Rough Draft of Supplemental Material

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Contents

S1 Top500 vs. Top8000 Reference Contours

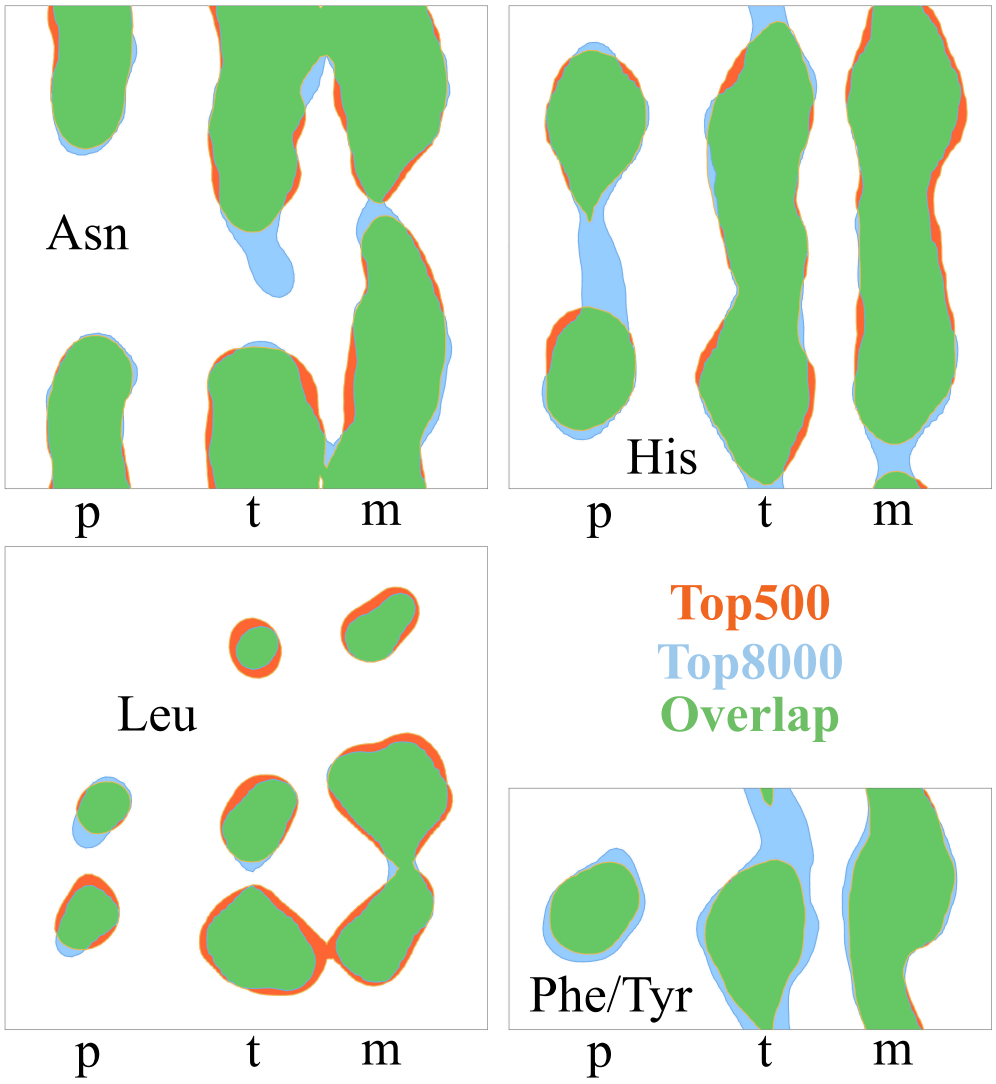

Figure S1: Areas in orange (from Top500 data) and in blue (from Top8000) fill the allowed regions for AsN, His, Leu, and Phe/Tyr. Phe and Tyr were done together as no significant difference was detected between their distributions. The extensive areas in green are where the two systems both declare allowed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

S2 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.

S3 Outlier Counts: Top500 vs. Top8000 Reference Contours

Residue	n	Top500 <= 0.3%	Top8000 <= 1.0%	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.

S4 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	-

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

S5 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.

S5.1 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

S5.2 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 **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

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

S5.3 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

S5.4 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

S5.5 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

S5.6 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

S5.7 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

S5.8 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

S5.9 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

S5.10 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

S5.11 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

S5.12 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

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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

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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

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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

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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

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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

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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