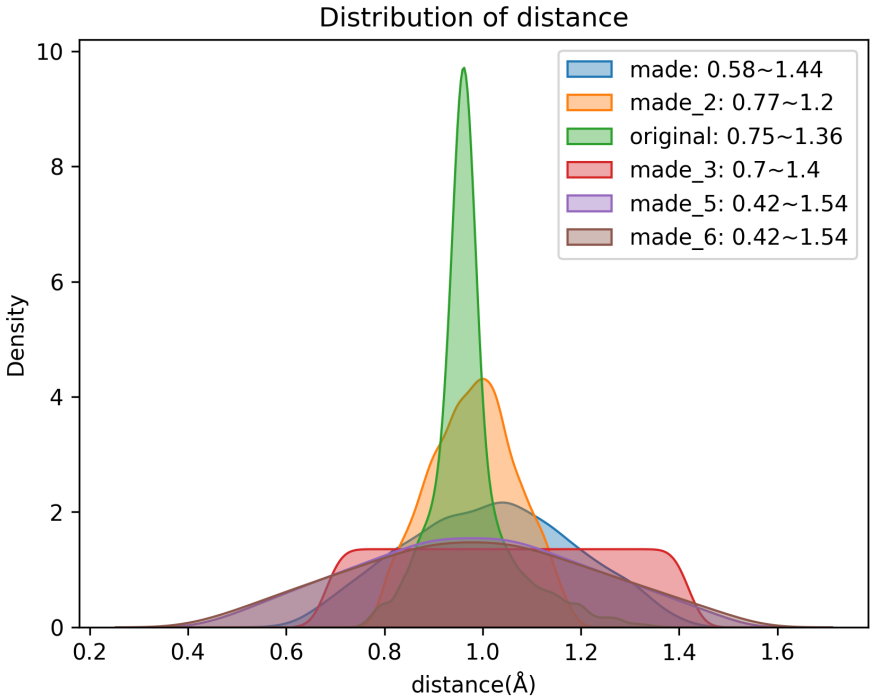
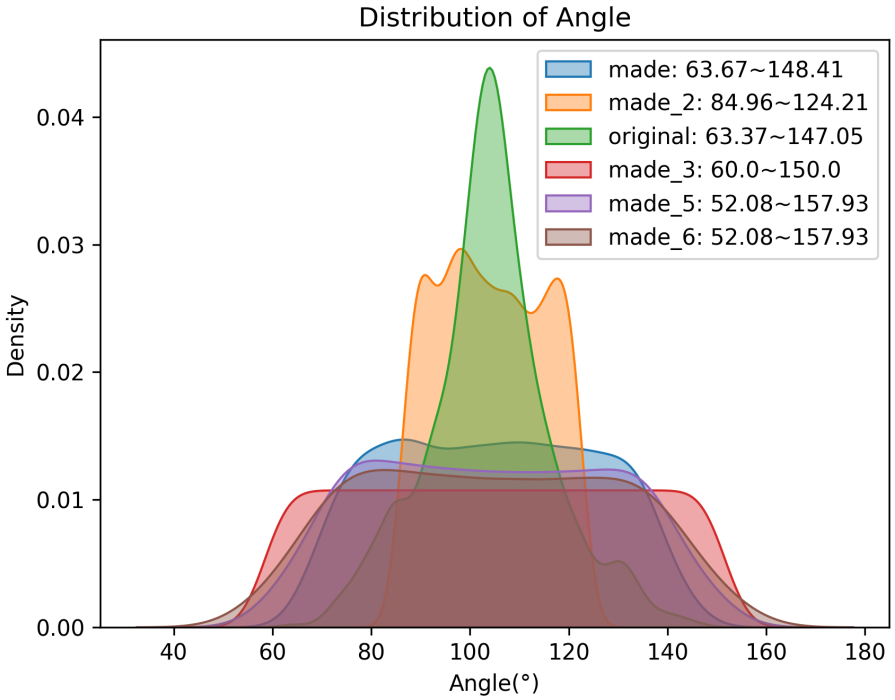
Data_name	Coordinates Type	Generation	region	structure #
Original	-	MD in various T (mostly near equi.)	-	5,213
made	Normal	Random	|c_1| < 0.8 |c_2| < 0.6 |c_3| < 0.8	3,000
Made_2	Normal	Random	|c_1| < 0.4 |c_2| < 0.3 |c_3| < 0.4	3,000
Made_3	Internal	Evenly-spaced	distance: 0.7 ~1.4 (20) angle: 60~150 (30)	20 x 20 x 30 = 12,000
Made_4	Internal	Evenly-spaced(2D)	distance: 0.7 ~1.4 (20) angle: 60~150 (30)	20 x30 =600
Made_5	Normal	Evenly-spaced	|c_1| < 0.8 (17) |c_2| < 0.6 (13) |c_3| < 0.8 (17)	17 x 13 x 17 =3,757
Made_6	Normal	Evenly-spaced	|c_1| < 0.8 (10) |c_2| < 0.6 (8) |c_3| < 0.8 (10)	10 x 8 x 10 =800
Made_7	Internal	Evenly-spaced(2D)	distance: 0.7 ~1.4 (30)	30x30 =900


Distribution of distance
made: 0.58~1.44
made_2: 0.77~1.2
original: 0.75~1.36
made_3: 0.7~1.4
made_5: 0.42~1.54
made_6: 0.42~1.54
Density
distance(Å)
0
2
4
6
8
10
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6


Distribution of Angle
made: 63.67~148.41
made_2: 84.96~124.21
original: 63.37~147.05
made_3: 60.0~150.0
made_5: 52.08~157.93
made_6: 52.08~157.93
Density
Angle(°)
0.00
0.01
0.02
0.03
0.04
40
60
80
100
120
140
160
180

Train` \ Test	Original	Made	Made_2	Made_3	Made_4	Made_5	Made_6	Made_7
Original 104 > full	**D 6 > 0.2**	D 154 > 69		D 130 > 60	D 90 > 30	D 1200 > 800		D 80 > 20
	H 50.2 > 41.3	H 304 > 109		H 400 > 408	H 468 > 423	H 1300 > 1000		H 100 > 60
	N 80.7 > 46.6	N 321 > 123		N 600 > 590	N 380 > 423	N 850 > 1000		N 300 > 150
	I 1.2 > 0.07	I 24 > 23		I 35 > 10	I 199 > 4.3	I 315 > 313		I 40 >20
Made 60 > full	D 10 > 0.4	D 20 > 1.7		D 40 > 11	D 24 >3.7	D 700 > 250		D 30 > 4
	H 65 > 67	H 26 > 1.7		H 350 > 350	H 322 > 324	H 500 > 200		H 50 > 40
	N 70 > 67	N 23 > 2.3		N 570 > 570	N 415 > 406	N 330 > 150		N 120 > 60
	I 2 > 0.8	I 8 > 1		I 20 > 10	I 9.4 > 3.1	I 200 > 90		I 11 > 8
Made_2 60 > full	D 10 > 2.4		D 3.7 > 0.6					
	H 71 > 69		H 4.2 > 1.2					
	N 80 > 71		N 4.4 > 1.1					
	I 3 > 1.3		I 0.3 > 0.05					
Made_3 120 > full	D 35 > 0.44			D 12 > 0.6	D 7.9 > 0.4			D 4.4 > 0.37
	H 168 > 60			H 340 >299	H 239 > 244			H 176 > 119
	N 85.7 > 44			N 543 > 475	N 351 > 341			N 176 > 67.7
	I 1.5 > 0.36			I 10 > 0.7	I 3.3 > 0.4			I 2.3 > 0.44
Made_5 37 > full	D 18.7 > 4					D 100 > 8		
	H 60 > 57					H 150 > 4.8		
	N 77 > 67.5					N 150 > 16.5		
	I 42 > 2					I 150 > 12		
Made_6 80 > full	D 88 > 18						D 102 > 51	
	H 67 > 59						H 114 > 42	
	N 80 > 73						N 154 > 39	
	I 14 > 3.8						I 74 > 13	