

## Force Field Data files:

**Note:** To run MoViES with your own force constants, you are recommended to only change the force constant marked in red in the following files. Please do not change the atom index.

### File1: *dtfctr*

This file contains bond stretch force constants and lengths of chemical bonds of the molecule in your input pdb file.

$$\sum_{\text{bond-stretch}} \frac{1}{2} K_i^r (r_i - \langle r_i \rangle)^2$$

#### Example *dtfctr* file:

Index	Atom 1 index	Atom 2 index				Force constant (mdyn/A)	Force constant (kcal/A <sup>2</sup> mol)	Equilibrium bond length (Å)	Real bond length (Å)	Name and residue of atom 1	Name and residue of atom 2	
1	1	2	0	0	0	4.6776	337.0	1.449	1.485	N ATHR	1 CA THR	1
2	2	3	0	0	0	4.4000	317.0	1.522	1.516	CA THR	1 C THR	1
3	2	5	0	0	0	3.6088	260.0	1.526	1.523	CA THR	1 CB ATHR	1
4	3	4	0	0	0	7.9116	570.0	1.229	1.247	C THR	1 O THR	1
5	3	8	0	0	0	6.8012	490.0	1.335	1.314	C THR	1 N THR	2
6	5	6	0	0	0	5.3577	386.0	1.425	1.417	CB ATHR	1 OGL1ATHR	1
7	5	7	0	0	0	3.6088	260.0	1.526	1.523	CB ATHR	1 CG2ATHR	1
8	8	9	0	0	0	4.6776	337.0	1.449	1.477	N THR	2 CA THR	2
9	9	10	0	0	0	4.4000	317.0	1.522	1.549	CA THR	2 C THR	2
10	9	12	0	0	0	3.6088	260.0	1.526	1.540	CA THR	2 CB ATHR	2

### File 2: *dtfcang*

This file contains angle bending force constants of chemical bonds of the molecule in your pdb file.

$$\sum_{\text{bond-angle}} \frac{1}{2} K_{im}^\theta (\theta_{im} - \langle \theta_{im} \rangle)^2$$

#### Example *dtfcang* file:

Index	Atom 1 index	Atom 2 index	Atom 3 index			Force constant (mdyn/A)	Force constant (kcal/A <sup>2</sup> mol)	Equilibrium bond angle (°)	Name and residue of atom 1	Name and residue of atom 2	Name and residue of atom	
1	1	2	3	0	0	0.8744	63.0	110.1	1.8 N ATHR	1 CA THR	1 C THR	1
2	1	2	5	0	0	1.1104	80.0	109.7	2.0 N ATHR	1 CA THR	1 CB ATHR	1
3	2	3	4	0	0	1.1104	80.0	120.4	2.1 CA THR	1 C THR	1 O THR	1
4	2	5	6	0	0	1.1104	80.0	109.5	1.9 CA THR	1 CB ATHR	1 OGL1ATHR	1
5	2	5	7	0	0	0.8744	63.0	111.5	1.9 CA THR	1 CB ATHR	1 CG2ATHR	1
6	2	3	8	0	0	0.9716	70.0	116.6	2.0 CA THR	1 C THR	1 N THR	2
7	3	2	5	0	0	0.8744	63.0	111.1	1.9 C THR	1 CA THR	1 CB ATHR	1
8	3	8	9	0	0	0.6940	50.0	121.9	2.1 C THR	1 N THR	2 CA THR	2
9	4	3	8	0	0	1.1104	80.0	122.9	2.2 O THR	1 C THR	1 N THR	2
10	6	5	7	0	0	1.1104	80.0	109.5	1.9 OGL1ATHR	1 CB ATHR	1 CG2ATHR	1

### File 3: *dtfactor*

This file contains torsion force constants of the chemical bonds of the molecule in your pdb file.

Torsion potential

$$\sum_{torsion} \frac{V_i}{2} [1 + \cos(n_i \phi_i - \gamma_i)]$$

Harmonic approximation:

$$\sum_{torsion} \frac{1}{2} K_i^\phi (\phi_i - \langle \phi_i \rangle)^2$$

#### Example *dtfactor* file:

Index	Atom 1 index	Atom 2 index	Atom 3 index	Atom 4 index	Force constant (mdyn/A)	Force constant (kcal/A <sup>2</sup> mol)	Equilibrium torsion angle phi (°)	gamma	n	
1	1	2	5	6	0.0694	5.0	1.0	1.0	2.0	2
2	1	2	5	7	0.0694	5.0	3.1	3.1	2.0	2

### File 4: *dtconnect*

This file provides the information about atom-atom connections.

#### Example *dtconnect* file:

Atom index	Connected atom 1	Connected atom 2	Connected atom3	.....	.....	.....	.....	.....	.....	.....	.....	.....
1	2	5	7	6	0	0	0	0	0	0	0	0
2	0	0	0	0	0	0	3	8	9	0	0	0
3	2	5	6	7	8	9	12	0	0	0	0	0
4	3	2	5	1	8	9	0	0	0	0	0	0
5	2	3	4	0	0	0	0	0	0	0	0	0
6	5	2	3	1	0	0	0	0	0	0	0	0
7	5	2	3	1	0	0	0	0	0	0	0	0
8	3	2	1	9	12	14	10	11	13	0	0	0
9	8	3	2	4	10	15	16	0	0	0	0	0
10	9	8	3	12	13	15	16	19	0	0	0	0

## File 5: *dthbond*

This file contains force constants and parameters of hydrogen bonds of the molecule in your pdb file.

H-bond potential

$$\sum_{H-bond} [V_i^H (1 - e^{-a_i(r_i - r_i^{min})})^2 - V_i^H]$$

Harmonic approximation

$$\sum_{H-bond} \frac{1}{2} K_i^H (r_i - \langle r_i \rangle)^2$$

### Example *dthbond* file:

Index	Atom 1 index	Atom 2 index	V0 (mdyn A)	a (A)	r0 (A)	Bond breaking length (A)	Real bond length (A)	Force constant (mdyn/A)	Name and residue of atom 1	Name and residue of atom 2
1	1	249	0.024	1.223	2.798	3.365	3.023	0.109	N ATHR	1 O ILE 35
2	6	264	0.024	1.225	2.800	3.366	2.580	0.234	OG1ATHR	1 O GLY 37
3	15	233	0.024	1.223	2.798	3.365	2.911	0.127	N CYS	3 O ILE 33
4	21	322	0.024	1.223	2.798	3.365	2.892	0.131	N CYS	4 O ASN 46
5	55	37	0.024	1.223	2.798	3.365	3.281	0.084	N ALA	9 O SER 6
6	60	37	0.024	1.223	2.798	3.365	3.081	0.101	N ARG	10 O SER 6
7	60	43	0.024	1.223	2.798	3.365	3.081	0.101	N ARG	10 O ILE 7
8	70	11	0.024	1.223	2.798	3.365	2.925	0.124	NH2AARG	10 O THR 2
9	70	322	0.024	1.223	2.798	3.365	2.952	0.120	NH2AARG	10 O ASN 46
10	71	43	0.024	1.223	2.798	3.365	2.837	0.143	N SER	11 O ILE 7