Rough Draft of Supplemental Material

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1 Filtered Top8000 Residue Counts

Residue Type	No Filter	Filter	%Kept
LYS	70035	34829	49.78%
GLU	88745	57462	64.82%
ARG	64333	46380	72.18%
GLN	50112	37119	74.14%
ASP	88822	72336	81.52%
ASN	63553	53650	84.57%
MET	21764	18382	84.62%
HIS	33910	29791	87.99%
SER	84656	76186	90.21%
LEU	126451	115053	91.22%
ILE	78547	71693	91.51%
TYR	51638	47243	91.61%
PRO	65013	59515	91.74%
THR	82124	75180	91.80%
PHE	60306	56282	93.52%
TRP	19966	18715	93.90%
VAL	103690	97050	93.92%
CYS	17808	16708	94.15%
Total	**1171473**	**983574**	**83.96%**

Table 1: Residue counts with and without residue-level filters ordered by % kept after filtering. 'No Filter' means no RSCC, $2mF_o$-DF_c sigma, and B filters but all other residue-level filters applied.

2 Top8000 Filtered Dataset: Rotamer Frequency

The following is a table describing counts of each of the 213 rotamers identified in the Top8000 filtered dataset. n is the count of each rotamer, % is the percent of the rotamer that occurs in the given residue type (e.g. 17.7% of CYS are **p**). Also noted is the *rarity* of each rotamer, defined at two levels – a singe and double checkmark. The rarity metric is normalized by both the number of residues and the number of rotamer types in a given residue type. If the empirical count for a rotamer is $< 8\%$ or $< 1\%$ of the *expected rotamer count* then the rarity is marked with a single or double checkmark, respectively. The *expected rotamer count* is the number of residues in a rotamer bin if all residues were distributed equally to all rotamer bins for a given residue type. e.g. if SER had 3000 residues in the dataset then the *expected count* for each of the three rotamers would be 1000. Further, if one of these rotamers had an empirical count < 80 or < 10, the *rarity* would be marked with a single or double checkmark respectively.

residue	rotamer	n	%	rarity
SER : TOTAL N = 76186				
SER	p	36901	48.44	-
SER	t	17502	22.97	-
SER	m	21558	28.30	-
SER	OUTLIER	225	0.30	-
CYS : TOTAL N = 16708				
CYS	p	2962	17.73	-
CYS	t	4399	26.33	-
CYS	m	9301	55.67	-
CYS	OUTLIER	46	0.28	-
THR : TOTAL N = 75180				
THR	p	36195	48.14	-
THR	t	5197	6.91	-
THR	m	33559	44.64	-
THR	OUTLIER	229	0.30	-
VAL : TOTAL N = 97050				
VAL	p	6015	6.20	-
VAL	t	73329	75.56	-
VAL	m	17410	17.94	-
VAL	OUTLIER	296	0.30	-
PRO : TOTAL N = 59515				
PRO	Cg_exo	30128	50.62	-
PRO	Cg_endo	29192	49.05	-
PRO	OUTLIER	195	0.33	-
LEU : TOTAL N = 115053				
LEU	pp	521	0.45	✓
LEU	pt	378	0.33	✓
LEU	tp	34655	30.12	-
LEU	tt	1576	1.37	-
LEU	tm	143	0.12	✓✓
LEU	mp	2711	2.36	-
LEU	mt	74252	64.54	-
LEU	mm	484	0.42	✓
LEU	OUTLIER	333	0.29	-
ILE : TOTAL N = 71693				
ILE	pp	254	0.35	✓
ILE	pt	8837	12.33	-
ILE	tp	1869	2.61	-
ILE	tt	4163	5.81	-
ILE	mp	623	0.87	✓
ILE	mt	44470	62.03	-
ILE	mm	11258	15.70	-
ILE	OUTLIER	219	0.31	-
ASN : TOTAL N = 53650				
ASN	p0	7513	14.00	-
ASN	t0	15610	29.10	-
ASN	t160	61	0.11	✓✓
ASN	m110	4003	7.46	-
ASN	m-40	26292	49.01	-
ASN	OUTLIER	171	0.32	-
ASP : TOTAL N = 72336				
ASP	p0	11746	16.24	-
ASP	t0	17107	23.65	-
ASP	t70	6029	8.33	-
ASP	m-30	37239	51.48	-
ASP	OUTLIER	215	0.30	-
HIS : TOTAL N = 29791				
HIS	p90	1492	5.01	-
HIS	p-80	2203	7.39	-
HIS	t70	5068	17.01	-
HIS	t-170	1332	4.47	-
HIS	t-90	3553	11.93	-
HIS	m170	2695	9.05	-
HIS	m90	3914	13.14	-
HIS	m-70	9453	31.73	-
HIS	OUTLIER	81	0.27	-
PHE : TOTAL N = 56282				
PHE	p90	6289	11.17	-
PHE	t80	19289	34.27	-
PHE	m-10	3880	6.89	-
PHE	m-80	26665	47.38	-
PHE	OUTLIER	159	0.28	-
TYR : TOTAL N = 47243				
TYR	p90	5466	11.57	-
TYR	t80	16312	34.53	-
TYR	m-10	2623	5.55	-
TYR	m-80	22683	48.01	-
TYR	OUTLIER	159	0.34	-
TRP : TOTAL N = 18715				
TRP	p90	971	5.19	-
TRP	p-90	1937	10.35	-
TRP	t60	3385	18.09	-
TRP	t-100	2893	15.46	-
TRP	m100	6319	33.76	-
TRP	m-10	2196	11.73	-
TRP	m-90	961	5.13	-
TRP	OUTLIER	53	0.28	-
MET : TOTAL N = 16794				
MET	ppp	50	0.30	✓
MET	pp-130	27	0.16	✓

residue	rotamer	n	%	rarity
MET	ptp	404	2.41	-
MET	ptt	260	1.55	-
MET	ptm	375	2.23	-
MET	pmt	7	0.04	✓✓
MET	pmm	42	0.25	✓
MET	tpp	1138	6.78	-
MET	tpt	388	2.31	-
MET	ttp	1246	7.42	-
MET	ttt	569	3.39	-
MET	ttm	1124	6.69	-
MET	tmt	34	0.20	✓
MET	tmm	276	1.64	-
MET	mpp	74	0.44	-
MET	mpt	34	0.20	✓
MET	mpm	13	0.08	✓
MET	mtp	2815	16.76	-
MET	mtt	1542	9.18	-
MET	mtm	1851	11.02	-
MET	mmp	520	3.10	-
MET	mmt	597	3.55	-
MET	mmm	3354	19.97	-
MET	OUTLIER	54	0.32	-
GLU : TOTAL N = 57462				
GLU	pp20	159	0.28	✓
GLU	pt0	2800	4.87	-
GLU	pm20	1485	2.58	-
GLU	tp30	4616	8.03	-
GLU	tt0	13610	23.69	-
GLU	tm-30	862	1.50	-
GLU	mp0	3671	6.39	-
GLU	mt-10	21021	36.58	-
GLU	mm-30	9080	15.80	-
GLU	OUTLIER	158	0.27	-
GLN : TOTAL N = 37119				
GLN	pp30	178	0.48	✓
GLN	pt0	1885	5.08	-
GLN	pm20	487	1.31	-
GLN	tp40	3618	9.75	-
GLN	tp-100	534	1.44	-
GLN	tt0	6936	18.69	-
GLN	tm130	55	0.15	✓
GLN	tm-30	547	1.47	-
GLN	mp10	1207	3.25	-
GLN	mp-120	87	0.23	✓
GLN	mt0	14370	38.71	-
GLN	mm110	1147	3.09	-
GLN	mm-40	5959	16.05	-
GLN	OUTLIER	109	0.29	-
ARG : TOTAL N = 46380				
ARG	ppp80	10	0.02	✓
ARG	ppp-140	4	0.01	✓✓
ARG	ppt170	57	0.12	✓
ARG	ppt90	19	0.04	✓
ARG	ppt-90	15	0.03	✓
ARG	ptp90	223	0.48	-
ARG	ptp-110	77	0.17	-
ARG	ptp-170	388	0.84	-
ARG	ptt180	820	1.77	-
ARG	ptt90	814	1.76	-
ARG	ptt-90	726	1.57	-

residue	rotamer	n	%	rarity
ARG	ptm160	502	1.08	-
ARG	ptm-80	215	0.46	-
ARG	pmt100	4	0.01	✓✓
ARG	pmt170	39	0.08	✓
ARG	pmt-80	27	0.06	✓
ARG	pmm150	12	0.03	✓
ARG	pmm-80	19	0.04	✓
ARG	tpp80	363	0.78	-
ARG	tpp-160	496	1.07	-
ARG	tpt170	825	1.78	-
ARG	tpt90	652	1.41	-
ARG	tpt-90	365	0.79	-
ARG	tpm170	110	0.24	-
ARG	tpm-80	20	0.04	✓
ARG	ttp80	1896	4.09	-
ARG	ttp-110	623	1.34	-
ARG	ttp-170	1533	3.31	-
ARG	ttt180	2339	5.04	-
ARG	ttt90	1057	2.28	-
ARG	ttt-90	1380	2.98	-
ARG	ttm110	725	1.56	-
ARG	ttm170	1317	2.84	-
ARG	ttm-80	1504	3.24	-
ARG	tmt170	104	0.22	-
ARG	tmt90	23	0.05	✓
ARG	tmt-80	62	0.13	-
ARG	tmm160	92	0.20	-
ARG	tmm-80	71	0.15	-
ARG	mpp80	54	0.12	✓
ARG	mpp-170	64	0.14	-
ARG	mpt180	245	0.53	-
ARG	mpt90	46	0.10	✓
ARG	mpt-90	85	0.18	-
ARG	mtp180	2504	5.40	-
ARG	mtp85	1857	4.00	-
ARG	mtp-110	470	1.01	-
ARG	mtt180	4592	9.90	-
ARG	mtt90	2460	5.30	-
ARG	mtt-85	2843	6.13	-
ARG	mtm110	781	1.68	-
ARG	mtm180	2407	5.19	-
ARG	mtm-85	2848	6.14	-
ARG	mmp80	164	0.35	-
ARG	mmp-170	123	0.27	-
ARG	mmt180	1203	2.59	-
ARG	mmt90	567	1.22	-
ARG	mmt-90	1428	3.08	-
ARG	mmm160	951	2.05	-
ARG	mmm-85	1022	2.20	-
ARG	OUTLIER	138	0.30	-
LYS : TOTAL N = 34829				
LYS	pptt	25	0.07	✓
LYS	ptpp	89	0.26	-
LYS	ptpt	148	0.42	-
LYS	pttp	240	0.69	-
LYS	pttt	1385	3.98	-
LYS	pttm	268	0.77	-
LYS	ptmt	187	0.54	-
LYS	ptmm	80	0.23	-
LYS	pmtt	10	0.03	✓

residue	rotamer	n	%	rarity
LYS	tppp	37	0.11	✓
LYS	tppt	272	0.78	-
LYS	tptp	409	1.17	-
LYS	tptt	1228	3.53	-
LYS	tptm	197	0.57	-
LYS	ttpp	229	0.66	-
LYS	ttpt	883	2.54	-
LYS	ttpm	4	0.01	✓✓
LYS	tttp	1233	3.54	-
LYS	tttt	5043	14.48	-
LYS	tttm	1176	3.38	-
LYS	ttmp	9	0.03	✓
LYS	ttmt	674	1.94	-
LYS	ttmm	197	0.57	-
LYS	tmtp	11	0.03	✓
LYS	tmtt	82	0.24	-
LYS	tmtm	20	0.06	✓
LYS	tmmt	33	0.09	✓
LYS	tmmm	8	0.02	✓
LYS	mppt	31	0.09	✓
LYS	mptp	26	0.07	✓
LYS	mptt	124	0.36	-
LYS	mptm	11	0.03	✓
LYS	mtpp	392	1.13	-
LYS	mtpt	1357	3.90	-
LYS	mtpm	17	0.05	✓
LYS	mttp	1414	4.06	-
LYS	mttt	8597	24.68	-
LYS	mttm	1829	5.25	-
LYS	mtmp	9	0.03	✓
LYS	mtmt	1314	3.77	-
LYS	mtmm	424	1.22	-
LYS	mmpt	31	0.09	✓
LYS	mmtp	463	1.33	-
LYS	mmtt	3137	9.01	-
LYS	mmtm	727	2.09	-
LYS	mmmt	544	1.56	-
LYS	mmmm	90	0.26	-
LYS	OUTLIER	114	0.33	-

3 χ and Covalent Bond Angle Central Values

The following tables report the central χ and covalent bond angles for each rotamer identified in the Top8000. The central χ values are calculated by taking the center-of-mass (COM) of the smoothed contours in the given rotamer bin as described in Section 2.4. The mean for the covalent bond angles is a simple mean.

3.1 SER

SER **p** n = 36901		
χ	Smooth COM	StdDev
chi1	65.916	8.614
Bond Angle	Mean	StdDev
Cα_Cβ_OG	111.001	1.348
Cα_C_O	120.458	0.922
Cβ_Cα_C	109.930	1.393
N_Cα_C	111.621	2.519
N_Cα_Cβ	110.666	1.118

SER **t** n = 17502		
χ	Smooth COM	StdDev
chi1	178.650	9.008
Bond Angle	Mean	StdDev
Cα_Cβ_OG	110.709	1.422
Cα_C_O	120.567	0.818
Cβ_Cα_C	109.799	1.449
N_Cα_C	110.491	2.405
N_Cα_Cβ	110.057	1.210

SER **m** n = 21558		
χ	Smooth COM	StdDev
chi1	-63.982	7.667
Bond Angle	Mean	StdDev
Cα_Cβ_OG	110.527	1.459
Cα_C_O	120.485	0.850
Cβ_Cα_C	109.476	1.447
N_Cα_C	111.471	2.440
N_Cα_Cβ	110.563	1.028

3.2 CYS

CYS **p** n = 2962		
χ	Smooth COM	StdDev
chi1	64.543	8.969
Bond Angle	Mean	StdDev
Cα_Cβ_SG	114.646	1.684
Cα_C_O	120.521	0.978
Cβ_Cα_C	110.473	1.502
N_Cα_C	111.297	2.778
N_Cα_Cβ	110.904	1.232

CYS **m** n = 9301		
χ	Smooth COM	StdDev
chi1	-65.374	8.203
Bond Angle	Mean	StdDev
Cα_Cβ_SG	113.554	1.864
Cα_C_O	120.431	0.871
Cβ_Cα_C	109.474	1.632
N_Cα_C	111.518	2.424
N_Cα_Cβ	110.613	1.065

CYS **t** n = 4399		
χ	Smooth COM	StdDev
chi1	-177.599	8.222
Bond Angle	Mean	StdDev
Cα_Cβ_SG	113.679	1.938
Cα_C_O	120.488	0.861
Cβ_Cα_C	110.333	1.295
N_Cα_C	109.702	2.435
N_Cα_Cβ	110.020	1.370

3.3 THR

THR **p** n = 36195		
χ	Smooth COM	StdDev
chi1	61.450	7.652
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ2	110.976	1.009
Cα_Cβ_OG1	109.502	0.971
Cα_C_O	120.473	0.956
Cβ_Cα_C	108.833	1.702
N_Cα_C	111.374	2.770
N_Cα_Cβ	111.784	1.258
OG1_Cβ_Cγ2	109.207	1.712

THR **t** n = 5197		
χ	Smooth COM	StdDev
chi1	-172.707	7.389
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ2	111.729	1.103
Cα_Cβ_OG1	109.533	0.990
Cα_C_O	120.619	0.834
Cβ_Cα_C	110.967	1.904
N_Cα_C	110.117	2.331
N_Cα_Cβ	111.298	1.337
OG1_Cβ_Cγ2	109.060	1.810

THR **m** n = 33559		
χ	Smooth COM	StdDev
chi1	-60.109	6.107
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ2	111.146	0.939
Cα_Cβ_OG1	108.916	0.972
Cα_C_O	120.533	0.810
Cβ_Cα_C	110.050	1.532
N_Cα_C	110.213	2.307
N_Cα_Cβ	110.718	1.188
OG1_Cβ_Cγ2	108.767	1.669

3.4 VAL

VAL **p** n = 6015		
χ	Smooth COM	StdDev
chi1	64.912	7.166
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	111.517	1.091
Cα_Cβ_Cγ2	110.755	1.020
Cα_C_O	120.598	0.828
Cβ_Cα_C	111.418	1.568
Cγ1_Cβ_Cγ2	111.030	1.204
N_Cα_C	110.312	2.482
N_Cα_Cβ	111.580	1.263

VAL **t** n = 73329		
χ	Smooth COM	StdDev
chi1	175.704	6.352
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	110.746	0.936
Cα_Cβ_Cγ2	110.161	0.946
Cα_C_O	120.549	0.788
Cβ_Cα_C	110.193	1.510
Cγ1_Cβ_Cγ2	110.464	1.126
N_Cα_C	109.421	2.363
N_Cα_Cβ	111.340	1.112

VAL **m** n = 17410		
χ	Smooth COM	StdDev
chi1	-61.900	5.694
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	110.354	0.917
Cα_Cβ_Cγ2	111.323	1.023
Cα_C_O	120.553	0.913
Cβ_Cα_C	109.824	1.600
Cγ1_Cβ_Cγ2	110.892	1.165
N_Cα_C	111.118	2.687
N_Cα_Cβ	112.271	1.177

3.5 PRO

PRO **Cg_exo** n = 30128		
χ	Smooth COM	StdDev
chi1	-24.512	7.169
chi2	35.520	7.825
chi3	-31.747	7.122
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	104.229	1.397
Cα_C_O	120.180	1.031
Cα_N_Cδ	111.654	0.806
Cβ_Cα_C	110.809	1.300
Cβ_Cγ_Cδ	104.701	2.311
N_Cα_C	112.655	2.417
N_Cα_Cβ	103.312	0.589
N_Cδ_Cγ	102.715	0.876

PRO **Cg_endo** n = 29192		
χ	Smooth COM	StdDev
chi1	26.645	7.653
chi2	-34.137	8.897
chi3	27.789	9.234
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	104.233	1.468
Cα_C_O	120.227	1.070
Cα_N_Cδ	111.798	0.843
Cβ_Cα_C	110.911	1.411
Cβ_Cγ_Cδ	105.301	2.361
N_Cα_C	112.933	2.596
N_Cα_Cβ	103.192	0.719
N_Cδ_Cγ	103.063	0.876

3.6 LEU

LEU **pp** n = 521		
χ	Smooth COM	StdDev
chi1	61.357	8.227
chi2	83.113	9.465
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	119.083	2.531
Cα_C_O	120.578	0.835
Cβ_Cα_C	111.537	1.381
Cβ_Cγ_Cδ1	111.539	1.890
Cβ_Cγ_Cδ2	109.789	1.678
Cδ1_Cγ_Cδ2	109.695	1.226
N_Cα_C	110.691	2.359
N_Cα_Cβ	111.107	1.151

LEU **pt** n = 378		
χ	Smooth COM	StdDev
chi1	72.738	8.508
chi2	164.797	10.798
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	118.709	2.155
Cα_C_O	120.802	0.831
Cβ_Cα_C	110.423	1.451
Cβ_Cγ_Cδ1	109.794	1.542
Cβ_Cγ_Cδ2	111.556	1.845
Cδ1_Cγ_Cδ2	110.437	1.240
N_Cα_C	110.447	2.450
N_Cα_Cβ	111.556	1.184

LEU **tp** n = 34655		
χ	Smooth COM	StdDev
chi1	-177.276	8.235
chi2	62.594	6.963
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.491	2.056
Cα_C_O	120.525	0.788
Cβ_Cα_C	110.192	1.205
Cβ_Cγ_Cδ1	111.069	1.554
Cβ_Cγ_Cδ2	109.781	1.495
Cδ1_Cγ_Cδ2	110.707	1.134
N_Cα_C	110.165	2.380
N_Cα_Cβ	110.303	1.147

LEU **tt** n = 1576		
χ	Smooth COM	StdDev
chi1	-172.476	8.492
chi2	153.401	10.535
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	117.300	2.706
Cα_C_O	120.592	0.860
Cβ_Cα_C	111.070	1.256
Cβ_Cγ_Cδ1	110.121	1.530
Cβ_Cγ_Cδ2	111.610	1.837
Cδ1_Cγ_Cδ2	110.437	1.320
N_Cα_C	109.108	2.499
N_Cα_Cβ	110.213	1.253

LEU **tm** n = 143		
χ	Smooth COM	StdDev
chi1	-171.753	5.901
chi2	-75.044	6.356
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	120.365	2.303
Cα_C_O	120.583	0.802
Cβ_Cα_C	111.264	1.174
Cβ_Cγ_Cδ1	112.297	1.918
Cβ_Cγ_Cδ2	111.622	1.690
Cδ1_Cγ_Cδ2	111.421	1.438
N_Cα_C	108.547	2.317
N_Cα_Cβ	109.930	1.129

LEU **mp** n = 2711		
χ	Smooth COM	StdDev
chi1	-77.359	12.530
chi2	71.504	15.741
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.579	2.638
Cα_C_O	120.462	0.850
Cβ_Cα_C	109.681	1.568
Cβ_Cγ_Cδ1	111.644	2.035
Cβ_Cγ_Cδ2	109.937	1.583
Cδ1_Cγ_Cδ2	110.503	1.455
N_Cα_C	110.165	2.644
N_Cα_Cβ	111.085	1.027

LEU **mt** n = 74252		
χ	Smooth COM	StdDev
chi1	-65.787	8.164
chi2	174.346	8.051
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.859	2.169
Cα_C_O	120.431	0.820
Cβ_Cα_C	109.811	1.421
Cβ_Cγ_Cδ1	109.882	1.466
Cβ_Cγ_Cδ2	110.965	1.547
Cδ1_Cγ_Cδ2	110.777	1.107
N_Cα_C	111.393	2.340
N_Cα_Cβ	110.599	0.985

LEU **mm** n = 484		
χ	Smooth COM	StdDev
chi1	-82.802	10.177
chi2	-63.907	9.998
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	117.810	2.626
Cα_C_O	120.323	0.893
Cβ_Cα_C	110.092	1.579
Cβ_Cγ_Cδ1	110.866	1.604
Cβ_Cγ_Cδ2	111.876	1.719
Cδ1_Cγ_Cδ2	110.701	1.403
N_Cα_C	111.081	2.614
N_Cα_Cβ	111.033	0.983

3.7 ILE

ILE **pp** n = 254		
χ	Smooth COM	StdDev
chi1	57.851	7.686
chi2	84.312	12.800
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	112.503	1.280
Cα_Cβ_Cγ2	109.866	1.145
Cα_C_O	120.547	0.873
Cβ_Cα_C	111.344	1.607
Cβ_Cγ1_Cδ1	115.059	1.803
Cγ1_Cβ_Cγ2	110.044	1.960
N_Cα_C	112.012	2.513
N_Cα_Cβ	112.286	1.249

ILE **pt** n = 8837		
χ	Smooth COM	StdDev
chi1	62.073	6.094
chi2	170.331	7.581
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	111.339	1.083
Cα_Cβ_Cγ2	110.176	0.938
Cα_C_O	120.535	0.937
Cβ_Cα_C	110.110	1.671
Cβ_Cγ1_Cδ1	113.605	1.254
Cγ1_Cβ_Cγ2	111.381	1.533
N_Cα_C	111.361	2.736
N_Cα_Cβ	112.260	1.195

ILE **tp** n = 1869		
χ	Smooth COM	StdDev
chi1	-167.339	7.836
chi2	65.770	7.313
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	111.105	1.130
Cα_Cβ_Cγ2	111.437	1.028
Cα_C_O	120.365	0.819
Cβ_Cα_C	111.532	1.459
Cβ_Cγ1_Cδ1	114.167	1.154
Cγ1_Cβ_Cγ2	110.819	1.695
N_Cα_C	111.577	2.333
N_Cα_Cβ	111.454	1.272

ILE **tt** n = 4163		
χ	Smooth COM	StdDev
chi1	-169.614	7.748
chi2	166.622	6.871
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	110.680	1.065
Cα_Cβ_Cγ2	111.396	1.038
Cα_C_O	120.604	0.827
Cβ_Cα_C	111.636	1.480
Cβ_Cγ1_Cδ1	113.490	1.268
Cγ1_Cβ_Cγ2	111.706	1.614
N_Cα_C	110.129	2.516
N_Cα_Cβ	111.350	1.316

ILE **mp** n = 623		
χ	Smooth COM	StdDev
chi1	-62.667	11.611
chi2	88.683	16.573
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	111.150	1.110
Cα_Cβ_Cγ2	110.473	1.090
Cα_C_O	120.462	0.812
Cβ_Cα_C	110.134	1.635
Cβ_Cγ1_Cδ1	114.582	1.667
Cγ1_Cβ_Cγ2	109.324	1.870
N_Cα_C	108.335	2.264
N_Cα_Cβ	111.949	1.287

ILE **mt** n = 44470		
χ	Smooth COM	StdDev
chi1	-62.999	6.427
chi2	169.237	7.398
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	109.984	1.081
Cα_Cβ_Cγ2	110.617	0.918
Cα_C_O	120.542	0.790
Cβ_Cα_C	110.366	1.581
Cβ_Cγ1_Cδ1	113.966	1.223
Cγ1_Cβ_Cγ2	110.762	1.437
N_Cα_C	109.405	2.337
N_Cα_Cβ	111.245	1.145

ILE **mm** n = 11258		
χ	Smooth COM	StdDev
chi1	-59.020	7.075
chi2	-61.129	7.343
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	110.904	1.123
Cα_Cβ_Cγ2	110.751	0.967
Cα_C_O	120.513	0.804
Cβ_Cα_C	109.837	1.605
Cβ_Cγ1_Cδ1	114.776	1.211
Cγ1_Cβ_Cγ2	111.277	1.468
N_Cα_C	109.449	2.450
N_Cα_Cβ	111.304	1.149

3.8 ASN

ASN **p0** n = 7513		
χ	Smooth COM	StdDev
chi1	63.756	7.767
chi2	6.662	43.284
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.139	0.878
Cα_C_O	120.389	0.966
Cβ_Cα_C	111.273	1.683
Cβ_Cγ_Nδ2	116.347	0.911
Cβ_Cγ_Oδ1	121.130	0.982
N_Cα_C	111.973	2.774
N_Cα_Cβ	111.073	1.286
Oδ1_Cγ_Nδ2	122.498	0.716

ASN **t0** n = 15610		
χ	Smooth COM	StdDev
chi1	-171.473	10.505
chi2	-1.493	54.857
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	112.733	0.917
Cα_C_O	120.615	0.874
Cβ_Cα_C	110.613	1.307
Cβ_Cγ_Nδ2	116.453	0.851
Cβ_Cγ_Oδ1	120.906	0.917
N_Cα_C	110.128	2.820
N_Cα_Cβ	110.094	1.446
Oδ1_Cγ_Nδ2	122.613	0.680

ASN **t160** n = 61		
χ	Smooth COM	StdDev
chi1	-161.337	7.377
chi2	163.600	9.123
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.235	1.524
Cα_C_O	120.433	0.848
Cβ_Cα_C	111.294	1.376
Cβ_Cγ_Nδ2	117.029	2.099
Cβ_Cγ_Oδ1	120.496	2.021
N_Cα_C	110.034	1.950
N_Cα_Cβ	109.281	1.457
Oδ1_Cγ_Nδ2	122.428	0.778

ASN **m110** n = 4003		
χ	Smooth COM	StdDev
chi1	-63.571	9.647
chi2	114.583	28.436
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	112.723	1.153
Cα_C_O	120.501	0.902
Cβ_Cα_C	109.543	1.841
Cβ_Cγ_Nδ2	116.643	1.136
Cβ_Cγ_Oδ1	120.710	1.173
N_Cα_C	112.046	2.783
N_Cα_Cβ	110.629	1.196
Oδ1_Cγ_Nδ2	122.607	0.825

ASN **m-40** n = 26292		
χ	Smooth COM	StdDev
chi1	-69.790	9.121
chi2	-41.669	26.314
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	112.457	0.918
Cα_C_O	120.432	0.869
Cβ_Cα_C	110.006	1.725
Cβ_Cγ_Nδ2	116.531	0.847
Cβ_Cγ_Oδ1	120.778	0.894
N_Cα_C	112.237	2.543
N_Cα_Cβ	110.546	1.096
Oδ1_Cγ_Nδ2	122.662	0.698

3.9 ASP

ASP **p0** n = 11746		
χ	Smooth COM	StdDev
chi1	62.914	7.504
chi2	-2.097	31.033
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.477	1.018
Cα_C_O	120.397	0.909
Cβ_Cα_C	111.293	1.647
Cβ_Cγ_Oδ1	119.658	1.560
Cβ_Cγ_Oδ2	118.192	1.768
N_Cα_C	112.193	2.551
N_Cα_Cβ	111.140	1.255
Oδ1_Cγ_Oδ2	122.124	1.639

ASP **t0** n = 17107		
χ	Smooth COM	StdDev
chi1	-171.502	10.156
chi2	-1.704	23.754
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.211	0.911
Cα_C_O	120.704	0.890
Cβ_Cα_C	110.867	1.230
Cβ_Cγ_Oδ1	119.520	1.387
Cβ_Cγ_Oδ2	118.084	1.734
N_Cα_C	108.896	2.647
N_Cα_Cβ	109.695	1.453
Oδ1_Cγ_Oδ2	122.372	1.580

ASP **t70** n = 6029		
χ	Smooth COM	StdDev
chi1	-174.210	9.206
chi2	74.194	19.764
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	112.428	0.833
Cα_C_O	120.495	0.800
Cβ_Cα_C	110.144	1.274
Cβ_Cγ_Oδ1	118.490	1.114
Cβ_Cγ_Oδ2	118.723	1.564
N_Cα_C	110.484	2.358
N_Cα_Cβ	110.212	1.370
Oδ1_Cγ_Oδ2	122.747	1.537

ASP **m-30** n = 37239		
χ	Smooth COM	StdDev
chi1	-68.819	8.157
chi2	-29.214	22.379
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	112.905	0.946
Cα_C_O	120.451	0.856
Cβ_Cα_C	109.353	1.669
Cβ_Cγ_Oδ1	119.179	1.363
Cβ_Cγ_Oδ2	118.242	1.703
N_Cα_C	111.690	2.296
N_Cα_Cβ	110.769	1.055
Oδ1_Cγ_Oδ2	122.553	1.556

3.10 HIS

HIS **p90** n = 1492		
χ	Smooth COM	StdDev
chi1	62.492	9.692
chi2	86.558	21.799
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.189	1.053
Cα_C_O	120.635	0.945
Cβ_Cα_C	110.826	1.567
Cβ_Cγ_Cδ2	131.000	0.858
Cβ_Cγ_Nδ1	122.773	0.915
Cϵ1_Nϵ2_Cδ2	108.808	0.592
Cγ_Cδ2_Nϵ2	107.271	0.501
Cγ_Nδ1_Cϵ1	109.201	0.717
Nδ1_Cϵ1_Nϵ2	108.528	0.659
Nδ1_Cγ_Cδ2	106.170	0.534
N_Cα_C	111.257	2.740
N_Cα_Cβ	110.998	1.361

HIS **p-80** n = 2203		
χ	Smooth COM	StdDev
chi1	64.769	9.896
chi2	-80.838	16.239
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.073	1.065
Cα_C_O	120.392	0.980
Cβ_Cα_C	110.369	1.531
Cβ_Cγ_Cδ2	131.015	0.802
Cβ_Cγ_Nδ1	122.746	0.806
Cϵ1_Nϵ2_Cδ2	108.828	0.584
Cγ_Cδ2_Nϵ2	107.240	0.521
Cγ_Nδ1_Cϵ1	109.201	0.610
Nδ1_Cϵ1_Nϵ2	108.521	0.605
Nδ1_Cγ_Cδ2	106.187	0.514
N_Cα_C	112.010	2.426
N_Cα_Cβ	111.016	1.324

HIS **t70** n = 5068		
χ	Smooth COM	StdDev
chi1	-178.423	10.035
chi2	73.865	17.323
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.614	1.068
Cα_C_O	120.573	0.830
Cβ_Cα_C	110.127	1.337
Cβ_Cγ_Cδ2	131.028	0.815
Cβ_Cγ_Nδ1	122.666	0.792
Cϵ1_Nϵ2_Cδ2	108.853	0.519
Cγ_Cδ2_Nϵ2	107.197	0.456
Cγ_Nδ1_Cϵ1	109.172	0.621
Nδ1_Cϵ1_Nϵ2	108.505	0.557
Nδ1_Cγ_Cδ2	106.248	0.497
N_Cα_C	110.682	2.354
N_Cα_Cβ	110.179	1.486

HIS **t-170** n = 1332		
χ	Smooth COM	StdDev
chi1	-173.314	9.701
chi2	-167.114	21.613
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.240	1.024
Cα_C_O	120.601	0.807
Cβ_Cα_C	110.900	1.306
Cβ_Cγ_Cδ2	131.372	0.975
Cβ_Cγ_Nδ1	122.414	1.049
Cϵ1_Nϵ2_Cδ2	108.773	0.553
Cγ_Cδ2_Nϵ2	107.239	0.449
Cγ_Nδ1_Cϵ1	109.216	0.658
Nδ1_Cϵ1_Nϵ2	108.565	0.625
Nδ1_Cγ_Cδ2	106.182	0.524
N_Cα_C	109.227	2.609
N_Cα_Cβ	109.644	1.519

HIS **t-90** n = 3553		
χ	Smooth COM	StdDev
chi1	-173.491	10.385
chi2	-86.784	18.450
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.698	1.010
Cα_C_O	120.474	0.846
Cβ_Cα_C	110.440	1.219
Cβ_Cγ_Cδ2	130.907	0.830
Cβ_Cγ_Nδ1	122.790	0.749
Cϵ1_Nϵ2_Cδ2	108.840	0.525
Cγ_Cδ2_Nϵ2	107.199	0.482
Cγ_Nδ1_Cϵ1	109.174	0.721
Nδ1_Cϵ1_Nϵ2	108.510	0.617
Nδ1_Cγ_Cδ2	106.247	0.554
N_Cα_C	109.908	2.468
N_Cα_Cβ	110.079	1.464

HIS **m170** n = 2695		
χ	Smooth COM	StdDev
chi1	-67.985	8.200
chi2	170.975	21.745
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.732	0.930
Cα_C_O	120.396	0.880
Cβ_Cα_C	109.708	1.788
Cβ_Cγ_Cδ2	131.144	0.993
Cβ_Cγ_Nδ1	122.596	1.037
Cϵ1_Nϵ2_Cδ2	108.792	0.528
Cγ_Cδ2_Nϵ2	107.215	0.471
Cγ_Nδ1_Cϵ1	109.180	0.692
Nδ1_Cϵ1_Nϵ2	108.559	0.624
Nδ1_Cγ_Cδ2	106.227	0.530
N_Cα_C	111.531	2.540
N_Cα_Cβ	110.742	1.152

HIS **m90** n = 3914		
χ	Smooth COM	StdDev
chi1	-65.658	9.782
chi2	88.477	17.472
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.467	1.110
Cα_C_O	120.484	0.896
Cβ_Cα_C	109.759	1.956
Cβ_Cγ_Cδ2	130.923	0.854
Cβ_Cγ_Nδ1	122.786	0.821
Cϵ1_Nϵ2_Cδ2	108.852	0.557
Cγ_Cδ2_Nϵ2	107.207	0.499
Cγ_Nδ1_Cϵ1	109.189	0.640
Nδ1_Cϵ1_Nϵ2	108.501	0.615
Nδ1_Cγ_Cδ2	106.226	0.511
N_Cα_C	111.473	2.734
N_Cα_Cβ	110.637	1.176

HIS **m-70** n = 9453		
χ	Smooth COM	StdDev
chi1	-64.458	10.014
chi2	-75.228	19.348
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.370	1.064
Cα_C_O	120.407	0.875
Cβ_Cα_C	109.866	1.886
Cβ_Cγ_Cδ2	131.054	0.818
Cβ_Cγ_Nδ1	122.620	0.801
Cϵ1_Nϵ2_Cδ2	108.856	0.517
Cγ_Cδ2_Nϵ2	107.184	0.469
Cγ_Nδ1_Cϵ1	109.178	0.630
Nδ1_Cϵ1_Nϵ2	108.498	0.562
Nδ1_Cγ_Cδ2	106.259	0.532
N_Cα_C	111.715	2.840
N_Cα_Cβ	110.397	1.175

3.11 PHE

PHE **p90** n = 6289		
χ	Smooth COM	StdDev
chi1	63.561	9.566
chi2	-89.699	9.411
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.408	0.965
Cα_C_O	120.711	0.891
Cβ_Cα_C	110.881	1.459
Cβ_Cγ_Cδ1	120.730	0.618
Cβ_Cγ_Cδ2	120.607	0.579
Cδ1_Cϵ1_Cζ	119.892	0.604
Cδ1_Cγ_Cδ2	118.617	0.534
Cϵ1_Cζ_Cϵ2	119.823	0.628
Cγ_Cδ1_Cϵ1	120.858	0.589
Cγ_Cδ2_Cϵ2	120.855	0.575
Cζ_Cϵ2_Cδ2	119.920	0.592
N_Cα_C	110.871	2.566
N_Cα_Cβ	111.393	1.319

PHE **t80** n = 19289		
χ	Smooth COM	StdDev
chi1	-178.297	9.973
chi2	75.767	17.432
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.786	1.072
Cα_C_O	120.598	0.802
Cβ_Cα_C	110.336	1.300
Cβ_Cγ_Cδ1	120.648	0.723
Cβ_Cγ_Cδ2	120.537	0.684
Cδ1_Cϵ1_Cζ	119.859	0.588
Cδ1_Cγ_Cδ2	118.764	0.551
Cϵ1_Cζ_Cϵ2	119.922	0.630
Cγ_Cδ1_Cϵ1	120.767	0.581
Cγ_Cδ2_Cϵ2	120.790	0.589
Cζ_Cϵ2_Cδ2	119.864	0.587
N_Cα_C	110.337	2.307
N_Cα_Cβ	110.203	1.503

PHE **m-10** n = 3880		
χ	Smooth COM	StdDev
chi1	-68.127	9.328
chi2	-14.743	19.837
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.792	0.955
Cα_C_O	120.423	0.872
Cβ_Cα_C	108.945	1.776
Cβ_Cγ_Cδ1	121.549	1.215
Cβ_Cγ_Cδ2	119.886	1.159
Cδ1_Cϵ1_Cζ	119.897	0.614
Cδ1_Cγ_Cδ2	118.521	0.565
Cϵ1_Cζ_Cϵ2	119.840	0.619
Cγ_Cδ1_Cϵ1	120.784	0.600
Cγ_Cδ2_Cϵ2	120.989	0.612
Cζ_Cϵ2_Cδ2	119.931	0.612
N_Cα_C	111.035	2.421
N_Cα_Cβ	111.200	1.109

PHE **m-80** n = 26665		
χ	Smooth COM	StdDev
chi1	-66.760	10.140
chi2	-80.589	16.828
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.517	1.023
Cα_C_O	120.453	0.861
Cβ_Cα_C	109.811	1.992
Cβ_Cγ_Cδ1	120.579	0.602
Cβ_Cγ_Cδ2	120.569	0.590
Cδ1_Cϵ1_Cζ	119.862	0.580
Cδ1_Cγ_Cδ2	118.798	0.527
Cϵ1_Cζ_Cϵ2	119.894	0.607
Cγ_Cδ1_Cϵ1	120.768	0.562
Cγ_Cδ2_Cϵ2	120.766	0.570
Cζ_Cϵ2_Cδ2	119.878	0.579
N_Cα_C	111.240	2.815
N_Cα_Cβ	110.549	1.107

3.12 TYR

TYR **p90** n = 5466		
χ	Smooth COM	StdDev
chi1	63.561	10.553
chi2	-89.699	10.123
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.846	1.875
Cα_C_O	120.663	0.933
Cβ_Cα_C	110.645	1.410
Cβ_Cγ_Cδ1	120.995	0.651
Cβ_Cγ_Cδ2	120.859	0.602
Cδ1_Cϵ1_Cζ	119.526	0.622
Cδ1_Cγ_Cδ2	118.104	0.554
Cϵ1_Cζ_Cϵ2	120.448	0.664
Cϵ1_Cζ_OH	119.792	1.246
Cγ_Cδ1_Cϵ1	121.166	0.582
Cγ_Cδ2_Cϵ2	121.163	0.550
Cζ_Cϵ2_Cδ2	119.562	0.624
N_Cα_C	111.069	2.657
N_Cα_Cβ	111.212	1.224
OH_Cζ_Cϵ2	119.743	1.241

TYR **t80** n = 16312		
χ	Smooth COM	StdDev
chi1	-178.297	10.473
chi2	75.767	16.674
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.708	2.135
Cα_C_O	120.621	0.799
Cβ_Cα_C	110.305	1.253
Cβ_Cγ_Cδ1	120.905	0.663
Cβ_Cγ_Cδ2	120.836	0.646
Cδ1_Cϵ1_Cζ	119.513	0.600
Cδ1_Cγ_Cδ2	118.209	0.523
Cϵ1_Cζ_Cϵ2	120.505	0.653
Cϵ1_Cζ_OH	119.748	1.279
Cγ_Cδ1_Cϵ1	121.095	0.555
Cγ_Cδ2_Cϵ2	121.137	0.560
Cζ_Cϵ2_Cδ2	119.508	0.628
N_Cα_C	110.391	2.248
N_Cα_Cβ	110.211	1.442
OH_Cζ_Cϵ2	119.729	1.278

TYR **m-10** n = 2623		
χ	Smooth COM	StdDev
chi1	-68.127	9.935
chi2	-14.743	20.169
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.769	1.568
Cα_C_O	120.432	0.845
Cβ_Cα_C	109.056	1.746
Cβ_Cγ_Cδ1	121.580	1.013
Cβ_Cγ_Cδ2	120.368	0.936
Cδ1_Cϵ1_Cζ	119.496	0.618
Cδ1_Cγ_Cδ2	118.010	0.570
Cϵ1_Cζ_Cϵ2	120.405	0.650
Cϵ1_Cζ_OH	120.080	1.320
Cγ_Cδ1_Cϵ1	121.075	0.598
Cγ_Cδ2_Cϵ2	121.325	0.575
Cζ_Cϵ2_Cδ2	119.652	0.642
N_Cα_C	111.382	2.346
N_Cα_Cβ	111.006	1.145
OH_Cζ_Cϵ2	119.496	1.345

TYR **m-80** n = 22683		
χ	Smooth COM	StdDev
chi1	-66.760	10.437
chi2	-80.589	16.848
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.205	2.043
Cα_C_O	120.442	0.877
Cβ_Cα_C	109.633	1.925
Cβ_Cγ_Cδ1	120.859	0.627
Cβ_Cγ_Cδ2	120.851	0.617
Cδ1_Cϵ1_Cζ	119.505	0.900
Cδ1_Cγ_Cδ2	118.240	0.580
Cϵ1_Cζ_Cϵ2	120.500	0.733
Cϵ1_Cζ_OH	119.719	1.238
Cγ_Cδ1_Cϵ1	121.099	0.856
Cγ_Cδ2_Cϵ2	121.096	0.860
Cζ_Cϵ2_Cδ2	119.515	0.903
N_Cα_C	111.429	2.763
N_Cα_Cβ	110.557	1.100
OH_Cζ_Cϵ2	119.764	1.250

3.13 TRP

TRP **p90** n = 971		
χ	Smooth COM	StdDev
chi1	60.293	9.937
chi2	87.822	14.661
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.031	2.042
Cα_C_O	120.569	0.863
Cβ_Cα_C	110.664	1.413
Cβ_Cγ_Cδ1	127.002	0.699
Cβ_Cγ_Cδ2	126.749	0.757
Cδ1_Cγ_Cδ2	106.201	0.376
Cδ1_Nϵ1_Cϵ2	108.926	0.597
Cδ2_Cϵ2_Cζ2	122.451	0.368
Cδ2_Cϵ3_Cζ3	118.690	0.344
Cϵ2_Cδ2_Cϵ3	118.827	0.360
Cϵ2_Cδ2_Cγ	107.259	0.313
Cϵ3_Cζ3_Cη2	121.028	0.417
Cγ_Cδ1_Nϵ1	110.152	0.498
Cγ_Cδ2_Cϵ3	133.896	0.337
Cη2_Cζ2_Cϵ2	117.467	0.446
Cζ3_Cη2_Cζ2	121.507	0.461
Nϵ1_Cϵ2_Cδ2	107.442	0.366
Nϵ1_Cϵ2_Cζ2	130.095	0.402
N_Cα_C	111.204	2.410
N_Cα_Cβ	111.115	1.260

TRP **p-90** n = 1937		
χ	Smooth COM	StdDev
chi1	61.771	9.829
chi2	-89.374	12.891
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.039	1.903
Cα_C_O	120.457	0.933
Cβ_Cα_C	110.457	1.434
Cβ_Cγ_Cδ1	126.859	0.673
Cβ_Cγ_Cδ2	126.898	0.711
Cδ1_Cγ_Cδ2	106.193	0.435
Cδ1_Nϵ1_Cϵ2	108.956	0.459
Cδ2_Cϵ2_Cζ2	122.437	0.342
Cδ2_Cϵ3_Cζ3	118.715	0.472
Cϵ2_Cδ2_Cϵ3	118.806	0.387
Cϵ2_Cδ2_Cγ	107.248	0.330
Cϵ3_Cζ3_Cη2	121.029	0.457
Cγ_Cδ1_Nϵ1	110.152	0.461
Cγ_Cδ2_Cϵ3	133.932	0.413
Cη2_Cζ2_Cϵ2	117.524	0.444
Cζ3_Cη2_Cζ2	121.463	0.462
Nϵ1_Cϵ2_Cδ2	107.431	0.341
Nϵ1_Cϵ2_Cζ2	130.118	0.406
N_Cα_C	112.137	2.597
N_Cα_Cβ	111.096	1.241

TRP **t60** n = 3385		
χ	Smooth COM	StdDev
chi1	-178.686	9.781
chi2	64.773	32.759
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.267	2.142
Cα_C_O	120.658	0.805
Cβ_Cα_C	110.556	1.354
Cβ_Cγ_Cδ1	127.131	0.791
Cβ_Cγ_Cδ2	126.521	0.816
Cδ1_Cγ_Cδ2	106.292	0.480
Cδ1_Nϵ1_Cϵ2	108.908	0.510
Cδ2_Cϵ2_Cζ2	122.396	0.397
Cδ2_Cϵ3_Cζ3	118.696	0.418
Cϵ2_Cδ2_Cϵ3	118.868	0.376
Cϵ2_Cδ2_Cγ	107.260	0.380
Cϵ3_Cζ3_Cη2	120.994	0.476
Cγ_Cδ1_Nϵ1	110.066	0.533
Cγ_Cδ2_Cϵ3	133.854	0.427
Cη2_Cζ2_Cϵ2	117.487	0.458
Cζ3_Cη2_Cζ2	121.531	0.477
Nϵ1_Cϵ2_Cδ2	107.451	0.384
Nϵ1_Cϵ2_Cζ2	130.137	0.461
N_Cα_C	110.136	2.153
N_Cα_Cβ	109.969	1.424

TRP **t-100** n = 2893		
χ	Smooth COM	StdDev
chi1	-177.069	11.596
chi2	-102.575	15.367
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.566	2.320
Cα_C_O	120.574	0.869
Cβ_Cα_C	110.338	1.328
Cβ_Cγ_Cδ1	126.901	0.685
Cβ_Cγ_Cδ2	126.744	0.710
Cδ1_Cγ_Cδ2	106.290	0.425
Cδ1_Nϵ1_Cϵ2	108.932	0.453
Cδ2_Cϵ2_Cζ2	122.411	0.363
Cδ2_Cϵ3_Cζ3	118.696	0.451
Cϵ2_Cδ2_Cϵ3	118.847	0.349
Cϵ2_Cδ2_Cγ	107.214	0.324
Cϵ3_Cζ3_Cη2	121.008	0.479
Cγ_Cδ1_Nϵ1	110.106	0.476
Cγ_Cδ2_Cϵ3	133.922	0.366
Cη2_Cζ2_Cϵ2	117.507	0.446
Cζ3_Cη2_Cζ2	121.503	0.457
Nϵ1_Cϵ2_Cδ2	107.437	0.338
Nϵ1_Cϵ2_Cζ2	130.137	0.434
N_Cα_C	110.511	2.424
N_Cα_Cβ	110.288	1.416

TRP **m100** n = 6319		
χ	Smooth COM	StdDev
chi1	-67.358	10.774
chi2	97.262	16.989
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.176	2.218
Cα_C_O	120.433	0.860
Cβ_Cα_C	109.632	1.917
Cβ_Cγ_Cδ1	127.022	0.664
Cβ_Cγ_Cδ2	126.590	0.685
Cδ1_Cγ_Cδ2	106.335	0.429
Cδ1_Nϵ1_Cϵ2	108.902	0.486
Cδ2_Cϵ2_Cζ2	122.401	0.364
Cδ2_Cϵ3_Cζ3	118.699	0.455
Cϵ2_Cδ2_Cϵ3	118.868	0.368
Cϵ2_Cδ2_Cγ	107.232	0.331
Cϵ3_Cζ3_Cη2	120.996	0.477
Cγ_Cδ1_Nϵ1	110.087	0.488
Cγ_Cδ2_Cϵ3	133.883	0.397
Cη2_Cζ2_Cϵ2	117.493	0.451
Cζ3_Cη2_Cζ2	121.514	0.456
Nϵ1_Cϵ2_Cδ2	107.423	0.349
Nϵ1_Cϵ2_Cζ2	130.160	0.431
N_Cα_C	111.436	2.636
N_Cα_Cβ	110.555	1.106

TRP **m-10** n = 2196		
χ	Smooth COM	StdDev
chi1	-68.163	8.989
chi2	-7.490	21.670
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.734	1.637
Cα_C_O	120.481	0.882
Cβ_Cα_C	109.190	1.715
Cβ_Cγ_Cδ1	127.548	0.711
Cβ_Cγ_Cδ2	126.108	0.767
Cδ1_Cγ_Cδ2	106.300	0.445
Cδ1_Nϵ1_Cϵ2	108.834	0.452
Cδ2_Cϵ2_Cζ2	122.350	0.407
Cδ2_Cϵ3_Cζ3	118.695	0.434
Cϵ2_Cδ2_Cϵ3	118.908	0.380
Cϵ2_Cδ2_Cγ	107.324	0.376
Cϵ3_Cζ3_Cη2	121.005	0.432
Cγ_Cδ1_Nϵ1	110.042	0.481
Cγ_Cδ2_Cϵ3	133.752	0.391
Cη2_Cζ2_Cϵ2	117.472	0.467
Cζ3_Cη2_Cζ2	121.543	0.462
Nϵ1_Cϵ2_Cδ2	107.478	0.366
Nϵ1_Cϵ2_Cζ2	130.159	0.453
N_Cα_C	111.431	2.538
N_Cα_Cβ	110.792	1.154

TRP **m-90** n = 961		
χ	Smooth COM	StdDev
chi1	-67.780	12.415
chi2	-89.279	13.788
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.837	2.475
Cα_C_O	120.475	0.855
Cβ_Cα_C	109.396	2.035
Cβ_Cγ_Cδ1	126.707	0.719
Cβ_Cγ_Cδ2	126.952	0.778
Cδ1_Cγ_Cδ2	106.279	0.441
Cδ1_Nϵ1_Cϵ2	108.930	0.474
Cδ2_Cϵ2_Cζ2	122.433	0.348
Cδ2_Cϵ3_Cζ3	118.702	0.453
Cϵ2_Cδ2_Cϵ3	118.842	0.382
Cϵ2_Cδ2_Cγ	107.196	0.323
Cϵ3_Cζ3_Cη2	121.019	0.460
Cγ_Cδ1_Nϵ1	110.124	0.496
Cγ_Cδ2_Cϵ3	133.947	0.378
Cη2_Cζ2_Cϵ2	117.505	0.430
Cζ3_Cη2_Cζ2	121.472	0.453
Nϵ1_Cϵ2_Cδ2	107.451	0.346
Nϵ1_Cϵ2_Cζ2	130.101	0.430
N_Cα_C	110.581	2.879
N_Cα_Cβ	110.698	1.125

3.14 MET

MET **ppp** n = 50		
χ	Smooth COM	StdDev
chi1	61.248	9.313
chi2	78.960	10.968
chi3	70.700	9.878
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.688	1.786
Cα_C_O	120.690	0.904
Cβ_Cα_C	111.199	1.571
Cβ_Cγ_SD	114.396	2.327
Cγ_SD_Cϵ	100.530	4.023
N_Cα_C	111.830	2.718
N_Cα_Cβ	110.925	1.021

MET **pp-130** n = 27		
χ	Smooth COM	StdDev
chi1	64.331	7.151
chi2	82.303	4.909
chi3	-154.200	27.756
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.400	1.176
Cα_C_O	120.921	0.655
Cβ_Cα_C	111.108	0.909
Cβ_Cγ_SD	113.705	2.013
Cγ_SD_Cϵ	100.847	1.954
N_Cα_C	110.987	1.836
N_Cα_Cβ	110.899	0.988

MET **ptp** n = 404		
χ	Smooth COM	StdDev
chi1	64.508	8.469
chi2	-176.358	11.392
chi3	73.220	11.597
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.589	1.803
Cα_C_O	120.674	0.921
Cβ_Cα_C	110.290	1.464
Cβ_Cγ_SD	112.889	2.185
Cγ_SD_Cϵ	100.792	1.939
N_Cα_C	110.626	2.559
N_Cα_Cβ	111.047	1.233

MET **ptt** n = 260		
χ	Smooth COM	StdDev
chi1	65.361	8.250
chi2	-178.195	9.143
chi3	179.354	15.601
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.719	1.689
Cα_C_O	120.592	0.945
Cβ_Cα_C	110.343	1.486
Cβ_Cγ_SD	111.033	2.395
Cγ_SD_Cϵ	99.817	2.318
N_Cα_C	111.139	2.697
N_Cα_Cβ	111.125	1.299

MET **ptm** n = 375		
χ	Smooth COM	StdDev
chi1	64.860	8.163
chi2	179.370	10.168
chi3	-72.053	11.599
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.625	1.646
Cα_C_O	120.634	0.935
Cβ_Cα_C	110.349	1.438
Cβ_Cγ_SD	112.773	2.109
Cγ_SD_Cϵ	100.903	1.820
N_Cα_C	110.872	2.766
N_Cα_Cβ	111.166	1.207

MET **pmt** n = 7		
χ	Smooth COM	StdDev
chi1	71.340	3.364
chi2	-74.720	3.186
chi3	-162.328	4.884
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.786	0.770
Cα_C_O	120.997	0.636
Cβ_Cα_C	111.122	1.130
Cβ_Cγ_SD	111.744	2.285
Cγ_SD_Cϵ	100.246	1.914
N_Cα_C	109.009	1.550
N_Cα_Cβ	111.648	1.281

MET **pmm** n = 42		
χ	Smooth COM	StdDev
chi1	72.629	7.847
chi2	-68.668	6.731
chi3	-68.863	8.148
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.484	0.858
Cα_C_O	120.618	0.788
Cβ_Cα_C	110.176	1.220
Cβ_Cγ_SD	115.246	2.537
Cγ_SD_Cϵ	101.108	1.585
N_Cα_C	112.287	2.688
N_Cα_Cβ	110.768	1.207

MET **tpp** n = 1138		
χ	Smooth COM	StdDev
chi1	-174.981	9.366
chi2	63.633	7.983
chi3	72.405	12.028
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.191	1.355
Cα_C_O	120.501	0.842
Cβ_Cα_C	110.324	1.130
Cβ_Cγ_SD	113.667	2.023
Cγ_SD_Cϵ	100.683	1.769
N_Cα_C	110.665	2.235
N_Cα_Cβ	110.488	1.169

MET **tpt** n = 388		
χ	Smooth COM	StdDev
chi1	-173.452	8.736
chi2	65.814	7.811
chi3	-156.289	31.222
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.077	1.391
Cα_C_O	120.521	0.742
Cβ_Cα_C	110.486	1.134
Cβ_Cγ_SD	112.447	1.994
Cγ_SD_Cϵ	100.425	2.088
N_Cα_C	110.446	2.248
N_Cα_Cβ	110.324	1.364

MET **ttp** n = 1246		
χ	Smooth COM	StdDev
chi1	-177.766	8.645
chi2	179.141	11.418
chi3	71.790	10.585
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.559	1.653
Cα_C_O	120.611	0.853
Cβ_Cα_C	110.039	1.168
Cβ_Cγ_SD	112.805	2.114
Cγ_SD_Cϵ	100.741	2.073
N_Cα_C	110.270	2.150
N_Cα_Cβ	110.378	1.313

MET **ttt** n = 569		
χ	Smooth COM	StdDev
chi1	-176.725	8.762
chi2	176.823	9.513
chi3	176.456	15.483
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.692	1.716
Cα_C_O	120.590	0.958
Cβ_Cα_C	110.139	1.307
Cβ_Cγ_SD	110.615	2.198
Cγ_SD_Cϵ	100.115	1.656
N_Cα_C	110.201	2.431
N_Cα_Cβ	110.091	1.385

MET **ttm** n = 1124		
χ	Smooth COM	StdDev
chi1	-175.045	9.346
chi2	179.637	8.225
chi3	-71.855	13.081
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.533	1.706
Cα_C_O	120.521	0.803
Cβ_Cα_C	109.956	1.173
Cβ_Cγ_SD	112.759	2.157
Cγ_SD_Cϵ	100.808	1.735
N_Cα_C	110.136	2.395
N_Cα_Cβ	110.414	1.331

MET **tmt** n = 34		
χ	Smooth COM	StdDev
chi1	-179.131	6.701
chi2	-85.941	7.575
chi3	173.719	24.401
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.856	1.126
Cα_C_O	120.669	0.563
Cβ_Cα_C	110.695	1.236
Cβ_Cγ_SD	112.753	1.775
Cγ_SD_Cϵ	100.340	1.369
N_Cα_C	110.002	2.892
N_Cα_Cβ	110.086	1.223

MET **tmm** n = 276		
χ	Smooth COM	StdDev
chi1	-177.257	7.306
chi2	-81.707	6.798
chi3	-72.167	10.514
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.995	1.371
Cα_C_O	120.520	0.782
Cβ_Cα_C	111.023	1.239
Cβ_Cγ_SD	114.026	2.121
Cγ_SD_Cϵ	100.840	1.640
N_Cα_C	109.902	2.105
N_Cα_Cβ	110.096	1.162

MET **mpp** n = 74		
χ	Smooth COM	StdDev
chi1	-76.610	13.735
chi2	73.172	12.266
chi3	73.993	11.907
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.617	1.359
Cα_C_O	120.531	0.886
Cβ_Cα_C	109.865	1.627
Cβ_Cγ_SD	114.327	2.245
Cγ_SD_Cϵ	101.176	2.262
N_Cα_C	110.743	2.686
N_Cα_Cβ	110.760	1.199

MET **mpt** n = 34		
χ	Smooth COM	StdDev
chi1	-69.557	11.736
chi2	74.032	10.961
chi3	167.387	18.642
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.581	0.956
Cα_C_O	120.388	0.881
Cβ_Cα_C	109.316	1.399
Cβ_Cγ_SD	113.183	2.024
Cγ_SD_Cϵ	100.105	2.397
N_Cα_C	110.123	2.780
N_Cα_Cβ	110.956	1.118

MET **mpm** n = 13		
χ	Smooth COM	StdDev
chi1	-77.183	5.132
chi2	63.994	5.469
chi3	-101.774	5.027
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.136	1.018
Cα_C_O	120.662	0.735
Cβ_Cα_C	109.135	1.274
Cβ_Cγ_SD	115.853	2.314
Cγ_SD_Cϵ	100.367	1.563
N_Cα_C	110.742	1.813
N_Cα_Cβ	111.036	1.046

MET **mtp** n = 2815		
χ	Smooth COM	StdDev
chi1	-66.650	7.058
chi2	177.074	9.262
chi3	70.464	10.090
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.148	1.645
Cα_C_O	120.492	0.844
Cβ_Cα_C	109.955	1.587
Cβ_Cγ_SD	112.850	2.081
Cγ_SD_Cϵ	100.766	1.731
N_Cα_C	111.257	2.348
N_Cα_Cβ	110.469	1.007

MET **mtt** n = 1542		
χ	Smooth COM	StdDev
chi1	-67.154	7.717
chi2	179.723	8.705
chi3	-176.816	16.539
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.586	1.708
Cα_C_O	120.527	0.825
Cβ_Cα_C	109.380	1.673
Cβ_Cγ_SD	110.388	2.192
Cγ_SD_Cϵ	100.144	1.974
N_Cα_C	111.150	2.271
N_Cα_Cβ	110.658	0.996

MET **mtm** n = 1851		
χ	Smooth COM	StdDev
chi1	-66.363	7.865
chi2	-177.825	10.672
chi3	-73.985	10.774
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.170	1.716
Cα_C_O	120.494	0.902
Cβ_Cα_C	109.943	1.631
Cβ_Cγ_SD	112.920	2.146
Cγ_SD_Cϵ	100.758	1.779
N_Cα_C	111.074	2.323
N_Cα_Cβ	110.665	1.072

MET **mmp** n = 520		
χ	Smooth COM	StdDev
chi1	-65.195	5.298
chi2	-61.634	6.333
chi3	102.180	9.255
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.212	1.410
Cα_C_O	120.324	0.802
Cβ_Cα_C	110.229	1.552
Cβ_Cγ_SD	113.849	2.144
Cγ_SD_Cϵ	101.224	2.184
N_Cα_C	111.490	2.153
N_Cα_Cβ	110.838	1.099

MET **mmt** n = 597		
χ	Smooth COM	StdDev
chi1	-64.971	8.734
chi2	-63.753	9.443
chi3	172.207	18.496
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.918	1.444
Cα_C_O	120.423	0.802
Cβ_Cα_C	109.926	1.551
Cβ_Cγ_SD	112.060	2.042
Cγ_SD_Cϵ	100.263	1.993
N_Cα_C	111.450	2.253
N_Cα_Cβ	110.610	0.944

MET **mmm** n = 3354		
χ	Smooth COM	StdDev
chi1	-65.551	8.867
chi2	-60.977	8.775
chi3	-69.165	10.156
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.003	1.286
Cα_C_O	120.359	0.857
Cβ_Cα_C	110.042	1.527
Cβ_Cγ_SD	113.654	1.948
Cγ_SD_Cϵ	100.895	1.737
N_Cα_C	111.629	2.379
N_Cα_Cβ	110.711	1.020

3.15 GLU

GLU **pp20** n = 159		
χ	Smooth COM	StdDev
chi1	61.255	8.074
chi2	85.644	7.983
chi3	19.654	17.191
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.555	1.282
Cα_C_O	120.440	0.848
Cβ_Cα_C	111.591	1.836
Cβ_Cγ_Cδ	114.078	1.297
Cγ_Cδ_Oϵ1	119.034	1.429
Cγ_Cδ_Oϵ2	118.356	1.340
N_Cα_C	110.829	2.541
N_Cα_Cβ	111.446	1.254
Oϵ1_Cδ_Oϵ2	122.590	1.020

GLU **pt0** n = 2800		
χ	Smooth COM	StdDev
chi1	65.363	8.357
chi2	-177.309	10.089
chi3	1.201	51.015
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.597	1.602
Cα_C_O	120.524	0.927
Cβ_Cα_C	110.513	1.498
Cβ_Cγ_Cδ	112.902	1.527
Cγ_Cδ_Oϵ1	118.928	1.384
Cγ_Cδ_Oϵ2	118.169	1.352
N_Cα_C	111.272	2.667
N_Cα_Cβ	111.061	1.180
Oϵ1_Cδ_Oϵ2	122.878	1.149

GLU **pm20** n = 1485		
χ	Smooth COM	StdDev
chi1	69.039	8.839
chi2	-84.712	8.551
chi3	15.811	21.665
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.558	1.350
Cα_C_O	120.191	0.834
Cβ_Cα_C	110.506	1.246
Cβ_Cγ_Cδ	114.466	1.447
Cγ_Cδ_Oϵ1	119.771	1.714
Cγ_Cδ_Oϵ2	117.692	1.688
N_Cα_C	112.900	1.826
N_Cα_Cβ	110.887	1.055
Oϵ1_Cδ_Oϵ2	122.520	1.102

GLU **tp30** n = 4616		
χ	Smooth COM	StdDev
chi1	-178.170	9.848
chi2	64.992	9.169
chi3	25.784	26.065
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.624	1.386
Cα_C_O	120.486	0.798
Cβ_Cα_C	110.645	1.209
Cβ_Cγ_Cδ	113.769	1.354
Cγ_Cδ_Oϵ1	119.284	1.459
Cγ_Cδ_Oϵ2	118.037	1.380
N_Cα_C	110.857	2.089
N_Cα_Cβ	110.284	1.123
Oϵ1_Cδ_Oϵ2	122.658	1.073

GLU **tt0** n = 13610		
χ	Smooth COM	StdDev
chi1	-176.677	8.634
chi2	177.900	10.314
chi3	1.122	41.445
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.479	1.738
Cα_C_O	120.579	0.766
Cβ_Cα_C	110.135	1.168
Cβ_Cγ_Cδ	113.090	1.500
Cγ_Cδ_Oϵ1	118.950	1.273
Cγ_Cδ_Oϵ2	117.962	1.269
N_Cα_C	110.583	2.260
N_Cα_Cβ	110.351	1.366
Oϵ1_Cδ_Oϵ2	123.063	1.067

GLU **tm-30** n = 862		
χ	Smooth COM	StdDev
chi1	-170.330	8.580
chi2	-83.400	9.158
chi3	-28.718	17.284
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.520	1.347
Cα_C_O	120.511	0.838
Cβ_Cα_C	110.969	1.333
Cβ_Cγ_Cδ	113.819	1.465
Cγ_Cδ_Oϵ1	119.014	1.362
Cγ_Cδ_Oϵ2	118.207	1.249
N_Cα_C	110.226	2.465
N_Cα_Cβ	110.236	1.156
Oϵ1_Cδ_Oϵ2	122.755	1.171

GLU **mp0** n = 3671		
χ	Smooth COM	StdDev
chi1	-66.877	7.274
chi2	82.550	9.362
chi3	3.347	27.520
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.352	1.344
Cα_C_O	120.431	0.818
Cβ_Cα_C	109.695	1.424
Cβ_Cγ_Cδ	114.166	1.404
Cγ_Cδ_Oϵ1	119.771	1.659
Cγ_Cδ_Oϵ2	117.760	1.471
N_Cα_C	112.041	1.999
N_Cα_Cβ	110.602	1.057
Oϵ1_Cδ_Oϵ2	122.450	1.179

GLU **mm-30** n = 9080		
χ	Smooth COM	StdDev
chi1	-66.002	8.689
chi2	-66.544	10.569
chi3	-31.662	26.859
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.037	1.414
Cα_C_O	120.415	0.828
Cβ_Cα_C	109.927	1.502
Cβ_Cγ_Cδ	113.361	1.338
Cγ_Cδ_Oϵ1	119.153	1.345
Cγ_Cδ_Oϵ2	118.206	1.265
N_Cα_C	111.483	2.356
N_Cα_Cβ	110.748	1.014
Oϵ1_Cδ_Oϵ2	122.622	1.092

GLU **mt-10** n = 21021		
χ	Smooth COM	StdDev
chi1	-66.989	7.750
chi2	179.213	11.417
chi3	-6.596	37.250
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.038	1.846
Cα_C_O	120.491	0.823
Cβ_Cα_C	110.020	1.731
Cβ_Cγ_Cδ	113.253	1.500
Cγ_Cδ_Oϵ1	119.081	1.288
Cγ_Cδ_Oϵ2	117.940	1.286
N_Cα_C	111.364	2.321
N_Cα_Cβ	110.595	1.004
Oϵ1_Cδ_Oϵ2	122.955	1.064

3.16 GLN

GLN **pp30** n = 178		
χ	Smooth COM	StdDev
chi1	62.991	7.802
chi2	83.801	8.473
chi3	29.841	20.903
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.880	1.278
Cα_C_O	120.321	0.946
Cβ_Cα_C	111.398	1.618
Cβ_Cγ_Cδ	113.604	1.401
Cγ_Cδ_Nϵ2	116.446	0.892
Cγ_Cδ_Oϵ1	120.885	0.949
N_Cα_C	111.003	2.550
N_Cα_Cβ	111.519	1.154
Oϵ1_Cδ_Nϵ2	122.630	0.669

GLN **pt0** n = 1885		
χ	Smooth COM	StdDev
chi1	64.891	8.125
chi2	-177.468	11.284
chi3	-2.755	75.227
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.518	1.528
Cα_C_O	120.546	0.962
Cβ_Cα_C	110.361	1.519
Cβ_Cγ_Cδ	112.497	1.466
Cγ_Cδ_Nϵ2	116.505	0.954
Cγ_Cδ_Oϵ1	120.841	0.973
N_Cα_C	111.263	2.631
N_Cα_Cβ	110.949	1.178
Oϵ1_Cδ_Nϵ2	122.629	0.748

GLN **pm20** n = 487		
χ	Smooth COM	StdDev
chi1	69.577	9.904
chi2	-84.394	9.313
chi3	16.576	32.336
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.686	1.408
Cα_C_O	120.304	0.925
Cβ_Cα_C	110.423	1.352
Cβ_Cγ_Cδ	113.925	1.430
Cγ_Cδ_Nϵ2	116.256	0.863
Cγ_Cδ_Oϵ1	121.254	0.986
N_Cα_C	112.420	2.222
N_Cα_Cβ	111.150	1.131
Oϵ1_Cδ_Nϵ2	122.470	0.718

GLN **tp40** n = 3618		
χ	Smooth COM	StdDev
chi1	-176.823	8.734
chi2	66.430	8.230
chi3	41.056	24.195
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.949	1.419
Cα_C_O	120.428	0.793
Cβ_Cα_C	110.237	1.153
Cβ_Cγ_Cδ	112.883	1.238
Cγ_Cδ_Nϵ2	116.593	0.838
Cγ_Cδ_Oϵ1	120.792	0.874
N_Cα_C	111.017	2.005
N_Cα_Cβ	110.571	1.130
Oϵ1_Cδ_Nϵ2	122.594	0.646

GLN **tp-100** n = 534		
χ	Smooth COM	StdDev
chi1	-176.963	8.680
chi2	62.135	8.823
chi3	-104.704	27.530
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.443	1.567
Cα_C_O	120.563	0.834
Cβ_Cα_C	110.517	1.240
Cβ_Cγ_Cδ	113.047	1.311
Cγ_Cδ_Nϵ2	116.553	0.949
Cγ_Cδ_Oϵ1	120.860	0.852
N_Cα_C	110.364	2.260
N_Cα_Cβ	110.382	1.236
Oϵ1_Cδ_Nϵ2	122.560	0.637

GLN **tt0** n = 6936		
χ	Smooth COM	StdDev
chi1	-176.317	8.500
chi2	177.556	10.804
chi3	2.032	60.871
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.566	1.797
Cα_C_O	120.576	0.762
Cβ_Cα_C	110.144	1.180
Cβ_Cγ_Cδ	112.612	1.504
Cγ_Cδ_Nϵ2	116.455	0.840
Cγ_Cδ_Oϵ1	120.819	0.883
N_Cα_C	110.448	2.271
N_Cα_Cβ	110.304	1.362
Oϵ1_Cδ_Nϵ2	122.701	0.714

GLN **tm130** n = 55		
χ	Smooth COM	StdDev
chi1	-171.730	9.735
chi2	-75.893	10.370
chi3	127.247	16.058
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.897	1.440
Cα_C_O	120.546	0.938
Cβ_Cα_C	111.262	1.629
Cβ_Cγ_Cδ	114.423	2.701
Cγ_Cδ_Nϵ2	117.082	1.285
Cγ_Cδ_Oϵ1	120.469	1.172
N_Cα_C	108.797	3.399
N_Cα_Cβ	110.136	1.370
Oϵ1_Cδ_Nϵ2	122.423	0.743

GLN **tm-30** n = 547		
χ	Smooth COM	StdDev
chi1	-171.950	10.144
chi2	-85.646	10.982
chi3	-29.401	20.284
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.618	1.348
Cα_C_O	120.534	0.826
Cβ_Cα_C	110.944	1.310
Cβ_Cγ_Cδ	113.510	1.404
Cγ_Cδ_Nϵ2	116.459	0.713
Cγ_Cδ_Oϵ1	120.874	0.812
N_Cα_C	110.153	2.506
N_Cα_Cβ	110.287	1.242
Oϵ1_Cδ_Nϵ2	122.641	0.676

GLN **mp10** n = 1207		
χ	Smooth COM	StdDev
chi1	-66.517	8.985
chi2	81.837	11.441
chi3	17.344	37.547
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.240	1.363
Cα_C_O	120.433	0.836
Cβ_Cα_C	109.775	1.525
Cβ_Cγ_Cδ	113.448	1.294
Cγ_Cδ_Nϵ2	116.318	0.819
Cγ_Cδ_Oϵ1	121.139	0.951
N_Cα_C	111.608	2.346
N_Cα_Cβ	110.830	1.095
Oϵ1_Cδ_Nϵ2	122.522	0.603

GLN **mp-120** n = 87		
χ	Smooth COM	StdDev
chi1	-72.531	9.965
chi2	69.333	11.372
chi3	-119.632	13.002
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.359	1.549
Cα_C_O	120.487	0.882
Cβ_Cα_C	109.672	1.790
Cβ_Cγ_Cδ	113.610	1.567
Cγ_Cδ_Nϵ2	116.625	0.650
Cγ_Cδ_Oϵ1	120.632	1.086
N_Cα_C	111.577	2.757
N_Cα_Cβ	110.738	1.006
Oϵ1_Cδ_Nϵ2	122.722	0.842

GLN **mt0** n = 14370		
χ	Smooth COM	StdDev
chi1	-66.588	7.494
chi2	179.220	11.203
chi3	-3.560	62.564
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.241	1.815
Cα_C_O	120.494	0.850
Cβ_Cα_C	109.919	1.708
Cβ_Cγ_Cδ	112.644	1.530
Cγ_Cδ_Nϵ2	116.444	0.847
Cγ_Cδ_Oϵ1	120.849	0.897
N_Cα_C	111.415	2.256
N_Cα_Cβ	110.567	1.042
Oϵ1_Cδ_Nϵ2	122.680	0.696

GLN **mm110** n = 1147		
χ	Smooth COM	StdDev
chi1	-65.092	8.598
chi2	-62.550	10.868
chi3	109.265	24.134
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.964	1.562
Cα_C_O	120.379	0.849
Cβ_Cα_C	109.984	1.528
Cβ_Cγ_Cδ	112.879	1.429
Cγ_Cδ_Nϵ2	116.587	0.920
Cγ_Cδ_Oϵ1	120.788	0.941
N_Cα_C	111.589	2.280
N_Cα_Cβ	110.721	1.066
Oϵ1_Cδ_Nϵ2	122.597	0.683

GLN **mm-40** n = 5959		
χ	Smooth COM	StdDev
chi1	-63.698	8.629
chi2	-66.032	10.427
chi3	-38.665	24.730
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.884	1.423
Cα_C_O	120.457	0.869
Cβ_Cα_C	109.908	1.491
Cβ_Cγ_Cδ	112.838	1.280
Cγ_Cδ_Nϵ2	116.518	0.909
Cγ_Cδ_Oϵ1	120.856	0.911
N_Cα_C	111.383	2.451
N_Cα_Cβ	110.631	1.036
Oϵ1_Cδ_Nϵ2	122.604	0.776

3.17 ARG

ARG **ppp80** n = 10		
χ	Smooth COM	StdDev
chi1	62.201	5.082
chi2	86.595	6.961
chi3	57.216	3.753
chi4	79.687	8.472
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.109	0.884
Cα_C_O	120.837	0.551
Cβ_Cα_C	111.013	1.509
Cβ_Cγ_Cδ	113.944	0.819
Cδ_Nϵ_Cζ	125.029	0.341
Cγ_Cδ_Nϵ	112.507	1.082
Nϵ_Cζ_Nη1	120.628	0.683
Nϵ_Cζ_Nη2	119.754	0.628
Nη1_Cζ_Nη2	119.607	0.318
N_Cα_C	111.134	2.176
N_Cα_Cβ	111.870	1.188

ARG **ppp-140** n = 4		
χ	Smooth COM	StdDev
chi1	58.431	3.025
chi2	91.756	4.604
chi3	62.263	10.579
chi4	-143.455	12.578
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.223	0.896
Cα_C_O	120.687	0.538
Cβ_Cα_C	111.973	1.456
Cβ_Cγ_Cδ	112.231	1.497
Cδ_Nϵ_Cζ	125.872	1.184
Cγ_Cδ_Nϵ	113.783	2.259
Nϵ_Cζ_Nη1	120.992	1.242
Nϵ_Cζ_Nη2	120.128	1.383
Nη1_Cζ_Nη2	118.855	0.611
N_Cα_C	113.626	2.343
N_Cα_Cβ	111.211	1.258

ARG **ppt170** n = 57		
χ	Smooth COM	StdDev
chi1	59.128	9.858
chi2	87.628	12.300
chi3	173.545	12.300
chi4	173.353	17.309
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.237	1.393
Cα_C_O	120.372	1.040
Cβ_Cα_C	111.948	1.371
Cβ_Cγ_Cδ	112.408	1.628
Cδ_Nϵ_Cζ	124.240	1.282
Cγ_Cδ_Nϵ	111.386	1.601
Nϵ_Cζ_Nη1	120.500	1.081
Nϵ_Cζ_Nη2	119.821	0.871
Nη1_Cζ_Nη2	119.657	0.701
N_Cα_C	110.844	2.504
N_Cα_Cβ	111.575	1.315

ARG **ppt90** n = 19		
χ	Smooth COM	StdDev
chi1	63.537	5.887
chi2	99.251	7.971
chi3	-179.890	9.835
chi4	87.261	12.995
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.366	1.885
Cα_C_O	120.762	0.834
Cβ_Cα_C	110.804	1.700
Cβ_Cγ_Cδ	111.852	2.407
Cδ_Nϵ_Cζ	125.397	1.126
Cγ_Cδ_Nϵ	113.143	2.891
Nϵ_Cζ_Nη1	120.860	1.089
Nϵ_Cζ_Nη2	119.873	1.094
Nη1_Cζ_Nη2	119.235	0.792
N_Cα_C	111.026	2.141
N_Cα_Cβ	110.842	1.298

ARG **ppt-90** n = 15		
χ	Smooth COM	StdDev
chi1	61.770	9.125
chi2	90.213	11.134
chi3	177.663	5.499
chi4	-92.246	14.372
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.763	1.382
Cα_C_O	120.637	0.931
Cβ_Cα_C	111.235	1.747
Cβ_Cγ_Cδ	113.040	1.278
Cδ_Nϵ_Cζ	124.988	0.738
Cγ_Cδ_Nϵ	111.689	1.956
Nϵ_Cζ_Nη1	120.569	1.315
Nϵ_Cζ_Nη2	119.890	1.166
Nη1_Cζ_Nη2	119.520	0.600
N_Cα_C	111.578	3.116
N_Cα_Cβ	111.579	1.236

ARG **ptp90** n = 223		
χ	Smooth COM	StdDev
chi1	65.165	9.396
chi2	178.845	11.322
chi3	64.039	8.635
chi4	87.873	11.117
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.956	1.706
Cα_C_O	120.464	0.957
Cβ_Cα_C	110.461	1.385
Cβ_Cγ_Cδ	111.807	1.560
Cδ_Nϵ_Cζ	124.916	1.152
Cγ_Cδ_Nϵ	112.153	2.179
Nϵ_Cζ_Nη1	120.771	1.065
Nϵ_Cζ_Nη2	119.714	0.970
Nη1_Cζ_Nη2	119.498	0.797
N_Cα_C	110.918	2.815
N_Cα_Cβ	111.106	1.187

ARG **ptp-110** n = 77		
χ	Smooth COM	StdDev
chi1	67.597	8.250
chi2	-179.670	11.900
chi3	64.784	10.049
chi4	-108.305	9.865
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.792	1.933
Cα_C_O	120.741	1.224
Cβ_Cα_C	110.403	1.416
Cβ_Cγ_Cδ	111.895	1.473
Cδ_Nϵ_Cζ	125.606	1.443
Cγ_Cδ_Nϵ	111.728	2.285
Nϵ_Cζ_Nη1	120.996	1.421
Nϵ_Cζ_Nη2	119.559	1.566
Nη1_Cζ_Nη2	119.421	1.129
N_Cα_C	111.045	2.373
N_Cα_Cβ	110.983	1.300

ARG **ptp-170** n = 388		
χ	Smooth COM	StdDev
chi1	67.375	7.654
chi2	-175.630	12.219
chi3	68.232	9.651
chi4	-172.286	15.957
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.528	1.455
Cα_C_O	120.563	0.963
Cβ_Cα_C	110.408	1.567
Cβ_Cγ_Cδ	111.291	1.743
Cδ_Nϵ_Cζ	124.582	1.140
Cγ_Cδ_Nϵ	111.416	1.628
Nϵ_Cζ_Nη1	120.454	0.937
Nϵ_Cζ_Nη2	119.760	0.930
Nη1_Cζ_Nη2	119.756	0.920
N_Cα_C	111.331	2.560
N_Cα_Cβ	110.785	1.148

ARG **ptt180** n = 820		
χ	Smooth COM	StdDev
chi1	65.305	8.301
chi2	-177.454	10.432
chi3	-179.814	10.417
chi4	179.152	17.466
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.577	1.525
Cα_C_O	120.578	1.008
Cβ_Cα_C	110.520	1.503
Cβ_Cγ_Cδ	111.129	2.013
Cδ_Nϵ_Cζ	124.433	1.099
Cγ_Cδ_Nϵ	110.745	1.990
Nϵ_Cζ_Nη1	120.477	0.941
Nϵ_Cζ_Nη2	119.617	0.893
Nη1_Cζ_Nη2	119.887	0.877
N_Cα_C	111.325	2.492
N_Cα_Cβ	111.010	1.124

ARG **ptt90** n = 814		
χ	Smooth COM	StdDev
chi1	64.935	7.600
chi2	178.802	12.292
chi3	176.614	8.719
chi4	87.625	9.814
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.818	1.433
Cα_C_O	120.575	0.864
Cβ_Cα_C	110.208	1.412
Cβ_Cγ_Cδ	110.988	1.946
Cδ_Nϵ_Cζ	124.876	0.920
Cγ_Cδ_Nϵ	111.873	2.472
Nϵ_Cζ_Nη1	120.762	0.988
Nϵ_Cζ_Nη2	119.679	0.912
Nη1_Cζ_Nη2	119.540	0.696
N_Cα_C	110.780	2.513
N_Cα_Cβ	111.050	1.153

ARG **ptt-90** n = 726		
χ	Smooth COM	StdDev
chi1	66.303	7.908
chi2	-175.118	12.037
chi3	-176.524	8.892
chi4	-87.098	11.825
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.840	1.508
Cα_C_O	120.486	0.935
Cβ_Cα_C	110.455	1.554
Cβ_Cγ_Cδ	110.983	2.037
Cδ_Nϵ_Cζ	124.865	1.144
Cγ_Cδ_Nϵ	111.656	2.664
Nϵ_Cζ_Nη1	120.763	1.014
Nϵ_Cζ_Nη2	119.688	1.138
Nη1_Cζ_Nη2	119.527	1.027
N_Cα_C	111.666	2.550
N_Cα_Cβ	110.954	1.159

ARG **ptm160** n = 502		
χ	Smooth COM	StdDev
chi1	63.484	8.731
chi2	-179.108	14.966
chi3	-67.148	9.716
chi4	165.337	25.706
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.588	1.635
Cα_C_O	120.504	0.978
Cβ_Cα_C	110.438	1.556
Cβ_Cγ_Cδ	111.713	1.805
Cδ_Nϵ_Cζ	124.678	1.394
Cγ_Cδ_Nϵ	111.548	2.110
Nϵ_Cζ_Nη1	120.580	1.282
Nϵ_Cζ_Nη2	119.717	1.123
Nη1_Cζ_Nη2	119.683	1.001
N_Cα_C	110.949	2.570
N_Cα_Cβ	111.004	1.273

ARG **ptm-80** n = 215		
χ	Smooth COM	StdDev
chi1	65.373	8.260
chi2	-178.472	14.370
chi3	-66.034	10.269
chi4	-84.515	10.828
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.564	1.281
Cα_C_O	120.421	0.844
Cβ_Cα_C	110.304	1.382
Cβ_Cγ_Cδ	111.894	1.743
Cδ_Nϵ_Cζ	124.963	1.432
Cγ_Cδ_Nϵ	112.362	2.279
Nϵ_Cζ_Nη1	120.717	1.214
Nϵ_Cζ_Nη2	119.898	1.456
Nη1_Cζ_Nη2	119.365	0.871
N_Cα_C	111.616	2.543
N_Cα_Cβ	110.971	1.307

ARG **pmt100** n = 4		
χ	Smooth COM	StdDev
chi1	70.210	7.245
chi2	-90.541	9.055
chi3	-174.190	5.432
chi4	97.849	2.006
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.830	0.421
Cα_C_O	120.581	0.283
Cβ_Cα_C	110.812	0.494
Cβ_Cγ_Cδ	112.728	0.575
Cδ_Nϵ_Cζ	125.083	0.125
Cγ_Cδ_Nϵ	111.181	0.920
Nϵ_Cζ_Nη1	120.967	0.288
Nϵ_Cζ_Nη2	119.634	0.266
Nη1_Cζ_Nη2	119.397	0.052
N_Cα_C	110.231	1.442
N_Cα_Cβ	111.390	0.423

ARG **pmt170** n = 39		
χ	Smooth COM	StdDev
chi1	73.963	11.193
chi2	-78.972	15.367
chi3	-169.420	10.139
chi4	-169.441	15.119
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.291	1.188
Cα_C_O	120.751	0.702
Cβ_Cα_C	110.782	1.123
Cβ_Cγ_Cδ	112.734	1.257
Cδ_Nϵ_Cζ	124.390	1.048
Cγ_Cδ_Nϵ	111.561	1.865
Nϵ_Cζ_Nη1	120.368	0.782
Nϵ_Cζ_Nη2	119.973	0.643
Nη1_Cζ_Nη2	119.646	0.558
N_Cα_C	110.725	2.400
N_Cα_Cβ	111.788	1.071

ARG **pmt-80** n = 27		
χ	Smooth COM	StdDev
chi1	81.229	9.292
chi2	-68.144	7.568
chi3	-176.905	10.963
chi4	-84.063	8.317
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.767	1.164
Cα_C_O	120.964	0.647
Cβ_Cα_C	110.281	1.017
Cβ_Cγ_Cδ	113.254	1.792
Cδ_Nϵ_Cζ	124.929	0.992
Cγ_Cδ_Nϵ	112.132	1.754
Nϵ_Cζ_Nη1	120.989	0.889
Nϵ_Cζ_Nη2	119.623	0.599
Nη1_Cζ_Nη2	119.368	0.601
N_Cα_C	110.720	2.032
N_Cα_Cβ	111.393	1.156

ARG **pmm150** n = 12		
χ	Smooth COM	StdDev
chi1	75.579	3.166
chi2	-75.440	5.561
chi3	-64.975	6.260
chi4	151.999	15.442
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.190	1.499
Cα_C_O	120.267	0.926
Cβ_Cα_C	110.409	1.045
Cβ_Cγ_Cδ	112.425	1.153
Cδ_Nϵ_Cζ	125.348	2.473
Cγ_Cδ_Nϵ	111.569	2.064
Nϵ_Cζ_Nη1	121.076	1.741
Nϵ_Cζ_Nη2	119.660	1.033
Nη1_Cζ_Nη2	119.218	1.385
N_Cα_C	109.038	0.995
N_Cα_Cβ	112.126	0.964

ARG **pmm-80** n = 19		
χ	Smooth COM	StdDev
chi1	73.642	12.608
chi2	-75.958	11.183
chi3	-56.789	8.115
chi4	-81.265	7.401
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.931	1.019
Cα_C_O	120.769	0.553
Cβ_Cα_C	110.942	1.227
Cβ_Cγ_Cδ	113.505	1.558
Cδ_Nϵ_Cζ	125.145	1.080
Cγ_Cδ_Nϵ	112.540	1.304
Nϵ_Cζ_Nη1	120.428	0.947
Nϵ_Cζ_Nη2	120.291	0.953
Nη1_Cζ_Nη2	119.271	0.671
N_Cα_C	109.672	2.434
N_Cα_Cβ	111.608	1.001

ARG **tpp80** n = 363		
χ	Smooth COM	StdDev
chi1	-177.765	10.251
chi2	65.211	10.679
chi3	59.806	9.544
chi4	84.211	9.112
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.925	1.369
Cα_C_O	120.516	0.750
Cβ_Cα_C	110.476	1.234
Cβ_Cγ_Cδ	112.970	1.585
Cδ_Nϵ_Cζ	124.999	1.053
Cγ_Cδ_Nϵ	112.587	2.062
Nϵ_Cζ_Nη1	120.720	0.868
Nϵ_Cζ_Nη2	119.749	0.827
Nη1_Cζ_Nη2	119.512	0.717
N_Cα_C	110.795	2.025
N_Cα_Cβ	110.349	1.121

ARG **tpp-160** n = 496		
χ	Smooth COM	StdDev
chi1	178.900	9.622
chi2	65.564	10.745
chi3	65.339	9.826
chi4	-167.680	19.748
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.753	1.301
Cα_C_O	120.521	0.835
Cβ_Cα_C	110.424	1.291
Cβ_Cγ_Cδ	112.686	1.753
Cδ_Nϵ_Cζ	124.533	1.383
Cγ_Cδ_Nϵ	111.868	1.817
Nϵ_Cζ_Nη1	120.495	1.034
Nϵ_Cζ_Nη2	119.796	1.090
Nη1_Cζ_Nη2	119.690	0.837
N_Cα_C	110.619	2.297
N_Cα_Cβ	110.242	1.093

ARG **tpt170** n = 825		
χ	Smooth COM	StdDev
chi1	-178.826	8.985
chi2	66.313	10.376
chi3	177.963	11.716
chi4	171.354	19.311
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.515	1.233
Cα_C_O	120.510	0.735
Cβ_Cα_C	110.571	1.154
Cβ_Cγ_Cδ	112.241	1.705
Cδ_Nϵ_Cζ	124.487	1.136
Cγ_Cδ_Nϵ	110.851	1.868
Nϵ_Cζ_Nη1	120.532	0.938
Nϵ_Cζ_Nη2	119.674	0.880
Nη1_Cζ_Nη2	119.775	0.857
N_Cα_C	110.743	1.989
N_Cα_Cβ	110.225	1.192

ARG **tpt90** n = 652		
χ	Smooth COM	StdDev
chi1	178.926	8.381
chi2	65.741	7.685
chi3	178.589	9.896
chi4	86.350	10.296
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.718	1.274
Cα_C_O	120.469	0.802
Cβ_Cα_C	110.288	1.182
Cβ_Cγ_Cδ	112.118	1.671
Cδ_Nϵ_Cζ	124.798	0.923
Cγ_Cδ_Nϵ	111.919	2.267
Nϵ_Cζ_Nη1	120.812	0.967
Nϵ_Cζ_Nη2	119.714	0.888
Nη1_Cζ_Nη2	119.453	0.822
N_Cα_C	111.449	2.056
N_Cα_Cβ	110.205	1.088

ARG **tpt-90** n = 365		
χ	Smooth COM	StdDev
chi1	179.343	8.403
chi2	67.144	10.829
chi3	-179.669	8.849
chi4	-89.385	12.210
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.741	1.251
Cα_C_O	120.494	0.717
Cβ_Cα_C	110.562	1.204
Cβ_Cγ_Cδ	112.371	1.618
Cδ_Nϵ_Cζ	124.855	1.145
Cγ_Cδ_Nϵ	111.131	2.518
Nϵ_Cζ_Nη1	120.736	1.033
Nϵ_Cζ_Nη2	119.671	1.050
Nη1_Cζ_Nη2	119.568	0.730
N_Cα_C	110.867	2.153
N_Cα_Cβ	110.203	1.187

ARG **tpm170** n = 110		
χ	Smooth COM	StdDev
chi1	178.317	8.113
chi2	70.416	10.901
chi3	-85.345	12.809
chi4	171.668	18.570
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.637	1.263
Cα_C_O	120.626	0.802
Cβ_Cα_C	110.602	1.333
Cβ_Cγ_Cδ	112.785	2.167
Cδ_Nϵ_Cζ	124.702	2.252
Cγ_Cδ_Nϵ	111.970	2.147
Nϵ_Cζ_Nη1	120.476	1.046
Nϵ_Cζ_Nη2	119.776	0.905
Nη1_Cζ_Nη2	119.734	0.745
N_Cα_C	111.099	1.434
N_Cα_Cβ	109.942	1.120

ARG **tpm-80** n = 20		
χ	Smooth COM	StdDev
chi1	-177.264	5.162
chi2	78.524	8.234
chi3	-80.359	10.382
chi4	-79.824	9.071
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.170	1.379
Cα_C_O	120.653	1.054
Cβ_Cα_C	110.318	1.131
Cβ_Cγ_Cδ	113.047	1.221
Cδ_Nϵ_Cζ	125.229	1.191
Cγ_Cδ_Nϵ	113.709	2.206
Nϵ_Cζ_Nη1	120.646	0.958
Nϵ_Cζ_Nη2	120.052	0.924
Nη1_Cζ_Nη2	119.284	0.631
N_Cα_C	110.800	1.483
N_Cα_Cβ	109.849	1.128

ARG **ttp80** n = 1896		
χ	Smooth COM	StdDev
chi1	-177.383	8.162
chi2	179.646	13.425
chi3	62.978	9.944
chi4	82.895	9.577
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.686	1.495
Cα_C_O	120.681	0.798
Cβ_Cα_C	110.045	1.208
Cβ_Cγ_Cδ	112.080	1.526
Cδ_Nϵ_Cζ	124.882	1.039
Cγ_Cδ_Nϵ	112.575	1.938
Nϵ_Cζ_Nη1	120.750	0.949
Nϵ_Cζ_Nη2	119.766	0.857
Nη1_Cζ_Nη2	119.465	0.753
N_Cα_C	110.748	2.056
N_Cα_Cβ	110.433	1.201

ARG **ttp-110** n = 623		
χ	Smooth COM	StdDev
chi1	-174.744	8.457
chi2	177.160	12.953
chi3	64.599	10.746
chi4	-113.458	9.867
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.826	1.633
Cα_C_O	120.605	0.798
Cβ_Cα_C	110.158	1.233
Cβ_Cγ_Cδ	112.012	1.748
Cδ_Nϵ_Cζ	125.367	1.360
Cγ_Cδ_Nϵ	111.876	2.159
Nϵ_Cζ_Nη1	121.079	1.283
Nϵ_Cζ_Nη2	119.474	1.161
Nη1_Cζ_Nη2	119.427	0.887
N_Cα_C	110.684	2.176
N_Cα_Cβ	110.314	1.287

ARG **ttp-170** n = 1533		
χ	Smooth COM	StdDev
chi1	-175.447	9.345
chi2	179.359	13.232
chi3	66.850	8.993
chi4	-171.036	17.274
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.660	1.651
Cα_C_O	120.595	0.757
Cβ_Cα_C	110.009	1.236
Cβ_Cγ_Cδ	111.642	1.683
Cδ_Nϵ_Cζ	124.480	1.169
Cγ_Cδ_Nϵ	111.497	1.581
Nϵ_Cζ_Nη1	120.455	0.896
Nϵ_Cζ_Nη2	119.763	0.881
Nη1_Cζ_Nη2	119.764	0.703
N_Cα_C	110.456	2.209
N_Cα_Cβ	110.433	1.313

ARG **ttt180** n = 2339		
χ	Smooth COM	StdDev
chi1	-176.225	9.097
chi2	176.468	11.186
chi3	178.543	11.535
chi4	179.245	18.746
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.475	1.785
Cα_C_O	120.570	0.812
Cβ_Cα_C	110.176	1.171
Cβ_Cγ_Cδ	111.351	2.189
Cδ_Nϵ_Cζ	124.329	1.194
Cγ_Cδ_Nϵ	110.653	1.920
Nϵ_Cζ_Nη1	120.399	0.902
Nϵ_Cζ_Nη2	119.608	0.915
Nη1_Cζ_Nη2	119.974	0.814
N_Cα_C	110.517	2.410
N_Cα_Cβ	110.183	1.389

ARG **ttt90** n = 1057		
χ	Smooth COM	StdDev
chi1	-176.157	9.260
chi2	176.118	10.807
chi3	176.454	9.628
chi4	86.745	10.847
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.859	1.696
Cα_C_O	120.572	0.794
Cβ_Cα_C	110.230	1.247
Cβ_Cγ_Cδ	111.326	2.078
Cδ_Nϵ_Cζ	124.757	1.007
Cγ_Cδ_Nϵ	111.615	2.616
Nϵ_Cζ_Nη1	120.741	1.016
Nϵ_Cζ_Nη2	119.607	0.998
Nη1_Cζ_Nη2	119.628	0.738
N_Cα_C	110.528	2.396
N_Cα_Cβ	110.355	1.373

ARG **ttt-90** n = 1380		
χ	Smooth COM	StdDev
chi1	-176.754	9.438
chi2	177.849	11.450
chi3	-178.261	9.915
chi4	-89.587	12.519
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.964	1.616
Cα_C_O	120.540	0.793
Cβ_Cα_C	110.272	1.256
Cβ_Cγ_Cδ	110.941	2.077
Cδ_Nϵ_Cζ	124.821	1.167
Cγ_Cδ_Nϵ	111.802	2.580
Nϵ_Cζ_Nη1	120.801	1.078
Nϵ_Cζ_Nη2	119.565	1.015
Nη1_Cζ_Nη2	119.613	0.869
N_Cα_C	110.382	2.296
N_Cα_Cβ	110.230	1.313

ARG **ttm110** n = 725		
χ	Smooth COM	StdDev
chi1	-175.260	8.991
chi2	178.639	9.463
chi3	-64.314	10.708
chi4	112.805	9.769
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.881	1.635
Cα_C_O	120.589	0.780
Cβ_Cα_C	110.255	1.228
Cβ_Cγ_Cδ	112.165	1.691
Cδ_Nϵ_Cζ	125.322	1.226
Cγ_Cδ_Nϵ	111.648	1.927
Nϵ_Cζ_Nη1	121.010	1.241
Nϵ_Cζ_Nη2	119.531	1.123
Nη1_Cζ_Nη2	119.435	0.817
N_Cα_C	110.499	2.138
N_Cα_Cβ	110.380	1.239

ARG **ttm170** n = 1317		
χ	Smooth COM	StdDev
chi1	-177.285	9.924
chi2	176.943	12.449
chi3	-67.797	9.912
chi4	171.206	17.554
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.752	1.740
Cα_C_O	120.583	0.815
Cβ_Cα_C	110.105	1.164
Cβ_Cγ_Cδ	111.482	1.826
Cδ_Nϵ_Cζ	124.437	1.166
Cγ_Cδ_Nϵ	111.263	1.652
Nϵ_Cζ_Nη1	120.519	0.959
Nϵ_Cζ_Nη2	119.735	0.929
Nη1_Cζ_Nη2	119.728	0.835
N_Cα_C	110.279	2.382
N_Cα_Cβ	110.267	1.337

ARG **ttm-80** n = 1504		
χ	Smooth COM	StdDev
chi1	-174.135	9.435
chi2	179.281	9.905
chi3	-64.732	10.575
chi4	-84.522	9.745
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.668	1.664
Cα_C_O	120.532	0.789
Cβ_Cα_C	110.241	1.238
Cβ_Cγ_Cδ	111.990	1.645
Cδ_Nϵ_Cζ	124.859	1.304
Cγ_Cδ_Nϵ	112.437	2.033
Nϵ_Cζ_Nη1	120.726	1.016
Nϵ_Cζ_Nη2	119.733	1.037
Nη1_Cζ_Nη2	119.521	0.763
N_Cα_C	110.578	2.257
N_Cα_Cβ	110.372	1.356

ARG **tmt170** n = 104		
χ	Smooth COM	StdDev
chi1	-173.869	12.307
chi2	-91.306	12.725
chi3	-173.542	9.380
chi4	-170.971	17.524
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.031	1.334
Cα_C_O	120.633	0.742
Cβ_Cα_C	110.891	1.069
Cβ_Cγ_Cδ	112.702	1.716
Cδ_Nϵ_Cζ	124.499	0.904
Cγ_Cδ_Nϵ	110.712	1.619
Nϵ_Cζ_Nη1	120.677	1.032
Nϵ_Cζ_Nη2	119.571	0.805
Nη1_Cζ_Nη2	119.736	0.716
N_Cα_C	108.533	3.170
N_Cα_Cβ	109.989	1.249

ARG **tmt90** n = 23		
χ	Smooth COM	StdDev
chi1	-178.402	9.228
chi2	-93.565	9.120
chi3	-177.879	11.168
chi4	87.027	11.977
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.152	1.485
Cα_C_O	120.604	0.982
Cβ_Cα_C	110.471	1.327
Cβ_Cγ_Cδ	112.863	2.341
Cδ_Nϵ_Cζ	125.096	1.261
Cγ_Cδ_Nϵ	111.403	2.847
Nϵ_Cζ_Nη1	120.873	1.858
Nϵ_Cζ_Nη2	119.647	1.458
Nη1_Cζ_Nη2	119.441	0.740
N_Cα_C	110.308	1.542
N_Cα_Cβ	109.926	1.134

ARG **tmt-80** n = 62		
χ	Smooth COM	StdDev
chi1	-174.441	10.751
chi2	-92.932	11.363
chi3	-177.757	10.023
chi4	-84.998	11.504
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.665	1.340
Cα_C_O	120.545	0.772
Cβ_Cα_C	111.341	1.330
Cβ_Cγ_Cδ	112.460	1.924
Cδ_Nϵ_Cζ	124.688	1.117
Cγ_Cδ_Nϵ	111.211	2.142
Nϵ_Cζ_Nη1	120.610	0.908
Nϵ_Cζ_Nη2	119.729	0.896
Nη1_Cζ_Nη2	119.637	0.627
N_Cα_C	110.062	2.449
N_Cα_Cβ	110.064	1.027

ARG **tmm160** n = 92		
χ	Smooth COM	StdDev
chi1	-172.150	10.890
chi2	-90.073	11.146
chi3	-61.282	11.279
chi4	163.764	18.601
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.825	1.323
Cα_C_O	120.627	0.803
Cβ_Cα_C	111.278	1.113
Cβ_Cγ_Cδ	112.552	1.822
Cδ_Nϵ_Cζ	124.630	1.190
Cγ_Cδ_Nϵ	111.887	1.925
Nϵ_Cζ_Nη1	120.655	1.000
Nϵ_Cζ_Nη2	119.705	0.893
Nη1_Cζ_Nη2	119.616	0.813
N_Cα_C	109.950	2.048
N_Cα_Cβ	110.061	1.132

ARG **tmm-80** n = 71		
χ	Smooth COM	StdDev
chi1	-174.294	9.153
chi2	-86.372	8.784
chi3	-56.434	10.717
chi4	-82.108	8.527
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.257	1.317
Cα_C_O	120.621	0.778
Cβ_Cα_C	111.061	1.008
Cβ_Cγ_Cδ	113.720	2.294
Cδ_Nϵ_Cζ	124.893	1.247
Cγ_Cδ_Nϵ	112.553	1.891
Nϵ_Cζ_Nη1	120.861	1.095
Nϵ_Cζ_Nη2	119.709	0.923
Nη1_Cζ_Nη2	119.397	0.720
N_Cα_C	109.672	1.698
N_Cα_Cβ	110.067	1.009

ARG **mpp80** n = 54		
χ	Smooth COM	StdDev
chi1	-76.744	11.753
chi2	81.853	11.964
chi3	57.995	7.391
chi4	84.630	10.143
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.469	1.724
Cα_C_O	120.418	1.087
Cβ_Cα_C	109.200	1.982
Cβ_Cγ_Cδ	113.558	1.616
Cδ_Nϵ_Cζ	124.998	1.163
Cγ_Cδ_Nϵ	113.125	2.284
Nϵ_Cζ_Nη1	120.782	1.174
Nϵ_Cζ_Nη2	119.773	1.129
Nη1_Cζ_Nη2	119.423	0.733
N_Cα_C	109.653	2.541
N_Cα_Cβ	111.451	1.261

ARG **mpp-170** n = 64		
χ	Smooth COM	StdDev
chi1	-78.876	12.884
chi2	81.734	17.402
chi3	65.059	7.427
chi4	-166.895	16.426
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.639	1.431
Cα_C_O	120.527	0.677
Cβ_Cα_C	109.707	1.574
Cβ_Cγ_Cδ	112.675	1.744
Cδ_Nϵ_Cζ	124.456	1.194
Cγ_Cδ_Nϵ	111.467	1.342
Nϵ_Cζ_Nη1	120.599	1.057
Nϵ_Cζ_Nη2	119.723	0.761
Nη1_Cζ_Nη2	119.659	0.703
N_Cα_C	109.974	3.124
N_Cα_Cβ	111.366	1.108

ARG **mpt180** n = 245		
χ	Smooth COM	StdDev
chi1	-84.592	7.996
chi2	69.331	13.073
chi3	173.629	9.351
chi4	174.437	16.771
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.779	1.423
Cα_C_O	120.561	0.858
Cβ_Cα_C	109.479	1.658
Cβ_Cγ_Cδ	113.013	1.809
Cδ_Nϵ_Cζ	124.423	1.453
Cγ_Cδ_Nϵ	110.690	1.999
Nϵ_Cζ_Nη1	120.410	1.021
Nϵ_Cζ_Nη2	119.733	0.916
Nη1_Cζ_Nη2	119.829	0.881
N_Cα_C	109.972	2.748
N_Cα_Cβ	111.150	1.151

ARG **mpt90** n = 46		
χ	Smooth COM	StdDev
chi1	-76.133	12.907
chi2	84.673	13.588
chi3	170.244	9.730
chi4	93.427	11.198
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.631	1.635
Cα_C_O	120.402	0.642
Cβ_Cα_C	109.251	1.434
Cβ_Cγ_Cδ	112.529	1.552
Cδ_Nϵ_Cζ	125.102	0.846
Cγ_Cδ_Nϵ	111.041	2.030
Nϵ_Cζ_Nη1	121.088	0.907
Nϵ_Cζ_Nη2	119.381	0.679
Nη1_Cζ_Nη2	119.512	0.586
N_Cα_C	109.965	2.682
N_Cα_Cβ	111.296	1.245

ARG **mpt-90** n = 85		
χ	Smooth COM	StdDev
chi1	-78.778	13.914
chi2	74.660	16.331
chi3	177.663	9.619
chi4	-87.847	13.667
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.921	1.261
Cα_C_O	120.436	0.752
Cβ_Cα_C	109.954	1.553
Cβ_Cγ_Cδ	112.861	2.301
Cδ_Nϵ_Cζ	124.891	0.998
Cγ_Cδ_Nϵ	111.632	2.525
Nϵ_Cζ_Nη1	120.590	1.067
Nϵ_Cζ_Nη2	119.828	0.834
Nη1_Cζ_Nη2	119.561	0.667
N_Cα_C	110.431	2.708
N_Cα_Cβ	110.866	1.019

ARG **mtp180** n = 2504		
χ	Smooth COM	StdDev
chi1	-66.448	8.145
chi2	178.975	13.041
chi3	66.423	9.133
chi4	-171.573	16.500
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.196	1.788
Cα_C_O	120.474	0.834
Cβ_Cα_C	110.040	1.648
Cβ_Cγ_Cδ	111.714	1.807
Cδ_Nϵ_Cζ	124.376	1.212
Cγ_Cδ_Nϵ	111.554	1.558
Nϵ_Cζ_Nη1	120.437	0.999
Nϵ_Cζ_Nη2	119.768	0.969
Nη1_Cζ_Nη2	119.779	0.774
N_Cα_C	111.426	2.415
N_Cα_Cβ	110.537	1.046

ARG **mtp85** n = 1857		
χ	Smooth COM	StdDev
chi1	-66.328	8.550
chi2	177.775	11.188
chi3	64.643	9.713
chi4	87.715	10.960
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.275	1.819
Cα_C_O	120.493	0.910
Cβ_Cα_C	110.136	1.676
Cβ_Cγ_Cδ	112.055	1.715
Cδ_Nϵ_Cζ	124.893	1.199
Cγ_Cδ_Nϵ	112.285	1.990
Nϵ_Cζ_Nη1	120.785	1.055
Nϵ_Cζ_Nη2	119.683	1.040
Nη1_Cζ_Nη2	119.513	0.811
N_Cα_C	111.102	2.410
N_Cα_Cβ	110.598	1.049

ARG **mtp-110** n = 470		
χ	Smooth COM	StdDev
chi1	-65.062	8.129
chi2	179.092	10.812
chi3	66.411	11.580
chi4	-109.636	9.635
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.354	1.662
Cα_C_O	120.369	0.947
Cβ_Cα_C	110.075	1.684
Cβ_Cγ_Cδ	112.354	1.634
Cδ_Nϵ_Cζ	125.306	2.055
Cγ_Cδ_Nϵ	111.671	1.878
Nϵ_Cζ_Nη1	121.057	1.200
Nϵ_Cζ_Nη2	119.441	1.295
Nη1_Cζ_Nη2	119.478	0.895
N_Cα_C	111.125	2.585
N_Cα_Cβ	110.743	1.052

ARG **mtt180** n = 4592		
χ	Smooth COM	StdDev
chi1	-67.383	7.802
chi2	179.853	11.020
chi3	-179.128	10.659
chi4	177.093	17.916
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	112.906	1.753
Cα_C_O	120.449	0.847
Cβ_Cα_C	109.969	1.657
Cβ_Cγ_Cδ	111.523	2.022
Cδ_Nϵ_Cζ	124.359	1.101
Cγ_Cδ_Nϵ	110.625	1.820
Nϵ_Cζ_Nη1	120.426	0.894
Nϵ_Cζ_Nη2	119.625	0.896
Nη1_Cζ_Nη2	119.931	0.794
N_Cα_C	111.576	2.328
N_Cα_Cβ	110.570	1.047

ARG **mtt90** n = 2460		
χ	Smooth COM	StdDev
chi1	-67.677	7.504
chi2	179.859	13.535
chi3	178.901	10.625
chi4	90.605	15.148
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.347	1.719
Cα_C_O	120.443	0.802
Cβ_Cα_C	109.894	1.726
Cβ_Cγ_Cδ	111.540	2.042
Cδ_Nϵ_Cζ	124.859	1.138
Cγ_Cδ_Nϵ	111.010	2.492
Nϵ_Cζ_Nη1	120.854	1.069
Nϵ_Cζ_Nη2	119.529	1.057
Nη1_Cζ_Nη2	119.591	0.803
N_Cα_C	111.444	2.403
N_Cα_Cβ	110.565	1.121

ARG **mtt-85** n = 2843		
χ	Smooth COM	StdDev
chi1	-67.013	7.843
chi2	-178.550	10.650
chi3	-176.240	9.240
chi4	-88.795	11.677
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.460	1.703
Cα_C_O	120.445	0.822
Cβ_Cα_C	109.838	1.651
Cβ_Cγ_Cδ	111.361	1.969
Cδ_Nϵ_Cζ	124.795	1.053
Cγ_Cδ_Nϵ	111.412	2.434
Nϵ_Cζ_Nη1	120.794	1.020
Nϵ_Cζ_Nη2	119.578	0.926
Nη1_Cζ_Nη2	119.609	0.768
N_Cα_C	111.436	2.299
N_Cα_Cβ	110.636	1.045

ARG **mtm110** n = 781		
χ	Smooth COM	StdDev
chi1	-68.128	8.152
chi2	-177.015	9.719
chi3	-68.916	10.245
chi4	112.867	10.583
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.128	1.811
Cα_C_O	120.427	0.902
Cβ_Cα_C	110.057	1.759
Cβ_Cγ_Cδ	112.410	1.719
Cδ_Nϵ_Cζ	125.312	1.518
Cγ_Cδ_Nϵ	112.087	1.885
Nϵ_Cζ_Nη1	121.057	1.278
Nϵ_Cζ_Nη2	119.445	1.122
Nη1_Cζ_Nη2	119.479	0.917
N_Cα_C	111.659	2.436
N_Cα_Cβ	110.673	1.037

ARG **mtm180** n = 2407		
χ	Smooth COM	StdDev
chi1	-66.409	8.111
chi2	179.025	12.715
chi3	-67.433	8.823
chi4	172.922	15.154
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.294	1.630
Cα_C_O	120.456	0.891
Cβ_Cα_C	109.865	1.623
Cβ_Cγ_Cδ	111.632	1.675
Cδ_Nϵ_Cζ	124.437	1.082
Cγ_Cδ_Nϵ	111.358	1.691
Nϵ_Cζ_Nη1	120.426	0.896
Nϵ_Cζ_Nη2	119.771	0.882
Nη1_Cζ_Nη2	119.785	0.768
N_Cα_C	111.291	2.634
N_Cα_Cβ	110.532	1.054

ARG **mtm-85** n = 2848		
χ	Smooth COM	StdDev
chi1	-68.282	8.114
chi2	-171.664	9.296
chi3	-63.903	9.515
chi4	-88.066	8.888
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.529	1.560
Cα_C_O	120.475	0.810
Cβ_Cα_C	110.037	1.494
Cβ_Cγ_Cδ	111.973	1.573
Cδ_Nϵ_Cζ	124.892	1.167
Cγ_Cδ_Nϵ	112.687	1.963
Nϵ_Cζ_Nη1	120.777	1.028
Nϵ_Cζ_Nη2	119.743	1.003
Nη1_Cζ_Nη2	119.464	0.785
N_Cα_C	111.343	1.972
N_Cα_Cβ	111.054	1.026

ARG **mmp80** n = 164		
χ	Smooth COM	StdDev
chi1	-62.526	6.654
chi2	-75.134	12.697
chi3	74.408	11.683
chi4	77.834	6.858
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.756	1.393
Cα_C_O	120.405	0.951
Cβ_Cα_C	109.795	1.486
Cβ_Cγ_Cδ	113.417	1.619
Cδ_Nϵ_Cζ	125.034	1.158
Cγ_Cδ_Nϵ	113.473	2.231
Nϵ_Cζ_Nη1	120.554	0.995
Nϵ_Cζ_Nη2	119.976	0.857
Nη1_Cζ_Nη2	119.450	0.642
N_Cα_C	111.399	1.818
N_Cα_Cβ	110.883	0.931

ARG **mmp-170** n = 123		
χ	Smooth COM	StdDev
chi1	-64.124	7.185
chi2	-65.485	14.262
chi3	85.873	9.711
chi4	-167.047	19.760
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.470	1.274
Cα_C_O	120.374	0.989
Cβ_Cα_C	109.451	1.525
Cβ_Cγ_Cδ	112.812	1.743
Cδ_Nϵ_Cζ	124.848	1.315
Cγ_Cδ_Nϵ	111.535	1.611
Nϵ_Cζ_Nη1	120.505	1.207
Nϵ_Cζ_Nη2	119.752	1.096
Nη1_Cζ_Nη2	119.724	1.141
N_Cα_C	111.010	2.146
N_Cα_Cβ	111.080	1.123

ARG **mmt180** n = 1203		
χ	Smooth COM	StdDev
chi1	-61.912	9.054
chi2	-68.373	12.909
chi3	-176.971	11.256
chi4	-176.339	17.437
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.493	1.380
Cα_C_O	120.394	0.872
Cβ_Cα_C	109.365	1.625
Cβ_Cγ_Cδ	112.048	1.715
Cδ_Nϵ_Cζ	124.422	1.187
Cγ_Cδ_Nϵ	110.995	1.829
Nϵ_Cζ_Nη1	120.487	0.873
Nϵ_Cζ_Nη2	119.663	0.872
Nη1_Cζ_Nη2	119.830	0.740
N_Cα_C	111.227	2.571
N_Cα_Cβ	110.702	1.071

ARG **mmt90** n = 567		
χ	Smooth COM	StdDev
chi1	-60.697	8.808
chi2	-68.408	12.498
chi3	179.437	10.449
chi4	90.018	12.895
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.636	1.391
Cα_C_O	120.470	0.870
Cβ_Cα_C	109.542	1.648
Cβ_Cγ_Cδ	112.219	1.613
Cδ_Nϵ_Cζ	124.948	1.236
Cγ_Cδ_Nϵ	111.566	2.487
Nϵ_Cζ_Nη1	120.843	1.216
Nϵ_Cζ_Nη2	119.554	1.095
Nη1_Cζ_Nη2	119.578	0.717
N_Cα_C	111.367	2.715
N_Cα_Cβ	110.685	1.076

ARG **mmt-90** n = 1428		
χ	Smooth COM	StdDev
chi1	-63.806	6.649
chi2	-68.992	8.052
chi3	-175.179	7.656
chi4	-91.022	11.109
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.535	1.429
Cα_C_O	120.522	0.849
Cβ_Cα_C	109.577	1.636
Cβ_Cγ_Cδ	112.031	1.668
Cδ_Nϵ_Cζ	124.921	0.997
Cγ_Cδ_Nϵ	111.800	2.277
Nϵ_Cζ_Nη1	120.940	0.997
Nϵ_Cζ_Nη2	119.615	0.880
Nη1_Cζ_Nη2	119.419	0.824
N_Cα_C	110.068	2.671
N_Cα_Cβ	110.879	1.109

ARG **mmm160** n = 951		
χ	Smooth COM	StdDev
chi1	-61.827	9.224
chi2	-66.167	13.742
chi3	-64.223	9.924
chi4	163.153	24.183
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.464	1.598
Cα_C_O	120.403	0.880
Cβ_Cα_C	109.780	1.544
Cβ_Cγ_Cδ	112.547	1.734
Cδ_Nϵ_Cζ	124.581	1.313
Cγ_Cδ_Nϵ	111.850	1.891
Nϵ_Cζ_Nη1	120.567	1.167
Nϵ_Cζ_Nη2	119.783	1.115
Nη1_Cζ_Nη2	119.627	0.771
N_Cα_C	111.421	2.426
N_Cα_Cβ	110.746	1.182

ARG **mmm-85** n = 1022		
χ	Smooth COM	StdDev
chi1	-63.497	9.155
chi2	-67.585	10.864
chi3	-60.741	9.180
chi4	-86.156	10.081
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.631	1.520
Cα_C_O	120.548	0.882
Cβ_Cα_C	109.688	1.537
Cβ_Cγ_Cδ	112.840	1.621
Cδ_Nϵ_Cζ	124.979	1.088
Cγ_Cδ_Nϵ	112.452	2.260
Nϵ_Cζ_Nη1	120.857	1.007
Nϵ_Cζ_Nη2	119.638	0.965
Nη1_Cζ_Nη2	119.485	0.827
N_Cα_C	111.267	2.645
N_Cα_Cβ	110.750	1.121

3.18 LYS

LYS **pptt** n = 25		
χ	Smooth COM	StdDev
chi1	64.183	7.527
chi2	89.871	8.334
chi3	175.578	11.861
chi4	179.092	7.380
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.057	1.244
Cα_C_O	120.408	0.698
Cβ_Cα_C	111.303	1.430
Cβ_Cγ_Cδ	112.212	1.704
Cδ_Cϵ_Nζ	111.319	1.822
Cγ_Cδ_Cϵ	110.556	1.940
N_Cα_C	111.714	2.089
N_Cα_Cβ	111.577	1.190

LYS **ptpp** n = 89		
χ	Smooth COM	StdDev
chi1	65.327	6.803
chi2	178.405	8.068
chi3	72.033	9.721
chi4	66.034	8.135
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.569	1.201
Cα_C_O	120.169	0.968
Cβ_Cα_C	110.070	1.280
Cβ_Cγ_Cδ	112.209	1.294
Cδ_Cϵ_Nζ	112.484	1.716
Cγ_Cδ_Cϵ	112.719	1.335
N_Cα_C	111.895	2.034
N_Cα_Cβ	110.924	1.307

LYS **ptpt** n = 148		
χ	Smooth COM	StdDev
chi1	64.802	8.153
chi2	179.088	11.802
chi3	72.966	10.396
chi4	174.545	11.210
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.721	1.636
Cα_C_O	120.525	0.854
Cβ_Cα_C	110.518	1.433
Cβ_Cγ_Cδ	112.144	1.650
Cδ_Cϵ_Nζ	111.436	2.103
Cγ_Cδ_Cϵ	112.378	1.854
N_Cα_C	111.237	2.936
N_Cα_Cβ	111.124	1.321

LYS **pttp** n = 240		
χ	Smooth COM	StdDev
chi1	67.562	8.269
chi2	-179.054	10.390
chi3	178.259	11.216
chi4	66.699	12.279
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.794	1.433
Cα_C_O	120.380	0.901
Cβ_Cα_C	110.362	1.449
Cβ_Cγ_Cδ	110.892	1.675
Cδ_Cϵ_Nζ	112.359	2.336
Cγ_Cδ_Cϵ	111.720	1.424
N_Cα_C	111.801	2.552
N_Cα_Cβ	110.983	1.091

LYS **pttt** n = 1385		
χ	Smooth COM	StdDev
chi1	65.436	7.578
chi2	-178.083	8.650
chi3	-179.332	9.673
chi4	-179.680	9.634
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.839	1.455
Cα_C_O	120.431	0.948
Cβ_Cα_C	110.437	1.381
Cβ_Cγ_Cδ	110.833	1.793
Cδ_Cϵ_Nζ	111.334	2.005
Cγ_Cδ_Cϵ	111.005	1.621
N_Cα_C	111.317	2.768
N_Cα_Cβ	111.134	1.099

LYS **pttm** n = 268		
χ	Smooth COM	StdDev
chi1	64.251	6.915
chi2	-177.627	9.133
chi3	-178.897	9.970
chi4	-67.053	11.673
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.862	1.467
Cα_C_O	120.393	0.977
Cβ_Cα_C	110.414	1.447
Cβ_Cγ_Cδ	110.696	2.050
Cδ_Cϵ_Nζ	112.324	2.369
Cγ_Cδ_Cϵ	111.942	1.508
N_Cα_C	111.970	2.550
N_Cα_Cβ	110.983	1.162

LYS **ptmt** n = 187		
χ	Smooth COM	StdDev
chi1	66.652	8.246
chi2	-175.856	12.044
chi3	-71.430	11.735
chi4	-175.836	10.337
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.548	1.572
Cα_C_O	120.513	0.972
Cβ_Cα_C	110.429	1.608
Cβ_Cγ_Cδ	112.146	1.576
Cδ_Cϵ_Nζ	111.541	2.110
Cγ_Cδ_Cϵ	112.363	1.870
N_Cα_C	111.050	2.718
N_Cα_Cβ	111.011	1.103

LYS **ptmm** n = 80		
χ	Smooth COM	StdDev
chi1	66.614	8.388
chi2	-177.929	9.983
chi3	-69.614	9.844
chi4	-66.129	7.000
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.458	1.301
Cα_C_O	120.630	1.032
Cβ_Cα_C	109.915	1.495
Cβ_Cγ_Cδ	112.342	1.435
Cδ_Cϵ_Nζ	112.989	1.776
Cγ_Cδ_Cϵ	112.999	1.154
N_Cα_C	110.495	2.702
N_Cα_Cβ	110.827	1.205

LYS **pmtt** n = 10		
χ	Smooth COM	StdDev
chi1	73.156	8.365
chi2	-74.065	10.515
chi3	-168.029	10.580
chi4	-174.606	10.738
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.445	1.641
Cα_C_O	120.801	0.552
Cβ_Cα_C	110.351	1.279
Cβ_Cγ_Cδ	112.587	2.234
Cδ_Cϵ_Nζ	111.694	2.248
Cγ_Cδ_Cϵ	111.327	1.312
N_Cα_C	109.953	2.378
N_Cα_Cβ	112.145	2.128

LYS **tppp** n = 37		
χ	Smooth COM	StdDev
chi1	-177.926	11.531
chi2	62.258	10.078
chi3	65.517	7.785
chi4	67.940	11.330
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.134	1.503
Cα_C_O	120.707	0.872
Cβ_Cα_C	110.330	0.746
Cβ_Cγ_Cδ	113.479	1.870
Cδ_Cϵ_Nζ	112.983	1.698
Cγ_Cδ_Cϵ	113.390	1.737
N_Cα_C	110.891	1.930
N_Cα_Cβ	110.228	1.115

LYS **tppt** n = 272		
χ	Smooth COM	StdDev
chi1	-178.194	7.887
chi2	63.490	8.924
chi3	69.535	9.197
chi4	177.447	9.361
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.823	1.234
Cα_C_O	120.535	0.743
Cβ_Cα_C	110.620	1.101
Cβ_Cγ_Cδ	113.177	1.543
Cδ_Cϵ_Nζ	111.201	1.842
Cγ_Cδ_Cϵ	112.378	1.445
N_Cα_C	110.638	2.080
N_Cα_Cβ	110.328	1.075

LYS **tptp** n = 409		
χ	Smooth COM	StdDev
chi1	-179.932	7.986
chi2	67.443	10.399
chi3	173.601	13.550
chi4	66.191	12.980
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.807	1.338
Cα_C_O	120.530	0.826
Cβ_Cα_C	110.226	1.227
Cβ_Cγ_Cδ	112.085	1.487
Cδ_Cϵ_Nζ	112.676	1.952
Cγ_Cδ_Cϵ	112.158	1.313
N_Cα_C	110.254	2.081
N_Cα_Cβ	110.339	1.125

LYS **tptt** n = 1228		
χ	Smooth COM	StdDev
chi1	-178.908	9.092
chi2	69.056	9.015
chi3	175.565	10.063
chi4	177.246	12.306
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.773	1.314
Cα_C_O	120.549	0.775
Cβ_Cα_C	110.423	1.219
Cβ_Cγ_Cδ	112.033	1.596
Cδ_Cϵ_Nζ	111.116	2.237
Cγ_Cδ_Cϵ	111.028	1.474
N_Cα_C	110.655	2.152
N_Cα_Cβ	110.224	1.113

LYS **tptm** n = 197		
χ	Smooth COM	StdDev
chi1	-177.928	7.615
chi2	67.158	9.702
chi3	-179.368	11.396
chi4	-66.243	13.423
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.983	1.451
Cα_C_O	120.391	0.767
Cβ_Cα_C	110.392	1.099
Cβ_Cγ_Cδ	111.930	1.409
Cδ_Cϵ_Nζ	112.550	2.065
Cγ_Cδ_Cϵ	111.891	1.350
N_Cα_C	110.288	2.061
N_Cα_Cβ	110.274	1.138

LYS **ttpp** n = 229		
χ	Smooth COM	StdDev
chi1	-178.427	8.557
chi2	174.058	14.474
chi3	71.618	11.151
chi4	68.201	10.487
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.658	1.575
Cα_C_O	120.629	0.777
Cβ_Cα_C	110.131	1.263
Cβ_Cγ_Cδ	112.134	1.677
Cδ_Cϵ_Nζ	112.810	2.349
Cγ_Cδ_Cϵ	112.800	1.569
N_Cα_C	110.229	2.480
N_Cα_Cβ	110.369	1.468

LYS **ttpt** n = 883		
χ	Smooth COM	StdDev
chi1	-178.343	8.129
chi2	174.555	12.116
chi3	73.017	11.886
chi4	175.105	11.316
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.777	1.645
Cα_C_O	120.604	0.755
Cβ_Cα_C	110.066	1.179
Cβ_Cγ_Cδ	112.121	1.474
Cδ_Cϵ_Nζ	111.088	2.074
Cγ_Cδ_Cϵ	112.173	1.575
N_Cα_C	110.329	2.318
N_Cα_Cβ	110.243	1.317

LYS **ttpm** n = 4		
χ	Smooth COM	StdDev
chi1	-176.905	10.026
chi2	175.311	6.851
chi3	87.099	18.038
chi4	-84.400	4.171
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.353	1.109
Cα_C_O	120.752	0.322
Cβ_Cα_C	110.281	0.444
Cβ_Cγ_Cδ	111.616	0.992
Cδ_Cϵ_Nζ	113.892	1.178
Cγ_Cδ_Cϵ	113.140	0.242
N_Cα_C	110.149	1.306
N_Cα_Cβ	110.149	0.835

LYS **tttp** n = 1233		
χ	Smooth COM	StdDev
chi1	-177.650	8.068
chi2	175.444	9.877
chi3	173.929	10.830
chi4	65.901	12.780
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.932	1.516
Cα_C_O	120.582	0.750
Cβ_Cα_C	110.189	1.092
Cβ_Cγ_Cδ	111.148	1.611
Cδ_Cϵ_Nζ	112.268	1.984
Cγ_Cδ_Cϵ	111.826	1.347
N_Cα_C	110.703	2.222
N_Cα_Cβ	110.410	1.138

LYS **tttt** n = 5043		
χ	Smooth COM	StdDev
chi1	-175.451	8.188
chi2	176.592	8.732
chi3	179.677	9.233
chi4	-179.889	10.261
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.874	1.525
Cα_C_O	120.583	0.778
Cβ_Cα_C	110.243	1.137
Cβ_Cγ_Cδ	111.148	1.744
Cδ_Cϵ_Nζ	111.156	1.986
Cγ_Cδ_Cϵ	111.042	1.543
N_Cα_C	110.545	2.283
N_Cα_Cβ	110.335	1.206

LYS **tttm** n = 1176		
χ	Smooth COM	StdDev
chi1	-176.393	8.096
chi2	177.818	9.663
chi3	-176.243	10.489
chi4	-67.353	12.094
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.887	1.596
Cα_C_O	120.552	0.824
Cβ_Cα_C	110.254	1.139
Cβ_Cγ_Cδ	111.029	1.702
Cδ_Cϵ_Nζ	112.329	1.971
Cγ_Cδ_Cϵ	111.847	1.465
N_Cα_C	110.514	2.115
N_Cα_Cβ	110.424	1.165

LYS **ttmp** n = 9		
χ	Smooth COM	StdDev
chi1	-174.170	4.238
chi2	-179.415	8.457
chi3	-95.701	18.562
chi4	76.743	25.218
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.206	1.243
Cα_C_O	120.593	0.500
Cβ_Cα_C	110.316	1.623
Cβ_Cγ_Cδ	112.630	1.745
Cδ_Cϵ_Nζ	114.038	1.362
Cγ_Cδ_Cϵ	112.905	0.737
N_Cα_C	110.754	1.510
N_Cα_Cβ	111.426	1.042

LYS **ttmt** n = 674		
χ	Smooth COM	StdDev
chi1	-174.573	9.441
chi2	-177.288	10.835
chi3	-73.479	11.719
chi4	-175.112	11.548
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.686	1.546
Cα_C_O	120.604	0.865
Cβ_Cα_C	110.214	1.180
Cβ_Cγ_Cδ	112.161	1.524
Cδ_Cϵ_Nζ	110.881	2.322
Cγ_Cδ_Cϵ	112.229	1.651
N_Cα_C	110.307	2.331
N_Cα_Cβ	110.339	1.250

LYS **ttmm** n = 197		
χ	Smooth COM	StdDev
chi1	-174.055	8.490
chi2	179.742	9.943
chi3	-71.028	11.891
chi4	-67.045	11.420
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.643	1.459
Cα_C_O	120.558	0.817
Cβ_Cα_C	110.229	1.285
Cβ_Cγ_Cδ	112.136	1.574
Cδ_Cϵ_Nζ	112.648	2.300
Cγ_Cδ_Cϵ	112.487	1.564
N_Cα_C	110.191	2.445
N_Cα_Cβ	110.327	1.394

LYS **tmtp** n = 11		
χ	Smooth COM	StdDev
chi1	-176.649	7.525
chi2	-97.994	8.314
chi3	-178.365	12.353
chi4	65.083	7.821
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.616	1.223
Cα_C_O	120.800	0.413
Cβ_Cα_C	110.486	0.704
Cβ_Cγ_Cδ	112.010	1.506
Cδ_Cϵ_Nζ	113.099	3.033
Cγ_Cδ_Cϵ	111.842	1.204
N_Cα_C	110.140	3.054
N_Cα_Cβ	110.368	0.871

LYS **tmtt** n = 82		
χ	Smooth COM	StdDev
chi1	-172.661	8.464
chi2	-91.117	9.621
chi3	-176.853	11.750
chi4	-178.511	10.695
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.500	1.145
Cα_C_O	120.778	0.610
Cβ_Cα_C	110.869	1.093
Cβ_Cγ_Cδ	111.882	1.443
Cδ_Cϵ_Nζ	110.842	2.070
Cγ_Cδ_Cϵ	111.015	1.375
N_Cα_C	110.180	1.891
N_Cα_Cβ	110.078	0.810

LYS **tmtm** n = 20		
χ	Smooth COM	StdDev
chi1	-172.233	10.447
chi2	-90.510	5.572
chi3	-172.543	15.072
chi4	-64.869	7.732
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.452	1.619
Cα_C_O	120.586	0.646
Cβ_Cα_C	110.984	0.853
Cβ_Cγ_Cδ	112.208	1.226
Cδ_Cϵ_Nζ	112.679	1.691
Cγ_Cδ_Cϵ	111.998	1.546
N_Cα_C	110.089	1.720
N_Cα_Cβ	109.782	0.789

LYS **tmmt** n = 33		
χ	Smooth COM	StdDev
chi1	-179.225	9.981
chi2	-93.418	12.058
chi3	-70.433	8.917
chi4	-179.549	10.245
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.020	1.846
Cα_C_O	120.544	0.877
Cβ_Cα_C	110.741	1.116
Cβ_Cγ_Cδ	113.459	1.734
Cδ_Cϵ_Nζ	110.756	2.859
Cγ_Cδ_Cϵ	112.411	2.864
N_Cα_C	109.953	2.155
N_Cα_Cβ	109.895	1.083

LYS **tmmm** n = 8		
χ	Smooth COM	StdDev
chi1	-177.527	11.864
chi2	-81.761	7.499
chi3	-63.102	8.026
chi4	-64.475	4.939
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.243	2.695
Cα_C_O	120.272	0.848
Cβ_Cα_C	111.246	1.126
Cβ_Cγ_Cδ	114.871	1.367
Cδ_Cϵ_Nζ	113.141	1.476
Cγ_Cδ_Cϵ	114.998	1.617
N_Cα_C	108.983	2.013
N_Cα_Cβ	109.523	1.258

LYS **mppt** n = 31		
χ	Smooth COM	StdDev
chi1	-82.599	8.918
chi2	73.518	14.873
chi3	69.157	8.044
chi4	177.385	5.414
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.111	1.987
Cα_C_O	120.424	0.890
Cβ_Cα_C	109.879	1.228
Cβ_Cγ_Cδ	113.688	1.564
Cδ_Cϵ_Nζ	111.358	1.922
Cγ_Cδ_Cϵ	112.185	1.373
N_Cα_C	108.768	1.973
N_Cα_Cβ	110.907	0.923

LYS **mptp** n = 26		
χ	Smooth COM	StdDev
chi1	-74.901	18.526
chi2	86.563	18.186
chi3	171.631	8.992
chi4	65.232	12.143
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.682	1.564
Cα_C_O	120.477	1.133
Cβ_Cα_C	110.099	1.428
Cβ_Cγ_Cδ	113.211	2.501
Cδ_Cϵ_Nζ	113.419	2.262
Cγ_Cδ_Cϵ	112.501	2.718
N_Cα_C	110.602	2.774
N_Cα_Cβ	110.868	1.039

LYS **mptt** n = 124		
χ	Smooth COM	StdDev
chi1	-79.911	13.282
chi2	72.964	17.284
chi3	176.124	12.429
chi4	175.095	11.920
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.896	1.389
Cα_C_O	120.553	0.785
Cβ_Cα_C	109.748	1.534
Cβ_Cγ_Cδ	112.619	2.029
Cδ_Cϵ_Nζ	110.877	2.274
Cγ_Cδ_Cϵ	111.162	1.603
N_Cα_C	110.579	2.594
N_Cα_Cβ	110.815	1.103

LYS **mptm** n = 11		
χ	Smooth COM	StdDev
chi1	-91.748	6.662
chi2	61.180	11.061
chi3	-173.655	5.358
chi4	-60.981	13.466
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.614	0.809
Cα_C_O	120.670	0.565
Cβ_Cα_C	110.693	0.842
Cβ_Cγ_Cδ	112.838	0.654
Cδ_Cϵ_Nζ	113.434	1.681
Cγ_Cδ_Cϵ	111.830	0.502
N_Cα_C	110.770	2.188
N_Cα_Cβ	110.642	0.906

LYS **mtpp** n = 392		
χ	Smooth COM	StdDev
chi1	-68.535	7.507
chi2	176.954	10.868
chi3	70.471	10.847
chi4	67.722	10.865
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.235	1.656
Cα_C_O	120.433	0.824
Cβ_Cα_C	110.157	1.514
Cβ_Cγ_Cδ	112.402	1.454
Cδ_Cϵ_Nζ	112.819	2.106
Cγ_Cδ_Cϵ	112.704	1.415
N_Cα_C	111.365	2.533
N_Cα_Cβ	110.495	1.009

LYS **mtpt** n = 1357		
χ	Smooth COM	StdDev
chi1	-69.197	8.061
chi2	174.242	11.340
chi3	70.524	11.811
chi4	175.197	10.445
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.256	1.539
Cα_C_O	120.481	0.839
Cβ_Cα_C	109.985	1.646
Cβ_Cγ_Cδ	112.293	1.551
Cδ_Cϵ_Nζ	110.841	2.155
Cγ_Cδ_Cϵ	112.343	1.491
N_Cα_C	111.357	2.211
N_Cα_Cβ	110.670	1.031

LYS **mtpm** n = 17		
χ	Smooth COM	StdDev
chi1	-70.323	6.135
chi2	174.831	15.490
chi3	90.638	14.675
chi4	-70.024	12.061
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.509	2.138
Cα_C_O	120.306	0.769
Cβ_Cα_C	109.783	2.273
Cβ_Cγ_Cδ	112.290	1.700
Cδ_Cϵ_Nζ	113.385	1.869
Cγ_Cδ_Cϵ	113.180	1.587
N_Cα_C	110.870	2.120
N_Cα_Cβ	110.511	1.029

LYS **mttp** n = 1414		
χ	Smooth COM	StdDev
chi1	-65.910	8.334
chi2	-179.442	10.679
chi3	176.319	11.179
chi4	66.691	13.607
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.442	1.732
Cα_C_O	120.510	0.841
Cβ_Cα_C	110.097	1.628
Cβ_Cγ_Cδ	111.258	1.746
Cδ_Cϵ_Nζ	112.223	1.982
Cγ_Cδ_Cϵ	111.751	1.466
N_Cα_C	111.268	2.491
N_Cα_Cβ	110.594	1.017

LYS **mttt** n = 8597		
χ	Smooth COM	StdDev
chi1	-67.654	7.111
chi2	-178.811	9.067
chi3	-179.106	9.781
chi4	179.484	10.347
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.453	1.623
Cα_C_O	120.467	0.827
Cβ_Cα_C	109.998	1.557
Cβ_Cγ_Cδ	111.143	1.850
Cδ_Cϵ_Nζ	111.119	2.099
Cγ_Cδ_Cϵ	111.049	1.601
N_Cα_C	111.334	2.236
N_Cα_Cβ	110.665	0.988

LYS **mttm** n = 1829		
χ	Smooth COM	StdDev
chi1	-66.855	7.320
chi2	-177.777	10.020
chi3	-176.656	10.842
chi4	-67.384	12.838
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.406	1.737
Cα_C_O	120.484	0.849
Cβ_Cα_C	110.086	1.544
Cβ_Cγ_Cδ	111.204	1.726
Cδ_Cϵ_Nζ	112.211	2.034
Cγ_Cδ_Cϵ	111.752	1.469
N_Cα_C	111.378	2.375
N_Cα_Cβ	110.611	1.003

LYS **mtmp** n = 9		
χ	Smooth COM	StdDev
chi1	-67.465	5.792
chi2	-175.781	8.346
chi3	-95.844	7.431
chi4	73.531	12.322
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.802	1.228
Cα_C_O	120.633	0.607
Cβ_Cα_C	109.891	1.198
Cβ_Cγ_Cδ	111.699	1.976
Cδ_Cϵ_Nζ	113.681	2.374
Cγ_Cδ_Cϵ	112.703	0.792
N_Cα_C	110.375	2.291
N_Cα_Cβ	110.828	0.914

LYS **mtmt** n = 1314		
χ	Smooth COM	StdDev
chi1	-66.838	6.886
chi2	-173.335	9.847
chi3	-73.733	11.654
chi4	-175.371	10.598
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.209	1.595
Cα_C_O	120.408	0.857
Cβ_Cα_C	110.085	1.557
Cβ_Cγ_Cδ	112.313	1.519
Cδ_Cϵ_Nζ	111.041	2.184
Cγ_Cδ_Cϵ	112.107	1.451
N_Cα_C	111.319	2.137
N_Cα_Cβ	110.673	0.960

LYS **mtmm** n = 424		
χ	Smooth COM	StdDev
chi1	-63.898	6.909
chi2	-177.154	10.058
chi3	-70.378	10.902
chi4	-66.004	9.830
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.456	1.534
Cα_C_O	120.488	0.838
Cβ_Cα_C	109.818	1.557
Cβ_Cγ_Cδ	112.288	1.374
Cδ_Cϵ_Nζ	112.759	2.097
Cγ_Cδ_Cϵ	112.869	1.500
N_Cα_C	111.524	2.392
N_Cα_Cβ	110.573	1.029

LYS **mmpt** n = 31		
χ	Smooth COM	StdDev
chi1	-60.371	7.013
chi2	-70.556	19.521
chi3	93.615	14.476
chi4	175.537	10.679
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.281	1.118
Cα_C_O	120.359	0.888
Cβ_Cα_C	109.807	1.683
Cβ_Cγ_Cδ	113.354	1.803
Cδ_Cϵ_Nζ	111.539	1.766
Cγ_Cδ_Cϵ	112.040	1.404
N_Cα_C	111.535	2.365
N_Cα_Cβ	111.168	1.386

LYS **mmtp** n = 463		
χ	Smooth COM	StdDev
chi1	-61.499	8.157
chi2	-68.646	12.048
chi3	179.724	11.913
chi4	67.912	13.158
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.716	1.514
Cα_C_O	120.405	0.904
Cβ_Cα_C	109.563	1.559
Cβ_Cγ_Cδ	112.024	1.545
Cδ_Cϵ_Nζ	112.649	2.339
Cγ_Cδ_Cϵ	111.879	1.343
N_Cα_C	111.141	2.596
N_Cα_Cβ	110.702	1.044

LYS **mmtt** n = 3137		
χ	Smooth COM	StdDev
chi1	-61.713	8.298
chi2	-67.230	9.794
chi3	-176.776	10.146
chi4	-178.237	10.966
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.531	1.322
Cα_C_O	120.435	0.906
Cβ_Cα_C	109.619	1.555
Cβ_Cγ_Cδ	111.910	1.487
Cδ_Cϵ_Nζ	111.069	2.082
Cγ_Cδ_Cϵ	111.132	1.533
N_Cα_C	111.465	2.473
N_Cα_Cβ	110.691	1.009

LYS **mmtm** n = 727		
χ	Smooth COM	StdDev
chi1	-60.188	8.246
chi2	-65.555	10.785
chi3	-173.090	11.157
chi4	-68.899	13.356
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.540	1.397
Cα_C_O	120.538	0.866
Cβ_Cα_C	109.750	1.568
Cβ_Cγ_Cδ	111.934	1.429
Cδ_Cϵ_Nζ	112.437	1.969
Cγ_Cδ_Cϵ	111.964	1.439
N_Cα_C	111.442	2.525
N_Cα_Cβ	110.623	1.025

LYS **mmmt** n = 544		
χ	Smooth COM	StdDev
chi1	-62.678	7.662
chi2	-64.116	10.733
chi3	-70.703	9.725
chi4	-176.812	9.766
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.613	1.313
Cα_C_O	120.383	0.968
Cβ_Cα_C	109.622	1.455
Cβ_Cγ_Cδ	113.105	1.508
Cδ_Cϵ_Nζ	111.154	2.215
Cγ_Cδ_Cϵ	112.301	1.533
N_Cα_C	111.767	2.314
N_Cα_Cβ	110.671	1.052

LYS **mmmm** n = 90		
χ	Smooth COM	StdDev
chi1	-61.396	8.320
chi2	-61.832	10.421
chi3	-66.893	10.843
chi4	-64.659	10.880
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.738	1.388
Cα_C_O	120.417	1.064
Cβ_Cα_C	109.517	1.525
Cβ_Cγ_Cδ	113.153	1.432
Cδ_Cϵ_Nζ	112.644	2.734
Cγ_Cδ_Cϵ	113.176	1.865
N_Cα_C	111.658	2.469
N_Cα_Cβ	110.501	1.112