Supplementary material for the paper “The New Method of Modeling of Conformational Changes of Multi Chain Proteins”

The percentage of covalent bond lengths and planar angles that lie outside the valid ranges and the percentage of amino acids with values of torsion angles ϕ and ψ in the disallowed regions of the Ramachandran plot for all intermediate conformations of the analyzed proteins are given in Tables 1-3.

PDB ID	MinActionPath	MENM	MCHAIN-PROMPT
2JUV	0.00	11.84	0.66
2LME	3.42	11.70	0.00
2MP2	12.25	13.15	0.00
2MW2	0.00	9.58	0.00
2MXR	0.00	11.66	0.00
2MXU	0.03	13.66	0.00
2RVB	22.56	12.15	0.00

Table 1: The portion of covalent bond lengths outside the valid range, %

PDB ID	MinActionPath	MENM	MCHAIN-PROMPT
2JUV	1.68	7.92	0.00
2LME	4.02	11.20	0.00
2MP2	18.45	15.81	0.00
2MW2	0.17	3.81	0.00
2MXR	1.55	4.79	0.00
2MXU	2.75	18.25	0.00
2RVB	19.55	19.615	0.00

Table 2: The portion of planar angles outside the valid range, %

PDB ID	MinActionPath	MENM	MCHAIN-PROMPT
2JUV	3.00	13.13	5.88
2LME	6.99	8.25	6.63
2MP2	6.44	17.23	11.63
2MW2	0.35	1.39	0.00
2MXR	2.33	8.48	5.11
2MXU	4.44	12.98	8.54
2RVB	7.30	12.64	10.76

Table 3: The portion of residues with torsion angles outside the valid range, %

Details about the virtual bonds chosen for each protein are presented in Table 4 (calculation method is labeled Approach 2 Implementation 2 in the paper). For example, insulin (PDB ID 2JUV) has two chains, the virtual bond between them connects the 32-nd atom of the second chain with the 55-th atom of the first chain.

PDB ID	Virtual bonds	
	Chain IDs	Atom numbers
2JUV	B – A	32 – 55
2LME	A – B	37 – 37
	A – C	37 – 37
2MP2	B – A	93 – 182
	B – C	93 – 2
2MW2	C – A	44 – 21
	C – B	44 – 124
2MXR	A – B	68 – 41
2MXU	B – A	38 – 29
	B – C	38 – 37
	B – D	38 – 80
	B – E	38 – 76
	B – F	38 – 30
	B – G	38 – 84
	B – H	38 – 50
	B – I	38 – 50
	B – J	38 – 49
	B – K	38 – 47
	B – L	38 – 62
2RVB	B – A	44 – 88

Table 4: Data about virtual bonds in analyzed proteins