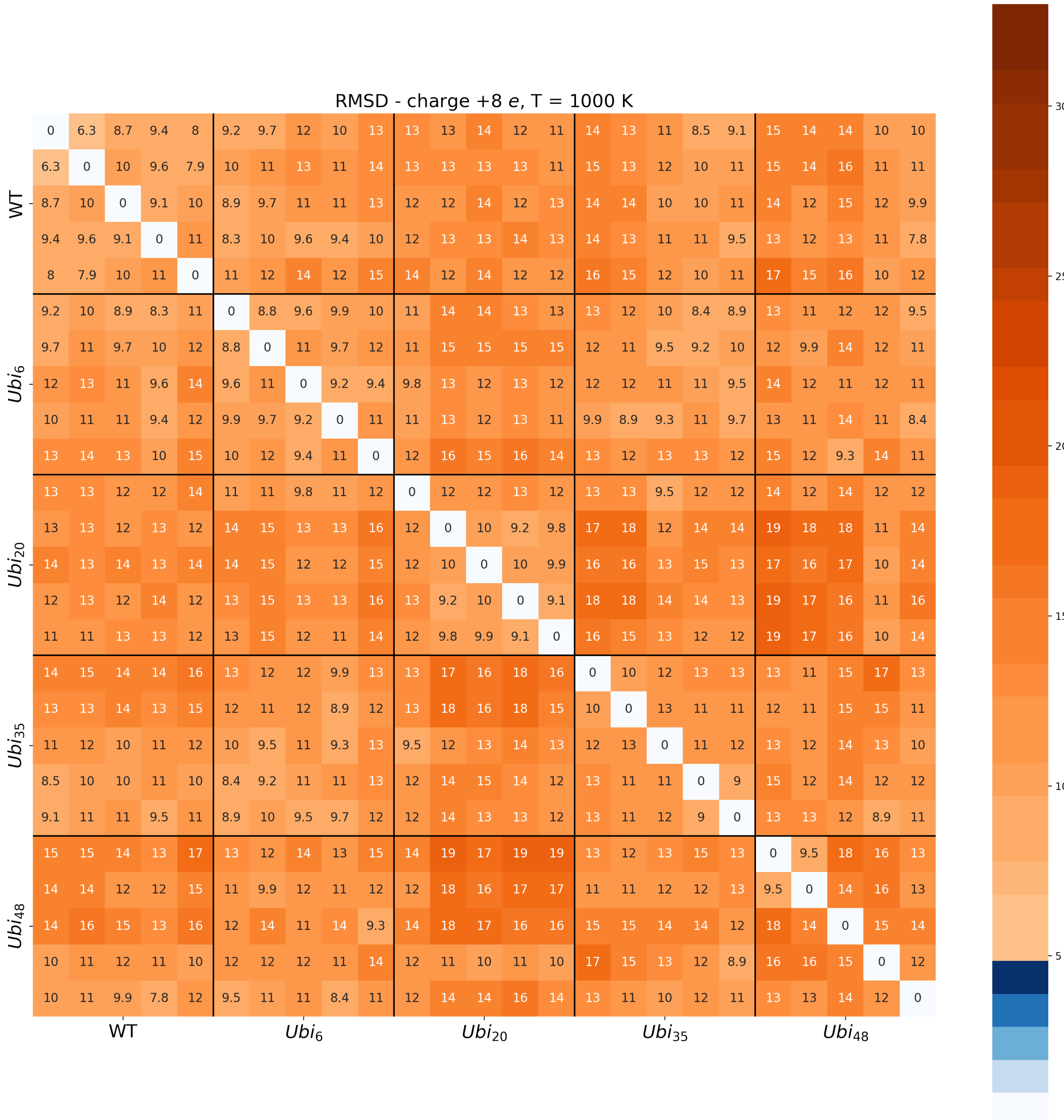

Fig. S16 RMSD matrix for simulations performed at 1000 K for systems of net charge +8 e. The values are expressed in units of Å.

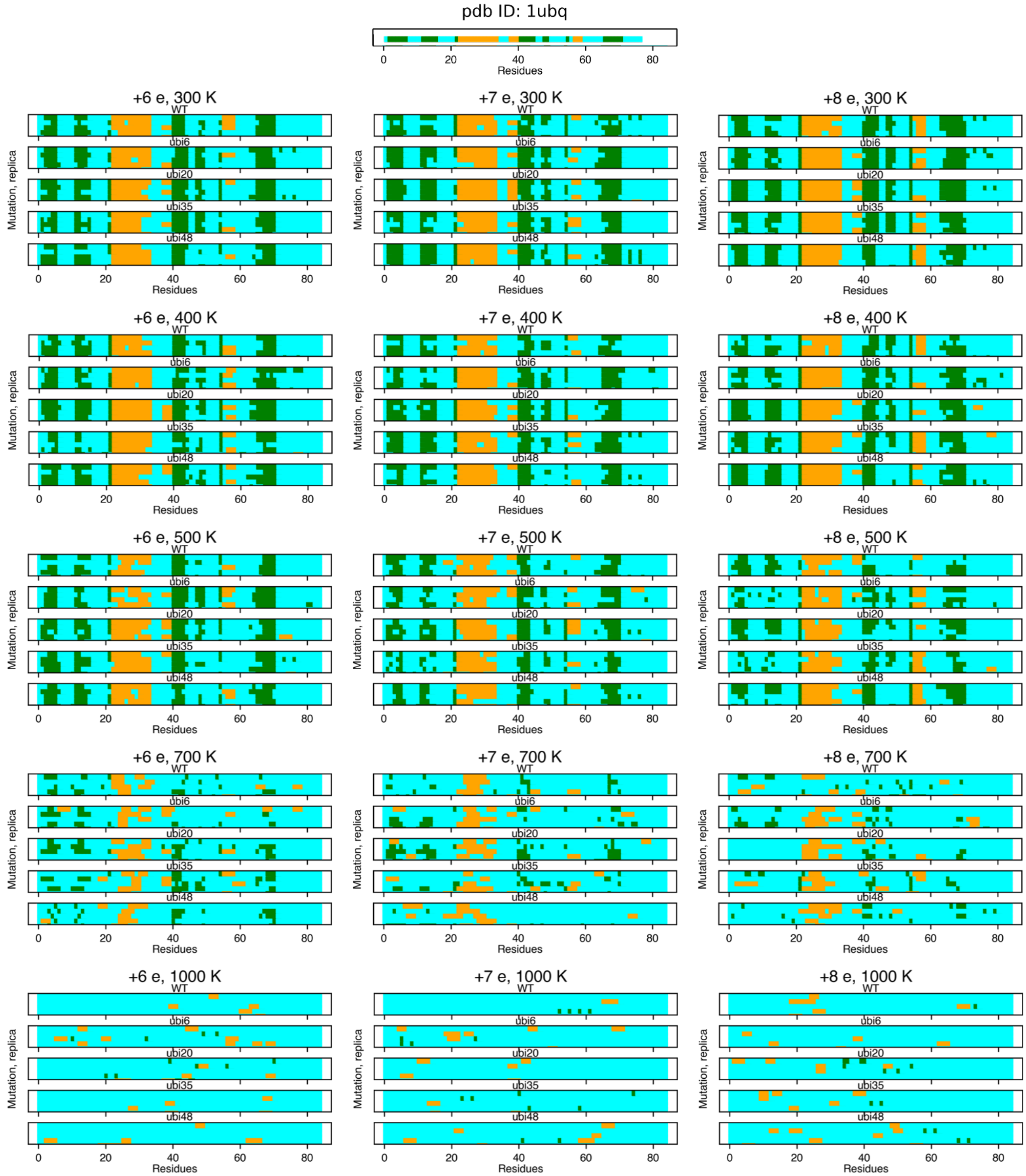

Fig. S17 Secondary structure analysis of ubiquitin is shown for the crystal structure (top subplot) and simulations performed at 300 K, 400 K, 500 K, 700 K, and 1000 K (bottom subplots). Each line represents a replica for a specific mutant and net charge of the systems,where coil, extended, and helix structures are depicted in cyan, green, and orange, respectively.

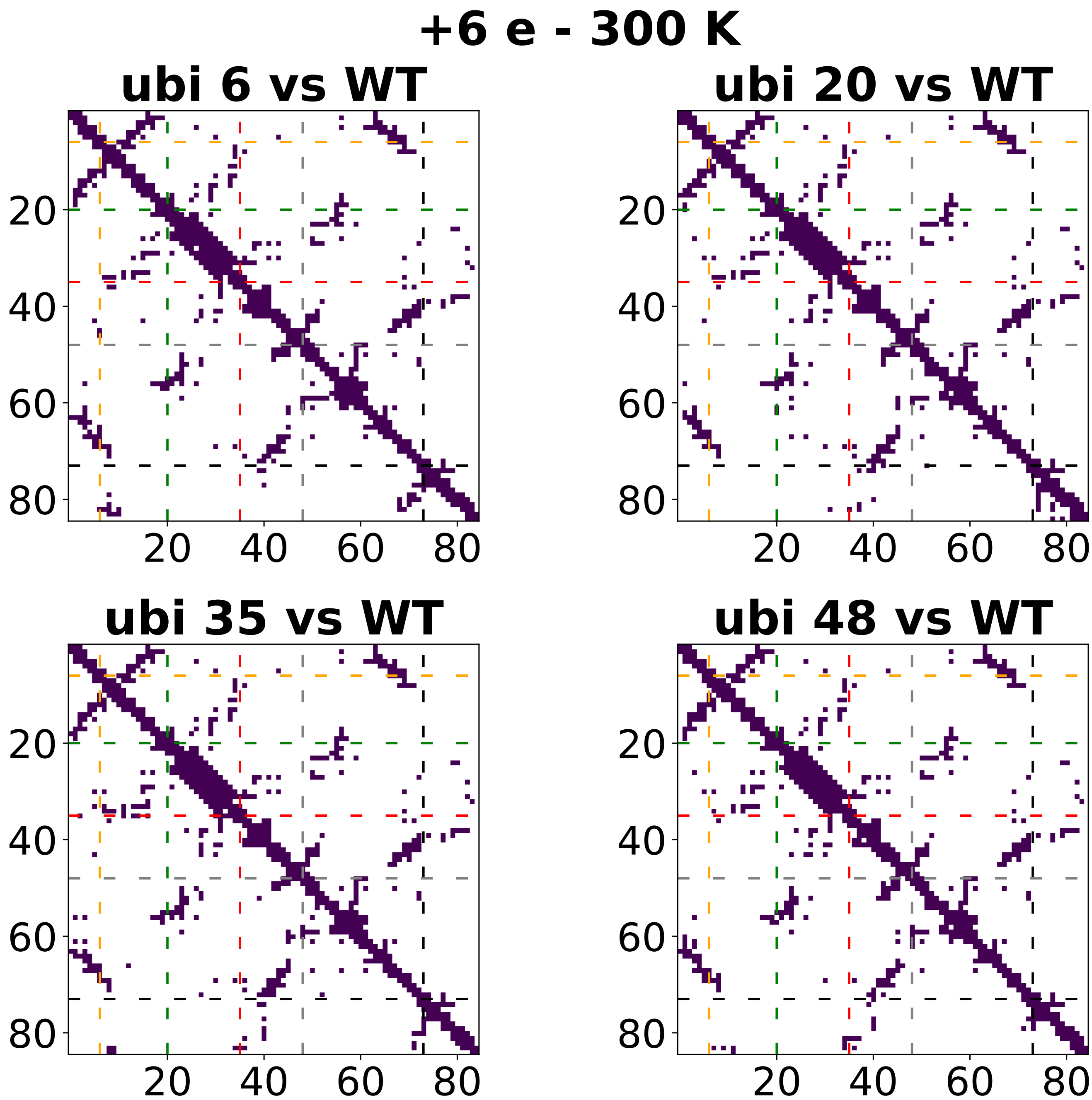

Fig. S18 Contacts matrix for simulations performed at 300 K for systems of net charge +6 *e*.

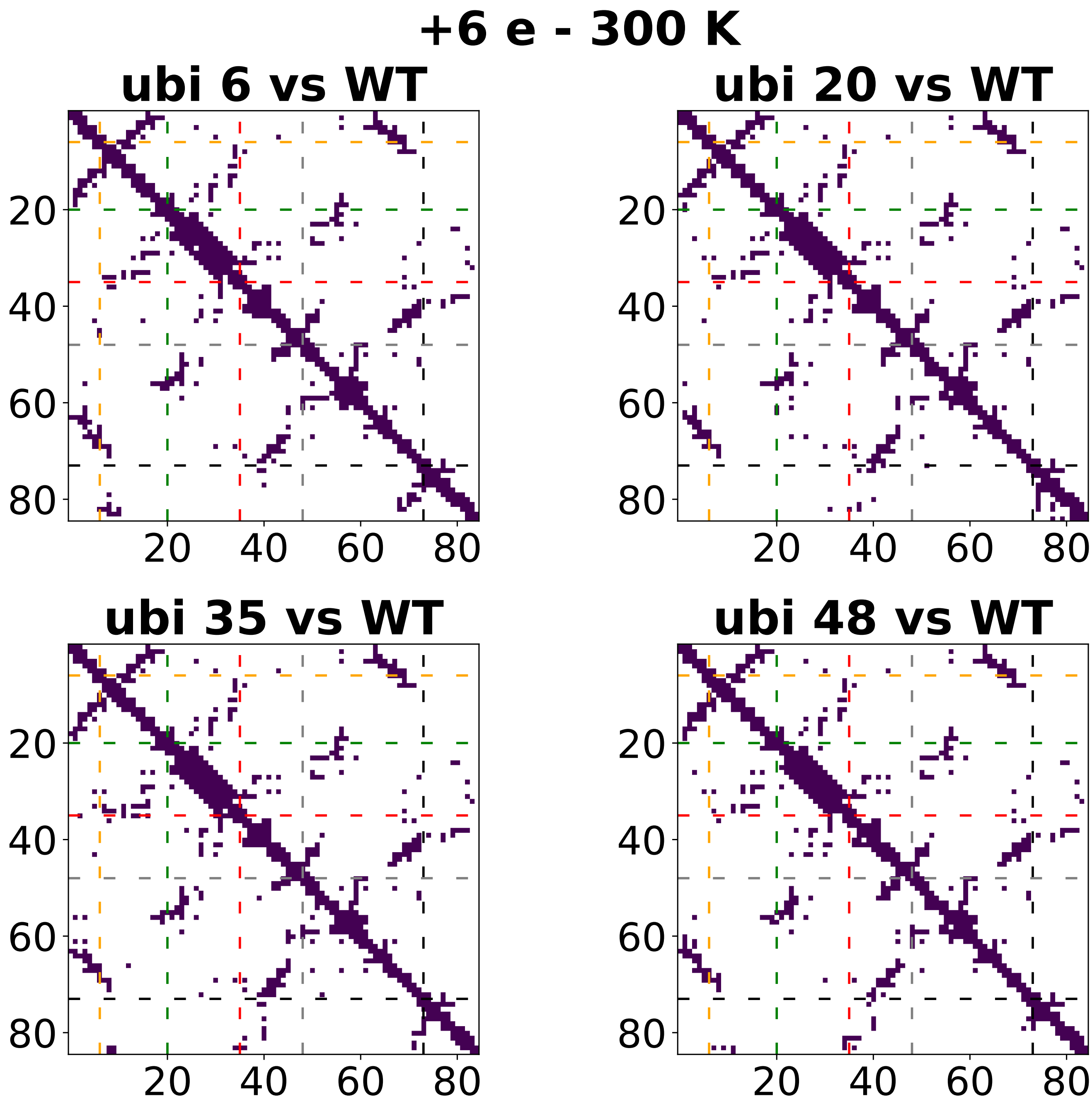

Fig. S19 Contacts matrix for simulations performed at 300 K for systems of net charge +6 *e*.

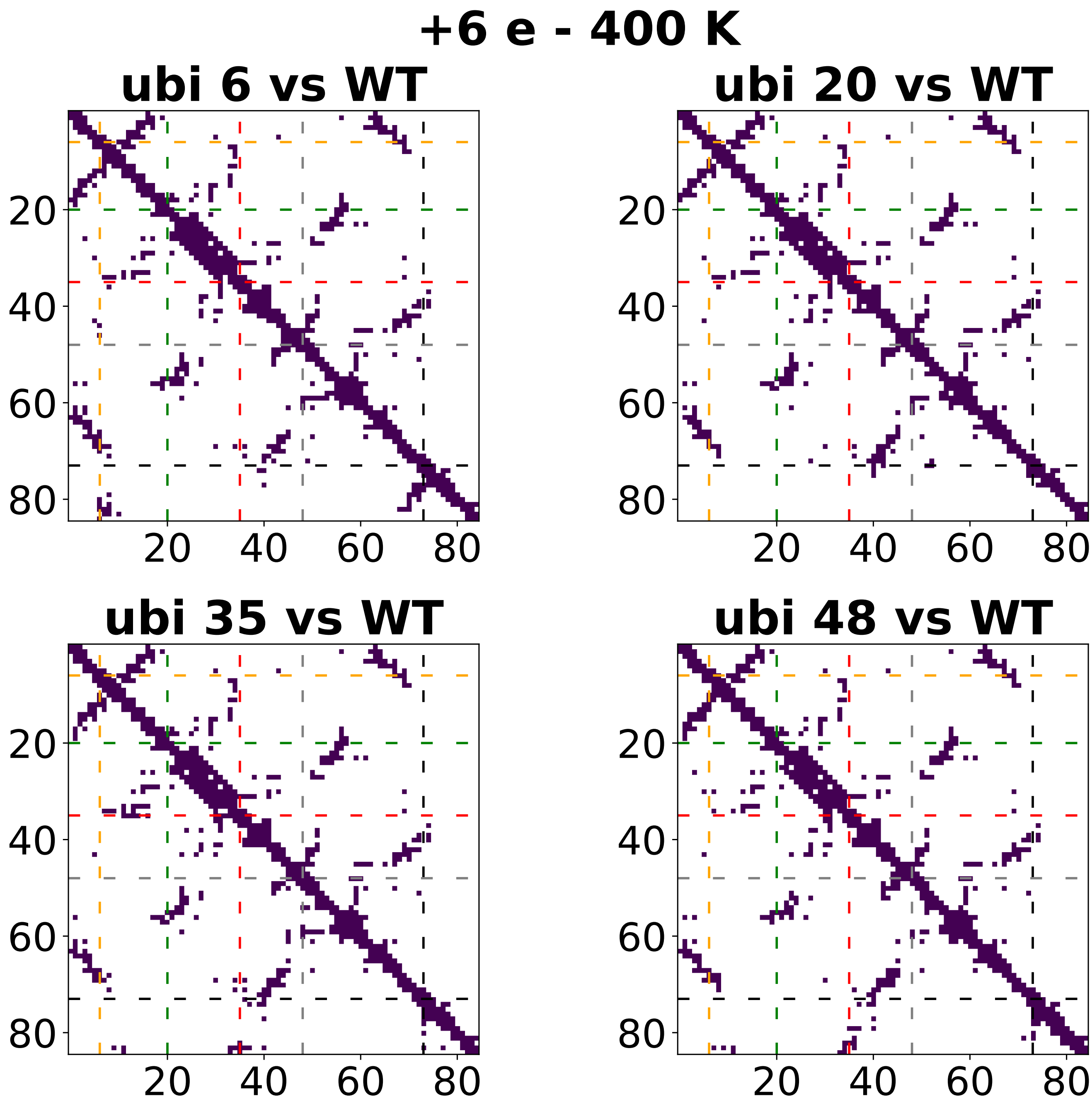

Fig. S20 Contacts matrix for simulations performed at 400 K for systems of net charge +6 *e*.

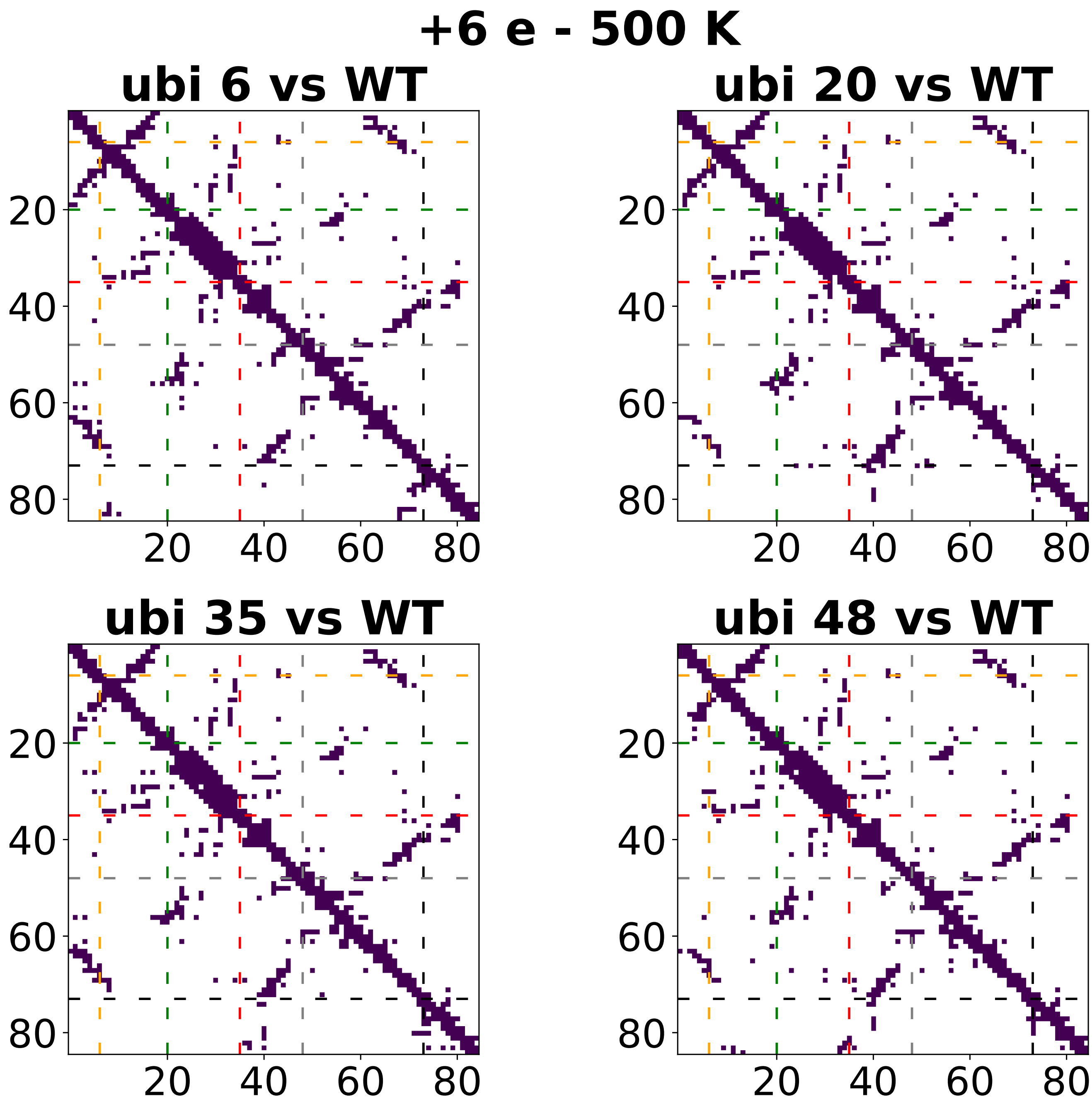

Fig. S21 Contacts matrix for simulations performed at 500 K for systems of net charge +6 *e*.

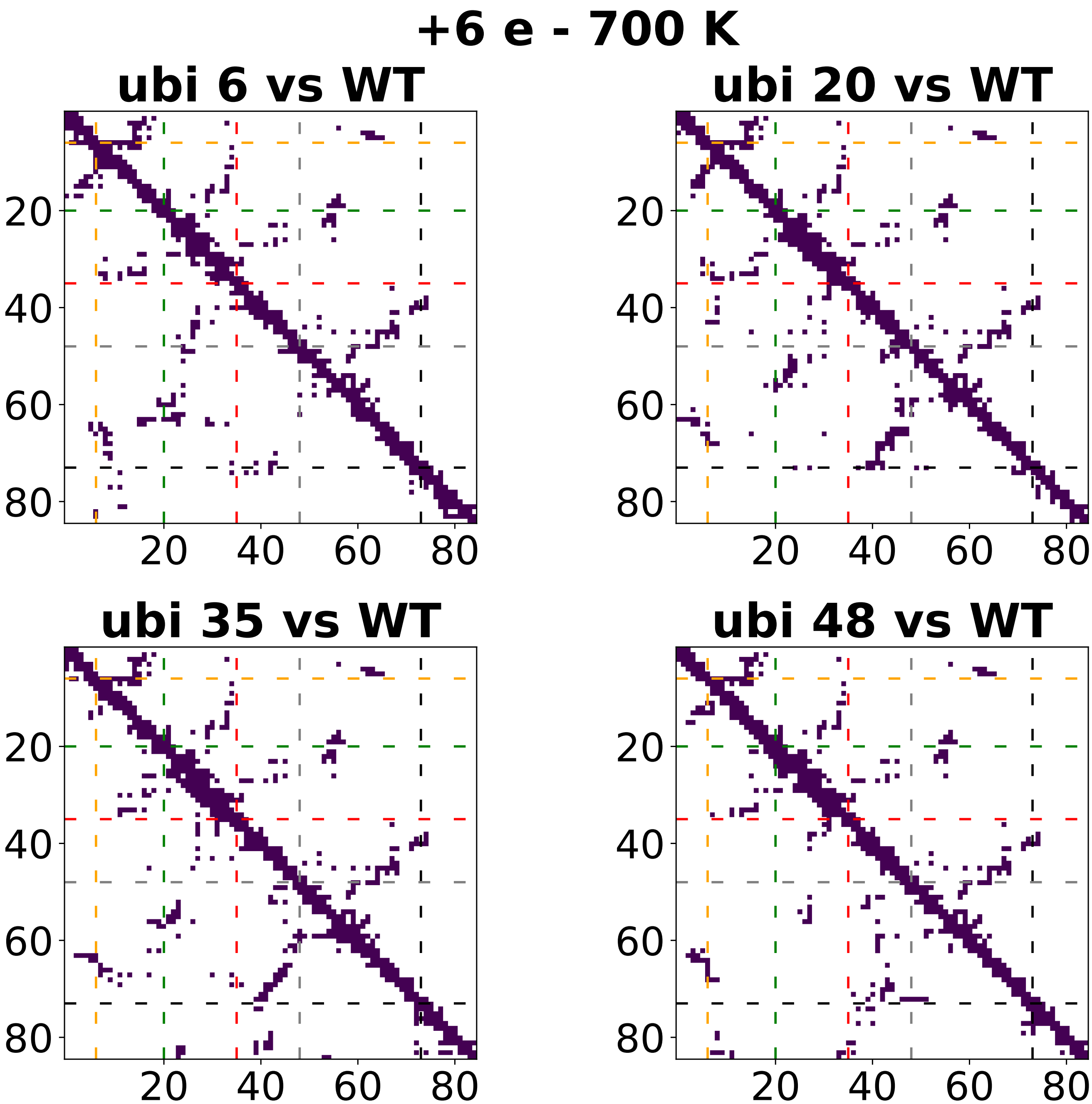

Fig. S22 Contacts matrix for simulations performed at 700 K for systems of net charge +6 *e*.

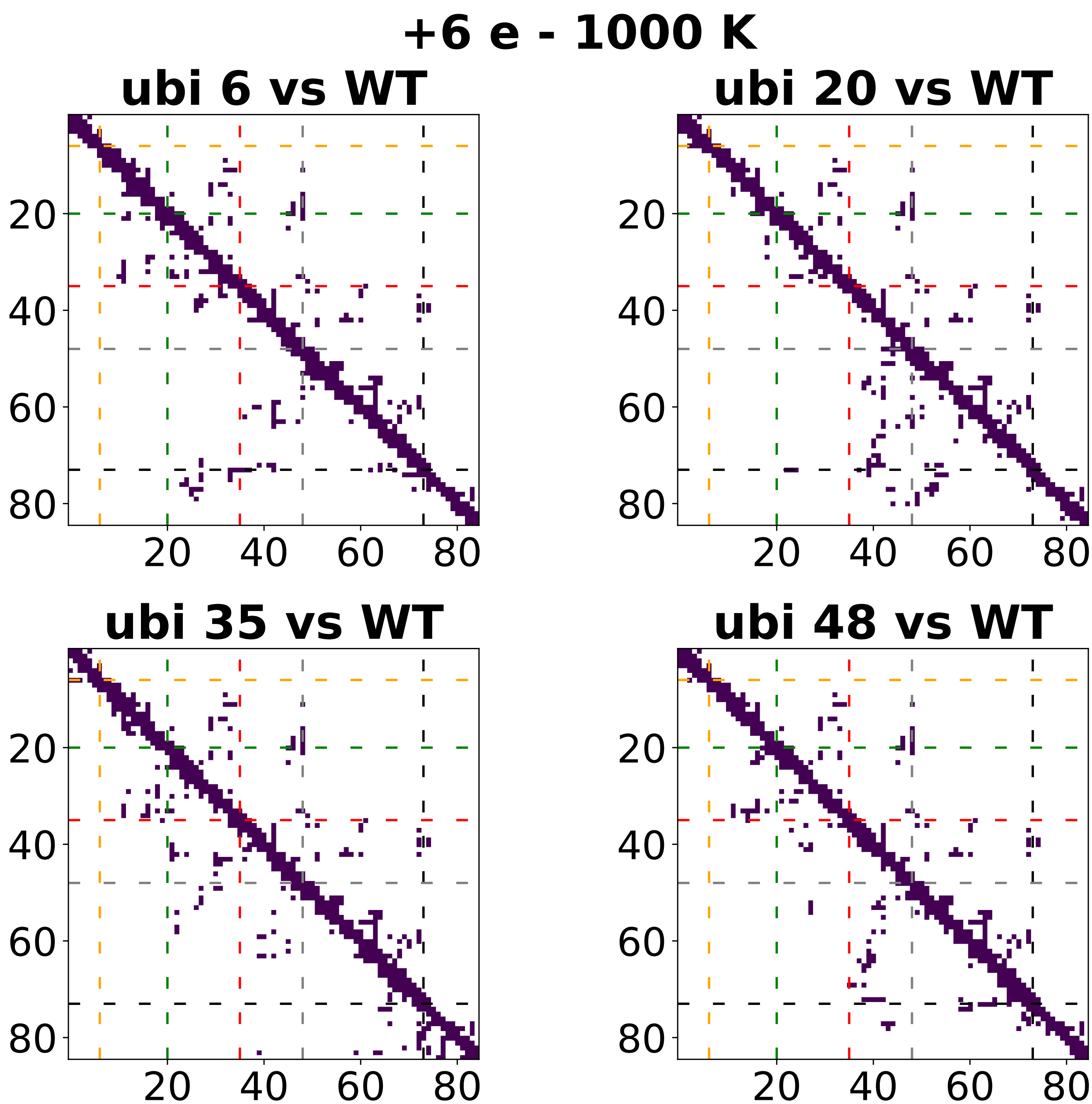

Fig. S23 Contacts matrix for simulations performed at 1000 K for systems of net charge +6 *e*.

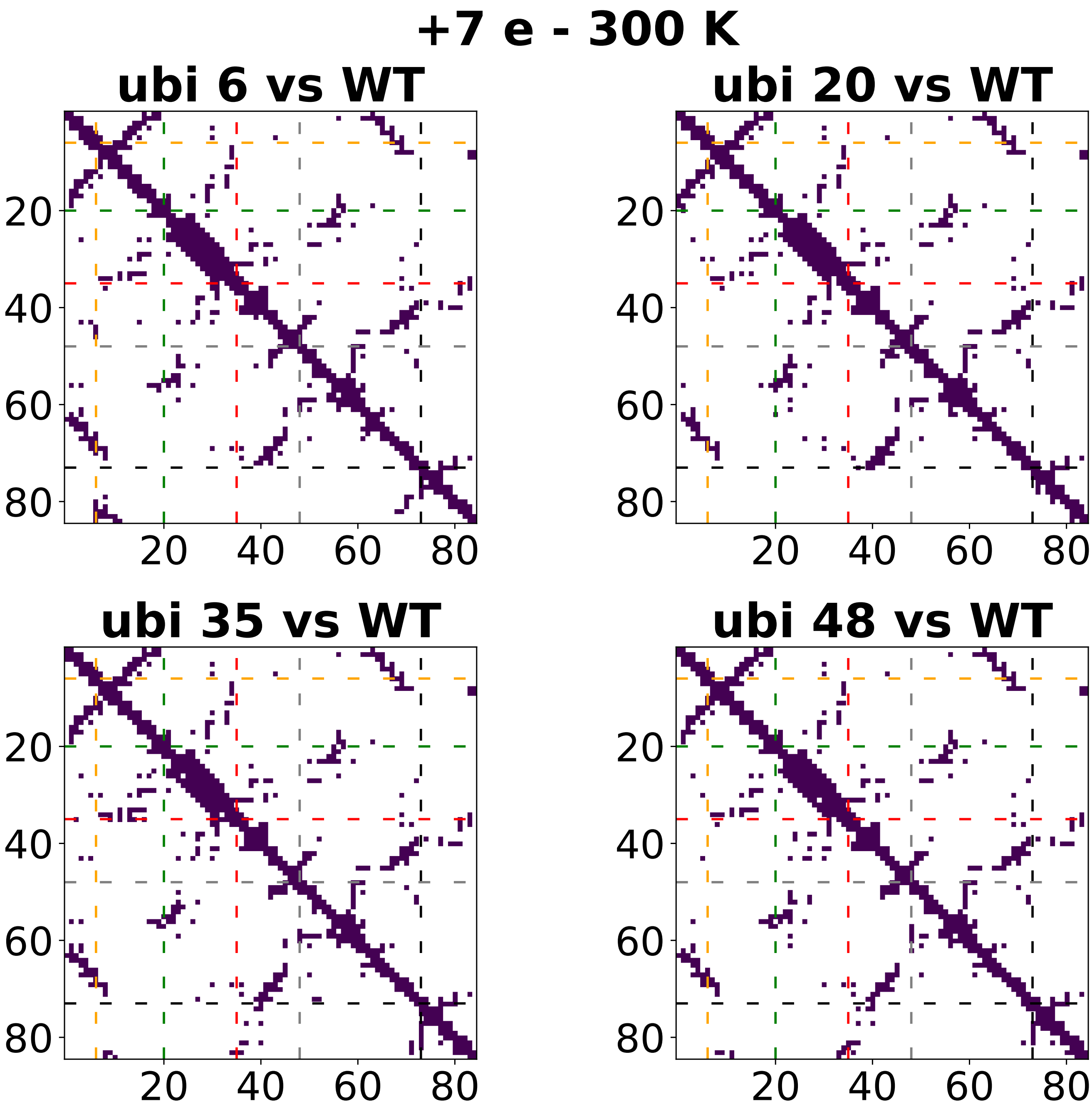

Fig. S24 Contacts matrix for simulations performed at 500 K for systems of net charge +7 *e*.

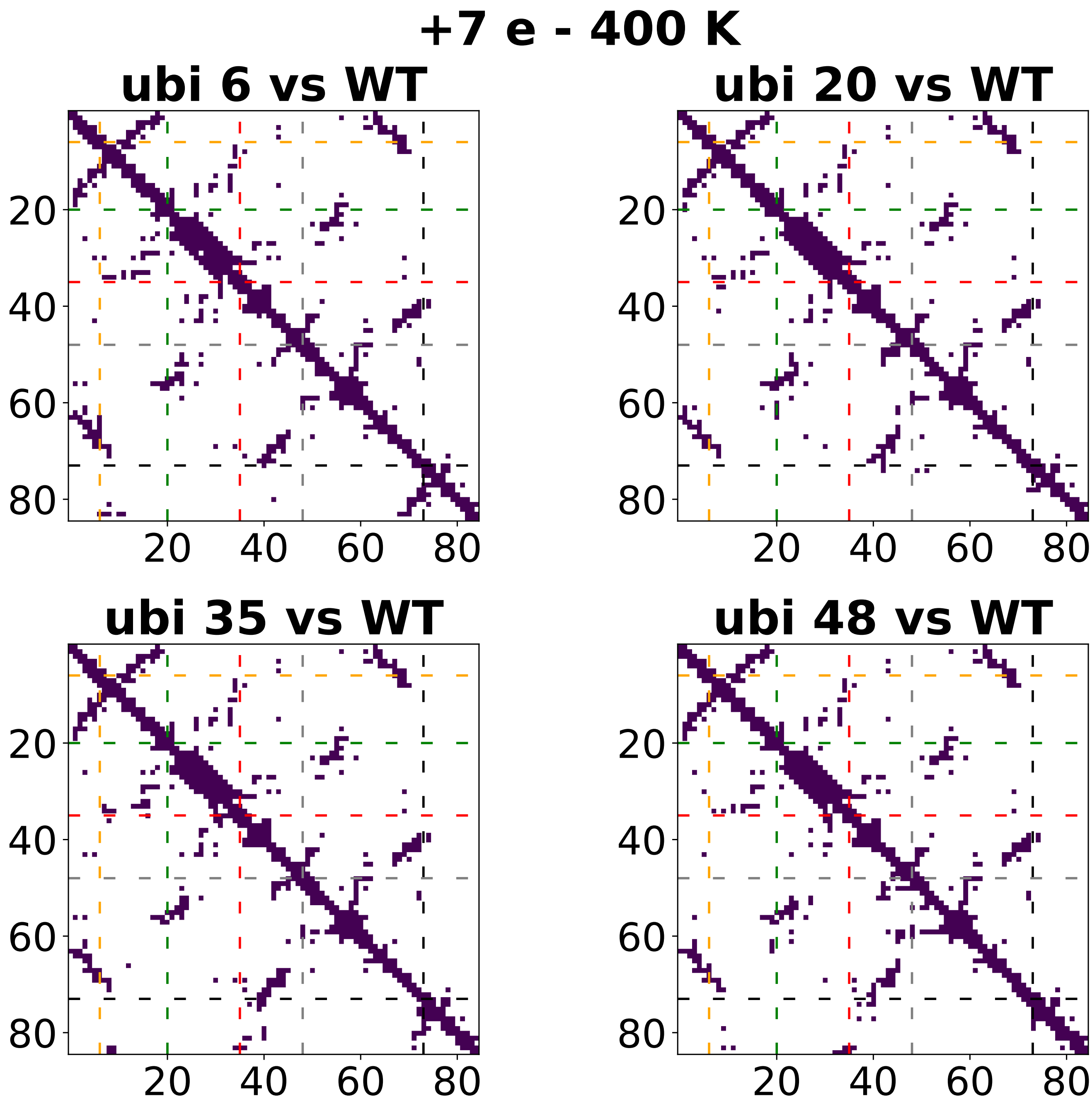

Fig. S25 Contacts matrix for simulations performed at 500 K for systems of net charge +7 *e*.

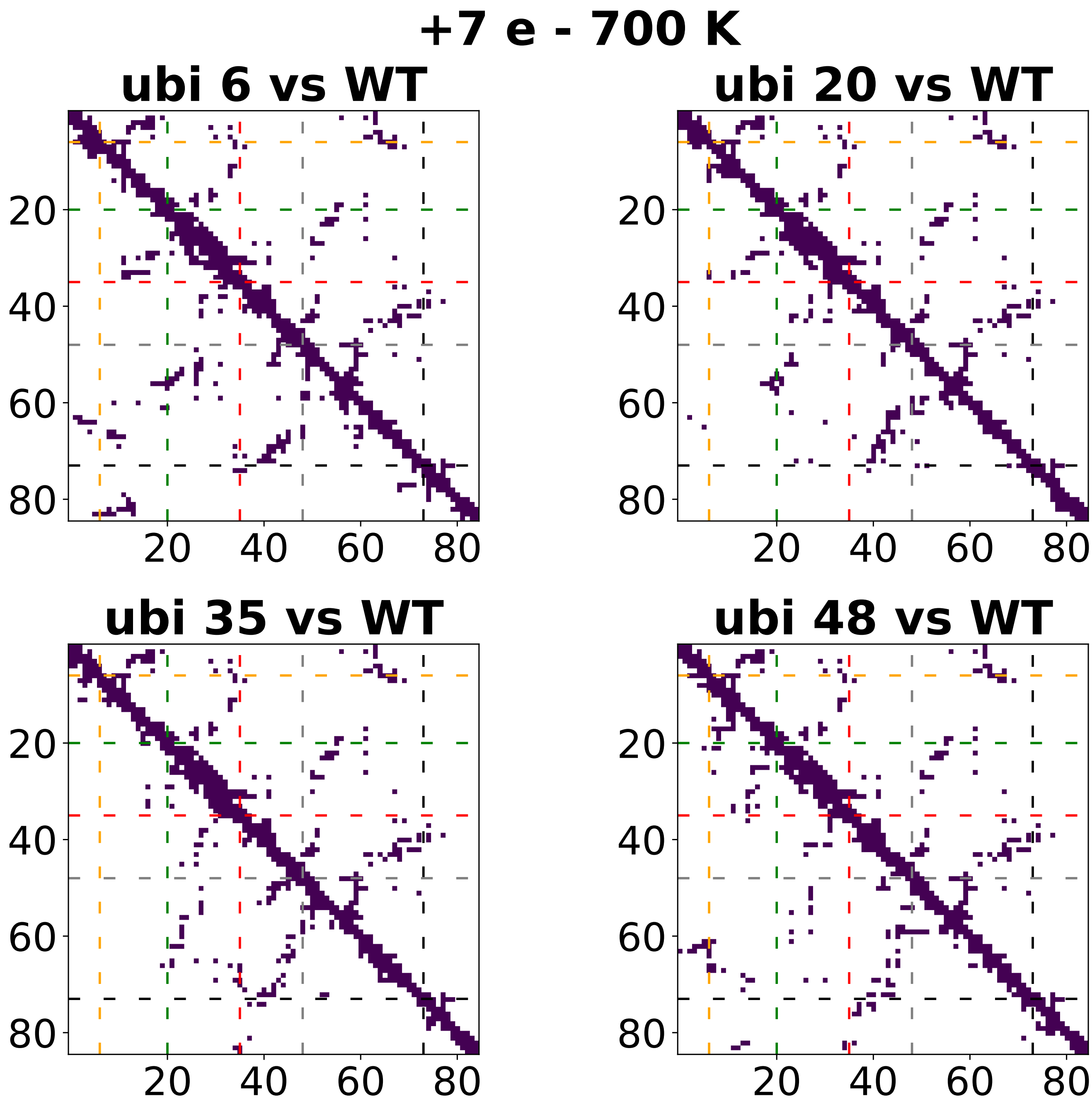

Fig. S26 Contacts matrix for simulations performed at 700 K for systems of net charge +7 *e*.

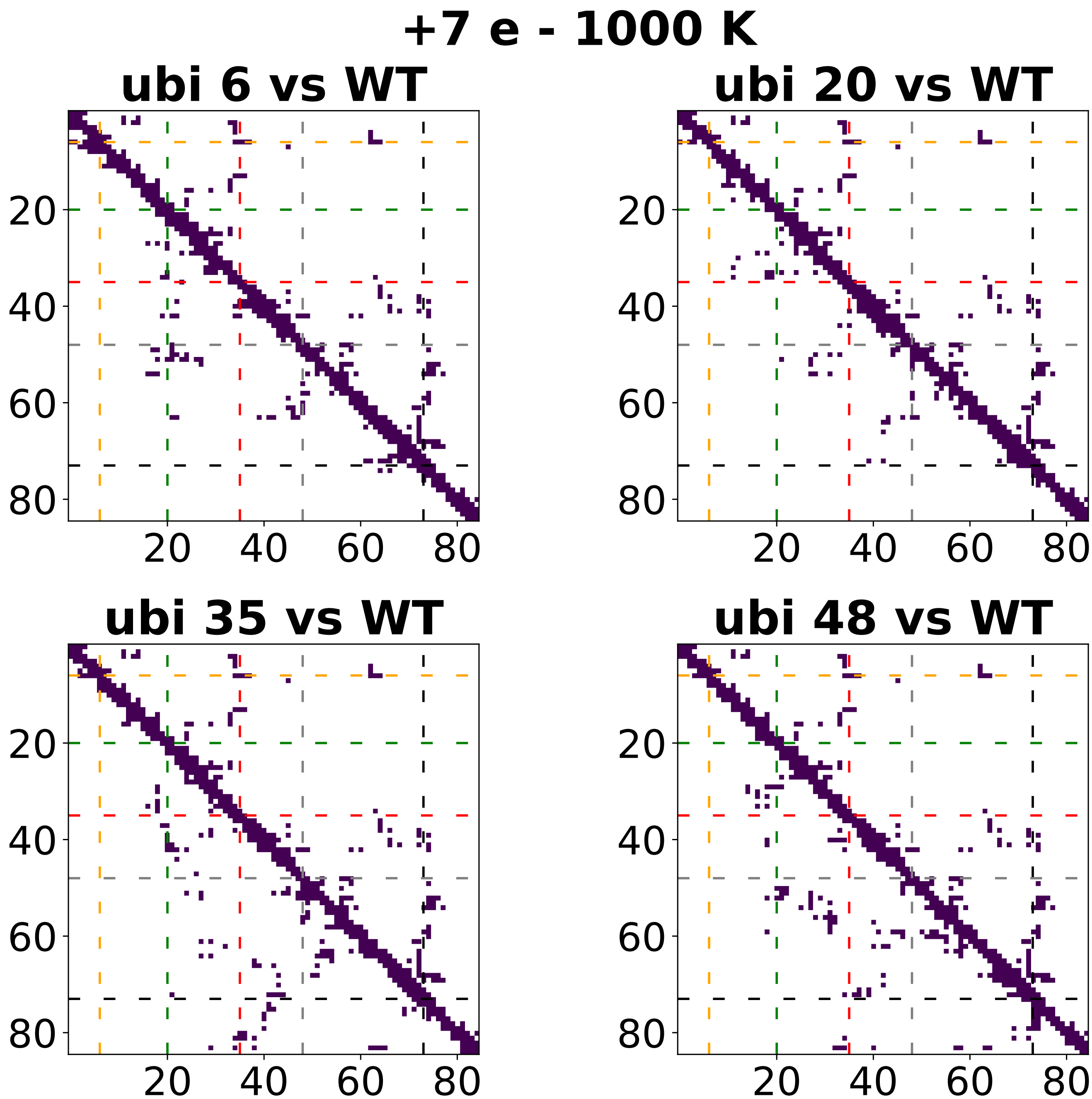

Fig. S27 Contacts matrix for simulations performed at 1000 K for systems of net charge +7 *e*.

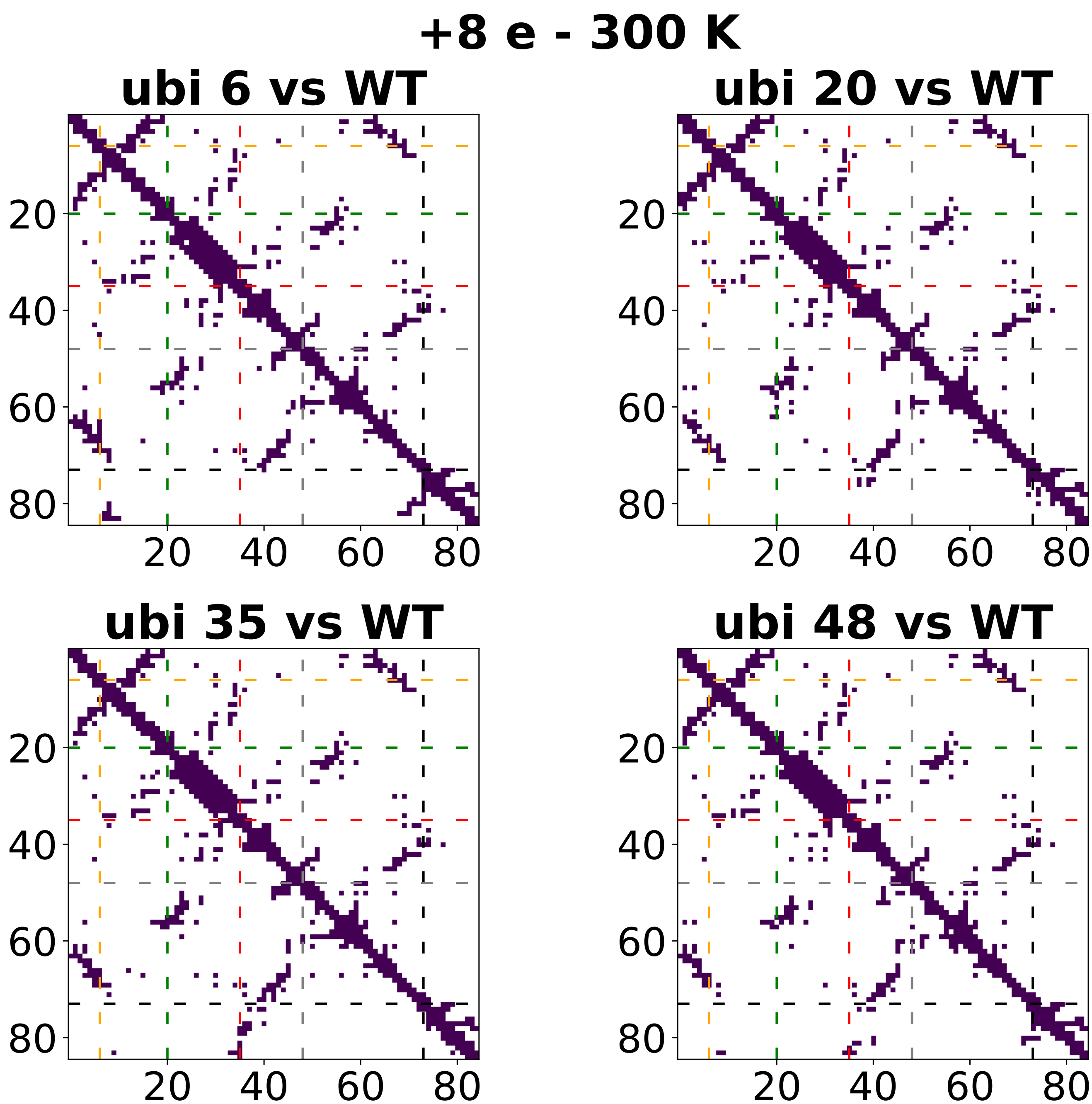

Fig. S28 Contacts matrix for simulations performed at 500 K for systems of net charge +8 *e*.

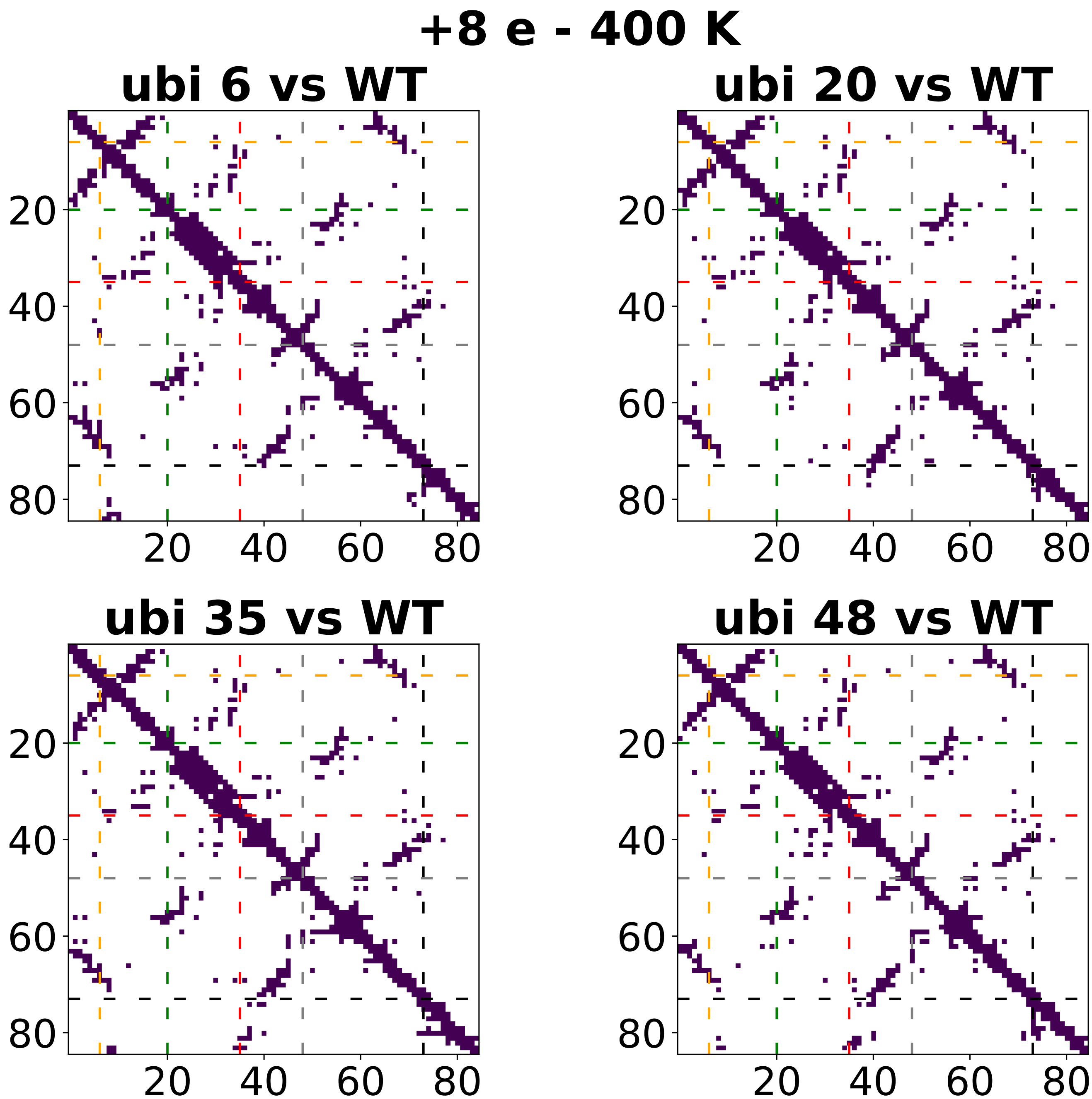

Fig. S29 Contacts matrix for simulations performed at 500 K for systems of net charge +8 *e*.

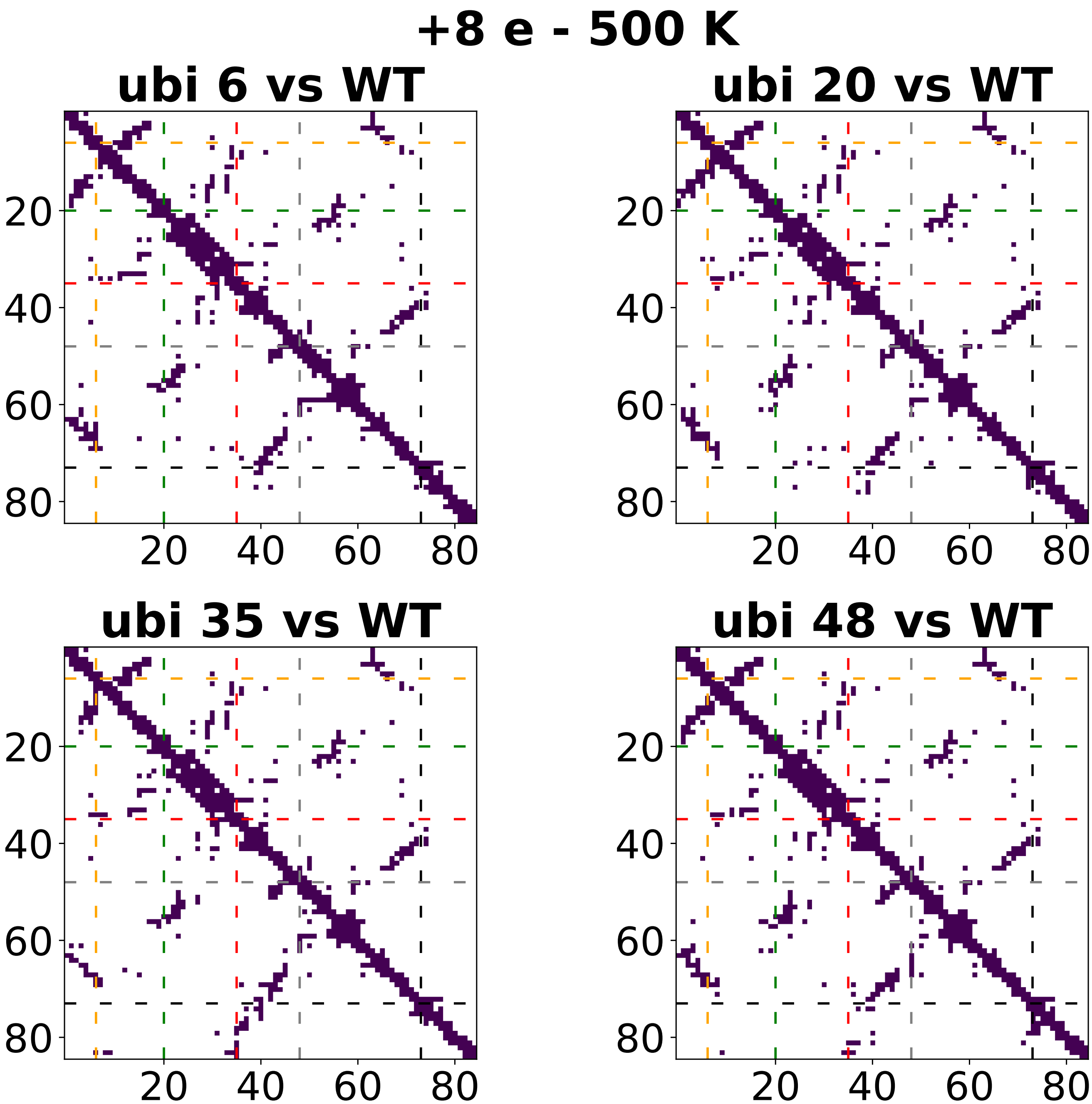

Fig. S30 Contacts matrix for simulations performed at 500 K for systems of net charge +8 *e*.

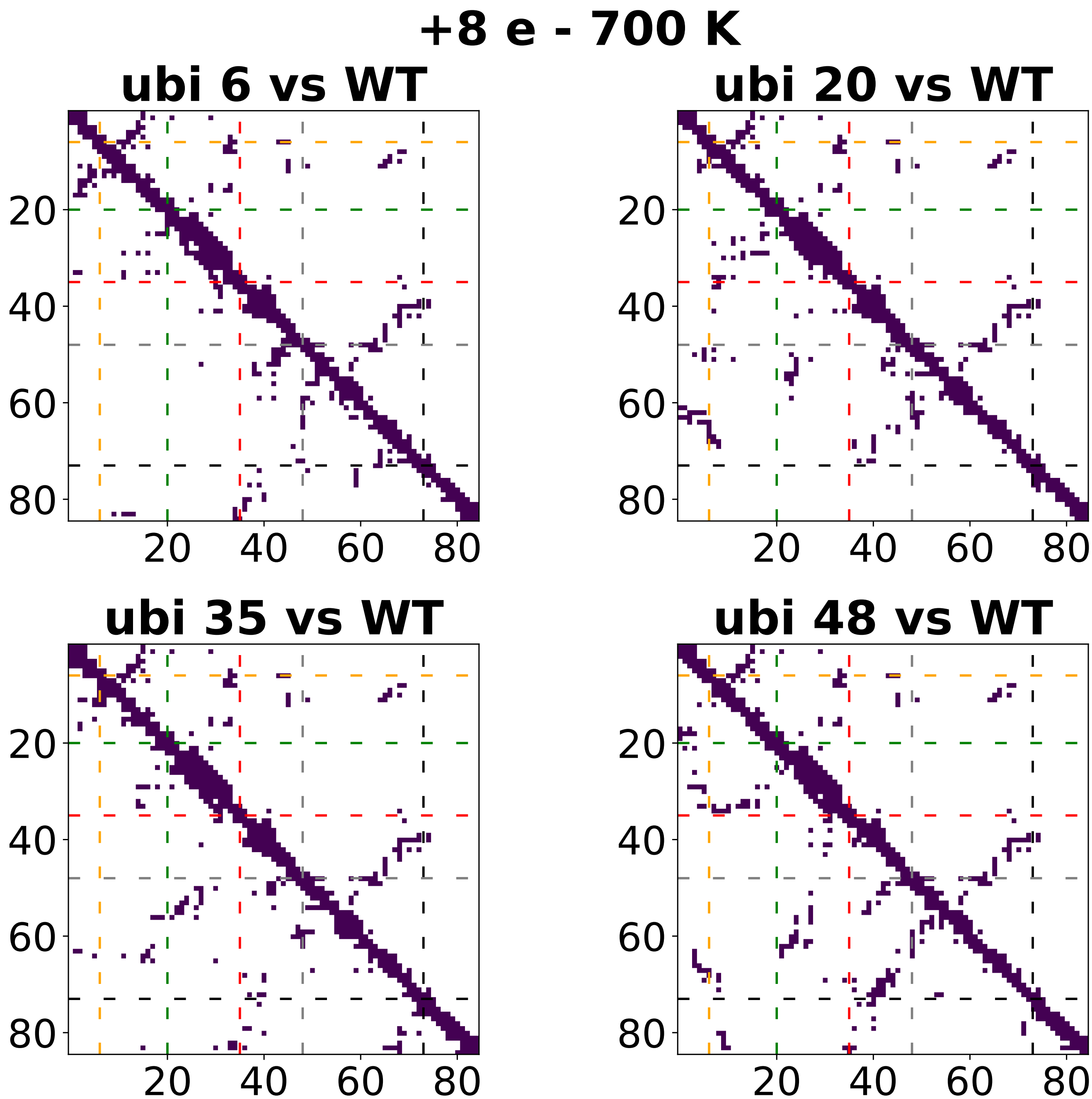

Fig. S31 Contacts matrix for simulations performed at 700 K for systems of net charge +8 *e*.

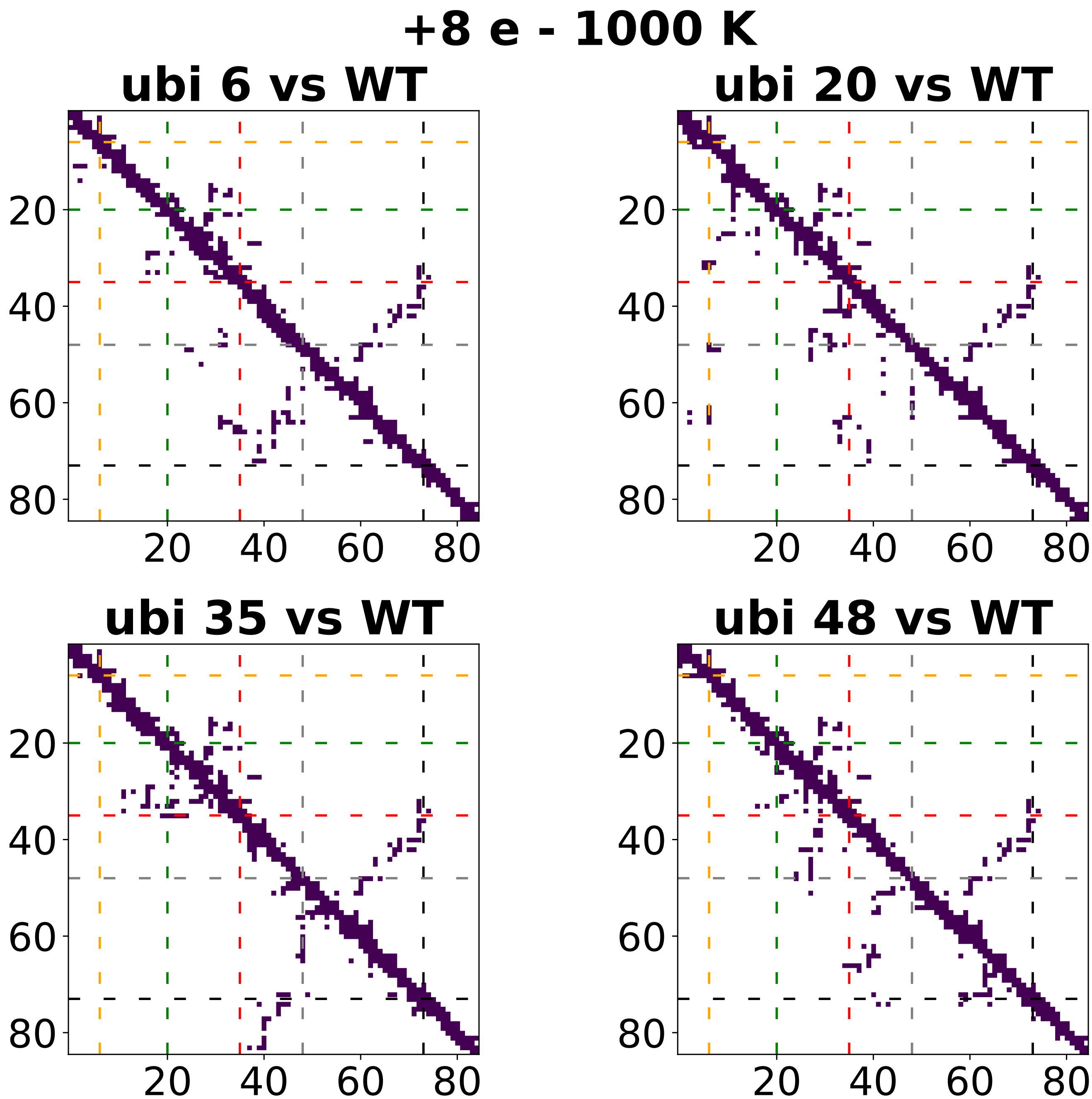

Fig. S32 Contacts matrix for simulations performed at 1000 K for systems of net charge +8 *e*.

2 ATTO520 parametrization

Atom types, bonded and non-bonded parameters are from the amber99sb-ildn standard force field implemented in GROMACS

[atoms]

N4 N2 -0.3623645569620253 1
C39 CA -0.3445645569620253 2
O1 OS -0.3535645569620253 3
C1 CA 0.30733544303797466 4
N1 N2 -0.7218645569620253 5
C2 CA -0.15756455696202532 6
N2 N -0.5496645569620253 7
C3 CA -0.008764556962025313 8
N3 N -0.5061645569620253 9
O3 O -0.6238645569620254 10
C4 CA -0.2760645569620253 11
O4 O -0.5562645569620253 12
C5 CA 0.4507354430379747 13
O5 O -0.6352645569620253 14
C6 CA 0.18693544303797469 15
C7 CA -0.2878645569620253 16
C8 CA 0.38543544303797467 17
C9 CA -0.3658645569620253 18
C10 CA 0.0030354430379746864 19
C11 CA -0.2410645569620253 20
C12 CA 0.4536354430379747 21
C13 CT -0.06206455696202531 22
C14 CT -0.0651645569620253 23
C15 CT 0.2035354430379747 24
C16 CT -0.11786455696202532 25
C17 CT 0.026035443037974688 26
C18 CT -0.11786455696202532 27
C21 CT -0.0738645569620253 28
C22 CT -0.1521645569620253 29
C26 C 0.6623354430379746 30
C30 CT 0.07523544303797469 31
C31 CT 0.07223544303797469 32
C32 C 0.7217354430379747 33
C33 CT -0.13816455696202531 34
C34 CT -0.08636455696202532 35
C35 C 0.7117354430379746 36
CA CT 0.025535443037974687 37
C38 CT -0.11886455696202532 38
S SH -0.3076645569620253 39
H0 HA 0.1772354430379747 40

[bonds]

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N4 C17
C39 C1
C39 C5
O1 C5
O1 C8
C1 N1
C1 C2
N1 C15
C2 C3
C2 C13
N2 C26
N2 C30
C3 C4
N3 C31
N3 C32
N3 C35
O3 C26
C4 C5
C4 C6
O4 C35
O5 C32
C6 C7
C6 C21
C7 C8
C7 C10
C8 C9
C9 C12
C10 C11
C11 C12
C11 C14
C15 C16
C17 C18
C21 C22
C22 C26
C30 C31
C32 C33
C33 C34
C34 C35
C34 S
CA C38
C38 S
N4 H4
C39 H0
N1 H5
N2 H05
C3 H1
C9 H2
C10 H3
C13 H6
C13 H7
C13 H8
C14 H9
C14 H10
C14 H11
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CA HA
CA C38
CA C
-C N
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C CA C38
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O5 C32 N3 C35 MKV_RRR_051
O5 C32 C33 C34 MKV_RRR_052
C6 C7 C8 C9 MKV_RRR_053
C6 C7 C10 C11 MKV_RRR_054
C6 C21 C22 C26 MKV_RRR_055
C7 C6 C21 C22 MKV_RRR_056
C7 C8 C9 C12 MKV_RRR_057
C7 C10 C11 C12 MKV_RRR_058

C7 C10 C11 C14 MKV_RRR_059
C8 C7 C6 C21 MKV_RRR_060
C8 C7 C10 C11 MKV_RRR_061
C8 C9 C12 C11 MKV_RRR_062
C9 C8 C7 C10 MKV_RRR_063
C17 N4 C12 C9 MKV_RRR_064
C9 C12 C11 C10 MKV_RRR_065
C9 C12 C11 C14 MKV_RRR_066
C10 C7 C6 C21 MKV_RRR_067
C17 N4 C12 C11 MKV_RRR_068
C12 N4 C17 C18 MKV_RRR_069
C22 C26 N2 C30 MKV_RRR_070
C22 C26 N2 C30 MKV_RRR_071
C26 N2 C30 C31 MKV_RRR_072
C26 N2 C30 C31 MKV_RRR_073
C26 N2 C30 C31 MKV_RRR_074
C26 N2 C30 C31 MKV_RRR_075
C30 C31 N3 C32 MKV_RRR_076
C30 C31 N3 C32 MKV_RRR_077
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C30 C31 N3 C35 MKV_RRR_081
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C30 C31 N3 C35 MKV_RRR_083
C31 N3 C32 C33 MKV_RRR_084
C31 N3 C32 C33 MKV_RRR_085
C31 N3 C35 C34 MKV_RRR_086
C31 N3 C35 C34 MKV_RRR_087
C32 N3 C35 C34 MKV_RRR_088
C32 C33 C34 C35 MKV_RRR_089
C32 C33 C34 S MKV_RRR_090
C33 C32 N3 C35 MKV_RRR_091
C33 C34 S C38 MKV_RRR_092
C34 S C38 CA MKV_RRR_093
C35 C34 S C38 MKV_RRR_094
C39 C2 C1 N1 MKV_RRR_095
C1 C3 C2 C13 MKV_RRR_096
C32 C35 N3 C31 MKV_RRR_097
C3 C5 C4 C6 MKV_RRR_098
C39 C4 C5 O1 MKV_RRR_099
C4 C7 C6 C21 MKV_RRR_100
C6 C8 C7 C10 MKV_RRR_101
C7 C9 C8 O1 MKV_RRR_102
C10 C12 C11 C14 MKV_RRR_103
N4 C12 C11 C9 MKV_RRR_104
C22 N2 C26 O3 MKV_RRR_105
C33 N3 C32 O5 MKV_RRR_106
C34 N3 C35 O4 MKV_RRR_107
N4 C12 C9 H2 MKV_RRR_108
N4 C17 C18 H19 MKV_RRR_109
N4 C17 C18 H20 MKV_RRR_110
N4 C17 C18 H21 MKV_RRR_111
C39 C1 N1 H5 MKV_RRR_112
O1 C5 C39 H0 MKV_RRR_113
O1 C8 C9 H2 MKV_RRR_114
C1 N1 C15 H12 MKV_RRR_115
C1 N1 C15 H13 MKV_RRR_116
C1 C2 C3 H1 MKV_RRR_117
C1 C2 C13 H6 MKV_RRR_118
C1 C2 C13 H7 MKV_RRR_119
C1 C2 C13 H8 MKV_RRR_120
N1 C1 C39 H0 MKV_RRR_121
N1 C15 C16 H14 MKV_RRR_122
N1 C15 C16 H15 MKV_RRR_123
N1 C15 C16 H16 MKV_RRR_124
C2 C1 C39 H0 MKV_RRR_125
C2 C1 N1 H5 MKV_RRR_126
N2 C26 C22 H01 MKV_RRR_127
N2 C26 C22 H02 MKV_RRR_128
N2 C30 C31 H35 MKV_RRR_129
N2 C30 C31 H36 MKV_RRR_130
C3 C2 C13 H6 MKV_RRR_131
C3 C2 C13 H7 MKV_RRR_132
C3 C2 C13 H8 MKV_RRR_133
N3 C31 C30 H33 MKV_RRR_134
N3 C31 C30 H34 MKV_RRR_135
N3 C32 C33 H06 MKV_RRR_136
N3 C32 C33 H07 MKV_RRR_137
N3 C35 C34 H08 MKV_RRR_138
O3 C26 N2 H05 MKV_RRR_139
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O3 C26 C22 H01 MKV_RRR_141
O3 C26 C22 H01 MKV_RRR_142
O3 C26 C22 H01 MKV_RRR_143
O3 C26 C22 H02 MKV_RRR_144
O3 C26 C22 H02 MKV_RRR_145
O3 C26 C22 H02 MKV_RRR_146
C4 C5 C39 H0 MKV_RRR_147
C4 C6 C21 H03 MKV_RRR_148
C4 C6 C21 H04 MKV_RRR_149
O4 C35 C34 H08 MKV_RRR_150
O4 C35 C34 H08 MKV_RRR_151
O4 C35 C34 H08 MKV_RRR_152
C5 C4 C3 H1 MKV_RRR_153
O5 C32 C33 H06 MKV_RRR_154
O5 C32 C33 H06 MKV_RRR_155
O5 C32 C33 H06 MKV_RRR_156
O5 C32 C33 H07 MKV_RRR_157
O5 C32 C33 H07 MKV_RRR_158
O5 C32 C33 H07 MKV_RRR_159
C6 C4 C3 H1 MKV_RRR_160
C6 C7 C10 H3 MKV_RRR_161
C6 C21 C22 H01 MKV_RRR_162
C6 C21 C22 H02 MKV_RRR_163
C7 C6 C21 H03 MKV_RRR_164
C7 C6 C21 H04 MKV_RRR_165
C7 C8 C9 H2 MKV_RRR_166
C8 C7 C10 H3 MKV_RRR_167
H4 N4 C12 C9 MKV_RRR_168
C10 C11 C14 H9 MKV_RRR_169
C10 C11 C14 H10 MKV_RRR_170

C10 C11 C14 H11 MKV_RRR_171
H4 N4 C12 C11 MKV_RRR_172
C11 C12 C9 H2 MKV_RRR_173
C12 N4 C17 H17 MKV_RRR_174
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C26 C22 C21 H03 MKV_RRR_187
C26 C22 C21 H04 MKV_RRR_188
C31 C30 N2 H05 MKV_RRR_189
C32 N3 C31 H35 MKV_RRR_190
C32 N3 C31 H36 MKV_RRR_191
C32 C33 C34 H08 MKV_RRR_192
C34 S C38 H09 MKV_RRR_193
C34 S C38 H22 MKV_RRR_194
C35 N3 C31 H35 MKV_RRR_195
C35 N3 C31 H36 MKV_RRR_196
C35 C34 C33 H06 MKV_RRR_197
C35 C34 C33 H07 MKV_RRR_198
C38 S C34 H08 MKV_RRR_199
S C34 C33 H06 MKV_RRR_200
S C34 C33 H07 MKV_RRR_201
H4 N4 C17 H17 MKV_RRR_205
H4 N4 C17 H18 MKV_RRR_206
H5 N1 C15 H12 MKV_RRR_207
H5 N1 C15 H13 MKV_RRR_208
H01 C22 C21 H03 MKV_RRR_209
H01 C22 C21 H04 MKV_RRR_210
H02 C22 C21 H03 MKV_RRR_211
H02 C22 C21 H04 MKV_RRR_212
H05 N2 C30 H33 MKV_RRR_213
H05 N2 C30 H34 MKV_RRR_214
H06 C33 C34 H08 MKV_RRR_215
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H33 C30 C31 H35 MKV_RRR_235
H33 C30 C31 H36 MKV_RRR_236
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H4 N4 C17 C12 MKV_RRR_239
C1 C5 C39 H0 MKV_RRR_240
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C26 C30 N2 H05 MKV_RRR_242
C2 C4 C3 H1 MKV_RRR_243
C8 C12 C9 H2 MKV_RRR_244
C7 C11 C10 H3 MKV_RRR_245
[impropers]
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