Supplemental Material for MolProbity's Ultimate Rotamer-Library Distributions for Model Validation

Bradley J. Hintze, Steven M. Lewis, Jane S. Richardson, and David C. Richardson

Department of Biochemistry, Duke University

List of Figures

List of Tables

Top500 vs. Top8000 Reference Contours

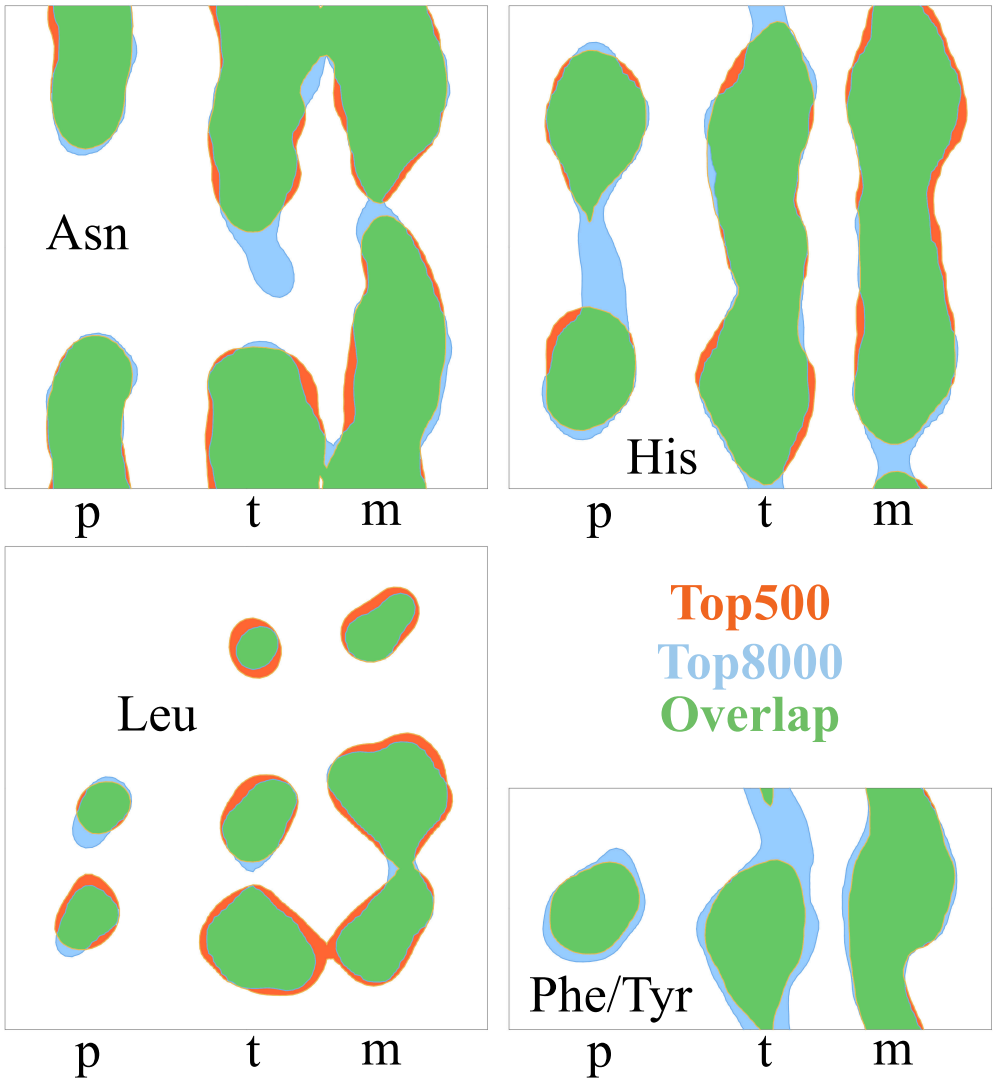

Figure S1: Areas in orange (from Top500 data) and in blue (from Top8000) fill the allowed regions for AsN, His, Leu, and Phe/Tyr. Phe and Tyr were done together as no significant difference was detected between their distributions. The extensive areas in green are where the two systems both declare allowed conformations. See Figure 2 for Asp, Trp, and Ile

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 S1: 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.

Outlier Counts: Top500 vs. Top8000 Reference Contours

Residue	n	Top500 $< 1.0\%$	Top8000 $< 0.3\%$	Δ
ARG	193295	7501	5643	-1858
ASN	161814	2143	1926	-217
ASP	225302	3745	2779	-966
CYS	50824	618	462	-156
GLN	140651	2751	2810	59
GLU	255560	4803	6334	1531
HIS	91316	1303	802	-501
ILE	222518	1766	3241	1475
LEU	347449	8245	9806	1561
LYS	209811	6501	7709	1208
MET	69395	1874	1830	-44
PHE	153564	1896	703	-1193
PRO	174910	849	800	-49
SER	236825	2640	2638	-2
THR	214960	2225	2787	562
TRP	53869	713	266	-447
TYR	134580	1757	696	-1061
VAL	280539	1633	3282	1649

Table S2: Showing differences between outlier counts in the unfiltered dataset using the Top500 and Top8000 reference contours.

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. as shown below, LEU has 115,053 examples in the filtered dataset and 8 rotamers. Thus LEU has an *expected rotamer count* of $115{,}053/8 \approx 14{,}382$. LEU **pp** has 521 examples which is 3.7% of the *expected rotamer count* thus gets a single checkmark. LEU **tm** has 143 examples which is 0.99% of the *expected rotamer count* thus gets a double checkmark.

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	-

residue	rotamer	n	%	rarity
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	-

residue	rotamer	n	%	rarity
TRP	OUTLIER	53	0.28	-
MET : TOTAL N = 16794				
MET	ppp	50	0.30	✓
MET	pp-130	27	0.16	✓
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	-

residue	rotamer	n	%	rarity
ARG	ptp-170	388	0.84	-
ARG	ptt180	820	1.77	-
ARG	ptt90	814	1.76	-
ARG	ptt-90	726	1.57	-
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	-

residue	rotamer	n	%	rarity
LYS	pttm	268	0.77	-
LYS	ptmt	187	0.54	-
LYS	ptmm	80	0.23	-
LYS	pmtt	10	0.03	✓
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	-

Table S3: Rotamer names, number of examples in the filtered data set, and frequency in its residue type.

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.

Table S4: SER Central Values

SER **p** n = 36901		
χ	Smooth COM	StdDev
chi1	65	8.6
Bond Angle	Mean	StdDev
Cα_Cβ_OG	111.0	1.35
Cα_C_O	120.5	0.92
Cβ_Cα_C	109.9	1.39
N_Cα_C	111.6	2.52
N_Cα_Cβ	110.7	1.12

SER **t** n = 17502		
χ	Smooth COM	StdDev
chi1	178	9.0
Bond Angle	Mean	StdDev
Cα_Cβ_OG	110.7	1.42
Cα_C_O	120.6	0.82
Cβ_Cα_C	109.8	1.45
N_Cα_C	110.5	2.40
N_Cα_Cβ	110.1	1.21

SER **m** n = 21558		
χ	Smooth COM	StdDev
chi1	-63	7.7
Bond Angle	Mean	StdDev
Cα_Cβ_OG	110.5	1.46
Cα_C_O	120.5	0.85
Cβ_Cα_C	109.5	1.45
N_Cα_C	111.5	2.44
N_Cα_Cβ	110.6	1.03

Table S5: CYS Central Values

CYS **p** n = 2962		
χ	Smooth COM	StdDev
chi1	64	9.0
Bond Angle	Mean	StdDev
Cα_Cβ_SG	114.6	1.68
Cα_C_O	120.5	0.98
Cβ_Cα_C	110.5	1.50
N_Cα_C	111.3	2.78
N_Cα_Cβ	110.9	1.23

CYS **t** n = 4399		
χ	Smooth COM	StdDev
chi1	-177	8.2
Bond Angle	Mean	StdDev
Cα_Cβ_SG	113.7	1.94
Cα_C_O	120.5	0.86
Cβ_Cα_C	110.3	1.30
N_Cα_C	109.7	2.44
N_Cα_Cβ	110.0	1.37

CYS **m** n = 9301		
χ	Smooth COM	StdDev
chi1	-65	8.2
Bond Angle	Mean	StdDev
Cα_Cβ_SG	113.6	1.86
Cα_C_O	120.4	0.87
Cβ_Cα_C	109.5	1.63
N_Cα_C	111.5	2.42
N_Cα_Cβ	110.6	1.07

Table S6: THR Central Values

THR **p** n = 36195		
χ	Smooth COM	StdDev
chi1	61	7.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ2	111.0	1.01
Cα_Cβ_OG1	109.5	0.97
Cα_C_O	120.5	0.96
Cβ_Cα_C	108.8	1.70
N_Cα_C	111.4	2.77
N_Cα_Cβ	111.8	1.26
OG1_Cβ_Cγ2	109.2	1.71

THR **t** n = 5197		
χ	Smooth COM	StdDev
chi1	-172	7.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ2	111.7	1.10
Cα_Cβ_OG1	109.5	0.99
Cα_C_O	120.6	0.83
Cβ_Cα_C	111.0	1.90
N_Cα_C	110.1	2.33
N_Cα_Cβ	111.3	1.34
OG1_Cβ_Cγ2	109.1	1.81

THR **m** n = 33559		
χ	Smooth COM	StdDev
chi1	-60	6.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ2	111.1	0.94
Cα_Cβ_OG1	108.9	0.97
Cα_C_O	120.5	0.81
Cβ_Cα_C	110.0	1.53
N_Cα_C	110.2	2.31
N_Cα_Cβ	110.7	1.19
OG1_Cβ_Cγ2	108.8	1.67

Table S7: VAL Central Values

VAL **p** n = 6015		
χ	Smooth COM	StdDev
chi1	64	7.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	111.5	1.09
Cα_Cβ_Cγ2	110.8	1.02
Cα_C_O	120.6	0.83
Cβ_Cα_C	111.4	1.57
Cγ1_Cβ_Cγ2	111.0	1.20
N_Cα_C	110.3	2.48
N_Cα_Cβ	111.6	1.26

VAL **t** n = 73329		
χ	Smooth COM	StdDev
chi1	175	6.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	110.7	0.94
Cα_Cβ_Cγ2	110.2	0.95
Cα_C_O	120.5	0.79
Cβ_Cα_C	110.2	1.51
Cγ1_Cβ_Cγ2	110.5	1.13
N_Cα_C	109.4	2.36
N_Cα_Cβ	111.3	1.11

VAL **m** n = 17410		
χ	Smooth COM	StdDev
chi1	-61	5.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	110.4	0.92
Cα_Cβ_Cγ2	111.3	1.02
Cα_C_O	120.6	0.91
Cβ_Cα_C	109.8	1.60
Cγ1_Cβ_Cγ2	110.9	1.16
N_Cα_C	111.1	2.69
N_Cα_Cβ	112.3	1.18

Table S8: PRO Central Values

PRO **Cg_exo** n = 30128		
χ	Smooth COM	StdDev
chi1	-24	7.2
chi2	35	7.8
chi3	-31	7.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	104.2	1.40
Cα_C_O	120.2	1.03
Cα_N_Cδ	111.7	0.81
Cβ_Cα_C	110.8	1.30
Cβ_Cγ_Cδ	104.7	2.31
N_Cα_C	112.7	2.42
N_Cα_Cβ	103.3	0.59
N_Cδ_Cγ	102.7	0.88

PRO **Cg_endo** n = 29192		
χ	Smooth COM	StdDev
chi1	26	7.7
chi2	-34	8.9
chi3	27	9.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	104.2	1.47
Cα_C_O	120.2	1.07
Cα_N_Cδ	111.8	0.84
Cβ_Cα_C	110.9	1.41
Cβ_Cγ_Cδ	105.3	2.36
N_Cα_C	112.9	2.60
N_Cα_Cβ	103.2	0.72
N_Cδ_Cγ	103.1	0.88

Table S9: LEU Central Values

LEU **pp** n = 521		
χ	Smooth COM	StdDev
chi1	61	8.2
chi2	83	9.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	119.1	2.53
Cα_C_O	120.6	0.83
Cβ_Cα_C	111.5	1.38
Cβ_Cγ_Cδ1	111.5	1.89
Cβ_Cγ_Cδ2	109.8	1.68
Cδ1_Cγ_Cδ2	109.7	1.23
N_Cα_C	110.7	2.36
N_Cα_Cβ	111.1	1.15

LEU **pt** n = 378		
χ	Smooth COM	StdDev
chi1	72	8.5
chi2	164	10.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	118.7	2.16
Cα_C_O	120.8	0.83
Cβ_Cα_C	110.4	1.45
Cβ_Cγ_Cδ1	109.8	1.54
Cβ_Cγ_Cδ2	111.6	1.84
Cδ1_Cγ_Cδ2	110.4	1.24
N_Cα_C	110.4	2.45
N_Cα_Cβ	111.6	1.18

LEU **tp** n = 34655		
χ	Smooth COM	StdDev
chi1	-177	8.2
chi2	62	7.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.5	2.06
Cα_C_O	120.5	0.79
Cβ_Cα_C	110.2	1.21
Cβ_Cγ_Cδ1	111.1	1.55
Cβ_Cγ_Cδ2	109.8	1.50
Cδ1_Cγ_Cδ2	110.7	1.13
N_Cα_C	110.2	2.38
N_Cα_Cβ	110.3	1.15

LEU **tt** n = 1576		
χ	Smooth COM	StdDev
chi1	-172	8.5
chi2	153	10.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	117.3	2.71
Cα_C_O	120.6	0.86
Cβ_Cα_C	111.1	1.26
Cβ_Cγ_Cδ1	110.1	1.53
Cβ_Cγ_Cδ2	111.6	1.84
Cδ1_Cγ_Cδ2	110.4	1.32
N_Cα_C	109.1	2.50
N_Cα_Cβ	110.2	1.25

LEU **tm** n = 143		
χ	Smooth COM	StdDev
chi1	-171	5.9
chi2	-75	6.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	120.4	2.30
Cα_C_O	120.6	0.80
Cβ_Cα_C	111.3	1.17
Cβ_Cγ_Cδ1	112.3	1.92
Cβ_Cγ_Cδ2	111.6	1.69
Cδ1_Cγ_Cδ2	111.4	1.44
N_Cα_C	108.5	2.32
N_Cα_Cβ	109.9	1.13

LEU **mp** n = 2711		
χ	Smooth COM	StdDev
chi1	-77	12.5
chi2	71	15.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.6	2.64
Cα_C_O	120.5	0.85
Cβ_Cα_C	109.7	1.57
Cβ_Cγ_Cδ1	111.6	2.04
Cβ_Cγ_Cδ2	109.9	1.58
Cδ1_Cγ_Cδ2	110.5	1.45
N_Cα_C	110.2	2.64
N_Cα_Cβ	111.1	1.03

LEU **mt** n = 74252		
χ	Smooth COM	StdDev
chi1	-65	8.2
chi2	174	8.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.9	2.17
Cα_C_O	120.4	0.82
Cβ_Cα_C	109.8	1.42
Cβ_Cγ_Cδ1	109.9	1.47
Cβ_Cγ_Cδ2	111.0	1.55
Cδ1_Cγ_Cδ2	110.8	1.11
N_Cα_C	111.4	2.34
N_Cα_Cβ	110.6	0.99

LEU **mm** n = 484		
χ	Smooth COM	StdDev
chi1	-82	10.2
chi2	-63	10.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	117.8	2.63
Cα_C_O	120.3	0.89
Cβ_Cα_C	110.1	1.58
Cβ_Cγ_Cδ1	110.9	1.60
Cβ_Cγ_Cδ2	111.9	1.72
Cδ1_Cγ_Cδ2	110.7	1.40
N_Cα_C	111.1	2.61
N_Cα_Cβ	111.0	0.98

Table S10: ILE Central Values

ILE **pp** n = 254		
χ	Smooth COM	StdDev
chi1	57	7.7
chi2	84	12.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	112.5	1.28
Cα_Cβ_Cγ2	109.9	1.15
Cα_C_O	120.5	0.87
Cβ_Cα_C	111.3	1.61
Cβ_Cγ1_Cδ1	115.1	1.80
Cγ1_Cβ_Cγ2	110.0	1.96
N_Cα_C	112.0	2.51
N_Cα_Cβ	112.3	1.25

ILE **pt** n = 8837		
χ	Smooth COM	StdDev
chi1	62	6.1
chi2	170	7.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	111.3	1.08
Cα_Cβ_Cγ2	110.2	0.94
Cα_C_O	120.5	0.94
Cβ_Cα_C	110.1	1.67
Cβ_Cγ1_Cδ1	113.6	1.25
Cγ1_Cβ_Cγ2	111.4	1.53
N_Cα_C	111.4	2.74
N_Cα_Cβ	112.3	1.20

ILE **tp** n = 1869		
χ	Smooth COM	StdDev
chi1	-167	7.8
chi2	65	7.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	111.1	1.13
Cα_Cβ_Cγ2	111.4	1.03
Cα_C_O	120.4	0.82
Cβ_Cα_C	111.5	1.46
Cβ_Cγ1_Cδ1	114.2	1.15
Cγ1_Cβ_Cγ2	110.8	1.70
N_Cα_C	111.6	2.33
N_Cα_Cβ	111.5	1.27

ILE **tt** n = 4163		
χ	Smooth COM	StdDev
chi1	-169	7.7
chi2	166	6.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	110.7	1.07
Cα_Cβ_Cγ2	111.4	1.04
Cα_C_O	120.6	0.83
Cβ_Cα_C	111.6	1.48
Cβ_Cγ1_Cδ1	113.5	1.27
Cγ1_Cβ_Cγ2	111.7	1.61
N_Cα_C	110.1	2.52
N_Cα_Cβ	111.4	1.32

ILE **mp** n = 623		
χ	Smooth COM	StdDev
chi1	-62	11.6
chi2	88	16.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	111.2	1.11
Cα_Cβ_Cγ2	110.5	1.09
Cα_C_O	120.5	0.81
Cβ_Cα_C	110.1	1.63
Cβ_Cγ1_Cδ1	114.6	1.67
Cγ1_Cβ_Cγ2	109.3	1.87
N_Cα_C	108.3	2.26
N_Cα_Cβ	111.9	1.29

ILE **mt** n = 44470		
χ	Smooth COM	StdDev
chi1	-62	6.4
chi2	169	7.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	110.0	1.08
Cα_Cβ_Cγ2	110.6	0.92
Cα_C_O	120.5	0.79
Cβ_Cα_C	110.4	1.58
Cβ_Cγ1_Cδ1	114.0	1.22
Cγ1_Cβ_Cγ2	110.8	1.44
N_Cα_C	109.4	2.34
N_Cα_Cβ	111.2	1.15

ILE **mm** n = 11258		
χ	Smooth COM	StdDev
chi1	-59	7.1
chi2	-61	7.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ1	110.9	1.12
Cα_Cβ_Cγ2	110.8	0.97
Cα_C_O	120.5	0.80
Cβ_Cα_C	109.8	1.61
Cβ_Cγ1_Cδ1	114.8	1.21
Cγ1_Cβ_Cγ2	111.3	1.47
N_Cα_C	109.4	2.45
N_Cα_Cβ	111.3	1.15

Table S11: ASN Central Values

ASN **p0** n = 7513		
χ	Smooth COM	StdDev
chi1	63	7.8
chi2	6	43.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.1	0.88
Cα_C_O	120.4	0.97
Cβ_Cα_C	111.3	1.68
Cβ_Cγ_Nδ2	116.3	0.91
Cβ_Cγ_Oδ1	121.1	0.98
N_Cα_C	112.0	2.77
N_Cα_Cβ	111.1	1.29
Oδ1_Cγ_Nδ2	122.5	0.72

ASN **t0** n = 15610		
χ	Smooth COM	StdDev
chi1	-171	10.5
chi2	-1	54.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	112.7	0.92
Cα_C_O	120.6	0.87
Cβ_Cα_C	110.6	1.31
Cβ_Cγ_Nδ2	116.5	0.85
Cβ_Cγ_Oδ1	120.9	0.92
N_Cα_C	110.1	2.82
N_Cα_Cβ	110.1	1.45
Oδ1_Cγ_Nδ2	122.6	0.68

ASN **t160** n = 61		
χ	Smooth COM	StdDev
chi1	-161	7.4
chi2	163	9.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.2	1.52
Cα_C_O	120.4	0.85
Cβ_Cα_C	111.3	1.38
Cβ_Cγ_Nδ2	117.0	2.10
Cβ_Cγ_Oδ1	120.5	2.02
N_Cα_C	110.0	1.95
N_Cα_Cβ	109.3	1.46
Oδ1_Cγ_Nδ2	122.4	0.78

ASN **m110** n = 4003		
χ	Smooth COM	StdDev
chi1	-63	9.6
chi2	114	28.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	112.7	1.15
Cα_C_O	120.5	0.90
Cβ_Cα_C	109.5	1.84
Cβ_Cγ_Nδ2	116.6	1.14
Cβ_Cγ_Oδ1	120.7	1.17
N_Cα_C	112.0	2.78
N_Cα_Cβ	110.6	1.20
Oδ1_Cγ_Nδ2	122.6	0.82

ASN **m-40** n = 26292		
χ	Smooth COM	StdDev
chi1	-69	9.1
chi2	-41	26.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	112.5	0.92
Cα_C_O	120.4	0.87
Cβ_Cα_C	110.0	1.72
Cβ_Cγ_Nδ2	116.5	0.85
Cβ_Cγ_Oδ1	120.8	0.89
N_Cα_C	112.2	2.54
N_Cα_Cβ	110.5	1.10
Oδ1_Cγ_Nδ2	122.7	0.70

Table S12: ASP Central Values

ASP **p0** n = 11746		
χ	Smooth COM	StdDev
chi1	62	7.5
chi2	-2	31.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.5	1.02
Cα_C_O	120.4	0.91
Cβ_Cα_C	111.3	1.65
Cβ_Cγ_Oδ1	119.7	1.56
Cβ_Cγ_Oδ2	118.2	1.77
N_Cα_C	112.2	2.55
N_Cα_Cβ	111.1	1.25
Oδ1_Cγ_Oδ2	122.1	1.64

ASP **t0** n = 17107		
χ	Smooth COM	StdDev
chi1	-171	10.2
chi2	-1	23.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.2	0.91
Cα_C_O	120.7	0.89
Cβ_Cα_C	110.9	1.23
Cβ_Cγ_Oδ1	119.5	1.39
Cβ_Cγ_Oδ2	118.1	1.73
N_Cα_C	108.9	2.65
N_Cα_Cβ	109.7	1.45
Oδ1_Cγ_Oδ2	122.4	1.58

ASP **t70** n = 6029		
χ	Smooth COM	StdDev
chi1	-174	9.2
chi2	74	19.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	112.4	0.83
Cα_C_O	120.5	0.80
Cβ_Cα_C	110.1	1.27
Cβ_Cγ_Oδ1	118.5	1.11
Cβ_Cγ_Oδ2	118.7	1.56
N_Cα_C	110.5	2.36
N_Cα_Cβ	110.2	1.37
Oδ1_Cγ_Oδ2	122.7	1.54

ASP **m-30** n = 37239		
χ	Smooth COM	StdDev
chi1	-68	8.2
chi2	-29	22.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	112.9	0.95
Cα_C_O	120.5	0.86
Cβ_Cα_C	109.4	1.67
Cβ_Cγ_Oδ1	119.2	1.36
Cβ_Cγ_Oδ2	118.2	1.70
N_Cα_C	111.7	2.30
N_Cα_Cβ	110.8	1.06
Oδ1_Cγ_Oδ2	122.6	1.56

Table S13: HIS Central Values

HIS **p90** n = 1492		
χ	Smooth COM	StdDev
chi1	62	9.7
chi2	86	21.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.2	1.05
Cα_C_O	120.6	0.95
Cβ_Cα_C	110.8	1.57
Cβ_Cγ_Cδ2	131.0	0.86
Cβ_Cγ_Nδ1	122.8	0.91
Cϵ1_Nϵ2_Cδ2	108.8	0.59
Cγ_Cδ2_Nϵ2	107.3	0.50
Cγ_Nδ1_Cϵ1	109.2	0.72
Nδ1_Cϵ1_Nϵ2	108.5	0.66
Nδ1_Cγ_Cδ2	106.2	0.53
N_Cα_C	111.3	2.74
N_Cα_Cβ	111.0	1.36

HIS **p-80** n = 2203		
χ	Smooth COM	StdDev
chi1	64	9.9
chi2	-80	16.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.1	1.06
Cα_C_O	120.4	0.98
Cβ_Cα_C	110.4	1.53
Cβ_Cγ_Cδ2	131.0	0.80
Cβ_Cγ_Nδ1	122.7	0.81
Cϵ1_Nϵ2_Cδ2	108.8	0.58
Cγ_Cδ2_Nϵ2	107.2	0.52
Cγ_Nδ1_Cϵ1	109.2	0.61
Nδ1_Cϵ1_Nϵ2	108.5	0.60
Nδ1_Cγ_Cδ2	106.2	0.51
N_Cα_C	112.0	2.43
N_Cα_Cβ	111.0	1.32

HIS **t70** n = 5068		
χ	Smooth COM	StdDev
chi1	-178	10.0
chi2	73	17.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.6	1.07
Cα_C_O	120.6	0.83
Cβ_Cα_C	110.1	1.34
Cβ_Cγ_Cδ2	131.0	0.82
Cβ_Cγ_Nδ1	122.7	0.79
Cϵ1_Nϵ2_Cδ2	108.9	0.52
Cγ_Cδ2_Nϵ2	107.2	0.46
Cγ_Nδ1_Cϵ1	109.2	0.62
Nδ1_Cϵ1_Nϵ2	108.5	0.56
Nδ1_Cγ_Cδ2	106.2	0.50
N_Cα_C	110.7	2.35
N_Cα_Cβ	110.2	1.49

HIS **t-170** n = 1332		
χ	Smooth COM	StdDev
chi1	-173	9.7
chi2	-167	21.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.2	1.02
Cα_C_O	120.6	0.81
Cβ_Cα_C	110.9	1.31
Cβ_Cγ_Cδ2	131.4	0.98
Cβ_Cγ_Nδ1	122.4	1.05
Cϵ1_Nϵ2_Cδ2	108.8	0.55
Cγ_Cδ2_Nϵ2	107.2	0.45
Cγ_Nδ1_Cϵ1	109.2	0.66
Nδ1_Cϵ1_Nϵ2	108.6	0.63
Nδ1_Cγ_Cδ2	106.2	0.52
N_Cα_C	109.2	2.61
N_Cα_Cβ	109.6	1.52

HIS **t-90** n = 3553		
χ	Smooth COM	StdDev
chi1	-173	10.4
chi2	-86	18.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.7	1.01
Cα_C_O	120.5	0.85
Cβ_Cα_C	110.4	1.22
Cβ_Cγ_Cδ2	130.9	0.83
Cβ_Cγ_Nδ1	122.8	0.75
Cϵ1_Nϵ2_Cδ2	108.8	0.52
Cγ_Cδ2_Nϵ2	107.2	0.48
Cγ_Nδ1_Cϵ1	109.2	0.72
Nδ1_Cϵ1_Nϵ2	108.5	0.62
Nδ1_Cγ_Cδ2	106.2	0.55
N_Cα_C	109.9	2.47
N_Cα_Cβ	110.1	1.46

HIS **m170** n = 2695		
χ	Smooth COM	StdDev
chi1	-67	8.2
chi2	170	21.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.7	0.93
Cα_C_O	120.4	0.88
Cβ_Cα_C	109.7	1.79
Cβ_Cγ_Cδ2	131.1	0.99
Cβ_Cγ_Nδ1	122.6	1.04
Cϵ1_Nϵ2_Cδ2	108.8	0.53
Cγ_Cδ2_Nϵ2	107.2	0.47
Cγ_Nδ1_Cϵ1	109.2	0.69
Nδ1_Cϵ1_Nϵ2	108.6	0.62
Nδ1_Cγ_Cδ2	106.2	0.53
N_Cα_C	111.5	2.54
N_Cα_Cβ	110.7	1.15

HIS **m90** n = 3914		
χ	Smooth COM	StdDev
chi1	-65	9.8
chi2	88	17.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.5	1.11
Cα_C_O	120.5	0.90
Cβ_Cα_C	109.8	1.96
Cβ_Cγ_Cδ2	130.9	0.85
Cβ_Cγ_Nδ1	122.8	0.82
Cϵ1_Nϵ2_Cδ2	108.9	0.56
Cγ_Cδ2_Nϵ2	107.2	0.50
Cγ_Nδ1_Cϵ1	109.2	0.64
Nδ1_Cϵ1_Nϵ2	108.5	0.61
Nδ1_Cγ_Cδ2	106.2	0.51
N_Cα_C	111.5	2.73
N_Cα_Cβ	110.6	1.18

HIS **m-70** n = 9453		
χ	Smooth COM	StdDev
chi1	-64	10.0
chi2	-75	19.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.4	1.06
Cα_C_O	120.4	0.87
Cβ_Cα_C	109.9	1.89
Cβ_Cγ_Cδ2	131.1	0.82
Cβ_Cγ_Nδ1	122.6	0.80
Cϵ1_Nϵ2_Cδ2	108.9	0.52
Cγ_Cδ2_Nϵ2	107.2	0.47
Cγ_Nδ1_Cϵ1	109.2	0.63
Nδ1_Cϵ1_Nϵ2	108.5	0.56
Nδ1_Cγ_Cδ2	106.3	0.53
N_Cα_C	111.7	2.84
N_Cα_Cβ	110.4	1.17

Table S14: PHE Central Values

PHE **p90** n = 6289		
χ	Smooth COM	StdDev
chi1	63	9.6
chi2	-89	9.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.4	0.97
Cα_C_O	120.7	0.89
Cβ_Cα_C	110.9	1.46
Cβ_Cγ_Cδ1	120.7	0.62
Cβ_Cγ_Cδ2	120.6	0.58
Cδ1_Cϵ1_Cζ	119.9	0.60
Cδ1_Cγ_Cδ2	118.6	0.53
Cϵ1_Cζ_Cϵ2	119.8	0.63
Cγ_Cδ1_Cϵ1	120.9	0.59
Cγ_Cδ2_Cϵ2	120.9	0.58
Cζ_Cϵ2_Cδ2	119.9	0.59
N_Cα_C	110.9	2.57
N_Cα_Cβ	111.4	1.32

PHE **t80** n = 19289		
χ	Smooth COM	StdDev
chi1	-178	10.0
chi2	75	17.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.8	1.07
Cα_C_O	120.6	0.80
Cβ_Cα_C	110.3	1.30
Cβ_Cγ_Cδ1	120.6	0.72
Cβ_Cγ_Cδ2	120.5	0.68
Cδ1_Cϵ1_Cζ	119.9	0.59
Cδ1_Cγ_Cδ2	118.8	0.55
Cϵ1_Cζ_Cϵ2	119.9	0.63
Cγ_Cδ1_Cϵ1	120.8	0.58
Cγ_Cδ2_Cϵ2	120.8	0.59
Cζ_Cϵ2_Cδ2	119.9	0.59
N_Cα_C	110.3	2.31
N_Cα_Cβ	110.2	1.50

PHE **m-10** n = 3880		
χ	Smooth COM	StdDev
chi1	-68	9.3
chi2	-14	19.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	0.96
Cα_C_O	120.4	0.87
Cβ_Cα_C	108.9	1.78
Cβ_Cγ_Cδ1	121.5	1.22
Cβ_Cγ_Cδ2	119.9	1.16
Cδ1_Cϵ1_Cζ	119.9	0.61
Cδ1_Cγ_Cδ2	118.5	0.56
Cϵ1_Cζ_Cϵ2	119.8	0.62
Cγ_Cδ1_Cϵ1	120.8	0.60
Cγ_Cδ2_Cϵ2	121.0	0.61
Cζ_Cϵ2_Cδ2	119.9	0.61
N_Cα_C	111.0	2.42
N_Cα_Cβ	111.2	1.11

PHE **m-80** n = 26665		
χ	Smooth COM	StdDev
chi1	-66	10.1
chi2	-80	16.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.5	1.02
Cα_C_O	120.5	0.86
Cβ_Cα_C	109.8	1.99
Cβ_Cγ_Cδ1	120.6	0.60
Cβ_Cγ_Cδ2	120.6	0.59
Cδ1_Cϵ1_Cζ	119.9	0.58
Cδ1_Cγ_Cδ2	118.8	0.53
Cϵ1_Cζ_Cϵ2	119.9	0.61
Cγ_Cδ1_Cϵ1	120.8	0.56
Cγ_Cδ2_Cϵ2	120.8	0.57
Cζ_Cϵ2_Cδ2	119.9	0.58
N_Cα_C	111.2	2.81
N_Cα_Cβ	110.5	1.11

Table S15: TYR Central Values

TYR **p90** n = 5466		
χ	Smooth COM	StdDev
chi1	63	10.6
chi2	-89	10.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	1.88
Cα_C_O	120.7	0.93
Cβ_Cα_C	110.6	1.41
Cβ_Cγ_Cδ1	121.0	0.65
Cβ_Cγ_Cδ2	120.9	0.60
Cδ1_Cϵ1_Cζ	119.5	0.62
Cδ1_Cγ_Cδ2	118.1	0.55
Cϵ1_Cζ_Cϵ2	120.4	0.66
Cϵ1_Cζ_OH	119.8	1.25
Cγ_Cδ1_Cϵ1	121.2	0.58
Cγ_Cδ2_Cϵ2	121.2	0.55
Cζ_Cϵ2_Cδ2	119.6	0.62
N_Cα_C	111.1	2.66
N_Cα_Cβ	111.2	1.22
OH_Cζ_Cϵ2	119.7	1.24

TYR **t80** n = 16312		
χ	Smooth COM	StdDev
chi1	-178	10.5
chi2	75	16.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.7	2.14
Cα_C_O	120.6	0.80
Cβ_Cα_C	110.3	1.25
Cβ_Cγ_Cδ1	120.9	0.66
Cβ_Cγ_Cδ2	120.8	0.65
Cδ1_Cϵ1_Cζ	119.5	0.60
Cδ1_Cγ_Cδ2	118.2	0.52
Cϵ1_Cζ_Cϵ2	120.5	0.65
Cϵ1_Cζ_OH	119.7	1.28
Cγ_Cδ1_Cϵ1	121.1	0.55
Cγ_Cδ2_Cϵ2	121.1	0.56
Cζ_Cϵ2_Cδ2	119.5	0.63
N_Cα_C	110.4	2.25
N_Cα_Cβ	110.2	1.44
OH_Cζ_Cϵ2	119.7	1.28

TYR **m-10** n = 2623		
χ	Smooth COM	StdDev
chi1	-68	9.9
chi2	-14	20.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.8	1.57
Cα_C_O	120.4	0.84
Cβ_Cα_C	109.1	1.75
Cβ_Cγ_Cδ1	121.6	1.01
Cβ_Cγ_Cδ2	120.4	0.94
Cδ1_Cϵ1_Cζ	119.5	0.62
Cδ1_Cγ_Cδ2	118.0	0.57
Cϵ1_Cζ_Cϵ2	120.4	0.65
Cϵ1_Cζ_OH	120.1	1.32
Cγ_Cδ1_Cϵ1	121.1	0.60
Cγ_Cδ2_Cϵ2	121.3	0.57
Cζ_Cϵ2_Cδ2	119.7	0.64
N_Cα_C	111.4	2.35
N_Cα_Cβ	111.0	1.14
OH_Cζ_Cϵ2	119.5	1.34

TYR **m-80** n = 22683		
χ	Smooth COM	StdDev
chi1	-66	10.4
chi2	-80	16.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.2	2.04
Cα_C_O	120.4	0.88
Cβ_Cα_C	109.6	1.92
Cβ_Cγ_Cδ1	120.9	0.63
Cβ_Cγ_Cδ2	120.9	0.62
Cδ1_Cϵ1_Cζ	119.5	0.90
Cδ1_Cγ_Cδ2	118.2	0.58
Cϵ1_Cζ_Cϵ2	120.5	0.73
Cϵ1_Cζ_OH	119.7	1.24
Cγ_Cδ1_Cϵ1	121.1	0.86
Cγ_Cδ2_Cϵ2	121.1	0.86
Cζ_Cϵ2_Cδ2	119.5	0.90
N_Cα_C	111.4	2.76
N_Cα_Cβ	110.6	1.10
OH_Cζ_Cϵ2	119.8	1.25

Table S16: TRP Central Values

TRP **p90** n = 971		
χ	Smooth COM	StdDev
chi1	60	9.9
chi2	87	14.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.0	2.04
Cα_C_O	120.6	0.86
Cβ_Cα_C	110.7	1.41
Cβ_Cγ_Cδ1	127.0	0.70
Cβ_Cγ_Cδ2	126.7	0.76
Cδ1_Cγ_Cδ2	106.2	0.38
Cδ1_Nϵ1_Cϵ2	108.9	0.60
Cδ2_Cϵ2_Cζ2	122.5	0.37
Cδ2_Cϵ3_Cζ3	118.7	0.34
Cϵ2_Cδ2_Cϵ3	118.8	0.36
Cϵ2_Cδ2_Cγ	107.3	0.31
Cϵ3_Cζ3_Cη2	121.0	0.42
Cγ_Cδ1_Nϵ1	110.2	0.50
Cγ_Cδ2_Cϵ3	133.9	0.34
Cη2_Cζ2_Cϵ2	117.5	0.45
Cζ3_Cη2_Cζ2	121.5	0.46
Nϵ1_Cϵ2_Cδ2	107.4	0.37
Nϵ1_Cϵ2_Cζ2	130.1	0.40
N_Cα_C	111.2	2.41
N_Cα_Cβ	111.1	1.26

TRP **p-90** n = 1937		
χ	Smooth COM	StdDev
chi1	61	9.8
chi2	-89	12.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.0	1.90
Cα_C_O	120.5	0.93
Cβ_Cα_C	110.5	1.43
Cβ_Cγ_Cδ1	126.9	0.67
Cβ_Cγ_Cδ2	126.9	0.71
Cδ1_Cγ_Cδ2	106.2	0.44
Cδ1_Nϵ1_Cϵ2	109.0	0.46
Cδ2_Cϵ2_Cζ2	122.4	0.34
Cδ2_Cϵ3_Cζ3	118.7	0.47
Cϵ2_Cδ2_Cϵ3	118.8	0.39
Cϵ2_Cδ2_Cγ	107.2	0.33
Cϵ3_Cζ3_Cη2	121.0	0.46
Cγ_Cδ1_Nϵ1	110.2	0.46
Cγ_Cδ2_Cϵ3	133.9	0.41
Cη2_Cζ2_Cϵ2	117.5	0.44
Cζ3_Cη2_Cζ2	121.5	0.46
Nϵ1_Cϵ2_Cδ2	107.4	0.34
Nϵ1_Cϵ2_Cζ2	130.1	0.41
N_Cα_C	112.1	2.60
N_Cα_Cβ	111.1	1.24

TRP **t60** n = 3385		
χ	Smooth COM	StdDev
chi1	-178	9.8
chi2	64	32.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.3	2.14
Cα_C_O	120.7	0.81
Cβ_Cα_C	110.6	1.35
Cβ_Cγ_Cδ1	127.1	0.79
Cβ_Cγ_Cδ2	126.5	0.82
Cδ1_Cγ_Cδ2	106.3	0.48
Cδ1_Nϵ1_Cϵ2	108.9	0.51
Cδ2_Cϵ2_Cζ2	122.4	0.40
Cδ2_Cϵ3_Cζ3	118.7	0.42
Cϵ2_Cδ2_Cϵ3	118.9	0.38
Cϵ2_Cδ2_Cγ	107.3	0.38
Cϵ3_Cζ3_Cη2	121.0	0.48
Cγ_Cδ1_Nϵ1	110.1	0.53
Cγ_Cδ2_Cϵ3	133.9	0.43
Cη2_Cζ2_Cϵ2	117.5	0.46
Cζ3_Cη2_Cζ2	121.5	0.48
Nϵ1_Cϵ2_Cδ2	107.5	0.38
Nϵ1_Cϵ2_Cζ2	130.1	0.46
N_Cα_C	110.1	2.15
N_Cα_Cβ	110.0	1.42

TRP **t-100** n = 2893		
χ	Smooth COM	StdDev
chi1	-177	11.6
chi2	-102	15.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.6	2.32
Cα_C_O	120.6	0.87
Cβ_Cα_C	110.3	1.33
Cβ_Cγ_Cδ1	126.9	0.69
Cβ_Cγ_Cδ2	126.7	0.71
Cδ1_Cγ_Cδ2	106.3	0.42
Cδ1_Nϵ1_Cϵ2	108.9	0.45
Cδ2_Cϵ2_Cζ2	122.4	0.36
Cδ2_Cϵ3_Cζ3	118.7	0.45
Cϵ2_Cδ2_Cϵ3	118.8	0.35
Cϵ2_Cδ2_Cγ	107.2	0.32
Cϵ3_Cζ3_Cη2	121.0	0.48
Cγ_Cδ1_Nϵ1	110.1	0.48
Cγ_Cδ2_Cϵ3	133.9	0.37
Cη2_Cζ2_Cϵ2	117.5	0.45
Cζ3_Cη2_Cζ2	121.5	0.46
Nϵ1_Cϵ2_Cδ2	107.4	0.34
Nϵ1_Cϵ2_Cζ2	130.1	0.43
N_Cα_C	110.5	2.42
N_Cα_Cβ	110.3	1.42

TRP **m100** n = 6319		
χ	Smooth COM	StdDev
chi1	-67	10.8
chi2	97	17.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.2	2.22
Cα_C_O	120.4	0.86
Cβ_Cα_C	109.6	1.92
Cβ_Cγ_Cδ1	127.0	0.66
Cβ_Cγ_Cδ2	126.6	0.69
Cδ1_Cγ_Cδ2	106.3	0.43
Cδ1_Nϵ1_Cϵ2	108.9	0.49
Cδ2_Cϵ2_Cζ2	122.4	0.36
Cδ2_Cϵ3_Cζ3	118.7	0.46
Cϵ2_Cδ2_Cϵ3	118.9	0.37
Cϵ2_Cδ2_Cγ	107.2	0.33
Cϵ3_Cζ3_Cη2	121.0	0.48
Cγ_Cδ1_Nϵ1	110.1	0.49
Cγ_Cδ2_Cϵ3	133.9	0.40
Cη2_Cζ2_Cϵ2	117.5	0.45
Cζ3_Cη2_Cζ2	121.5	0.46
Nϵ1_Cϵ2_Cδ2	107.4	0.35
Nϵ1_Cϵ2_Cζ2	130.2	0.43
N_Cα_C	111.4	2.64
N_Cα_Cβ	110.6	1.11

TRP **m-10** n = 2196		
χ	Smooth COM	StdDev
chi1	-68	9.0
chi2	-7	21.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.7	1.64
Cα_C_O	120.5	0.88
Cβ_Cα_C	109.2	1.71
Cβ_Cγ_Cδ1	127.5	0.71
Cβ_Cγ_Cδ2	126.1	0.77
Cδ1_Cγ_Cδ2	106.3	0.45
Cδ1_Nϵ1_Cϵ2	108.8	0.45
Cδ2_Cϵ2_Cζ2	122.3	0.41
Cδ2_Cϵ3_Cζ3	118.7	0.43
Cϵ2_Cδ2_Cϵ3	118.9	0.38
Cϵ2_Cδ2_Cγ	107.3	0.38
Cϵ3_Cζ3_Cη2	121.0	0.43
Cγ_Cδ1_Nϵ1	110.0	0.48
Cγ_Cδ2_Cϵ3	133.8	0.39
Cη2_Cζ2_Cϵ2	117.5	0.47
Cζ3_Cη2_Cζ2	121.5	0.46
Nϵ1_Cϵ2_Cδ2	107.5	0.37
Nϵ1_Cϵ2_Cζ2	130.2	0.45
N_Cα_C	111.4	2.54
N_Cα_Cβ	110.8	1.15

TRP **m-90** n = 961		
χ	Smooth COM	StdDev
chi1	-67	12.4
chi2	-89	13.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.8	2.48
Cα_C_O	120.5	0.86
Cβ_Cα_C	109.4	2.04
Cβ_Cγ_Cδ1	126.7	0.72
Cβ_Cγ_Cδ2	127.0	0.78
Cδ1_Cγ_Cδ2	106.3	0.44
Cδ1_Nϵ1_Cϵ2	108.9	0.47
Cδ2_Cϵ2_Cζ2	122.4	0.35
Cδ2_Cϵ3_Cζ3	118.7	0.45
Cϵ2_Cδ2_Cϵ3	118.8	0.38
Cϵ2_Cδ2_Cγ	107.2	0.32
Cϵ3_Cζ3_Cη2	121.0	0.46
Cγ_Cδ1_Nϵ1	110.1	0.50
Cγ_Cδ2_Cϵ3	133.9	0.38
Cη2_Cζ2_Cϵ2	117.5	0.43
Cζ3_Cη2_Cζ2	121.5	0.45
Nϵ1_Cϵ2_Cδ2	107.5	0.35
Nϵ1_Cϵ2_Cζ2	130.1	0.43
N_Cα_C	110.6	2.88
N_Cα_Cβ	110.7	1.12

Table S17: MET Central Values

MET **ppp** n = 50		
χ	Smooth COM	StdDev
chi1	61	9.3
chi2	78	11.0
chi3	70	9.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.7	1.79
Cα_C_O	120.7	0.90
Cβ_Cα_C	111.2	1.57
Cβ_Cγ_SD	114.4	2.33
Cγ_SD_Cϵ	100.5	4.02
N_Cα_C	111.8	2.72
N_Cα_Cβ	110.9	1.02

MET **pp-130** n = 27		
χ	Smooth COM	StdDev
chi1	64	7.2
chi2	82	4.9
chi3	-154	27.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.4	1.18
Cα_C_O	120.9	0.65
Cβ_Cα_C	111.1	0.91
Cβ_Cγ_SD	113.7	2.01
Cγ_SD_Cϵ	100.8	1.95
N_Cα_C	111.0	1.84
N_Cα_Cβ	110.9	0.99

MET **ptp** n = 404		
χ	Smooth COM	StdDev
chi1	64	8.5
chi2	-176	11.4
chi3	73	11.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.80
Cα_C_O	120.7	0.92
Cβ_Cα_C	110.3	1.46
Cβ_Cγ_SD	112.9	2.19
Cγ_SD_Cϵ	100.8	1.94
N_Cα_C	110.6	2.56
N_Cα_Cβ	111.0	1.23

MET **ptt** n = 260		
χ	Smooth COM	StdDev
chi1	65	8.2
chi2	-178	9.1
chi3	179	15.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.7	1.69
Cα_C_O	120.6	0.94
Cβ_Cα_C	110.3	1.49
Cβ_Cγ_SD	111.0	2.39
Cγ_SD_Cϵ	99.8	2.32
N_Cα_C	111.1	2.70
N_Cα_Cβ	111.1	1.30

MET **ptm** n = 375		
χ	Smooth COM	StdDev
chi1	64	8.2
chi2	179	10.2
chi3	-72	11.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.65
Cα_C_O	120.6	0.93
Cβ_Cα_C	110.3	1.44
Cβ_Cγ_SD	112.8	2.11
Cγ_SD_Cϵ	100.9	1.82
N_Cα_C	110.9	2.77
N_Cα_Cβ	111.2	1.21

MET **pmt** n = 7		
χ	Smooth COM	StdDev
chi1	71	3.4
chi2	-74	3.2
chi3	-162	4.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	0.77
Cα_C_O	121.0	0.64
Cβ_Cα_C	111.1	1.13
Cβ_Cγ_SD	111.7	2.28
Cγ_SD_Cϵ	100.2	1.91
N_Cα_C	109.0	1.55
N_Cα_Cβ	111.6	1.28

MET **pmm** n = 42		
χ	Smooth COM	StdDev
chi1	72	7.8
chi2	-68	6.7
chi3	-68	8.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.5	0.86
Cα_C_O	120.6	0.79
Cβ_Cα_C	110.2	1.22
Cβ_Cγ_SD	115.2	2.54
Cγ_SD_Cϵ	101.1	1.58
N_Cα_C	112.3	2.69
N_Cα_Cβ	110.8	1.21

MET **tpp** n = 1138		
χ	Smooth COM	StdDev
chi1	-174	9.4
chi2	63	8.0
chi3	72	12.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.2	1.35
Cα_C_O	120.5	0.84
Cβ_Cα_C	110.3	1.13
Cβ_Cγ_SD	113.7	2.02
Cγ_SD_Cϵ	100.7	1.77
N_Cα_C	110.7	2.23
N_Cα_Cβ	110.5	1.17

MET **tpt** n = 388		
χ	Smooth COM	StdDev
chi1	-173	8.7
chi2	65	7.8
chi3	-156	31.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.1	1.39
Cα_C_O	120.5	0.74
Cβ_Cα_C	110.5	1.13
Cβ_Cγ_SD	112.4	1.99
Cγ_SD_Cϵ	100.4	2.09
N_Cα_C	110.4	2.25
N_Cα_Cβ	110.3	1.36

MET **ttp** n = 1246		
χ	Smooth COM	StdDev
chi1	-177	8.6
chi2	179	11.4
chi3	71	10.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.6	1.65
Cα_C_O	120.6	0.85
Cβ_Cα_C	110.0	1.17
Cβ_Cγ_SD	112.8	2.11
Cγ_SD_Cϵ	100.7	2.07
N_Cα_C	110.3	2.15
N_Cα_Cβ	110.4	1.31

MET **ttt** n = 569		
χ	Smooth COM	StdDev
chi1	-176	8.8
chi2	176	9.5
chi3	176	15.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.7	1.72
Cα_C_O	120.6	0.96
Cβ_Cα_C	110.1	1.31
Cβ_Cγ_SD	110.6	2.20
Cγ_SD_Cϵ	100.1	1.66
N_Cα_C	110.2	2.43
N_Cα_Cβ	110.1	1.39

MET **ttm** n = 1124		
χ	Smooth COM	StdDev
chi1	-175	9.3
chi2	179	8.2
chi3	-71	13.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.5	1.71
Cα_C_O	120.5	0.80
Cβ_Cα_C	110.0	1.17
Cβ_Cγ_SD	112.8	2.16
Cγ_SD_Cϵ	100.8	1.74
N_Cα_C	110.1	2.40
N_Cα_Cβ	110.4	1.33

MET **tmt** n = 34		
χ	Smooth COM	StdDev
chi1	-179	6.7
chi2	-85	7.6
chi3	173	24.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.9	1.13
Cα_C_O	120.7	0.56
Cβ_Cα_C	110.7	1.24
Cβ_Cγ_SD	112.8	1.77
Cγ_SD_Cϵ	100.3	1.37
N_Cα_C	110.0	2.89
N_Cα_Cβ	110.1	1.22

MET **tmm** n = 276		
χ	Smooth COM	StdDev
chi1	-177	7.3
chi2	-81	6.8
chi3	-72	10.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.0	1.37
Cα_C_O	120.5	0.78
Cβ_Cα_C	111.0	1.24
Cβ_Cγ_SD	114.0	2.12
Cγ_SD_Cϵ	100.8	1.64
N_Cα_C	109.9	2.10
N_Cα_Cβ	110.1	1.16

MET **mpp** n = 74		
χ	Smooth COM	StdDev
chi1	-76	13.7
chi2	73	12.3
chi3	73	11.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.36
Cα_C_O	120.5	0.89
Cβ_Cα_C	109.9	1.63
Cβ_Cγ_SD	114.3	2.25
Cγ_SD_Cϵ	101.2	2.26
N_Cα_C	110.7	2.69
N_Cα_Cβ	110.8	1.20

MET **mpt** n = 34		
χ	Smooth COM	StdDev
chi1	-69	11.7
chi2	74	11.0
chi3	167	18.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	0.96
Cα_C_O	120.4	0.88
Cβ_Cα_C	109.3	1.40
Cβ_Cγ_SD	113.2	2.02
Cγ_SD_Cϵ	100.1	2.40
N_Cα_C	110.1	2.78
N_Cα_Cβ	111.0	1.12

MET **mpm** n = 13		
χ	Smooth COM	StdDev
chi1	-77	5.1
chi2	63	5.5
chi3	-101	5.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.1	1.02
Cα_C_O	120.7	0.73
Cβ_Cα_C	109.1	1.27
Cβ_Cγ_SD	115.9	2.31
Cγ_SD_Cϵ	100.4	1.56
N_Cα_C	110.7	1.81
N_Cα_Cβ	111.0	1.05

MET **mtp** n = 2815		
χ	Smooth COM	StdDev
chi1	-66	7.1
chi2	177	9.3
chi3	70	10.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.1	1.64
Cα_C_O	120.5	0.84
Cβ_Cα_C	110.0	1.59
Cβ_Cγ_SD	112.8	2.08
Cγ_SD_Cϵ	100.8	1.73
N_Cα_C	111.3	2.35
N_Cα_Cβ	110.5	1.01

MET **mtt** n = 1542		
χ	Smooth COM	StdDev
chi1	-67	7.7
chi2	179	8.7
chi3	-176	16.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.6	1.71
Cα_C_O	120.5	0.82
Cβ_Cα_C	109.4	1.67
Cβ_Cγ_SD	110.4	2.19
Cγ_SD_Cϵ	100.1	1.97
N_Cα_C	111.1	2.27
N_Cα_Cβ	110.7	1.00

MET **mtm** n = 1851		
χ	Smooth COM	StdDev
chi1	-66	7.9
chi2	-177	10.7
chi3	-73	10.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.2	1.72
Cα_C_O	120.5	0.90
Cβ_Cα_C	109.9	1.63
Cβ_Cγ_SD	112.9	2.15
Cγ_SD_Cϵ	100.8	1.78
N_Cα_C	111.1	2.32
N_Cα_Cβ	110.7	1.07

MET **mmp** n = 520		
χ	Smooth COM	StdDev
chi1	-65	5.3
chi2	-61	6.3
chi3	102	9.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.2	1.41
Cα_C_O	120.3	0.80
Cβ_Cα_C	110.2	1.55
Cβ_Cγ_SD	113.8	2.14
Cγ_SD_Cϵ	101.2	2.18
N_Cα_C	111.5	2.15
N_Cα_Cβ	110.8	1.10

MET **mmt** n = 597		
χ	Smooth COM	StdDev
chi1	-64	8.7
chi2	-63	9.4
chi3	172	18.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.9	1.44
Cα_C_O	120.4	0.80
Cβ_Cα_C	109.9	1.55
Cβ_Cγ_SD	112.1	2.04
Cγ_SD_Cϵ	100.3	1.99
N_Cα_C	111.5	2.25
N_Cα_Cβ	110.6	0.94

MET **mmm** n = 3354		
χ	Smooth COM	StdDev
chi1	-65	8.9
chi2	-60	8.8
chi3	-69	10.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.0	1.29
Cα_C_O	120.4	0.86
Cβ_Cα_C	110.0	1.53
Cβ_Cγ_SD	113.7	1.95
Cγ_SD_Cϵ	100.9	1.74
N_Cα_C	111.6	2.38
N_Cα_Cβ	110.7	1.02

Table S18: GLU Central Values

GLU **pp20** n = 159		
χ	Smooth COM	StdDev
chi1	61	8.1
chi2	85	8.0
chi3	19	17.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.6	1.28
Cα_C_O	120.4	0.85
Cβ_Cα_C	111.6	1.84
Cβ_Cγ_Cδ	114.1	1.30
Cγ_Cδ_Oϵ1	119.0	1.43
Cγ_Cδ_Oϵ2	118.4	1.34
N_Cα_C	110.8	2.54
N_Cα_Cβ	111.4	1.25
Oϵ1_Cδ_Oϵ2	122.6	1.02

GLU **pt0** n = 2800		
χ	Smooth COM	StdDev
chi1	65	8.4
chi2	-177	10.1
chi3	1	51.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.60
Cα_C_O	120.5	0.93
Cβ_Cα_C	110.5	1.50
Cβ_Cγ_Cδ	112.9	1.53
Cγ_Cδ_Oϵ1	118.9	1.38
Cγ_Cδ_Oϵ2	118.2	1.35
N_Cα_C	111.3	2.67
N_Cα_Cβ	111.1	1.18
Oϵ1_Cδ_Oϵ2	122.9	1.15

GLU **pm20** n = 1485		
χ	Smooth COM	StdDev
chi1	69	8.8
chi2	-84	8.6
chi3	15	21.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.6	1.35
Cα_C_O	120.2	0.83
Cβ_Cα_C	110.5	1.25
Cβ_Cγ_Cδ	114.5	1.45
Cγ_Cδ_Oϵ1	119.8	1.71
Cγ_Cδ_Oϵ2	117.7	1.69
N_Cα_C	112.9	1.83
N_Cα_Cβ	110.9	1.05
Oϵ1_Cδ_Oϵ2	122.5	1.10

GLU **tp30** n = 4616		
χ	Smooth COM	StdDev
chi1	-178	9.8
chi2	64	9.2
chi3	25	26.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.39
Cα_C_O	120.5	0.80
Cβ_Cα_C	110.6	1.21
Cβ_Cγ_Cδ	113.8	1.35
Cγ_Cδ_Oϵ1	119.3	1.46
Cγ_Cδ_Oϵ2	118.0	1.38
N_Cα_C	110.9	2.09
N_Cα_Cβ	110.3	1.12
Oϵ1_Cδ_Oϵ2	122.7	1.07

GLU **tt0** n = 13610		
χ	Smooth COM	StdDev
chi1	-176	8.6
chi2	177	10.3
chi3	1	41.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.5	1.74
Cα_C_O	120.6	0.77
Cβ_Cα_C	110.1	1.17
Cβ_Cγ_Cδ	113.1	1.50
Cγ_Cδ_Oϵ1	119.0	1.27
Cγ_Cδ_Oϵ2	118.0	1.27
N_Cα_C	110.6	2.26
N_Cα_Cβ	110.4	1.37
Oϵ1_Cδ_Oϵ2	123.1	1.07

GLU **tm-30** n = 862		
χ	Smooth COM	StdDev
chi1	-170	8.6
chi2	-83	9.2
chi3	-28	17.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.5	1.35
Cα_C_O	120.5	0.84
Cβ_Cα_C	111.0	1.33
Cβ_Cγ_Cδ	113.8	1.47
Cγ_Cδ_Oϵ1	119.0	1.36
Cγ_Cδ_Oϵ2	118.2	1.25
N_Cα_C	110.2	2.46
N_Cα_Cβ	110.2	1.16
Oϵ1_Cδ_Oϵ2	122.8	1.17

GLU **mp0** n = 3671		
χ	Smooth COM	StdDev
chi1	-66	7.3
chi2	82	9.4
chi3	3	27.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.4	1.34
Cα_C_O	120.4	0.82
Cβ_Cα_C	109.7	1.42
Cβ_Cγ_Cδ	114.2	1.40
Cγ_Cδ_Oϵ1	119.8	1.66
Cγ_Cδ_Oϵ2	117.8	1.47
N_Cα_C	112.0	2.00
N_Cα_Cβ	110.6	1.06
Oϵ1_Cδ_Oϵ2	122.4	1.18

GLU **mm-30** n = 9080		
χ	Smooth COM	StdDev
chi1	-66	8.7
chi2	-66	10.6
chi3	-31	26.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.0	1.41
Cα_C_O	120.4	0.83
Cβ_Cα_C	109.9	1.50
Cβ_Cγ_Cδ	113.4	1.34
Cγ_Cδ_Oϵ1	119.2	1.35
Cγ_Cδ_Oϵ2	118.2	1.26
N_Cα_C	111.5	2.36
N_Cα_Cβ	110.7	1.01
Oϵ1_Cδ_Oϵ2	122.6	1.09

GLU **mt-10** n = 21021		
χ	Smooth COM	StdDev
chi1	-66	7.7
chi2	179	11.4
chi3	-6	37.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.0	1.85
Cα_C_O	120.5	0.82
Cβ_Cα_C	110.0	1.73
Cβ_Cγ_Cδ	113.3	1.50
Cγ_Cδ_Oϵ1	119.1	1.29
Cγ_Cδ_Oϵ2	117.9	1.29
N_Cα_C	111.4	2.32
N_Cα_Cβ	110.6	1.00
Oϵ1_Cδ_Oϵ2	123.0	1.06

Table S19: GLN Central Values

GLN **pp30** n = 178		
χ	Smooth COM	StdDev
chi1	62	7.8
chi2	83	8.5
chi3	29	20.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.9	1.28
Cα_C_O	120.3	0.95
Cβ_Cα_C	111.4	1.62
Cβ_Cγ_Cδ	113.6	1.40
Cγ_Cδ_Nϵ2	116.4	0.89
Cγ_Cδ_Oϵ1	120.9	0.95
N_Cα_C	111.0	2.55
N_Cα_Cβ	111.5	1.15
Oϵ1_Cδ_Nϵ2	122.6	0.67

GLN **pt0** n = 1885		
χ	Smooth COM	StdDev
chi1	64	8.1
chi2	-177	11.3
chi3	-2	75.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.5	1.53
Cα_C_O	120.5	0.96
Cβ_Cα_C	110.4	1.52
Cβ_Cγ_Cδ	112.5	1.47
Cγ_Cδ_Nϵ2	116.5	0.95
Cγ_Cδ_Oϵ1	120.8	0.97
N_Cα_C	111.3	2.63
N_Cα_Cβ	110.9	1.18
Oϵ1_Cδ_Nϵ2	122.6	0.75

GLN **pm20** n = 487		
χ	Smooth COM	StdDev
chi1	69	9.9
chi2	-84	9.3
chi3	16	32.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.7	1.41
Cα_C_O	120.3	0.93
Cβ_Cα_C	110.4	1.35
Cβ_Cγ_Cδ	113.9	1.43
Cγ_Cδ_Nϵ2	116.3	0.86
Cγ_Cδ_Oϵ1	121.3	0.99
N_Cα_C	112.4	2.22
N_Cα_Cβ	111.2	1.13
Oϵ1_Cδ_Nϵ2	122.5	0.72

GLN **tp40** n = 3618		
χ	Smooth COM	StdDev
chi1	-176	8.7
chi2	66	8.2
chi3	41	24.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.9	1.42
Cα_C_O	120.4	0.79
Cβ_Cα_C	110.2	1.15
Cβ_Cγ_Cδ	112.9	1.24
Cγ_Cδ_Nϵ2	116.6	0.84
Cγ_Cδ_Oϵ1	120.8	0.87
N_Cα_C	111.0	2.01
N_Cα_Cβ	110.6	1.13
Oϵ1_Cδ_Nϵ2	122.6	0.65

GLN **tp-100** n = 534		
χ	Smooth COM	StdDev
chi1	-176	8.7
chi2	62	8.8
chi3	-104	27.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.4	1.57
Cα_C_O	120.6	0.83
Cβ_Cα_C	110.5	1.24
Cβ_Cγ_Cδ	113.0	1.31
Cγ_Cδ_Nϵ2	116.6	0.95
Cγ_Cδ_Oϵ1	120.9	0.85
N_Cα_C	110.4	2.26
N_Cα_Cβ	110.4	1.24
Oϵ1_Cδ_Nϵ2	122.6	0.64

GLN **tt0** n = 6936		
χ	Smooth COM	StdDev
chi1	-176	8.5
chi2	177	10.8
chi3	2	60.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.6	1.80
Cα_C_O	120.6	0.76
Cβ_Cα_C	110.1	1.18
Cβ_Cγ_Cδ	112.6	1.50
Cγ_Cδ_Nϵ2	116.5	0.84
Cγ_Cδ_Oϵ1	120.8	0.88
N_Cα_C	110.4	2.27
N_Cα_Cβ	110.3	1.36
Oϵ1_Cδ_Nϵ2	122.7	0.71

GLN **tm130** n = 55		
χ	Smooth COM	StdDev
chi1	-171	9.7
chi2	-75	10.4
chi3	127	16.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.9	1.44
Cα_C_O	120.5	0.94
Cβ_Cα_C	111.3	1.63
Cβ_Cγ_Cδ	114.4	2.70
Cγ_Cδ_Nϵ2	117.1	1.28
Cγ_Cδ_Oϵ1	120.5	1.17
N_Cα_C	108.8	3.40
N_Cα_Cβ	110.1	1.37
Oϵ1_Cδ_Nϵ2	122.4	0.74

GLN **tm-30** n = 547		
χ	Smooth COM	StdDev
chi1	-171	10.1
chi2	-85	11.0
chi3	-29	20.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.35
Cα_C_O	120.5	0.83
Cβ_Cα_C	110.9	1.31
Cβ_Cγ_Cδ	113.5	1.40
Cγ_Cδ_Nϵ2	116.5	0.71
Cγ_Cδ_Oϵ1	120.9	0.81
N_Cα_C	110.2	2.51
N_Cα_Cβ	110.3	1.24
Oϵ1_Cδ_Nϵ2	122.6	0.68

GLN **mp10** n = 1207		
χ	Smooth COM	StdDev
chi1	-66	9.0
chi2	81	11.4
chi3	17	37.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.2	1.36
Cα_C_O	120.4	0.84
Cβ_Cα_C	109.8	1.52
Cβ_Cγ_Cδ	113.4	1.29
Cγ_Cδ_Nϵ2	116.3	0.82
Cγ_Cδ_Oϵ1	121.1	0.95
N_Cα_C	111.6	2.35
N_Cα_Cβ	110.8	1.10
Oϵ1_Cδ_Nϵ2	122.5	0.60

GLN **mp-120** n = 87		
χ	Smooth COM	StdDev
chi1	-72	10.0
chi2	69	11.4
chi3	-119	13.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.4	1.55
Cα_C_O	120.5	0.88
Cβ_Cα_C	109.7	1.79
Cβ_Cγ_Cδ	113.6	1.57
Cγ_Cδ_Nϵ2	116.6	0.65
Cγ_Cδ_Oϵ1	120.6	1.09
N_Cα_C	111.6	2.76
N_Cα_Cβ	110.7	1.01
Oϵ1_Cδ_Nϵ2	122.7	0.84

GLN **mt0** n = 14370		
χ	Smooth COM	StdDev
chi1	-66	7.5
chi2	179	11.2
chi3	-3	62.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.2	1.82
Cα_C_O	120.5	0.85
Cβ_Cα_C	109.9	1.71
Cβ_Cγ_Cδ	112.6	1.53
Cγ_Cδ_Nϵ2	116.4	0.85
Cγ_Cδ_Oϵ1	120.8	0.90
N_Cα_C	111.4	2.26
N_Cα_Cβ	110.6	1.04
Oϵ1_Cδ_Nϵ2	122.7	0.70

GLN **mm110** n = 1147		
χ	Smooth COM	StdDev
chi1	-65	8.6
chi2	-62	10.9
chi3	109	24.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.0	1.56
Cα_C_O	120.4	0.85
Cβ_Cα_C	110.0	1.53
Cβ_Cγ_Cδ	112.9	1.43
Cγ_Cδ_Nϵ2	116.6	0.92
Cγ_Cδ_Oϵ1	120.8	0.94
N_Cα_C	111.6	2.28
N_Cα_Cβ	110.7	1.07
Oϵ1_Cδ_Nϵ2	122.6	0.68

GLN **mm-40** n = 5959		
χ	Smooth COM	StdDev
chi1	-63	8.6
chi2	-66	10.4
chi3	-38	24.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.9	1.42
Cα_C_O	120.5	0.87
Cβ_Cα_C	109.9	1.49
Cβ_Cγ_Cδ	112.8	1.28
Cγ_Cδ_Nϵ2	116.5	0.91
Cγ_Cδ_Oϵ1	120.9	0.91
N_Cα_C	111.4	2.45
N_Cα_Cβ	110.6	1.04
Oϵ1_Cδ_Nϵ2	122.6	0.78

Table S20: ARG Central Values

ARG **ppp80** n = 10		
χ	Smooth COM	StdDev
chi1	62	5.1
chi2	86	7.0
chi3	57	3.8
chi4	79	8.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.1	0.88
Cα_C_O	120.8	0.55
Cβ_Cα_C	111.0	1.51
Cβ_Cγ_Cδ	113.9	0.82
Cδ_Nϵ_Cζ	125.0	0.34
Cγ_Cδ_Nϵ	112.5	1.08
Nϵ_Cζ_Nη1	120.6	0.68
Nϵ_Cζ_Nη2	119.8	0.63
Nη1_Cζ_Nη2	119.6	0.32
N_Cα_C	111.1	2.18
N_Cα_Cβ	111.9	1.19

ARG **ppp-140** n = 4		
χ	Smooth COM	StdDev
chi1	58	3.0
chi2	91	4.6
chi3	62	10.6
chi4	-143	12.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.2	0.90
Cα_C_O	120.7	0.54
Cβ_Cα_C	112.0	1.46
Cβ_Cγ_Cδ	112.2	1.50
Cδ_Nϵ_Cζ	125.9	1.18
Cγ_Cδ_Nϵ	113.8	2.26
Nϵ_Cζ_Nη1	121.0	1.24
Nϵ_Cζ_Nη2	120.1	1.38
Nη1_Cζ_Nη2	118.9	0.61
N_Cα_C	113.6	2.34
N_Cα_Cβ	111.2	1.26

ARG **ppt170** n = 57		
χ	Smooth COM	StdDev
chi1	59	9.9
chi2	87	12.3
chi3	173	12.3
chi4	173	17.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.2	1.39
Cα_C_O	120.4	1.04
Cβ_Cα_C	111.9	1.37
Cβ_Cγ_Cδ	112.4	1.63
Cδ_Nϵ_Cζ	124.2	1.28
Cγ_Cδ_Nϵ	111.4	1.60
Nϵ_Cζ_Nη1	120.5	1.08
Nϵ_Cζ_Nη2	119.8	0.87
Nη1_Cζ_Nη2	119.7	0.70
N_Cα_C	110.8	2.50
N_Cα_Cβ	111.6	1.32

ARG **ppt90** n = 19		
χ	Smooth COM	StdDev
chi1	63	5.9
chi2	99	8.0
chi3	-179	9.8
chi4	87	13.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.4	1.89
Cα_C_O	120.8	0.83
Cβ_Cα_C	110.8	1.70
Cβ_Cγ_Cδ	111.9	2.41
Cδ_Nϵ_Cζ	125.4	1.13
Cγ_Cδ_Nϵ	113.1	2.89
Nϵ_Cζ_Nη1	120.9	1.09
Nϵ_Cζ_Nη2	119.9	1.09
Nη1_Cζ_Nη2	119.2	0.79
N_Cα_C	111.0	2.14
N_Cα_Cβ	110.8	1.30

ARG **ppt-90** n = 15		
χ	Smooth COM	StdDev
chi1	61	9.1
chi2	90	11.1
chi3	177	5.5
chi4	-92	14.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.8	1.38
Cα_C_O	120.6	0.93
Cβ_Cα_C	111.2	1.75
Cβ_Cγ_Cδ	113.0	1.28
Cδ_Nϵ_Cζ	125.0	0.74
Cγ_Cδ_Nϵ	111.7	1.96
Nϵ_Cζ_Nη1	120.6	1.31
Nϵ_Cζ_Nη2	119.9	1.17
Nη1_Cζ_Nη2	119.5	0.60
N_Cα_C	111.6	3.12
N_Cα_Cβ	111.6	1.24

ARG **ptp90** n = 223		
χ	Smooth COM	StdDev
chi1	65	9.4
chi2	178	11.3
chi3	64	8.6
chi4	87	11.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.0	1.71
Cα_C_O	120.5	0.96
Cβ_Cα_C	110.5	1.39
Cβ_Cγ_Cδ	111.8	1.56
Cδ_Nϵ_Cζ	124.9	1.15
Cγ_Cδ_Nϵ	112.2	2.18
Nϵ_Cζ_Nη1	120.8	1.06
Nϵ_Cζ_Nη2	119.7	0.97
Nη1_Cζ_Nη2	119.5	0.80
N_Cα_C	110.9	2.82
N_Cα_Cβ	111.1	1.19

ARG **ptp-110** n = 77		
χ	Smooth COM	StdDev
chi1	67	8.2
chi2	-179	11.9
chi3	64	10.0
chi4	-108	9.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	1.93
Cα_C_O	120.7	1.22
Cβ_Cα_C	110.4	1.42
Cβ_Cγ_Cδ	111.9	1.47
Cδ_Nϵ_Cζ	125.6	1.44
Cγ_Cδ_Nϵ	111.7	2.29
Nϵ_Cζ_Nη1	121.0	1.42
Nϵ_Cζ_Nη2	119.6	1.57
Nη1_Cζ_Nη2	119.4	1.13
N_Cα_C	111.0	2.37
N_Cα_Cβ	111.0	1.30

ARG **ptp-170** n = 388		
χ	Smooth COM	StdDev
chi1	67	7.7
chi2	-175	12.2
chi3	68	9.7
chi4	-172	16.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.5	1.46
Cα_C_O	120.6	0.96
Cβ_Cα_C	110.4	1.57
Cβ_Cγ_Cδ	111.3	1.74
Cδ_Nϵ_Cζ	124.6	1.14
Cγ_Cδ_Nϵ	111.4	1.63
Nϵ_Cζ_Nη1	120.5	0.94
Nϵ_Cζ_Nη2	119.8	0.93
Nη1_Cζ_Nη2	119.8	0.92
N_Cα_C	111.3	2.56
N_Cα_Cβ	110.8	1.15

ARG **ptt180** n = 820		
χ	Smooth COM	StdDev
chi1	65	8.3
chi2	-177	10.4
chi3	-179	10.4
chi4	179	17.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.53
Cα_C_O	120.6	1.01
Cβ_Cα_C	110.5	1.50
Cβ_Cγ_Cδ	111.1	2.01
Cδ_Nϵ_Cζ	124.4	1.10
Cγ_Cδ_Nϵ	110.7	1.99
Nϵ_Cζ_Nη1	120.5	0.94
Nϵ_Cζ_Nη2	119.6	0.89
Nη1_Cζ_Nη2	119.9	0.88
N_Cα_C	111.3	2.49
N_Cα_Cβ	111.0	1.12

ARG **ptt90** n = 814		
χ	Smooth COM	StdDev
chi1	64	7.6
chi2	178	12.3
chi3	176	8.7
chi4	87	9.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	1.43
Cα_C_O	120.6	0.86
Cβ_Cα_C	110.2	1.41
Cβ_Cγ_Cδ	111.0	1.95
Cδ_Nϵ_Cζ	124.9	0.92
Cγ_Cδ_Nϵ	111.9	2.47
Nϵ_Cζ_Nη1	120.8	0.99
Nϵ_Cζ_Nη2	119.7	0.91
Nη1_Cζ_Nη2	119.5	0.70
N_Cα_C	110.8	2.51
N_Cα_Cβ	111.0	1.15

ARG **ptt-90** n = 726		
χ	Smooth COM	StdDev
chi1	66	7.9
chi2	-175	12.0
chi3	-176	8.9
chi4	-87	11.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	1.51
Cα_C_O	120.5	0.94
Cβ_Cα_C	110.5	1.55
Cβ_Cγ_Cδ	111.0	2.04
Cδ_Nϵ_Cζ	124.9	1.14
Cγ_Cδ_Nϵ	111.7	2.66
Nϵ_Cζ_Nη1	120.8	1.01
Nϵ_Cζ_Nη2	119.7	1.14
Nη1_Cζ_Nη2	119.5	1.03
N_Cα_C	111.7	2.55
N_Cα_Cβ	111.0	1.16

ARG **ptm160** n = 502		
χ	Smooth COM	StdDev
chi1	63	8.7
chi2	-179	15.0
chi3	-67	9.7
chi4	165	25.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.63
Cα_C_O	120.5	0.98
Cβ_Cα_C	110.4	1.56
Cβ_Cγ_Cδ	111.7	1.80
Cδ_Nϵ_Cζ	124.7	1.39
Cγ_Cδ_Nϵ	111.5	2.11
Nϵ_Cζ_Nη1	120.6	1.28
Nϵ_Cζ_Nη2	119.7	1.12
Nη1_Cζ_Nη2	119.7	1.00
N_Cα_C	110.9	2.57
N_Cα_Cβ	111.0	1.27

ARG **ptm-80** n = 215		
χ	Smooth COM	StdDev
chi1	65	8.3
chi2	-178	14.4
chi3	-66	10.3
chi4	-84	10.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.28
Cα_C_O	120.4	0.84
Cβ_Cα_C	110.3	1.38
Cβ_Cγ_Cδ	111.9	1.74
Cδ_Nϵ_Cζ	125.0	1.43
Cγ_Cδ_Nϵ	112.4	2.28
Nϵ_Cζ_Nη1	120.7	1.21
Nϵ_Cζ_Nη2	119.9	1.46
Nη1_Cζ_Nη2	119.4	0.87
N_Cα_C	111.6	2.54
N_Cα_Cβ	111.0	1.31

ARG **pmt100** n = 4		
χ	Smooth COM	StdDev
chi1	70	7.2
chi2	-90	9.1
chi3	-174	5.4
chi4	97	2.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.8	0.42
Cα_C_O	120.6	0.28
Cβ_Cα_C	110.8	0.49
Cβ_Cγ_Cδ	112.7	0.57
Cδ_Nϵ_Cζ	125.1	0.12
Cγ_Cδ_Nϵ	111.2	0.92
Nϵ_Cζ_Nη1	121.0	0.29
Nϵ_Cζ_Nη2	119.6	0.27
Nη1_Cζ_Nη2	119.4	0.05
N_Cα_C	110.2	1.44
N_Cα_Cβ	111.4	0.42

ARG **pmt170** n = 39		
χ	Smooth COM	StdDev
chi1	73	11.2
chi2	-78	15.4
chi3	-169	10.1
chi4	-169	15.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.3	1.19
Cα_C_O	120.8	0.70
Cβ_Cα_C	110.8	1.12
Cβ_Cγ_Cδ	112.7	1.26
Cδ_Nϵ_Cζ	124.4	1.05
Cγ_Cδ_Nϵ	111.6	1.87
Nϵ_Cζ_Nη1	120.4	0.78
Nϵ_Cζ_Nη2	120.0	0.64
Nη1_Cζ_Nη2	119.6	0.56
N_Cα_C	110.7	2.40
N_Cα_Cβ	111.8	1.07

ARG **pmt-80** n = 27		
χ	Smooth COM	StdDev
chi1	81	9.3
chi2	-68	7.6
chi3	-176	11.0
chi4	-84	8.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.8	1.16
Cα_C_O	121.0	0.65
Cβ_Cα_C	110.3	1.02
Cβ_Cγ_Cδ	113.3	1.79
Cδ_Nϵ_Cζ	124.9	0.99
Cγ_Cδ_Nϵ	112.1	1.75
Nϵ_Cζ_Nη1	121.0	0.89
Nϵ_Cζ_Nη2	119.6	0.60
Nη1_Cζ_Nη2	119.4	0.60
N_Cα_C	110.7	2.03
N_Cα_Cβ	111.4	1.16

ARG **pmm150** n = 12		
χ	Smooth COM	StdDev
chi1	75	3.2
chi2	-75	5.6
chi3	-64	6.3
chi4	151	15.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.2	1.50
Cα_C_O	120.3	0.93
Cβ_Cα_C	110.4	1.04
Cβ_Cγ_Cδ	112.4	1.15
Cδ_Nϵ_Cζ	125.3	2.47
Cγ_Cδ_Nϵ	111.6	2.06
Nϵ_Cζ_Nη1	121.1	1.74
Nϵ_Cζ_Nη2	119.7	1.03
Nη1_Cζ_Nη2	119.2	1.39
N_Cα_C	109.0	1.00
N_Cα_Cβ	112.1	0.96

ARG **pmm-80** n = 19		
χ	Smooth COM	StdDev
chi1	73	12.6
chi2	-75	11.2
chi3	-56	8.1
chi4	-81	7.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.9	1.02
Cα_C_O	120.8	0.55
Cβ_Cα_C	110.9	1.23
Cβ_Cγ_Cδ	113.5	1.56
Cδ_Nϵ_Cζ	125.1	1.08
Cγ_Cδ_Nϵ	112.5	1.30
Nϵ_Cζ_Nη1	120.4	0.95
Nϵ_Cζ_Nη2	120.3	0.95
Nη1_Cζ_Nη2	119.3	0.67
N_Cα_C	109.7	2.43
N_Cα_Cβ	111.6	1.00

ARG **tpp80** n = 363		
χ	Smooth COM	StdDev
chi1	-177	10.3
chi2	65	10.7
chi3	59	9.5
chi4	84	9.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.9	1.37
Cα_C_O	120.5	0.75
Cβ_Cα_C	110.5	1.23
Cβ_Cγ_Cδ	113.0	1.59
Cδ_Nϵ_Cζ	125.0	1.05
Cγ_Cδ_Nϵ	112.6	2.06
Nϵ_Cζ_Nη1	120.7	0.87
Nϵ_Cζ_Nη2	119.7	0.83
Nη1_Cζ_Nη2	119.5	0.72
N_Cα_C	110.8	2.03
N_Cα_Cβ	110.3	1.12

ARG **tpp-160** n = 496		
χ	Smooth COM	StdDev
chi1	178	9.6
chi2	65	10.7
chi3	65	9.8
chi4	-167	19.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	1.30
Cα_C_O	120.5	0.84
Cβ_Cα_C	110.4	1.29
Cβ_Cγ_Cδ	112.7	1.75
Cδ_Nϵ_Cζ	124.5	1.38
Cγ_Cδ_Nϵ	111.9	1.82
Nϵ_Cζ_Nη1	120.5	1.03
Nϵ_Cζ_Nη2	119.8	1.09
Nη1_Cζ_Nη2	119.7	0.84
N_Cα_C	110.6	2.30
N_Cα_Cβ	110.2	1.09

ARG **tpt170** n = 825		
χ	Smooth COM	StdDev
chi1	-178	9.0
chi2	66	10.4
chi3	177	11.7
chi4	171	19.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.5	1.23
Cα_C_O	120.5	0.74
Cβ_Cα_C	110.6	1.15
Cβ_Cγ_Cδ	112.2	1.71
Cδ_Nϵ_Cζ	124.5	1.14
Cγ_Cδ_Nϵ	110.9	1.87
Nϵ_Cζ_Nη1	120.5	0.94
Nϵ_Cζ_Nη2	119.7	0.88
Nη1_Cζ_Nη2	119.8	0.86
N_Cα_C	110.7	1.99
N_Cα_Cβ	110.2	1.19

ARG **tpt90** n = 652		
χ	Smooth COM	StdDev
chi1	178	8.4
chi2	65	7.7
chi3	178	9.9
chi4	86	10.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.7	1.27
Cα_C_O	120.5	0.80
Cβ_Cα_C	110.3	1.18
Cβ_Cγ_Cδ	112.1	1.67
Cδ_Nϵ_Cζ	124.8	0.92
Cγ_Cδ_Nϵ	111.9	2.27
Nϵ_Cζ_Nη1	120.8	0.97
Nϵ_Cζ_Nη2	119.7	0.89
Nη1_Cζ_Nη2	119.5	0.82
N_Cα_C	111.4	2.06
N_Cα_Cβ	110.2	1.09

ARG **tpt-90** n = 365		
χ	Smooth COM	StdDev
chi1	179	8.4
chi2	67	10.8
chi3	-179	8.8
chi4	-89	12.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.7	1.25
Cα_C_O	120.5	0.72
Cβ_Cα_C	110.6	1.20
Cβ_Cγ_Cδ	112.4	1.62
Cδ_Nϵ_Cζ	124.9	1.15
Cγ_Cδ_Nϵ	111.1	2.52
Nϵ_Cζ_Nη1	120.7	1.03
Nϵ_Cζ_Nη2	119.7	1.05
Nη1_Cζ_Nη2	119.6	0.73
N_Cα_C	110.9	2.15
N_Cα_Cβ	110.2	1.19

ARG **tpm170** n = 110		
χ	Smooth COM	StdDev
chi1	178	8.1
chi2	70	10.9
chi3	-85	12.8
chi4	171	18.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.6	1.26
Cα_C_O	120.6	0.80
Cβ_Cα_C	110.6	1.33
Cβ_Cγ_Cδ	112.8	2.17
Cδ_Nϵ_Cζ	124.7	2.25
Cγ_Cδ_Nϵ	112.0	2.15
Nϵ_Cζ_Nη1	120.5	1.05
Nϵ_Cζ_Nη2	119.8	0.90
Nη1_Cζ_Nη2	119.7	0.74
N_Cα_C	111.1	1.43
N_Cα_Cβ	109.9	1.12

ARG **tpm-80** n = 20		
χ	Smooth COM	StdDev
chi1	-177	5.2
chi2	78	8.2
chi3	-80	10.4
chi4	-79	9.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.2	1.38
Cα_C_O	120.7	1.05
Cβ_Cα_C	110.3	1.13
Cβ_Cγ_Cδ	113.0	1.22
Cδ_Nϵ_Cζ	125.2	1.19
Cγ_Cδ_Nϵ	113.7	2.21
Nϵ_Cζ_Nη1	120.6	0.96
Nϵ_Cζ_Nη2	120.1	0.92
Nη1_Cζ_Nη2	119.3	0.63
N_Cα_C	110.8	1.48
N_Cα_Cβ	109.8	1.13

ARG **ttp80** n = 1896		
χ	Smooth COM	StdDev
chi1	-177	8.2
chi2	179	13.4
chi3	62	9.9
chi4	82	9.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.7	1.50
Cα_C_O	120.7	0.80
Cβ_Cα_C	110.0	1.21
Cβ_Cγ_Cδ	112.1	1.53
Cδ_Nϵ_Cζ	124.9	1.04
Cγ_Cδ_Nϵ	112.6	1.94
Nϵ_Cζ_Nη1	120.7	0.95
Nϵ_Cζ_Nη2	119.8	0.86
Nη1_Cζ_Nη2	119.5	0.75
N_Cα_C	110.7	2.06
N_Cα_Cβ	110.4	1.20

ARG **ttp-110** n = 623		
χ	Smooth COM	StdDev
chi1	-174	8.5
chi2	177	13.0
chi3	64	10.7
chi4	-113	9.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.8	1.63
Cα_C_O	120.6	0.80
Cβ_Cα_C	110.2	1.23
Cβ_Cγ_Cδ	112.0	1.75
Cδ_Nϵ_Cζ	125.4	1.36
Cγ_Cδ_Nϵ	111.9	2.16
Nϵ_Cζ_Nη1	121.1	1.28
Nϵ_Cζ_Nη2	119.5	1.16
Nη1_Cζ_Nη2	119.4	0.89
N_Cα_C	110.7	2.18
N_Cα_Cβ	110.3	1.29

ARG **ttp-170** n = 1533		
χ	Smooth COM	StdDev
chi1	-175	9.3
chi2	179	13.2
chi3	66	9.0
chi4	-171	17.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.7	1.65
Cα_C_O	120.6	0.76
Cβ_Cα_C	110.0	1.24
Cβ_Cγ_Cδ	111.6	1.68
Cδ_Nϵ_Cζ	124.5	1.17
Cγ_Cδ_Nϵ	111.5	1.58
Nϵ_Cζ_Nη1	120.5	0.90
Nϵ_Cζ_Nη2	119.8	0.88
Nη1_Cζ_Nη2	119.8	0.70
N_Cα_C	110.5	2.21
N_Cα_Cβ	110.4	1.31

ARG **ttt180** n = 2339		
χ	Smooth COM	StdDev
chi1	-176	9.1
chi2	176	11.2
chi3	178	11.5
chi4	179	18.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.5	1.78
Cα_C_O	120.6	0.81
Cβ_Cα_C	110.2	1.17
Cβ_Cγ_Cδ	111.4	2.19
Cδ_Nϵ_Cζ	124.3	1.19
Cγ_Cδ_Nϵ	110.7	1.92
Nϵ_Cζ_Nη1	120.4	0.90
Nϵ_Cζ_Nη2	119.6	0.92
Nη1_Cζ_Nη2	120.0	0.81
N_Cα_C	110.5	2.41
N_Cα_Cβ	110.2	1.39

ARG **ttt90** n = 1057		
χ	Smooth COM	StdDev
chi1	-176	9.3
chi2	176	10.8
chi3	176	9.6
chi4	86	10.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.9	1.70
Cα_C_O	120.6	0.79
Cβ_Cα_C	110.2	1.25
Cβ_Cγ_Cδ	111.3	2.08
Cδ_Nϵ_Cζ	124.8	1.01
Cγ_Cδ_Nϵ	111.6	2.62
Nϵ_Cζ_Nη1	120.7	1.02
Nϵ_Cζ_Nη2	119.6	1.00
Nη1_Cζ_Nη2	119.6	0.74
N_Cα_C	110.5	2.40
N_Cα_Cβ	110.4	1.37

ARG **ttt-90** n = 1380		
χ	Smooth COM	StdDev
chi1	-176	9.4
chi2	177	11.5
chi3	-178	9.9
chi4	-89	12.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.0	1.62
Cα_C_O	120.5	0.79
Cβ_Cα_C	110.3	1.26
Cβ_Cγ_Cδ	110.9	2.08
Cδ_Nϵ_Cζ	124.8	1.17
Cγ_Cδ_Nϵ	111.8	2.58
Nϵ_Cζ_Nη1	120.8	1.08
Nϵ_Cζ_Nη2	119.6	1.01
Nη1_Cζ_Nη2	119.6	0.87
N_Cα_C	110.4	2.30
N_Cα_Cβ	110.2	1.31

ARG **ttm110** n = 725		
χ	Smooth COM	StdDev
chi1	-175	9.0
chi2	178	9.5
chi3	-64	10.7
chi4	112	9.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.9	1.64
Cα_C_O	120.6	0.78
Cβ_Cα_C	110.3	1.23
Cβ_Cγ_Cδ	112.2	1.69
Cδ_Nϵ_Cζ	125.3	1.23
Cγ_Cδ_Nϵ	111.6	1.93
Nϵ_Cζ_Nη1	121.0	1.24
Nϵ_Cζ_Nη2	119.5	1.12
Nη1_Cζ_Nη2	119.4	0.82
N_Cα_C	110.5	2.14
N_Cα_Cβ	110.4	1.24

ARG **ttm170** n = 1317		
χ	Smooth COM	StdDev
chi1	-177	9.9
chi2	176	12.4
chi3	-67	9.9
chi4	171	17.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.8	1.74
Cα_C_O	120.6	0.81
Cβ_Cα_C	110.1	1.16
Cβ_Cγ_Cδ	111.5	1.83
Cδ_Nϵ_Cζ	124.4	1.17
Cγ_Cδ_Nϵ	111.3	1.65
Nϵ_Cζ_Nη1	120.5	0.96
Nϵ_Cζ_Nη2	119.7	0.93
Nη1_Cζ_Nη2	119.7	0.83
N_Cα_C	110.3	2.38
N_Cα_Cβ	110.3	1.34

ARG **ttm-80** n = 1504		
χ	Smooth COM	StdDev
chi1	-174	9.4
chi2	179	9.9
chi3	-64	10.6
chi4	-84	9.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.7	1.66
Cα_C_O	120.5	0.79
Cβ_Cα_C	110.2	1.24
Cβ_Cγ_Cδ	112.0	1.64
Cδ_Nϵ_Cζ	124.9	1.30
Cγ_Cδ_Nϵ	112.4	2.03
Nϵ_Cζ_Nη1	120.7	1.02
Nϵ_Cζ_Nη2	119.7	1.04
Nη1_Cζ_Nη2	119.5	0.76
N_Cα_C	110.6	2.26
N_Cα_Cβ	110.4	1.36

ARG **tmt170** n = 104		
χ	Smooth COM	StdDev
chi1	-173	12.3
chi2	-91	12.7
chi3	-173	9.4
chi4	-170	17.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.0	1.33
Cα_C_O	120.6	0.74
Cβ_Cα_C	110.9	1.07
Cβ_Cγ_Cδ	112.7	1.72
Cδ_Nϵ_Cζ	124.5	0.90
Cγ_Cδ_Nϵ	110.7	1.62
Nϵ_Cζ_Nη1	120.7	1.03
Nϵ_Cζ_Nη2	119.6	0.80
Nη1_Cζ_Nη2	119.7	0.72
N_Cα_C	108.5	3.17
N_Cα_Cβ	110.0	1.25

ARG **tmt90** n = 23		
χ	Smooth COM	StdDev
chi1	-178	9.2
chi2	-93	9.1
chi3	-177	11.2
chi4	87	12.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.2	1.49
Cα_C_O	120.6	0.98
Cβ_Cα_C	110.5	1.33
Cβ_Cγ_Cδ	112.9	2.34
Cδ_Nϵ_Cζ	125.1	1.26
Cγ_Cδ_Nϵ	111.4	2.85
Nϵ_Cζ_Nη1	120.9	1.86
Nϵ_Cζ_Nη2	119.6	1.46
Nη1_Cζ_Nη2	119.4	0.74
N_Cα_C	110.3	1.54
N_Cα_Cβ	109.9	1.13

ARG **tmt-80** n = 62		
χ	Smooth COM	StdDev
chi1	-174	10.8
chi2	-92	11.4
chi3	-177	10.0
chi4	-84	11.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.7	1.34
Cα_C_O	120.5	0.77
Cβ_Cα_C	111.3	1.33
Cβ_Cγ_Cδ	112.5	1.92
Cδ_Nϵ_Cζ	124.7	1.12
Cγ_Cδ_Nϵ	111.2	2.14
Nϵ_Cζ_Nη1	120.6	0.91
Nϵ_Cζ_Nη2	119.7	0.90
Nη1_Cζ_Nη2	119.6	0.63
N_Cα_C	110.1	2.45
N_Cα_Cβ	110.1	1.03

ARG **tmm160** n = 92		
χ	Smooth COM	StdDev
chi1	-172	10.9
chi2	-90	11.1
chi3	-61	11.3
chi4	163	18.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	1.32
Cα_C_O	120.6	0.80
Cβ_Cα_C	111.3	1.11
Cβ_Cγ_Cδ	112.6	1.82
Cδ_Nϵ_Cζ	124.6	1.19
Cγ_Cδ_Nϵ	111.9	1.92
Nϵ_Cζ_Nη1	120.7	1.00
Nϵ_Cζ_Nη2	119.7	0.89
Nη1_Cζ_Nη2	119.6	0.81
N_Cα_C	110.0	2.05
N_Cα_Cβ	110.1	1.13

ARG **tmm-80** n = 71		
χ	Smooth COM	StdDev
chi1	-174	9.2
chi2	-86	8.8
chi3	-56	10.7
chi4	-82	8.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.3	1.32
Cα_C_O	120.6	0.78
Cβ_Cα_C	111.1	1.01
Cβ_Cγ_Cδ	113.7	2.29
Cδ_Nϵ_Cζ	124.9	1.25
Cγ_Cδ_Nϵ	112.6	1.89
Nϵ_Cζ_Nη1	120.9	1.10
Nϵ_Cζ_Nη2	119.7	0.92
Nη1_Cζ_Nη2	119.4	0.72
N_Cα_C	109.7	1.70
N_Cα_Cβ	110.1	1.01

ARG **mpp80** n = 54		
χ	Smooth COM	StdDev
chi1	-76	11.8
chi2	81	12.0
chi3	57	7.4
chi4	84	10.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.5	1.72
Cα_C_O	120.4	1.09
Cβ_Cα_C	109.2	1.98
Cβ_Cγ_Cδ	113.6	1.62
Cδ_Nϵ_Cζ	125.0	1.16
Cγ_Cδ_Nϵ	113.1	2.28
Nϵ_Cζ_Nη1	120.8	1.17
Nϵ_Cζ_Nη2	119.8	1.13
Nη1_Cζ_Nη2	119.4	0.73
N_Cα_C	109.7	2.54
N_Cα_Cβ	111.5	1.26

ARG **mpp-170** n = 64		
χ	Smooth COM	StdDev
chi1	-78	12.9
chi2	81	17.4
chi3	65	7.4
chi4	-166	16.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.43
Cα_C_O	120.5	0.68
Cβ_Cα_C	109.7	1.57
Cβ_Cγ_Cδ	112.7	1.74
Cδ_Nϵ_Cζ	124.5	1.19
Cγ_Cδ_Nϵ	111.5	1.34
Nϵ_Cζ_Nη1	120.6	1.06
Nϵ_Cζ_Nη2	119.7	0.76
Nη1_Cζ_Nη2	119.7	0.70
N_Cα_C	110.0	3.12
N_Cα_Cβ	111.4	1.11

ARG **mpt180** n = 245		
χ	Smooth COM	StdDev
chi1	-84	8.0
chi2	69	13.1
chi3	173	9.4
chi4	174	16.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	1.42
Cα_C_O	120.6	0.86
Cβ_Cα_C	109.5	1.66
Cβ_Cγ_Cδ	113.0	1.81
Cδ_Nϵ_Cζ	124.4	1.45
Cγ_Cδ_Nϵ	110.7	2.00
Nϵ_Cζ_Nη1	120.4	1.02
Nϵ_Cζ_Nη2	119.7	0.92
Nη1_Cζ_Nη2	119.8	0.88
N_Cα_C	110.0	2.75
N_Cα_Cβ	111.1	1.15

ARG **mpt90** n = 46		
χ	Smooth COM	StdDev
chi1	-76	12.9
chi2	84	13.6
chi3	170	9.7
chi4	93	11.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.63
Cα_C_O	120.4	0.64
Cβ_Cα_C	109.3	1.43
Cβ_Cγ_Cδ	112.5	1.55
Cδ_Nϵ_Cζ	125.1	0.85
Cγ_Cδ_Nϵ	111.0	2.03
Nϵ_Cζ_Nη1	121.1	0.91
Nϵ_Cζ_Nη2	119.4	0.68
Nη1_Cζ_Nη2	119.5	0.59
N_Cα_C	110.0	2.68
N_Cα_Cβ	111.3	1.24

ARG **mpt-90** n = 85		
χ	Smooth COM	StdDev
chi1	-78	13.9
chi2	74	16.3
chi3	177	9.6
chi4	-87	13.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.9	1.26
Cα_C_O	120.4	0.75
Cβ_Cα_C	110.0	1.55
Cβ_Cγ_Cδ	112.9	2.30
Cδ_Nϵ_Cζ	124.9	1.00
Cγ_Cδ_Nϵ	111.6	2.53
Nϵ_Cζ_Nη1	120.6	1.07
Nϵ_Cζ_Nη2	119.8	0.83
Nη1_Cζ_Nη2	119.6	0.67
N_Cα_C	110.4	2.71
N_Cα_Cβ	110.9	1.02

ARG **mtp180** n = 2504		
χ	Smooth COM	StdDev
chi1	-66	8.1
chi2	178	13.0
chi3	66	9.1
chi4	-171	16.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.2	1.79
Cα_C_O	120.5	0.83
Cβ_Cα_C	110.0	1.65
Cβ_Cγ_Cδ	111.7	1.81
Cδ_Nϵ_Cζ	124.4	1.21
Cγ_Cδ_Nϵ	111.6	1.56
Nϵ_Cζ_Nη1	120.4	1.00
Nϵ_Cζ_Nη2	119.8	0.97
Nη1_Cζ_Nη2	119.8	0.77
N_Cα_C	111.4	2.42
N_Cα_Cβ	110.5	1.05

ARG **mtp85** n = 1857		
χ	Smooth COM	StdDev
chi1	-66	8.6
chi2	177	11.2
chi3	64	9.7
chi4	87	11.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.3	1.82
Cα_C_O	120.5	0.91
Cβ_Cα_C	110.1	1.68
Cβ_Cγ_Cδ	112.1	1.71
Cδ_Nϵ_Cζ	124.9	1.20
Cγ_Cδ_Nϵ	112.3	1.99
Nϵ_Cζ_Nη1	120.8	1.05
Nϵ_Cζ_Nη2	119.7	1.04
Nη1_Cζ_Nη2	119.5	0.81
N_Cα_C	111.1	2.41
N_Cα_Cβ	110.6	1.05

ARG **mtp-110** n = 470		
χ	Smooth COM	StdDev
chi1	-65	8.1
chi2	179	10.8
chi3	66	11.6
chi4	-109	9.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.4	1.66
Cα_C_O	120.4	0.95
Cβ_Cα_C	110.1	1.68
Cβ_Cγ_Cδ	112.4	1.63
Cδ_Nϵ_Cζ	125.3	2.05
Cγ_Cδ_Nϵ	111.7	1.88
Nϵ_Cζ_Nη1	121.1	1.20
Nϵ_Cζ_Nη2	119.4	1.29
Nη1_Cζ_Nη2	119.5	0.90
N_Cα_C	111.1	2.59
N_Cα_Cβ	110.7	1.05

ARG **mtt180** n = 4592		
χ	Smooth COM	StdDev
chi1	-67	7.8
chi2	179	11.0
chi3	-179	10.7
chi4	177	17.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	112.9	1.75
Cα_C_O	120.4	0.85
Cβ_Cα_C	110.0	1.66
Cβ_Cγ_Cδ	111.5	2.02
Cδ_Nϵ_Cζ	124.4	1.10
Cγ_Cδ_Nϵ	110.6	1.82
Nϵ_Cζ_Nη1	120.4	0.89
Nϵ_Cζ_Nη2	119.6	0.90
Nη1_Cζ_Nη2	119.9	0.79
N_Cα_C	111.6	2.33
N_Cα_Cβ	110.6	1.05

ARG **mtt90** n = 2460		
χ	Smooth COM	StdDev
chi1	-67	7.5
chi2	179	13.5
chi3	178	10.6
chi4	90	15.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.3	1.72
Cα_C_O	120.4	0.80
Cβ_Cα_C	109.9	1.73
Cβ_Cγ_Cδ	111.5	2.04
Cδ_Nϵ_Cζ	124.9	1.14
Cγ_Cδ_Nϵ	111.0	2.49
Nϵ_Cζ_Nη1	120.9	1.07
Nϵ_Cζ_Nη2	119.5	1.06
Nη1_Cζ_Nη2	119.6	0.80
N_Cα_C	111.4	2.40
N_Cα_Cβ	110.6	1.12

ARG **mtt-85** n = 2843		
χ	Smooth COM	StdDev
chi1	-67	7.8
chi2	-178	10.6
chi3	-176	9.2
chi4	-88	11.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.5	1.70
Cα_C_O	120.4	0.82
Cβ_Cα_C	109.8	1.65
Cβ_Cγ_Cδ	111.4	1.97
Cδ_Nϵ_Cζ	124.8	1.05
Cγ_Cδ_Nϵ	111.4	2.43
Nϵ_Cζ_Nη1	120.8	1.02
Nϵ_Cζ_Nη2	119.6	0.93
Nη1_Cζ_Nη2	119.6	0.77
N_Cα_C	111.4	2.30
N_Cα_Cβ	110.6	1.04

ARG **mtm110** n = 781		
χ	Smooth COM	StdDev
chi1	-68	8.2
chi2	-177	9.7
chi3	-68	10.2
chi4	112	10.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.1	1.81
Cα_C_O	120.4	0.90
Cβ_Cα_C	110.1	1.76
Cβ_Cγ_Cδ	112.4	1.72
Cδ_Nϵ_Cζ	125.3	1.52
Cγ_Cδ_Nϵ	112.1	1.88
Nϵ_Cζ_Nη1	121.1	1.28
Nϵ_Cζ_Nη2	119.4	1.12
Nη1_Cζ_Nη2	119.5	0.92
N_Cα_C	111.7	2.44
N_Cα_Cβ	110.7	1.04

ARG **mtm180** n = 2407		
χ	Smooth COM	StdDev
chi1	-66	8.1
chi2	179	12.7
chi3	-67	8.8
chi4	172	15.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.3	1.63
Cα_C_O	120.5	0.89
Cβ_Cα_C	109.9	1.62
Cβ_Cγ_Cδ	111.6	1.68
Cδ_Nϵ_Cζ	124.4	1.08
Cγ_Cδ_Nϵ	111.4	1.69
Nϵ_Cζ_Nη1	120.4	0.90
Nϵ_Cζ_Nη2	119.8	0.88
Nη1_Cζ_Nη2	119.8	0.77
N_Cα_C	111.3	2.63
N_Cα_Cβ	110.5	1.05

ARG **mtm-85** n = 2848		
χ	Smooth COM	StdDev
chi1	-68	8.1
chi2	-171	9.3
chi3	-63	9.5
chi4	-88	8.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.5	1.56
Cα_C_O	120.5	0.81
Cβ_Cα_C	110.0	1.49
Cβ_Cγ_Cδ	112.0	1.57
Cδ_Nϵ_Cζ	124.9	1.17
Cγ_Cδ_Nϵ	112.7	1.96
Nϵ_Cζ_Nη1	120.8	1.03
Nϵ_Cζ_Nη2	119.7	1.00
Nη1_Cζ_Nη2	119.5	0.78
N_Cα_C	111.3	1.97
N_Cα_Cβ	111.1	1.03

ARG **mmp80** n = 164		
χ	Smooth COM	StdDev
chi1	-62	6.7
chi2	-75	12.7
chi3	74	11.7
chi4	77	6.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	1.39
Cα_C_O	120.4	0.95
Cβ_Cα_C	109.8	1.49
Cβ_Cγ_Cδ	113.4	1.62
Cδ_Nϵ_Cζ	125.0	1.16
Cγ_Cδ_Nϵ	113.5	2.23
Nϵ_Cζ_Nη1	120.6	0.99
Nϵ_Cζ_Nη2	120.0	0.86
Nη1_Cζ_Nη2	119.5	0.64
N_Cα_C	111.4	1.82
N_Cα_Cβ	110.9	0.93

ARG **mmp-170** n = 123		
χ	Smooth COM	StdDev
chi1	-64	7.2
chi2	-65	14.3
chi3	85	9.7
chi4	-167	19.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.5	1.27
Cα_C_O	120.4	0.99
Cβ_Cα_C	109.5	1.52
Cβ_Cγ_Cδ	112.8	1.74
Cδ_Nϵ_Cζ	124.8	1.32
Cγ_Cδ_Nϵ	111.5	1.61
Nϵ_Cζ_Nη1	120.5	1.21
Nϵ_Cζ_Nη2	119.8	1.10
Nη1_Cζ_Nη2	119.7	1.14
N_Cα_C	111.0	2.15
N_Cα_Cβ	111.1	1.12

ARG **mmt180** n = 1203		
χ	Smooth COM	StdDev
chi1	-61	9.1
chi2	-68	12.9
chi3	-176	11.3
chi4	-176	17.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.5	1.38
Cα_C_O	120.4	0.87
Cβ_Cα_C	109.4	1.62
Cβ_Cγ_Cδ	112.0	1.71
Cδ_Nϵ_Cζ	124.4	1.19
Cγ_Cδ_Nϵ	111.0	1.83
Nϵ_Cζ_Nη1	120.5	0.87
Nϵ_Cζ_Nη2	119.7	0.87
Nη1_Cζ_Nη2	119.8	0.74
N_Cα_C	111.2	2.57
N_Cα_Cβ	110.7	1.07

ARG **mmt90** n = 567		
χ	Smooth COM	StdDev
chi1	-60	8.8
chi2	-68	12.5
chi3	179	10.4
chi4	90	12.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.39
Cα_C_O	120.5	0.87
Cβ_Cα_C	109.5	1.65
Cβ_Cγ_Cδ	112.2	1.61
Cδ_Nϵ_Cζ	124.9	1.24
Cγ_Cδ_Nϵ	111.6	2.49
Nϵ_Cζ_Nη1	120.8	1.22
Nϵ_Cζ_Nη2	119.6	1.09
Nη1_Cζ_Nη2	119.6	0.72
N_Cα_C	111.4	2.72
N_Cα_Cβ	110.7	1.08

ARG **mmt-90** n = 1428		
χ	Smooth COM	StdDev
chi1	-63	6.6
chi2	-68	8.1
chi3	-175	7.7
chi4	-91	11.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.5	1.43
Cα_C_O	120.5	0.85
Cβ_Cα_C	109.6	1.64
Cβ_Cγ_Cδ	112.0	1.67
Cδ_Nϵ_Cζ	124.9	1.00
Cγ_Cδ_Nϵ	111.8	2.28
Nϵ_Cζ_Nη1	120.9	1.00
Nϵ_Cζ_Nη2	119.6	0.88
Nη1_Cζ_Nη2	119.4	0.82
N_Cα_C	110.1	2.67
N_Cα_Cβ	110.9	1.11

ARG **mmm160** n = 951		
χ	Smooth COM	StdDev
chi1	-61	9.2
chi2	-66	13.7
chi3	-64	9.9
chi4	163	24.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.5	1.60
Cα_C_O	120.4	0.88
Cβ_Cα_C	109.8	1.54
Cβ_Cγ_Cδ	112.5	1.73
Cδ_Nϵ_Cζ	124.6	1.31
Cγ_Cδ_Nϵ	111.9	1.89
Nϵ_Cζ_Nη1	120.6	1.17
Nϵ_Cζ_Nη2	119.8	1.11
Nη1_Cζ_Nη2	119.6	0.77
N_Cα_C	111.4	2.43
N_Cα_Cβ	110.7	1.18

ARG **mmm-85** n = 1022		
χ	Smooth COM	StdDev
chi1	-63	9.2
chi2	-67	10.9
chi3	-60	9.2
chi4	-86	10.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.52
Cα_C_O	120.5	0.88
Cβ_Cα_C	109.7	1.54
Cβ_Cγ_Cδ	112.8	1.62
Cδ_Nϵ_Cζ	125.0	1.09
Cγ_Cδ_Nϵ	112.5	2.26
Nϵ_Cζ_Nη1	120.9	1.01
Nϵ_Cζ_Nη2	119.6	0.96
Nη1_Cζ_Nη2	119.5	0.83
N_Cα_C	111.3	2.64
N_Cα_Cβ	110.8	1.12

Table S21: LYS Central Values

LYS **pptt** n = 25		
χ	Smooth COM	StdDev
chi1	64	7.5
chi2	89	8.3
chi3	175	11.9
chi4	179	7.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.1	1.24
Cα_C_O	120.4	0.70
Cβ_Cα_C	111.3	1.43
Cβ_Cγ_Cδ	112.2	1.70
Cδ_Cϵ_Nζ	111.3	1.82
Cγ_Cδ_Cϵ	110.6	1.94
N_Cα_C	111.7	2.09
N_Cα_Cβ	111.6	1.19

LYS **ptpp** n = 89		
χ	Smooth COM	StdDev
chi1	65	6.8
chi2	178	8.1
chi3	72	9.7
chi4	66	8.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.20
Cα_C_O	120.2	0.97
Cβ_Cα_C	110.1	1.28
Cβ_Cγ_Cδ	112.2	1.29
Cδ_Cϵ_Nζ	112.5	1.72
Cγ_Cδ_Cϵ	112.7	1.34
N_Cα_C	111.9	2.03
N_Cα_Cβ	110.9	1.31

LYS **ptpt** n = 148		
χ	Smooth COM	StdDev
chi1	64	8.2
chi2	179	11.8
chi3	72	10.4
chi4	174	11.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.7	1.64
Cα_C_O	120.5	0.85
Cβ_Cα_C	110.5	1.43
Cβ_Cγ_Cδ	112.1	1.65
Cδ_Cϵ_Nζ	111.4	2.10
Cγ_Cδ_Cϵ	112.4	1.85
N_Cα_C	111.2	2.94
N_Cα_Cβ	111.1	1.32

LYS **pttp** n = 240		
χ	Smooth COM	StdDev
chi1	67	8.3
chi2	-179	10.4
chi3	178	11.2
chi4	66	12.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	1.43
Cα_C_O	120.4	0.90
Cβ_Cα_C	110.4	1.45
Cβ_Cγ_Cδ	110.9	1.68
Cδ_Cϵ_Nζ	112.4	2.34
Cγ_Cδ_Cϵ	111.7	1.42
N_Cα_C	111.8	2.55
N_Cα_Cβ	111.0	1.09

LYS **pttt** n = 1385		
χ	Smooth COM	StdDev
chi1	65	7.6
chi2	-178	8.7
chi3	-179	9.7
chi4	-179	9.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	1.46
Cα_C_O	120.4	0.95
Cβ_Cα_C	110.4	1.38
Cβ_Cγ_Cδ	110.8	1.79
Cδ_Cϵ_Nζ	111.3	2.00
Cγ_Cδ_Cϵ	111.0	1.62
N_Cα_C	111.3	2.77
N_Cα_Cβ	111.1	1.10

LYS **pttm** n = 268		
χ	Smooth COM	StdDev
chi1	64	6.9
chi2	-177	9.1
chi3	-178	10.0
chi4	-67	11.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.9	1.47
Cα_C_O	120.4	0.98
Cβ_Cα_C	110.4	1.45
Cβ_Cγ_Cδ	110.7	2.05
Cδ_Cϵ_Nζ	112.3	2.37
Cγ_Cδ_Cϵ	111.9	1.51
N_Cα_C	112.0	2.55
N_Cα_Cβ	111.0	1.16

LYS **ptmt** n = 187		
χ	Smooth COM	StdDev
chi1	66	8.2
chi2	-175	12.0
chi3	-71	11.7
chi4	-175	10.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.5	1.57
Cα_C_O	120.5	0.97
Cβ_Cα_C	110.4	1.61
Cβ_Cγ_Cδ	112.1	1.58
Cδ_Cϵ_Nζ	111.5	2.11
Cγ_Cδ_Cϵ	112.4	1.87
N_Cα_C	111.0	2.72
N_Cα_Cβ	111.0	1.10

LYS **ptmm** n = 80		
χ	Smooth COM	StdDev
chi1	66	8.4
chi2	-177	10.0
chi3	-69	9.8
chi4	-66	7.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.5	1.30
Cα_C_O	120.6	1.03
Cβ_Cα_C	109.9	1.49
Cβ_Cγ_Cδ	112.3	1.44
Cδ_Cϵ_Nζ	113.0	1.78
Cγ_Cδ_Cϵ	113.0	1.15
N_Cα_C	110.5	2.70
N_Cα_Cβ	110.8	1.21

LYS **pmtt** n = 10		
χ	Smooth COM	StdDev
chi1	73	8.4
chi2	-74	10.5
chi3	-168	10.6
chi4	-174	10.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.4	1.64
Cα_C_O	120.8	0.55
Cβ_Cα_C	110.4	1.28
Cβ_Cγ_Cδ	112.6	2.23
Cδ_Cϵ_Nζ	111.7	2.25
Cγ_Cδ_Cϵ	111.3	1.31
N_Cα_C	110.0	2.38
N_Cα_Cβ	112.1	2.13

LYS **tppp** n = 37		
χ	Smooth COM	StdDev
chi1	-177	11.5
chi2	62	10.1
chi3	65	7.8
chi4	67	11.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.1	1.50
Cα_C_O	120.7	0.87
Cβ_Cα_C	110.3	0.75
Cβ_Cγ_Cδ	113.5	1.87
Cδ_Cϵ_Nζ	113.0	1.70
Cγ_Cδ_Cϵ	113.4	1.74
N_Cα_C	110.9	1.93
N_Cα_Cβ	110.2	1.12

LYS **tppt** n = 272		
χ	Smooth COM	StdDev
chi1	-178	7.9
chi2	63	8.9
chi3	69	9.2
chi4	177	9.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	1.23
Cα_C_O	120.5	0.74
Cβ_Cα_C	110.6	1.10
Cβ_Cγ_Cδ	113.2	1.54
Cδ_Cϵ_Nζ	111.2	1.84
Cγ_Cδ_Cϵ	112.4	1.45
N_Cα_C	110.6	2.08
N_Cα_Cβ	110.3	1.07

LYS **tptp** n = 409		
χ	Smooth COM	StdDev
chi1	-179	8.0
chi2	67	10.4
chi3	173	13.6
chi4	66	13.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	1.34
Cα_C_O	120.5	0.83
Cβ_Cα_C	110.2	1.23
Cβ_Cγ_Cδ	112.1	1.49
Cδ_Cϵ_Nζ	112.7	1.95
Cγ_Cδ_Cϵ	112.2	1.31
N_Cα_C	110.3	2.08
N_Cα_Cβ	110.3	1.12

LYS **tptt** n = 1228		
χ	Smooth COM	StdDev
chi1	-178	9.1
chi2	69	9.0
chi3	175	10.1
chi4	177	12.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.8	1.31
Cα_C_O	120.5	0.78
Cβ_Cα_C	110.4	1.22
Cβ_Cγ_Cδ	112.0	1.60
Cδ_Cϵ_Nζ	111.1	2.24
Cγ_Cδ_Cϵ	111.0	1.47
N_Cα_C	110.7	2.15
N_Cα_Cβ	110.2	1.11

LYS **tptm** n = 197		
χ	Smooth COM	StdDev
chi1	-177	7.6
chi2	67	9.7
chi3	-179	11.4
chi4	-66	13.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.0	1.45
Cα_C_O	120.4	0.77
Cβ_Cα_C	110.4	1.10
Cβ_Cγ_Cδ	111.9	1.41
Cδ_Cϵ_Nζ	112.5	2.06
Cγ_Cδ_Cϵ	111.9	1.35
N_Cα_C	110.3	2.06
N_Cα_Cβ	110.3	1.14

LYS **ttpp** n = 229		
χ	Smooth COM	StdDev
chi1	-178	8.6
chi2	174	14.5
chi3	71	11.2
chi4	68	10.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.7	1.58
Cα_C_O	120.6	0.78
Cβ_Cα_C	110.1	1.26
Cβ_Cγ_Cδ	112.1	1.68
Cδ_Cϵ_Nζ	112.8	2.35
Cγ_Cδ_Cϵ	112.8	1.57
N_Cα_C	110.2	2.48
N_Cα_Cβ	110.4	1.47

LYS **ttpt** n = 883		
χ	Smooth COM	StdDev
chi1	-178	8.1
chi2	174	12.1
chi3	73	11.9
chi4	175	11.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.8	1.64
Cα_C_O	120.6	0.75
Cβ_Cα_C	110.1	1.18
Cβ_Cγ_Cδ	112.1	1.47
Cδ_Cϵ_Nζ	111.1	2.07
Cγ_Cδ_Cϵ	112.2	1.58
N_Cα_C	110.3	2.32
N_Cα_Cβ	110.2	1.32

LYS **ttpm** n = 4		
χ	Smooth COM	StdDev
chi1	-176	10.0
chi2	175	6.9
chi3	87	18.0
chi4	-84	4.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.4	1.11
Cα_C_O	120.8	0.32
Cβ_Cα_C	110.3	0.44
Cβ_Cγ_Cδ	111.6	0.99
Cδ_Cϵ_Nζ	113.9	1.18
Cγ_Cδ_Cϵ	113.1	0.24
N_Cα_C	110.1	1.31
N_Cα_Cβ	110.1	0.84

LYS **tttp** n = 1233		
χ	Smooth COM	StdDev
chi1	-177	8.1
chi2	175	9.9
chi3	173	10.8
chi4	65	12.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.9	1.52
Cα_C_O	120.6	0.75
Cβ_Cα_C	110.2	1.09
Cβ_Cγ_Cδ	111.1	1.61
Cδ_Cϵ_Nζ	112.3	1.98
Cγ_Cδ_Cϵ	111.8	1.35
N_Cα_C	110.7	2.22
N_Cα_Cβ	110.4	1.14

LYS **tttt** n = 5043		
χ	Smooth COM	StdDev
chi1	-175	8.2
chi2	176	8.7
chi3	179	9.2
chi4	-179	10.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.9	1.52
Cα_C_O	120.6	0.78
Cβ_Cα_C	110.2	1.14
Cβ_Cγ_Cδ	111.1	1.74
Cδ_Cϵ_Nζ	111.2	1.99
Cγ_Cδ_Cϵ	111.0	1.54
N_Cα_C	110.5	2.28
N_Cα_Cβ	110.3	1.21

LYS **tttm** n = 1176		
χ	Smooth COM	StdDev
chi1	-176	8.1
chi2	177	9.7
chi3	-176	10.5
chi4	-67	12.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.9	1.60
Cα_C_O	120.6	0.82
Cβ_Cα_C	110.3	1.14
Cβ_Cγ_Cδ	111.0	1.70
Cδ_Cϵ_Nζ	112.3	1.97
Cγ_Cδ_Cϵ	111.8	1.47
N_Cα_C	110.5	2.11
N_Cα_Cβ	110.4	1.16

LYS **ttmp** n = 9		
χ	Smooth COM	StdDev
chi1	-174	4.2
chi2	-179	8.5
chi3	-95	18.6
chi4	76	25.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.2	1.24
Cα_C_O	120.6	0.50
Cβ_Cα_C	110.3	1.62
Cβ_Cγ_Cδ	112.6	1.74
Cδ_Cϵ_Nζ	114.0	1.36
Cγ_Cδ_Cϵ	112.9	0.74
N_Cα_C	110.8	1.51
N_Cα_Cβ	111.4	1.04

LYS **ttmt** n = 674		
χ	Smooth COM	StdDev
chi1	-174	9.4
chi2	-177	10.8
chi3	-73	11.7
chi4	-175	11.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.7	1.55
Cα_C_O	120.6	0.86
Cβ_Cα_C	110.2	1.18
Cβ_Cγ_Cδ	112.2	1.52
Cδ_Cϵ_Nζ	110.9	2.32
Cγ_Cδ_Cϵ	112.2	1.65
N_Cα_C	110.3	2.33
N_Cα_Cβ	110.3	1.25

LYS **ttmm** n = 197		
χ	Smooth COM	StdDev
chi1	-174	8.5
chi2	179	9.9
chi3	-71	11.9
chi4	-67	11.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.6	1.46
Cα_C_O	120.6	0.82
Cβ_Cα_C	110.2	1.29
Cβ_Cγ_Cδ	112.1	1.57
Cδ_Cϵ_Nζ	112.6	2.30
Cγ_Cδ_Cϵ	112.5	1.56
N_Cα_C	110.2	2.45
N_Cα_Cβ	110.3	1.39

LYS **tmtp** n = 11		
χ	Smooth COM	StdDev
chi1	-176	7.5
chi2	-97	8.3
chi3	-178	12.4
chi4	65	7.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.22
Cα_C_O	120.8	0.41
Cβ_Cα_C	110.5	0.70
Cβ_Cγ_Cδ	112.0	1.51
Cδ_Cϵ_Nζ	113.1	3.03
Cγ_Cδ_Cϵ	111.8	1.20
N_Cα_C	110.1	3.05
N_Cα_Cβ	110.4	0.87

LYS **tmtt** n = 82		
χ	Smooth COM	StdDev
chi1	-172	8.5
chi2	-91	9.6
chi3	-176	11.7
chi4	-178	10.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.5	1.14
Cα_C_O	120.8	0.61
Cβ_Cα_C	110.9	1.09
Cβ_Cγ_Cδ	111.9	1.44
Cδ_Cϵ_Nζ	110.8	2.07
Cγ_Cδ_Cϵ	111.0	1.37
N_Cα_C	110.2	1.89
N_Cα_Cβ	110.1	0.81

LYS **tmtm** n = 20		
χ	Smooth COM	StdDev
chi1	-172	10.4
chi2	-90	5.6
chi3	-172	15.1
chi4	-64	7.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.5	1.62
Cα_C_O	120.6	0.65
Cβ_Cα_C	111.0	0.85
Cβ_Cγ_Cδ	112.2	1.23
Cδ_Cϵ_Nζ	112.7	1.69
Cγ_Cδ_Cϵ	112.0	1.55
N_Cα_C	110.1	1.72
N_Cα_Cβ	109.8	0.79

LYS **tmmt** n = 33		
χ	Smooth COM	StdDev
chi1	-179	10.0
chi2	-93	12.1
chi3	-70	8.9
chi4	-179	10.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.0	1.85
Cα_C_O	120.5	0.88
Cβ_Cα_C	110.7	1.12
Cβ_Cγ_Cδ	113.5	1.73
Cδ_Cϵ_Nζ	110.8	2.86
Cγ_Cδ_Cϵ	112.4	2.86
N_Cα_C	110.0	2.15
N_Cα_Cβ	109.9	1.08

LYS **tmmm** n = 8		
χ	Smooth COM	StdDev
chi1	-177	11.9
chi2	-81	7.5
chi3	-63	8.0
chi4	-64	4.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	116.2	2.69
Cα_C_O	120.3	0.85
Cβ_Cα_C	111.2	1.13
Cβ_Cγ_Cδ	114.9	1.37
Cδ_Cϵ_Nζ	113.1	1.48
Cγ_Cδ_Cϵ	115.0	1.62
N_Cα_C	109.0	2.01
N_Cα_Cβ	109.5	1.26

LYS **mppt** n = 31		
χ	Smooth COM	StdDev
chi1	-82	8.9
chi2	73	14.9
chi3	69	8.0
chi4	177	5.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.1	1.99
Cα_C_O	120.4	0.89
Cβ_Cα_C	109.9	1.23
Cβ_Cγ_Cδ	113.7	1.56
Cδ_Cϵ_Nζ	111.4	1.92
Cγ_Cδ_Cϵ	112.2	1.37
N_Cα_C	108.8	1.97
N_Cα_Cβ	110.9	0.92

LYS **mptp** n = 26		
χ	Smooth COM	StdDev
chi1	-74	18.5
chi2	86	18.2
chi3	171	9.0
chi4	65	12.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.7	1.56
Cα_C_O	120.5	1.13
Cβ_Cα_C	110.1	1.43
Cβ_Cγ_Cδ	113.2	2.50
Cδ_Cϵ_Nζ	113.4	2.26
Cγ_Cδ_Cϵ	112.5	2.72
N_Cα_C	110.6	2.77
N_Cα_Cβ	110.9	1.04

LYS **mptt** n = 124		
χ	Smooth COM	StdDev
chi1	-79	13.3
chi2	72	17.3
chi3	176	12.4
chi4	175	11.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.9	1.39
Cα_C_O	120.6	0.78
Cβ_Cα_C	109.7	1.53
Cβ_Cγ_Cδ	112.6	2.03
Cδ_Cϵ_Nζ	110.9	2.27
Cγ_Cδ_Cϵ	111.2	1.60
N_Cα_C	110.6	2.59
N_Cα_Cβ	110.8	1.10

LYS **mptm** n = 11		
χ	Smooth COM	StdDev
chi1	-91	6.7
chi2	61	11.1
chi3	-173	5.4
chi4	-60	13.5
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	0.81
Cα_C_O	120.7	0.57
Cβ_Cα_C	110.7	0.84
Cβ_Cγ_Cδ	112.8	0.65
Cδ_Cϵ_Nζ	113.4	1.68
Cγ_Cδ_Cϵ	111.8	0.50
N_Cα_C	110.8	2.19
N_Cα_Cβ	110.6	0.91

LYS **mtpp** n = 392		
χ	Smooth COM	StdDev
chi1	-68	7.5
chi2	176	10.9
chi3	70	10.8
chi4	67	10.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.2	1.66
Cα_C_O	120.4	0.82
Cβ_Cα_C	110.2	1.51
Cβ_Cγ_Cδ	112.4	1.45
Cδ_Cϵ_Nζ	112.8	2.11
Cγ_Cδ_Cϵ	112.7	1.41
N_Cα_C	111.4	2.53
N_Cα_Cβ	110.5	1.01

LYS **mtpt** n = 1357		
χ	Smooth COM	StdDev
chi1	-69	8.1
chi2	174	11.3
chi3	70	11.8
chi4	175	10.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.3	1.54
Cα_C_O	120.5	0.84
Cβ_Cα_C	110.0	1.65
Cβ_Cγ_Cδ	112.3	1.55
Cδ_Cϵ_Nζ	110.8	2.15
Cγ_Cδ_Cϵ	112.3	1.49
N_Cα_C	111.4	2.21
N_Cα_Cβ	110.7	1.03

LYS **mtpm** n = 17		
χ	Smooth COM	StdDev
chi1	-70	6.1
chi2	174	15.5
chi3	90	14.7
chi4	-70	12.1
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.5	2.14
Cα_C_O	120.3	0.77
Cβ_Cα_C	109.8	2.27
Cβ_Cγ_Cδ	112.3	1.70
Cδ_Cϵ_Nζ	113.4	1.87
Cγ_Cδ_Cϵ	113.2	1.59
N_Cα_C	110.9	2.12
N_Cα_Cβ	110.5	1.03

LYS **mttp** n = 1414		
χ	Smooth COM	StdDev
chi1	-65	8.3
chi2	-179	10.7
chi3	176	11.2
chi4	66	13.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.4	1.73
Cα_C_O	120.5	0.84
Cβ_Cα_C	110.1	1.63
Cβ_Cγ_Cδ	111.3	1.75
Cδ_Cϵ_Nζ	112.2	1.98
Cγ_Cδ_Cϵ	111.8	1.47
N_Cα_C	111.3	2.49
N_Cα_Cβ	110.6	1.02

LYS **mttt** n = 8597		
χ	Smooth COM	StdDev
chi1	-67	7.1
chi2	-178	9.1
chi3	-179	9.8
chi4	179	10.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.5	1.62
Cα_C_O	120.5	0.83
Cβ_Cα_C	110.0	1.56
Cβ_Cγ_Cδ	111.1	1.85
Cδ_Cϵ_Nζ	111.1	2.10
Cγ_Cδ_Cϵ	111.0	1.60
N_Cα_C	111.3	2.24
N_Cα_Cβ	110.7	0.99

LYS **mttm** n = 1829		
χ	Smooth COM	StdDev
chi1	-66	7.3
chi2	-177	10.0
chi3	-176	10.8
chi4	-67	12.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.4	1.74
Cα_C_O	120.5	0.85
Cβ_Cα_C	110.1	1.54
Cβ_Cγ_Cδ	111.2	1.73
Cδ_Cϵ_Nζ	112.2	2.03
Cγ_Cδ_Cϵ	111.8	1.47
N_Cα_C	111.4	2.37
N_Cα_Cβ	110.6	1.00

LYS **mtmp** n = 9		
χ	Smooth COM	StdDev
chi1	-67	5.8
chi2	-175	8.3
chi3	-95	7.4
chi4	73	12.3
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.8	1.23
Cα_C_O	120.6	0.61
Cβ_Cα_C	109.9	1.20
Cβ_Cγ_Cδ	111.7	1.98
Cδ_Cϵ_Nζ	113.7	2.37
Cγ_Cδ_Cϵ	112.7	0.79
N_Cα_C	110.4	2.29
N_Cα_Cβ	110.8	0.91

LYS **mtmt** n = 1314		
χ	Smooth COM	StdDev
chi1	-66	6.9
chi2	-173	9.8
chi3	-73	11.7
chi4	-175	10.6
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.2	1.59
Cα_C_O	120.4	0.86
Cβ_Cα_C	110.1	1.56
Cβ_Cγ_Cδ	112.3	1.52
Cδ_Cϵ_Nζ	111.0	2.18
Cγ_Cδ_Cϵ	112.1	1.45
N_Cα_C	111.3	2.14
N_Cα_Cβ	110.7	0.96

LYS **mtmm** n = 424		
χ	Smooth COM	StdDev
chi1	-63	6.9
chi2	-177	10.1
chi3	-70	10.9
chi4	-66	9.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	113.5	1.53
Cα_C_O	120.5	0.84
Cβ_Cα_C	109.8	1.56
Cβ_Cγ_Cδ	112.3	1.37
Cδ_Cϵ_Nζ	112.8	2.10
Cγ_Cδ_Cϵ	112.9	1.50
N_Cα_C	111.5	2.39
N_Cα_Cβ	110.6	1.03

LYS **mmpt** n = 31		
χ	Smooth COM	StdDev
chi1	-60	7.0
chi2	-70	19.5
chi3	93	14.5
chi4	175	10.7
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	115.3	1.12
Cα_C_O	120.4	0.89
Cβ_Cα_C	109.8	1.68
Cβ_Cγ_Cδ	113.4	1.80
Cδ_Cϵ_Nζ	111.5	1.77
Cγ_Cδ_Cϵ	112.0	1.40
N_Cα_C	111.5	2.37
N_Cα_Cβ	111.2	1.39

LYS **mmtp** n = 463		
χ	Smooth COM	StdDev
chi1	-61	8.2
chi2	-68	12.0
chi3	179	11.9
chi4	67	13.2
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.7	1.51
Cα_C_O	120.4	0.90
Cβ_Cα_C	109.6	1.56
Cβ_Cγ_Cδ	112.0	1.55
Cδ_Cϵ_Nζ	112.6	2.34
Cγ_Cδ_Cϵ	111.9	1.34
N_Cα_C	111.1	2.60
N_Cα_Cβ	110.7	1.04

LYS **mmtt** n = 3137		
χ	Smooth COM	StdDev
chi1	-61	8.3
chi2	-67	9.8
chi3	-176	10.1
chi4	-178	11.0
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.5	1.32
Cα_C_O	120.4	0.91
Cβ_Cα_C	109.6	1.56
Cβ_Cγ_Cδ	111.9	1.49
Cδ_Cϵ_Nζ	111.1	2.08
Cγ_Cδ_Cϵ	111.1	1.53
N_Cα_C	111.5	2.47
N_Cα_Cβ	110.7	1.01

LYS **mmtm** n = 727		
χ	Smooth COM	StdDev
chi1	-60	8.2
chi2	-65	10.8
chi3	-173	11.2
chi4	-68	13.4
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.5	1.40
Cα_C_O	120.5	0.87
Cβ_Cα_C	109.7	1.57
Cβ_Cγ_Cδ	111.9	1.43
Cδ_Cϵ_Nζ	112.4	1.97
Cγ_Cδ_Cϵ	112.0	1.44
N_Cα_C	111.4	2.53
N_Cα_Cβ	110.6	1.02

LYS **mmmt** n = 544		
χ	Smooth COM	StdDev
chi1	-62	7.7
chi2	-64	10.7
chi3	-70	9.7
chi4	-176	9.8
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.6	1.31
Cα_C_O	120.4	0.97
Cβ_Cα_C	109.6	1.46
Cβ_Cγ_Cδ	113.1	1.51
Cδ_Cϵ_Nζ	111.2	2.21
Cγ_Cδ_Cϵ	112.3	1.53
N_Cα_C	111.8	2.31
N_Cα_Cβ	110.7	1.05

LYS **mmmm** n = 90		
χ	Smooth COM	StdDev
chi1	-61	8.3
chi2	-61	10.4
chi3	-66	10.8
chi4	-64	10.9
Bond Angle	Mean	StdDev
Cα_Cβ_Cγ	114.7	1.39
Cα_C_O	120.4	1.06
Cβ_Cα_C	109.5	1.53
Cβ_Cγ_Cδ	113.2	1.43
Cδ_Cϵ_Nζ	112.6	2.73
Cγ_Cδ_Cϵ	113.2	1.87
N_Cα_C	111.7	2.47
N_Cα_Cβ	110.5	1.11