

# Investigation of Binding Affinity between Potential Antiviral Agents and PB2 Protein of Influenza A: Non-equilibrium Molecular Dynamics Simulation Approach

Tri Pham<sup>1,2</sup>, Hoang Linh Nguyen<sup>1,2</sup>, Tuyn Phan-Toai<sup>1</sup>, and Hung Nguyen<sup>1,\*</sup>

<sup>1</sup>*Institute for Computational Science and Technology, Ho Chi Minh City, Vietnam.*

<sup>2</sup>*VNUHCM-University of Technology, Ho Chi Minh City, Vietnam.*

\*Email: [hung.nv@icst.org.vn](mailto:hung.nv@icst.org.vn)

## SUPPORTING INFORMATION

The parameterization scheme used for three compounds is shown below:

1) The inhibitor (4):

[ atomtypes ]

; name	at.num	mass	charge	ptype	sigma	epsilon
CB	6	12.0110	0.0	A	0.355005	0.292880
NPYD	7	14.0067	0.0	A	0.329632	0.836800
C5B	6	12.0110	0.0	A	0.363487	0.209200
C5A	6	12.0110	0.0	A	0.363487	0.209200
NPYL	7	14.0067	0.0	A	0.306469	0.376560
F	9	18.9984	0.0	A	0.290433	0.564840
NM	7	14.0067	0.0	A	0.329632	0.836800
CR	6	12.0110	0.0	A	0.387541	0.230120
CO2M	6	12.0110	0.0	A	0.356359	0.292880
O2CM	8	15.9994	0.0	A	0.302905	0.502080
CR4R	6	12.0110	0.0	A	0.333196	0.589944
HCMM	1	1.0079	0.0	A	0.235197	0.092048
HNR	1	1.0079	0.0	A	0.040001	0.192464

[ pairtypes ]

; i	j	func	sigma1-4	epsilon1-4	; THESE ARE 1-4 INTERACTIONS
CR	CB	1	0.346773	0.110698	
CR	NPYD	1	0.334087	0.187114	
CR	C5B	1	0.351014	0.093557	
CR	C5A	1	0.351014	0.093557	
CR	NPYL	1	0.322505	0.125520	
CR	F	1	0.314487	0.153730	
CR	NM	1	0.334087	0.187114	
CR	CR	1	0.338541	0.041840	
CR	CO2M	1	0.347450	0.110698	
CR	O2CM	1	0.320723	0.144938	
CR	CR4R	1	0.335869	0.157109	
CR	HCMM	1	0.286869	0.062059	
CR	HNR	1	0.189271	0.089737	

[ moleculetype ]

; Name nrexcl

## [ atoms ]

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; nr type resnr resid atom cgnr charge mass
 1 CB  1 LIG C    1 0.1900 12.0110
 2 CB  1 LIG C1   2 0.1600 12.0110
 3 NPYD 1 LIG N   3 -0.6200 14.0067
 4 CB  1 LIG C2   4 0.6740 12.0110
 5 NPYD 1 LIG N1  5 -0.6200 14.0067
 6 CB  1 LIG C3   6 0.0580 12.0110
 7 C5B 1 LIG C12  7 -0.0540 12.0110
 8 C5B 1 LIG C13  8 0.0000 12.0110
 9 CB  1 LIG C14  9 -0.1500 12.0110
10 CB  1 LIG C15 10 0.1900 12.0110
11 CB  1 LIG C16 11 0.1600 12.0110
12 NPYD 1 LIG N3 12 -0.5670 14.0067
13 C5A 1 LIG C17 13 0.1054 12.0110
14 NPYL 1 LIG N4 14 0.0332 14.0067
15 C5A 1 LIG C18 15 -0.3016 12.0110
16 F   1 LIG F   16 -0.1900 18.9984
17 NM  1 LIG N2  17 -0.6980 14.0067
18 CR  1 LIG C4  18 -0.0500 12.0110
19 CR  1 LIG C5  19 -0.1060 12.0110
20 CO2M 1 LIG C6 20 0.9060 12.0110
21 O2CM 1 LIG O  21 -0.9000 15.9994
22 O2CM 1 LIG O1 22 -0.9000 15.9994
23 CR4R 1 LIG C7 23 0.0000 12.0110
24 CR4R 1 LIG C8 24 0.0000 12.0110
25 CR4R 1 LIG C9 25 0.0000 12.0110
26 CR4R 1 LIG C10 26 0.0000 12.0110
27 CR  1 LIG C11 27 0.0000 12.0110
28 F   1 LIG F1  28 -0.1900 18.9984
29 HCMM 1 LIG H   29 0.1500  1.0079
30 HCMM 1 LIG H1  30 0.0000  1.0079
31 HCMM 1 LIG H2  31 0.0000  1.0079
32 HCMM 1 LIG H3  32 0.0000  1.0079
33 HCMM 1 LIG H4  33 0.0000  1.0079
34 HCMM 1 LIG H5  34 0.0000  1.0079
35 HCMM 1 LIG H6  35 0.0000  1.0079
36 HCMM 1 LIG H7  36 0.0000  1.0079
37 HCMM 1 LIG H8  37 0.0000  1.0079
38 HCMM 1 LIG H9  38 0.0000  1.0079
39 HCMM 1 LIG H10 39 0.0000  1.0079
40 HCMM 1 LIG H11 40 0.0000  1.0079
41 HCMM 1 LIG H12 41 0.0000  1.0079
42 HCMM 1 LIG H13 42 0.1500  1.0079
43 HCMM 1 LIG H14 43 0.1500  1.0079
44 HNR  1 LIG H15 44 0.2700  1.0079
45 HCMM 1 LIG H16 45 0.1500  1.0079

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## [ bonds ]

```

; ai aj fu b0 kb, b0 kb
20 21 1 0.12610 587519.8 0.12610 587519.8
20 22 1 0.12610 587519.8 0.12610 587519.8
44 14 1 0.10120 428294.3 0.10120 428294.3
14 13 1 0.13640 379454.5 0.13640 379454.5
14 15 1 0.13640 379454.5 0.13640 379454.5

```

12 13 1 0.13300 439556.0 0.13300 439556.0  
12 11 1 0.13330 345489.6 0.13330 345489.6  
43 11 1 0.10840 319534.6 0.10840 319534.6  
13 8 1 0.13770 428655.8 0.13770 428655.8  
45 15 1 0.10800 333084.1 0.10800 333084.1  
11 10 1 0.13740 335613.7 0.13740 335613.7  
15 7 1 0.13770 428655.8 0.13770 428655.8  
8 7 1 0.14180 259734.4 0.14180 259734.4  
8 9 1 0.13790 371023.7 0.13790 371023.7  
7 4 1 0.13790 371023.7 0.13790 371023.7  
10 9 1 0.13740 335613.7 0.13740 335613.7  
10 28 1 0.13420 392101.0 0.13420 392101.0  
9 42 1 0.10840 319534.6 0.10840 319534.6  
3 4 1 0.13330 345489.6 0.13330 345489.6  
3 2 1 0.13330 345489.6 0.13330 345489.6  
4 5 1 0.13330 345489.6 0.13330 345489.6  
5 6 1 0.13330 345489.6 0.13330 345489.6  
29 2 1 0.10840 319534.6 0.10840 319534.6  
2 1 1 0.13740 335613.7 0.13740 335613.7  
20 19 1 0.15100 230648.0 0.15100 230648.0  
6 1 1 0.13740 335613.7 0.13740 335613.7  
6 17 1 0.13350 429799.7 0.13350 429799.7  
30 18 1 0.10930 287014.9 0.10930 287014.9  
1 16 1 0.13420 392101.0 0.13420 392101.0  
35 25 1 0.10930 292193.8 0.10930 292193.8  
18 19 1 0.15080 256422.3 0.15080 256422.3  
18 17 1 0.14440 268346.7 0.14440 268346.7  
18 23 1 0.15040 280029.3 0.15040 280029.3  
19 32 1 0.10930 287014.9 0.10930 287014.9  
19 31 1 0.10930 287014.9 0.10930 287014.9  
38 26 1 0.10930 292193.8 0.10930 292193.8  
33 24 1 0.10930 292193.8 0.10930 292193.8  
25 36 1 0.10930 292193.8 0.10930 292193.8  
25 26 1 0.15260 220590.5 0.15260 220590.5  
25 24 1 0.15260 220590.5 0.15260 220590.5  
26 23 1 0.15260 220590.5 0.15260 220590.5  
26 37 1 0.10930 292193.8 0.10930 292193.8  
24 23 1 0.15260 220590.5 0.15260 220590.5  
24 34 1 0.10930 292193.8 0.10930 292193.8  
23 27 1 0.15040 280029.3 0.15040 280029.3  
40 27 1 0.10930 287014.9 0.10930 287014.9  
27 41 1 0.10930 287014.9 0.10930 287014.9  
27 39 1 0.10930 287014.9 0.10930 287014.9

[ pairs ]

; ai aj fu

1 4 1  
1 18 1  
2 5 1  
2 17 1  
2 7 1  
3 6 1  
3 16 1  
3 8 1  
3 15 1  
4 29 1  
4 17 1

4 9 1  
4 13 1  
4 14 1  
4 45 1  
5 8 1  
5 15 1  
5 16 1  
5 18 1  
6 29 1  
6 7 1  
6 19 1  
6 23 1  
6 30 1  
7 10 1  
7 42 1  
7 12 1  
7 44 1  
8 45 1  
8 11 1  
8 28 1  
8 44 1  
9 15 1  
9 12 1  
9 14 1  
9 43 1  
10 13 1  
11 42 1  
11 14 1  
12 28 1  
12 15 1  
12 44 1  
13 42 1  
13 43 1  
13 45 1  
16 29 1  
16 17 1  
17 20 1  
17 31 1  
17 32 1  
17 24 1  
17 26 1  
17 27 1  
18 21 1  
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18 25 1  
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18 40 1  
18 41 1  
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19 27 1  
20 23 1  
20 30 1

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 27 38 1  
 28 42 1  
 28 43 1  
 30 31 1  
 30 32 1  
 33 35 1  
 33 36 1  
 34 35 1  
 34 36 1  
 35 37 1  
 35 38 1  
 36 37 1  
 36 38 1  
 44 45 1

[ angles ]

; ai aj ak fu th0 kth ub0 kub th0 kth ub0 kub

2	1	6	1	119.9770	402.88	119.9770	402.88
2	1	16	1	118.0650	658.81	118.0650	658.81
6	1	16	1	118.0650	658.81	118.0650	658.81
1	2	3	1	126.1390	358.92	126.1390	358.92
1	2	29	1	120.5710	339.05	120.5710	339.05
3	2	29	1	115.5880	417.33	115.5880	417.33
2	3	4	1	115.4060	653.40	115.4060	653.40
3	4	5	1	128.9380	436.60	128.9380	436.60
3	4	7	1	128.9380	436.60	128.9380	436.60
5	4	7	1	128.9380	436.60	128.9380	436.60
4	5	6	1	115.4060	653.40	115.4060	653.40
1	6	5	1	126.1390	358.92	126.1390	358.92
1	6	17	1	124.3840	566.68	124.3840	566.68
5	6	17	1	118.3490	691.34	118.3490	691.34
4	7	8	1	128.6730	464.91	128.6730	464.91

4	7	15	1	120.0000	602.21	120.0000	602.21
8	7	15	1	108.2390	521.51	108.2390	521.51
7	8	9	1	128.6730	464.91	128.6730	464.91
7	8	13	1	108.2390	521.51	108.2390	521.51
9	8	13	1	120.0000	602.21	120.0000	602.21
8	9	10	1	112.5670	254.73	112.5670	254.73
8	9	42	1	121.4460	314.95	121.4460	314.95
10	9	42	1	120.5710	339.05	120.5710	339.05
9	10	11	1	119.9770	402.88	119.9770	402.88
9	10	28	1	118.0650	658.81	118.0650	658.81
11	10	28	1	118.0650	658.81	118.0650	658.81
10	11	12	1	126.1390	358.92	126.1390	358.92
10	11	43	1	120.5710	339.05	120.5710	339.05
12	11	43	1	115.5880	417.33	115.5880	417.33
11	12	13	1	110.1810	740.72	110.1810	740.72
8	13	12	1	126.5130	548.01	126.5130	548.01
8	13	14	1	107.2550	489.59	107.2550	489.59
12	13	14	1	124.8140	615.46	124.8140	615.46
13	14	15	1	109.5990	693.74	109.5990	693.74
13	14	44	1	127.7700	331.82	127.7700	331.82
15	14	44	1	127.7700	331.82	127.7700	331.82
7	15	14	1	107.2550	489.59	107.2550	489.59
7	15	45	1	131.7210	347.47	131.7210	347.47
14	15	45	1	121.1270	371.56	121.1270	371.56
6	17	18	1	120.0000	602.21	120.0000	602.21
17	18	19	1	109.5000	602.21	109.5000	602.21
17	18	23	1	109.5000	602.21	109.5000	602.21
17	18	30	1	113.0350	394.45	113.0350	394.45
19	18	23	1	108.6590	614.86	108.6590	614.86
19	18	30	1	110.5490	383.00	110.5490	383.00
23	18	30	1	111.0000	425.16	111.0000	425.16
18	19	20	1	98.4220	198.73	98.4220	198.73
18	19	31	1	110.5490	383.00	110.5490	383.00
18	19	32	1	110.5490	383.00	110.5490	383.00
20	19	31	1	108.9040	316.16	108.9040	316.16
20	19	32	1	108.9040	316.16	108.9040	316.16
31	19	32	1	108.8360	310.74	108.8360	310.74
19	20	21	1	114.6890	728.07	114.6890	728.07
19	20	22	1	114.6890	728.07	114.6890	728.07
21	20	22	1	130.6000	711.20	130.6000	711.20
18	23	24	1	113.3130	302.31	113.3130	302.31
18	23	26	1	113.3130	302.31	113.3130	302.31
18	23	27	1	113.1310	567.89	113.1310	567.89
24	23	26	1	108.6440	607.02	108.6440	607.02
24	23	27	1	113.3130	302.31	113.3130	302.31
26	23	27	1	113.3130	302.31	113.3130	302.31
23	24	25	1	108.6440	607.02	108.6440	607.02
23	24	33	1	113.9400	339.65	113.9400	339.65
23	24	34	1	113.9400	339.65	113.9400	339.65
25	24	33	1	113.9400	339.65	113.9400	339.65
25	24	34	1	113.9400	339.65	113.9400	339.65
33	24	34	1	109.1070	264.37	109.1070	264.37
24	25	26	1	108.6440	607.02	108.6440	607.02
24	25	35	1	113.9400	339.65	113.9400	339.65
24	25	36	1	113.9400	339.65	113.9400	339.65
26	25	35	1	113.9400	339.65	113.9400	339.65
26	25	36	1	113.9400	339.65	113.9400	339.65

35	25	36	1	109.1070	264.37	109.1070	264.37
23	26	25	1	108.6440	607.02	108.6440	607.02
23	26	37	1	113.9400	339.65	113.9400	339.65
23	26	38	1	113.9400	339.65	113.9400	339.65
25	26	37	1	113.9400	339.65	113.9400	339.65
25	26	38	1	113.9400	339.65	113.9400	339.65
37	26	38	1	109.1070	264.37	109.1070	264.37
23	27	39	1	111.0000	425.16	111.0000	425.16
23	27	40	1	111.0000	425.16	111.0000	425.16
23	27	41	1	111.0000	425.16	111.0000	425.16
39	27	40	1	108.8360	310.74	108.8360	310.74
39	27	41	1	108.8360	310.74	108.8360	310.74
40	27	41	1	108.8360	310.74	108.8360	310.74

[ dihedrals ]

; ai aj ak al fu phi0 kphi mult phi0 kphi mult

1	2	3	4	9	180.00	14.6440	2	180.00	14.6440	2
1	6	5	4	9	180.00	14.6440	2	180.00	14.6440	2
1	6	17	18	9	180.00	7.5312	2	180.00	7.5312	2
2	1	6	5	9	180.00	14.6440	2	180.00	14.6440	2
2	1	6	17	9	180.00	14.6440	2	180.00	14.6440	2
2	3	4	5	9	180.00	14.6440	2	180.00	14.6440	2
2	3	4	7	9	180.00	14.6440	2	180.00	14.6440	2
3	2	1	6	9	180.00	14.6440	2	180.00	14.6440	2
3	2	1	16	9	180.00	14.6440	2	180.00	14.6440	2
3	4	5	6	9	180.00	14.6440	2	180.00	14.6440	2
3	4	7	8	9	180.00	14.6440	2	180.00	14.6440	2
3	4	7	15	9	180.00	14.6440	2	180.00	14.6440	2
4	3	2	29	9	180.00	14.6440	2	180.00	14.6440	2
4	5	6	17	9	180.00	14.6440	2	180.00	14.6440	2
4	7	8	9	9	180.00	3.7656	2	180.00	3.7656	2
4	7	8	13	9	180.00	3.7656	2	180.00	3.7656	2
5	4	7	8	9	180.00	14.6440	2	180.00	14.6440	2
5	4	7	15	9	180.00	14.6440	2	180.00	14.6440	2
5	6	1	16	9	180.00	14.6440	2	180.00	14.6440	2
5	6	17	18	9	180.00	7.5312	2	180.00	7.5312	2
6	1	2	29	9	180.00	14.6440	2	180.00	14.6440	2
6	5	4	7	9	180.00	14.6440	2	180.00	14.6440	2
6	17	18	19	9	0.00	0.5230	3	0.00	0.5230	3
6	17	18	23	9	0.00	0.5230	3	0.00	0.5230	3
6	17	18	30	9	0.00	0.5230	3	0.00	0.5230	3
7	8	9	10	9	180.00	14.6440	2	180.00	14.6440	2
7	8	9	42	9	180.00	14.6440	2	180.00	14.6440	2
7	8	13	12	9	180.00	14.6440	2	180.00	14.6440	2
7	8	13	14	9	180.00	14.6440	2	180.00	14.6440	2
7	15	14	13	9	180.00	8.3680	2	180.00	8.3680	2
7	15	14	44	9	180.00	8.3680	2	180.00	8.3680	2
8	7	15	14	9	180.00	14.6440	2	180.00	14.6440	2
8	7	15	45	9	180.00	14.6440	2	180.00	14.6440	2
8	9	10	11	9	180.00	14.6440	2	180.00	14.6440	2
8	9	10	28	9	180.00	14.6440	2	180.00	14.6440	2
8	13	12	11	9	180.00	14.6440	2	180.00	14.6440	2
8	13	14	15	9	180.00	8.3680	2	180.00	8.3680	2
8	13	14	44	9	180.00	8.3680	2	180.00	8.3680	2
9	8	7	15	9	180.00	3.7656	2	180.00	3.7656	2
9	8	13	12	9	180.00	14.6440	2	180.00	14.6440	2
9	10	11	12	9	180.00	14.6440	2	180.00	14.6440	2

9 10 11 43 9 180.00 14.6440 2 180.00 14.6440 2  
10 9 8 13 9 180.00 14.6440 2 180.00 14.6440 2  
10 11 12 13 9 180.00 14.6440 2 180.00 14.6440 2  
11 10 9 42 9 180.00 14.6440 2 180.00 14.6440 2  
11 12 13 14 9 180.00 14.6440 2 180.00 14.6440 2  
12 11 10 28 9 180.00 14.6440 2 180.00 14.6440 2  
12 13 14 15 9 180.00 8.3680 2 180.00 8.3680 2  
12 13 14 44 9 180.00 8.3680 2 180.00 8.3680 2  
13 8 7 15 9 180.00 14.6440 2 180.00 14.6440 2  
13 8 9 42 9 180.00 14.6440 2 180.00 14.6440 2  
13 12 11 43 9 180.00 14.6440 2 180.00 14.6440 2  
13 14 15 45 9 180.00 8.3680 2 180.00 8.3680 2  
16 1 2 29 9 180.00 14.6440 2 180.00 14.6440 2  
16 1 6 17 9 180.00 14.6440 2 180.00 14.6440 2  
17 18 19 20 9 0.00 0.6276 3 0.00 0.6276 3  
17 18 19 31 9 0.00 0.6276 3 0.00 0.6276 3  
17 18 19 32 9 0.00 0.6276 3 0.00 0.6276 3  
17 18 23 24 9 0.00 0.7322 3 0.00 0.7322 3  
17 18 23 26 9 0.00 0.7322 3 0.00 0.7322 3  
17 18 23 27 9 0.00 0.7322 3 0.00 0.7322 3  
18 19 20 21 9 180.00 2.6401 2 180.00 2.6401 2  
18 19 20 22 9 180.00 2.6401 2 180.00 2.6401 2  
18 23 24 25 9 0.00 -0.1339 1 0.00 -0.1339 1  
18 23 24 25 9 180.00 -0.1339 2 180.00 -0.1339 2  
18 23 24 25 9 0.00 0.2929 3 0.00 0.2929 3  
18 23 24 33 9 0.00 0.1423 1 0.00 0.1423 1  
18 23 24 33 9 180.00 0.1715 2 180.00 0.1715 2  
18 23 24 33 9 0.00 0.7238 3 0.00 0.7238 3  
18 23 24 34 9 0.00 0.1423 1 0.00 0.1423 1  
18 23 24 34 9 180.00 0.1715 2 180.00 0.1715 2  
18 23 24 34 9 0.00 0.7238 3 0.00 0.7238 3  
18 23 26 25 9 0.00 -0.1339 1 0.00 -0.1339 1  
18 23 26 25 9 180.00 -0.1339 2 180.00 -0.1339 2  
18 23 26 25 9 0.00 0.2929 3 0.00 0.2929 3  
18 23 26 37 9 0.00 0.1423 1 0.00 0.1423 1  
18 23 26 37 9 180.00 0.1715 2 180.00 0.1715 2  
18 23 26 37 9 0.00 0.7238 3 0.00 0.7238 3  
18 23 26 38 9 0.00 0.1423 1 0.00 0.1423 1  
18 23 26 38 9 180.00 0.1715 2 180.00 0.1715 2  
18 23 26 38 9 0.00 0.7238 3 0.00 0.7238 3  
18 23 27 39 9 0.00 0.7322 3 0.00 0.7322 3  
18 23 27 40 9 0.00 0.7322 3 0.00 0.7322 3  
18 23 27 41 9 0.00 0.7322 3 0.00 0.7322 3  
19 18 23 24 9 0.00 0.7322 3 0.00 0.7322 3  
19 18 23 26 9 0.00 0.7322 3 0.00 0.7322 3  
19 18 23 27 9 0.00 0.7322 3 0.00 0.7322 3  
20 19 18 23 9 0.00 0.6276 3 0.00 0.6276 3  
20 19 18 30 9 0.00 -0.2929 3 0.00 -0.2929 3  
21 20 19 31 9 0.00 -0.2218 3 0.00 -0.2218 3  
21 20 19 32 9 0.00 -0.2218 3 0.00 -0.2218 3  
22 20 19 31 9 0.00 -0.2218 3 0.00 -0.2218 3  
22 20 19 32 9 0.00 -0.2218 3 0.00 -0.2218 3  
23 18 19 31 9 0.00 0.6276 3 0.00 0.6276 3  
23 18 19 32 9 0.00 0.6276 3 0.00 0.6276 3  
23 24 25 26 9 0.00 0.4184 3 0.00 0.4184 3  
23 24 25 35 9 0.00 -0.1213 1 0.00 -0.1213 1  
23 24 25 35 9 0.00 0.6402 3 0.00 0.6402 3



23	24	25	36	9	0.00	-0.1213	1	0.00	-0.1213	1
23	24	25	36	9	0.00	0.6402	3	0.00	0.6402	3
23	26	25	24	9	0.00	0.4184	3	0.00	0.4184	3
23	26	25	35	9	0.00	-0.1213	1	0.00	-0.1213	1
23	26	25	35	9	0.00	0.6402	3	0.00	0.6402	3
23	26	25	36	9	0.00	-0.1213	1	0.00	-0.1213	1
23	26	25	36	9	0.00	0.6402	3	0.00	0.6402	3
24	23	18	30	9	0.00	0.7531	3	0.00	0.7531	3
24	23	26	25	9	0.00	0.4184	3	0.00	0.4184	3
24	23	26	37	9	0.00	-0.1213	1	0.00	-0.1213	1
24	23	26	37	9	0.00	0.6402	3	0.00	0.6402	3
24	23	26	38	9	0.00	-0.1213	1	0.00	-0.1213	1
24	23	26	38	9	0.00	0.6402	3	0.00	0.6402	3
24	23	27	39	9	0.00	0.7531	3	0.00	0.7531	3
24	23	27	40	9	0.00	0.7531	3	0.00	0.7531	3
24	23	27	41	9	0.00	0.7531	3	0.00	0.7531	3
24	25	26	37	9	0.00	-0.1213	1	0.00	-0.1213	1
24	25	26	37	9	0.00	0.6402	3	0.00	0.6402	3
24	25	26	38	9	0.00	-0.1213	1	0.00	-0.1213	1
24	25	26	38	9	0.00	0.6402	3	0.00	0.6402	3
25	24	23	26	9	0.00	0.4184	3	0.00	0.4184	3
25	24	23	27	9	0.00	-0.1339	1	0.00	-0.1339	1
25	24	23	27	9	180.00	-0.1339	2	180.00	-0.1339	2
25	24	23	27	9	0.00	0.2929	3	0.00	0.2929	3
25	26	23	27	9	0.00	-0.1339	1	0.00	-0.1339	1
25	26	23	27	9	180.00	-0.1339	2	180.00	-0.1339	2
25	26	23	27	9	0.00	0.2929	3	0.00	0.2929	3
26	23	18	30	9	0.00	0.7531	3	0.00	0.7531	3
26	23	24	33	9	0.00	-0.1213	1	0.00	-0.1213	1
26	23	24	33	9	0.00	0.6402	3	0.00	0.6402	3
26	23	24	34	9	0.00	-0.1213	1	0.00	-0.1213	1
26	23	24	34	9	0.00	0.6402	3	0.00	0.6402	3
26	23	27	39	9	0.00	0.7531	3	0.00	0.7531	3
26	23	27	40	9	0.00	0.7531	3	0.00	0.7531	3
26	23	27	41	9	0.00	0.7531	3	0.00	0.7531	3
26	25	24	33	9	0.00	-0.1213	1	0.00	-0.1213	1
26	25	24	33	9	0.00	0.6402	3	0.00	0.6402	3
26	25	24	34	9	0.00	-0.1213	1	0.00	-0.1213	1
26	25	24	34	9	0.00	0.6402	3	0.00	0.6402	3
27	23	18	30	9	0.00	0.7322	3	0.00	0.7322	3
27	23	24	33	9	0.00	0.1423	1	0.00	0.1423	1
27	23	24	33	9	180.00	0.1715	2	180.00	0.1715	2
27	23	24	33	9	0.00	0.7238	3	0.00	0.7238	3
27	23	24	34	9	0.00	0.1423	1	0.00	0.1423	1
27	23	24	34	9	180.00	0.1715	2	180.00	0.1715	2
27	23	24	34	9	0.00	0.7238	3	0.00	0.7238	3
27	23	26	37	9	0.00	0.1423	1	0.00	0.1423	1
27	23	26	37	9	180.00	0.1715	2	180.00	0.1715	2
27	23	26	37	9	0.00	0.7238	3	0.00	0.7238	3
27	23	26	38	9	0.00	0.1423	1	0.00	0.1423	1
27	23	26	38	9	180.00	0.1715	2	180.00	0.1715	2
27	23	26	38	9	0.00	0.7238	3	0.00	0.7238	3
28	10	9	42	9	180.00	14.6440	2	180.00	14.6440	2
28	10	11	43	9	180.00	14.6440	2	180.00	14.6440	2
30	18	19	31	9	0.00	0.5941	1	0.00	0.5941	1
30	18	19	31	9	180.00	-2.8995	2	180.00	-2.8995	2
30	18	19	31	9	0.00	0.6569	3	0.00	0.6569	3

30	18	19	32	9	0.00	0.5941	1	0.00	0.5941	1
30	18	19	32	9	180.00	-2.8995	2	180.00	-2.8995	2
30	18	19	32	9	0.00	0.6569	3	0.00	0.6569	3
33	24	25	35	9	0.00	0.8870	3	0.00	0.8870	3
33	24	25	36	9	0.00	0.8870	3	0.00	0.8870	3
34	24	25	35	9	0.00	0.8870	3	0.00	0.8870	3
34	24	25	36	9	0.00	0.8870	3	0.00	0.8870	3
35	25	26	37	9	0.00	0.8870	3	0.00	0.8870	3
35	25	26	38	9	0.00	0.8870	3	0.00	0.8870	3
36	25	26	37	9	0.00	0.8870	3	0.00	0.8870	3
36	25	26	38	9	0.00	0.8870	3	0.00	0.8870	3
44	14	15	45	9	180.00	8.3680	2	180.00	8.3680	2

[ dihedrals ]

```
; ai aj ak al fu xi0 kxi xi0 kxi
1 2 6 16 2 0.00 21.0790 0.00 21.0790
2 3 1 29 2 0.00 27.6981 0.00 27.6981
4 7 3 5 2 0.00 21.0790 0.00 21.0790
7 8 4 15 2 0.00 -6.6275 0.00 -6.6275
8 9 7 13 2 0.00 -6.6275 0.00 -6.6275
9 10 8 42 2 0.00 7.2300 0.00 7.2300
10 11 9 28 2 0.00 21.0790 0.00 21.0790
13 14 8 12 2 0.00 30.1081 0.00 30.1081
6 5 1 17 2 0.00 21.0790 0.00 21.0790
18 23 17 19 2 0.00 0.0000 0.00 0.0000
18 19 17 30 2 0.00 0.0000 0.00 0.0000
19 20 18 32 2 0.00 0.0000 0.00 0.0000
19 20 18 31 2 0.00 0.0000 0.00 0.0000
20 21 19 22 2 0.00 107.1941 0.00 107.1941
23 24 18 26 2 0.00 0.0000 0.00 0.0000
23 26 18 27 2 0.00 0.0000 0.00 0.0000
26 25 23 38 2 0.00 0.0000 0.00 0.0000
26 38 23 37 2 0.00 0.0000 0.00 0.0000
24 25 23 33 2 0.00 0.0000 0.00 0.0000
24 33 23 34 2 0.00 0.0000 0.00 0.0000
25 24 26 35 2 0.00 0.0000 0.00 0.0000
25 35 26 36 2 0.00 0.0000 0.00 0.0000
27 40 23 41 2 0.00 0.0000 0.00 0.0000
27 40 23 39 2 0.00 0.0000 0.00 0.0000
11 12 10 43 2 0.00 27.6981 0.00 27.6981
14 15 13 44 2 0.00 -8.4349 0.00 -8.4349
15 14 7 45 2 0.00 11.4391 0.00 11.4391
```

2) The inhibitor (12):

[ atomtypes ]

```
; name at.num mass charge ptype sigma epsilon
NPYD 7 14.0067 0.0 A 0.329632 0.836800
CB 6 12.0110 0.0 A 0.355005 0.292880
C5A 6 12.0110 0.0 A 0.363487 0.209200
NPYL 7 14.0067 0.0 A 0.306469 0.376560
C5B 6 12.0110 0.0 A 0.363487 0.209200
OR 8 15.9994 0.0 A 0.315378 0.636386
F 9 18.9984 0.0 A 0.290433 0.564840
CR 6 12.0110 0.0 A 0.387541 0.230120
NM 7 14.0067 0.0 A 0.329632 0.836800
C=O 6 12.0110 0.0 A 0.356359 0.460240
```

O=C	8	15.9994	0.0	A	0.302905	0.502080
NC=O	7	14.0067	0.0	A	0.329632	0.836800
HCMM	1	1.0079	0.0	A	0.235197	0.092048
HOR	1	1.0079	0.0	A	0.040001	0.192464
HNR	1	1.0079	0.0	A	0.040001	0.192464

[ pairtypes ]

; i j func sigma1-4 epsilon1-4 ; THESE ARE 1-4 INTERACTIONS

CR	NPYD	1	0.334087	0.187114
CR	CB	1	0.346773	0.110698
CR	C5A	1	0.351014	0.093557
CR	NPYL	1	0.322505	0.125520
CR	C5B	1	0.351014	0.093557
CR	OR	1	0.326960	0.163176
CR	F	1	0.314487	0.153730
CR	CR	1	0.338541	0.041840
CR	NM	1	0.334087	0.187114
CR	C=O	1	0.347450	0.138768
CR	O=C	1	0.293997	0.144938
CR	NC=O	1	0.334087	0.187114
CR	HCMM	1	0.286869	0.062059
CR	HOR	1	0.189271	0.089737
CR	HNR	1	0.189271	0.089737
O=C	NPYD	1	0.289542	0.648182
O=C	CB	1	0.302228	0.383470
O=C	C5A	1	0.306469	0.324091
O=C	NPYL	1	0.277960	0.434814
O=C	C5B	1	0.306469	0.324091
O=C	OR	1	0.282415	0.565258
O=C	F	1	0.269942	0.532536
O=C	NM	1	0.289542	0.648182
O=C	C=O	1	0.302905	0.480705
O=C	O=C	1	0.249452	0.502080
O=C	NC=O	1	0.289542	0.648182
O=C	HCMM	1	0.242324	0.214978
O=C	HOR	1	0.144726	0.310857
O=C	HNR	1	0.144726	0.310857

[ moleculetype ]

; Name nrexcl

12 3

[ atoms ]

; nr	type	resnr	resid	atom	cgnr	charge	mass
1	NPYD	1	LIG	N	1	-0.5670	14.0067
2	CB	1	LIG	C	2	-0.1500	12.0110
3	CB	1	LIG	C1	3	0.1900	12.0110
4	CB	1	LIG	C2	4	0.1600	12.0110
5	C5A	1	LIG	C3	5	0.1054	12.0110
6	NPYL	1	LIG	N1	6	0.0332	14.0067
7	C5A	1	LIG	CA	7	-0.3316	12.0110
8	C5B	1	LIG	C5	8	-0.0540	12.0110
9	C5B	1	LIG	C6	9	0.0000	12.0110
10	CB	1	LIG	C7	10	0.6740	12.0110
11	NPYD	1	LIG	N2	11	-0.6200	14.0067
12	CB	1	LIG	C8	12	0.0580	12.0110

13 CB 1 LIG C9 13 0.1900 12.0110  
 14 CB 1 LIG C10 14 0.1600 12.0110  
 15 NPYD 1 LIG N3 15 -0.6200 14.0067  
 16 OR 1 LIG O 16 -0.6800 15.9994  
 17 F 1 LIG F 17 -0.1900 18.9984  
 18 CR 1 LIG C4 18 0.4600 12.0110  
 19 F 1 LIG F1 19 -0.1900 18.9984  
 20 NM 1 LIG N4 20 -0.6980 14.0067  
 21 CR 1 LIG C11 21 -0.0500 12.0110  
 22 CR 1 LIG C12 22 0.0000 12.0110  
 23 CR 1 LIG C13 23 -0.0500 12.0110  
 24 CR 1 LIG C14 24 0.0000 12.0110  
 25 CR 1 LIG C15 25 0.0000 12.0110  
 26 CR 1 LIG C16 26 0.0000 12.0110  
 27 NM 1 LIG N5 27 -0.7300 14.0067  
 28 C=O 1 LIG C17 28 0.4100 12.0110  
 29 O=C 1 LIG O1 29 -0.5700 15.9994  
 30 NC=O 1 LIG N6 30 -0.6602 14.0067  
 31 CR 1 LIG C18 31 0.3001 12.0110  
 32 CR 1 LIG C19 32 0.0000 12.0110  
 33 CR 1 LIG C20 33 0.0000 12.0110  
 34 CR 1 LIG C21 34 0.3001 12.0110  
 35 HCMM 1 LIG H 35 0.1500 1.0079  
 36 HOR 1 LIG H3 36 0.4000 1.0079  
 37 HCMM 1 LIG H4 37 0.1500 1.0079  
 38 HNR 1 LIG H5 38 0.2700 1.0079  
 39 HCMM 1 LIG H1 39 0.0000 1.0079  
 40 HCMM 1 LIG H2 40 0.0000 1.0079  
 41 HCMM 1 LIG H6 41 0.1500 1.0079  
 42 HCMM 1 LIG H7 42 0.0000 1.0079  
 43 HCMM 1 LIG H8 43 0.0000 1.0079  
 44 HCMM 1 LIG H9 44 0.0000 1.0079  
 45 HCMM 1 LIG H10 45 0.0000 1.0079  
 46 HCMM 1 LIG H11 46 0.0000 1.0079  
 47 HCMM 1 LIG H12 47 0.0000 1.0079  
 48 HCMM 1 LIG H13 48 0.0000 1.0079  
 49 HCMM 1 LIG H14 49 0.0000 1.0079  
 50 HCMM 1 LIG H15 50 0.0000 1.0079  
 51 HCMM 1 LIG H16 51 0.0000 1.0079  
 52 HCMM 1 LIG H17 52 0.0000 1.0079  
 53 HCMM 1 LIG H18 53 0.0000 1.0079  
 54 HCMM 1 LIG H19 54 0.0000 1.0079  
 55 HCMM 1 LIG H20 55 0.0000 1.0079  
 56 HCMM 1 LIG H21 56 0.0000 1.0079  
 57 HCMM 1 LIG H22 57 0.0000 1.0079  
 58 HCMM 1 LIG H23 58 0.0000 1.0079  
 59 HCMM 1 LIG H24 59 -0.0000 1.0079

[ bonds ]

; ai aj fu b0 kb, b0 kb

38 6 1 0.10120 428294.3 0.10120 428294.3  
 36 16 1 0.09720 469365.3 0.09720 469365.3  
 16 18 1 0.14180 303937.5 0.14180 303937.5  
 6 5 1 0.13640 379454.5 0.13640 379454.5  
 6 7 1 0.13640 379454.5 0.13640 379454.5  
 1 5 1 0.13300 439556.0 0.13300 439556.0  
 1 4 1 0.13330 345489.6 0.13330 345489.6

39 18 1 0.10930 287014.9 0.10930 287014.9  
37 4 1 0.10840 319534.6 0.10840 319534.6  
18 7 1 0.14710 269852.1 0.14710 269852.1  
18 40 1 0.10930 287014.9 0.10930 287014.9  
5 9 1 0.13770 428655.8 0.13770 428655.8  
4 3 1 0.13740 335613.7 0.13740 335613.7  
7 8 1 0.13770 428655.8 0.13770 428655.8  
9 8 1 0.14180 259734.4 0.14180 259734.4  
9 2 1 0.13790 371023.7 0.13790 371023.7  
8 10 1 0.13790 371023.7 0.13790 371023.7  
3 2 1 0.13740 335613.7 0.13740 335613.7  
3 17 1 0.13420 392101.0 0.13420 392101.0  
2 35 1 0.10840 319534.6 0.10840 319534.6  
15 10 1 0.13330 345489.6 0.13330 345489.6  
15 14 1 0.13330 345489.6 0.13330 345489.6  
10 11 1 0.13330 345489.6 0.13330 345489.6  
11 12 1 0.13330 345489.6 0.13330 345489.6  
14 41 1 0.10840 319534.6 0.10840 319534.6  
14 13 1 0.13740 335613.7 0.13740 335613.7  
12 13 1 0.13740 335613.7 0.13740 335613.7  
12 20 1 0.13350 429799.7 0.13350 429799.7  
42 21 1 0.10930 287014.9 0.10930 287014.9  
13 19 1 0.13420 392101.0 0.13420 392101.0  
48 25 1 0.10930 287014.9 0.10930 287014.9  
51 26 1 0.10930 287014.9 0.10930 287014.9  
21 20 1 0.14440 268346.7 0.14440 268346.7  
21 26 1 0.15080 256422.3 0.15080 256422.3  
21 22 1 0.15080 256422.3 0.15080 256422.3  
45 23 1 0.10930 287014.9 0.10930 287014.9  
29 28 1 0.12220 779866.6 0.12220 779866.6  
26 25 1 0.15080 256422.3 0.15080 256422.3  
26 50 1 0.10930 287014.9 0.10930 287014.9  
43 22 1 0.10930 287014.9 0.10930 287014.9  
25 49 1 0.10930 287014.9 0.10930 287014.9  
25 24 1 0.15080 256422.3 0.15080 256422.3  
22 23 1 0.15080 256422.3 0.15080 256422.3  
22 44 1 0.10930 287014.9 0.10930 287014.9  
23 24 1 0.15080 256422.3 0.15080 256422.3  
23 27 1 0.14440 268346.7 0.14440 268346.7  
53 31 1 0.10930 287014.9 0.10930 287014.9  
46 24 1 0.10930 287014.9 0.10930 287014.9  
24 47 1 0.10930 287014.9 0.10930 287014.9  
28 27 1 0.13220 455755.6 0.13220 455755.6  
28 30 1 0.13690 351030.1 0.13690 351030.1  
31 52 1 0.10930 287014.9 0.10930 287014.9  
31 30 1 0.14360 280872.8 0.14360 280872.8  
31 32 1 0.15080 256422.3 0.15080 256422.3  
30 34 1 0.14360 280872.8 0.14360 280872.8  
55 32 1 0.10930 287014.9 0.10930 287014.9  
32 54 1 0.10930 287014.9 0.10930 287014.9  
32 33 1 0.15080 256422.3 0.15080 256422.3  
58 34 1 0.10930 287014.9 0.10930 287014.9  
34 59 1 0.10930 287014.9 0.10930 287014.9  
34 33 1 0.15080 256422.3 0.15080 256422.3  
33 56 1 0.10930 287014.9 0.10930 287014.9  
33 57 1 0.10930 287014.9 0.10930 287014.9

[ pairs ]  
; ai aj fu  
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5 10 1  
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57 59 1

[ angles ]

; ai aj ak fu th0 kth ub0 kub th0 kth ub0 kub

4	1	5	1	110.1810	740.72	110.1810	740.72
3	2	9	1	112.5670	254.73	112.5670	254.73
3	2	35	1	120.5710	339.05	120.5710	339.05
9	2	35	1	121.4460	314.95	121.4460	314.95
2	3	4	1	119.9770	402.88	119.9770	402.88
2	3	17	1	118.0650	658.81	118.0650	658.81
4	3	17	1	118.0650	658.81	118.0650	658.81
1	4	3	1	126.1390	358.92	126.1390	358.92
1	4	37	1	115.5880	417.33	115.5880	417.33
3	4	37	1	120.5710	339.05	120.5710	339.05
1	5	6	1	124.8140	615.46	124.8140	615.46
1	5	9	1	126.5130	548.01	126.5130	548.01
6	5	9	1	107.2550	489.59	107.2550	489.59



5	6	7	1	109.5990	693.74	109.5990	693.74
5	6	38	1	127.7700	331.82	127.7700	331.82
7	6	38	1	127.7700	331.82	127.7700	331.82
6	7	8	1	107.2550	489.59	107.2550	489.59
6	7	18	1	121.8320	563.07	121.8320	563.07
8	7	18	1	131.3780	443.83	131.3780	443.83
7	8	9	1	108.2390	521.51	108.2390	521.51
7	8	10	1	120.0000	602.21	120.0000	602.21
9	8	10	1	128.6730	464.91	128.6730	464.91
2	9	5	1	120.0000	602.21	120.0000	602.21
2	9	8	1	128.6730	464.91	128.6730	464.91
5	9	8	1	108.2390	521.51	108.2390	521.51
8	10	11	1	128.6730	464.91	128.6730	464.91
8	10	15	1	128.6730	464.91	128.6730	464.91
11	10	15	1	128.9380	436.60	128.9380	436.60
10	11	12	1	115.4060	653.40	115.4060	653.40
11	12	13	1	126.1390	358.92	126.1390	358.92
11	12	20	1	118.3490	691.34	118.3490	691.34
13	12	20	1	124.3840	566.68	124.3840	566.68
12	13	14	1	119.9770	402.88	119.9770	402.88
12	13	19	1	118.0650	658.81	118.0650	658.81
14	13	19	1	118.0650	658.81	118.0650	658.81
13	14	15	1	126.1390	358.92	126.1390	358.92
13	14	41	1	120.5710	339.05	120.5710	339.05
15	14	41	1	115.5880	417.33	115.5880	417.33
10	15	14	1	115.4060	653.40	115.4060	653.40
18	16	36	1	106.5030	477.55	106.5030	477.55
7	18	16	1	106.5350	813.59	106.5350	813.59
7	18	39	1	110.4670	373.97	110.4670	373.97
7	18	40	1	110.4670	373.97	110.4670	373.97
16	18	39	1	108.5770	470.32	108.5770	470.32
16	18	40	1	108.5770	470.32	108.5770	470.32
39	18	40	1	108.8360	310.74	108.8360	310.74
12	20	21	1	120.0000	602.21	120.0000	602.21
20	21	22	1	109.5000	602.21	109.5000	602.21
20	21	26	1	109.5000	602.21	109.5000	602.21
20	21	42	1	113.0350	394.45	113.0350	394.45
22	21	26	1	109.6080	512.48	109.6080	512.48
22	21	42	1	110.5490	383.00	110.5490	383.00
26	21	42	1	110.5490	383.00	110.5490	383.00
21	22	23	1	109.6080	512.48	109.6080	512.48
21	22	43	1	110.5490	383.00	110.5490	383.00
21	22	44	1	110.5490	383.00	110.5490	383.00
23	22	43	1	110.5490	383.00	110.5490	383.00
23	22	44	1	110.5490	383.00	110.5490	383.00
43	22	44	1	108.8360	310.74	108.8360	310.74
22	23	24	1	109.6080	512.48	109.6080	512.48
22	23	27	1	109.5000	602.21	109.5000	602.21
22	23	45	1	110.5490	383.00	110.5490	383.00
24	23	27	1	109.5000	602.21	109.5000	602.21
24	23	45	1	110.5490	383.00	110.5490	383.00
27	23	45	1	113.0350	394.45	113.0350	394.45
23	24	25	1	109.6080	512.48	109.6080	512.48
23	24	46	1	110.5490	383.00	110.5490	383.00
23	24	47	1	110.5490	383.00	110.5490	383.00
25	24	46	1	110.5490	383.00	110.5490	383.00
25	24	47	1	110.5490	383.00	110.5490	383.00

46	24	47	1	108.8360	310.74	108.8360	310.74
24	25	26	1	109.6080	512.48	109.6080	512.48
24	25	48	1	110.5490	383.00	110.5490	383.00
24	25	49	1	110.5490	383.00	110.5490	383.00
26	25	48	1	110.5490	383.00	110.5490	383.00
26	25	49	1	110.5490	383.00	110.5490	383.00
48	25	49	1	108.8360	310.74	108.8360	310.74
21	26	25	1	109.6080	512.48	109.6080	512.48
21	26	50	1	110.5490	383.00	110.5490	383.00
21	26	51	1	110.5490	383.00	110.5490	383.00
25	26	50	1	110.5490	383.00	110.5490	383.00
25	26	51	1	110.5490	383.00	110.5490	383.00
50	26	51	1	108.8360	310.74	108.8360	310.74
23	27	28	1	120.0000	602.21	120.0000	602.21
27	28	29	1	129.3490	679.89	129.3490	679.89
27	28	30	1	120.0000	602.21	120.0000	602.21
29	28	30	1	127.1520	546.20	127.1520	546.20
28	30	31	1	119.6000	494.41	119.6000	494.41
28	30	34	1	119.6000	494.41	119.6000	494.41
31	30	34	1	117.9090	672.67	117.9090	672.67
30	31	32	1	109.9600	632.32	109.9600	632.32
30	31	52	1	107.6460	445.64	107.6460	445.64
30	31	53	1	107.6460	445.64	107.6460	445.64
32	31	52	1	110.5490	383.00	110.5490	383.00
32	31	53	1	110.5490	383.00	110.5490	383.00
52	31	53	1	108.8360	310.74	108.8360	310.74
31	32	33	1	109.6080	512.48	109.6080	512.48
31	32	54	1	110.5490	383.00	110.5490	383.00
31	32	55	1	110.5490	383.00	110.5490	383.00
33	32	54	1	110.5490	383.00	110.5490	383.00
33	32	55	1	110.5490	383.00	110.5490	383.00
54	32	55	1	108.8360	310.74	108.8360	310.74
32	33	34	1	109.6080	512.48	109.6080	512.48
32	33	56	1	110.5490	383.00	110.5490	383.00
32	33	57	1	110.5490	383.00	110.5490	383.00
34	33	56	1	110.5490	383.00	110.5490	383.00
34	33	57	1	110.5490	383.00	110.5490	383.00
56	33	57	1	108.8360	310.74	108.8360	310.74
30	34	33	1	109.9600	632.32	109.9600	632.32
30	34	58	1	107.6460	445.64	107.6460	445.64
30	34	59	1	107.6460	445.64	107.6460	445.64
33	34	58	1	110.5490	383.00	110.5490	383.00
33	34	59	1	110.5490	383.00	110.5490	383.00
58	34	59	1	108.8360	310.74	108.8360	310.74

[ dihedrals ]

; ai aj ak al fu phi0 kphi mult phi0 kphi mult

1	4	3	2	9	180.00	14.6440	2	180.00	14.6440	2
1	4	3	17	9	180.00	14.6440	2	180.00	14.6440	2
1	5	6	7	9	180.00	8.3680	2	180.00	8.3680	2
1	5	6	38	9	180.00	8.3680	2	180.00	8.3680	2
1	5	9	2	9	180.00	14.6440	2	180.00	14.6440	2
1	5	9	8	9	180.00	14.6440	2	180.00	14.6440	2
2	3	4	37	9	180.00	14.6440	2	180.00	14.6440	2
2	9	5	6	9	180.00	14.6440	2	180.00	14.6440	2
2	9	8	7	9	180.00	14.6440	2	180.00	14.6440	2
2	9	8	10	9	180.00	14.6440	2	180.00	14.6440	2

3	2	9	5	9	180.00	14.6440	2	180.00	14.6440	2
3	2	9	8	9	180.00	14.6440	2	180.00	14.6440	2
3	4	1	5	9	180.00	14.6440	2	180.00	14.6440	2
4	1	5	6	9	180.00	14.6440	2	180.00	14.6440	2
4	1	5	9	9	180.00	14.6440	2	180.00	14.6440	2
4	3	2	9	9	180.00	14.6440	2	180.00	14.6440	2
4	3	2	35	9	180.00	14.6440	2	180.00	14.6440	2
5	1	4	37	9	180.00	14.6440	2	180.00	14.6440	2
5	6	7	8	9	180.00	8.3680	2	180.00	8.3680	2
5	6	7	18	9	180.00	8.3680	2	180.00	8.3680	2
5	9	2	35	9	180.00	14.6440	2	180.00	14.6440	2
5	9	8	7	9	180.00	14.6440	2	180.00	14.6440	2
5	9	8	10	9	180.00	14.6440	2	180.00	14.6440	2
6	5	9	8	9	180.00	14.6440	2	180.00	14.6440	2
6	7	8	9	9	180.00	14.6440	2	180.00	14.6440	2
6	7	8	10	9	180.00	14.6440	2	180.00	14.6440	2
7	6	5	9	9	180.00	8.3680	2	180.00	8.3680	2
7	8	10	11	9	180.00	3.7656	2	180.00	3.7656	2
7	8	10	15	9	180.00	3.7656	2	180.00	3.7656	2
7	18	16	36	9	0.00	0.4184	3	0.00	0.4184	3
8	7	6	38	9	180.00	8.3680	2	180.00	8.3680	2
8	9	2	35	9	180.00	14.6440	2	180.00	14.6440	2
9	2	3	17	9	180.00	14.6440	2	180.00	14.6440	2
9	5	6	38	9	180.00	8.3680	2	180.00	8.3680	2
9	8	7	18	9	180.00	14.6440	2	180.00	14.6440	2
9	8	10	11	9	180.00	3.7656	2	180.00	3.7656	2
9	8	10	15	9	180.00	3.7656	2	180.00	3.7656	2
10	11	12	13	9	180.00	14.6440	2	180.00	14.6440	2
10	11	12	20	9	180.00	14.6440	2	180.00	14.6440	2
10	15	14	13	9	180.00	14.6440	2	180.00	14.6440	2
10	15	14	41	9	180.00	14.6440	2	180.00	14.6440	2
11	10	15	14	9	180.00	14.6440	2	180.00	14.6440	2
11	12	13	14	9	180.00	14.6440	2	180.00	14.6440	2
11	12	13	19	9	180.00	14.6440	2	180.00	14.6440	2
11	12	20	21	9	180.00	7.5312	2	180.00	7.5312	2
12	11	10	15	9	180.00	14.6440	2	180.00	14.6440	2
12	13	14	15	9	180.00	14.6440	2	180.00	14.6440	2
12	13	14	41	9	180.00	14.6440	2	180.00	14.6440	2
12	20	21	22	9	0.00	0.5230	3	0.00	0.5230	3
12	20	21	26	9	0.00	0.5230	3	0.00	0.5230	3
12	20	21	42	9	0.00	0.5230	3	0.00	0.5230	3
13	12	20	21	9	180.00	7.5312	2	180.00	7.5312	2
14	13	12	20	9	180.00	14.6440	2	180.00	14.6440	2
15	14	13	19	9	180.00	14.6440	2	180.00	14.6440	2
17	3	2	35	9	180.00	14.6440	2	180.00	14.6440	2
17	3	4	37	9	180.00	14.6440	2	180.00	14.6440	2
18	7	6	38	9	180.00	8.3680	2	180.00	8.3680	2
19	13	12	20	9	180.00	14.6440	2	180.00	14.6440	2
19	13	14	41	9	180.00	14.6440	2	180.00	14.6440	2
20	21	22	23	9	0.00	0.6276	3	0.00	0.6276	3
20	21	22	43	9	0.00	0.6276	3	0.00	0.6276	3
20	21	22	44	9	0.00	0.6276	3	0.00	0.6276	3
20	21	26	25	9	0.00	0.6276	3	0.00	0.6276	3
20	21	26	50	9	0.00	0.6276	3	0.00	0.6276	3
20	21	26	51	9	0.00	0.6276	3	0.00	0.6276	3
21	22	23	24	9	0.00	0.2134	1	0.00	0.2134	1
21	22	23	24	9	180.00	1.4267	2	180.00	1.4267	2

21 22 23 24 9 0.00 0.6945 3 0.00 0.6945 3  
21 22 23 27 9 0.00 0.6276 3 0.00 0.6276 3  
21 22 23 45 9 0.00 1.3389 1 0.00 1.3389 1  
21 22 23 45 9 180.00 -1.3180 2 180.00 -1.3180 2  
21 22 23 45 9 0.00 0.5523 3 0.00 0.5523 3  
21 26 25 24 9 0.00 0.2134 1 0.00 0.2134 1  
21 26 25 24 9 180.00 1.4267 2 180.00 1.4267 2  
21 26 25 24 9 0.00 0.6945 3 0.00 0.6945 3  
21 26 25 48 9 0.00 1.3389 1 0.00 1.3389 1  
21 26 25 48 9 180.00 -1.3180 2 180.00 -1.3180 2  
21 26 25 48 9 0.00 0.5523 3 0.00 0.5523 3  
21 26 25 49 9 0.00 1.3389 1 0.00 1.3389 1  
21 26 25 49 9 180.00 -1.3180 2 180.00 -1.3180 2  
21 26 25 49 9 0.00 0.5523 3 0.00 0.5523 3  
22 21 26 25 9 0.00 0.2134 1 0.00 0.2134 1  
22 21 26 25 9 180.00 1.4267 2 180.00 1.4267 2  
22 21 26 25 9 0.00 0.6945 3 0.00 0.6945 3  
22 21 26 50 9 0.00 1.3389 1 0.00 1.3389 1  
22 21 26 50 9 180.00 -1.3180 2 180.00 -1.3180 2  
22 21 26 50 9 0.00 0.5523 3 0.00 0.5523 3  
22 21 26 51 9 0.00 1.3389 1 0.00 1.3389 1  
22 21 26 51 9 180.00 -1.3180 2 180.00 -1.3180 2  
22 21 26 51 9 0.00 0.5523 3 0.00 0.5523 3  
22 23 24 25 9 0.00 0.2134 1 0.00 0.2134 1  
22 23 24 25 9 180.00 1.4267 2 180.00 1.4267 2  
22 23 24 25 9 0.00 0.6945 3 0.00 0.6945 3  
22 23 24 46 9 0.00 1.3389 1 0.00 1.3389 1  
22 23 24 46 9 180.00 -1.3180 2 180.00 -1.3180 2  
22 23 24 46 9 0.00 0.5523 3 0.00 0.5523 3  
22 23 24 47 9 0.00 1.3389 1 0.00 1.3389 1  
22 23 24 47 9 180.00 -1.3180 2 180.00 -1.3180 2  
22 23 24 47 9 0.00 0.5523 3 0.00 0.5523 3  
22 23 27 28 9 0.00 0.5230 3 0.00 0.5230 3  
23 22 21 26 9 0.00 0.2134 1 0.00 0.2134 1  
23 22 21 26 9 180.00 1.4267 2 180.00 1.4267 2  
23 22 21 26 9 0.00 0.6945 3 0.00 0.6945 3  
23 22 21 42 9 0.00 1.3389 1 0.00 1.3389 1  
23 22 21 42 9 180.00 -1.3180 2 180.00 -1.3180 2  
23 22 21 42 9 0.00 0.5523 3 0.00 0.5523 3  
23 24 25 26 9 0.00 0.2134 1 0.00 0.2134 1  
23 24 25 26 9 180.00 1.4267 2 180.00 1.4267 2  
23 24 25 26 9 0.00 0.6945 3 0.00 0.6945 3  
23 24 25 48 9 0.00 1.3389 1 0.00 1.3389 1  
23 24 25 48 9 180.00 -1.3180 2 180.00 -1.3180 2  
23 24 25 48 9 0.00 0.5523 3 0.00 0.5523 3  
23 24 25 49 9 0.00 1.3389 1 0.00 1.3389 1  
23 24 25 49 9 180.00 -1.3180 2 180.00 -1.3180 2  
23 24 25 49 9 0.00 0.5523 3 0.00 0.5523 3  
23 27 28 29 9 180.00 7.5312 2 180.00 7.5312 2  
23 27 28 30 9 180.00 7.5312 2 180.00 7.5312 2  
24 23 22 43 9 0.00 1.3389 1 0.00 1.3389 1  
24 23 22 43 9 180.00 -1.3180 2 180.00 -1.3180 2  
24 23 22 43 9 0.00 0.5523 3 0.00 0.5523 3  
24 23 22 44 9 0.00 1.3389 1 0.00 1.3389 1  
24 23 22 44 9 180.00 -1.3180 2 180.00 -1.3180 2  
24 23 22 44 9 0.00 0.5523 3 0.00 0.5523 3  
24 23 27 28 9 0.00 0.5230 3 0.00 0.5230 3

24 25 26 50 9 0.00 1.3389 1 0.00 1.3389 1  
24 25 26 50 9 180.00 -1.3180 2 180.00 -1.3180 2  
24 25 26 50 9 0.00 0.5523 3 0.00 0.5523 3  
24 25 26 51 9 0.00 1.3389 1 0.00 1.3389 1  
24 25 26 51 9 180.00 -1.3180 2 180.00 -1.3180 2  
24 25 26 51 9 0.00 0.5523 3 0.00 0.5523 3  
25 24 23 27 9 0.00 0.6276 3 0.00 0.6276 3  
25 24 23 45 9 0.00 1.3389 1 0.00 1.3389 1  
25 24 23 45 9 180.00 -1.3180 2 180.00 -1.3180 2  
25 24 23 45 9 0.00 0.5523 3 0.00 0.5523 3  
25 26 21 42 9 0.00 1.3389 1 0.00 1.3389 1  
25 26 21 42 9 180.00 -1.3180 2 180.00 -1.3180 2  
25 26 21 42 9 0.00 0.5523 3 0.00 0.5523 3  
26 21 22 43 9 0.00 1.3389 1 0.00 1.3389 1  
26 21 22 43 9 180.00 -1.3180 2 180.00 -1.3180 2  
26 21 22 43 9 0.00 0.5523 3 0.00 0.5523 3  
26 21 22 44 9 0.00 1.3389 1 0.00 1.3389 1  
26 21 22 44 9 180.00 -1.3180 2 180.00 -1.3180 2  
26 21 22 44 9 0.00 0.5523 3 0.00 0.5523 3  
26 25 24 46 9 0.00 1.3389 1 0.00 1.3389 1  
26 25 24 46 9 180.00 -1.3180 2 180.00 -1.3180 2  
26 25 24 46 9 0.00 0.5523 3 0.00 0.5523 3  
26 25 24 47 9 0.00 1.3389 1 0.00 1.3389 1  
26 25 24 47 9 180.00 -1.3180 2 180.00 -1.3180 2  
26 25 24 47 9 0.00 0.5523 3 0.00 0.5523 3  
27 23 22 43 9 0.00 0.6276 3 0.00 0.6276 3  
27 23 22 44 9 0.00 0.6276 3 0.00 0.6276 3  
27 23 24 46 9 0.00 0.6276 3 0.00 0.6276 3  
27 23 24 47 9 0.00 0.6276 3 0.00 0.6276 3  
27 28 30 31 9 180.00 12.5520 2 180.00 12.5520 2  
27 28 30 34 9 180.00 12.5520 2 180.00 12.5520 2  
28 27 23 45 9 0.00 0.5230 3 0.00 0.5230 3  
28 30 31 32 9 0.00 -2.1464 1 0.00 -2.1464 1  
28 30 31 32 9 180.00 1.4518 2 180.00 1.4518 2  
28 30 31 32 9 0.00 1.9832 3 0.00 1.9832 3  
28 30 31 52 9 0.00 -4.3932 1 0.00 -4.3932 1  
28 30 31 52 9 180.00 2.8493 2 180.00 2.8493 2  
28 30 31 52 9 0.00 0.0460 3 0.00 0.0460 3  
28 30 31 53 9 0.00 -4.3932 1 0.00 -4.3932 1  
28 30 31 53 9 180.00 2.8493 2 180.00 2.8493 2  
28 30 31 53 9 0.00 0.0460 3 0.00 0.0460 3  
28 30 34 33 9 0.00 -2.1464 1 0.00 -2.1464 1  
28 30 34 33 9 180.00 1.4518 2 180.00 1.4518 2  
28 30 34 33 9 0.00 1.9832 3 0.00 1.9832 3  
28 30 34 58 9 0.00 -4.3932 1 0.00 -4.3932 1  
28 30 34 58 9 180.00 2.8493 2 180.00 2.8493 2  
28 30 34 58 9 0.00 0.0460 3 0.00 0.0460 3  
28 30 34 59 9 0.00 -4.3932 1 0.00 -4.3932 1  
28 30 34 59 9 180.00 2.8493 2 180.00 2.8493 2  
28 30 34 59 9 0.00 0.0460 3 0.00 0.0460 3  
29 28 30 31 9 0.00 -0.6694 1 0.00 -0.6694 1  
29 28 30 31 9 180.00 13.1670 2 180.00 13.1670 2  
29 28 30 31 9 0.00 -0.3054 3 0.00 -0.3054 3  
29 28 30 34 9 0.00 -0.6694 1 0.00 -0.6694 1  
29 28 30 34 9 180.00 13.1670 2 180.00 13.1670 2  
29 28 30 34 9 0.00 -0.3054 3 0.00 -0.3054 3  
30 31 32 33 9 0.00 0.6276 3 0.00 0.6276 3

30	31	32	54	9	0.00	0.8912	3	0.00	0.8912	3
30	31	32	55	9	0.00	0.8912	3	0.00	0.8912	3
30	34	33	32	9	0.00	0.6276	3	0.00	0.6276	3
30	34	33	56	9	0.00	0.8912	3	0.00	0.8912	3
30	34	33	57	9	0.00	0.8912	3	0.00	0.8912	3
31	30	34	33	9	0.00	0.6276	3	0.00	0.6276	3
31	30	34	58	9	0.00	1.6318	3	0.00	1.6318	3
31	30	34	59	9	0.00	1.6318	3	0.00	1.6318	3
31	32	33	34	9	0.00	0.2134	1	0.00	0.2134	1
31	32	33	34	9	180.00	1.4267	2	180.00	1.4267	2
31	32	33	34	9	0.00	0.6945	3	0.00	0.6945	3
31	32	33	56	9	0.00	1.3389	1	0.00	1.3389	1
31	32	33	56	9	180.00	-1.3180	2	180.00	-1.3180	2
31	32	33	56	9	0.00	0.5523	3	0.00	0.5523	3
31	32	33	57	9	0.00	1.3389	1	0.00	1.3389	1
31	32	33	57	9	180.00	-1.3180	2	180.00	-1.3180	2
31	32	33	57	9	0.00	0.5523	3	0.00	0.5523	3
32	31	30	34	9	0.00	0.6276	3	0.00	0.6276	3
32	33	34	58	9	0.00	1.3389	1	0.00	1.3389	1
32	33	34	58	9	180.00	-1.3180	2	180.00	-1.3180	2
32	33	34	58	9	0.00	0.5523	3	0.00	0.5523	3
32	33	34	59	9	0.00	1.3389	1	0.00	1.3389	1
32	33	34	59	9	180.00	-1.3180	2	180.00	-1.3180	2
32	33	34	59	9	0.00	0.5523	3	0.00	0.5523	3
33	32	31	52	9	0.00	1.3389	1	0.00	1.3389	1
33	32	31	52	9	180.00	-1.3180	2	180.00	-1.3180	2
33	32	31	52	9	0.00	0.5523	3	0.00	0.5523	3
33	32	31	53	9	0.00	1.3389	1	0.00	1.3389	1
33	32	31	53	9	180.00	-1.3180	2	180.00	-1.3180	2
33	32	31	53	9	0.00	0.5523	3	0.00	0.5523	3
34	30	31	52	9	0.00	1.6318	3	0.00	1.6318	3
34	30	31	53	9	0.00	1.6318	3	0.00	1.6318	3
34	33	32	54	9	0.00	1.3389	1	0.00	1.3389	1
34	33	32	54	9	180.00	-1.3180	2	180.00	-1.3180	2
34	33	32	54	9	0.00	0.5523	3	0.00	0.5523	3
34	33	32	55	9	0.00	1.3389	1	0.00	1.3389	1
34	33	32	55	9	180.00	-1.3180	2	180.00	-1.3180	2
34	33	32	55	9	0.00	0.5523	3	0.00	0.5523	3
36	16	18	39	9	0.00	1.2468	1	0.00	1.2468	1
36	16	18	39	9	180.00	-0.5774	2	180.00	-0.5774	2
36	16	18	39	9	0.00	0.7238	3	0.00	0.7238	3
36	16	18	40	9	0.00	1.2468	1	0.00	1.2468	1
36	16	18	40	9	180.00	-0.5774	2	180.00	-0.5774	2
36	16	18	40	9	0.00	0.7238	3	0.00	0.7238	3
42	21	22	43	9	0.00	0.5941	1	0.00	0.5941	1
42	21	22	43	9	180.00	-2.8995	2	180.00	-2.8995	2
42	21	22	43	9	0.00	0.6569	3	0.00	0.6569	3
42	21	22	44	9	0.00	0.5941	1	0.00	0.5941	1
42	21	22	44	9	180.00	-2.8995	2	180.00	-2.8995	2
42	21	22	44	9	0.00	0.6569	3	0.00	0.6569	3
42	21	26	50	9	0.00	0.5941	1	0.00	0.5941	1
42	21	26	50	9	180.00	-2.8995	2	180.00	-2.8995	2
42	21	26	50	9	0.00	0.6569	3	0.00	0.6569	3
42	21	26	51	9	0.00	0.5941	1	0.00	0.5941	1
42	21	26	51	9	180.00	-2.8995	2	180.00	-2.8995	2
42	21	26	51	9	0.00	0.6569	3	0.00	0.6569	3
43	22	23	45	9	0.00	0.5941	1	0.00	0.5941	1

43 22 23 45 9 180.00 -2.8995 2 180.00 -2.8995 2  
43 22 23 45 9 0.00 0.6569 3 0.00 0.6569 3  
44 22 23 45 9 0.00 0.5941 1 0.00 0.5941 1  
44 22 23 45 9 180.00 -2.8995 2 180.00 -2.8995 2  
44 22 23 45 9 0.00 0.6569 3 0.00 0.6569 3  
45 23 24 46 9 0.00 0.5941 1 0.00 0.5941 1  
45 23 24 46 9 180.00 -2.8995 2 180.00 -2.8995 2  
45 23 24 46 9 0.00 0.6569 3 0.00 0.6569 3  
45 23 24 47 9 0.00 0.5941 1 0.00 0.5941 1  
45 23 24 47 9 180.00 -2.8995 2 180.00 -2.8995 2  
45 23 24 47 9 0.00 0.6569 3 0.00 0.6569 3  
46 24 25 48 9 0.00 0.5941 1 0.00 0.5941 1  
46 24 25 48 9 180.00 -2.8995 2 180.00 -2.8995 2  
46 24 25 48 9 0.00 0.6569 3 0.00 0.6569 3  
46 24 25 49 9 0.00 0.5941 1 0.00 0.5941 1  
46 24 25 49 9 180.00 -2.8995 2 180.00 -2.8995 2  
46 24 25 49 9 0.00 0.6569 3 0.00 0.6569 3  
47 24 25 48 9 0.00 0.5941 1 0.00 0.5941 1  
47 24 25 48 9 180.00 -2.8995 2 180.00 -2.8995 2  
47 24 25 48 9 0.00 0.6569 3 0.00 0.6569 3  
47 24 25 49 9 0.00 0.5941 1 0.00 0.5941 1  
47 24 25 49 9 180.00 -2.8995 2 180.00 -2.8995 2  
47 24 25 49 9 0.00 0.6569 3 0.00 0.6569 3  
48 25 26 50 9 0.00 0.5941 1 0.00 0.5941 1  
48 25 26 50 9 180.00 -2.8995 2 180.00 -2.8995 2  
48 25 26 50 9 0.00 0.6569 3 0.00 0.6569 3  
48 25 26 51 9 0.00 0.5941 1 0.00 0.5941 1  
48 25 26 51 9 180.00 -2.8995 2 180.00 -2.8995 2  
48 25 26 51 9 0.00 0.6569 3 0.00 0.6569 3  
49 25 26 50 9 0.00 0.5941 1 0.00 0.5941 1  
49 25 26 50 9 180.00 -2.8995 2 180.00 -2.8995 2  
49 25 26 50 9 0.00 0.6569 3 0.00 0.6569 3  
49 25 26 51 9 0.00 0.5941 1 0.00 0.5941 1  
49 25 26 51 9 180.00 -2.8995 2 180.00 -2.8995 2  
49 25 26 51 9 0.00 0.6569 3 0.00 0.6569 3  
52 31 32 54 9 0.00 0.5941 1 0.00 0.5941 1  
52 31 32 54 9 180.00 -2.8995 2 180.00 -2.8995 2  
52 31 32 54 9 0.00 0.6569 3 0.00 0.6569 3  
52 31 32 55 9 0.00 0.5941 1 0.00 0.5941 1  
52 31 32 55 9 180.00 -2.8995 2 180.00 -2.8995 2  
52 31 32 55 9 0.00 0.6569 3 0.00 0.6569 3  
53 31 32 54 9 0.00 0.5941 1 0.00 0.5941 1  
53 31 32 54 9 180.00 -2.8995 2 180.00 -2.8995 2  
53 31 32 54 9 0.00 0.6569 3 0.00 0.6569 3  
53 31 32 55 9 0.00 0.5941 1 0.00 0.5941 1  
53 31 32 55 9 180.00 -2.8995 2 180.00 -2.8995 2  
53 31 32 55 9 0.00 0.6569 3 0.00 0.6569 3  
54 32 33 56 9 0.00 0.5941 1 0.00 0.5941 1  
54 32 33 56 9 180.00 -2.8995 2 180.00 -2.8995 2  
54 32 33 56 9 0.00 0.6569 3 0.00 0.6569 3  
54 32 33 57 9 0.00 0.5941 1 0.00 0.5941 1  
54 32 33 57 9 180.00 -2.8995 2 180.00 -2.8995 2  
54 32 33 57 9 0.00 0.6569 3 0.00 0.6569 3  
55 32 33 56 9 0.00 0.5941 1 0.00 0.5941 1  
55 32 33 56 9 180.00 -2.8995 2 180.00 -2.8995 2  
55 32 33 56 9 0.00 0.6569 3 0.00 0.6569 3  
55 32 33 57 9 0.00 0.5941 1 0.00 0.5941 1

```

55 32 33 57 9 180.00 -2.8995 2 180.00 -2.8995 2
55 32 33 57 9 0.00 0.6569 3 0.00 0.6569 3
56 33 34 58 9 0.00 0.5941 1 0.00 0.5941 1
56 33 34 58 9 180.00 -2.8995 2 180.00 -2.8995 2
56 33 34 58 9 0.00 0.6569 3 0.00 0.6569 3
56 33 34 59 9 0.00 0.5941 1 0.00 0.5941 1
56 33 34 59 9 180.00 -2.8995 2 180.00 -2.8995 2
56 33 34 59 9 0.00 0.6569 3 0.00 0.6569 3
57 33 34 58 9 0.00 0.5941 1 0.00 0.5941 1
57 33 34 58 9 180.00 -2.8995 2 180.00 -2.8995 2
57 33 34 58 9 0.00 0.6569 3 0.00 0.6569 3
57 33 34 59 9 0.00 0.5941 1 0.00 0.5941 1
57 33 34 59 9 180.00 -2.8995 2 180.00 -2.8995 2
57 33 34 59 9 0.00 0.6569 3 0.00 0.6569 3

```

[ dihedrals ]

```

; ai aj ak al fu xi0 kxi xi0 kxi
4 3 1 37 2 0.00 27.6981 0.00 27.6981
3 2 4 17 2 0.00 21.0790 0.00 21.0790
5 9 1 6 2 0.00 30.1081 0.00 30.1081
6 7 5 38 2 0.00 -8.4349 0.00 -8.4349
7 8 6 18 2 0.00 30.1081 0.00 30.1081
8 9 7 10 2 0.00 -6.6275 0.00 -6.6275
10 11 8 15 2 0.00 21.0790 0.00 21.0790
12 20 11 13 2 0.00 21.0790 0.00 21.0790
18 16 7 39 2 0.00 0.0000 0.00 0.0000
18 16 7 40 2 0.00 0.0000 0.00 0.0000
13 14 12 19 2 0.00 21.0790 0.00 21.0790
21 22 20 26 2 0.00 0.0000 0.00 0.0000
21 26 20 42 2 0.00 0.0000 0.00 0.0000
22 23 21 43 2 0.00 0.0000 0.00 0.0000
22 43 21 44 2 0.00 0.0000 0.00 0.0000
23 27 22 24 2 0.00 0.0000 0.00 0.0000
23 24 22 45 2 0.00 0.0000 0.00 0.0000
26 25 21 51 2 0.00 0.0000 0.00 0.0000
26 51 21 50 2 0.00 0.0000 0.00 0.0000
28 30 27 29 2 0.00 78.2910 0.00 78.2910
30 31 28 34 2 0.00 -12.0416 0.00 -12.0416
31 32 30 53 2 0.00 0.0000 0.00 0.0000
31 53 30 52 2 0.00 0.0000 0.00 0.0000
32 33 31 55 2 0.00 0.0000 0.00 0.0000
32 55 31 54 2 0.00 0.0000 0.00 0.0000
2 9 3 35 2 0.00 7.2300 0.00 7.2300
14 13 15 41 2 0.00 27.6981 0.00 27.6981
24 25 23 46 2 0.00 0.0000 0.00 0.0000
24 25 23 47 2 0.00 0.0000 0.00 0.0000
25 24 26 48 2 0.00 0.0000 0.00 0.0000
25 48 26 49 2 0.00 0.0000 0.00 0.0000
33 34 32 56 2 0.00 0.0000 0.00 0.0000
33 34 32 57 2 0.00 0.0000 0.00 0.0000
34 33 30 58 2 0.00 0.0000 0.00 0.0000
34 58 30 59 2 0.00 0.0000 0.00 0.0000

```

3) The inhibitor (16):

[ atomtypes ]

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; name at.num mass charge ptype sigma epsilon

```



NPYD	7	14.0067	0.0	A	0.329632	0.836800
CB	6	12.0110	0.0	A	0.355005	0.292880
C5A	6	12.0110	0.0	A	0.363487	0.209200
NPYL	7	14.0067	0.0	A	0.306469	0.376560
C5B	6	12.0110	0.0	A	0.363487	0.209200
F	9	18.9984	0.0	A	0.290433	0.564840
CR	6	12.0110	0.0	A	0.387541	0.230120
NM	7	14.0067	0.0	A	0.329632	0.836800
C=O	6	12.0110	0.0	A	0.356359	0.460240
O=C	8	15.9994	0.0	A	0.302905	0.502080
NC=O	7	14.0067	0.0	A	0.329632	0.836800
HCMM	1	1.0079	0.0	A	0.235197	0.092048
HNR	1	1.0079	0.0	A	0.040001	0.192464

[ pairtypes ]

; i j func sigmal-4 epsilon1-4 ; THESE ARE 1-4 INTERACTIONS

CR	NPYD	1	0.334087	0.187114
CR	CB	1	0.346773	0.110698
CR	C5A	1	0.351014	0.093557
CR	NPYL	1	0.322505	0.125520
CR	C5B	1	0.351014	0.093557
CR	F	1	0.314487	0.153730
CR	CR	1	0.338541	0.041840
CR	NM	1	0.334087	0.187114
CR	C=O	1	0.347450	0.138768
CR	O=C	1	0.293997	0.144938
CR	NC=O	1	0.334087	0.187114
CR	HCMM	1	0.286869	0.062059
CR	HNR	1	0.189271	0.089737
O=C	NPYD	1	0.289542	0.648182
O=C	CB	1	0.302228	0.383470
O=C	C5A	1	0.306469	0.324091
O=C	NPYL	1	0.277960	0.434814
O=C	C5B	1	0.306469	0.324091
O=C	F	1	0.269942	0.532536
O=C	NM	1	0.289542	0.648182
O=C	C=O	1	0.302905	0.480705
O=C	O=C	1	0.249452	0.502080
O=C	NC=O	1	0.289542	0.648182
O=C	HCMM	1	0.242324	0.214978
O=C	HNR	1	0.144726	0.310857

[ moleculetype ]

; Name nrexcl

16 3

[ atoms ]

; nr type resnr resid atom cgnr charge mass

1	NPYD	1	LIG	N	1	-0.5670	14.0067
2	CB	1	LIG	C	2	-0.1500	12.0110
3	CB	1	LIG	C1	3	0.1900	12.0110
4	CB	1	LIG	C2	4	0.1600	12.0110
5	C5A	1	LIG	C3	5	0.1054	12.0110
6	NPYL	1	LIG	N1	6	0.0332	14.0067
7	C5A	1	LIG	C4	7	-0.3316	12.0110
8	C5B	1	LIG	C6	8	-0.0540	12.0110

9 C5B 1 LIG C7 9 0.0000 12.0110  
10 CB 1 LIG C8 10 0.6740 12.0110  
11 NPYD 1 LIG N2 11 -0.6200 14.0067  
12 CB 1 LIG C9 12 0.0580 12.0110  
13 CB 1 LIG C10 13 0.1900 12.0110  
14 CB 1 LIG C11 14 0.1600 12.0110  
15 NPYD 1 LIG N3 15 -0.6200 14.0067  
16 F 1 LIG F 16 -0.1900 18.9984  
17 CR 1 LIG C5 17 0.1800 12.0110  
18 F 1 LIG F1 18 -0.1900 18.9984  
19 NM 1 LIG N4 19 -0.6980 14.0067  
20 CR 1 LIG C12 20 -0.0500 12.0110  
21 CR 1 LIG C13 21 0.0000 12.0110  
22 CR 1 LIG C14 22 -0.0500 12.0110  
23 CR 1 LIG C15 23 0.0000 12.0110  
24 CR 1 LIG C16 24 0.0000 12.0110  
25 CR 1 LIG C17 25 0.0000 12.0110  
26 NM 1 LIG N5 26 -0.7300 14.0067  
27 C=O 1 LIG C18 27 0.4100 12.0110  
28 O=C 1 LIG O 28 -0.5700 15.9994  
29 NC=O 1 LIG N6 29 -0.6602 14.0067  
30 CR 1 LIG C19 30 0.3001 12.0110  
31 CR 1 LIG C20 31 0.0000 12.0110  
32 CR 1 LIG C21 32 0.0000 12.0110  
33 CR 1 LIG C22 33 0.3001 12.0110  
34 HCMM 1 LIG H 34 0.1500 1.0079  
35 HCMM 1 LIG H1 35 0.1500 1.0079  
36 HNR 1 LIG H2 36 0.2700 1.0079  
37 HCMM 1 LIG H3 37 0.0000 1.0079  
38 HCMM 1 LIG H4 38 0.0000 1.0079  
39 HCMM 1 LIG H5 39 0.0000 1.0079  
40 HCMM 1 LIG H6 40 0.1500 1.0079  
41 HCMM 1 LIG H7 41 0.0000 1.0079  
42 HCMM 1 LIG H8 42 0.0000 1.0079  
43 HCMM 1 LIG H9 43 0.0000 1.0079  
44 HCMM 1 LIG H10 44 0.0000 1.0079  
45 HCMM 1 LIG H11 45 0.0000 1.0079  
46 HCMM 1 LIG H12 46 0.0000 1.0079  
47 HCMM 1 LIG H13 47 0.0000 1.0079  
48 HCMM 1 LIG H14 48 0.0000 1.0079  
49 HCMM 1 LIG H15 49 0.0000 1.0079  
50 HCMM 1 LIG H16 50 0.0000 1.0079  
51 HCMM 1 LIG H17 51 0.0000 1.0079  
52 HCMM 1 LIG H18 52 0.0000 1.0079  
53 HCMM 1 LIG H19 53 0.0000 1.0079  
54 HCMM 1 LIG H20 54 0.0000 1.0079  
55 HCMM 1 LIG H21 55 0.0000 1.0079  
56 HCMM 1 LIG H22 56 0.0000 1.0079  
57 HCMM 1 LIG H23 57 0.0000 1.0079  
58 HCMM 1 LIG H24 58 0.0000 1.0079

[ bonds ]

; ai aj fu b0 kb, b0 kb

36 6 1 0.10120 428294.3 0.10120 428294.3  
39 17 1 0.10930 287014.9 0.10930 287014.9  
6 5 1 0.13640 379454.5 0.13640 379454.5  
6 7 1 0.13640 379454.5 0.13640 379454.5

17 38 1 0.10930 287014.9 0.10930 287014.9  
17 37 1 0.10930 287014.9 0.10930 287014.9  
17 7 1 0.14710 269852.1 0.14710 269852.1  
1 5 1 0.13300 439556.0 0.13300 439556.0  
1 4 1 0.13330 345489.6 0.13330 345489.6  
5 9 1 0.13770 428655.8 0.13770 428655.8  
7 8 1 0.13770 428655.8 0.13770 428655.8  
35 4 1 0.10840 319534.6 0.10840 319534.6  
4 3 1 0.13740 335613.7 0.13740 335613.7  
8 9 1 0.14180 259734.4 0.14180 259734.4  
8 10 1 0.14320 317065.2 0.14320 317065.2  
9 2 1 0.14320 317065.2 0.14320 317065.2  
3 2 1 0.13740 335613.7 0.13740 335613.7  
3 16 1 0.13420 392101.0 0.13420 392101.0  
2 34 1 0.10840 319534.6 0.10840 319534.6  
15 10 1 0.13330 345489.6 0.13330 345489.6  
15 14 1 0.13330 345489.6 0.13330 345489.6  
10 11 1 0.13330 345489.6 0.13330 345489.6  
40 14 1 0.10840 319534.6 0.10840 319534.6  
14 13 1 0.13740 335613.7 0.13740 335613.7  
11 12 1 0.13330 345489.6 0.13330 345489.6  
13 12 1 0.13740 335613.7 0.13740 335613.7  
13 18 1 0.13420 392101.0 0.13420 392101.0  
12 19 1 0.13350 429799.7 0.13350 429799.7  
41 20 1 0.10930 287014.9 0.10930 287014.9  
19 20 1 0.14440 268346.7 0.14440 268346.7  
50 25 1 0.10930 287014.9 0.10930 287014.9  
20 25 1 0.15080 256422.3 0.15080 256422.3  
20 21 1 0.15080 256422.3 0.15080 256422.3  
42 21 1 0.10930 287014.9 0.10930 287014.9  
47 24 1 0.10930 287014.9 0.10930 287014.9  
44 22 1 0.10930 287014.9 0.10930 287014.9  
25 24 1 0.15080 256422.3 0.15080 256422.3  
25 49 1 0.10930 287014.9 0.10930 287014.9  
21 22 1 0.15080 256422.3 0.15080 256422.3  
21 43 1 0.10930 287014.9 0.10930 287014.9  
24 48 1 0.10930 287014.9 0.10930 287014.9  
24 23 1 0.15080 256422.3 0.15080 256422.3  
22 23 1 0.15080 256422.3 0.15080 256422.3  
22 26 1 0.14440 268346.7 0.14440 268346.7  
57 33 1 0.10930 287014.9 0.10930 287014.9  
23 45 1 0.10930 287014.9 0.10930 287014.9  
23 46 1 0.10930 287014.9 0.10930 287014.9  
26 27 1 0.13220 455755.6 0.13220 455755.6  
58 33 1 0.10930 287014.9 0.10930 287014.9  
33 29 1 0.14360 280872.8 0.14360 280872.8  
33 32 1 0.15080 256422.3 0.15080 256422.3  
27 29 1 0.13690 351030.1 0.13690 351030.1  
27 28 1 0.12220 779866.6 0.12220 779866.6  
56 32 1 0.10930 287014.9 0.10930 287014.9  
29 30 1 0.14360 280872.8 0.14360 280872.8  
55 32 1 0.10930 287014.9 0.10930 287014.9  
32 31 1 0.15080 256422.3 0.15080 256422.3  
52 30 1 0.10930 287014.9 0.10930 287014.9  
30 31 1 0.15080 256422.3 0.15080 256422.3  
30 51 1 0.10930 287014.9 0.10930 287014.9  
31 53 1 0.10930 287014.9 0.10930 287014.9

31 54 1 0.10930 287014.9 0.10930 287014.9

[ pairs ]

; ai aj fu

1 2 1  
1 16 1  
1 7 1  
1 36 1  
1 8 1  
2 35 1  
2 6 1  
2 7 1  
2 10 1  
3 5 1  
3 8 1  
4 6 1  
4 9 1  
4 34 1  
5 35 1  
5 17 1  
5 34 1  
5 10 1  
6 10 1  
6 37 1  
6 38 1  
6 39 1  
7 11 1  
7 15 1  
8 36 1  
8 37 1  
8 38 1  
8 39 1  
8 34 1  
8 12 1  
8 14 1  
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[ angles ]

; ai aj ak fu th0 kth ub0 kub th0 kth ub0 kub

4	1	5	1	110.1810	740.72	110.1810	740.72
3	2	9	1	112.5670	254.73	112.5670	254.73
3	2	34	1	120.5710	339.05	120.5710	339.05
9	2	34	1	121.4460	314.95	121.4460	314.95
2	3	4	1	119.9770	402.88	119.9770	402.88
2	3	16	1	118.0650	658.81	118.0650	658.81
4	3	16	1	118.0650	658.81	118.0650	658.81
1	4	3	1	126.1390	358.92	126.1390	358.92
1	4	35	1	115.5880	417.33	115.5880	417.33
3	4	35	1	120.5710	339.05	120.5710	339.05
1	5	6	1	124.8140	615.46	124.8140	615.46
1	5	9	1	126.5130	548.01	126.5130	548.01
6	5	9	1	107.2550	489.59	107.2550	489.59
5	6	7	1	109.5990	693.74	109.5990	693.74

5	6	36	1	127.7700	331.82	127.7700	331.82
7	6	36	1	127.7700	331.82	127.7700	331.82
6	7	8	1	107.2550	489.59	107.2550	489.59
6	7	17	1	121.8320	563.07	121.8320	563.07
8	7	17	1	131.3780	443.83	131.3780	443.83
7	8	9	1	108.2390	521.51	108.2390	521.51
7	8	10	1	120.0000	602.21	120.0000	602.21
9	8	10	1	128.6730	464.91	128.6730	464.91
2	9	5	1	120.0000	602.21	120.0000	602.21
2	9	8	1	128.6730	464.91	128.6730	464.91
5	9	8	1	108.2390	521.51	108.2390	521.51
8	10	11	1	128.6730	464.91	128.6730	464.91
8	10	15	1	128.6730	464.91	128.6730	464.91
11	10	15	1	128.9380	436.60	128.9380	436.60
10	11	12	1	115.4060	653.40	115.4060	653.40
11	12	13	1	126.1390	358.92	126.1390	358.92
11	12	19	1	118.3490	691.34	118.3490	691.34
13	12	19	1	124.3840	566.68	124.3840	566.68
12	13	14	1	119.9770	402.88	119.9770	402.88
12	13	18	1	118.0650	658.81	118.0650	658.81
14	13	18	1	118.0650	658.81	118.0650	658.81
13	14	15	1	126.1390	358.92	126.1390	358.92
13	14	40	1	120.5710	339.05	120.5710	339.05
15	14	40	1	115.5880	417.33	115.5880	417.33
10	15	14	1	115.4060	653.40	115.4060	653.40
7	17	37	1	110.4670	373.97	110.4670	373.97
7	17	38	1	110.4670	373.97	110.4670	373.97
7	17	39	1	110.4670	373.97	110.4670	373.97
37	17	38	1	108.8360	310.74	108.8360	310.74
37	17	39	1	108.8360	310.74	108.8360	310.74
38	17	39	1	108.8360	310.74	108.8360	310.74
12	19	20	1	120.0000	602.21	120.0000	602.21
19	20	21	1	109.5000	602.21	109.5000	602.21
19	20	25	1	109.5000	602.21	109.5000	602.21
19	20	41	1	113.0350	394.45	113.0350	394.45
21	20	25	1	109.6080	512.48	109.6080	512.48
21	20	41	1	110.5490	383.00	110.5490	383.00
25	20	41	1	110.5490	383.00	110.5490	383.00
20	21	22	1	109.6080	512.48	109.6080	512.48
20	21	42	1	110.5490	383.00	110.5490	383.00
20	21	43	1	110.5490	383.00	110.5490	383.00
22	21	42	1	110.5490	383.00	110.5490	383.00
22	21	43	1	110.5490	383.00	110.5490	383.00
42	21	43	1	108.8360	310.74	108.8360	310.74
21	22	23	1	109.6080	512.48	109.6080	512.48
21	22	26	1	109.5000	602.21	109.5000	602.21
21	22	44	1	110.5490	383.00	110.5490	383.00
23	22	26	1	109.5000	602.21	109.5000	602.21
23	22	44	1	110.5490	383.00	110.5490	383.00
26	22	44	1	113.0350	394.45	113.0350	394.45
22	23	24	1	109.6080	512.48	109.6080	512.48
22	23	45	1	110.5490	383.00	110.5490	383.00
22	23	46	1	110.5490	383.00	110.5490	383.00
24	23	45	1	110.5490	383.00	110.5490	383.00
24	23	46	1	110.5490	383.00	110.5490	383.00
45	23	46	1	108.8360	310.74	108.8360	310.74
23	24	25	1	109.6080	512.48	109.6080	512.48

23	24	47	1	110.5490	383.00	110.5490	383.00
23	24	48	1	110.5490	383.00	110.5490	383.00
25	24	47	1	110.5490	383.00	110.5490	383.00
25	24	48	1	110.5490	383.00	110.5490	383.00
47	24	48	1	108.8360	310.74	108.8360	310.74
20	25	24	1	109.6080	512.48	109.6080	512.48
20	25	49	1	110.5490	383.00	110.5490	383.00
20	25	50	1	110.5490	383.00	110.5490	383.00
24	25	49	1	110.5490	383.00	110.5490	383.00
24	25	50	1	110.5490	383.00	110.5490	383.00
49	25	50	1	108.8360	310.74	108.8360	310.74
22	26	27	1	120.0000	602.21	120.0000	602.21
26	27	28	1	129.3490	679.89	129.3490	679.89
26	27	29	1	120.0000	602.21	120.0000	602.21
28	27	29	1	127.1520	546.20	127.1520	546.20
27	29	30	1	119.6000	494.41	119.6000	494.41
27	29	33	1	119.6000	494.41	119.6000	494.41
30	29	33	1	117.9090	672.67	117.9090	672.67
29	30	31	1	109.9600	632.32	109.9600	632.32
29	30	51	1	107.6460	445.64	107.6460	445.64
29	30	52	1	107.6460	445.64	107.6460	445.64
31	30	51	1	110.5490	383.00	110.5490	383.00
31	30	52	1	110.5490	383.00	110.5490	383.00
51	30	52	1	108.8360	310.74	108.8360	310.74
30	31	32	1	109.6080	512.48	109.6080	512.48
30	31	53	1	110.5490	383.00	110.5490	383.00
30	31	54	1	110.5490	383.00	110.5490	383.00
32	31	53	1	110.5490	383.00	110.5490	383.00
32	31	54	1	110.5490	383.00	110.5490	383.00
53	31	54	1	108.8360	310.74	108.8360	310.74
31	32	33	1	109.6080	512.48	109.6080	512.48
31	32	55	1	110.5490	383.00	110.5490	383.00
31	32	56	1	110.5490	383.00	110.5490	383.00
33	32	55	1	110.5490	383.00	110.5490	383.00
33	32	56	1	110.5490	383.00	110.5490	383.00
55	32	56	1	108.8360	310.74	108.8360	310.74
29	33	32	1	109.9600	632.32	109.9600	632.32
29	33	57	1	107.6460	445.64	107.6460	445.64
29	33	58	1	107.6460	445.64	107.6460	445.64
32	33	57	1	110.5490	383.00	110.5490	383.00
32	33	58	1	110.5490	383.00	110.5490	383.00
57	33	58	1	108.8360	310.74	108.8360	310.74

[ dihedrals ]

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1	4	3	2	9	180.00	14.6440	2	180.00	14.6440	2
1	4	3	16	9	180.00	14.6440	2	180.00	14.6440	2
1	5	6	7	9	180.00	8.3680	2	180.00	8.3680	2
1	5	6	36	9	180.00	8.3680	2	180.00	8.3680	2
1	5	9	2	9	180.00	14.6440	2	180.00	14.6440	2
1	5	9	8	9	180.00	14.6440	2	180.00	14.6440	2
2	3	4	35	9	180.00	14.6440	2	180.00	14.6440	2
2	9	5	6	9	180.00	14.6440	2	180.00	14.6440	2
2	9	8	7	9	180.00	14.6440	2	180.00	14.6440	2
2	9	8	10	9	180.00	14.6440	2	180.00	14.6440	2
3	2	9	5	9	180.00	14.6440	2	180.00	14.6440	2
3	2	9	8	9	180.00	14.6440	2	180.00	14.6440	2



3	4	1	5	9	180.00	14.6440	2	180.00	14.6440	2
4	1	5	6	9	180.00	14.6440	2	180.00	14.6440	2
4	1	5	9	9	180.00	14.6440	2	180.00	14.6440	2
4	3	2	9	9	180.00	14.6440	2	180.00	14.6440	2
4	3	2	34	9	180.00	14.6440	2	180.00	14.6440	2
5	1	4	35	9	180.00	14.6440	2	180.00	14.6440	2
5	6	7	8	9	180.00	8.3680	2	180.00	8.3680	2
5	6	7	17	9	180.00	8.3680	2	180.00	8.3680	2
5	9	2	34	9	180.00	14.6440	2	180.00	14.6440	2
5	9	8	7	9	180.00	14.6440	2	180.00	14.6440	2
5	9	8	10	9	180.00	14.6440	2	180.00	14.6440	2
6	5	9	8	9	180.00	14.6440	2	180.00	14.6440	2
6	7	8	9	9	180.00	14.6440	2	180.00	14.6440	2
6	7	8	10	9	180.00	14.6440	2	180.00	14.6440	2
7	6	5	9	9	180.00	8.3680	2	180.00	8.3680	2
7	8	10	11	9	180.00	3.7656	2	180.00	3.7656	2
7	8	10	15	9	180.00	3.7656	2	180.00	3.7656	2
8	7	6	36	9	180.00	8.3680	2	180.00	8.3680	2
8	9	2	34	9	180.00	14.6440	2	180.00	14.6440	2
9	2	3	16	9	180.00	14.6440	2	180.00	14.6440	2
9	5	6	36	9	180.00	8.3680	2	180.00	8.3680	2
9	8	7	17	9	180.00	14.6440	2	180.00	14.6440	2
9	8	10	11	9	180.00	3.7656	2	180.00	3.7656	2
9	8	10	15	9	180.00	3.7656	2	180.00	3.7656	2
10	11	12	13	9	180.00	14.6440	2	180.00	14.6440	2
10	11	12	19	9	180.00	14.6440	2	180.00	14.6440	2
10	15	14	13	9	180.00	14.6440	2	180.00	14.6440	2
10	15	14	40	9	180.00	14.6440	2	180.00	14.6440	2
11	10	15	14	9	180.00	14.6440	2	180.00	14.6440	2
11	12	13	14	9	180.00	14.6440	2	180.00	14.6440	2
11	12	13	18	9	180.00	14.6440	2	180.00	14.6440	2
11	12	19	20	9	180.00	7.5312	2	180.00	7.5312	2
12	11	10	15	9	180.00	14.6440	2	180.00	14.6440	2
12	13	14	15	9	180.00	14.6440	2	180.00	14.6440	2
12	13	14	40	9	180.00	14.6440	2	180.00	14.6440	2
12	19	20	21	9	0.00	0.5230	3	0.00	0.5230	3
12	19	20	25	9	0.00	0.5230	3	0.00	0.5230	3
12	19	20	41	9	0.00	0.5230	3	0.00	0.5230	3
13	12	19	20	9	180.00	7.5312	2	180.00	7.5312	2
14	13	12	19	9	180.00	14.6440	2	180.00	14.6440	2
15	14	13	18	9	180.00	14.6440	2	180.00	14.6440	2
16	3	2	34	9	180.00	14.6440	2	180.00	14.6440	2
16	3	4	35	9	180.00	14.6440	2	180.00	14.6440	2
17	7	6	36	9	180.00	8.3680	2	180.00	8.3680	2
18	13	12	19	9	180.00	14.6440	2	180.00	14.6440	2
18	13	14	40	9	180.00	14.6440	2	180.00	14.6440	2
19	20	21	22	9	0.00	0.6276	3	0.00	0.6276	3
19	20	21	42	9	0.00	0.6276	3	0.00	0.6276	3
19	20	21	43	9	0.00	0.6276	3	0.00	0.6276	3
19	20	25	24	9	0.00	0.6276	3	0.00	0.6276	3
19	20	25	49	9	0.00	0.6276	3	0.00	0.6276	3
19	20	25	50	9	0.00	0.6276	3	0.00	0.6276	3
20	21	22	23	9	0.00	0.2134	1	0.00	0.2134	1
20	21	22	23	9	180.00	1.4267	2	180.00	1.4267	2
20	21	22	23	9	0.00	0.6945	3	0.00	0.6945	3
20	21	22	26	9	0.00	0.6276	3	0.00	0.6276	3
20	21	22	44	9	0.00	1.3389	1	0.00	1.3389	1

20 21 22 44 9 180.00 -1.3180 2 180.00 -1.3180 2  
20 21 22 44 9 0.00 0.5523 3 0.00 0.5523 3  
20 25 24 23 9 0.00 0.2134 1 0.00 0.2134 1  
20 25 24 23 9 180.00 1.4267 2 180.00 1.4267 2  
20 25 24 23 9 0.00 0.6945 3 0.00 0.6945 3  
20 25 24 47 9 0.00 1.3389 1 0.00 1.3389 1  
20 25 24 47 9 180.00 -1.3180 2 180.00 -1.3180 2  
20 25 24 47 9 0.00 0.5523 3 0.00 0.5523 3  
20 25 24 48 9 0.00 1.3389 1 0.00 1.3389 1  
20 25 24 48 9 180.00 -1.3180 2 180.00 -1.3180 2  
20 25 24 48 9 0.00 0.5523 3 0.00 0.5523 3  
21 20 25 24 9 0.00 0.2134 1 0.00 0.2134 1  
21 20 25 24 9 180.00 1.4267 2 180.00 1.4267 2  
21 20 25 24 9 0.00 0.6945 3 0.00 0.6945 3  
21 20 25 49 9 0.00 1.3389 1 0.00 1.3389 1  
21 20 25 49 9 180.00 -1.3180 2 180.00 -1.3180 2  
21 20 25 49 9 0.00 0.5523 3 0.00 0.5523 3  
21 20 25 50 9 0.00 1.3389 1 0.00 1.3389 1  
21 20 25 50 9 180.00 -1.3180 2 180.00 -1.3180 2  
21 20 25 50 9 0.00 0.5523 3 0.00 0.5523 3  
21 22 23 24 9 0.00 0.2134 1 0.00 0.2134 1  
21 22 23 24 9 180.00 1.4267 2 180.00 1.4267 2  
21 22 23 24 9 0.00 0.6945 3 0.00 0.6945 3  
21 22 23 45 9 0.00 1.3389 1 0.00 1.3389 1  
21 22 23 45 9 180.00 -1.3180 2 180.00 -1.3180 2  
21 22 23 45 9 0.00 0.5523 3 0.00 0.5523 3  
21 22 23 46 9 0.00 1.3389 1 0.00 1.3389 1  
21 22 23 46 9 180.00 -1.3180 2 180.00 -1.3180 2  
21 22 23 46 9 0.00 0.5523 3 0.00 0.5523 3  
21 22 26 27 9 0.00 0.5230 3 0.00 0.5230 3  
22 21 20 25 9 0.00 0.2134 1 0.00 0.2134 1  
22 21 20 25 9 180.00 1.4267 2 180.00 1.4267 2  
22 21 20 25 9 0.00 0.6945 3 0.00 0.6945 3  
22 21 20 41 9 0.00 1.3389 1 0.00 1.3389 1  
22 21 20 41 9 180.00 -1.3180 2 180.00 -1.3180 2  
22 21 20 41 9 0.00 0.5523 3 0.00 0.5523 3  
22 23 24 25 9 0.00 0.2134 1 0.00 0.2134 1  
22 23 24 25 9 180.00 1.4267 2 180.00 1.4267 2  
22 23 24 25 9 0.00 0.6945 3 0.00 0.6945 3  
22 23 24 47 9 0.00 1.3389 1 0.00 1.3389 1  
22 23 24 47 9 180.00 -1.3180 2 180.00 -1.3180 2  
22 23 24 47 9 0.00 0.5523 3 0.00 0.5523 3  
22 23 24 48 9 0.00 1.3389 1 0.00 1.3389 1  
22 23 24 48 9 180.00 -1.3180 2 180.00 -1.3180 2  
22 23 24 48 9 0.00 0.5523 3 0.00 0.5523 3  
22 26 27 28 9 180.00 7.5312 2 180.00 7.5312 2  
22 26 27 29 9 180.00 7.5312 2 180.00 7.5312 2  
23 22 21 42 9 0.00 1.3389 1 0.00 1.3389 1  
23 22 21 42 9 180.00 -1.3180 2 180.00 -1.3180 2  
23 22 21 42 9 0.00 0.5523 3 0.00 0.5523 3  
23 22 21 43 9 0.00 1.3389 1 0.00 1.3389 1  
23 22 21 43 9 180.00 -1.3180 2 180.00 -1.3180 2  
23 22 21 43 9 0.00 0.5523 3 0.00 0.5523 3  
23 22 26 27 9 0.00 0.5230 3 0.00 0.5230 3  
23 24 25 49 9 0.00 1.3389 1 0.00 1.3389 1  
23 24 25 49 9 180.00 -1.3180 2 180.00 -1.3180 2  
23 24 25 49 9 0.00 0.5523 3 0.00 0.5523 3

23 24 25 50 9 0.00 1.3389 1 0.00 1.3389 1  
23 24 25 50 9 180.00 -1.3180 2 180.00 -1.3180 2  
23 24 25 50 9 0.00 0.5523 3 0.00 0.5523 3  
24 23 22 26 9 0.00 0.6276 3 0.00 0.6276 3  
24 23 22 44 9 0.00 1.3389 1 0.00 1.3389 1  
24 23 22 44 9 180.00 -1.3180 2 180.00 -1.3180 2  
24 23 22 44 9 0.00 0.5523 3 0.00 0.5523 3  
24 25 20 41 9 0.00 1.3389 1 0.00 1.3389 1  
24 25 20 41 9 180.00 -1.3180 2 180.00 -1.3180 2  
24 25 20 41 9 0.00 0.5523 3 0.00 0.5523 3  
25 20 21 42 9 0.00 1.3389 1 0.00 1.3389 1  
25 20 21 42 9 180.00 -1.3180 2 180.00 -1.3180 2  
25 20 21 42 9 0.00 0.5523 3 0.00 0.5523 3  
25 20 21 43 9 0.00 1.3389 1 0.00 1.3389 1  
25 20 21 43 9 180.00 -1.3180 2 180.00 -1.3180 2  
25 20 21 43 9 0.00 0.5523 3 0.00 0.5523 3  
25 24 23 45 9 0.00 1.3389 1 0.00 1.3389 1  
25 24 23 45 9 180.00 -1.3180 2 180.00 -1.3180 2  
25 24 23 45 9 0.00 0.5523 3 0.00 0.5523 3  
25 24 23 46 9 0.00 1.3389 1 0.00 1.3389 1  
25 24 23 46 9 180.00 -1.3180 2 180.00 -1.3180 2  
25 24 23 46 9 0.00 0.5523 3 0.00 0.5523 3  
26 22 21 42 9 0.00 0.6276 3 0.00 0.6276 3  
26 22 21 43 9 0.00 0.6276 3 0.00 0.6276 3  
26 22 23 45 9 0.00 0.6276 3 0.00 0.6276 3  
26 22 23 46 9 0.00 0.6276 3 0.00 0.6276 3  
26 27 29 30 9 180.00 12.5520 2 180.00 12.5520 2  
26 27 29 33 9 180.00 12.5520 2 180.00 12.5520 2  
27 26 22 44 9 0.00 0.5230 3 0.00 0.5230 3  
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29 30 31 32 9 0.00 0.6276 3 0.00 0.6276 3  
29 30 31 53 9 0.00 0.8912 3 0.00 0.8912 3  
29 30 31 54 9 0.00 0.8912 3 0.00 0.8912 3  
29 33 32 31 9 0.00 0.6276 3 0.00 0.6276 3

29 33 32 55 9 0.00 0.8912 3 0.00 0.8912 3  
29 33 32 56 9 0.00 0.8912 3 0.00 0.8912 3  
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3 2 4 16 2 0.00 21.0790 0.00 21.0790  
5 9 1 6 2 0.00 30.1081 0.00 30.1081  
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